Computational fluid dynamics analysis of air-water bubble columns

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Computational fluid dynamics analysis of air-water bubble columns

by

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A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

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\textbf{Nomenclature}

\begin{itemize}
\item $a_k$ coefficient used in determining partition coefficient $\beta_{kl}$ in the $k$-$\varepsilon$ model
\item $c^0_\mu$ $k$-$\varepsilon$ model constant equal to 0.09
\item $c_{\mu k}$ $k$-$\varepsilon$ model expression dependent on $k$, $\varepsilon$, energy exchange rate, and density
\item $C_{\varepsilon 1}$ constant in turbulence energy decay ($\varepsilon$) equation equal to 1.44
\item $C_{\varepsilon 2}$ constant in turbulence energy decay ($\varepsilon$) equation equal to 1.92
\item $c_0$ speed of sound, cm/s (Section 3.2.2)
\item $Ca_\gamma$ capillary number (Section 3.1.3)
\item $C_{att}$ attraction coefficient
\item $C_{BP}$ proportionality constant for bubble pressure model
\item $C_{BT}$ proportionality constant for bubble-induced turbulence model
\item $C_D$ drag coefficient
\item $C_L$ lift coefficient
\item $c_p$ constant pressure specific heat (Section 3.2)
\item $\tilde{C}_r$ net repulsive coefficient (Eqs. 3.9a and 3.9b)
\item $C_{rep}$ repulsion coefficient
\item $C_{rot}$ rotation coefficient
\item $C_S$ strain coefficient
\item $c_v$ constant volume specific heat (Section 3.2)
\item $\tilde{C}_v$ net viscous coefficient (Eqs. 3.9a and 3.9b)
\item $C_{vm}$ virtual-mass coefficient
\item $C_{x0}$ adjustable term in drag coefficient $C_D(Re)$ in Eqs. 3.25a, 5.9
\item $d_b$ bubble diameter, mm or cm
\item $E$ total energy (Section 3.2.2)
\item $e_k$ internal energy of material $k$ (Secs. 3.2.2 and 3.2.3)
\item $E_{kl}$ turbulence energy exchange rate coefficient for $k$-$\varepsilon$ model
\item $E_0$ Eötvös number, dimensionless
\item $f$ statistical distribution function (Section 3.2.2)
\item $F_{att}$ attraction force
\item $f_c, f_d$ bubble-bubble-interaction forces (Eqs. 3.9a and 3.9b)
\end{itemize}
\( F_D \) drag force
\( F_{fk} \) sum of interphase forces
\( F_L \) lift force
\( F_{rep} \) repulsion force
\( F_{rot} \) rotation force
\( F_S \) strain force
\( F_{vm} \) virtual-mass force
\( g \) gravitational force
\( G \) sum of symmetric and antisymmetric tensors to calculate \( F_{att} \) and \( F_{rep} \)
\( h_{gassed} \) liquid level obtained after gas enters bubble column (Chapter 7)
\( h_{ungassed} \) initial liquid level in bubble column (Chapter 7)
\( h_v \) close-spacing function for separation between spheres (Eqs. 3.9a and 3.9b)
\( i \) imaginary number (Chapter 6)
\( i \) unit vector in the upward vertical direction
\( I \) identity tensor
\( j \) plane index for plane-average and running-average routines (Chapter 6)
\( k \) wave vector (Chapter 6)
\( k \) wavenumber or frequency, magnitude of wave vector (Chapter 6)
\( k_k \) turbulence kinetic energy for phase \( k \)
\( K_{kl} \) momentum exchange coefficient in \( k-\varepsilon \) model
\( k_{max} \) largest wavenumber resolved on the computational grid (Chapter 6)
\( l \) wavelength (Chapter 6)
\( m_k \) mass of material \( k \)
\( n \) unit normal vector
\( p, p_0 \) pressure \( \left( p = \langle p_0 \rangle \right) \)
\( p_0' \) pressure fluctuations (Section 3.2.2)
\( p^0_k \) pressure for pure material \( k \) (Secs. 3.2.2 and 3.2.3)
\( P_d \) bubble pressure model applied to dispersed phase
\( Q_0 \) function of state vector \( \Gamma_0 \); represents mass, momentum, and total energy of material in \( V \) (Section 3.2.2)
\( q_0 \) heat flux (Section 3.2.2)
arbitrary field variable in volume \( V \) (Section 3.2.3)

\( Re \) bubble Reynolds number, dimensionless

\( Re_0 \) bubble Reynolds number for zero-order terms, dimensionless (Chapter 6)

\( R_k \) ideal gas constant (Section 3.2.2)

\( R_k \) Reynolds stress tensor for phase \( k \) (Section 3.1.2)

\( S \) surface, e.g., a face of a cell (Section 3.2.3)

\( S_i \) surface vector of side or face \( i \) (Section 3.2.3)

\( t \) time, seconds

\( T_1 \) final time (sec) for running-average calculation (Chapter 6)

\( T_2 \) final time (sec) for plane-average calculation (Chapter 6)

\( T_k \) temperature of material \( k \)

\( u_c \) velocity of continuous phase, \( \text{cm/s} \)

\( u_{d0} \) rise velocity, \( \text{cm/s} \)

\( u_d \) velocity of dispersed phase, \( \text{cm/s} \)

\( u_{d0} \) rise velocity in the uniform state, \( \text{cm/s} \) (Chapter 6)

\( u_g \) superficial gas velocity, \( \text{cm/s} \)

\( u_k \) velocity of phase \( k \) or material \( k \), \( \text{cm/s} \)

\( u'_k \) velocity fluctuations (Secs. 3.2.2 and 3.2.3)

\( u'_f \) face-centered or fluxing velocity, \( \text{cm/s} \) (Section 3.2.3)

\( u_i \) inlet water velocity, \( \text{cm/s} \)

\( u_m \) mesh velocity, \( \text{cm/s} \) (Section 3.2.3)

\( U_S \) slip velocity, \( \text{cm/s} \) (Chapter 4)

\( u_v \) phase-averaged velocity, \( \text{cm/s} \)

\( V \) total volume

\( v_k \) volume of material \( k \) per unit total volume (Secs. 3.2.2 and 3.2.3)

\( x \) position vector (Secs. 3.2.2 and 3.2.3); vertical vector (Chapter 6)

\( X \) generic variable expression (Chapter 6)

\( \alpha_c \) volume fraction of continuous phase, dimensionless

\( \alpha_d \) volume fraction of dispersed phase, dimensionless
\( \bar{\alpha}_d \) average dispersed-phase volume fraction, dimensionless

\( \alpha_{d0} \) volume fraction of dispersed phase in uniform state, dimensionless

\( \alpha_{dcp} \) gas volume fraction at close packing, dimensionless

\( \alpha_{\text{height}} \) average gas volume fraction determined by change in liquid level, dimensionless (Chapter 7)

\( \alpha_k \) volume fraction of phase \( k \), dimensionless

\( \beta_0 \) coefficient in zero-order drag term (Chapter 6)

\( \beta_1 \) coefficient in drag term for perturbed state (Chapter 6)

\( \beta_{kl} \) partition coefficient in \( k-\varepsilon \) model

\( \varepsilon_k \) turbulence energy decay for phase \( k \)

\( \phi_{\varepsilon} \) turbulent Prandtl number for turbulence energy decay

\( \phi_k \) turbulent Prandtl number for turbulence kinetic energy diffusion

\( \gamma \) ratio of constant pressure specific heat to constant volume specific heat (Secs. 3.2.2 and 3.2.3)

\( \Gamma_0 \) single phase state vector (Section 3.2.2)

\( \Gamma_N \) multiphase state vector (Section 3.2.2)

\( \lambda \) disturbance growth rate (Chapter 6)

\( \mu_{0,c} \) molecular viscosity of continuous phase

\( \mu_{0,d} \) molecular viscosity of dispersed phase

\( \mu_{0,k} \) molecular viscosity of phase \( k \)

\( \mu_{\text{eff},c} \) effective viscosity of continuous phase

\( \mu_{\text{eff},d} \) effective viscosity of dispersed phase

\( \mu_{\text{eff},k} \) effective viscosity of phase \( k \)

\( \mu_{c,c} \) pseudo-turbulent viscosity for continuous phase

\( \mu_{k,k} \) turbulent viscosity for phase \( k \)

\( \nu_c \) kinematic molecular viscosity for continuous phase

\( \nu_k \) kinematic viscosity for phase \( k \)

\( \nu_t \) kinematic turbulent viscosity

\( \theta \) slip velocity fluctuations (Chapter 4)

\( \theta_k \) expected value or average value of \( \alpha_k \) (Secs. 3.2.2 and 3.2.3)

\( \rho_c \) density of continuous phase
\( \rho_d \) density of dispersed phase
\( \rho_k \) density of phase \( k \) or material \( k \)
\( \rho_v \) phase-averaged density
\( \rho_{v0} \) phase-averaged density in uniform state (Chapter 6)
\( \sigma \) gas holdup fluctuations (Chapter 4)
\( \sigma \) surface tension, 72.8 dyne/cm (Chapter 5)
\( \tau_0 \) deviatoric stress (Section 3.2.2)
\( \tau_{dl} \) empirically determined time constant in turbulence energy decay (\( \varepsilon \)) equation (Chapter 3)
\( \nu \) velocity of propagation, cm/s (Chapter 6)
\( \zeta_0 \) rate of strain tensor (Secs. 3.2.2 and 3.2.3)

**Subscripts**
0 zero-order term (Chapter 6)
1 perturbation value (Chapter 6)
c continuous phase
d dispersed phase
\( f \) index for sum of interfacial forces
\( k, l \) general phase or material \( k \) or \( l \)

**Superscripts**
c cell-centered operator
eq equilibrium
\( L \) Lagrangian value (Section 3.2.3)
n Eulerian value (Section 3.2.3)
n+1 Eulerian value at next time level (Section 3.2.3)
\( Ttl \) total mass, velocity, and temperature mapped (Section 3.2.3)
u upwind, cell-centered (Section 3.2.3)
* face-centered quantity (Section 3.2.3)
Chapter 1. Introduction

1.1 Background, Motivation, and Objectives

Bubble columns are widely used in the chemical industry for processes including Fischer-Tropsch reactions, oxidation, alkylation, fermentation, hydrogenation, halogenation, water treatment, and coal liquefaction (Sanyal et al., 1999; Joshi, 2001). Buoyancy drives the typically two-phase flow pattern in which gas bubbles are dispersed within a continuous liquid phase (Pan et al., 2000). Bubble columns possess superior heat-and mass-transfer properties due to the large interfacial area available, and they have relatively high values of liquid holdup. These characteristics make bubble columns suitable for slow chemical reactions and exothermic or endothermic processes. Reactor performance depends on factors including gas holdup, bubble size, bubble rise velocity, bubble-bubble interactions, rate of mixing, and the amount of interfacial area (Sanyal et al., 1999; Joshi, 2001). Figure 1.1 illustrates a basic schematic of a bubble column.

Figure 1.1. Basic schematic of a bubble column.
The inlet flow conditions determine which of the primary flow regimes, homogeneous or heterogeneous, will be observed in the bubble column. Small, uniform, spherical bubbles and low superficial gas velocities are typical of the homogeneous, or bubbly-flow, regime. Bubbles travel upwards with nearly the same rise velocities and do not tend to interact with neighboring bubbles. An increase in inlet gas velocity leads to a transition to the heterogeneous regime (Shah and Deckwer, 1983). This regime is characterized by bubbles of different sizes and shapes, high gas holdup, bubble-bubble interaction, and liquid circulation (Chen et al., 1994).

The design and scale-up of bubble columns depend upon the column hydrodynamics, the study of which is often complicated since these reactors use multiphase flows. Computational fluid dynamics (CFD) aids design, optimization, and scale-up by predicting the hydrodynamics for various complex geometries, allowing engineers to investigate a large number of design alternatives at a relatively low cost. Two notable methods for the numerical simulation of bubble columns are Eulerian-Eulerian, in which the two-fluid model describes both the gas and liquid phases, and Eulerian-Lagrangian, in which the liquid phase is considered a continuum, while the gas phase is described by tracking individual bubbles (Pan et al., 2000). Successful design of a bubble column reactor requires consideration of the following key issues:

- Determining a suitable means for modeling interphase momentum transfer
- Calculating forces acting upon individual bubbles
- Modeling turbulence in two-phase flows
- Comparing 2D and 3D simulations and the resulting flow structures
- Compromising between sufficient grid resolution and necessary computational effort
- Determining the effect of bubble-bubble interaction and coalescence
- Validating the model with experimental data

Sokolichin et al. (2004) have noted in their recent review paper that over approximately the last ten years, an increase in computer power has allowed simulations of systems to progress from highly simplified fluid-flow models to detailed yet efficient
simulation codes. These codes produce suitable agreement between experimental and simulated results, demonstrating that CFD simulations can yield increasingly reliable predictions of bubble flow. However, Sokolichin et al. (2004) also state that there is still discussion regarding which physical effects are most significant and what are appropriate ways to model these effects. Thus, there is no clear agreement on which models are necessary for CFD simulations of bubble columns. For example, this work brings attention to the interaction terms proposed by Kashiwa (1998). According to a detailed survey, these terms have not been reported in the two-fluid models previously discussed in the literature. In the original derivation, these interaction forces are expressed in two parts: attraction and repulsion. Each part takes the form of a second-order tensor that is multiplied by the difference in velocity between gas and liquid. In this work, an alternative representation of these interaction forces is presented in three parts—lift, rotation, and strain.

The numerical studies presented in this work provide a detailed analysis of the interaction terms, the effective viscosity, and the bubble pressure in the two-fluid model formulation. A fundamental simulation study consisting of numerical “experiments” illustrates how various two-fluid model parameters affect the CFD predictions for bubble columns. The findings from this fundamental study motivated subsequent studies for which simulations are based on the experiments performed by Harteveld et al. (2003, 2004, 2005). These experiments utilized a geometry similar to that applied in the fundamental study. Additionally, the operating conditions of these experiments were such that the assumption of non-coalescing spherical bubbles having approximately the same size was reasonable for the simulations. Finally, the linear stability of the two-fluid model is analyzed to determine what roles the effective viscosity, the bubble pressure, and the interaction terms have in determining whether or not a solution is linearly stable. Overall, the numerical studies presented in this work demonstrate that the effective viscosity model, the bubble-pressure model, and the interaction terms proposed by Kashiwa (1998) should all be considered and included, but that further study may be needed.
1.2 Outline

This thesis includes seven chapters. Chapter 2 provides a review of bubble column simulations reported in the literature. Chapter 3 contains a detailed description of the two-fluid model implemented in CFDLib with an emphasis on the closure models applied in our numerical studies. Additionally, the major subroutines and the discretization scheme within CFDLib are explained. Chapter 4 discusses the characteristics of the homogeneous, transitional, and heterogeneous flow regimes, and then focuses on the ability of the two-fluid model to predict the behavior of these flow regimes. A detailed analysis shows that the flow predictions are highly dependent on the model formulation (i.e., bubble-induced turbulence, drag, lift, rotation, strain, virtual-mass), as well as parameters such as bubble size and liquid coflow. Scale-up to larger column diameters for the flow regimes is also studied. Chapter 5 presents a further analysis of the effect of the two-fluid model formulation on bubble-column flow-regime predictions. Simulations are presented in the form of flow maps, which show the flow behavior expected for a particular value of the bubble Reynolds number and the average void fraction. A particular set of model parameters shows qualitative agreement with experiments performed at Delft University of Technology. Chapter 6 describes how linear stability analysis can be used to determine the stability of the two-fluid model applied toward the CFD predictions. The derivation of the dispersion relations corresponding to the two-fluid model used in this work is presented. Chapter 7 presents a validation study of our results against those of the experimental research group at Delft University of Technology. Specifically, we focus on their rectangular pseudo-two-dimensional column in which non-homogeneous flow can be obtained by changing the aeration pattern. Chapter 8 summarizes the major conclusions and discusses recommendations for future work.
Chapter 2. Literature Review

Factors such as the bubble-rise velocity, bubble-bubble interactions, bubble-fluid interactions, bubble shape and size distribution, gas holdup, and interstitial liquid velocities determine the hydrodynamic behavior of a bubble column. Reliable design and scale-up of a bubble column requires a thorough understanding of the column hydrodynamics, which is difficult due to the complex nature of the flow. Since this complexity has hindered design development, computational fluid dynamics (CFD) has been utilized over the last few decades in order to better understand bubble-column flow behavior (Joshi, 2001). Several authors, including Jakobsen et al. (1997), Joshi (2001), Joshi et al. (2002), Lain et al. (2002), Sokolichin et al. (2004), and Chen and Fan (2004), have discussed recent developments in the fields of modeling and CFD simulation.

A survey of recent papers shows various approaches toward modeling bubble columns, including simple one-dimensional models (Rice and Geary, 1990; Geary and Rice, 1992; Burns and Rice, 1997; Vitankar and Joshi, 2002), two-dimensional gas-liquid mixture models (Sokolichin and Eigenberger, 1994; Sokolichin et al., 1997; Sanyal et al., 1999; Buscaglia et al., 2002), two- and three-dimensional turbulent CFD approaches for flow field computations combined with a compartmental model for handling chemistry computations (Rigopoulos and Jones, 2003), two- and three-dimensional, two-fluid turbulent models with variations in the formulation of the Euler-Euler or the Euler-Lagrangian approach (Torvik and Svendsen, 1990; Lapin and Lübbert, 1994; Grevskott et al., 1996; Delnoij et al., 1997a, b, c; Sokolichin and Eigenberger, 1999; Mudde and Simonin, 1999; Pan et al., 1999; Pan et al., 2000; Pfleger and Becker, 2001; Buwa and Ranade, 2002; Lehr et al., 2002; Michele and Hempel, 2002; Zhou et al., 2002; Oey et al., 2003; Olmos et al., 2003b; Politano et al., 2003; Behzadi et al., 2004; Schallenberg et al., 2005; Wang et al., 2005), and large-eddy simulation (LES) attempts (Deen et al., 2001; Bove et al., 2004).

According to Joshi (2001), the developments made in modeling bubble column flows can be grouped into three classifications. The first classification includes early models that assumed either creeping flow or inviscid flow, and that did not consider the role of turbulence in momentum transfer. The second classification includes models that
account for turbulence, but use simplified assumptions in order to determine eddy diffusivity. However, phase interaction, turbulent dispersion effects, and added-mass effects were not considered. The third classification includes work that utilizes closure models and stresses completeness of the continuity and momentum equations.

2.1 Early Modeling Attempts

The following examples show that while the earliest attempts (the first classification) to model bubble columns applied simplifying assumptions, these works still greatly contributed to understanding the complex flow pattern in bubble columns. Crabtree and Bridgwater (1969) studied how a chain, or vertical line, of bubbles in a viscous liquid would generate bulk motion of the liquid. The chain forms as gas is bubbled in at the center of the bottom of the column. Their model suggests that the bubble chain exerts a force analogous to a line force acting vertically upwards along the central axis of the column. The model gave sufficient predictions of the liquid velocity profile and the induced pressure gradient, and showed that the extent of liquid circulation generated by the gas flow was dependent on gas flow rate, gas volume fraction, and liquid kinematic viscosity. Freedman and Davidson (1969) studied the effect of gas distributor design on gas volume fraction in bubble columns. Their study revealed that poor gas distribution resulted in liquid recirculation and a decrease in gas volume fraction. Additionally, they found that surface active properties have an effect on the minimum gas volume fraction for which bubble coalescence occurs. Rietema and Ottengraf (1970) studied bubble street formation and showed that when the flow was purely laminar and inertial forces could be neglected, bubble column circulation could be predicted through the use of the principle of minimum energy dissipation. Bhavaraju et al. (1978) studied liquid circulation in bubble columns and showed that bubble breakup depends on liquid turbulence in the column rather than the turbulence of the gas entering the column. They called for the development of models that would take into account liquid turbulence.
2.2 Inclusion of Turbulence via Simplified Models

Simplified models that began to account for turbulence are included in the second classification of works to model bubble column flow behavior. These models generally assumed one-dimensional flow and required either a value of velocity near the wall or a value of centerline velocity in order to solve the equation of motion. However, these models also came with several limitations: assuming constant eddy diffusivity, or turbulent kinematic viscosity ($\nu_t$), throughout the column; tuning $\nu_t$ to satisfy either the value of velocity near the wall or the value of the centerline velocity; failing to satisfy the energy balance; inability to apply the correlation for $\nu_t$ toward unknown systems or toward the limiting case of zero superficial velocity; neglecting to consider net liquid flow; neglecting to check the gas phase mass balance; and calculating wall shear stress values that did not satisfy the energy balance (Joshi, 2001).

Hills (1974) demonstrated that local values of gas volume fraction and circulation velocities could be measured, and suggested that the variation of the local radial dispersion coefficient with column radius was indicative of dispersion caused by large-scale eddies. Joshi (1980) found that the liquid phase axial dispersion coefficient was dependent on column diameter and average liquid circulation velocity. For bubble columns, they found that the circulation velocity was dependent on average gas volume fraction, terminal bubble velocity, and superficial gas velocity. Walter and Blanch (1983) used microscopic and macroscopic balances to predict the liquid velocity profile and the average liquid velocity. They found that when liquid velocity is low, the boundary layer at the wall is large, so the velocity profile is controlled by the shear stress at the column walls, resulting in no slip at the wall. Under turbulent flow conditions, the boundary layer at the column wall is very small, so the stress at the wall no longer has an effect on the velocity profile.

Several authors accounted for the radial variation of $\nu_t$ in order to overcome some of the limitations mentioned previously (Joshi, 2001). Sato and Sekoguchi (1975) developed a bubble-induced turbulence (BIT) model for bubbly flows, in which $\nu_t$ caused by bubble-bubble interaction is proportional to the local gas volume fraction, the mean bubble diameter, and the mean relative velocity of the bubbles. Given that the
characteristic length scale is the bubble diameter, Sato’s BIT model can be interpreted as a description of momentum transport induced by the bubble wakes. Sato et al. (1981) then extended the theory toward determining a turbulent heat flux due to bubble-bubble interaction. Rice and Geary (1990) developed a model based on the assumption of two primary zones—a turbulent central core and an adjacent thin viscous wall layer. Their model was used to predict liquid circulation for bubbly and near bubbly flows. The locally varying mixing length was considered to be proportional to both bubble diameter and gas volume fraction. Geary and Rice (1991) then corrected this model to include distorted bubbles. The model was then extended to account for turbulence originating at the column walls (Geary and Rice, 1992). They found that a mixing length scale dependent on bubble size was best for small columns, while a mixing length proportional to the column diameter was appropriate for larger columns. Kumar et al. (1994) acquired gas volume fraction data via computer tomography and liquid velocity data via computer automated radioactive particle tracking for five different column sizes. They found that for identical gas-liquid systems, gas volume fraction and velocity measurements made in smaller columns (yet no smaller than 0.15 m in diameter) could be used to determine a mixing length scale that would sufficiently predict the liquid velocity profiles in larger columns, provided the radial holdup distribution is known. Burns and Rice (1997) utilized an energy dissipation model to determine $\nu_t$ as a function of superficial gas velocity and length scale. A scale based on bubble diameter was used for bubbly flows and a scale based on column diameter was used for turbulent flows. The model resulted in plug-shaped flow profiles in the column core. Additionally, they found that lowering the surface tension allowed uniform circulation to occur in the bubbly flow regime.

2.3 Recent Modeling Contributions

The third classification of bubble column flow modeling focused on the completeness of the continuity and momentum equations. In general, this classification includes the most recent modeling studies (publications from approximately the last 15-20 years). Analyses tend to consider turbulence in two-dimensional (2D) or three-dimensional (3D) two-phase flows, the behavior of circulation cells, interphase energy
transfer, the effect of turbulent dispersion on gas holdup, appropriate closure models, and the effects of the interfacial drag, virtual-mass, and lift forces (Joshi, 2001).

2.3.1 Force Models and Parameters

Our previous work with the two-fluid model (Monahan and Fox, 2002, 2007) has illustrated that high-resolution CFD simulations of air-water bubble columns are sensitive to the physical models and chosen parameters employed in the simulations. A similar conclusion is stated in the recent review paper of Joshi (2001). The recent review paper from Sokolichin et al. (2004), however, suggests that only pressure and drag are the relevant forces for bubble column simulations, and notes that there is no general consensus in the literature regarding how to correctly formulate the two-fluid model for gas-liquid flows, or on the ability of CFD models to predict experimentally observed flow regimes (Sokolichin et al., 2004). The following examples comprise a chronological review of the effects of force models and their associated parameters.

Sokolichin and Eigenberger (1994) and Becker et al. (1994) used a quasi-steady gas phase momentum balance, neglected virtual-mass and lift forces, and assumed a constant value for the drag coefficient. Delnoij et al. (1997a, b, c) accounted for bubble-bubble interactions via an interaction model similar to a collision model, and considered the contributions of liquid phase pressure gradient, drag, lift, virtual-mass, liquid vorticity, and gravity in their 2D Euler-Lagrangian simulations of bubble columns. Delnoij et al. (1997b) found that the virtual-mass force had a significant effect near the gas distributor region. Enabling the virtual-mass force prevented bubbles from initially accelerating at unrealistically high rates. They also showed that when the lift force, directed toward the column walls, was exerted on bubbles in a plume in the center of the column, the plume would widen as expected. If the lift force was not enabled, unrealistic narrow plumes were observed in the column.

Sokolichin and Eigenberger (1999) obtained results similar to those of Delnoij (1997b) with a highly simplified version of the gas-phase momentum balance. Their model assumed a constant slip velocity, and expressed the gas velocity as the sum of the liquid velocity and the slip velocity. They neglected the virtual-mass, lift, and hydrodynamic forces, and did not consider bubble-bubble interactions, but utilized a finer...
grid. Meanwhile, Delnoij (1999) performed 3D simulations in which they continued to account for pressure gradient, drag, lift, virtual-mass, and gravitational forces, but focused on collisions between bubbles and the column walls instead of bubble-bubble collisions. Overall, the flow structures observed from the 3D simulations appeared more complex than those observed from the 2D simulations, as expected.

Pan et al. (1999) utilized both the drag and virtual-mass forces, and suggested that rotational and internal motion could be neglected since individual bubbles move as whole entities. Mudde and Simonin (1999) performed 2D and 3D simulations of a bubble plume, either using only the drag force to account for interfacial momentum transfer, or using drag, virtual-mass, and turbulent pressure effects. Their model utilizes a drag force that includes both a contribution from the mean phase velocity difference and an additional contribution from a drifting velocity. This drifting velocity accounts for the dispersion of bubbles caused by transport by liquid turbulence. They found that if only the drag force is used, the lower part of the plume would not oscillate and the plume would move along the left column wall. Fluctuations were observed in the middle of the plume, but the amplitude and oscillation period of the plume were much smaller than expected. Including virtual-mass resulted in oscillations with an amplitude and period in agreement with experimentally observed behavior. Vortices moved downward with one at the left side of the column and then one at the right side of the column after half a period had passed. The 3D simulations performed by Deen et al. (2001) did not reflect a strong effect of the virtual-mass force. Using only the drag force resulted in a bubble plume that would rise vertically upward with no spreading in other directions. Including the virtual-mass force did not noticeably change the plume behavior. Using only the drag and lift force resulted in a plume that would spread across the column, as similarly observed by Delnoij (1997b). Adding the virtual-mass force yielded only small differences to the flow behavior. Deen et al. (2001) suggested that the minimal effect of the virtual-mass force was due to the fact that the simulations produce a quasi-stationary state in which acceleration is minimal. Bove et al. (2004) modeled the drag coefficient using a drag-distorted model and a drag force model for a bubble in contaminated water.
The latter model improved predictions of slip velocity, but underestimated gas and liquid velocity profiles.

Krishna and van Baten (2001) only considered the drag force in their elevated pressure turbulent flow simulations. They noted a high degree of uncertainty when considering lift forces for both small and large bubbles, and claimed that the virtual-mass force would not be applicable as the large bubbles present in this flow regime experience a high degree of recirculation and do not have closed wakes. Jakobsen (2001) considered the importance of both steady drag and transversal lift forces for phase distribution in bubble columns, and finally concluded that numerical models required further improvements in accuracy and stability. Oey et al. (2003) found that the drag force resulted in suitable representations of global bubble column dynamics, while the virtual-mass force could be used to tune the simulation results. They also noted that further research regarding the importance of the lift force was necessary.

Lucas et al. (2005, 2006) studied the effect of the lift force on the stability of a homogeneous bubble column, and found that a positive lift coefficient (corresponding to small bubbles) would stabilize the flow, while a negative lift coefficient (corresponding to large bubbles) would lead to instability and the onset of heterogeneous flow. A subsequent stability analysis for a monodispersed case showed that the influence of the lift force was higher than that of the turbulent dispersion force. Dijkhuizen et al. (2005) calculated the drag and virtual-mass forces using a 3D front tracking model and a 2D volume-of-fluid (VOF) model, the latter used to determine the influence of the third dimension. Bubbles with equivalent diameter ranging from 1 mm to 10 mm were considered. Terminal bubble rise velocities calculated with the 3D front tracking model agreed well with experimental data, while the 2D VOF model showed disagreement for bubbles smaller than 3 mm, caused by an underestimation of surface tension forces. The 3D front tracking model successfully predicted values for the mean bubble aspect ratio, while the 2D VOF model overestimated the values of mean aspect ratio for larger bubbles. Both the 3D front tracking model and the 2D VOF model yielded values of the drag and virtual-mass coefficients that were comparable to theoretical values.
2.3.2 Turbulence Modeling and Grid Resolution

As mentioned previously, the most recent attempts to model bubble column behavior involved the use of detailed closure models to account for turbulence (Joshi, 2001). Several researchers have utilized the standard $k$-$\varepsilon$ model developed for single-phase flows in order to model turbulence in the liquid phase. However, the fact that turbulence generated by the gas phase is not considered is a notable limitation. Such turbulence can be accounted for through other means such as Sato’s bubble-induced turbulence model, discussed in Section 2.2, or modifications to the $k$-$\varepsilon$ model (Sokolichin et al., 2004). It should be noted that even at low gas flow rates, where the liquid phase is laminar away from the bubble wakes, the Reynolds number based on the bubble rise velocity is typically large ($\sim 10^1$-$10^3$). Thus, Sato’s BIT model can still be applied to these gas-liquid flows. However, at high gas flow rates, the momentum transfer from the gas phase can be high enough to generate large-scale turbulence in the liquid phase. In fully turbulent two-phase flows, this contribution to the liquid-phase turbulence can be modeled through an extra source term in the $k$-$\varepsilon$ turbulence model. A discussion of several recent notable contributions to turbulence modeling in bubble column simulations follows, and an overview of the mathematical approaches and turbulence models can be found in Table 2.1.

Several researchers studied the use of the standard $k$-$\varepsilon$ model. For example, Becker et al. (1994) found that using the 2D, two-fluid model with constant viscosity, increased by a factor of 100, would sufficiently represent both steady and transient flow patterns in 2D bubble columns, while the standard $k$-$\varepsilon$ model yielded very high values of turbulent viscosity, which in turn dampened out vortices. Sokolichin and Eigenberger (1999) utilized a 2D laminar model, a 2D standard $k$-$\varepsilon$ model, and a 3D standard $k$-$\varepsilon$ model. For the 2D laminar case, the results depended strongly on grid resolution. The 2D $k$-$\varepsilon$ model produced an overestimate of the effective viscosity by one order of magnitude, and the expected vortices were dampened. Sokolichin and Eigenberger (1999) believed that the small column depth resulted in decreased turbulence intensity. The expected oscillating plumes and vortices were obtained with the 3D $k$-$\varepsilon$ model. Mudde and Simonin (1999) used the standard $k$-$\varepsilon$ model on both 2D and 3D domains.
The 2D case resulted in a single stationary liquid circulation cell, in which turbulent viscosity was overestimated and oscillations were subsequently damped. The 3D $k$-$\varepsilon$ simulations resulted in a transient solution. Using a low Reynolds $k$-$\varepsilon$ model did not result in any significant changes in flow behavior.

Including the BIT model developed by Sato et al. (1975) is one of the simplest ways to consider the effect of bubble-generated turbulence (Sokolichin et al., 2004). Pan et al. (1999) found that including both interphase momentum transfer models and Sato’s bubble-induced turbulent viscosity yielded sufficient predictions for mean flow values in the dispersed flow regime, or for low gas superficial velocities. Deen et al. (2001) performed both large-eddy simulations and simulations using the standard $k$-$\varepsilon$ model. Sato’s BIT model was included in both simulation cases in order to consider the effect of turbulence produced by bubble movement. However, they did not observe any significant effects from including the BIT model. Bove et al. (2004) performed very large-eddy simulations (VLES) and studied Sato’s model on the flow behavior. They found that bubble-induced turbulence was of particular importance near the gas inlet when large inlet gas velocities are used.

Additional source terms could be added to the $k$-$\varepsilon$ model to account for bubble-generated turbulence. Sanyal et al. (1999) modeled liquid phase turbulence with a modified $k$-$\varepsilon$ model, in which extra terms accounting for interphase turbulent momentum transfer were included. These additional terms were dependent on liquid-gas velocity covariance. While the model provided reasonable predictions of kinetic energy profiles, Sanyal et al. (1999) noted that further improvements to turbulence modeling were needed. Pfleger and Becker (2001) included an additional term in the $k$-$\varepsilon$ model to account for the generation of turbulence by local shear forces in the liquid phase, and this term assumed that bubble-induced turbulence is proportional to the interphase momentum exchange. The proportionality constant was equal to 1.44 in the $k$-equation and 1.92 in the $\varepsilon$-equation. Accounting for bubble-induced turbulence improved the radial profiles of axial velocities, but worsened predictions of local and global gas volume fraction. Lain et al. (2002) developed a consistent Lagrangian formulation in which the standard $k$-$\varepsilon$ model was modified to include source terms in the $k$ and $\varepsilon$ equations to allow for the
effect of bubble-generated turbulence. It was assumed that the pressure gradient and the drag, virtual-mass, and lift forces affected turbulent quantities, so these forces were considered in the source terms added to the $k$-$\epsilon$ model. Lain et al. (2002) found that the production and dissipation of fluctuating liquid kinetic energy is caused by the bubble source. They subsequently concluded further research toward modeling of the bubble source terms in the $k$ and $\epsilon$ equations was necessary to properly model the flow behavior in bubble columns.

Other researchers have proposed different methods in order to model turbulence. Delnoij et al. (1997a, b, c) assumed a 2D laminar flow model and included a hard sphere collision model to account for bubble-bubble interactions. Oscillating bubble plumes and liquid phase vortices were observed. Politano et al. (2003) developed a polydisperse two-phase model to study the effect of bubble size on radial phase distribution in vertical channels. A $k$-$\epsilon$ model for two-phase flows was applied, and a model for potential flow around a bubble accounted for bubble-induced turbulence. The authors noted that the two-phase $k$-$\epsilon$ model must reduce to the single-phase model when the gas volume fraction approached zero; thus, the constants used in the two-phase $k$-$\epsilon$ model were the same as those used in the standard $k$-$\epsilon$ model. In order to determine near-wall boundary conditions for the two-fluid and $k$-$\epsilon$ models, Politano et al. (2003) developed a logarithmic wall law for two-phase flows. The two-phase flow was accounted for by adding a first-order correction to the logarithmic law of the wall. Near-wall turbulence was determined by analyzing the asymptotic behavior of the $k$-$\epsilon$ model. Politano et al. (2003) found good agreement with several experiments; however, they noted that their model was only applicable for low superficial velocities, and that further examination of near-wall turbulence was necessary to assure consistent predictions of turbulent viscosity in the presence of bubbles in the near-wall region.

Behzadi et al. (2004) used an Eulerian two-fluid model for studying two-phase flow at high dispersed-phase volume fractions. The authors noted that as the dispersed-phase volume fraction increases, turbulence becomes increasingly less dominated by the continuous phase. Behzadi et al. (2004) presented a $k$-$\epsilon$ turbulence model based on the mixture of the continuous and dispersed phases. The model was applicable for all
volume fraction values and thus reduced to the single-phase $k$-$\varepsilon$ model when only one of the two phases was present. The turbulent fluctuations of the continuous and dispersed phases were related by a response function dependent on the dispersed-phase volume fraction. Behzadi et al. (2004) observed improved agreement with experiments, but also noted that further research into turbulence modeling was needed for more accurate predictions.

Grid resolution can have a significant effect on simulation accuracy; however, an increase in grid refinement requires an increase in computational cost. The following examples illustrate the role of grid resolution in bubble column simulations, and a comparison among grid resolutions used by various researchers can be found in Table 2.2.

Becker et al. (1994) obtained a stationary result with a coarse grid (6 x 2.78 cm$^2$); whereas with a finer grid (3 x 1.39 cm$^2$), a transient solution was obtained that reflected experimentally observed bubble swarm behavior. Sokolichin and Eigenberger (1999) also investigated the effect of grid size for the laminar model using five different grids for their 2D simulations (2 x 2; 1 x 1; 0.5 x 0.5; 0.25 x 0.25; 0.125 x 0.125 cm$^2$) and three different grids for their 3D simulations (2 x 2 x 2; 1 x 1 x 1; 0.667 x 0.667 x 0.667 cm$^3$). The number of circulation cells resolved by the simulations was found to increase with the increased spatial resolution. Pfleger and Becker (2001) performed 3D cylindrical simulations for several different grid resolutions. The amount of grid cells ranged from 6150 to 62,400, with a 12300-cell grid considered the standard. While the finer grids improved the accuracy of the results, they required extensive computational effort. Pfleger and Becker (2001) utilized the standard grid size as a compromise between simulation accuracy and computational cost. Lain et al. (2002) used two different grids (0.433 x 0.28; 0.295 x 0.2 cm$^2$) in order to test for grid independence. They found only slight differences between the resulting flow profiles from each domain, and concluded that the coarser grid was sufficient.
<table>
<thead>
<tr>
<th>Author</th>
<th>Approach</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Becker et al. (1994)</td>
<td>Euler-Euler</td>
<td>2D, Laminar viscosity increased by factor of 100</td>
</tr>
<tr>
<td>Sokolichin &amp; Eigenberger (1994)</td>
<td>Euler-Euler</td>
<td>Laminar, 2D</td>
</tr>
<tr>
<td>Delnoij et al. (1997 a, b)</td>
<td>Euler-Lagrange</td>
<td>Laminar, 2D, hard-sphere collision model</td>
</tr>
<tr>
<td>Delnoij et al. (1997c)</td>
<td>Euler-Lagrange</td>
<td>Laminar, Pseudo-2D, hard-sphere collision</td>
</tr>
<tr>
<td>Jakobsen et al. (1997)</td>
<td>Euler-Euler</td>
<td>2D axisymmetric, modified k-ε model</td>
</tr>
<tr>
<td>Delnoij et al. (1999)</td>
<td>Euler-Lagrange</td>
<td>Laminar, 3D</td>
</tr>
<tr>
<td>Krishna et al. (1999)</td>
<td>Three phase Euler-Euler</td>
<td>3D cylindrical, standard k-ε model</td>
</tr>
<tr>
<td>Mudde &amp; Simonin (1999)</td>
<td>Euler-Euler</td>
<td>2D, 3D, Standard or low Reynolds k-ε models</td>
</tr>
<tr>
<td>Pan et al. (1999)</td>
<td>Euler-Euler</td>
<td>2D, Sato’s model</td>
</tr>
<tr>
<td>Pfleger et al. (1999)</td>
<td>Euler-Euler</td>
<td>2D, 3D, Standard k-ε model</td>
</tr>
<tr>
<td>Sanyal et al. (1999)</td>
<td>Euler-Euler</td>
<td>2D axisymmetric, Modified k-ε model</td>
</tr>
<tr>
<td>Sokolichin &amp; Eigenberger (1999)</td>
<td>Euler-Euler</td>
<td>2D, 3D, Laminar, and standard k-ε model</td>
</tr>
<tr>
<td>Padial et al. (2000)</td>
<td>Euler-Euler</td>
<td>3D conical domain, multiphase k-ε model</td>
</tr>
<tr>
<td>Deen et al. (2001)</td>
<td>Euler-Euler</td>
<td>3D, Standard k-ε model &amp; LES, each combined with Sato’s BIT model</td>
</tr>
<tr>
<td>Pfleger &amp; Becker (2001)</td>
<td>Euler-Euler</td>
<td>3D, k-ε model with bubble-induced turbulence via additional production terms in k-ε equations</td>
</tr>
<tr>
<td>Lain et al. (2002)</td>
<td>Euler-Lagrange</td>
<td>2D axisymmetric, modified k-ε model</td>
</tr>
<tr>
<td>Lehr et al. (2002)</td>
<td>Euler-Euler</td>
<td>3D, k-ε model with shear and bubble-induced terms</td>
</tr>
<tr>
<td>Monahan &amp; Fox (2002)</td>
<td>Euler-Euler</td>
<td>2D, Laminar</td>
</tr>
<tr>
<td>Olmos et al. (2003)</td>
<td>Multiple gas phase Euler-Euler</td>
<td>Population balance, 2D axisymmetric, modified k-ε model or Sato’s model</td>
</tr>
<tr>
<td>Politano et al. (2003)</td>
<td>Polydisperse model based on Euler-Euler two-fluid model</td>
<td>2D axisymmetric, N groups of constant mass to represent polydispersity, k-ε model for two-phase flows</td>
</tr>
<tr>
<td>Behzadi et al. (2004)</td>
<td>Euler-Euler</td>
<td>2D, mixture k-ε model with turbulent response function</td>
</tr>
<tr>
<td>Bove et al. (2004)</td>
<td>Euler-Euler</td>
<td>3D, VLES with Sato’s model</td>
</tr>
<tr>
<td>Dijkhuizen et al. (2005)</td>
<td>Euler-Lagrange Euler-Euler</td>
<td>3D front-tracking method and 2D volume-of-fluid method</td>
</tr>
<tr>
<td>Schallenberg et al. (2005)</td>
<td>Three phase Euler-Euler</td>
<td>3D, modified k-ε model to account for bubble-induced turbulence</td>
</tr>
</tbody>
</table>
Table 2.2. Comparison of grid resolutions used in bubble column simulations.

<table>
<thead>
<tr>
<th>Author</th>
<th>Grid cell size in cm (H x W x D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Becker et al. (1994)</td>
<td>6 x 2.78; 3 x 1.39</td>
</tr>
<tr>
<td>Sokolichin &amp; Eigenberger (1994)</td>
<td>1 x 0.6</td>
</tr>
<tr>
<td>Delnoij et al. (1997 a, b)</td>
<td>1.5 x 1</td>
</tr>
<tr>
<td>Delnoij et al. (1997c)</td>
<td>0.875 x 0.875</td>
</tr>
<tr>
<td>Jakobsen et al. (1997)</td>
<td>15 x 29 cells in computational grid</td>
</tr>
<tr>
<td>Delnoij et al. (1999)</td>
<td>0.875 x 0.875 x 0.875</td>
</tr>
<tr>
<td>Krishna et al. (1999)</td>
<td>4800 total cells. Radial: 10 cells in central core region, 20 cells near wall region</td>
</tr>
<tr>
<td></td>
<td>Axial: 1 cm cells in first 20 cm at column bottom, 2 cm cells for remainder of column</td>
</tr>
<tr>
<td>Mudde &amp; Simonin (1999)</td>
<td>3 x 2; 3 x 1.39; 3 x 2 x 1; 3 x 1.39 x 0.5</td>
</tr>
<tr>
<td>Pan et al. (1999)</td>
<td>0.8 x 0.5 in general, more refined near air injectors</td>
</tr>
<tr>
<td>Pfleger et al. (1999)</td>
<td>Standard grid has 40000 cells; coarsest is 45 x 22 x 5 cells and finest is 90 x 44 x 15 cells</td>
</tr>
<tr>
<td>Sanyal et al. (1999)</td>
<td>0.66 x 0.5</td>
</tr>
<tr>
<td>Sokolichin &amp; Eigenberger (1999)</td>
<td>2D: 2 x 2; 1 x 1; 0.5 x 0.5; 0.25 x 0.25; 0.125 x 0.125</td>
</tr>
<tr>
<td></td>
<td>3D: 2 x 2 x 2; 1 x 1 x 1; 0.667 x 0.667 x 0.667</td>
</tr>
<tr>
<td>Deen et al. (2001)</td>
<td>1 x 1 x 1</td>
</tr>
<tr>
<td>Padial et al. (2000)</td>
<td>Cells have 8 vertices and 6 faces; mesh uses 67 blocks with 4620 real cells, with 20280 ghost cells to aid communication between blocks</td>
</tr>
<tr>
<td>Pfleger &amp; Becker (2001)</td>
<td>Quadrilateral cells in number ranging from 6150 (coarsest) to 62400 (finest); standard is 123000 cells</td>
</tr>
<tr>
<td>Buscaglia et al. (2002)</td>
<td>3.2 x 1.4; 1.6 x 0.7</td>
</tr>
<tr>
<td>Buwa &amp; Ranade (2002)</td>
<td>Quadrilateral cells in number ranging from 2975 (coarsest) to 106628 (finest); mid-range is 16544 cells</td>
</tr>
<tr>
<td>Lain et al. (2002)</td>
<td>0.433 x 0.28; 0.295 x 0.2</td>
</tr>
<tr>
<td>Lehr et al. (2002)</td>
<td>Block structured grid; edges of volume elements are 1-2 cm long</td>
</tr>
<tr>
<td>Michele &amp; Hempel (2002)</td>
<td>Coarse grid with average cell length of 5.9 cm, resulting in 13600 total cells</td>
</tr>
<tr>
<td>Monahan &amp; Fox (2002)</td>
<td>1 x 1; 0.5 x 0.5; 0.25 x 0.25</td>
</tr>
<tr>
<td>Olmos et al. (2003)</td>
<td>0.5 x 0.5</td>
</tr>
<tr>
<td>Behzadi et al. (2004)</td>
<td>Domain describes sudden expansion in a pipe; grids of 40 x 210 cells and 80 x 420 cells used; mesh is graded such that it is more refined near the sudden expansion</td>
</tr>
<tr>
<td>Bove et al. (2004)</td>
<td>1.5 x 2.5 x 2.5; 1.5 x 1.67 x 1.67; 1 x 1 x 1</td>
</tr>
<tr>
<td>Dijkhuizen et al. (2005)</td>
<td>2D VOF: 160 x 320 cells</td>
</tr>
<tr>
<td></td>
<td>3D front-tracking: 80 x 80 x 80 cells</td>
</tr>
<tr>
<td>Schallenberg et al. (2005)</td>
<td>3D domain with 0.6 m diameter and 5 m height; 36000 calculation nodes on an unstructured grid</td>
</tr>
</tbody>
</table>
2.3.3 Predictions for Flow Regimes and Transitions

As noted in Chapter 1, the inlet flow conditions determine whether homogeneous or heterogeneous flow will be observed in the bubble column. In general, most literature studies have been limited to the prediction of one particular flow regime. Several researchers, however, have developed models to predict flow-regime transitions, usually caused by changes in the gas flow rate and/or the column dimensions. The effects of bubble coalescence and breakup may also be considered. Recent contributions that focus on modeling transitional flow behavior are given in the following examples.

Shnip et al. (1992) used linear stability theory to develop criteria for the transition from homogeneous to heterogeneous flow for 2D bubble columns operating in either the semibatch or the continuous mode. They found that the maximum critical gas volume fraction, an indicator of transitional behavior, was approximately 0.42. Additionally, they found that cocurrent liquid flow hindered transition to the heterogeneous regime, while countercurrent liquid flow aided transitional behavior. Ruzicka et al. (2001a) developed a physical model based on the hydrodynamic coupling between the gas and liquid phases. Numerical expressions described the gas volume fraction-gas flow dependence observed in the homogeneous, transitional, and heterogeneous regimes. The model also provided a stability condition for the homogeneous regime, predicted the critical gas flow-rate that signaled transitional behavior, and predicted the maximum possible gas holdup. Ruzicka et al. (2001) validated their model with data from four individual air-water bubble column experiments, and found that the model agreed with the linear stability theory previously presented by Shnip et al. (1992). Ruzicka et al. (2001b) then extended their work to examine the effect of column geometry on flow-regime transitions. They found that an increase in both the column height and width resulted in a loss of stability in the homogeneous regime and thus facilitated the transition to the heterogeneous regime.

The recent works of Olmos et al. (2001, 2003a, b) are notable for their examination of more than one bubble column flow regime. They first combined the Euler-Euler two-fluid model with a population balance model, allowing bubbles to be distributed into 10 different diameter classes and yielding predictions for liquid velocity
and gas volume fraction profiles. Comparison with experiments showed good agreement in the homogeneous regime. The onset of transitional behavior was marked by an underestimate of the global gas volume fraction. When superficial gas velocity $u_g$ was less than 4.7-4.8 cm/s, the sparger had the most influence on the flow behavior, and a narrow bubble size distribution was observed. When $u_g$ was greater than 4.7-4.8 cm/s, bubble breakup became more prominent, resulting in a broader bubble size distribution (Olmos et al., 2001). In order to achieve a better representation of flow regime transitions, Olmos et al. (2003b) developed a two-step calculation. In the first step, a population balance model combined with a single gas phase Euler-Euler model was used to determine bubble size distributions, and in the second step, the distributions were applied in a multiple gas phase Euler-Euler model. Bubble-induced turbulence was also considered, first via Sato and Sekoguchi’s (1975) model, and then by adding source terms to the $k-\varepsilon$ equations to account for turbulence produced in bubble wakes. It was concluded that the latter provided the better representation of liquid turbulence and energy dissipation. Comparison with experiments showed that the model successfully predicted flow regime transitions, hydrodynamic properties, and turbulence (Olmos et al., 2003b).

Wang et al. (2005) applied a population balance model to determine bubble size distributions. Their model accounted for bubble coalescence caused by turbulent eddies, a difference in bubble rise velocities, and/or bubble wake entrainment, and bubble breakup arising from eddy collisions and/or instability of large bubbles. The population balance model successfully calculated bubble size distributions in the homogeneous and heterogeneous regimes. A sudden decrease in the volume fraction of small bubbles indicated transitional behavior, which occurred for a superficial gas velocity of approximately 4 cm/s for an air-water system.

2.4 Summary

This review has illustrated that important characteristics such as bubble-bubble interactions, two-phase turbulence modeling, gas-liquid interfacial mass, momentum, and energy-transfer mechanisms, coupling between the phases, and the required grid resolution still need to be resolved. For example, at low gas velocities, homogeneous
bubbly flow regimes have been observed experimentally. The gas phase is uniformly distributed and moves vertically upward with no large-scale flow structures (Garnier et al. 2002a, b; Harteveld, 2005). In contrast, grid-independent CFD simulations for this case using the standard two-fluid model approach exhibit highly turbulent, inhomogeneous two-phase flow (Monahan and Fox, 2002). Such disagreement between simulations and experiments shows that the two-fluid CFD models for gas-liquid flows as presently formulated is in need of further validation, and provides motivation for a careful investigation of the capabilities of CFD models.
Chapter 3. Model Theory and Computational Background

There are two primary methods that can be applied toward the numerical simulation of bubble columns: Eulerian-Eulerian and Eulerian-Lagrangian. The Eulerian-Eulerian method uses the two-fluid model to describe both the gas and the liquid phases. The system is considered to be a continuum with averaged transport equations to describe the flow behavior. In the Eulerian-Lagrangian method, only the liquid phase is treated as a continuum (serving as the continuous phase), while the dispersed phase (gas) is described by solving equations of motion for individual bubbles, or bubble tracking. This method is best for fundamental studies, including the effects of bubble-bubble or bubble-liquid interaction. However, the Eulerian-Lagrangian method is limited to cases having low superficial gas velocity and low gas holdup. Meanwhile, the Eulerian-Eulerian method is preferred for modeling industrial applications, since these columns tend to operate with high superficial gas velocity, in turn producing higher values of gas holdup and turbulent flow (Pan et al., 2000).

In this work, the Eulerian two-fluid model is employed to simulate bubble column flow dynamics. CFDLib, a cell-centered, finite-volume Fortran code developed by Los Alamos National Laboratory, is used for all simulations (Kashiwa et al., 1994). The first part of this chapter focuses on the two-fluid model implemented in CFDLib and the relevant closure models, and the second part of this chapter describes the CFDLib code and its discretization method.

3.1 Two-Fluid Model

The basic model equations for multi-component flows used in CFD codes can be found in Drew and Passman (1999). Note, however, that only a small subset of these equations is included in most CFD simulations for gas-liquid flows reported in the literature. For example, it is generally accepted that the terms describing drag and viscous stress must be included. As discussed later in this section, several forces modeled in CFDLib differ slightly from the description in Drew and Passman (1999).

For consistency, the subscript \( c \) denotes the continuous phase (water), and the subscript \( d \) represents the dispersed phase (air). Volume fraction, density, and velocity of
each phase are represented by $\alpha$, $\rho$, and $u$, respectively. The physical parameters correspond to air and water at room temperature and pressure. The bubble diameter is an input value and is assumed to be uniform and constant.

The continuity equations for the continuous and dispersed phases are, respectively

$$\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c u_c) = 0,$$  

(3.1)

and

$$\frac{\partial \alpha_d \rho_d}{\partial t} + \nabla \cdot (\alpha_d \rho_d u_d) = 0.$$

(3.2)

The momentum balances for the continuous and dispersed phases are, respectively

$$\alpha_c \rho_c \frac{\partial u_c}{\partial t} + \alpha_c \rho_c u_c \cdot \nabla u_c = -\alpha_c \nabla p + \nabla \cdot \alpha_c \mu_{eff,c} \left[ \nabla u_c + (\nabla u_c)^T \right] + \sum F_{fc} + \alpha_c \rho_c g$$  

(3.3)

and

$$\alpha_d \rho_d \frac{\partial u_d}{\partial t} + \alpha_d \rho_d u_d \cdot \nabla u_d = -\alpha_d \nabla p - \nabla P_d + \nabla \cdot \alpha_d \mu_{eff,d} \left[ \nabla u_d + (\nabla u_d)^T \right] + \sum F_{fd} + \alpha_d \rho_d g.$$  

(3.4)

The terms on the right-hand sides of Eqs. 3.3 and 3.4 represent, from left to right, the pressure gradient, effective stress, interfacial momentum exchange, and the gravitational force. The $\nabla P_d$ expression in Eq. 3.4 represents the bubble pressure model, which is only considered in the dispersed phase. The closures for the bubble pressure model, effective stress, and interfacial momentum exchange are discussed below.

It is of course necessary that $\alpha_c + \alpha_d = 1$. Additionally, the phase densities $\rho_c$ and $\rho_d$ are assumed to be constant in this work. Therefore, the phase-average velocity

$$(u_v = \alpha_c u_c + \alpha_d u_d)$$

is solenoidal: $\nabla \cdot u_v = 0$. This statement can be used to determine the governing equation for the pressure $p$ in Eqs. 3.3 and 3.4. Both phases are assumed to share the same pressure $p$ expressed in the momentum balances. Appendix A demonstrates how the mass and momentum balance equations and the following relevant closures in the two-fluid model can be made dimensionless.
3.1.1 Bubble Pressure Model

The bubble pressure model represents the transport of momentum due to bubble velocity fluctuations, collisions, and hydrodynamic interactions. It is believed to be a significant factor in bubble-phase stability (Spelt and Sangani, 1998). The bubble-phase pressure is composed of a kinetic component caused by fluctuations in bubble motion, a collisional component due to collisions between bubbles, and a hydrodynamic component due to the relative motion of the bubbles and the spatial and velocity distribution of the bubbles (Spelt and Sangani, 1998).

A study performed by Spelt and Sangani (1998) demonstrates that as $\alpha_d$ increases from zero, the bubble-phase pressure will increase from zero, attain a maximum value, and then decrease. As a result, if $\alpha_d$ is suitably small, then $dP_d/d\alpha_d$ is both positive and proportional to relative velocity and $\alpha_d$, and the collisional and hydrodynamic components are not considered. These assumptions give rise to the following expression for the bubble-phase pressure:

$$ P_d = \rho_c C_{BP} \alpha_d \left( u_d - u_c \right) \cdot \left( u_d - u_c \right). $$

(3.5)

A positive value of $dP_d/d\alpha_d$ tends to force bubbles to move from areas of higher $\alpha_d$ to areas of lower $\alpha_d$. This helps to stabilize the bubbly-flow regime. However, as $\alpha_d$ increases, the collisional and the hydrodynamic components become significant (Sankaranarayanan and Sundaresan, 2002).

Biesheuvel and Gorissen (1990) proposed a bubble pressure model with the following form:

$$ P_d = \rho_c C_{BP} \alpha_d \left( u_d - u_c \right) \cdot \left( u_d - u_c \right) H(\alpha_d), $$

(3.6a)

where (Batchelor, 1988)

$$ H(\alpha_d) = \left( \frac{\alpha_d}{\alpha_{dcp}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dcp}} \right). $$

(3.6b)

In Eq. 3.6a, $C_{BP}$ is a proportionality constant, and $\alpha_{dcp}$ in Eq. 3.6b represents the gas void fraction at close packing, which is set equal to 1.0 in this work. The closures defined in
Eqs. 3.5 and 3.6a suggest that \( P_d \) approaches zero as \( \alpha_d \) approaches zero. When examining the change in \( P_d \) as defined in Eq. 3.5 with respect to \( \alpha_d \),

\[
\frac{dP_d}{d\alpha_d} = \rho_c C_{BP} (\mathbf{u}_d - \mathbf{u}_c) \cdot (\mathbf{u}_d - \mathbf{u}_c),
\]

(3.7)

it can be seen that Eq. 3.7 suggests that \( \frac{dP_d}{d\alpha_d} \) continues to be nonzero as \( \alpha_d \) approaches zero. However, the change in \( P_d \) as defined in Eq. 3.6a with respect to \( \alpha_d \) is given by

\[
\frac{dP_d}{d\alpha_d} = \rho_c C_{BP} (\mathbf{u}_d - \mathbf{u}_c) \cdot (\mathbf{u}_d - \mathbf{u}_c) \left[ \frac{2\alpha_d}{\alpha_{dep}} \left( 1 - \frac{\alpha_d}{\alpha_{dep}} \right) + \left( \frac{\alpha_d^2}{\alpha_{dep}} \right) \left( 0 - \frac{1}{\alpha_{dep}} \right) \right].
\]

(3.8)

Eq. 3.8 suggests that \( \frac{dP_d}{d\alpha_d} \) approaches zero as \( \alpha_d \) approaches zero (Sankaranarayanan and Sundaresan, 2002). For this reason, Eq. 3.6a is used to represent the bubble pressure model in this work.

It should be noted that Kashiwa and Rauenzahn (2004) have recently proposed a zero-order (in terms of velocity gradients) addition to the two-fluid model that can be written in the form of forces similar to the bubble-pressure model, but for both phases:

\[
f_d = -\tilde{C}_r \rho_c \left| \mathbf{u}_d - \mathbf{u}_c \right|^2 \nabla \alpha_d - \tilde{C}_v h_v \rho_c (\mathbf{u}_d - \mathbf{u}_c) \cdot (\mathbf{u}_d - \mathbf{u}_c) \cdot \nabla \alpha_d
\]

(3.9a)

and

\[
f_c = -\tilde{C}_r \rho_c \left| \mathbf{u}_d - \mathbf{u}_c \right|^2 \nabla \alpha_c - \tilde{C}_v h_v \rho_c (\mathbf{u}_d - \mathbf{u}_c) \cdot (\mathbf{u}_d - \mathbf{u}_c) \cdot \nabla \alpha_c,
\]

(3.9b)

where \( \tilde{C}_r \) is the net repulsive coefficient found in the limit of potential flow, \( \tilde{C}_v \) is the net viscous coefficient, and \( h_v \) is a close-spacing function that depends on the separation distance between two spheres. A discussion on how the values of these parameters are determined can be found in Kashiwa and Rauenzahn (2004). Note that \( f_d + f_c = 0 \) so that these bubble-bubble-interaction terms will cancel in the phase-average momentum equation. Eqs. 3.9a and 3.9b cannot truly be represented as pressure gradients since the right-hand sides need not be irrotational. However, they do account for bubble-bubble
interactions similar to the bubble-pressure models defined by Eqs. 3.5 and 3.6a. Kashiwa and Rauenzahn (2004) show that these terms will have a stabilizing effect on the uniform-flow solution in the limit of zero viscosity (i.e., they show that the 1D two-fluid model is unconditionally hyperbolic). However, Eqs. 3.9a and 3.9b have not yet been implemented into the CFDLib code, and are thus not considered in the simulations discussed in this work.

3.1.2 Effective Viscosity and Turbulence Modeling

The stress term for phase \( k (k = c, d) \) is expressed as

\[ \nabla \cdot \alpha_k \mu_{eff,k} \begin{bmatrix} \nabla u_k + (\nabla u_k)^T \end{bmatrix}, \]

(3.10)

where \( \mu_{eff,k} \) represents the effective viscosity, which is the sum of the molecular viscosity of phase \( k \) and the turbulent viscosity:

\[ \mu_{eff,k} = \mu_{0,k} + \mu_{r,k}. \]

(3.11)

The majority of the simulations in this work assume that the effective viscosity for the continuous phase is the sum of the molecular viscosity of the continuous phase and the turbulent viscosity, or \( \mu_{eff,c} = \mu_{0,c} + \mu_{t,c} \), and that the effective viscosity for the dispersed phase is equal to the molecular viscosity of the dispersed phase, or \( \mu_{eff,d} = \mu_{0,d} \).

However, additional studies are performed in which the effective viscosity for the dispersed phase is also assumed equal to the sum of the molecular viscosity of the dispersed phase and the turbulent viscosity, or \( \mu_{eff,d} = \mu_{0,d} + \mu_{r,d} \).

The inclusion and modeling of the turbulent viscosity is one possible method to account for bubble-bubble interactions, which have a significant effect on the flow behavior observed in bubble columns. For example, the experiments of Duineveld (1994) focused on how either the rise velocity of bubbles or the approach velocity of bubbles affects bouncing and coalescence phenomena. The experiments showed that the liquid between two bubbles opposes the relative motion caused by the two bubbles approaching each other. The relative motion leads to an increase in the pressure in the film between the bubbles, and this pressure increase pushes the liquid out from the film. The bubbles will bounce if the pressure in the liquid film becomes high enough to stop
the relative motion of the bubbles. Otherwise, the bubbles will coalesce (Delnoij et al., 1997b). These interactions result in additional turbulence in the liquid phase. As bubbles travel upward in the column, a portion of the energy released is dissipated at the gas-liquid interface, while the remaining energy passes to the liquid phase, where it is finally dissipated at very small scales in the wakes of the bubbles (Joshi, 2001).

There are several models that attempt to account for this bubble-induced turbulence (Sokolichin et al., 2004). This work utilizes the bubble-induced turbulence (BIT) model proposed by Sato and Sekoguchi (1975), which yields a turbulent viscosity that is proportional to the bubble diameter and slip velocity of the rising bubbles:

$$\mu_{t,c} = \rho_c C_{BT} C_{d} \alpha d |u_d - u_c|,$$

where the proportionality constant $C_{BT}$ is equal to 0.6 (Sato et al., 1981). Generally, the turbulent viscosity for the continuous (liquid) phase calculated in Eq. 3.12 is then added to the molecular viscosity in the continuous phase, resulting in an effective viscosity in the continuous phase, as seen in Eq. 3.11. Additional studies are performed to determine the effect when the BIT model is also applied for the dispersed (bubble) phase.

Several researchers, including Pan et al. (1999), have included Sato’s BIT model in their simulations. Pfleger and Becker (2001) observed an improvement in the simulation of radial profiles of axial velocities, but were less successful when predicting gas holdup. Deen et al. (2001) carried out simulations on square cross-sectioned bubble columns, and combined the BIT model with either a large-eddy-simulation (LES), or the $k$-$\varepsilon$ model. However, they found that the BIT model did not have a significant effect on their results.

The turbulent viscosity can be determined through other methods, such as the $k$-$\varepsilon$ model or LES (Sokolichin et al., 2004). The turbulent viscosity for a general phase $k$ that is calculated from the $k$-$\varepsilon$ model (Padial et al., 2000) is

$$\mu_{t,k} = c_{\mu,k} \rho_k \left( \frac{k^2_k}{\varepsilon_k} \right),$$

where (Padial et al., 2000)
The constant $c_{\mu}^0$ is equal to 0.09 and $E_{kl}$ represents the turbulence energy exchange rate coefficient (Padial et al., 2000) defined as

$$E_{kl} = a_k a_l \left( \frac{\rho_k \rho_l}{\rho_k + \rho_l} \right) \frac{\sqrt{k_k + k_l}}{d_b} \left( 1 + Re_e^{0.6} \right).$$

Padial et al. (2000) state that the $k$-$\varepsilon$ model presented in CFDLib calculates the turbulence generated at the gas-liquid interface in the form of a slip-production energy term. The turbulence kinetic energy ($k$) and turbulence energy decay rate ($\varepsilon$) equations, respectively, for a general phase $k$ are expressed as (Padial et al., 2000)

$$\rho_k \frac{dk_k}{dt} = \nabla \cdot \left( \frac{\rho_k \nu_k \nabla k_k}{\phi_k} \right) - \rho_k R_k : \nabla u_k - \rho_k \varepsilon_k + \sum_{l \neq k} \beta_{kl} K_{kl} \left| u_k - u_l \right|^2 + 2 \sum_{l \neq k} E_{kl} \left( k_l - k_k \right)$$

and

$$\rho_k \frac{d\varepsilon_k}{dt} = \nabla \cdot \left( \frac{\rho_k \nu_k \nabla \varepsilon_k}{\phi_k} \right) - \frac{\varepsilon_k}{k_k} \left( C_{1e} \rho_k R_k : \nabla u_k + C_{2e} \rho_k \varepsilon_k \right) + \frac{1}{\tau_{sl}} \left( \sum_{l \neq k} \beta_{kl} K_{kl} \left| u_k - u_l \right|^2 \right),$$

where $\rho_k R_k$, the Reynolds stress tensor for phase $k$, is defined as

$$\rho_k R_k = \frac{2}{3} \rho_k k_k I - \rho_k \nu_k \left[ \nabla u_k + (\nabla u_k)^T - \frac{2}{3} (\nabla \cdot u_k) I \right].$$

The terms on the right-hand side of Eq. 3.16 represent turbulent diffusion, mean flow shear production, decay of turbulence kinetic energy of phase $k$, production of turbulence energy caused by slip between phases, and interphase turbulence energy exchange. The turbulent Prandtl number for turbulence kinetic energy diffusion is denoted by $\phi_k$ and is set equal to 1.0. The coefficient $\beta_{kl}$ is defined as (Padial et al., 2000)

$$\beta_{kl} = \frac{a_k}{a_k + a_l},$$
where
\[ a_k = \frac{\alpha_k^{\frac{1}{3}}}{\rho_k + \rho_c}, \quad (3.20) \]
with \( \rho_k \) representing the density of phase \( k \) and \( \rho_c \) representing the continuous fluid density. Finally, the momentum exchange coefficient \( K_{kl} \) is given as (Padial et al., 2000):
\[ K_{kl} = \frac{3}{4} \rho_c C_{D}(Re) \frac{|u_i - u_k|}{d_b}, \quad (3.21) \]
where \( C_{D}(Re) \) is the drag coefficient (to be discussed in Sec. 3.1.3).

The terms on the right-hand side of Eq. 3.17 represent turbulent diffusion of the decay rate, the production of decay caused by momentum exchange from mean slip between phases, and the effect of fluctuations in momentum transfer (Padial et al., 2000). \( \phi_c \) represents the Prandtl number, equal to 1.3, and \( C_{el} \) and \( C_{el2} \) are constants equal to 1.44 and 1.92, respectively. The time constant, \( \tau_{kl} \), is found empirically and depends on the materials being simulated (Padial et al., 2000).

It should be noted that the \( k-\varepsilon \) model was tested for the homogeneous flow cases presented in Chapter 4. However, the resulting flow predictions were in disagreement with the experiments that motivated our work (see Chapter 4). For this reason, simulations using the \( k-\varepsilon \) model are not discussed in this work. The description of the \( k-\varepsilon \) model is included to provide a more complete discussion of turbulence modeling.

### 3.1.3 Interfacial Momentum Exchange

The flow of liquid around a bubble generates relative motion between individual bubbles and the surrounding liquid. This behavior produces local-level variations in pressure and stress, and these variations in turn cause interaction between the continuous and dispersed phases (Clift et al., 1978). The interfacial momentum exchange describes this interaction, and in CFDLib, the total interfacial force acting on either of the phases (\( k = c, d \)) is expressed by a sum of five individual forces:
\[ \sum_j F_{jk} = F_{D,k} + F_{\text{vm},k} + F_{L,k} + F_{\text{rot},k} + F_{S,k}, \quad (3.22) \]
Note that Eq. 3.22 is presented and discussed as it appears in the momentum balance for the dispersed phase (Eq. 3.4). The opposite sign is used when Eq. 3.22 is defined for the continuous phase. For example, $F_{D,d} = -F_{D,c} = F_D$.

The drag force is exerted on bubbles traveling steadily through a fluid, and is defined in CFDLib as

$$F_D = -\alpha_d \alpha_c \rho_c C_D \left( \frac{3}{4d_b} | \mathbf{u}_d - \mathbf{u}_c | (\mathbf{u}_d - \mathbf{u}_c) \right),$$  \hspace{1cm} (3.23)

where $\text{Re}$ denotes the bubble Reynolds number:

$$\text{Re} = \frac{d_b | \mathbf{u}_d - \mathbf{u}_c |}{\nu_c}.$$  \hspace{1cm} (3.24)

As seen in Eq. 3.23, the drag coefficient, $C_D$, is a function of the bubble Reynolds number, and there are various functional relationships described in the literature (Joshi, 2001; Joshi et al., 2002; Sokolichin et al., 2004). CFDLib uses the following relationship (Kashiwa et al., 1994):

$$C_D (\text{Re}) = C_a + \frac{24}{\text{Re}} + \frac{6}{1 + \sqrt{\text{Re}}},$$  \hspace{1cm} (3.25a)

where $C_a$ has a nominal value of 0.5. It should be noted, however, that Eq. 3.25a is not specific to bubbly flows. In order to test the effect of the drag correlation on the flow structures and transitions observed in our simulations, we also considered the following correlation, which corresponds to the drag coefficient of a bubble in a sufficiently contaminated system (Tomiyama et al., 1995):

$$C_D = \max \left[ \frac{24}{\text{Re}} \left( 1 + 0.15 \text{Re}^{0.687} \right), \frac{8 \text{Eo}}{3 \left( \text{Eo} + 4 \right)} \right],$$  \hspace{1cm} (3.25b)

where

$$\text{Eo} = \frac{g \rho_c d_b^2}{\sigma}.$$  \hspace{1cm} (3.25c)

This drag correlation has also been applied by Tsuchiya et al. (1997), Pan et al. (1999), and Buwa and Ranade (2002).

It should be noted that several correlations for the drag coefficient discussed in the literature are for isolated bubbles and therefore do not take into account bubble-
bubble interaction. This is because direct experimental measurements can be limited to the terminal rise velocity of a single bubble in a stagnant liquid. A possible method for considering bubble-bubble interaction is to multiply the drag correlation by a correction factor dependent on gas holdup $\alpha_d$ (Sokolichin et al., 2004).

For example, Sankaranarayanan et al. (2002) developed a closure dependent on holdup, bubble Reynolds number, Eötvös number, and Morton number. Their closure model is applicable for both hindered rise and cooperative rise, is valid for $0 < \alpha_d < 0.2$, and is restricted to bubbles in cubic arrays. Behzadi et al. (2004) applied a correlation in which the drag coefficient is equal to the product of a correction term and the drag coefficient for a single bubble, where the correction term is a function of gas holdup. Their drag correlation allowed the model to account for high holdup values. When modeling three-phase (air, water, and solid particles) bubble columns, Schallenberg et al. (2005) included a volume-fraction-dependent correction term in the drag coefficient for the gas phase. This correction accounted for both bubble-bubble interactions and the influence of solid particles on the motion of gas bubbles.

The drag force accounts for the interaction between the continuous and dispersed phases under non-accelerating conditions. Another component, the added-mass or virtual-mass force, is considered when the bubbles accelerate. The virtual-mass force is exerted on a moving bubble when it accelerates and causes the surrounding fluid to accelerate (Drew and Passman, 1999). It is defined in CFDLib as

$$F_{vm} = -\alpha_d \rho_v \frac{\partial u_d}{\partial t} \left[ \frac{\hat{c} u_d}{\alpha} + u_d \cdot \nabla u_d \right] = \left[ \frac{\hat{c} u_c}{\alpha} + u_c \cdot \nabla u_c \right],$$

(3.26)

where $\rho_v$ denotes the phase-averaged density, $\rho_v = \rho_c \alpha_c + \rho_d \alpha_d$. Additionally, this definition includes the volume fractions for each phase, instead of only the dispersed phase volume fraction as described in Drew and Passman (1999). These definitions ensure that the model equations treat each phase in an analogous manner at very high and very low bubble volume fractions.

There are several values of the virtual-mass coefficient, $C_{vm}$, that have been reported in the literature. For example, Drew et al. (1979) have used 0.5 for rigid spherical particles, and Cook and Harlow (1986) have used 0.25 for bubbles in water.
Jakobsen et al. (1997) have used a value of 0.2. In this work, the virtual-mass coefficient is set equal to 0.5, which is the value for dilute suspensions of spheres in a fluid (Drew and Passman, 1999). This value has also been reported by Padial et al. (2000), Deen et al. (2001), Lain et al. (2004), and Bove et al. (2004).

Other studies reported in the literature suggest that $C_{vm}$ is a function of gas holdup. For example, Homsy et al. (1980) define $C_{vm}$ as

$$C_{vm} = \frac{3 - 2\alpha_c}{2\alpha_c}$$

(3.27)

and Biesheuvel and Spoelstra (1989) define $C_{vm}$ as

$$C_{vm} = 1 + 3.32\alpha_d + O(\alpha_d^2),$$

(3.28)
a definition also applied by Pan et al. (1999). Sankaranarayanan et al. (2002) developed a model for the virtual-mass coefficient, and observed that $C_{vm}$ increased nearly linearly with increasing $\alpha_d$, for both spherical and distorted bubbles. Additionally, they found a correlation between $C_{vm}$ for isolated bubbles and the aspect ratio of isolated bubbles.

A bubble moving within a fluid in shearing motion will be subjected to a lift force transverse to the direction of motion (Drew and Passman, 1999). For a spherical bubble, the lift force is given by

$$F_L = \alpha_c \alpha_d \rho_c C_L (u_d - u_c) \times \nabla \times u_c.$$  

(3.29)

There has been considerable debate regarding the appropriate value of the lift coefficient, $C_L$, and the significance of the lift force in simulations. Delnoij et al. (1997b) have claimed that including the lift force in Eulerian-Lagrangian models is necessary for the realistic representation of flow behavior in bubble columns. Auton (1987) has shown that the lift coefficient, $C_L$, has a value of 0.5. This value has also been reported in more recent studies, including Deen et al. (2001), Lain et al. (2002), and Bove et al. (2004). Delnoij et al. (1997c, 1999) have reported a value of 0.53. Behzadi et al. (2004) accounted for the behavior of the lift force at high holdup by utilizing a correlation for which $C_L$ is a function of local holdup values.

Tomiyama et al. (2002) determined an empirical correlation for a net transverse lift coefficient, where for $d_b < 4.4$ mm, $C_L$ was found to be a function of the bubble Reynolds number, while for $d_b > 4.4$ mm, $C_L$ was found to be a function of a modified
Eötvös number, where the characteristic length used was the maximum horizontal dimension of the bubble. The sign of $C_L$ changed from positive to negative when $d_b = 5.8$ mm. Tomiyama et al. (2002) suggested three possible regimes for lateral bubble movement in a vertical pipe: (i) the wall regime ($0.4 \text{ mm} < d_b < 5 \text{ mm}$), in which $C_L$ has a large positive value and bubbles move toward the wall, (ii) the core regime ($d_b > 6 \text{ mm}$), in which $C_L$ has a large negative value and bubbles move toward the center of the pipe, and (iii) a neutral regime ($d_b < 0.4 \text{ mm}$; $5 \text{ mm} < d_b < 6 \text{ mm}$), in which $C_L$ has a small magnitude and bubble movement is influenced by factors such as turbulence or bubble residence time.

Sankaranarayanan and Sundaresan (2002) developed a closure for the lift force, valid for $Ca_\gamma < 0.01$ and $\alpha_d < 0.15$, where $Ca_\gamma$ is the capillary number based on dimensionless shear rate. They observed that for $Ca_\gamma < 0.01$, the lateral drift velocity exhibited a linear relationship with $Ca_\gamma$. As $Ca_\gamma$ was increased, the relationship eventually became nonlinear and $C_L$ became a function of $Ca_\gamma$. It was also observed that $C_L$ gradually decreases with increasing $Ca_\gamma$, and that the sign of $C_L$ would change from positive to negative when $Ca_\gamma \approx 10^{-1}$. However, Sankaranarayanan and Sundaresan (2002) noted that for air-water systems in which $1 \text{ mm} < d_b < 10 \text{ mm}$, $Ca_\gamma \approx 10^{-3} - 10^{-2}$. Therefore, $C_L$ was expected to remain positive for bubble column flows. Such disagreement regarding the lift force has led Sokolichin et al. (2004) to question the significance of this force in bubble column simulations.

It can be seen in Eq. 3.29 that the lift force depends on the vorticity of the continuous phase. Drew and Passman’s (1999) discussion of the constitutive equations for multiphase flow also includes a term proportional to $(u_d - u_c) \times \nabla \times u_d$. Consequently, the rotation force, which depends on the vorticity of the dispersed phase, may also be considered in the interfacial momentum exchange:

$$F_{rot} = \alpha_c \alpha_d \rho_v C_{rot} (u_d - u_c) \times \nabla \times u_d.$$  \hfill (3.30)

Arnold et al. (1989) suggest that gradients within the dispersed phase have a significant effect on the direction and magnitude of the interfacial force. Clift et al. (1978) suggest that particles or fluids can rotate about axes either normal or parallel to
the direction of relative motion. The first case is known as top spin, when rotation is caused by fluid shear or collisions. A basic example involves a nearly spherical object, such as a bubble or particle, in a uniform shear flow field in the plane of the object (here, the $xy$-plane). The center of the object will move with the velocity that the continuous fluid would have at that same location if no object was present. Meanwhile, the axis of the object will experience rotation in a periodic path, in which the angular velocities depend on the angle between the object’s axis of symmetry and the $z$-axis, the angle between the $yz$-plane and the plane containing both the $z$-axis and the object’s axis of symmetry, the shear rate, and the shape of the object (Clift et al., 1978). An example of top spin is shown in Figure 3.1.

Figure 3.1. Diagram of a spherical object rotating in a fluid in uniform shear. In this example, the sphere rotates about an axis normal to the direction of motion, and thus the sphere experiences top spin. (Adapted from Fig. 10.7 in Clift et al., 1978.)
Rotation about axes parallel to the direction of relative motion is called screw motion, which is characterized by the Reynolds number and the ratio of surface speed to approach velocity. Bubbles experiencing screw motion tend to become flatter as the angular velocity increases (Clift et al., 1978). An example of screw motion is shown in Figure 3.2.

Figure 3.2. Diagram of a bubble experiencing screw motion.
It is important to note that the two-fluid model in CFDLib includes interaction terms developed by Kashiwa (1998) that, to our knowledge, have not appeared in two-fluid models previously discussed in the literature. In the original derivation in CFDLib, these interaction forces are separated into two parts, attraction and repulsion, and take the form of a second-order tensor, constructed from the deformation rates of the velocity fields, and multiplied by the velocity difference between the two phases. These interaction terms appearing in CFDLib can also be expressed (Monahan et al., 2005) as a lift force, a rotation force, and a strain force. Thus, it should also be noted that the lift force arising from the interaction terms has the same form, but not the same origin, as the standard lift force involving a single bubble (Eq. 3.29). Similarly, the rotation term arising from the interaction terms has the same form, but not the same origin, as the rotation force expressed in Eq. 3.30.

The strain force (assuming incompressible flow) is defined as

$$\mathbf{F}_s = \alpha_d \alpha_c \rho_c \nabla \cdot \left[ \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right) + \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right)^T \right] \cdot \left( \mathbf{u}_c - \mathbf{u}_d \right). \quad (3.31)$$

We have observed that including these interaction terms suppresses flow transitions (Monahan et al., 2005) up to relatively large values (~0.5) for the average gas volume fraction.

As discussed below, CFDLib assigns equal values to the lift coefficient, $C_L$, and the rotation coefficient, $C_{rot}$. Additionally, like the definition for the virtual-mass force, the definitions for the lift and rotation forces also apply the phase-averaged density and include the volume fractions for each phase, instead of only the dispersed phase volume fraction as described in Drew and Passman (1999).

The following derivation shows how the interaction terms in CFDLib can be expressed as a lift force, a rotation force, and a strain force. As noted previously, the interaction terms are represented in CFDLib as the sum of attraction and repulsion forces:

$$\mathbf{F}_{att} + \mathbf{F}_{rep} = \alpha_c \alpha_d \rho_c \mathbf{G} \cdot \left( \mathbf{u}_c - \mathbf{u}_d \right), \quad (3.32)$$

where the matrix $\mathbf{G}$ is equal to

$$\mathbf{G} = \left( \frac{C_{rep}}{2} \right) \left[ \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right) + \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right)^T \right] - C_{att} \left[ \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right) - \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right)^T \right]. \quad (3.33)$$
A velocity gradient $\nabla u$ can be expressed as the sum of a symmetric tensor and an antisymmetric tensor

$$\nabla u = \frac{1}{2} \left[ \nabla u + (\nabla u)^T \right] + \frac{1}{2} \left[ \nabla u - (\nabla u)^T \right],$$

(3.34)
in which the symmetric tensor is related to the local rate of deformation and the antisymmetric tensor is related to the local rate of rotation (Deen, 1998). Note that $G$ also represents the sum of a symmetric tensor and an antisymmetric tensor. The symmetric tensor in $G$ represents the sum of the rate-of-strain tensors (assuming incompressible flow) for each phase and therefore appears in the equation for the strain force (Eq. 3.31). Hence, the strain coefficient $C_S$ is equal to $C_{rep}/2$. The antisymmetric part of $G$ represents the sum of the vorticity tensors for each phase. The dot product of the antisymmetric tensor in $G$ with $(u_c - u_d)$ results in the alternate representation of the sum of the lift and rotation forces presented in Eqs. 3.29 and 3.30. In other words,

$$\alpha_c \alpha_d \rho_v \left(-C_{att}\right) \left[ (\nabla u_c + \nabla u_d) - (\nabla u_c + \nabla u_d)^T \right] (u_c - u_d)$$

$$= \alpha_c \alpha_d \rho_v \left(-C_{att}\right) (u_c - u_d) \times \nabla (u_c + u_d)$$

$$= \alpha_c \alpha_d \rho_v \left(C_{att}\right) (u_d - u_c) \times \nabla (u_c + u_d).$$

(3.35)

The following process proves Eq. 3.35. The left-hand side of Eq. 3.35 is equal to

$$\alpha_c \alpha_d \rho_v \left(-C_{att}\right) \left[ \begin{array}{c}
\frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} \\
\frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} \\
\frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z}
\end{array} \right]$$

$$- \left[ \begin{array}{c}
\frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} + \frac{\partial u_c}{\partial x} \\
\frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} + \frac{\partial u_c}{\partial y} \\
\frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z} + \frac{\partial u_c}{\partial z}
\end{array} \right] \cdot (u_c - u_d),$$

(3.36a)

which simplifies to
\[ \alpha_c \alpha_d \rho_v (-C_{an})^* \]

\[
\begin{bmatrix}
0 & \frac{\partial (u_{cy} + u_{dy})}{\partial y} - \frac{\partial (u_{cx} + u_{dx})}{\partial x} & \frac{\partial (u_{cz} + u_{dz})}{\partial z} - \frac{\partial (u_{cx} + u_{dx})}{\partial x} \\
\frac{\partial (u_{cx} + u_{dx})}{\partial y} - \frac{\partial (u_{cy} + u_{dy})}{\partial x} & 0 & \frac{\partial (u_{cz} + u_{dz})}{\partial z} - \frac{\partial (u_{cy} + u_{dy})}{\partial y} \\
\frac{\partial (u_{cx} + u_{dx})}{\partial z} - \frac{\partial (u_{cz} + u_{dz})}{\partial x} & \frac{\partial (u_{cx} + u_{dx})}{\partial y} - \frac{\partial (u_{cy} + u_{dy})}{\partial z} & 0
\end{bmatrix} \begin{bmatrix} u_{cx} - u_{dx} \\ u_{cy} - u_{dy} \\ u_{cz} - u_{dz} \end{bmatrix} = (3.36b)
\]

In order to simplify the dot product calculation, the substitutions \( a = u_c + u_d \) and \( b = u_c - u_d \) are made. In component form,

\[ a = \left( a_1 = u_{cx} + u_{dx}, \ a_2 = u_{cy} + u_{dy}, \ a_3 = u_{cz} + u_{dz} \right) \]  \hspace{1cm} (3.37a)

and

\[ b = \left( b_1 = u_{cx} - u_{dx}, \ b_2 = u_{cy} - u_{dy}, \ b_3 = u_{cz} - u_{dz} \right). \]  \hspace{1cm} (3.37b)

Thus, Eq. 3.36b is rewritten as

\[ \alpha_c \alpha_d \rho_v (-C_{an}) \begin{bmatrix} \frac{\partial a_2}{\partial y} - \frac{\partial a_1}{\partial x} \\ \frac{\partial a_3}{\partial z} - \frac{\partial a_1}{\partial y} \\ \frac{\partial a_3}{\partial z} - \frac{\partial a_2}{\partial y} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} \frac{\partial a_2}{\partial x} - \frac{\partial a_1}{\partial y} \\ \frac{\partial a_3}{\partial y} - \frac{\partial a_1}{\partial z} \\ \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \end{bmatrix}. \]  \hspace{1cm} (3.38)

Once the dot product is calculated, Eq. 3.38 simplifies to

\[
\alpha_c \alpha_d \rho_v (-C_{an}) \left[ \left( \frac{\partial a_2}{\partial x} - \frac{\partial a_1}{\partial y} \right) b_2 + \left( \frac{\partial a_3}{\partial x} - \frac{\partial a_1}{\partial z} \right) b_1 \right] + \left[ \left( \frac{\partial a_1}{\partial y} - \frac{\partial a_2}{\partial x} \right) b_2 + \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) b_1 \right]\left( \frac{\partial a_2}{\partial y} - \frac{\partial a_1}{\partial x} \right)
\]

\[
\alpha_c \alpha_d \rho_v (-C_{an}) \left[ \left( \frac{\partial a_2}{\partial x} - \frac{\partial a_1}{\partial y} \right) b_2 + \left( \frac{\partial a_3}{\partial x} - \frac{\partial a_1}{\partial z} \right) b_1 \right] + \left[ \left( \frac{\partial a_1}{\partial y} - \frac{\partial a_2}{\partial x} \right) b_2 + \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) b_1 \right] = (3.39)
\]

Returning to the original notation, Eq. 3.39 is now expressed by
\[ \alpha_c \alpha_d \rho_v (-C_{att})^* \]

\[
\begin{bmatrix}
\left( \frac{\partial (u_{cx} + u_{dx})}{\partial x} - \frac{\partial (u_{cy} + u_{dy})}{\partial y} \right) (u_{cy} - u_{dy}) + \left( \frac{\partial (u_{cx} + u_{dx})}{\partial x} - \frac{\partial (u_{cz} + u_{dz})}{\partial z} \right) (u_{cz} - u_{dz}) \\
\left( \frac{\partial (u_{cx} + u_{dx})}{\partial y} - \frac{\partial (u_{cy} + u_{dy})}{\partial x} \right) (u_{cx} - u_{dx}) + \left( \frac{\partial (u_{cx} + u_{dx})}{\partial y} - \frac{\partial (u_{cy} + u_{dy})}{\partial z} \right) (u_{cx} - u_{dx}) \\
\left( \frac{\partial (u_{cx} + u_{dx})}{\partial z} - \frac{\partial (u_{cz} + u_{dz})}{\partial x} \right) (u_{cx} - u_{dx}) + \left( \frac{\partial (u_{cz} + u_{dz})}{\partial z} - \frac{\partial (u_{cy} + u_{dy})}{\partial y} \right) (u_{cy} - u_{dy})
\end{bmatrix}
\]  

(3.40)

The right-hand side of Eq. 3.35 yields the same result as Eq. 3.40, as shown in the following steps. First, as done previously, to simplify the calculation, the substitutions \( a = u_c + u_d \) and \( b = u_c - u_d \) are made. Thus, the right-hand side of Eq. 3.35 becomes

\[ \alpha_c \alpha_d \rho_v (-C_{att}) (u_c - u_d) \times \nabla \times (u_c + u_d) = \alpha_c \alpha_d \rho_v (-C_{att}) \left[ b \times (\nabla \times a) \right]. \]  

(3.41)

Note that \( a \) and \( b \) are again described by Eqs. 3.37a and 3.37b, respectively, in order to calculate the cross products. By the definition of the curl of a vector (Deen, 1998),

\[ \nabla \times a = \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) x + \left( \frac{\partial a_1}{\partial z} - \frac{\partial a_3}{\partial x} \right) y + \left( \frac{\partial a_2}{\partial x} - \frac{\partial a_1}{\partial y} \right) z. \]  

(3.42)

In turn,

\[ b \times (\nabla \times a) = (b_1 x + b_2 y + b_3 z) \times \left[ \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) x + \left( \frac{\partial a_1}{\partial z} - \frac{\partial a_3}{\partial x} \right) y + \left( \frac{\partial a_2}{\partial x} - \frac{\partial a_1}{\partial y} \right) z \right], \]  

(3.43)

which is equal to

\[
\begin{bmatrix}
 b_2 \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) - b_3 \left( \frac{\partial a_3}{\partial z} - \frac{\partial a_2}{\partial x} \right) \\
 b_3 \left( \frac{\partial a_1}{\partial x} - \frac{\partial a_2}{\partial y} \right) - b_1 \left( \frac{\partial a_1}{\partial y} - \frac{\partial a_2}{\partial z} \right) \\
 b_1 \left( \frac{\partial a_3}{\partial z} - \frac{\partial a_2}{\partial x} \right) - b_2 \left( \frac{\partial a_3}{\partial x} - \frac{\partial a_1}{\partial y} \right)
\end{bmatrix}
\]  

\[
\begin{bmatrix}
 b_2 \left( \frac{\partial a_3}{\partial y} - \frac{\partial a_2}{\partial z} \right) + b_3 \left( \frac{\partial a_3}{\partial z} - \frac{\partial a_2}{\partial x} \right) \\
 b_3 \left( \frac{\partial a_1}{\partial x} - \frac{\partial a_2}{\partial y} \right) + b_1 \left( \frac{\partial a_1}{\partial y} - \frac{\partial a_2}{\partial z} \right) \\
 b_1 \left( \frac{\partial a_3}{\partial z} - \frac{\partial a_2}{\partial x} \right) + b_2 \left( \frac{\partial a_3}{\partial x} - \frac{\partial a_1}{\partial y} \right)
\end{bmatrix}
\]  

(3.44)
where the rightmost matrix in Eq. 3.44 is the same as that calculated in Eq. 3.39. Returning to the original notation, Eq. 3.44 can be expressed as

\[ \mathbf{b} \times (\nabla \times \mathbf{a}) \]

\[
= \left[ \begin{array}{c}
\frac{\partial (u_{cy} + u_{dy})}{\partial x} - \frac{\partial (u_{cx} + u_{dx})}{\partial y} (u_{cy} - u_{dy}) + \frac{\partial (u_{cx} + u_{dx})}{\partial z} (u_{cz} - u_{dz}) \\
\frac{\partial (u_{cx} + u_{dx})}{\partial y} - \frac{\partial (u_{cy} + u_{dy})}{\partial x} (u_{cx} - u_{dx}) + \frac{\partial (u_{cy} + u_{dy})}{\partial z} (u_{cz} - u_{dz}) \\
\frac{\partial (u_{cx} + u_{dx})}{\partial z} - \frac{\partial (u_{cy} + u_{dy})}{\partial x} (u_{cx} - u_{dx}) + \frac{\partial (u_{cy} + u_{dy})}{\partial y} (u_{cz} - u_{dz})
\end{array} \right] (u_e - u_d) \\
= \nabla \times (u_e + u_d) \times (u_e - u_d).
\]

Therefore,

\[ \alpha_c \alpha_d \rho_v (-C_{att}) (u_e - u_d) \times \nabla \times (u_e + u_d) \]

\[ = \alpha_c \alpha_d \rho_v (-C_{att})^*\]

which is the same final expression achieved in Eq. 3.40. Therefore,

\[ \alpha_c \alpha_d \rho_v (-C_{att}) \left[ (\nabla u_e + \nabla u_d) - (\nabla u_e + \nabla u_d)^T \right] (u_e - u_d) \]

\[ = \alpha_c \alpha_d \rho_v (-C_{att}) (u_e - u_d) \times \nabla \times (u_e + u_d) \]

\[ = \alpha_c \alpha_d \rho_v (C_{att}) (u_d - u_e) \times \nabla \times (u_e + u_d), \]

in which the final term in the equality in Eq. 3.47 represents the sum of the lift and rotation forces (Eqs. 3.29 and 3.30), with \( C_{att} = C_L = C_{rot} \).
3.2 CFDLib: Code Overview and Discretization Scheme

3.2.1 Description of Code Operation

CFDLib is a multiphase simulation library developed at Los Alamos National Laboratory, USA (Kashiwa et al., 1994; Kashiwa and Rauenzahn, 1994), and it uses a finite-volume technique to integrate the time-dependent equations of motion that govern multiphase flows. This code has also been used by Pan et al. (1999, 2000), Padial et al. (2000), and Chen and Fan (2004) for simulating gas-liquid bubble columns. The majority of the simulations discussed in this work were performed with CFDLib version 99.2, since the more recent versions of the code continue to be tested.

Operation of CFDLib is as follows. The program utilizes an input file, either in2d for a 2D simulation or in3d for a 3D simulation. CFDLib is block structured and therefore the domain geometry, including the number of blocks, the appropriate coordinate system, the origin of each block, the number of sections in a particular direction within each block, the number of cells in each section, and the grid resolution must be specified in the input file. Boundary conditions and inter-block communication information must be supplied. Additionally, data such as the initial volume fraction, initial density, initial temperature, force model coefficients, bubble size, and inlet velocity are specified. Output such as pressure, density, temperature, volume fraction, and velocity data for each fluid class are written to Tecplot files. The user selects the initial time, final time, and time increment for Tecplot output.

The following example describes how the simulation domain is specified. Figure 3.3 shows a 2D Cartesian domain with two blocks. Direction 1 is assigned to the X-direction and direction 2 is assigned to the Y-direction. (For a 3D simulation, direction 3 denotes the Z-direction.) The number of blocks is specified as nblks = 2 in the input file. Additionally, Block 1 has three sections in direction 1 and two sections in direction 2. These sections are specified in the input file as nsect(1,1) = 3 and nsect(2,1) = 2, where the first index denotes the direction number and the second index denotes the block number. Similarly, for Block 2, nsect(1,2) = 1,1.
Next, the number of cells in each section, direction, and block are specified. For simplicity, assume that cells are 1 cm in each direction. For Block 1, direction 1, $n_{cell}(1,1,1) = 10$, $n_{cell}(2,1,1) = 10$, and $n_{cell}(3,1,1) = 10$, where the first index is the section number, the second index is the direction number, and the third index is the block number. Similarly, for Block 1, direction 2, $n_{cell}(1,2,1) = 25$ and $n_{cell}(2,2,1) = 25$. Block 2 is not divided into individual sections; therefore $n_{cell}(1,1,2) = 30$ and $n_{cell}(1,2,2) = 20$.

Origins of blocks are denoted by $x_0$. The origin of Block 1 is $(0, 0)$, so $x_0(1,1) = 0$ and $x_0(2,1) = 0$, where the first index is the direction number and the second index is the block number. The origin of Block 2 is $(0, 50)$, so $x_0(1,2) = 0$ and $x_0(2,2) = 50$. Cell spacing is denoted by $dx$. 1 cm cells are used. For Block 1, direction 1, $dx(1,1,1) = 1$, $dx(2,1,1) = 1$, and $dx(3,1,1) = 1$, where the first index is the section number, the second index is the direction number, and the third index is the block number. For Block 1, direction 2, $dx(1,2,1) = 1$ and $dx(2,2,1) = 1$. For Block 2, $dx(1,1,2) = 1$ and $dx(1,2,2) = 1$. 

Figure 3.3. Basic example for CFDLib domain specification.
3.2.2 Ensemble Averaged Equations

CFDLib uses ensemble-averaged equations. The description of the derivation of these equations is found in Kashiwa and Rauenzahn (1994). They first consider a statistical distribution function \( f(t, x, \Gamma_0) \), which depends on time, position \( x \), and state vector \( \Gamma_0 \). If a material state is described by the mass \( m_0 \), velocity \( dx/dt \) or \( u_0 \), and internal energy \( e_0 \), then

\[
\Gamma_0 = (m_0, u_0, e_0) \quad (3.48a)
\]

and

\[
d\Gamma_0 = (dm_0, du_0, de_0) \quad (3.48b)
\]

It is assumed that volume \( V \) and mass \( m_0 \) are fixed, and that \( V \) acts as a continuum. The total variation of \( f(t, x, \Gamma_0) \) is defined as (Kashiwa and Rauenzahn, 1994):

\[
\frac{\partial f}{\partial t} + u_0 \cdot \nabla f + \dot{\Gamma}_0 \cdot \frac{\partial f}{\partial \Gamma_0} = \frac{Df}{Dt} \quad (3.48c)
\]

The vector \( \mathbf{Q}_0 \), where

\[
\mathbf{Q}_0 = \{ m_0, m_0 u_0, m_0 [e_0 + (u_0^2/2)] \}
\]

represents the mass, momentum, and total energy of the material in \( V \), where \( E_0 = e_0 + (u_0^2/2) \). The moment of \( f \) corresponding to the average of \( \mathbf{Q}_0(\Gamma_0) \) is defined as

\[
\langle \mathbf{Q}_0 \rangle = \int \mathbf{Q}_0 f \, d\Gamma_0 \quad (3.49b)
\]

The balance equation for \( \langle \mathbf{Q}_0 \rangle \) is given as (Kashiwa and Rauenzahn, 1994):

\[
\frac{\partial \langle \mathbf{Q}_0 \rangle}{\partial t} + \mathbf{V} \cdot \langle \mathbf{Q}_0 \rangle = \left( \dot{\Gamma}_0 \cdot \frac{\partial \mathbf{Q}_0}{\partial \Gamma_0} \right) + \int \mathbf{Q}_0 \frac{Df}{Dt} \, d\Gamma_0\quad (3.49c)
\]

It should be noted that \( m_0, m_0 u_0 \), and \( m_0 E_0 \) are defined to be invariants that make the \( \int \mathbf{Q}_0 \frac{Df}{Dt} \, d\Gamma_0 \) term on the right-hand side of Eq. 3.49c equal to zero (Kashiwa and Rauenzahn, 1994).

Thus, the momentum equations become:
\[
\frac{\partial}{\partial t} \begin{bmatrix} \langle m_0 \rangle \\ \langle m_0 u_0 \rangle \\ \langle m_0 E_0 \rangle/V \end{bmatrix} + \nabla \cdot \begin{bmatrix} \langle m_0 \rangle \\ \langle m_0 u_0 \rangle \\ \langle m_0 E_0 \rangle/V \end{bmatrix} = \begin{bmatrix} m_0 \rho \\ m_0 u_0 \\ m_0 \left( e_0 + \frac{u_0^2}{2} \right) \end{bmatrix}
\]

Letting \( u_0 = u + u_0' \) yields:

\[
\frac{\partial}{\partial t} \begin{bmatrix} \langle m_0 \rangle \\ \langle m_0 u_0 \rangle \\ \langle m_0 E_0 \rangle/V \end{bmatrix} + \nabla \cdot \begin{bmatrix} \langle m_0 (u + u_0') \rangle \\ \frac{\langle m_0 (u + u_0')(u + u_0') \rangle}{V} \\ \frac{\langle m_0 E_0 (u + u_0') \rangle}{V} \end{bmatrix} = \begin{bmatrix} m_0 \rho \\ m_0 u_0 \\ m_0 \left( e_0 + \frac{u_0^2}{2} \right) \end{bmatrix},
\]

which simplifies to

\[
\frac{\partial}{\partial t} \begin{bmatrix} \langle m_0 \rangle \\ \langle m_0 u_0 \rangle \\ \langle m_0 E_0 \rangle/V \end{bmatrix} + \nabla \cdot \begin{bmatrix} \langle m_0 u \rangle + \langle m_0 u_0' \rangle \\ \frac{\langle m_0 uu \rangle + 2 \langle m_0 u_0'u \rangle + \langle m_0 u_0'u_0' \rangle}{V} \\ \frac{\langle m_0 E_0 u \rangle + \langle m_0 E_0 u_0' \rangle}{V} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{\langle m_0 \frac{du_0}{dt} \rangle}{V} \\ \langle m_0 \left( \frac{de_0}{dt} + u_0 \frac{du_0}{dt} \right) \rangle \end{bmatrix}
\]

Note that (Kashiwa and Rauenzahn, 1994)

\[
\langle m_0 u_0' \rangle = 0,
\]

\[
\langle m_0 u_0'u \rangle = 0,
\]

\[
\rho = \langle m_0 \rangle/V,
\]
\[ \rho u = \frac{\langle m_0 u_0 \rangle}{V}, \] (3.51d)

and

\[ \rho E = \frac{\langle m_0 E_0 \rangle}{V}. \] (3.51e)

Thus, the balance equations in Eq. 3.50c simplify to

\[ \frac{\partial}{\partial t} \left[ \rho \begin{bmatrix} \rho u \\ \rho \end{bmatrix} \right] + \nabla \cdot \left[ \begin{bmatrix} \rho u \\ \rho \end{bmatrix} \begin{bmatrix} \langle m_0 u \rangle/V \\ \langle m_0 E_0 u + \langle m_0 E_0 u' \rangle \rangle/V \end{bmatrix} \right] = \begin{bmatrix} 0 \\ \langle m_0 (\dot{e}_0 + u_0 \cdot \dot{u}_0) \rangle/V \end{bmatrix} \] (3.52a)

\[ \rightarrow \frac{\partial}{\partial t} \left[ \rho \begin{bmatrix} \rho u \\ \rho \end{bmatrix} \right] + \nabla \cdot \left[ \rho \begin{bmatrix} \rho uu + \langle \rho \dot{u}_0 \rangle \langle u_0 \rangle + \langle \rho \dot{u} u_0 \rangle \rangle \\ \rho E u + \langle \rho \dot{E} \rangle \langle u_0 \rangle \rangle \right] = \begin{bmatrix} 0 \\ \langle m_0 (\dot{e}_0 + u_0 \cdot \dot{u}_0) \rangle/V \end{bmatrix}. \] (3.52b)

The right-hand side of Eq. 3.52b can be simplified via the Euler equations (Kashiwa and Rauenzahn, 1994) as follows. First,

\[ m_0 \dot{u}_0 = m_0 \frac{d u_0}{d t} = m_0 \frac{d x}{d t} \frac{d u_0}{d x} \Rightarrow m_0 u_0 \cdot \nabla u_0 \Rightarrow m_0 \left( -\frac{1}{\rho_0} \nabla p_0 \right) \Rightarrow -V \nabla p. \] (3.52c)

Thus,

\[ \frac{\langle m_0 \dot{u}_0 \rangle}{V} = -\frac{\langle V \nabla p_0 \rangle}{V} = -\langle \nabla p \rangle = -\nabla p. \] (3.52d)

Similarly,

\[ m_0 \dot{e}_0 = -p_0 V \nabla \cdot u_0 = \gamma^{-1} V \dot{p}_0; \] (3.52e)

\[ \therefore \frac{\langle m_0 \dot{e}_0 \rangle}{V} = \frac{\langle \gamma^{-1} V \dot{p}_0 \rangle}{V} = \langle \gamma^{-1} \dot{p}_0 \rangle, \] (3.52f)

where \( \gamma = c_p/c_v \). Note that \( p_0 = p + p' \) and in turn, \( p'_0 = p_0 - p \), which gives:

\[ \langle \gamma^{-1} \dot{p}_0 \rangle = \langle \gamma^{-1} (p + p' \rangle \rangle = \langle \gamma^{-1} \dot{p} \rangle + \langle \gamma^{-1} \dot{p}' \rangle = \gamma^{-1} \dot{p} + \langle \gamma^{-1} (p_0 - p) \rangle. \] (3.52g)

Additionally,

\[ \frac{\langle m_0 u_0 \cdot \dot{u}_0 \rangle}{V} = \frac{\langle u_0 \cdot m_0 \dot{u}_0 \rangle}{V} = -\frac{\langle u_0 \cdot V \nabla p_0 \rangle}{V} = -\langle u_0 \cdot \nabla p \rangle. \] (3.53a)

If \( u_0 = u + u'_0 \) and \( p_0 = p + p'_0 \), then

\[ -\langle u_0 \cdot \nabla p \rangle = -\langle (u + u'_0) \cdot \nabla (p + p'_0) \rangle \] (3.53b)

\[ \rightarrow -\langle u \cdot \nabla p \rangle - \langle u'_0 \cdot \nabla p \rangle - \langle u \cdot \nabla p_0 \rangle - \langle u'_0 \cdot \nabla p_0 \rangle = -u \cdot \nabla p - \langle u'_0 \cdot \nabla p_0 \rangle. \] (3.53c)
The momentum equations in Eq. 3.52b are now expressed as:

\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{uu} + \langle \rho \rho_0 \mathbf{u} \mathbf{u}_0 \rangle \\ \rho E \mathbf{u} + \langle \rho \rho_0 E \mathbf{u} \mathbf{u}_0 \rangle \end{bmatrix} = \begin{bmatrix} 0 \\ -\nabla P \\ \gamma^{-1} \hat{P} + \gamma^{-1} (\rho_0 - P)^* - \mathbf{u} \cdot \nabla P - \langle \mathbf{u} ' \cdot \nabla P_0 \rangle \end{bmatrix},
\]

(3.54a)

and can be rearranged by recalling that \( E = e + (u^2/2) \):

\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho \left( e + \frac{u^2}{2} \right) \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{uu} + \langle \rho \rho_0 \mathbf{u} \mathbf{u}_0 \rangle \\ \rho \left( e + \frac{u^2}{2} \right) + \langle \rho \rho_0 E \mathbf{u} \mathbf{u}_0 \rangle \end{bmatrix} = \begin{bmatrix} 0 \\ -\nabla P \\ \gamma^{-1} \hat{P} + \gamma^{-1} (\rho_0 - P)^* \end{bmatrix}.
\]

(3.54b)

It can be shown that the expression

\[
\frac{\partial}{\partial t} \left( \frac{\rho u^2}{2} \right) + \nabla \cdot \left( \frac{\rho \mathbf{uu}}{2} \right) = -\mathbf{u} \cdot \nabla P
\]

(3.54c)

can be subtracted out of Eq. 3.54b. Expanding Eq. 3.54c gives:

\[
\left( \frac{u^2}{2} \right) \frac{\partial \rho}{\partial t} + \rho \mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial t} + \left( \frac{u^2}{2} \right) \nabla \cdot (\rho \mathbf{u}) + \rho \mathbf{u} \cdot \nabla \cdot \left( \frac{u^2}{2} \right) = -\mathbf{u} \cdot \nabla P.
\]

(3.54d)

Note that (Tannehill et al., 1997)

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,
\]

(3.54e)

and therefore

\[
\left( \frac{u^2}{2} \right) \frac{\partial \rho}{\partial t} + \left( \frac{u^2}{2} \right) \nabla \cdot (\rho \mathbf{u}) = 0.
\]

(3.54f)

Thus, Eq. 3.54d becomes:

\[
\rho \mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \cdot \left( \frac{u^2}{2} \right) = -\mathbf{u} \cdot \nabla P,
\]

(3.54g)

or
\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \left( \frac{u^2}{2} \right) = -\frac{1}{\rho} \nabla p ,
\]

(3.54h)

which holds true if body forces are not considered (Tannehill et al., 1997). The momentum equations are ultimately defined as (Kashiwa and Rauenzahn, 1994)

\[
\begin{bmatrix}
\frac{\partial \rho \mathbf{u}}{\partial t} \\
\frac{\partial \rho u u}{\partial t} \\
\frac{\partial \rho u}{\partial t} \\
\frac{\partial \rho E_0 u'_0}{\partial t}
\end{bmatrix} + \nabla \cdot \begin{bmatrix}
\rho u u + \langle \rho_0 u'_0 u'_0 \rangle \\
\rho uu + \langle \rho_0 E_0 u'_0 \rangle \\
\rho u + \langle \rho_0 E_0 \rangle \\
\rho E_0 u'_0 + \langle \rho_0 E_0 u'_0 \rangle + \langle \rho_0 \rangle
\end{bmatrix} = \begin{bmatrix}
0 \\
-\nabla p \\
\gamma^{-1} \dot{p} + \left[ \gamma^{-1} (p_0 - p) \right] - \langle \mathbf{u}'_0 \cdot \nabla p'_0 \rangle
\end{bmatrix} .
\]

(3.55)

For a multimaterial case, the derivation is similar to the single-material case previously outlined. However, now the statistical distribution function \( f \) is represented by

\[
f(t, \mathbf{x}, m_0, \mathbf{u}_0, e_0, \alpha_1, \alpha_2, \ldots, \alpha_N) ,
\]

where \( \alpha_k \) is the volume fraction of material \( k \), and the state vector becomes

\[
\Gamma_N = (m_0, \mathbf{u}_0, e_0, \alpha_1, \alpha_2, \ldots, \alpha_N) ,
\]

(3.56a)

where

\[
d\Gamma_N = (dm_0 d\mathbf{u}_0 de_0 d\alpha_1 d\alpha_2 \ldots d\alpha_N)
\]

(3.56b)

or

\[
d\Gamma_N = (d\Gamma_0 d\alpha_1 d\alpha_2 \ldots d\alpha_N) .
\]

(3.56c)

The moment of \( f \) that is average of the function \( \mathbf{Q}_0 \) is now represented as

\[
\langle \alpha_k \mathbf{Q}_0 \rangle = \int \alpha_k \mathbf{Q}_0 f d\Gamma_N ,
\]

(3.56d)

to reflect the dependence on a particular material \( k \) (Kashiwa and Rauenzahn, 1994). Eq. 3.49c is rewritten for the multimaterial case as:

\[
\frac{\partial }{\partial t} \langle \alpha_k \mathbf{Q}_0 \rangle + \nabla \cdot \langle \alpha_k \mathbf{Q}_0 \mathbf{u}_0 \rangle = \left( \Gamma_N \cdot \frac{\partial \alpha_k \mathbf{Q}_0}{\partial \Gamma_N} \right) + \int \alpha_k \mathbf{Q}_0 \frac{Df}{Dt} d\Gamma_N .
\]

(3.56e)

Additionally, if \( \mathbf{Q}_0 \) is an invariant, then (Kashiwa and Rauenzahn, 1994):

\[
\int \alpha_k \mathbf{Q}_0 \frac{Df}{Dt} d\Gamma_N = \int \alpha_k \int \mathbf{Q}_0 \frac{Df}{Dt} d\Gamma_0 d\alpha_1 d\alpha_2 \ldots d\alpha_N = 0 .
\]

(3.56f)

The momentum equations are now represented as
\[ \frac{\partial}{\partial t} \begin{bmatrix} \frac{\langle \alpha_i m_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 u_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 \rangle}{V} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \frac{\langle \alpha_i m_0 u_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 u_0 u_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 u_0 \rangle}{V} \end{bmatrix} = \begin{bmatrix} \frac{\alpha_i m_0}{V} \\ \frac{\alpha_i m_0 u_0}{V} \\ \frac{\alpha_i m_0 e_0}{V} \end{bmatrix}. \]

(3.57a)

Let \( u_0 = u_k + u'_k \), which gives:

\[ \frac{\partial}{\partial t} \begin{bmatrix} \frac{\langle \alpha_i m_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 u_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 \rangle}{V} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \frac{\langle \alpha_i m_0 (u_k + u'_k) \rangle}{V} \\ \frac{\langle \alpha_i m_0 (u_k + u'_k) (u_k + u'_k) \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 (u_k + u'_k) \rangle}{V} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial t} \frac{\alpha_i m_0}{V} \\ \frac{\alpha_i m_0 u_0}{V} \\ \frac{\alpha_i m_0 e_0}{V} \end{bmatrix}, \]

(3.57b)

which simplifies to

\[ \frac{\partial}{\partial t} \begin{bmatrix} \frac{\langle \alpha_i m_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 u_0 \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 \rangle}{V} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \frac{\langle \alpha_i m_0 u_k \rangle + \langle \alpha_i m_0 u'_k \rangle}{V} \\ \frac{\langle \alpha_i m_0 u_k u_k \rangle + 2 \langle \alpha_i m_0 u'_k u_k \rangle}{V} \\ \frac{\langle \alpha_i m_0 e_0 u_k \rangle + \langle \alpha_i m_0 e_0 u'_k \rangle}{V} \end{bmatrix} = \begin{bmatrix} \frac{\langle m_0 d\alpha_k \rangle}{dt} \\ \frac{\langle m_0 u_k d\alpha_k \rangle}{dt} + \frac{\langle m_0 u_0 d\alpha_k \rangle}{dt} \\ \frac{\langle m_0 e_0 d\alpha_k \rangle}{dt} + \frac{\langle m_0 e_0 d\alpha_k \rangle}{dt} \end{bmatrix}. \]

(3.57c)

Note that (Kashiwa and Rauenzahn, 1994)
\[ \langle \alpha_k m_0 \mathbf{u}_k \rangle = 0, \]  
\[ \langle \alpha_k m_0 \mathbf{u}_k' \mathbf{u}_k \rangle = 0, \]  
\[ \rho_k = \langle \alpha_k m_0 \rangle / V, \]  
\[ \rho_k \mathbf{u}_k = \langle \alpha_k m_0 \mathbf{u}_0 \rangle / V, \]  
and
\[ \rho_k e_k = \langle \alpha_k m_0 e_0 \rangle / V. \]  

The balance equations in Eq. 3.57c simplify to:

\[ \frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \rho_k \mathbf{u}_k \\ \rho_k \mathbf{e}_k \end{bmatrix} + \nabla \cdot \begin{bmatrix} \langle \alpha_k m_0 \mathbf{u}_k \rangle / V \\ \langle \alpha_k m_0 \mathbf{e}_0 \mathbf{u}_k + (\alpha_k m_0 \mathbf{u}_0') \mathbf{u}_k' \rangle / V \end{bmatrix} = \begin{bmatrix} \langle m_0 \dot{\alpha}_k \rangle / V \\ \langle m_0 \dot{\alpha}_k \rangle \end{bmatrix} \]  
\[ \rightarrow \frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \rho_k \mathbf{u}_k \\ \rho_k \mathbf{e}_k \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho_k \mathbf{u}_k \\ \rho_k \mathbf{e}_k \end{bmatrix} = \begin{bmatrix} \rho_k \dot{\mathbf{u}}_k \\ \rho_k \dot{\mathbf{e}}_k \end{bmatrix}. \]  

(3.59a)

As done previously for the single-material case, the Euler equations are applied to the right-hand side of Eq. 3.59b. Recall from Eqs. 3.52c and 3.52d that

\[ \langle m_0 \dot{\mathbf{u}}_0 \rangle / V = -\langle \nabla \rho_0 \rangle. \]  

(3.60a)

Therefore,

\[ \langle \alpha_k m_0 \dot{\mathbf{u}}_0 \rangle / V = -\langle \alpha_k \nabla \rho_0 \rangle. \]  

(3.60b)

This term is expanded:

\[ -\langle \alpha_k \nabla \rho_0 \rangle = -\nabla \langle \alpha_k \rho_0 \rangle - \langle \rho_0 \nabla \alpha_k \rangle = -\nabla \langle \alpha_k \rho_0 \rangle + \langle \rho_0 \nabla \alpha_k \rangle = -\nabla p_k + \langle \rho_0 \nabla \alpha_k \rangle. \]  

(3.60c)

Note that \( p_0 = p + p_o' \) and in turn, \( p_o' = p_0 - p \):

\[ -\nabla p_k + \langle \rho_0 \nabla \alpha_k \rangle = -\nabla p_k + \langle (p + p_o') \nabla \alpha_k \rangle = -\nabla p_k + \langle p \nabla \alpha_k \rangle + \langle p_o' \nabla \alpha_k \rangle = -\nabla p_k + p \nabla \langle \alpha_k \rangle + \langle (p_0 - p) \nabla \alpha_k \rangle. \]  

(3.60d)
Kashiwa and Rauenzahn (1994) define $\theta_k = \langle \alpha_k \rangle$. Eq. 3.60d becomes:

$$-\nabla p_k + p \nabla \theta_k + \langle (p_0 - p) \nabla \alpha_k \rangle = -\nabla p_k + \nabla (\theta_k p) - \theta_k \nabla p + \langle (p_0 - p) \nabla \alpha_k \rangle$$

$$= -\nabla (p_k - \theta_k p) - \theta_k \nabla p + \langle (p_0 - p) \nabla \alpha_k \rangle.$$  \hspace{1cm} (3.60e)

Recall from Eq. 3.52f that

$$\langle m_i \dot{v}_i \rangle / V = \langle \gamma^{-1} \dot{p}_0 \rangle.$$ \hspace{1cm} (3.61a)

Thus,

$$\langle \alpha_k m_i \dot{v}_i \rangle / V = \langle \alpha_k \gamma^{-1} \dot{p}_0 \rangle.$$ \hspace{1cm} (3.61b)

The expansion of this term yields:

$$\langle \alpha_k \gamma^{-1} \dot{p}_0 \rangle = \langle \alpha_k \gamma^{-1} (p + p'_0) \rangle = \langle \alpha_k \gamma^{-1} \dot{p} \rangle + \langle \alpha_k \gamma^{-1} \dot{p}' \rangle$$

$$= \langle \alpha_k \gamma^{-1} \dot{p} \rangle + \langle \alpha_k \gamma^{-1} (p_0 - p) \rangle \Rightarrow \gamma^{-1} \dot{p} + \langle \alpha_k \gamma^{-1} (p_0 - p) \rangle.$$ \hspace{1cm} (3.61c)

After the Euler equations are applied, the momentum equations in Eq. 3.59b can be expressed as (Kashiwa and Rauenzahn, 1994):

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \rho_k \dot{u}_k \\ \rho_k \dot{e}_k \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho_k \dot{u}_k \\ \rho_k \dot{u}_k + \langle \alpha_k \rho_k u'_k \rangle \\ \rho_k \dot{e}_k + \langle \alpha_k \rho_k e'_k \rangle \end{bmatrix} = \begin{bmatrix} \langle \rho_0 \dot{\alpha}_k \rangle \\ -\nabla (p_k - \theta_k p) - \theta_k \nabla p + \langle (p_0 - p) \nabla \alpha_k \rangle + \langle \rho_0 \dot{u}_k \rangle \\ \gamma^{-1} \dot{p} + \langle \alpha_k \gamma^{-1} (p_0 - p) \rangle + \langle \rho_0 \dot{e}_k \rangle \end{bmatrix}. \hspace{1cm} (3.62)$$

Kashiwa and Rauenzahn (1994) assume that the pressure $p$ in the above equations is equal to the equilibration pressure, and that the expected value for the volume fraction at equilibrium, $\theta^eq_k$, can be represented as

$$\theta^eq_k = \rho_k v_k \left(p, T_k\right), \hspace{1cm} (3.63a)$$

where $\rho_k v_k$ represents volume of material $k$ per unit total volume. If one assumes ideal gas behavior and that $\theta^eq_k = \theta_k$, then $\theta_k / v_k = \rho_k$ and

$$p_k = \rho_k R_k T_k = (\theta_k / v_k) R_k T_k = (\theta_k R_k T_k) / v_k, \hspace{1cm} (3.63b)$$
where $R_k$ is the gas constant. The quantity $(R_k T_k)/v_k$ remains unchanged for all $k$ materials at equilibrium. Therefore, at equilibrium (Kashiwa and Rauenzahn, 1994),

$$\frac{(\theta_k R_k T_k)}{v_k} - \theta_k p = 0,$$

(3.63c)

or

$$\frac{(\theta_k R_k T_k)}{v_k} = \theta_k p,$$

(3.63d)

and

$$\frac{(R_k T_k)}{v_k} = p^0_k,$$

(3.63e)

where $p^0_k$ represents the pressure for a pure material $k$. Therefore,

$$p_k = \frac{(\theta_k R_k T_k)}{v_k} = \theta_k p^0_k.$$  

(3.63f)

The $\nabla(p_k - \theta_k p)$ term in the momentum equations in Eq. 3.62 can then be expressed as

$$\nabla(p_k - \theta_k p) = \nabla \theta_k (p^0_k - p).$$  

(3.63g)

The previous derivations are simplified versions of the momentum equations since the Euler equations are used to define $m_\alpha \dot{u}_0$ and $m_\alpha \dot{e}_0$. If the Navier-Stokes equations are used instead, the expressions become (Kashiwa and Rauenzahn, 1994):

$$m_\alpha \dot{u}_0 = -V \nabla p_0 + V \nabla \cdot \tau_0 + \rho_0 V g,$$

(3.64)

and

$$m_\alpha \dot{e}_0 = \gamma_0^{-1} V p_0 + \left[ V (\tau_0 : \xi_0)/2 \right] - V \nabla \cdot q_0,$$

(3.65)

where $\tau_0$ denotes the deviatoric stress, $q_0$ denotes the heat flux, and $\xi_0$ denotes the rate-of-strain tensor (Kashiwa and Rauenzahn, 1994):

$$\xi_0 = \nabla u_0 + (\nabla u_0)^\top - (2/3)(\nabla \cdot u_0) I.$$  

(3.66)

Thus, $\langle \alpha_k m_\alpha \dot{u}_0 \rangle / \rho$ can be expressed as the following:

$$\frac{\langle \alpha_k m_\alpha \dot{u}_0 \rangle}{\rho} = \frac{-\langle \alpha_k V \nabla p_0 \rangle + \langle \alpha_k \nabla \cdot \tau_0 \rangle + \langle \alpha_k \rho_0 V g \rangle}{\rho} = \langle -\alpha_k \nabla p_0 \rangle + \langle \alpha_k \nabla \cdot \tau_0 \rangle + \langle \alpha_k \rho_0 g \rangle,$$

(3.67a)

where, from Eqs. 3.60c, d, and e,

$$-\langle \alpha_k \nabla p_0 \rangle = -\nabla(p_k - \theta_k p) - \theta_k \nabla p + \left( (p_0 - p) \nabla \alpha_k \right),$$

(3.67b)

and therefore
\[ \langle \alpha_k m_k \dot{u}_k \rangle/V = -\nabla (p_k - \theta_k p) - \theta_k \nabla p + \langle (p_k - p) \nabla \alpha_k \rangle + \langle \alpha_k \nabla \cdot \tau_k \rangle + \langle \alpha_k \rho_0 \mathbf{g} \rangle \\
= -\nabla \theta_k (p_k^0 - p) - \theta_k \nabla p + \langle (p_k^0 - p) \cdot \nabla \alpha_k \rangle + \langle \nabla \cdot (\alpha_k \tau_k) \rangle - \langle (\nabla \alpha_k) \cdot \tau_k \rangle + \rho_k \mathbf{g} \\
= -\nabla \theta_k (p_k^0 - p) - \theta_k \nabla p + \left[ \left( (p_k^0 - p) \mathbf{I} - \tau_k \right) \nabla \alpha_k \right] + \nabla \cdot (\alpha_k \tau_k) + \rho_k \mathbf{g} . \quad (3.67c) \]

Similarly, \( \langle \alpha_k m_k \dot{e}_k \rangle/V \) can be expressed as the following:
\[
\frac{\langle \alpha_k m_k \dot{e}_k \rangle}{V} = \frac{\langle \alpha_k \gamma_k^{-1} \dot{p}_k \rangle}{V} + \frac{\left[ \langle \alpha_k V (\tau_k : \xi_0) / 2 \rangle \right]}{V} - \langle \alpha_k \nabla \cdot \mathbf{q}_k \rangle, \quad (3.68a)
\]
where, from Eq. 3.61c,
\[
\langle \alpha_k \gamma_k^{-1} \dot{p}_k \rangle = \langle \alpha_k \gamma_k^{-1} p \rangle + \langle \alpha_k \gamma_k^{-1} (p_0 - p)^* \rangle . \quad (3.68b)
\]
Assuming ideal gas behavior,
\[
\langle \alpha_k \gamma_k^{-1} \rangle = \langle \alpha_k p_0 / (\rho_0 c_v^2) \rangle = \left( p_k v_k / c_v^2 \right) , \quad (3.68c)
\]
where \( c_0 \) denotes the speed of sound (Kashiwa and Rauenzahn, 1994). Also note that
\[
-\langle \alpha_k \nabla \cdot \mathbf{q}_k \rangle = -\langle \nabla \cdot (\alpha_k \mathbf{q}_k) \rangle + \langle \mathbf{q}_k \cdot \nabla \alpha_k \rangle . \quad (3.68d)
\]
Therefore,
\[
\frac{\langle \alpha_k m_k \dot{e}_k \rangle}{V} = \left[ \left( p_k v_k / c_v^2 \right) \dot{p} + \left( \alpha_k \gamma_k^{-1} (p_0 - p)^* \right) \right] + \left( \alpha_k \left( \tau_0 : \xi_0 \right) \right) / 2 - \nabla \cdot (\alpha_k \mathbf{q}_0) + \langle \mathbf{q}_0 \cdot \nabla \alpha_k \rangle . \quad (3.68e)
\]

Finally, the unclosed ensemble-averaged equations for the multimaterial case are (Kashiwa and Rauenzahn, 1994):
\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \rho_k \mathbf{u}_k \\ \rho_k \mathbf{e}_k \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho_k \mathbf{u}_k \\ \alpha_k \rho_0 \mathbf{u}_k \mathbf{u}_k' \\ \alpha_k \rho_0 \mathbf{e}_k \mathbf{u}_k' \end{bmatrix} = \begin{bmatrix} \langle \rho_0 \dot{\alpha}_k \rangle \\ -\nabla \theta_k (p_k^0 - p) - \theta_k \nabla p + \left[ \left( (p_k^0 - p) \mathbf{I} - \tau_0 \right) \nabla \alpha_k \right] + \nabla \cdot (\alpha_k \tau_k) + \rho_k \mathbf{g} + \langle \rho_0 \mathbf{u}_0 \dot{\alpha}_k \rangle \\
\left( p_k v_k / c_v^2 \right) \dot{p} + \left( \alpha_k \gamma_k^{-1} (p_0 - p)^* \right) \right] + \left( \alpha_k \left( \tau_0 : \xi_0 \right) \right) / 2 - \nabla \cdot (\alpha_k \mathbf{q}_0) + \langle \mathbf{q}_0 \cdot \nabla \alpha_k \rangle + \langle \rho_0 \mathbf{e}_0 \dot{\alpha}_k \rangle \end{bmatrix} , \quad (3.69)
where (Kashiwa and Rauenzahn, 1994)

\[
\dot{\rho} = \left( \sum v_k \rho_0 \alpha_k \right) - \left( \sum \nabla \cdot \theta_k u_k \right) / \left( \sum \theta_k v_k / c_k^2 \right).
\]  

(3.70)

3.2.3 Numerical Calculation Scheme and Finite Volume Discretization

CFDLib is based on an Arbitrary-Lagrangian-Eulerian (ALE) scheme as described by Hirt et al. (1974). The ALE scheme is known for its flexibility since it allows the computational mesh either to be moved along with the fluid (Lagrangian), to remain in a fixed position (Eulerian), or to be moved in another way as selected by the user. Including an implicit formulation similar to that in the implicit continuous-fluid Eulerian (ICE) method enables the ALE scheme to handle flows at any speed, including the limiting cases of fully incompressible flow and hypersonic flow (Hirt et al., 1974). Therefore, the numerical method implemented in CFDLib is a generalization of the implicit continuous-fluid Eulerian (ICE) scheme proposed by Harlow and Amsden (1975), which is stable for any value of the Courant number based on the speed of sound (Kashiwa et al., 1994). In CFDLib, however, the classical ICE method is extended to consider multi-fluid and multiphase calculations for an arbitrary number of fluid fields. According to Kashiwa et al. (1994), when the limiting case of incompressible flow is considered, the ICE method will in effect become identical to the Marker and Cell (MAC) method. The limiting case of incompressible flow is applied in this work.

The computational cycle includes three main parts: the primary phase, the Lagrangian phase, and the Eulerian phase. Auxiliary quantities are calculated in the primary phase, effects of physical processes are calculated in the Lagrangian phase, and all states and components of the state vector are remapped to one common control volume in the Eulerian phase. Since the calculation method uses only one common control volume, all the state quantities are regarded as cell-centered quantities. The computational cycle is carried out as long as the time-dependent state advances in increments of \( \Delta t \) (Kashiwa et al., 1994).

Figure 3.4 is a flowchart that displays the sequence in which the major subroutines in CFDLib are called. A description of the functions in each major subroutine follows Figure 3.4.
Figure 3.4. Flowchart of major CFDLib subroutines.
WHOCompile—This routine writes information about the code and checks code options, including if the calculation is for a multifluid case or a single fluid case; if the calculation is sequential, auto-parallel, or MPI; and the preferred calculation method (e.g., ICE or MAC).

RDInput—This routine reads problem input from the input file, reads the problem title, sets default values, checks for changes when a problem is restarted, checks the number of fields needed for equation of state calculations, and verifies if diffusion will be calculated.

DIMCheck—This routine checks dimension limits and will stop the program if these limits are exceeded. The program also stops if required input values such as number of blocks, number of sections, number of cells per section, initial densities, initial volume fractions, and/or density values at certain boundaries are not specified.

SESSEt—This routine initializes the SESAME tables if required, and also initializes some equation of state variables.

BCOMSEt—This routine generates the data required for inter-block communication, initializes boundary communication arrays and checks these arrays for consistency, and checks the mesh dimensions on each face of a block.

GRPHINIT—This routine initializes graphics and sets timing parameters for output.

NEWPROB—This routine prepares a new problem. It sets up the mesh, loads cell-centered flags, initializes the Lagrangian-phase calculations, checks array dimensions, tests for negative density values (and stops the program if such values are found), and initializes velocity, temperature, species density, phase density, and volume fraction values.

NRESTART—This determines from what time a program must be restarted. CFDLib writes dump files, named dp2d or dp3d, at time increments specified in the input file. These files contain all data needed to restart a calculation from the most recent simulation time. The time step at which a dump file is written is assigned a dump number, which is printed in the output file. In the input file, nrestart is set equal to the most recent dump number to restart the calculation. (nrestart = 0 for a new problem.) Finally, the dp3d files must be renamed rs3d, or dp2d files must be renamed rs2d.

RESTART—This routine reads restart data from the rs3d or rs2d file, creates arrays needed to resume the calculation, and initializes the boundary communication routine.

NCYC—This parameter denotes the current calculation cycle. The maximum number of cycles, ncyemax, can be specified in the input file. A new calculation cycle begins when a new time step value is determined.
NEWCYC—This routine finds the new time step in preparation for the next cycle through the subroutine HYDRO.

HYDROOUT—At specified times, this routine provides output information, such as the cycle number, current simulation time, and value of the time step.

DIFFUSION_DRV—This is the driver for mass and temperature diffusion calculations.

HYDRO—This driver for the Lagrangian-phase calculation calls routines that calculate surface tension, momentum exchange, pressure, divergence, the boundary force vector, and acceleration. The driver also calls routines that handle turbulence production.

REMAP—This driver for the remapping (Eulerian) phase calls routines that perform advection calculations.

EXCHANGE_NL—This driver for the nonlinear exchange processes calls for mass exchange and volume exchange.

UPDATE—This routine updates the state and the state variables.

TIMNG—This routine outputs timing information, such as CPU seconds used for key subroutines.

The following description of the discretization method in CFDLib is found in Kashiwa et al. (1994). Their example utilizes a fixed reference frame and a finite-volume computational mesh that moves with velocity $\mathbf{u}_m$. Their example works backward to describe the computational cycle; it first discusses the Eulerian phase, then the Lagrangian phase, and finally the primary phase.

If $q_k(x,t)$ represents an arbitrary field variable in volume $V$, the change in volume caused by physical processes is expressed as

$$\int_V \frac{\partial q_k}{\partial t} dV + \int_S \mathbf{n} \cdot \mathbf{q}_k dS = \frac{d}{dt} \int_V q_k dV, \quad (3.71a)$$

where $S$ denotes the surface $S(x,t)$, $\mathbf{n}$ denotes the unit normal vector, and $\mathbf{u}_k$ denotes the velocity for material $k$. Kashiwa et al. (1994) consider $q_k$ to be the average value in $V$, such that

$$\int_V q_k dV = q_k V \quad (3.71b)$$

and
\[
\frac{d}{dt} \int_V q_k \, dV = \frac{\Delta (q_k V)}{\Delta t}.
\] (3.71c)

The change in volume resulting from material transport, denoted by \(\frac{d_m}{dt}\), is defined as
\[
\int_V \frac{\partial q_k}{\partial t} dV + \int_n n \cdot q_k u_m \, dS = \frac{d_m}{dt} \int_V q_k \, dV,
\] (3.72)
and the total change in \(q_k\) on the computational mesh, moving with velocity \(u_m\), is the difference between Eqs. 3.71a and 3.72:
\[
\left( \int_V \frac{\partial q_k}{\partial t} \, dV - \int_V \frac{\partial q_k}{\partial t} \, dV \right) + \left( \int_n n \cdot q_k u_k \, dS - \int_n n \cdot q_k u_m \, dS \right) = \left[ \frac{\Delta (q_k V)}{\Delta t} - \frac{d_m}{dt} \int_V q_k \, dV \right],
\] (3.73a)

or
\[
\frac{d_m}{dt} \int_V q_k \, dV + \int_n n \cdot q_k (u_k - u_m) \, dS = \frac{\Delta (q_k V)}{\Delta t}.
\] (3.73b)

The discretization of Eq. 3.73b involves a summation that takes place over all surfaces (i.e., cell faces) that define the volume \(V\). The discretized form of Eq. 3.73b is
\[
q_k^{n+1} V^{n+1} - q_k^n V^n + \left[ \sum_i \Delta t S_i \cdot (u_k^* - u_m) \right] \left\langle q_k \right\rangle_i^u = q_k^L V_k^L - q_k^n V^n,
\] (3.74a)

where the superscript \(L\) denotes Lagrangian values; \(V^n\) is determined by the surfaces (faces), which are in turn determined by the cell vertices; \(S_i\) denotes the surface vector (area times outward normal) of a side or face \(i\); vertices on the computational mesh travel with \(u_m\); \(\left\langle q_k \right\rangle_i^u\) denotes an upwind, cell-centered value of \(q_k\); and \(u_k^*\) is a face-centered velocity representing the rate at which the volume of material \(k\) passes through face \(i\).

Kashiwa et al. (1994) state that the sum over all the surfaces defining \(V^n\) can also be expressed in terms of an advection operator, \(A\), that utilizes Lagrangian time values:
\[
\Delta t A(q_k) = \sum_i \Delta t S_i \cdot (u_k^* - u_m) \left\langle q_k \right\rangle_i^u.
\] (3.74b)

Thus, Eq. 3.74a can be rewritten as:
\[
q_k^{n+1} V^{n+1} - q_k^n V^n + \Delta t A(q_k) = q_k^L V_k^L - q_k^n V^n,
\] (3.75a)

or
\[
q_k^{n+1} V^{n+1} + \Delta t A(q_k) = q_k^L V_k^L.
\] (3.75b)
The solution for $V^{n+1}$ is obtained from the equation for volume change caused by material transport (Eq. 3.72):

$$\int_v \frac{\partial q_k}{\partial t} dV + \int_k n \cdot q_k u_m dS = \frac{d}{dt} \int_v q_k dV \Rightarrow \int_v \frac{\partial q_k}{\partial t} dV + \int_k n \cdot q_k u_m dS = \frac{d}{dt} \left( q_k V \right).$$

(Eq. 3.76a)

Eq. 3.76a is divided by $q_k$:

$$\int_v \frac{\partial}{\partial t} dV + \int_k n \cdot u_m dS = \frac{d}{dt} (V) \Rightarrow \Delta t \int_k n \cdot u_m dS = V^{n+1} - V^n. \quad (3.76b)$$

Discretization is performed, with the required summation over all faces:

$$\Delta t \sum_i \left( S \cdot u_m \right)^i = V^{n+1} - V^n \Rightarrow V^{n+1} = V^n + \Delta t \sum_i \left( S \cdot u_m \right)^i. \quad (3.76c)$$

Similarly, the solution for $V^L_k$ is obtained from the equation for volume change caused by physical processes (Eq. 3.71a):

$$\int_v \frac{\partial}{\partial t} dV + \int_k n \cdot q_k u_k dS = \frac{d}{dt} \int_v q_k dV \Rightarrow \int_v \frac{\partial q_k}{\partial t} dV + \int_k n \cdot q_k u_k dS = \frac{d}{dt} (q_k V).$$

(Eq. 3.77a)

Eq. 3.77a is divided by $q_k$:

$$\int_v \frac{\partial}{\partial t} dV + \int_k n \cdot u_k dS = \frac{d}{dt} (V) \Rightarrow \int_k n \cdot u_k dS = \frac{\Delta V}{\Delta t} \Rightarrow \Delta t \int_k n \cdot u_k dS = \Delta V. \quad (3.77b)$$

Discretization is performed, with the required summation over all faces:

$$\Delta t \sum_i \left( S \cdot u_k^* \right)^i = V^L_k - V^n \Rightarrow V^L_k = V^n + \Delta t \sum_i \left( S \cdot u_k^* \right)^i. \quad (3.77c)$$

Kashiwa et al. (1994) set $q_k$ equal to the state vector $(\rho_k, u_k, T_k)^{Ttl}$. (The superscript $Ttl$ will be discussed shortly.) Placing this state vector in Eq. 3.75b yields:

$$\rho_k^{n+1} V^{n+1} + \Delta t A(\rho_k) = \rho^L_k V^L_k, \quad (3.78a)$$

$$u_k^{n+1} V^{n+1} + \Delta t A(u_k) = u^L_k V^L_k, \quad (3.78b)$$

and

$$T_k^{n+1} V^{n+1} + \Delta t A(T_k) = T^L_k V^L_k. \quad (3.78c)$$
Solving for $\rho_{k}^{n+1}, u_{k}^{n+1},$ and $T_{k}^{n+1}$ yields:

$$\rho_{k}^{n+1} = \frac{\rho_{k}^{L} V_{k}^{L} - \Delta t A(\rho_{k})}{V^{n+1}},$$  \hspace{1cm} (3.79a)$$

$$u_{k}^{n+1} = \frac{u_{k}^{L} V_{k}^{L} - \Delta t A(u_{k})}{V^{n+1}},$$  \hspace{1cm} (3.79b)$$

and

$$T_{k}^{n+1} = \frac{T_{k} V_{k}^{L} - \Delta t A(T_{k})}{V^{n+1}}.$$  \hspace{1cm} (3.79c)$$

The Lagrangian values of the state vector, $(\rho_{k}^{L}, u_{k}^{L}, T_{k}^{L})^{Tl}$, are solved for in the Lagrangian calculation phase. The superscript $Tl$ indicates that the total mass, the velocity, and the temperature are mapped instead of the total mass, total momentum, and total energy. This designation improves the performance of the algorithm and reduces numerical noise (Kashiwa et al., 1994). Thus, the state vector can also be represented as

$$q_{k} = (\rho_{k}, \rho_{k} u_{k}, \rho_{k} e_{k}).$$  \hspace{1cm} (3.80a)$$

Recalling that

$$\frac{d}{d t} \int_{y} q_{k} d V = \frac{\Delta(q_{k} V)}{\Delta t},$$  \hspace{1cm} (3.80b)$$

and multiplying by $\Delta t$ gives

$$\frac{\Delta(q_{k} V)}{\Delta t} \Delta t = \Delta m_{k},$$  \hspace{1cm} (3.80c)$$

$$\frac{\Delta(q_{k} u_{k} V)}{\Delta t} \Delta t = \Delta(m_{k} u_{k}),$$  \hspace{1cm} (3.80d)$$

and

$$\frac{\Delta(q_{k} e_{k} V)}{\Delta t} \Delta t = \Delta(m_{k} e_{k}).$$  \hspace{1cm} (3.80e)$$

The property $\Delta q_{k} = q_{k}^{L} - q_{k}^{n}$ is applied to $\Delta m_{k}, \Delta(m_{k} u_{k}),$ and $\Delta(m_{k} e_{k})$ to determine $\rho_{k}^{L}, u_{k}^{L},$ and $T_{k}^{L}$:

$$\Delta m_{k} = m_{k}^{L} - m_{k}^{n} = \rho_{k}^{L} V_{k}^{L} - \rho_{k}^{n} V_{k}^{n}$$

$$\Rightarrow \rho_{k}^{L} V_{k}^{L} = \rho_{k}^{n} V_{k}^{n} + \Delta m_{k} \Rightarrow \rho_{k}^{L} = \frac{\rho_{k}^{n} V_{k}^{n} + \Delta m_{k}}{V_{k}^{L}}.$$  \hspace{1cm} (3.81a)$$
\[ \Delta (m_k u_k) = m_k^i u_k^i - m_k^u u_k^u \Rightarrow m_k^i u_k^i = m_k^u u_k^u + \Delta (m_k u_k) \]

\[ \rightarrow m_k^i u_k^i = \left( m_k^i - \Delta m_k \right) u_k^u + \Delta (m_k u_k) \]

\[ \rightarrow u_k^i = \frac{\left( m_k^i - \Delta m_k \right) u_k^u}{m_k^i} + \frac{\Delta (m_k u_k)}{m_k^i}, \quad (3.81b) \]

and

\[ \Delta (m_k e_k) = m_k^i e_k^i - m_k^u e_k^u \Rightarrow m_k^i e_k^i = m_k^u e_k^u + \Delta (m_k e_k) \]

\[ \rightarrow m_k^i \left( e_k^u + \Delta e_k \right) = \left( m_k^i - \Delta m_k \right) e_k^u + \Delta (m_k e_k), \quad (3.81c) \]

where

\[ \Delta e_k = c_{vk} \Delta T_k, \quad (3.81d) \]

and \( c_{vk} \) is the constant volume specific heat of \( k \) (Kashiwa et al., 1994). This substitution is placed into Eq. 3.81c to yield

\[ m_k^i \left( e_k^u + c_{vk} \Delta T_k \right) = \left( m_k^i - \Delta m_k \right) e_k^u + \Delta (m_k e_k) \]

\[ \rightarrow m_k^i e_k^u + m_k^i c_{vk} \left( T_k^i - T_k^u \right) = m_k^i e_k^u - (\Delta m_k) e_k^u + \Delta (m_k e_k) \]

\[ \rightarrow m_k^i c_{vk} \left( T_k^i - T_k^u \right) = -(\Delta m_k) e_k^u + \Delta (m_k e_k) \]

\[ \rightarrow m_k^i c_{vk} T_k^i = m_k^i c_{vk} T_k^u - (\Delta m_k) e_k^u + \Delta (m_k e_k) \]

\[ \rightarrow c_{vk} T_k^i = c_{vk} T_k^u - \frac{(\Delta m_k) e_k^u}{m_k^i} + \frac{\Delta (m_k e_k)}{m_k^i} \]

\[ \rightarrow c_{vk} T_k^i = c_{vk} T_k^u \left( 1 - \frac{e_k^u}{c_{vk} T_k^u m_k^i} \frac{\Delta m_k}{m_k^i} \right) + \frac{\Delta (m_k e_k)}{c_{vk} m_k^i} \]

\[ \rightarrow T_k^i = T_k^u \left( 1 - \frac{e_k^u}{c_{vk} T_k^u m_k^i} \frac{\Delta m_k}{m_k^i} \right) + \frac{\Delta (m_k e_k)}{c_{vk} m_k^i}. \quad (3.81e) \]

The values of \( \Delta m_k \), \( \Delta (m_k u_k) / m_k^i \), and \( \Delta (m_k e_k) / m_k^i \) come from the right-hand side of Eq. 3.69 multiplied by \( \Delta t V^n \), with the use of a cell-centered operator, \( \nabla^c \), wherever \( \nabla \) is required in the equations (Kashiwa et al., 1994):

\[ \Delta m_k = \Delta t V^n \left( \rho_0 \dot{\alpha}_k \right) = \Delta t \left( m_k \dot{\alpha}_k \right), \quad (3.82a) \]
The primary calculation phase is responsible for the auxiliary quantities required by the Lagrangian and Eulerian calculation phases. These are $u^*_k$, the face-centered velocity or fluxing velocity; $p^*$, the face-centered equilibration pressure; and $\dot{p}\Delta t$ or $\Delta p$, the cell-centered change in the equilibration pressure. The details for their complex derivations can be found in Kashiwa et al. (1994). It also should be noted that the mass exchange terms, having the form $\langle \dot{\alpha}_k \rangle$, comprise by themselves a set of ordinary differential equations that is solved separately. The resulting value of $\Delta m_k$ represents the change in the mass of material $k$ and provides a volume source needed to solve for the pressure (Kashiwa et al., 1994).

The calculation method can be summarized as follows. The primary calculation phase calculates the equations of state, determines the equilibration pressure $p$, determines the pressure $p^0_k$ of pure material $k$ for all materials, sets $\theta_k = \theta_k^{eq}$ if material $k$ is in pressure equilibrium, solves the set of ordinary differential equations responsible for the mass exchange terms, calculates the change in equilibration pressure $\Delta p$, and determines the fluxing velocity $u^*_k$. It also determines $p^*$, the face-centered equilibration pressure, and the value of $V^L_k$ to be used in the Lagrangian calculation phase. The Lagrangian phase calculates the Lagrangian values of the state vector, $\left( \rho^L_k, u^L_k, T^L_k \right)^T$. The Eulerian calculation phase finds the mesh velocity $u_m$ and the value of $V^{n+1}$, and then determines $\rho^{n+1}_k$, $u^{n+1}_k$, and $T^{n+1}_k$ to update the state.
Chapter 4. CFD Predictions for Flow-Regime Transitions in Bubble Columns

Chapter 4 demonstrates the ability of the two-fluid model to predict known flow regimes in air-water bubble columns. A review of these flow regimes is provided in Section 4.1, along with a discussion of two recent experiments on homogeneous bubbly flow that motivated this work. Simulation results are presented in Section 4.2. The simulations can be considered as numerical experiments in which parameters are adjusted via changing model coefficient values in order to determine the effects on homogeneous flow transition.

It should be noted that the majority of this chapter is adapted from the *AIChE Journal* paper “CFD Predictions for Flow-Regime Transitions in Bubble Columns” by Monahan et al. (2005). Specifically, Section 4.1 of this chapter is adapted from the section titled “Bubble-Column Flow Regimes” in Monahan et al. (2005), and Section 4.2 of this chapter is adapted from the section titled “Results and Discussions” in Monahan et al. (2005). Any changes to the text are made to correspond to the equation numbers, chapter and section numbers, tables and table numbers, or figures and figure numbers presented in this thesis. It should also be noted that additional figures are presented in this thesis chapter. To accommodate for these additional figures, the numbers of various figures in this thesis chapter may differ from their appearance in Monahan et al. (2005).

4.1 Bubble-Column Flow Regimes

Depending on the inlet flow conditions, two primary flow regimes can be identified for bubble-column flows: homogeneous and heterogeneous. A flow-regime map for air-water bubble columns, based on column diameter and inlet air velocity ($u_g$), is given in Fig. 4.1. (Both Figs. 4.1 and 4.2 are adapted from Shah and Deckwer, 1983.) Note that the flow-regime map does not account for bubble diameter; however, Shah and Deckwer (1983) suggest that the representative stable bubble diameter is near 4 mm. It should be noted that the map is overall qualitative and is utilized primarily to define the difference between homogeneous and heterogeneous flow. Figure 4.2 illustrates qualitative representations of homogeneous flow, slug flow, and churn-turbulent flow,
each of which will be discussed in this section. Note that for slug and churn-turbulent flows bubble coalescence is significant and most likely has a predominate effect on these flows. Markers are superimposed onto Fig. 4.1 in order to designate the expected flow regimes for the cases studied in the present work. The homogeneous, or bubbly-flow, regime is characterized by low gas velocities (less than 5 cm/s) and bubbles that tend to be small, uniform, and approximately spherical in shape. In this regime, the bubbles have nearly equal rise velocities, travel rectilinearly upwards, and exhibit little interaction with neighboring bubbles (Shah and Deckwer, 1983).

Figure 4.1. Flow-regime map (adapted from Shah and Deckwer, 1983) and markers indicating cases studied in the present work. A: 6-cm column with inlet air velocity of 2 cm/s. B: 6-cm column with inlet air velocity of 6.2 cm/s. C: 6-cm column with inlet air velocity of 12 cm/s. D: 20-cm column with inlet air velocity of 2 cm/s. E: 40-cm column with inlet air velocity of 2 cm/s. F: 40-cm column with inlet air velocity of 12 cm/s. Note that this map does not account for the effect of bubble size.
Recent experiments have demonstrated that the use of low air inlet flow rates and uniform feed in small-diameter bubble columns results in homogeneous flow behavior. Garnier et al. (2002a, b) utilized a cylindrical air-water bubble column with a diameter of 8 cm. The column height was fixed at 31 cm for this particular experiment. Air was injected through a system of needles at the bottom of the column, and the injection device was designed to maintain a nearly uniform distribution of air. Water was introduced perpendicular to the needles, and then traveled upward through the column. Experiments were conducted for four values of the superficial liquid velocity: 1.6, 3.3, 4.4, and 6.2 cm/s. Velocity and holdup profiles were overall uniform for these experiments. By suppressing bubble coalescence, Garnier et al. (2002a, b) were able to observe the transition from laminar to turbulent flow by increasing the gas velocity. Unlike the slug-flow regime shown in Fig. 4.2, the turbulent-flow regime exhibits large velocity fluctuations due to the rapid, coherent motion of “bubble swarms.”

In an independent experimental study, Harteveld et al. (2003) utilized a 15-cm cylindrical bubble column, initially filled with tap water to a height of 130 cm. Air injection needles were organized in groups to allow both uniform and non-uniform feed. For uniform aeration, air was introduced at 2.3 cm/s. As expected from Fig. 4.2, the resulting radial gas holdup profiles were uniform except at the column walls. Most inhomogeneous flow behavior caused by the bubble injection system disappeared at a height of 15 cm (i.e., the homogeneous flow was stable to initial fluctuations). However, these authors show that the bubble-flow behavior is strongly influenced by non-uniform feed (i.e., by changing the inlet boundary conditions for the gas phase). For example, when bubbles are injected uniformly except for a region near the wall where no bubbles are introduced, a transition to swirling bubbly flow is observed. Although beyond the scope of the work presented in this chapter, this sensitivity of homogeneous flow to the inlet boundary conditions offers a valuable database for testing the predictive abilities of two-fluid CFD models.
Figure 4.2. Representations of flow regimes observed in bubble columns.

As the gas flow rate is increased, transition to the heterogeneous-flow regime will eventually occur. Bubbles of different sizes and shapes and intense liquid circulation are typical for this regime (Chen et al., 1994). The relatively high gas holdup and vigorous velocity fluctuations lead to bubble coalescence, which further enhances flow instabilities. At high gas velocities, slug flow occurs in small-diameter columns, while churn-turbulent flow occurs in large-diameter columns (Shah and Deckwer, 1983). Churn-turbulent flow is observed in most industrial applications, and is characterized by large bubbles traveling primarily in the center of the column. As gas velocity increases, gas is more likely to be transported by large bubbles and bubble clusters (Shah and Deckwer, 1983). Slug flow occurs in small-diameter columns when large bubbles are stabilized by the column walls to form slugs, as shown in Fig. 4.2. Such behavior usually is not observed for columns of industrial size. While bubble clusters approximately 10 cm in diameter can be observed in bubble columns, slugs typically do not form in columns larger than approximately 15 cm in diameter (Shah and Deckwer, 1983).

Olmos et al. (2003a) observed two transitional regimes in between the homogeneous- and heterogeneous-flow regimes. Their experiments for a 20-cm column
demonstrated that homogeneous flow was dominant for superficial gas velocities less than 3.2 cm/s. For gas velocities between 3.2-4.4 cm/s (the first transitional regime), holdup increased at a slower rate, and coalescence occurred near the sparger, resulting in a plume. However, this plume broke apart after reaching a definitive liquid height, after which the flow regime again appeared homogeneous. Holdup values remained nearly constant when the superficial gas velocity was between 4.4-5.5 cm/s (the second transitional regime), and the height of the plume increased with increasing superficial velocity. The heterogeneous regime was observed for superficial gas velocities larger than 5.5 cm/s, and was characterized by varied bubble sizes, with the largest bubbles located in the center of the column, as described by Shah and Deckwer (1983).

As noted previously, much of the recent CFD work on bubble columns has focused on the predictions of time-averaged quantities such as gas holdup in the churn-turbulent regime (Krishna et al., 1999; Pan et al., 1999; Buwa and Ranade, 2002; Zhou et al., 2002; Sokolichin et al., 2004). As shown in this work, such studies are of limited utility for determining the predictive ability of two-fluid CFD models for gas-liquid flows, and for discriminating between different model formulations. For example, we show that the drag-force model primarily determines the time-averaged gas holdup, and thus the same value is obtained for laminar, homogeneous flow and for turbulent, heterogeneous flow. Hence, since the drag-force model is a correlation that must be input into the CFD model, comparison of time-averaged gas holdup only confirms the adequacy of the correlation while resting mute on the predictive abilities of the two-fluid model. For this reason, we focus our attention in this work on the ability of CFD models to predict instantaneous flow patterns and transitions between known flow regimes with uniform inlet boundary conditions as observed in the experiments of Garnier et al. (2002a, b) and Harteveld et al. (2003). In particular, we seek to answer the question of whether or not the two-fluid model can predict the homogeneous- and transitional-flow regimes shown in Fig. 4.1. In our opinion, only after answering this question in the affirmative can CFD model validation for non-uniform inlet boundary conditions and for the churn-turbulent regime be undertaken with any confidence in the generality of the conclusions.
4.2 Simulation Results and Discussion

The first set of simulations is based on the small-column-diameter experiments performed by Garnier et al. (2002a, b), but with slight differences from their experimental setup described previously. Unless stated otherwise, the simulations are performed on a two-dimensional (2D) Cartesian grid with free-slip boundary conditions at the column walls. Additionally, the column height is extended to 50 cm in order to provide sufficient freeboard at the top of the column. The column is initially filled with water, and uniform aeration is turned on at the beginning of the simulations. After several seconds of real time, the simulations reach a statistically steady-state flow regime. All results presented are taken for flows in this regime. The two-fluid model in CFDLib as discussed in Chapter 3 is applied, and Table 4.1 summarizes the conditions and model parameters for all simulations reported in this work. It should be noted that in some simulations the bubble diameter is held constant at the value reported in the experiments. In other cases, simulations are run for different bubble diameters to determine its effect on the flow predictions. Also note that changing the bubble diameter corresponds to changing the bubble Reynolds number. In this work we consider bubble Reynolds numbers in the range \(25 \leq Re \leq 1100\). In all cases, bubble coalescence is neglected and the physical properties of air and water at room temperature are employed. Finally, recall that the lift, rotation, and strain forces come from the interaction forces (i.e., attraction and repulsion) in the original derivation in CFDLib, as described in Chapter 3, Section 3.1.3.

Our numerical results are divided into the following categories. First, commentary on the effect of the wall boundary conditions is given. Then, the effect of grid resolution on laminar-flow simulations is discussed. Next, the effects of force-model parameters on both laminar-flow simulations and simulations applying the bubble-induced turbulence (BIT) model are presented for the homogeneous flow regime. Then, the combined effect of force-model parameters and the BIT model on transitional-flow behavior in 6-cm columns is studied. Subsequently, for high-flow-rate simulations both the effect of bubble size on flow structures and the effect of liquid coflow on the flow stability are discussed. Finally, flow predictions for scale-up in terms of column diameter are analyzed.
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**Homogeneous Flow**

| Column width | 6 cm |
| Inlet velocities | Air: 2 cm/s, Water: 0 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.75, 0.75, 0.25); (0.5, 0.375, 0.375, 0.125); or (0, 0, 0, 0) |
| Vertical boundary conditions | Free-slip: all cases; Periodic: \( (C_{vm}, C_L, C_{rot}, C_S) = (0.5, 0.375, 0.375, 0.125) \) only |

**Transitional Flow**

| Column width | 6 cm |
| Inlet velocities | Air: 2, 6.2, and 12 cm/s; Water: 1.6 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.75, 0.75, 0.25); (0.5, 0.375, 0.375, 0.125); or (0, 0, 0, 0) |
| Vertical boundary conditions | Free-slip: all cases; Periodic: \( (C_{vm}, C_L, C_{rot}, C_S) = (0.5, 0.375, 0.375, 0.125) \) only |

**Effect of Bubble Size on Flow Structures**

| Column width | 6 cm |
| Inlet velocities | Air: 12 cm/s, Water: 1.6 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.375, 0.375, 0.125) |
| Vertical boundary conditions | Free-slip and periodic |

**Effect of Liquid Coflow**

| Column width | 6 cm |
| Inlet velocities | Air: 12 cm/s, Water: 0, 1.6, and 3.3 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.375, 0.375, 0.125) |
| Vertical boundary conditions | Free-slip |

**Effect of Column Diameter (Homogeneous Flow)**

| Column width | 6, 20, 40 cm |
| Inlet velocities | Air: 2 cm/s, Water: 0 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.75, 0.75, 0.25); (0.5, 0.375, 0.375, 0.125); or (0, 0, 0, 0) |
| Vertical boundary conditions | Free-slip |

**Effect of Column Diameter (Transitional Flow)**

| Column width | 6, 40 cm |
| Inlet velocities | Air: 2 and 12 cm/s; Water: 1.6 cm/s |
| \( (C_{vm}, C_L, C_{rot}, C_S) \) | (0.5, 0.375, 0.375, 0.125) |
| Vertical boundary conditions | Free-slip |
4.2.1 Effect of Wall Boundary Conditions

The two types of wall boundary conditions considered for our numerical studies are free-slip, for which velocity gradients at the wall are assumed to be null, and periodic, for which a pseudo-infinite domain is assumed. As shown in Fig. 4.3, the use of periodic boundary conditions results in (presumably) unphysical bands in the velocity vector fields. Figure 4.3 illustrates this phenomenon for a 6-cm column using (i) an air inlet flow rate of 2 cm/s with $d_b$ set to 0.5 mm, and (ii) an air inlet flow rate of 12 cm/s with $d_b$ again set to 0.5 mm. The velocity bands are not observed for simulations utilizing free-slip boundary conditions. For this reason, the majority of the simulations discussed in the present work are performed with free-slip boundary conditions at the column walls. It is interesting to observe that when the gas phase is introduced as a point source (instead of uniformly) in bubble-column experiments, meandering plumes are observed (Sokolichin et al., 2004). We can thus speculate that the wavelength of the banded velocity structures seen with periodic walls will be related to the meandering frequency found in simulations with non-uniform inlet boundary conditions (Pfleger and Becker, 2001).

It should be noted that the presence of velocity bands is dependent on the flow domain used. For example, we show in Figure 4.4 that the use of periodic boundary conditions for a flow domain of 500 x 500 cm$^2$ generates circulation cells separated by approximately 100-150 cm, instead of bands. This suggests that the liquid level most likely determines the circulation-cell spacing. Additionally, circulation cells are found with 2D periodic boundary conditions when the flow-domain width is larger than the liquid level, suggesting that periodic boundary conditions should not be used for cases with large height/width ratios. Finally, we note that the appearance of banded velocity fields is not unique to air-water bubble columns or an artifact of our simulation code. We have observed analogous banded structures when simulating gas-solid fluidized beds with other two-fluid simulation codes that use very different numerics. Moreover, at this point we find that they are very robust and do not depend on the details of force models or grid resolution. We can thus speculate here that banded velocity fields are a generic property of the two-fluid model equations for 2D periodic domains. For a 3D case, due to symmetry, banded velocity fields would not be expected.
Figure 4.3. Water velocity vector fields for simulations utilizing periodic boundary conditions. Left: Inlet air velocity of 2 cm/s. Right: Inlet air velocity of 12 cm/s. The horizontal bands are observed only with periodic boundary conditions.
4.2.2 Grid Resolution

As shown in our earlier work (Monahan and Fox, 2002), domain size and grid resolution have a significant effect on flow simulations. In the present case, grid-resolution studies were carried out for a 6-cm column using 2D and 3D grids. Cell spacing is uniform in each direction; thus the cells are uniform squares on a 2D grid or uniform cubes on a 3D grid. Figure 4.5 illustrates typical water volume-fraction profiles at different grid resolutions. The simulations were performed using an air inflow rate of 2 cm/s and a water inflow rate of 1.6 cm/s. Figure 4.5A shows that a coarse grid (albeit
typical of previous studies, see Chapter 2) results in a near uniform flow pattern without any flow structures. Such behavior is caused by numerical diffusion which smoothes out velocity and volume-fraction gradients on coarse grids. Sokolichin and Eigenberger (1999) have reported similar effects of numerical diffusion.

With a refined grid of 0.25 cm (Fig. 4.5B), large-scale plume structures are obtained and persist throughout nearly the entire column length. Further grid refinement to 0.1 cm (Fig. 4.5C) shows even finer-scale vertical plumes, primarily at the bottom of the column. At a height between 25 and 30 cm, these plumes break up into smaller structures. Similar structures have been observed in gas-solid flow simulations using the two-fluid model (Sundaresan, 2000). One can safely assume that further grid refinement will result in even finer structures. Monahan and Fox (2002) have observed such behavior, and also find that the flow structures depend on the force models employed. However, it is also worth noting that such fine grids may be impractical for simulating industrial-scale bubble columns. In this case, sub-grid models would be needed to perform large-eddy simulations of industrial bubble columns (Sundaresan, 2000).

To justify the use of a 2D grid, 3D simulations were carried out on a grid using 0.25-cm spacing in each direction. Figure 4.5D shows a 2D slice of the 3D domain. It can be seen that these 3D flow structures are comparable with those shown in Fig. 4.5B. Furthermore, no significant change in the volume-averaged gas holdup was observed when using either a more refined grid or a 3D domain, both of which greatly increase the computational cost. Hence, unless otherwise noted, all further simulations reported in this work are performed on 2D domains using a 0.25-cm grid (uniform square cells). Finally, it should be noted that when refined grids are used (Figs. 4.5B, 4.5C, 4.5D), the laminar two-fluid model does not predict the homogeneous flow regime expected for the air inflow rate used (2 cm/s). Thus, the next step in our investigation is to examine what additional terms are needed in the two-fluid model in order to predict homogeneous flow on refined grids.
4.2.3 Homogeneous Flow

According to the flow-regime map shown in Fig. 4.1, a 6-cm wide column with 2 cm/s inlet air velocity should operate in the homogeneous-flow regime. Initially, the bubble pressure (BP) model (Eq. 3.6a) was incorporated into the two-fluid model in an attempt to obtain homogeneous flow. As discussed in Chapter 3, the BP model should help to maintain the uniform-bubbling state by driving the bubbles from higher- to lower-
holdup regions. Although the flow dynamics changed slightly when the proportionality constant $C_{BP}$ was varied, no significant effect of the BP model on the holdup distribution was observed. $C_{BP}$ was set equal to 0.2 for all subsequent simulations discussed in this chapter.

As noted in Chapter 3, bubble wakes result in enhanced turbulence in the liquid phase. Hence, to reduce the circulation and vortical structures observed in the laminar-flow simulations (i.e., $\mu_{eff,c} = \mu_{0,c}$), the bubble-induced turbulence (BIT) model (Eq. 3.12) was introduced in the continuous phase momentum balance and tested. However, it was determined that the addition of the BIT model alone (with or without the BP model) is not sufficient to generate homogeneous flow on refined grids.

Thus, a study of the force models and parameter values is undertaken in order to determine if the two-fluid model can produce homogeneous flow. This study is carried out for 6-cm columns with an air inflow rate of 2 cm/s and a water inflow rate of 0 cm/s. The value for the bubble diameter is varied from 0.5 to 4 mm, corresponding to bubble Reynolds numbers of approximately 25 and 1100, respectively. Both laminar-flow simulations ($\mu_{eff,c} = \mu_{0,c}$) and simulations applying the BIT model are performed for several bubble diameter (or Reynolds number) values in this range. Three main force model combinations are considered:

(i) All forces (virtual-mass, drag, lift, rotation, and strain) enabled with nominal coefficient values. The virtual-mass coefficient is equal to 0.5, the lift and rotation coefficients are equal to 0.75, and the strain coefficient is equal to 0.25. This is the same combination that was applied toward the laminar-flow grid-resolution study.

(ii) All forces enabled with the virtual-mass coefficient equal to 0.5. The lift and rotation coefficients are equal to 0.375, and the strain coefficient is equal to 0.125 (i.e., half the nominal values).

(iii) Only drag force enabled, where the virtual-mass, lift, rotation, and strain coefficients are all equal to zero.

Table 4.1 summarizes the conditions for these simulations.
A quantitative analysis of the simulation results can be performed by plotting the volume-averaged gas holdup ($\bar{\alpha}_d$) and the volume-averaged slip velocity ($\bar{U}_s$) as functions of the bubble diameter ($d_b$), and the holdup fluctuations ($\sigma$) and slip-velocity fluctuations ($\theta$) as functions of the bubble Reynolds number $Re$ (see Figs. 4.6 and 4.8). The volume-averaged quantities are obtained by taking an average over all the nodes in the calculation domain at the final time step of the simulation. It should be noted that determining the values for $\bar{U}_s$ is required to calculate the values of $Re$. Studying the deviations from these averaged quantities allows further insight into the stability of the flow. Smaller values for $\sigma$ and $\theta$ indicate higher stability, or a tendency toward homogeneous flow (i.e., the deviations from the volume-averaged quantities are small).

The expressions for $\sigma$ and $\theta$ are given by

$$\sigma = \frac{\sqrt{\alpha'_d \alpha'_d}}{\bar{\alpha}_d}; \quad \theta = \frac{\sqrt{U'_s U'_s}}{\bar{U}_s}, \quad (4.1)$$

where $\alpha'_d = \alpha_d - \bar{\alpha}_d$ and $U'_s = U_s - \bar{U}_s$. Values of $\sigma$ and $\theta$ are calculated in the following manner. First, the local deviation values, $\alpha'_d$ and $U'_s$, are determined by subtracting the volume-averaged value from the local value for each node in the domain. Then each local deviation value is squared, and an average of these squares is taken over the domain. The square root of this average is finally divided by the volume-averaged mean. (For our purposes, $U_s = u_{d,y} - u_{e,y}$.)

Figure 4.6 presents the quantitative analysis for the 6-cm column using the laminar-flow model. It can be seen that when the laminar-flow model is applied, the line plots for the volume-averaged gas holdup and slip velocity are in agreement, regardless of the force models and parameter values used. Additionally, the fluctuation data for the laminar-flow simulations tend to be high, with the values of $\sigma$ and $\theta$ increasing with increasing bubble $Re$. For nearly all bubble $Re$, enabling all force models with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$ resulted in lower values of $\sigma$ and $\theta$ than for the other force-model combinations, sometimes by nearly an order of magnitude. These results indicate that using $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$ is an improvement
towards predicting homogeneous flow. However, even when these parameter values are used, the highest values of $\sigma$ and $\theta$ observed are approximately $10^{-1}$ and $10^{-2}$, respectively, indicating higher deviations from the average than we expected for homogeneous flow. Qualitatively, all laminar-flow simulations predict water volume-fraction profiles similar to Fig. 4.5B. Figure 4.7 provides the qualitative representation of the laminar-flow simulations for each of the force model cases. An examination of these water volume-fraction profiles further confirms that using $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$ comes the closest to predicting homogeneous flow for all $Re$ values in the range considered for the laminar-flow simulations.

Figure 4.7. Qualitative comparison of three force model cases for simulations in which the laminar-flow model is applied.
Figure 4.8. Quantitative analysis for a 6-cm column with the BIT model. A: volume-averaged holdup. B: volume-averaged slip velocity. C: holdup fluctuations. D: slip-velocity fluctuations.

Figure 4.8 presents the quantitative analysis for the 6-cm column with the BIT model. As seen for the cases in which the laminar-flow model was used (Fig. 4.6), the volume-averaged quantities are nearly equal regardless of force models enabled or parameter values used. However, it is clear from the plots for $\sigma$ and $\theta$ that varying the force models enabled or their coefficients affects the flow stability. As the bubble $Re$ decreases, the values for $\sigma$ and $\theta$ for each simulation approach the limiting value observed in the laminar-flow simulations. This result is not unexpected as the BIT model is directly proportional to the bubble diameter, and thus has no effect at zero bubble diameter, or zero bubble $Re$. With the BIT model and all forces enabled with $C_L = C_{rot} = 0.75$ and $C_S = 0.25$, the values for $\sigma$ and $\theta$ tend to decrease with increasing bubble $Re$. 
until $Re$ is approximately equal to 210, after which both $\sigma$ and $\theta$ increase with increasing bubble $Re$. A similar trend is observed when $C_L = C_{rot} = 0.375$ and $C_S = 0.125$; however, the values of $\sigma$ and $\theta$ are overall lower, sometimes by up to two orders of magnitude. The transition observed when $Re \approx 210$ occurs because the viscous term becomes more influential than the combined effect of the force models when $Re$ is greater than approximately 210. The opposite trend is observed when only the BIT model and the drag force are enabled. Values of $\sigma$ and $\theta$ increase with increasing bubble diameter until $Re$ is approximately equal to 275, after which both $\sigma$ and $\theta$ decrease with increasing bubble $Re$. For $Re$ higher than approximately 275, the viscous term becomes of equal or higher influence when compared with the drag term, resulting in dampened fluctuations from average values. Additionally, for $Re \geq 275$, values of $\sigma$ and $\theta$ are at least an order of magnitude lower than when the laminar model is used (Fig. 4.6). While simulations with the BIT model and virtual-mass and drag forces enabled were also performed (i.e., no lift, rotation or strain), these were found to be numerically unstable and did not appear to follow a general trend. Thus, such cases were not further investigated for this study.

It should be noted that the case for which all forces are enabled, with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$, was performed first with free-slip boundary conditions at the column walls, and then with periodic boundary conditions. Overall, as seen in Fig. 4.8, the change in boundary conditions does not result in large differences in the quantitative analysis. However, the fluctuating quantities tend to be slightly smaller with periodic boundary conditions (most notably when $Re \approx 25$).

It may be noted that Deen et al. (2001) did not observe any significant effect when using Sato’s BIT model. On the other hand, Pfleger and Becker (2001) observed a remarkable effect when considering bubble-induced turbulence via applying additional production terms in their $k$ and $\varepsilon$ equations. They observed a marked improvement on the simulation of radial profiles of axial velocities, but had less successful predictions of local and overall gas holdup. The present work demonstrates that the use of the BIT model (Fig. 4.8) generally results in lower values of $\sigma$ and $\theta$ than when the laminar model is used (Fig. 4.6). For this reason, all remaining simulations reported below utilize the BIT model to stabilize the flow.
Figure 4.9. Qualitative comparison of three force model cases, for simulations in which the BIT model is applied.
Figures 4.6A and 4.8A, and Figs. 4.6B and 4.8B, illustrate that the volume-averaged holdup and slip velocity, respectively, are determined by the drag coefficient alone, and are quite independent of the instantaneous flow fields. Furthermore, since the drag model and its dependence on the bubble Reynolds number are inputs into the two-fluid model, comparisons of volume-averaged holdup and volume-averaged slip velocity with experimental data are of little use for validating the predictive abilities of two-fluid CFD models. In other words, changes in the force models can yield instantaneous flow fields that range from highly turbulent to nearly time-invariant, but which have exactly the same average holdup and average slip velocity. It would appear from Fig. 4.8 that including the BIT model, enabling all force models, and using $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$ are sufficient requirements for the two-fluid model to yield homogeneous-flow predictions. This conclusion is further strengthened by the results presented in Figure 4.9, a qualitative comparison of the force model cases for the simulations in which the BIT model is applied. Case (ii), with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$, results in the closest representation of homogeneous flow throughout the range of bubble Re values considered.

4.2.4 Transitional Flow

The next goal is to determine if the two-fluid model, with the inclusion of the BIT model and parameter settings of $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$, will yield reasonable predictions for transitional-flow behavior in 6-cm columns. In order to do this, 2D simulations are carried out for three inlet air velocities: 2, 6.2, and 12 cm/s. As in the experiments of Garnier et al. (2002a, b), an inlet water velocity of 1.6 cm/s is used, and the bubble diameter is set to 4 mm ($Re \approx 1093$). Finally, as discussed previously, three model formulations are studied: (i) all forces enabled, with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.75$, and $C_S = 0.25$; (ii) all forces enabled, with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$; and (iii) only drag force enabled, with $C_{vm} = C_L = C_{rot} = C_S = 0.0$. Conditions for these simulations are summarized in Table 4.1.
Figure 4.10. Quantitative analysis for transitional-flow study in 6-cm columns with the BIT model. A: volume-averaged holdup. B: volume-averaged slip velocity. C: holdup fluctuations. D: slip-velocity fluctuations.

Figure 4.10 presents the quantitative analysis for transitional flow in 6-cm columns. The values for volume-averaged gas holdup ($\bar{\alpha}_d$), volume-averaged slip velocity ($\bar{U}_S$), holdup fluctuations ($\sigma$), and slip-velocity fluctuations ($\theta$) are calculated in the same manner as described beforehand. However, for this study, $\bar{\alpha}_d$ and $\bar{U}_S$ are plotted as functions of inlet gas velocity $u_g$, and $\sigma$ and $\theta$ are plotted as functions of $\bar{\alpha}_d$. It can be seen in Figs. 4.10A and 4.10B that when all forces are enabled, the volume-averaged quantities are in agreement. However, the curve when only the drag force is enabled shows volume-averaged quantities that deviate from the other two curves at higher gas velocities. Only for the lowest inlet air velocity (2 cm/s) do all force-model
combinations yield equal values for the volume-averaged quantities. It should be noted that since a constant bubble diameter is used, the average slip velocity (and hence the bubble Reynolds number) does not change significantly with an increase in inlet air velocity. In other words, the gas flow rate controls $\bar{\alpha}_d$ and bubble diameter controls $Re$. Overall, the time-averaged quantities are again insensitive to the instantaneous flow profiles occurring in the bubble column, and thus cannot be used to discriminate between different model formulations.

At high gas velocities, highly turbulent flow with irregular structures is expected from experiments (Chen et al., 1994). Therefore, it would be expected that as the gas flow rate, and in turn $\bar{\alpha}_d$, increases, the values for $\sigma$ and $\theta$ would also increase, indicating a tendency away from homogeneous flow. Such a trend is observed when only the drag force is enabled, and also when all forces are enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ (Figs. 4.10C and 4.10D). However, when all forces are enabled with $C_L = C_{rot} = 0.75$ and $C_S = 0.25$, the opposite trend is observed; i.e., the lowest values of $\sigma$ and $\theta$ are obtained for the highest value of $\bar{\alpha}_d$. (Note that a linear scale is used for $\sigma$ in Fig. 4.10C in order to highlight the change from homogeneous to transitional flow.) The results for the force-model combination of $C_L = C_{rot} = 0.75$ and $C_S = 0.25$ are unexpected and viewed (at this point) as an incorrect representation of transitional-flow behavior. (This force-model combination is revisited in Chapter 6.) When considering flow stability, it would appear that enabling all forces with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ yields the most reasonable representation of transitional flow in 6-cm columns. This model combination results in lower values for $\sigma$ and $\theta$ than when only the drag force is enabled. This conclusion is further strengthened by a qualitative analysis of the water volume-fraction profiles.

Figures 4.11 and 4.12 provide this qualitative analysis of transitional-flow behavior by showing, respectively, the water volume-fraction profiles for the case in which only the drag force is enabled (Fig. 4.11), and the case in which all forces are enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ (Fig. 4.12). According to the flow-regime map in Fig. 4.1, for a 6-cm column, an inlet air velocity of 2 cm/s should result in a
A homogeneous-flow profile, an inlet air velocity of 6.2 cm/s should yield a transitional-flow profile, and an inlet air velocity of 12 cm/s should yield slug flow. When only the drag force is enabled, an inlet air velocity of 2 cm/s (Fig. 4.11A) yields the expected homogeneous-flow profile. Increasing the inlet velocity to 6.2 cm/s (Fig. 4.11B) results in a non-uniform profile with a high volume fraction of water along the column walls and small plumes of air in the center of the column. The profile for an inlet flow of 6.2 cm/s (Fig. 4.11B) could be considered transitional, as it shows a higher degree of non-uniform behavior than the profile for an inlet flow of 2 cm/s (Fig. 4.11A), but a lower degree of non-uniform behavior than the profile for an inlet flow of 12 cm/s (Fig. 4.11C).

Figure 4.11. Water volume-fraction profiles for transitional-flow study with only drag force enabled ($C_{vm} = C_L = C_{rot} = C_S = 0.0$).
Using an inlet velocity of 12 cm/s does not yield the expected slug-flow profile, but instead results in a profile with a pronounced bubble plume at the bottom of the column. This plume travels upward before breaking into smaller, air-rich structures in the middle of the column. In contrast, regions of high water volume fraction are confined to the walls. With only drag enabled, the predicted instantaneous flow field thus has a “core-annular” structure that one would normally associate with much higher gas flow rates. Moreover, the transition from homogeneous to core-annular flow is very abrupt (see Fig. 4.10C), unlike the large transitional range expected from Fig. 4.1. We thus conclude that the use of the BIT and drag-force model alone cannot adequately represent flow-regime transitions in bubble columns.

When all forces are enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$, an inlet air velocity of 2 cm/s (Fig. 4.12A) yields the expected homogeneous-flow profile. Using an inlet flow of 6.2 cm/s (Fig. 4.12B) yields a transitional-flow profile, which appears uniform in the bottom half of the column and reveals faint, horizontally banded structures in the top half of the column. The bands can also be considered as rising plane waves, indicating a transition from uniform flow to non-uniform behavior. It may be noted that Olmos et al. (2001) reported radially uniform gas holdup profiles for low superficial gas velocities characteristic of homogeneous flow. These profiles appeared parabolic as gas velocity increased, indicative of either transitional or heterogeneous flow. Additionally, Michele and Hempel (2002) observed a superficial gas velocity of 6 cm/s indicated the start of the heterogeneous-flow regime. Increasing the inlet air velocity to 12 cm/s (Fig. 4.12C) results in a flow profile with more pronounced banded structures that originate as horizontal bands near the bottom of the column. As these bands progress upward, they become parabolic in appearance, and seem to represent bubble swarms that extend across the column diameter. The bands maintain nearly the same width, except at the top of the column, where outflow effects become significant. In our opinion, this is the closest qualitative representation of slug flow that can be achieved when neglecting bubble coalescence. Such a profile would be expected for a 6-cm column with an inlet air velocity of 12 cm/s.
Figure 4.12. Water volume-fraction profiles for transitional-flow study with all forces enabled \((C_{vm} = 0.5, C_L = C_{rot} = 0.375, C_S = 0.125)\). A-C correspond to simulations with free-slip boundary conditions, while D corresponds to a simulation with periodic boundary conditions.

Figure 4.12D illustrates the flow profile for the 6-cm column with an inlet air velocity of 12 cm/s, but with periodic boundary conditions for the column walls. This flow profile also has pronounced banded structures originating as horizontal bands near the bottom of the column. However, these structures remain horizontal as they progress upward. Unlike the parabolic bands observed when free-slip boundary conditions are used (Fig. 4.12C), the bands have different widths when periodic boundary conditions are used (Fig. 4.12D). For both cases, these bands rise on average with a velocity of about 1 cm/s (compared to a bubble rise velocity near 27 cm/s). Studying how the centerline
values of $\alpha_d$ vary with column height revealed that the width of the bands is approximately 2 cm. Extracting data for both $\alpha_d$ and $u_{dy}$ at a fixed height of 40 cm and determining how both quantities oscillate with time produced wavelengths corresponding to a frequency of approximately 2 seconds. Dividing the average bandwidth (2 cm) by the average frequency (2 sec) results in an average band rise velocity of 1 cm/s.

Note that the blue bands in Figs. 4.12C and 4.12D have bubble volume fractions near 0.5. If bubble coalescence were included in the model, it can be expected that coalescence rates would be relatively large at such high volume fractions, and thus that slugs (similar to those shown in Fig. 4.2) would form in these regions. Therefore, we can conclude that the combination of the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ yields a reasonable representation of transitional-flow behavior in small (6-cm) columns.

4.2.5 Effect of Bubble Size on Flow Structures

The banded flow structures observed in Figs. 4.12C and 4.12D resulted from simulations in which the bubble diameter was set to 4 mm ($Re \approx 1093$). As discussed earlier, varying the bubble $Re$ plays an important role in the stability of the simulations utilizing a 2 cm/s inlet air velocity. Thus, we want to determine the effect of bubble $Re$ on the flow structures resulting from high-flow-rate (12 cm/s) simulations. Since the use of the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ results in acceptable representations of homogeneous and transitional flow, only this combination of parameters is applied toward this study. The liquid inlet velocity is held constant at 1.6 cm/s, and both boundary-condition cases (free-slip and periodic) are considered. The value for the bubble diameter is varied from 0.5 to 4 mm, corresponding to $Re$ ranging from approximately 25 to 1100. Simulation conditions are summarized in Table 4.1.

Figure 4.13 presents the quantitative analysis for high-flow-rate simulations in 6-cm columns. The values for volume-averaged gas holdup ($\bar{\alpha}_d$), volume-averaged slip velocity ($\bar{U}_s$), holdup fluctuations ($\sigma$), and slip-velocity fluctuations ($\theta$) were computed as discussed previously. Both $\bar{\alpha}_d$ and $\bar{U}_s$ are plotted as functions of bubble diameter ($d_b$), and $\sigma$ and $\theta$ are plotted as functions of $Re$. Overall, changing the boundary
conditions from free-slip to periodic does not result in large differences in the quantitative analysis. On the other hand, volume-averaged holdup decreases with increasing \( d_b \), while the volume-averaged slip velocity increases with increasing \( d_b \) in nearly the same way as seen previously for the homogeneous-flow predictions (Figs. 4.6B and 4.8B). These results further confirm that the volume-averaged quantities are determined solely by the drag coefficient, which in turn depends on \( Re \) via input bubble diameter. Thus, even for high-flow-rate simulations, comparisons of the average holdup and average slip velocity with experimental data will not greatly aid in validating the predictive capabilities of the two-fluid model.

Figure 4.13. Quantitative analysis for high-flow-rate (12 cm/s) study in 6-cm columns with the BIT model. All forces are enabled with \( C_{vm} = 0.5, C_L = C_{rot} = 0.375 \), and \( C_S = 0.125 \). A: volume-averaged holdup. B: volume-averaged slip velocity. C: holdup fluctuations. D: slip-velocity fluctuations.
The dependence of stability upon bubble $Re$ for the high-flow-rate simulations is illustrated in the plots for $\sigma$ and $\theta$ (Figs. 4.13C and 4.13D). As $Re$ increases, the values for $\sigma$ and $\theta$ decrease until $Re$ is approximately equal to 500, after which both $\sigma$ and $\theta$ increase with increasing bubble $Re$. A similar trend was observed for the homogeneous-flow simulations (see Fig. 4.8); however, for the homogeneous-flow predictions, $\sigma$ and $\theta$ reached minimum values when $Re \approx 210$ (Figs. 4.8C and 4.8D). Additionally, the maximum values of $\sigma$ and $\theta$ computed are on the order of 0.1, higher overall than those computed from the homogeneous-flow predictions that used the same parameter values (BIT, all forces enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$). This tendency away from stability is expected as an increase in the gas flow rate typically results in unstable flow (Shah and Deckwer, 1983). However, when $200 \leq Re \leq 500$ ($d_b \approx 1.5 - 2.5$ mm), the values of $\sigma$ and $\theta$ indicate a degree of stability closer to that observed for homogeneous flow. To our knowledge, there exists no experimental data for varying bubble size, and in turn bubble $Re$, that can be used to validate the transition from homogeneous to unstable flow shown in Fig. 4.13. However, given the sensitivity of the model predictions to the bubble diameter, such experiments would be extremely useful for testing the force models.

Figure 4.14 illustrates the effect of bubble $Re$ on the banded flow structures, such as those presented in Figs. 4.12C and 4.12D. In Fig. 4.14, the centerline values of the instantaneous gas holdup ($\alpha_i$) are plotted as a function of column height. The water volume-fraction profiles presented in Figure 4.15 show the corresponding qualitative representations of the flow structures observed in these high-flow-rate simulations. When $Re$ is approximately 26, corresponding to the smallest bubble size studied, the centerline values of $\alpha_i$ vary randomly as column height increases. These fluctuations correspond to the random vortical structures seen in Fig. 4.15 in the volume-fraction profile for $Re \approx 26$ that are similar to low-Reynolds-number turbulence observed in single-phase flows. Note that the average gas holdup for such small bubbles is extremely high (0.8) for this gas flow rate. Since the holdup corresponding to close-packed spheres is approximately 0.64, it is unlikely that such a high holdup could be observed experimentally.
In Fig. 4.14, the centerline holdup profiles for medium-sized bubbles ($Re \approx 210$ and 504) are flat, corresponding to the smaller computed values of $\sigma$ and $\theta$ (Figs. 4.13C and 4.13D) for these bubble $Re$ and indicating the absence of banded flow structures. Accordingly, the corresponding volume-fraction profiles in Fig. 4.15 appear uniform. Increasing $Re$ to approximately 880 produces oscillations in $\alpha_d$ along the column centerline after a column height of approximately 10 cm. These oscillations correspond to banded structures as seen in Fig. 4.15 for $Re \approx 880$ and have a wavelength of about 2 cm. Their amplitude increases with increasing column height until a height of approximately 30 cm, after which the amplitude remains constant. This behavior corresponds to the sudden increase in the values of $\sigma$ and $\theta$ (Figs. 4.13C and 4.13D). As seen in Figs. 4.12C and 4.12D, the periodicity of the banded structures is enhanced by the use of free-slip (as opposed to periodic) boundary conditions.

Figure 4.14. Effect of bubble diameter on the stability and appearance of flow structures observed for high-flow-rate (12 cm/s) simulations using free-slip boundary conditions. All forces are enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$. 
In Fig. 4.14, further increasing \( Re \) to approximately 1093, corresponding to the largest bubble size studied, again produces oscillations that originate after a column height of approximately 10 cm and have a wavelength of about 2 cm. However, these oscillations have higher amplitude and are less ordered than those resulting from \( Re \approx 880 \). Fig. 4.15 shows the corresponding banded structures for \( Re \approx 1093 \). Such behavior corresponds to the highest values of \( \sigma \) and \( \theta \) presented in Figs. 4.13C and 4.13D. It is therefore concluded that the bubble Reynolds number plays a significant role in the stability of high-flow-rate simulations and the appearance of flow structures. The bands, presumed to be indicative of slug flow as expected for a 6-cm column with an air inlet flow rate of 12 cm/s, only occur for bubbles for which the Reynolds number is greater than approximately 500.

**Figure 4.15.** Water volume-fraction profiles for high-flow-rate study, with all forces enabled (\( C_{vm} = 0.5, C_L = C_{rot} = 0.375, C_S = 0.125 \)).
4.2.6 Effect of Liquid Coflow

The previously discussed high-flow-rate simulations (e.g., Figs. 4.14 and 4.15) utilized a constant inlet liquid velocity of 1.6 cm/s, one of the inlet values used in the small-column-diameter experiments performed by Garnier et al. (2002a, b). These experiments studied the effect of liquid coflow by considering four different values of the superficial liquid velocity \( u_l \). They observed that for high values of dispersed-phase holdup, large-scale, downward motions would occur at the column outlet for \( u_l \) equal to 1.6 cm/s. Such instabilities were not observed experimentally for larger values of \( u_l \). In order to study the effect of liquid coflow on flow stability, 2D simulations are carried out for three inlet liquid velocities: 0, 1.6, and 3.3 cm/s. In these simulations, the bubble diameter is set to 4 mm \((Re \approx 1093)\), and the inlet air velocity is held constant at 12 cm/s. The BIT model and all force models with \( C_L = C_{rot} = 0.375 \) and \( C_S = 0.125 \) are applied in this study. Note that as liquid coflow is increased, average gas holdup will slightly decrease.

Figure 4.16 presents the centerline values of the holdup \((\alpha_d)\) as a function of column height for each value of \( u_l \) in order to demonstrate the effect of liquid coflow on the banded flow structures. When no coflow is applied, oscillations in \( \alpha_d \) originate at a column height of 4 cm, and are not consistent in either wavelength or amplitude as column height increases. Increasing \( u_l \) to 1.6 cm/s results in oscillations in \( \alpha_d \) that originate at a column height of approximately 10 cm. The wavelength of the banded structures is about 2 cm, and the amplitude increases with column height until a height of approximately 30 cm, after which the amplitude is nearly constant. At a height of about 40 cm, however, both the wavelength and amplitude of the oscillations vary again, reflecting instability at the column outlet. Further increasing \( u_l \) to 3.3 cm/s produces oscillations that originate at a column height of approximately 12 cm. These oscillations maintain a wavelength of about 2 cm, while the amplitude increases with column height until a height of 40 cm, after which the amplitude is nearly constant. Average band rise velocity was determined again by dividing the average bandwidth by the average frequency, and for all three cases the bands rise on average with a velocity of about 1 cm/s, therefore showing no significant dependence on liquid coflow. However, the
behavior of the oscillations of the centerline values of $\alpha_d$ with respect to variations in liquid coflow further confirm that an increase in $u_l$ results in enhanced stability of the high-gas-flow-rate simulations.

Figure 4.16. Effect of liquid coflow on the stability and appearance of flow structures observed for high-flow-rate (12 cm/s) simulations. All forces are enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$. The bubble Reynolds number $Re$ is approximately equal to 1093 for this case.
4.2.7 Effect of Column Diameter

Our final goal is to determine if the combined use of the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ will predict the correct behavior for larger column diameters (see Fig. 4.1). Scale-up is an important aspect in the design of a bubble column. Krishna et al. (1999) have shown the limitations in the applicability of the empirical correlations over a range of column diameters. As the column diameter is increased, the length scales of the flow eddies also increase, resulting in enhanced turbulence in the churn-turbulent regime. Turbulence models for multiphase flows should scale accordingly. On the other hand, in the homogeneous regime the flow remains stable for all column diameters (see Fig. 4.1). Hence, the applicability of two-fluid CFD models to larger column diameters must be tested. First, simulations for 20- and 40-cm columns, using an inlet air velocity of 2 cm/s and an inlet water velocity of 0 cm/s, are reported. As discussed previously, three force-model combinations are used: (i) all forces enabled, with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.75$, and $C_S = 0.25$; (ii) all forces enabled, with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$; and (iii) only drag force enabled, with $C_{vm} = C_L = C_{rot} = C_S = 0$. Quantitative analysis is performed as described in earlier sections. The values for volume-averaged gas holdup ($\bar{\alpha}$) and volume-averaged slip velocity ($\bar{U}_S$) are plotted as functions of bubble diameter ($d_b$), and the holdup fluctuations ($\sigma$) and slip-velocity fluctuations ($\theta$) are plotted as functions of bubble $Re$. Conditions for these simulations are summarized in Table 4.1. Figure 4.17 presents the quantitative analysis for this scale-up study.

According to the flow-regime map (Fig. 4.1), columns of 6, 20, or 40 cm in diameter using an inlet air velocity of 2 cm/s should all operate in the homogeneous-flow regime. It may be noted that the experiments of Chen et al. (2001), performed on columns of 20, 40, and 80 cm in diameter, showed that the power spectrum was not affected by varying the column diameter. However, Kolmogorov entropy decreased with increasing column diameter, and uniform radial holdup profiles were observed only in the widest column (Chen et al., 2001). Ruzicka et al. (2001b) carried out experiments on 14-, 29-, and 40-cm columns, and reported that an increase in column size decreased
homogeneous-flow stability and enhanced flow regime transitions. However, Forret et al. (2003) performed experiments on columns of 15, 40, and 100 cm in diameter and found that average holdup was independent of column diameter, while liquid velocity and the axial dispersion coefficient increased with column diameter. Our work, presented in Fig. 4.17, shows that regardless of column diameter, forces enabled, or parameter values, the volume-averaged quantities calculated for each bubble diameter are nearly the same. Thus, as discussed previously, experimental and computational data for average holdup and slip velocity are useful for parameterizing the drag coefficient, but not for validating the scale-up of two-fluid CFD models.

Since enabling all forces with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ results in homogeneous-flow profiles for 6-cm columns, only this force-model combination is shown in the curves for $\sigma$ and $\theta$ (Figs. 4.17C and 4.17D). Values of $\sigma$ and $\theta$ decrease with increasing bubble Reynolds number until $Re$ is approximately equal to 210, after which both $\sigma$ and $\theta$ increase slightly with increasing bubble $Re$. Additionally, as $Re$ decreases both $\sigma$ and $\theta$ approach a constant value between $10^{-1}$ and $10^{-2}$. Such behavior was also observed in Fig. 4.8 for the 6-cm column. There does not appear to be a significant difference among column diameters for $\sigma$ and $\theta$ in Fig. 4.17 (i.e., with the BIT model, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$). Overall, we can conclude that the two-fluid model with the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ correctly predicts homogeneous flow for all values of the column diameter. We note, however, that it would be very difficult to introduce bubbles uniformly in a large-diameter column, which inevitably would yield inhomogeneous flow (Harteveld et al., 2003).

Figure 4.18 shows a qualitative comparison between a 6-cm and a 40-cm column, both utilizing an inlet air velocity of 12 cm/s and an inlet water velocity of 1.6 cm/s. For these simulations, the bubble diameter is set to 4 mm ($Re \approx 1093$), coalescence is neglected, the BIT model is included, and all forces are enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$. Simulation conditions are summarized in Table 4.1. According to the flow-regime map (Fig. 4.1), a 6-cm column with an inlet air velocity of 12 cm/s should exhibit slug flow, while a 40-cm column with the same inlet flow rate should exhibit churn-turbulent flow. The 6-cm column, as seen previously in Fig. 4.12C, shows horizontal banded structures that are originally flat near the bottom of the column, and become parabolic in appearance as they travel upward. Since these bands appeared to represent bubble swarms of the width of the column diameter, it was concluded previously that the 6-cm column would exhibit slug flow (as predicted by the flow-regime map in Fig. 4.1) if bubble coalescence were included in the model. The simulation for the 40-cm column does not yield churn-turbulent flow as predicted by the flow-regime map. Instead, as seen in the 6-cm column, horizontal bands form and persist throughout the column, becoming increasingly pronounced as they reach the top of the
column. As in the 6-cm column, the bubble volume fraction in these bands is near 0.5, and thus relatively large coalescence rates would be expected. Moreover, since the thickness of the bands in the 40-cm column is approximately the same as in the 6-cm column, it can be expected that the average bubble sizes generated by coalescence in the two columns will be approximately the same. Hence, in the 40-cm column, the average bubble size would be much smaller than the column diameter. Therefore, since such bubbles would not span the entire column, it may indeed be possible to generate churn-turbulent flow in the 40-cm column if a bubble coalescence model, such as that described by Sanyal et al. (2004), were included in the two-fluid model.

Figure 4.18. Qualitative analysis of the effect of column diameter on the water volume-fraction profiles in the heterogeneous-flow regime. Left: 6-cm column. Right: 40-cm column.
4.3 Summary and Conclusions for CFD Predictions

Multiphase CFD flow regime predictions depend significantly on grid resolution and model formulation. Cell spacing of 0.25 cm provides sufficient grid resolution. The bubble Reynolds number $Re$, the BIT model, and the two-fluid model parameters have a combined effect on the flow profiles observed in bubble column simulations. For example, using the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ yielded the expected homogeneous-flow predictions for 6-, 20-, and 40-cm columns with low air flow rates (e.g., 2 cm/s), successfully predicting column scale-up in the homogeneous-flow regime. The same formulation also yielded a reasonable representation of transitional-flow behavior in small (e.g., 6-cm) columns. The numerical studies also show that the inlet gas flow rate controls $\bar{\alpha}_d$ and the bubble diameter controls $Re$.

For high-flow-rate simulations (e.g., 12 cm/s), the flow structures observed in 6-cm columns have a strong dependence on the bubble diameter. Small bubbles ($d_b = 0.5$ mm, $Re \approx 26$) yield random flow structures, while large bubbles ($d_b = 3.5 – 4.0$ mm, $Re \approx 880 – 1100$) give rise to ordered horizontal bands or swarms. It also appears that the stability of these flow structures, as well as the overall stability of the high-flow-rate simulations, is enhanced by increasing the liquid coflow. However, using the BIT model and all force models with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$ does not result in the expected churn-turbulent profile when the column diameter is increased for high-flow-rate simulations. This may be due to the absence of a bubble-coalescence model.
Chapter 5. Effect of Two-Fluid Model Formulation on Flow-Regime Predictions for Bubble-Column Simulations

As shown in Chapter 4, bubble-column flow-regime predictions have a strong dependence on the CFD model formulation. A particular set of model parameters yielded the expected homogeneous-flow profiles for low gas flow rates over a range of values of the bubble Reynolds number, and the same set was then examined for transitional-flow behavior. The complete set of interphase force models includes drag, virtual-mass, lift, rotation, and strain. When the two-fluid model including all interphase forces is applied for uniformly aerated simulations, homogeneous flow is observed in the same range of inlet-gas flow rates as experiments performed at Delft University (Harteveld et al., 2004, 2005). These simulations are carried out assuming the bubbles are uniformly sized (non-coalescing) and remain spherical. Results are presented in the form of flow maps parameterized by the bubble Reynolds number and the average gas volume fraction. As expected, the flow maps show a strong dependence on the model formulation. Additionally, selected force-model components are analyzed to show how their behaviors change according to the flow structures observed.

It should be noted that portions of this chapter are adapted from the AIChe Journal paper “Effect of Model Formulation on Flow-Regime Predictions for Bubble Columns” by Monahan and Fox (2007). Changes to the text are made to correspond to equation numbers, chapter and section numbers, tables and table numbers, or figures and figure numbers presented in this thesis. It should also be noted that additional figures are presented in this thesis chapter. To accommodate for these additional figures, the numbers of several figures in this chapter may differ from their appearance in Monahan and Fox (2007).

5.1 Motivation

Before proceeding, several clarifications should be discussed. Recall that a goal for the numerical studies presented in Chapter 4 was to determine whether the two-fluid model could predict the homogeneous- and transitional-flow regimes classified in Figure 4.1. The flow map shown in Figure 4.1 was generally regarded as qualitative and used
mainly to distinguish between homogeneous and heterogeneous flow. In those studies, flow profiles that were considered “homogeneous” had very small spatial gradients (i.e., appeared nearly uniform) and the local values for gas holdup and slip velocity showed little fluctuation and did not deviate significantly from the average values. However, a slight change has been made to the terminology for the studies presented in this chapter. “Homogeneous” flow refers to conditions for which the average gas holdup is a (nearly) linear function of the inlet gas velocity, and “uniform” flow refers to flow that contains no spatial gradients. Note that these designations imply that a flow need not be “uniform” in order to be “homogeneous.” Similarly, “heterogeneous” flow refers to conditions for which the linear relationship between average gas holdup and inlet gas velocity is no longer observed. In most cases, the heterogeneous-flow profiles observed in the simulations are representative of turbulent flow characterized by chaotic behavior and large gradients in the local volume fraction. The examples presented in Section 5.3.2 illustrate these different flow profiles.

There are numerous studies reported in literature that have focused on the prediction of flow-regime transitions using numerical simulations (Olmos et al., 2001; 2003a, b) or linear stability analysis of various model equations (Pauchon and Banerjee, 1986, 1988; Biesheuvel and Gorissen, 1990; Van Wijngaarden and Kapteyn, 1990; Shnip et al., 1992; Minev et al., 1999; León-Becerril and Liné, 2001; Ruzicka et al., 2001a, b; Sankaranarayanan and Sundaresan, 2002; Ruzicka and Thomas, 2003; Thorat and Joshi, 2004; Lucas et al., 2005; Bhole and Joshi, 2005). The modes of instability observed can usually be classified in one of two ways: (1) a transition from uniform to non-uniform flow by way of rising plane waves, called hindered rise; or (2) a transition from uniform to heterogeneous flow by way of rising vertical bubble plumes, called cooperative rise (Sankaranarayanan and Sundaresan, 2002).

It may be noted that rising plane waves can be difficult to study experimentally since these structures are dense and opaque (Zenit et al., 2001; Figueroza-Espinoza and Zenit, 2005; Mudde, 2005a). It is also worth noting that, as discussed in Section 5.3, flows exhibiting rising plane waves can still show a linear dependence between the average gas holdup and the inlet gas flow rate. Thus, the rising plane waves are an
example of flow that is considered “homogeneous” yet not “uniform” in this study. A linear dependence between average gas holdup and inlet gas flow rate is not observed for rising bubble plumes where, due to cooperative rise, the “effective” bubble rise velocity is higher than for an isolated bubble, resulting in a lower average gas holdup than would otherwise be observed at the same inlet gas flow rate. The cooperative-rise instability observed in two-dimensional models does lead to large-scale turbulent flow structures, and would be considered as leading to heterogeneous flow.

The Eulerian two-fluid models for homogeneous bubbly flow tend to predict transitions to non-uniform and heterogeneous flow at very low values of the average gas holdup (usually much less than 0.2). An opposite trend was observed in the recent experiments of Harteveld (2005), which clearly showed that homogeneous bubbly flow could be observed up to average gas holdups greater than 0.5. This disagreement between theory and experiments suggests that important physics are not included in the two-fluid models currently used to model bubble columns. Recall that the work presented in Chapter 4 examined the effect of adding force models arising from interaction terms (Kashiwa, 1998) and showed that the transition to heterogeneous flow could be suppressed up to much larger average gas holdups. Without these interaction terms, homogeneous flow would transition to heterogeneous flow very quickly (Monahan et al., 2005). Therefore, it is worthwhile to investigate the role of model formulation on flow transitions in greater detail, using numerical simulations to determine the “minimal” model required for predicting stable homogenous flow at high gas holdups.

The carefully designed experiments of Harteveld et al. (2003, 2004, 2005) are a good choice for comparison with our numerical studies. All experiments were performed using simple column geometries (e.g., cylindrical or rectangular). The aeration system consisted of constant flow-rate air injection needles organized into groups, allowing for both uniform feed and well-defined non-uniform aeration patterns. The bubble size distribution from this aeration system was very narrow (average size about 4 mm), allowing for the assumption that all bubbles have the same diameter in the simulations. Considering the bubble size and strong interactions with nearby bubbles (at least at gas holdups above 0.1-0.2), it is possible to approximate the bubble shape as a sphere in the
simulations. At the high gas holdups reached in the experiments, bubble coalescence could become significant and result in a rapid transition to heterogeneous flow. However, Harteveald (2005) was able to suppress bubble coalescence by using “aged” or “contaminated” water, since coalescence occurs more readily in pure liquids. Any flow transitions observed in the experiments were therefore not caused by bubble coalescence. Thus, coalescence need not be considered in the simulations.

This chapter is organized as follows. First, a brief review of the two-fluid model is given in Section 5.2. In the model formulation, the bubble Reynolds number \((Re)\) is controlled by bubble diameter and average gas holdup \((\bar{\alpha}_d)\) is controlled by the inlet gas flow rate. In Section 5.3, flow maps are presented to identify the regions in \(Re-\bar{\alpha}_d\) space where the flow profiles exhibit a particular behavior and to clearly illustrate where flow transitions occur. We show how these maps depend on the model formulation used, first by varying selected model parameters, and then by checking the sensitivity to the drag correlation. An additional examination of selected force-model components shows how their behaviors change for the flow transitions described in the flow maps. Finally, conclusions are drawn in Section 5.4.

5.2 Review of Two-Fluid Model

As in Chapter 4, the numerical studies reported here are performed with CFDLib v. 99.2. A full description of the Eulerian two-fluid model applied can be found in Chapter 3. A review of the notable terms follows.

The mass balance for phase \(k (= c, d)\) is expressed as

\[
\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0 . \tag{5.1}
\]

The momentum balance for phase \(k\) is given by

\[
\alpha_k \rho_k \frac{\partial \mathbf{u}_k}{\partial t} + \alpha_k \rho_k \mathbf{u}_k \cdot \nabla \mathbf{u}_k = -\alpha_k \nabla p - \nabla P_k + \nabla \cdot \alpha_k \mu_{ef,k} \left[ \nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T \right] + \sum_f \mathbf{F}_{fk} + \alpha_k \rho_k \mathbf{g} . \tag{5.2}
\]

The terms on the right-hand side of Eq. 5.2 represent, from left to right, the pressure gradient, bubble pressure, effective stress, interphase momentum exchange, and the
gravitational force. The closures for bubble pressure, effective stress, and interphase momentum exchange are defined as follows.

5.2.1 Bubble Pressure

The bubble-pressure model represents the transport of momentum due to bubble-velocity fluctuations, collisions, and hydrodynamic interactions, and is assumed to play an important role in bubble-phase stability (Spelt and Sangani, 1998). In this work, we apply the bubble-pressure model proposed by Biesheuvel and Gorissen (1990):

\[ P_d = \rho_c C_{BP} \alpha_d \left| \mathbf{u}_d - \mathbf{u}_c \right|^2 H(\alpha_d), \]  

(5.3a)

where (Batchelor, 1988)

\[ H(\alpha_d) = \left( \frac{\alpha_d}{\alpha_{dcp}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dcp}} \right). \]  

(5.3b)

In Eq. 5.3a, \( C_{BP} \) is a proportionality constant (set to 0.2 in this study), and \( \alpha_{dcp} \) in Eq. 5.3b is the void fraction at close packing (set to 1.0 in this study). Recall that the bubble-pressure model appears only in the dispersed-phase momentum balance (i.e., \( P_c = 0 \)).

5.2.2 Effective Viscosity

The effective stress term for phase \( k = (c, d) \) is expressed as

\[ \nabla \cdot \alpha_k \mu_{eff,k} \left[ \nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T \right], \]

(5.4)

where \( \mu_{eff,k} \) represents the effective viscosity. In this study, the effective viscosity for the continuous phase is equal to the sum of the molecular viscosity of the continuous phase and a value for “turbulent viscosity”: \( \mu_{eff,c} = \mu_{0,c} + \mu_{t,c} \). Note that in homogeneous flow, only so-called “pseudo-turbulence” and not large-scale turbulence is present, and these differ by an order of magnitude in energy (Harteveld, 2005). It would thus be inappropriate to model the turbulent viscosity in homogeneous flow by applying a multiphase turbulence model such as the \( k-\varepsilon \) model. In Chapter 4, the effective viscosity for the dispersed phase was equal to the molecular viscosity of the dispersed phase, or \( \mu_{eff,d} = \mu_{0,d} \). Additional studies are performed to determine changes in flow behavior when the effective viscosity is also used for the dispersed phase, or \( \mu_{eff,d} = \mu_{0,d} + \mu_{t,d} \).
Sato’s bubble-induced turbulence (BIT) model (Sato and Sekoguchi, 1975) is used to determine the pseudo-turbulent effective viscosity:

$$\mu_{t,c}, \mu_{t,d} = C_{BT} \rho_{c} d_{b} \alpha_{d} |u_{d} - u_{c}|. \quad (5.5)$$

The designation BIT1 is used when Eq. 5.5 applies to just $$\mu_{t,c}$$, and the designation BIT2 is used when Eq. 5.5 applies to both $$\mu_{t,c}$$ and $$\mu_{t,d}$$. The model constant $$C_{BT}$$ is equal to 0.6 (Sato et al., 1981). Note that at low bubble Reynolds numbers (or small $$d_{b}$$), the BIT model has diminishing effect on the flow. However, the numerical studies (Monahan et al., 2005) have shown that including a BIT model is effective when predicting homogeneous flow at higher bubble Reynolds numbers.

5.2.3 Interphase Momentum Exchange

The interphase momentum exchange describes the interaction between the continuous and dispersed phases. The total interfacial force acting on either of the phases can be expressed by the sum of the drag, virtual-mass, lift, rotation, and strain forces:

$$\sum_{f} F_{fk} = F_{D,k} + F_{vm,k} + F_{L,k} + F_{rot,k} + F_{S,k}. \quad (5.6)$$

Note that Eq. 5.6 is defined as it appears in the momentum balance for the dispersed phase (Eq. 5.2), and the opposite sign is used for the continuous phase.

The drag force is exerted on bubbles traveling steadily through a fluid, and is defined in CFDLib as

$$F_{D} = -\alpha_{d} \alpha_{c} \rho_{c} \rho_{d} C_{D}(Re) \frac{3}{4d_{b}} |u_{d} - u_{c}| (u_{d} - u_{c}), \quad (5.7)$$

where the bubble Reynolds number is defined by

$$Re = \frac{d_{b} |u_{d} - u_{c}|}{\nu_{c}}. \quad (5.8)$$

For the drag coefficient, CFDLib uses the following relationship (Kashiwa et al., 1994):

$$C_{D}(Re) = C_{\infty} + \frac{24}{Re} + \frac{6}{1 + \sqrt{Re}}, \quad (5.9)$$

where $$C_{\infty}$$ has a nominal value of 0.5. However, as described below, $$C_{\infty}$$ can be adjusted in order to predict the experimentally observed (Harteveld et al., 2004) average gas
holdup for a given value of the inlet gas velocity. For this study, we also tested another
drag coefficient that is more appropriate for bubbly flow (Tomiyama et al., 1995):

\[
C_D = \max \left[ \frac{24}{Re} \left( 1 + 0.15 Re^{0.687} \right), \frac{8}{3} \frac{Eo}{Eo + 4} \right],
\]  

(5.10)

where the Eötvös number is defined by

\[
Eo = \frac{g \rho_d d_b^2}{\sigma}.
\]  

(5.11)

This drag correlation differs primarily from Eq. 5.9 by its behavior at medium to high
Reynolds numbers. We can also note that the form of Eq. 5.7 corresponds to a
Richardson-Zaki exponent of \( n = 1 \), and thus the drag force is neutral to both hindered
(\( n > 1 \)) and cooperative (\( n < 1 \)) bubble rise (Sankaranarayanan and Sundaresan, 2002).
The choice of \( n = 1 \) also corresponds to the linear relation between the average gas
holdup (in the range of 0.06 to 0.25) and the inlet gas flow rate that is observed in the
experiments (Harteveld et al., 2004).

The virtual-mass force is defined in CFDLib as

\[
F_{vm} = -\alpha_d \alpha_c \rho_v C_{vm} \left( \frac{\partial u_d}{\partial t} + u_d \cdot \nabla u_d \right) - \left( \frac{\partial u_c}{\partial t} + u_c \cdot \nabla u_c \right),
\]  

(5.12)

where \( \rho_v \) denotes the volume-averaged density, \( \rho_v = \alpha_c \rho_c + \alpha_d \rho_d \). In this work, the
virtual-mass coefficient \( C_{vm} \) is assumed to be 0.5.

Finally, as discussed in Chapter 3, the interaction terms appearing in CFDLib can
be expressed as a lift force:

\[
F_L = \alpha_c \alpha_d \rho_c C_L \left( u_d - u_c \right) \times \nabla \times u_c,
\]  

(5.13)
a rotation force:

\[
F_{rot} = \alpha_c \alpha_d \rho_c C_{rot} \left( u_d - u_c \right) \times \nabla \times u_d,
\]  

(5.14)

where \( C_L = C_{rot} \), and a strain force:

\[
F_S = \alpha_d \alpha_c \rho_c C_S \left[ \nabla u_c + \nabla u_d \right] \cdot \left[ \nabla u_c + \nabla u_d \right] \cdot \left( u_c - u_d \right).
\]  

(5.15)

In the implementation in CFDLib, it is possible to use (i) only the lift and rotation forces,
(ii) only the strain force, or (iii) all three—lift, rotation, and strain. Since numerical
simulations using (i) only lift and rotation or (ii) only strain typically generate
heterogeneous flow at relatively low volume fractions, only option (iii)—cases with or without the lift, rotation, and strain forces—is considered. Thus, in this study, we have applied fixed values for the force coefficients and focused on the effect of enabling or disabling particular force terms.

5.3 Simulation Results and Discussion

The studies presented in Chapter 4 showed that homogeneous- and transitional-flow behavior could be predicted in 6-cm columns with the BIT model and all interphase force models enabled with $C_L = C_{rot} = 0.375$ and $C_S = 0.125$. Additionally, we demonstrated that the bubble Reynolds number $Re$ is controlled by bubble diameter, and average gas holdup $\bar{\alpha}_d$ is controlled by inlet gas velocity $u_g$. Thus, we conjecture in this study that for given values of $Re$ and $\bar{\alpha}_d$, the flow behavior will be the same for a particular set of force models. To test this conjecture, we have used numerical simulations to construct flow maps to find the regions in $Re-\bar{\alpha}_d$ space where the flow exhibits a particular behavior.

5.3.1 Preliminary Analysis

As noted earlier, our numerical simulations are based on the experiments performed by Harteveld et al. (2004, 2005). In these experiments, uniform aeration yielded homogeneous flow in the range shown in Table 5.1, while having non-aerated sections near the column walls resulted in large-scale structures.

Table 5.1. Inlet gas velocity and average gas holdup for Delft bubble column.

<table>
<thead>
<tr>
<th>$u_g$ (cm/s)</th>
<th>$\bar{\alpha}_d$ (Exp)</th>
<th>$\bar{\alpha}_d$ (Eq. 5.16)</th>
<th>$\bar{\alpha}_d$ (Eq. 5.17)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>0.061</td>
<td>0.061</td>
<td>0.084</td>
</tr>
<tr>
<td>1.7</td>
<td>0.076</td>
<td>0.073</td>
<td>0.095</td>
</tr>
<tr>
<td>2.5</td>
<td>0.11</td>
<td>0.118</td>
<td>0.140</td>
</tr>
<tr>
<td>3.2</td>
<td>0.16</td>
<td>0.157</td>
<td>0.180</td>
</tr>
<tr>
<td>3.9</td>
<td>0.20</td>
<td>0.196</td>
<td>0.219</td>
</tr>
<tr>
<td>4.9</td>
<td>0.25</td>
<td>0.252</td>
<td>0.275</td>
</tr>
</tbody>
</table>

Since the transition from homogeneous to heterogeneous flow by way of bubble plumes requires two spatial dimensions, we opted to investigate a 2D geometry in order
to validate whether our model predicts homogeneous flow in the range described in Table 5.1. However, it was first necessary to select an appropriate value for the input bubble diameter \( d_b \) and to adjust \( C_\infty \) in the drag model (Eq. 5.9) in order to give the correct value of \( \bar{\alpha}_d \) as a function of superficial gas velocity \( u_g \) in the range given in Table 5.1. Since bubbles observed experimentally range between 3.5 and 4.5 mm in diameter, a value of 4 mm (0.4 cm) was selected for \( d_b \), and \( C_\infty \) was adjusted as follows.

The experimental data in Table 5.1 is linear and described by

\[
\bar{\alpha}_d = 0.056115 u_g - 0.022705. \tag{5.16}
\]

If \( u_g = 0 \), \( \bar{\alpha}_d \) should theoretically also be zero; hence, the line intercept \((-0.022705)\) is regarded as a systematic experimental error (e.g., a slight variation of bubble size with inlet flow rate (Harteveld, 2005)) or evidence of hindered rise at very low gas holdup, and is not further considered. The desired relationship is then

\[
\bar{\alpha}_d = 0.056115 u_g. \tag{5.17}
\]

Note that the homogeneous flow simulations in Chapter 4 used \( u_g = 2 \) cm/s, for which Eq. 5.17 yields \( \bar{\alpha}_d = 0.11 \). The mass balance can be used to determine the rise velocity, \( u_d \):

\[
u_g = \bar{\alpha}_d u_d, \tag{5.18}
\]

which yields \( u_d = 17.82 \) cm/s for \( u_g = 2 \) cm/s and \( \bar{\alpha}_d = 0.11 \).

The uniform state of the two-fluid model produces a relation between drag and buoyancy, where only the drag coefficient is unknown:

\[
0 = \frac{F_D}{1 - \bar{\alpha}_d} + \bar{\alpha}_d (\rho_d - \rho_c) g, \tag{5.19}
\]

and

\[
F_D = -\bar{\alpha}_d (1 - \bar{\alpha}_d) \rho_c \frac{3}{4d_b} u_d (u_d \bar{\alpha}_d) C_D. \tag{5.20}
\]

Solving for the drag coefficient yields

\[
C_D = -\left(\frac{4}{3}\right) \frac{(\rho_d - \rho_c) g d_b}{\rho_c u_d^2} = -\left(\frac{4}{3}\right) \frac{(\rho_d - \rho_c) g}{\rho_c u_d^2} \left(\frac{Re \nu_c}{u_d}\right). \tag{5.21}
\]
For \( u_d = 17.82 \text{ cm/s} \), Eq. 5.21 yields \( C_D = C_D(Re) = 1.644 \). From Eq. 5.8 for \( Re \), setting \( d_b = 0.4 \text{ cm} \) and \( u_d = 17.82 \text{ cm/s} \) results in \( Re = 712.82 \). In turn, from Eq. 5.9 with \( C_\infty = 0.5 \), \( Re = 712.82 \) yields \( C_D(Re) = 0.7503 \). The difference between the two \( C_D(Re) \) results is about 0.9; thus we set \( C_\infty \) equal to 1.4 (nominal value 0.5 plus 0.9) in Eq. 5.9 so the drag coefficient will agree with the experiments.

To assure that the CFDLib drag force model has been adjusted properly, two initial test-case simulations are presented: one at the lowest inlet-gas velocity used in the Delft experiments (1.5 cm/s) and one at the highest inlet-gas velocity (4.9 cm/s). Our simulations utilized a 2D domain of width 24.3 cm and height 48.6 cm (twice the column width), as noted in Table 5.2, with free-slip boundary conditions at the vertical walls. BIT and all interphase forces were included.

### Table 5.2. Simulation parameters for numerical studies discussed in Chapter 5.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column width</td>
<td>24.3 cm</td>
</tr>
<tr>
<td>Column height</td>
<td>48.6 cm</td>
</tr>
<tr>
<td>Number of cells in x-direction</td>
<td>100</td>
</tr>
<tr>
<td>Number of cells in y-direction</td>
<td>200</td>
</tr>
<tr>
<td>Grid cell spacing (square cells)</td>
<td>0.243 cm</td>
</tr>
<tr>
<td></td>
<td>0.1215 cm (for grid-resolution study only)</td>
</tr>
<tr>
<td>Input bubble diameter</td>
<td>4 mm</td>
</tr>
</tbody>
</table>

A grid-resolution study was carried out first, with uniform cell spacing. Cell sizes considered were 0.243 cm and 0.1215 cm. Figures 5.1 and 5.2 show the liquid volume fraction profiles for the 1.5 cm/s inlet-gas velocity case and the 4.9 cm/s inlet-gas velocity case, respectively. As seen in Figures 5.1 and 5.2, the average gas holdup values are approximately equal for both grid resolutions. It appears that refining the grid does not reveal significant changes in the flow; thus, the cell spacing of 0.243 cm is probably sufficient. Since a cell spacing of 0.243 cm was found to yield grid-independent flow structures, it was therefore used for all other simulation results reported in this chapter.
Figure 5.1. Water volume fraction profiles for test-case simulations with $u_g = 1.5$ cm/s. Left: Cell spacing of 0.243 cm. Right: Cell spacing of 0.1215 cm.

Figure 5.2. Water volume fraction profiles for test-case simulations with $u_g = 4.9$ cm/s. Left: Cell spacing of 0.243 cm. Right: Cell spacing of 0.1215 cm.
Table 5.3. Gas holdup and rise velocity from simulations.

<table>
<thead>
<tr>
<th></th>
<th>Case 1, $u_g = 1.5$ cm/s</th>
<th>Case 2, $u_g = 4.9$ cm/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average gas holdup, simulation</td>
<td>0.0843</td>
<td>0.274</td>
</tr>
<tr>
<td>Average gas holdup, experiments</td>
<td>0.061</td>
<td>0.25</td>
</tr>
<tr>
<td>Average rise velocity, simulation</td>
<td>17.79</td>
<td>17.77</td>
</tr>
</tbody>
</table>

Table 5.3 shows the quantitative comparison between the simulation results and the Delft experimental data (Harteveld et al., 2004). It can be seen in Table 5.3 that the simulations predict slightly higher average holdup values than those observed in experiments (which is expected due to the difference between Eqs. 5.16 and 5.17). The flow profiles obtained for the simulations are homogeneous over the range of gas-flow rates used in these experiments (i.e., average gas holdup up to 0.25). Note also that the bubble rise velocity is independent of the inlet-gas flow for both the experiments and the simulations, which is consistent with using a Richardson-Zaki exponent of unity in the drag force (Eq. 5.7).

5.3.2 Flow Maps

In order to cover the entire range where flow transitions occur, simulations were performed with fixed values of the Reynolds number and the inlet-gas flow rate. $Re$ is fixed at 100, 400, 700, 1000, 1300, 1600, and 1900; while the values considered for the average gas holdup $\bar{\alpha}_d$ are 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 0.7. The computational domain is the same as described in Section 5.3.1. Each fully resolved, 2D, time-dependent simulation was run for a total of 15 seconds in order to ensure that the flow statistics were independent of the initial conditions, and thus approximately 150 CPU hours on a 16-processor SunFire 6800 were needed for each of the points on a flow map. Three force-model cases are considered:

Case (i): All forces enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$ and $C_S = 0.125$.

Case (ii): Only drag force enabled.

Case (iii): Drag and virtual-mass forces enabled.

Case (i) is the baseline model that includes all force terms used in Chapter 4 for homogeneous flow. Case (ii) is a “minimal” model that includes only drag (which cannot
be neglected), and Case (iii) includes the virtual-mass term that is known to be important in gas-liquid flow.

Determining the input bubble diameter to yield the desired $Re$ and the input value of $u_g$ to yield the desired $\bar{\alpha}_d$ was done in the following manner. First, $C_D(Re)$ was calculated from Eq. 5.9, with $C_\infty = 1.4$, for each value of $Re$ in the range considered. Next, the value of $C_D = C_D(Re)$ was used in Eq. 5.21 to determine the rise velocity $u_d$. Once $u_d$ was known, the expression for $Re$ (Eq. 5.8) was used to determine the $d_b$ value corresponding to $Re$ and $u_d$. Finally, the mass balance (Eq. 5.18) was used to determine the appropriate input value for $u_g$ to obtain the desired $\bar{\alpha}_d$ value. In general, the simulations returned the target values for $Re$ and $\bar{\alpha}_d$, except when the flow transitioned to heterogeneous flow.

![Continuous-phase volume-fraction profiles illustrating the representative flow structures observed in two-fluid simulations.](image-url)
Carrying out the simulations for the flow maps revealed that six different structure classifications could be observed as shown in Fig. 5.3. In this figure, contour plots of the water volume fraction are plotted at the end of the simulation (15 seconds). Because the amplitude of the fluctuations in the local holdup depends on the flow regime, we have not used the same scaling in all plots. In general, the amplitude in the homogeneous regime is on the order of a few percent, while in the turbulent regime it is much larger. The profiles of swirls are characterized by small spatial inhomogeneities in the volume fraction. These structures tend to be no larger than 2 cm in width or length, and the change in local volume fraction with respect to position is gradual, not a steep gradient. It is important to also note that while the profiles of swirls or bands do not reflect uniform-flow behavior, the $\alpha_d$ values that resulted from these profiles yielded a linear relationship between $\alpha_d$ and $u_g$, which in experimental studies is taken as evidence of homogeneous flow. Only for transitional and turbulent flow profiles did the $\alpha_d$ values deviate from linearity. It can also be seen in Fig. 5.3 that the particular example of transitional flow shows both bands as well as more turbulent behavior. The reader can appreciate that the exact structure varies with time, and depends on the model formulation and $Re$.

Figures 5.4a and 5.4b illustrate the flow maps for Case (i), in which all force models are enabled. Figure 5.4a corresponds to cases in which BIT1 is considered, and Figure 5.4b corresponds to cases in which BIT2 is considered. Recall that the CFDLib drag model was adjusted at $Re = 713$ in order to predict an average gas holdup in the range described in Table 5.1. Thus, the flow maps agree with the Delft experiments for $Re = 713$, which showed that the flow was homogeneous for average gas holdups up to 0.5. According to the flow maps, when $Re \approx 700$, transition to turbulence occurs for $\alpha_d$ near 0.5. Note that the widest range of homogeneous flow is observed (without fitting any parameters except the drag model) for the Reynolds number (700) corresponding to approximately 4 mm bubbles in air-water systems. Additionally, the flow maps reflect that Case (i) results in the greatest variation in possible flow structures, as the behavior progresses from uniform flow or swirls to horizontal bands to turbulence, with increasing
In general, for larger Reynolds numbers banded structures are observed, while for small Reynolds numbers transition to turbulent flow occurs directly from the uniform state. It is also worth noting that while some of the individual $\alpha_d$-$Re$ points differ slightly between the map for BIT1 and the map for BIT2, overall applying BIT2 does not change the general location of the transition points on the flow map.

![Flow map for Case (i), BIT1 model applied.](image)

Several simulations discussed in Chapter 4 also applied all force models and the BIT1 model. However, these simulations utilized the drag model with $C_\infty = 0.5$, and a uniform flow was obtained for $Re = 504$ and $\alpha_d \approx 0.5$. This disagreement with the flow maps presented in Figs. 5.4a and 5.4b is due to the adjustment to the drag model (setting $C_\infty = 1.4$). As mentioned earlier, the observed flow regimes will depend on the form of
the drag correlation (Eq. 5.9), which (in Figs. 5.4a and 5.4b) is fit for data at $Re = 713$ as discussed above.

![Figure 5.4b. Flow map for Case (i), BIT2 model applied.](image)

In experimental investigations of bubble columns, plots of the gas holdup versus the inlet-gas velocity are often used to pinpoint the transition from homogeneous to heterogeneous flow (Zahradnik et al., 1997; Ruzicka et al., 2001a, b; Olmos et al., 2001; Olmos et al., 2003 a, b). Figures 5.5a and 5.5b show the relationship between gas holdup and inlet-gas velocity for cases in which BIT1 and BIT2, respectively, are applied. As seen in Figs. 5.5a and 5.5b, the value of $\bar{\alpha}_d$ falls below a straight line with respect to $u_g$ at the transition to heterogeneous flow. In the (linear) homogenous regime, the slope of the line is a decreasing function of Reynolds number. In Figs. 5.5a and 5.5b, circular symbols correspond to $\bar{\alpha}_d$ obtained from simulations, while the solid lines correspond to
the linear relationship between $\bar{\alpha}_d$ and $u_g$ that applies for homogeneous flow. As noted earlier, the banded structures do not deviate from this linear behavior. The deviation from linear behavior (signifying the transition to heterogeneous flow) is slightly less for $Re = 1000$, 1300, and 1600 when BIT2 is applied. Overall, however, there does not seem to be a significant difference between the line plots for BIT1 and BIT2.

At the transition to turbulence the slope decreases continuously, indicating that the effective drag coefficient for the bubbles decreases in the turbulent regime. Note that unlike in many experiments where churn turbulence is observed (Ruzicka et al., 2001a, b; Olmos et al., 2003a, b), the slope never becomes negative (nor is there a discontinuous jump to a lower line). We speculate that such behavior is due to bubble coalescence (which is not represented in our model), leading to an increase in the effective bubble diameter (and hence an increase in $Re$ and a decrease in the drag coefficient).

**BIT1**

![Figure 5.5a. Average gas holdup $\bar{\alpha}_d$ as a function of $u_g$ for Case (i), BIT1 applied. Red: $Re = 100$. Green: $Re = 400$. Blue: $Re = 700$. Light blue: $Re = 1000$. Orange: $Re = 1300$. Gray: $Re = 1600$. Pink: $Re = 1900$. Symbols correspond to $\bar{\alpha}_d$ obtained from simulations, and solid lines correspond to the linear relationship between $\bar{\alpha}_d$ and $u_g$ that applies for homogeneous flow.](image-url)
Figure 5.5b. Average gas holdup $\overline{\alpha}_d$ as a function of $u_g$ for Case (i), BIT2 applied. Red: $Re = 100$. Green: $Re = 400$. Blue: $Re = 700$. Light blue: $Re = 1000$. Orange: $Re = 1300$. Gray: $Re = 1600$. Pink: $Re = 1900$. Symbols correspond to $\overline{\alpha}_d$ obtained from simulations, and solid lines correspond to the linear relationship between $\overline{\alpha}_d$ and $u_g$ that applies for homogeneous flow.

Note that since the qualitative behavior is nearly the same for BIT1 and BIT2, we present only the cases for which BIT1 is considered for the remainder of the discussion.

In the literature on the two-fluid simulation of air-water bubble columns (Sokolichin et al., 2004), several researchers have concluded (often based on under-resolved simulations) that only the drag force is needed to adequately describe the fluid dynamics. Figure 5.6 illustrates the flow map for Case (ii), in which only the drag force is enabled. The map shows that the transition to the turbulent regime occurs for $\overline{\alpha}_d$ near 0.2 for all Reynolds numbers. Thus, using only the drag force is not in qualitative agreement with the Delft experiments, which showed that homogeneous flow could be obtained for gas holdup values up to at least 0.5. Figure 5.7 shows the volume-averaged holdup $\overline{\alpha}_d$ as a function of $u_g$ for Case (ii). The transition to turbulent flow again results in a deviation from linearity as seen previously in Figs. 5.5a and 5.5b, except it now occurs at a much lower value of the average gas holdup than observed for Case (i).
Figure 5.6. Flow map for Case (ii).

Figure 5.7. Average gas holdup $\alpha_d$ as a function of $u_g$ for Case (ii). Red: $Re = 100$. Green: $Re = 400$. Blue: $Re = 700$. Light blue: $Re = 1000$. Orange: $Re = 1300$. Gray: $Re = 1600$. Pink: $Re = 1900$. Symbols correspond to $\alpha_d$ obtained from simulations, and solid lines correspond to the linear relationship between $\alpha_d$ and $u_g$ that applies for homogeneous flow.
Figure 5.8. Flow map for Case (iii).

While drag is insufficient by itself to stabilize the flow, in bubbly flows the density of the continuous phase is large relative to the dispersed phase, and it can be argued that the virtual-mass term cannot be neglected (Delnoij et al., 1997b). Figure 5.8
illustrates the flow map for Case (iii), in which the drag and virtual-mass forces are enabled. According to this map, transition to turbulent flow occurs for $\bar{\alpha}_d$ approximately equal to 0.1-0.2. Again, the map agrees with the corresponding line plots presented in Fig. 5.9, which show that transition to turbulent flow occurs for $\bar{\alpha}_d$ approximately equal to 0.1-0.2. Both Cases (ii) and (iii) do not result in much variation of the possible flow structures observed, since the onset of turbulence occurs for smaller values of $\bar{\alpha}_d$ than observed for Case (i). Overall, the flow maps illustrate that the structures observed for a given value of $Re$ and $\bar{\alpha}_d$ are highly dependent on the model parameters applied in the simulations, and that only Case (i) is in qualitative agreement with the Delft experiments.

5.3.3 Effect of Drag Correlation

As noted earlier, the drag correlation in Eq. 5.9 is not specific to bubbly flows. In order to test the effect of the drag correlation on the flow structures and transitions observed in our simulations, we have also constructed a flow map using Eq. 5.10. Note that $Eo$ can be expressed in terms of $Re$:

$$Eo = \left(\frac{g \rho c^2}{\sigma} \right) \left(\frac{Re}{u_d}\right)^2,$$

where all terms in the first set of parentheses are held constant. Thus, for each value of $Re$ in the range studied, we used this expression to find a corresponding value of $Eo$. It should be noted that for this study, no adjustments were made to the drag correlation at $Re = 713$ in order to predict gas holdup in the range described in Table 5.1.

Figure 5.10 illustrates the flow map with all force models enabled and the drag correlation defined in Eq. 5.10. As expected, a change to the drag correlation results in a small change to the structures observed for several values of $Re$ and $\bar{\alpha}_d$. The first notable difference is that bands are observed for smaller values of $Re$. When the original correlation (Eq. 5.9) was applied, horizontal bands extending across the column width were first observed for $Re = 1000$ and $\bar{\alpha}_d = 0.3$ and 0.4. When the correlation given by Eq. 5.10 is applied, the same horizontal bands are first observed for $Re = 400$ and $\bar{\alpha}_d =$
0.3, and for $Re = 700$ and $\bar{\alpha}_d = 0.2$. These data points corresponded to either uniform flow or swirls when the original correlation (Eq. 5.9) was applied. Subsequently, horizontal bands that are smaller than the column width are observed for smaller values of $Re$. Such structures were first observed with Eq. 5.9 when $Re = 1300$ and $\bar{\alpha}_d = 0.3$ or 0.4. When the drag correlation given by Eq. 5.10 is applied, such structures are first observed for $Re = 700$ and $\bar{\alpha}_d = 0.3$ or 0.4. The second notable difference resulting from the change in drag correlation is that for $Re = 1600$ and 1900, transitional behavior does not occur until $\bar{\alpha}_d$ is approximately 0.6. When the original correlation was applied, transitional behavior for these $Re$ values was observed when $\bar{\alpha}_d$ was approximately 0.5.

Figure 5.10. Flow map for drag correlation described by Eq. 5.10 with all forces enabled.
Figure 5.11 shows $\bar{\alpha}_d$ as a function of $u_g$ for all force models and the drag correlation defined in Eq. 5.10. As seen in the previous line plots, the transition to turbulence is marked by a deviation from linearity. The deviations observed on the line plots shown in Fig. 5.11 correspond to the values of $\bar{\alpha}_d$ in the flow map in Fig. 5.10 at which the transitional behavior occurs. It should be noted that while no adjustments were made to the drag correlation given by Eq. 5.10, the transition to heterogeneous flow also occurs for $\bar{\alpha}_d \approx 0.5$ when $Re \approx 700$, as seen in Figs. 5.10 and 5.11. Thus, including all interphase forces and applying the drag correlation given by Eq. 5.10 agrees qualitatively with the Delft experiments at $Re = 713$. Also note that in Fig. 5.11 at higher Reynolds numbers, all curves fall on nearly the same line. This is due to the fact that the drag correlation in Eq. 5.10 becomes nearly independent of Reynolds number for large values of this parameter.

![Figure 5.11. Average gas holdup $\bar{\alpha}_d$ as a function of $u_g$ for drag correlation in Eq. 5.10 with all forces enabled. Red: $Re = 100$. Green: $Re = 400$. Blue: $Re = 700$. Light blue: $Re = 1000$. Orange: $Re = 1300$. Gray: $Re = 1600$. Pink: $Re = 1900$. Symbols correspond to $\bar{\alpha}_d$ obtained from simulations, and solid lines correspond to the linear relationship between $\bar{\alpha}_d$ and $u_g$ that applies for homogeneous flow.](image-url)
5.3.4 Examination of Force Components

The flow maps and line plots presented in the previous section show that the force models have a significant effect on the transition regions observed, and that they determine the type of flow structures observed as the gas-flow rate, and in turn $\overline{\alpha_d}$, increases. Thus, it is worthwhile to examine how selected force-model components behave for a particular model formulation. In this study, the average values of selected force-model components were determined for each of the horizontal planes in the column. We first plot the plane-averaged values of these force-model components as a function of column height for $Re = 1300$ and $\overline{\alpha_d} \approx 0.1$ for Cases (i)-(iii), and then do the same for $Re = 1300$ and $\overline{\alpha_d} \approx 0.2$ for Cases (i)-(iii). In order to show how the behavior of the force components reflects the behavior of the flow structures observed as $\overline{\alpha_d}$ increases, we then plot the plane-averaged values of the force-model components as a function of column height for $Re = 1300$ and $\overline{\alpha_d} \approx 0.3, 0.4, \text{ and } 0.5$ for Case (i).

Post-processing software was used to calculate all spatial derivatives from the simulation data in order to calculate the horizontal and vertical components of the drag, lift, rotation, and strain forces (Eqs. 5.7, 5.13, 5.14, 5.15). It should be noted that for Cases (ii) and (iii), in which certain force models are disabled (i.e., the force-model coefficient was set to zero in the simulation), spatial derivatives and thus the force-model components can still be calculated during post-processing. In other words, the force model may not have been included during the simulation, but the post-processing analysis allows us to calculate what the force-model components would have been for a given set of data obtained during the simulation. Subsequently, we can show how the force components would have behaved for each type of flow at approximately the same $Re$ and $\overline{\alpha_d}$.

Finally, two scaling issues are addressed. First, the uniform-flow drag term (Eq. 5.20) was subtracted from the vertical component of the drag force calculated from Eq. 5.7, or $F_{Dy,\text{net}} = F_{Dy} - F_{D0}$. In uniform flow, we would thus expect $F_{Dy,\text{net}}$ to be null. Considering only the net vertical drag force component allows for an examination of the effect of drag on an order of magnitude more comparable to those of the other force-
model components. In these comparisons, the drag coefficient is defined by Eq. 5.9 with $C_w$ equal to 1.4. Second, if the uniform rise velocity $u_d$ is considered the characteristic velocity, the bubble diameter $d_b$ is considered the characteristic length, and the continuous phase density $\rho_c$ is considered the characteristic density, the force components can be made dimensionless by dividing by $(\rho_c u_d^2/d_b)$. All the force components discussed below have been made dimensionless in this manner.

![Graphs showing force components for Case (i), when $Re = 1300$ and $\bar{\alpha}_d = 0.1$. Uniform flow is observed.](image)

Figure 5.12. Force components for Case (i), when $Re = 1300$ and $\bar{\alpha}_d = 0.1$. Uniform flow is observed.

We first examine how the force-model components behave for Cases (i)-(iii) with $Re = 1300$ and $\bar{\alpha}_d \approx 0.1$. Figure 5.12 illustrates the force-model component behavior for Case (i), when homogeneous flow is observed. As column height increases, the plane-averaged values of the net vertical drag component are approximately $5.0 \times 10^{-5}$ on
average, and the plane-averaged values of all the other force-model components remain approximately zero (within the accuracy of the code). Any variations observed are on the order of $10^{-5}$ to $10^{-4}$ for the net drag force, and on the order of $10^{-6}$ for the lift, rotation, and strain forces. Such behavior corresponds to the uniform flow observed for $Re = 1300$ and $\bar{\alpha}_d = 0.1$.

Figure 5.13. Force components for Case (ii) with $Re = 1300$ and $\bar{\alpha}_d = 0.1$. Uniform flow is observed.

Figure 5.13 shows how the force-model components behave for Case (ii) with $Re = 1300$ and $\bar{\alpha}_d \approx 0.1$, when uniform flow is also observed. The horizontal drag component is approximately zero along the column height, while the net vertical drag component varies weakly. Note that when the net vertical drag component is positive, it
corresponds to $F_{D0} > F_{Dy}$ on average for a particular plane. The lift and rotation components are relatively small along the column height. The plane-averaged vertical component of the strain force also remains small as column height increases, while the horizontal component varies weakly along the column height. Any variations among the plane-averaged force components are small ($\sim 10^{-4}$), corresponding to the expected uniform profile designated by the flow map for Case (ii) (Fig. 5.6).

![Graphs showing force components](image)

**Figure 5.14.** Force components for Case (iii) with $Re = 1300$ and $\overline{\alpha}_d \approx 0.1$. Transitional behavior is observed.

For Case (iii) with $Re = 1300$ and $\overline{\alpha}_d \approx 0.1$, transitional behavior is observed. Figure 5.14 shows that the plane-averaged components of all the forces vary significantly with increasing column height. The maximum variations observed are $\sim 10^{-2}$ for the net...
drag force, $\sim 5 \times 10^{-3}$ for the lift and rotation forces, and $\sim 2.5 \times 10^{-3}$ for the strain terms. The higher degree of variation observed for all the components reflects that the flow is transitioning from uniform behavior. Additionally, note that the net vertical drag component is largely positive throughout much of the column. This corresponds to $F_{D0} > F_{Dy}$ on average for most of the horizontal planes examined within the column. As discussed previously, the effective drag coefficient in $F_{Dy}$ for the bubbles is decreasing upon transition from uniform flow, and thus an increase in rise velocity occurs. Note from Eq. 5.18 that $\bar{\alpha}_d = u_d / u_d$. Therefore, the increase in rise velocity corresponds to the smaller $\bar{\alpha}_d$ value for which transitional or turbulent behavior is observed.

Figure 5.15. Force components for Case (i), when $Re = 1300$ and $\bar{\alpha}_d = 0.2$. Banded flow structures are observed.
Figures 5.15, 5.16, and 5.17 show how the force-model components behave for Cases (i), (ii), and (iii), respectively, when \( Re = 1300 \) and \( \bar{\alpha}_d \approx 0.2 \). For Case (i), bands are observed. It can be seen in Fig. 5.15 that the plane-averaged values of the net vertical drag component and the vertical strain component oscillate as column height increases, and such behavior corresponds to the ordered banded structures observed. These components have a magnitude of approximately \( 10^{-3} \) to \( 10^{-2} \). Note that the strain force is approximately 90 degrees out of phase with the drag force. This suggests that the strain force is somehow modulating growth of the instability manifested in the drag force. The plane-averaged values of the horizontal lift and rotation components show negligible variations (\( \sim 10^{-5} \)) along the column height. The horizontal components of the drag and strain forces and the vertical components of the lift and rotation forces remain approximately zero as column height increases. Nevertheless, we should note that based on numerical simulations (for which the flow maps are not shown due to their similarity to Fig. 5.6), if the lift and rotation forces are eliminated, the strain force is not sufficient to stabilize the flow.

Transitional flow is observed for Case (ii) when \( Re = 1300 \) and \( \bar{\alpha}_d \approx 0.2 \). Figure 5.16 shows that the plane-averaged components of all the forces vary randomly with increasing column height. These variations are on the order of \( 5 \times 10^{-2} \) for the net drag force, \( 10^{-2} \) for the lift and rotation forces, and \( 5 \times 10^{-3} \) for the strain terms. Both the randomness of these variations (as opposed to ordered oscillations) and the increases in the orders of magnitude (from \( 10^{-4} \) to \( \sim 10^{-3} - 10^{-2} \)) are indicative of transitional behavior. Additionally, the net vertical drag component is positive throughout much of the column, corresponding to \( F_{D0} > F_{Dy} \) on average. As discussed previously, the effective drag coefficient in \( F_{Dy} \) for the bubbles is decreasing, resulting in an increase in rise velocity. Consequently, transitional behavior is observed for a smaller value of \( \bar{\alpha}_d \).

Turbulent flow is observed for Case (iii) when \( Re = 1300 \) and \( \bar{\alpha}_d \approx 0.2 \). Figure 5.17 shows that the plane-averaged components of all the forces vary randomly with increasing column height. The net vertical drag component varies between zero and approximately \( 7.5 \times 10^{-2} \), while the horizontal drag component varies between
approximately $-2.5 \times 10^{-2}$ and zero. The horizontal components of the lift, rotation, and strain forces vary between $-10^{-2}$ and $2.0 \times 10^{-2}$, while the vertical components vary approximately between $-10^{-2}$ and $5 \times 10^{-3}$. The random variations at a higher order of magnitude correspond to the random flow structures observed in a turbulent flow profile. Note again that the net vertical drag component is positive throughout the column, corresponding to $F_{D0} > F_{Dy}$ on average. The net vertical drag component for Case (iii) also has a higher magnitude than observed for Case (ii). Presumably, this corresponds to an even greater decrease in the effective drag coefficient in $F_{Dy}$ and therefore a greater increase in the rise velocity. Consequently, turbulent, and not transitional, behavior is observed for $\overline{\alpha}_d \approx 0.2$ for Case (iii).

Figure 5.16. Force components for Case (ii), when $Re = 1300$ and $\overline{\alpha}_d \approx 0.2$. Transitional behavior is observed.
We next illustrate how the force-model components behave for Case (i) with $Re = 1300$ as the average volume fraction $\alpha_d$ is increased. Recall from Figure 5.15 that when $\alpha_d \approx 0.2$, banded flow structures are observed. The plane-averaged values of the net vertical drag component and the vertical strain component oscillated as column height increased, while the plane-averaged values of the horizontal lift and rotation components exhibited minor variations ($\sim 10^{-5}$) along the column height. Figures 5.18-5.20 show how the force-model components behave for Case (i) with $Re = 1300$ and $\alpha_d \approx 0.3, 0.4,$ and $0.5$, respectively.

According to the flow maps for Case (i) (Figs. 5.4a and 5.4b), when $\alpha_d$ is approximately 0.3, horizontal bands are still observed; however, these bands tend to be...
shorter, bent, or broken apart instead of ordered structures extending straight across the width of the column. The aperiodic oscillations shown in Fig. 5.18 for the plane-averaged net vertical drag component and the vertical strain component correspond to the type of bands observed. The aperiodicity is more prominent at greater column heights, which is expected since (as seen in Fig. 5.3) the bands become gradually shorter or more disordered as they move upward in the column. The increase in $\overline{\alpha}$ from 0.2 (Fig. 5.15) to 0.3 also results in an increase by a factor of 2 for the maximum oscillation amplitude in the vertical drag and strain components, and an increase from $\sim 10^{-5}$ to $\sim 10^{-4}$ in the fluctuations in the lift and rotation components. The latter may be due to the onset of damped cooperative-rise instabilities (Sankaranarayanan and Sundaresan, 2002) that eventually lead to the transition to heterogeneous flow.

![Figure 5.18. Force components for Case (i) with $Re = 1300$ and $\overline{\alpha} \approx 0.3$. Small, disordered banded structures are observed.](image-url)
Figure 5.19 shows how the force-model components behave with $Re = 1300$ and $\bar{\alpha}_d \approx 0.4$, for which the shorter, more disordered bands are observed. Accordingly, the plane-averaged net vertical drag component and the vertical strain component exhibit significant aperiodic oscillations. However, the aperiodicity is now observed at all column heights, instead of appearing most prominently at larger column heights. Additionally, the fluctuations in the plane-averaged lift and rotation forces have increased from $\sim 10^{-4}$ to $\sim 10^{-3}$. The higher degree of variation exhibited by all the force components is expected since the flow gradually approaches the transition to heterogeneous flow as $\bar{\alpha}_d$ increases.

Figure 5.19. Force components for Case (i) with $Re = 1300$ and $\bar{\alpha}_d \approx 0.4$. Small, random banded structures are observed.
Finally, note that the horizontal drag component increases in magnitude as column height increases, instead of remaining nearly zero as observed in previous figures. The graphs presented in Figs. 5.18-5.20 show the components at a particular time (15 seconds). At other times, the magnitude of the horizontal drag component either remains near zero or decreases from zero as column height increases, due to instability in the flow near the top of the column. In other words, the time-averaged horizontal drag component is zero as expected, but the large-scale flow structures form at the top of the column so that the instantaneous horizontal drag is nonzero.

Figure 5.20. Force components for Case (i) with $Re = 1300$ and $\bar{\alpha}_d \approx 0.5$. Transitional flow behavior is observed.

Figure 5.20 shows how the force-model components behave with $Re = 1300$ and $\bar{\alpha}_d \approx 0.5$, for which fully transitional behavior is observed. The plane-averaged
components of all the forces vary significantly with increasing column height, with fluctuations on the order of $10^{-2}$ for the net drag force, and on the order of $10^{-3}$ for the lift, rotation, and strain forces. Aperiodic oscillations are observed in the vertical strain component along the column height, and in the net vertical drag component when the column height is less than 20 cm. However, the magnitude of these oscillations is much smaller than in the previous figures. The overall disordered behavior exhibited by all the force components corresponds to the structures observed in the transitional flow profile (Fig. 5.3). Note again that the magnitude of the horizontal drag component increases as column height increases. As discussed previously, Fig. 5.20 is shown for 15 seconds. At other times, the instability in the flow near the top of the column causes the magnitude of the horizontal drag component to change values accordingly. Nevertheless, the time-averaged horizontal drag component is null as expected.

Several final remarks should be stated regarding the behavior of the instabilities observed in our simulations. First, in all simulations presented, the lift-force coefficient (if applied) was positive. Based on an analysis of the role of the lift force by Lucas et al. (2005), Harteveld (2005) has speculated that the instability observed in his experiments was due to a change in sign of the lift force near the walls at the top of the bubble column. A change in the sign of the lift force cannot be the cause of the transition from homogeneous to turbulent flow observed in Case (i) of our study because the lift coefficient was held constant. Second, because free-slip boundary conditions were used at the walls, the instability in Case (i) did not begin at the column walls, although it did originate near the top of the column. For this reason, the effect of the velocity profile near the walls in the simulations cannot be examined directly. Third, it can be concluded that all of the force terms, combined with a bubble-induced turbulence model, must be included in order to observe homogeneous flow up to high average gas holdup. Our studies clearly show that if any one of these components is not included, the transition to turbulent flow occurs at considerably lower values of the average gas holdup. However, it must be noted that when all forces are present, the transition to turbulent flow arises from the banded structures, a non-uniform though “homogeneous” state. Such behavior
complicates further studies such as linear stability analysis. It is clear that further study is necessary regarding transitional behavior and the effects the various forces may have.

5.4 Summary and Conclusions

The overall conclusion from this study is that flow-regime predictions for bubble-column simulations must include the full set of force models in order to predict homogeneous flow at high average gas holdup as observed in the experiments of Harteveld (2005). Applying all the interphase force models results in homogeneous flow in the same range of inlet flow rates as those used in the Delft experiments (Harteveld et al., 2003, 2004, 2005; Mudde, 2005b). Simulations over a wide range of bubble diameters and inlet gas flow rates were carried out in order to construct flow maps of the regions in $Re-\bar{\alpha}$ space where flow transitions occur. Using drag only or drag and virtual-mass, we illustrated the strong dependence of the predicted flow maps on the two-fluid model formulation.

An analysis of selected force-model components showed that the overall behavior of the force components corresponds to the flow structures expected from the flow maps. An examination of the net vertical drag component provides insight as to why transitional or turbulent behavior is observed for smaller values of $\bar{\alpha}_d$ in a particular model formulation. It would seem that the role of the strain term is to modulate the instability exhibited by the non-uniform drag components, allowing for a transition from uniform flow to banded structures. As the transition to turbulent flow is approached, these banded structures gradually break down, while “bubble-rich” plumes appear near the top of the column. A qualitative examination of how the flow behaves at different times suggests that large-scale structures originate near the top of the flow domain and eventually propagate through the entire bubble column. Such behavior is consistent with the experimental observations of Harteveld (2005). However, our understanding of the nature of flow transitions would benefit from further study regarding the effect of inhomogeneous velocity and gas holdup profiles near the column walls and the effect of the choice of boundary conditions used.
Chapter 6. Linear Stability Analysis of a Two-Fluid Model for Air-Water Bubble Columns

As seen in Chapters 4 and 5, the predictions of known bubble-column flow regimes were found to be highly dependent on the model formulation, which includes drag, virtual-mass, lift, rotation, and strain forces, and bubble-induced turbulence (BIT). At low gas velocities, nearly uniform flow profiles were obtained when the BIT model and all force models were applied using a particular set of model coefficients. This model formulation appeared to stabilize the flow, as the profiles presented in Chapter 4 showed only small fluctuations ($\sim 10^{-4} - 10^{-3}$) about the spatial averages for gas holdup ($\alpha_d \sim 0.1 - 0.4$) and relative velocity. As shown in Chapter 5, the flow-regime predictions for bubble-column simulations must include the full set of force models in order to predict homogeneous flow at high average holdup as observed in the experiments of Harteveld (2005). An increase in both the bubble Reynolds number and the inlet gas velocity resulted in a transition from uniform flow to rising plane waves and eventually turbulent flow. A linear stability analysis is performed in order to examine the role of individual model parameters in determining the flow dynamics.

It should be noted that portions of this chapter are adapted from the Chemical Engineering Science paper “Linear Stability Analysis of a Two-Fluid Model for Air-Water Bubble Columns” by Monahan and Fox (2007). Any changes to the text are made to correspond to the equation numbers, chapter and section numbers, tables and table numbers, or figures and figure numbers presented in this thesis.

6.1 Introduction

6.1.1 Literature Review for Linear Stability Analysis

A literature survey shows that researchers have utilized linear stability analysis in order to determine stability conditions for their multiphase systems, or to identify the characteristics of transitional behavior. Biesheuvel and van Wijngaarden (1984) applied ensemble averaging to develop a system of equations for bubbly flows and to account for hydrodynamic fluctuations. It was assumed that the suspension was dilute and that the motion of a single bubble caused velocity fluctuations at a particular position. The
system of equations was hyperbolic, with one characteristic velocity equal to zero, two characteristic velocities associated with sound waves, and one characteristic velocity associated with concentration waves. Bubble-bubble interactions needed to be considered in order to determine the effect of volume fraction on the propagation velocity of the concentration waves.

Jones and Prosperetti (1985) performed a linear stability analysis on a general class of one-dimensional models for two-phase flow, for the case of steady uniform flow. The model equations contained only first-order derivatives and algebraic expressions, and accounted for the virtual-mass force, the drag force, phase interaction, and differences in phase pressures. It was assumed that both phases were incompressible. The analysis showed that stability properties had no dependence on perturbation wavelength, and therefore hyperbolicity was a necessary stability condition. This was an unphysical result indicating that the general model was incomplete. Extending their work to include higher-order derivatives in the general class of one-dimensional models resulted in stability properties with the expected dependence on perturbation wavelength (Prosperetti and Jones, 1987). However, they also found that adding higher-order derivatives would not improve the long-wavelength stability behavior of a first-order hyperbolic model. The long-wavelength stability condition was sensitive to the drag formulation used.

Batchelor (1988) developed a one-dimensional (vertical) model to describe the unsteady motion of particles in a fluidized bed. The two dependent variables were local particle volume fraction and local mean particle velocity. Several parameters were functions of the particle volume fraction and particle Reynolds number, including mean particle velocity, mean-square particle velocity fluctuation, gradient diffusivity of particles, and particle viscosity. The bed became unstable when the particle Froude number surpassed the critical value. Disturbances were characterized by vertically propagating sinusoidal deviations in the local particle velocity and local particle volume fraction. An extension of this work (Batchelor, 1993) illustrated the conditions for which a fluidized bed undergoing a planar (primary) instability would then be subject to secondary instabilities in the transverse direction.
Biesheuvel and Gorissen (1990) described gas bubbles dispersed in a liquid with a one-dimensional model that accounted for inertial forces on the bubbles. Their linear stability analysis showed that above a critical void fraction, void-fraction disturbances would cause a uniform fluid to become linearly unstable. The effect of planar disturbances on bubbly-flow stability was also considered. The presence of column walls caused non-uniformities in the circular column cross-sections, and these non-uniformities affected the transition to the slug-flow regime. Lammers and Biesheuvel (1996) determined that Batchelor’s (1988) equations describing planar disturbances in fluidized beds could also be used to describe instabilities in bubbly flows. Experiments showed that changes in gas or liquid flow rate or changes in vessel height affected the size of the bubbles, and that the critical gas volume concentration varied with superficial liquid velocity. Such behavior suggested that the critical gas volume concentration had a strong dependence on bubble size. Experiments also showed that during flow transition, the radial concentration profile first appeared uniform, and then exhibited a parabolic shape before the flow became turbulent (Lammers and Biesheuvel, 1996).

Minev et al. (1999) investigated the linear stability of a general formulation for five different models, including an earlier model from Jackson (1971) and the model of Biesheuvel and Gorissen (1990), and studied their significance to bubbly flows. They found that the form of the convection term, in particular the form of the virtual-mass force, appearing in the momentum equations had a critical effect on the stability of the uniform-flow solution.

Johri and Glasser (2002) performed a linear stability analysis of model equations for a fluidized bed. Their analysis illustrated that the uniform state of the compressible-flow equations could become unstable, resulting in plane density waves. These waves materialized from a Hopf bifurcation of the uniform state and proceeded to move through the bed. Subsequent bifurcation analysis illustrated that these waves were sinusoidal at low amplitudes, but became unstable in the lateral direction as the amplitude increased. Johri and Glasser (2002) ultimately concluded that the primary and secondary instabilities of a fluidized bed could be represented qualitatively by the compressible-flow equations, but that quantitative results were dependent on the closures applied.
Sankaranarayanan and Sundaresan (2002) performed a linear stability analysis of the uniformly-bubbling state for a bubble column. Their lattice-Boltzmann simulations of bubble rise in periodic boxes illustrated both hindered rise, characterized by nearly spherical bubbles, and cooperative rise, characterized by highly distorted bubbles. In the hindered-rise regime, the bubble rise velocity in a periodic array of bubbles decreases with increasing bubble volume fraction, while in the cooperative-rise regime, bubble rise velocity increases with increasing bubble volume fraction. Their linear stability analysis showed that for the hindered-rise regime, the uniformly-bubbling state initially became unstable in the form of vertically traveling waves, while for the cooperative-rise regime, instabilities first occurred in the form of vertical column-like structures. For both regimes, the uniform state became unstable at very low bubble volume fractions ($\alpha_d = 0.0334$ for hindered rise, $\alpha_d = 0.0257$ for cooperative rise), which suggested that experimentally obtained bubbly flows were not truly uniform states. Additionally, the lift force was found to have a significant role in the destabilization of the uniform state in the cooperative-rise regime. Further analysis showed that in the hindered-rise regime, the vertically traveling waves would then experience transverse instabilities and yield two- and three-dimensional flow structures. However, in the cooperative-rise regime, the alternating bubble-rich and bubble-lean vertical columns would gradually form bubble plumes. The plumes would then experience secondary instabilities, resulting in a meandering two-dimensional structure or a vortical three-dimensional structure.

Thorat and Joshi (2004) developed a mathematical model that utilized linear stability analysis to predict the critical gas volume fraction that indicated the transition regime in a bubble column. A stability criterion was derived for which positive values indicated stable gas-liquid dispersions, negative values indicated unstable dispersions, and a value of zero corresponded to neutrally stable dispersions. Experimental results showed that the critical gas volume fraction increased with decreasing sparger free area and decreasing sparger hole diameter, and that critical gas volume fraction decreased with an increase in the ratio of gas dispersion height to column diameter. A lower degree of bubble coalescence tended to yield an increase in the critical gas volume fraction, indicating a delay in transitions from homogeneous to heterogeneous flow. Predictions
obtained from linear stability theory were found to be in good agreement with the experimental values of the critical gas volume fraction.

Lucas et al. (2005, 2006) studied the effect of the lift force on the stability of a uniform bubble column, and found that the influence of the lift force on flow stability was higher than that of the turbulent dispersion force. In addition, the authors concluded that a positive lift coefficient (corresponding to small bubbles) would stabilize the flow, while a negative lift coefficient (corresponding to large bubbles) would lead to instability and the transition to heterogeneous flow. Stability criteria were determined for monodispersed flow, flow with two different bubble sizes, and flow with \( N \) different bubble sizes. Their criteria agreed well with CFD simulations, and also with the experiments of Harteveld (2005).

6.1.2 Motivation

The numerical studies presented in Chapters 4 and 5 showed that the predictions of bubble-column flow regimes are highly dependent on the model formulation. We are thus motivated to investigate in detail the linear stability of our two-fluid model, and the effect of selected model parameters. Jackson (2000) has performed such an analysis for fluidized beds to examine how small perturbations affect the stability of the uniformly fluidized state. He has determined the dispersion relations that describe the growth (or decay) rates for small-amplitude disturbance waves. We extend Jackson’s procedure to include the additional forces present in gas-liquid flow. Our primary interest is to determine how the two-fluid model formulation affects the transition from homogeneous to heterogeneous flow.

This study is organized as follows. First, we derive the dispersion relations corresponding to the two-fluid model applied toward our bubble-column simulations. For simplicity, the derivation presented is for a two-dimensional case (i.e., vertical and horizontal). Based on symmetry, it is assumed that the equations describing the third dimension would have the same form as those for the second (horizontal) dimension. Various combinations of model parameters are then tested to determine their effects on the growth rate \( \lambda \) and the propagation velocity \( \nu \) for small-amplitude disturbances. We organize these studies primarily into cases of vertical and horizontal modes. Simulation
results are used to illustrate changes in linear stability. Either two- or three-dimensional transient simulations allow enough degrees of freedom to examine flow transitions. Finally, conclusions are drawn in the closing section of the chapter.

6.2 Review of Two-Fluid Model

A review of the two-fluid model equations is presented below. The subscript $c$ denotes the continuous phase (water), and the subscript $d$ represents the dispersed phase (air). Volume fraction, density, and velocity of each phase are represented by $\alpha$, $\rho$, and $u$, respectively. The physical parameters correspond to air and water at room temperature and pressure, and the bubble diameter is assumed constant. A detailed discussion of the two-fluid model is in Chapter 3.

The continuity equations for the continuous and dispersed phases are, respectively

$$\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c u_c) = 0$$

and

$$\frac{\partial \alpha_d \rho_d}{\partial t} + \nabla \cdot (\alpha_d \rho_d u_d) = 0.$$  (6.2)

The momentum balances for the continuous and dispersed phases are, respectively

$$\alpha_c \rho_c \frac{\partial u_c}{\partial t} + \alpha_c \rho_c u_c \cdot \nabla u_c = -\alpha_c \nabla p + \nabla \cdot [\alpha_c \mu_{\text{eff},c} \left( \nabla u_c + (\nabla u_c)^T \right)] + \sum_f F_{fc} + \alpha_c \rho_c g$$

and

$$\alpha_d \rho_d \frac{\partial u_d}{\partial t} + \alpha_d \rho_d u_d \cdot \nabla u_d$$

$$= -\alpha_d \nabla p - \nabla P_d + \nabla \cdot [\alpha_d \mu_{\text{eff},d} \left( \nabla u_d + (\nabla u_d)^T \right)] + \sum_f F_{fd} + \alpha_d \rho_d g.$$  (6.4)

The terms on the right-hand-sides of Eqs. 6.3 and 6.4 represent, from left to right, the pressure gradient, the effective stress, the interphase momentum exchange, and the gravitational force. Several closures in Eqs. 6.3 and 6.4 are reviewed below.

First, $\nabla P_d$ represents a bubble-pressure model applied only in the dispersed-phase momentum balance (Eq. 6.4), where (Biesheuvel and Gorissen, 1990)
\[ P_d = \rho_d C_{BP} \alpha_d \left( u_d - u_c \right) \cdot \left( u_d - u_c \right) \left( \frac{\alpha_d}{\alpha_{d,p}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{d,p}} \right), \quad (6.5) \]

\( \alpha_{d,p} \) is the gas volume fraction at close packing, and \( C_{BP} \) is a proportionality constant.

Second, the effective viscosity for the continuous phase is equal to the sum of the molecular viscosity of the continuous phase and a value for turbulent viscosity, or \( \mu_{eff,c} = \mu_{0,c} + \mu_{t,c} \). The studies in Chapter 5 included cases in which the effective viscosity for the dispersed phase is equal to the molecular viscosity of the dispersed phase, or \( \mu_{eff,d} = \mu_{0,d} \), as well as cases in which the effective viscosity for the dispersed phase is set equal to the sum of the molecular viscosity of the dispersed phase and the turbulent viscosity, or \( \mu_{eff,d} = \mu_{0,d} + \mu_{t,d} \). In this work, Sato’s bubble-induced turbulence (BIT) model (Sato and Sekoguchi, 1975) is used to determine both \( \mu_{t,c} \) and \( \mu_{t,d} \):

\[ \mu_{t,c}, \mu_{t,d} = C_{BT} \rho_d d, \alpha_d \left| u_d - u_c \right|, \quad (6.6) \]

where \( C_{BT} \) is a proportionality constant equal to 0.6 (Sato et al., 1981). When the BIT model is not used, \( C_{BT} \) is set equal to 0 and we refer to such cases as “laminar.” Note that Eq. 6.6 is a model for momentum transfer by the wake of an isolated bubble. At large gas holdups, bubble-bubble interactions are likely to suppress wake formation and thus \( C_{BT} \) would perhaps be more accurately modeled as a decreasing function of gas holdup.

Finally, note that

\[ \sum_f F_{fc} = -\sum_f F_{jd} , \quad (6.7a) \]

which is the sum of the drag, virtual-mass, lift, rotation, and strain forces:

\[ \sum_f F_{jd} = F_d + F_{vm} + F_L + F_{rot} + F_S = -\alpha_d \alpha_c \rho_c C_D \left( \frac{Re}{4d_b} \right) \left[ u_d - u_c \right] \left( u_d - u_c \right) \]

\[ -\alpha_d \alpha_c \left( \alpha_c \rho_c + \alpha_d \rho_d \right) C_{vm} \left[ \left( \frac{\partial u_c}{\partial t} + u_d \cdot \nabla u_c \right) - \left( \frac{\partial u_d}{\partial t} + u_c \cdot \nabla u_d \right) \right] \]

\[ +\alpha_d \alpha_c \left( \alpha_c \rho_c + \alpha_d \rho_d \right) C_L \left( u_d - u_c \right) \times \nabla \times u_c \]

\[ +\alpha_d \alpha_c \left( \alpha_c \rho_c + \alpha_d \rho_d \right) C_{rot} \left( u_d - u_c \right) \times \nabla \times u_d \]

\[ +\alpha_d \alpha_c \left( \alpha_c \rho_c + \alpha_d \rho_d \right) C_S \left[ \left( \nabla u_c + \nabla u_d \right) + \left( \nabla u_c + \nabla u_d \right)^T \right] \left( u_c - u_d \right). \quad (6.7b) \]
Recall from Chapter 3 that the lift, rotation, and strain terms in this model arise from the interaction terms proposed by Kashiwa (1998). Additionally, note that the drag coefficient $C_D(Re)$ is a function of the Reynolds number:

$$C_D(Re) = C_\infty + \frac{24}{Re} + \frac{6}{1 + \sqrt{Re}},$$  \hspace{1em} (6.8a)

where $C_\infty$ is set equal to 1.4 in order to agree with the experiments of Harteveld (2003, 2004, 2005), and the bubble Reynolds number is defined as

$$Re = \frac{d_b |u_d - u_c|}{\nu_c}.$$  \hspace{1em} (6.8b)

### 6.3 Derivation of Dispersion Relations

The derivation described in this section focuses on linear stability analysis of the uniform state. First, several simplifying assumptions are given. Then, the continuous- and dispersed-phase mass and momentum balances are determined for the uniform state. Perturbations to the uniform state are made, resulting in a set of linear partial differential equations. These equations are solved to yield a set of algebraic equations from which the dispersion relations are obtained. Both the growth rate $\lambda$ and the propagation velocity $\nu$ are determined for small-amplitude disturbances. In Section 6.3, the most important steps of the derivation are highlighted. Additional details are given in the Appendices.

#### 6.3.1 Bubbly Flow Equations

Both $\rho_c$ and $\rho_d$ are assumed to be constant in this work, and are subsequently divided out of the continuity equations (Eqs. 6.1 and 6.2). Additionally, the substitution $\alpha_c = 1 - \alpha_d$ is made in Eq. 6.1. Thus, the continuity equations are rewritten as

$$\frac{\partial}{\partial t} (1 - \alpha_d) + \nabla \cdot \left[ (1 - \alpha_d) \mathbf{u}_c \right] = 0$$  \hspace{1em} (6.9)

and

$$\frac{\partial \alpha_d}{\partial t} + \nabla \cdot (\alpha_d \mathbf{u}_d) = 0.$$  \hspace{1em} (6.10)
Next, it can be seen in Eqs. 6.3 and 6.4 that both phases share the pressure \( p \) in the expression \(-\nabla p\), which is unknown. The continuous-phase momentum balance (Eq. 6.3) is used to solve for \(-\nabla p\):

\[
-\nabla p = \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c - \frac{1}{\alpha_c} \nabla \cdot \mathbf{u}_c \mu_{\text{eff}} \left[ \nabla \mathbf{u}_c + \left( \nabla \mathbf{u}_c \right)^T \right] + \frac{1}{\alpha_c} \sum_f F_{fd} - \rho_c g,
\]

(6.11)

and the resulting expression for \(-\nabla p\) (Eq. 6.11) is substituted into the dispersed-phase momentum balance (Eq. 6.4).

Note that the drag term is nonlinear:

\[
F_D = -\alpha_d (1 - \alpha_d) \rho_c \left[ \frac{7}{5} + \frac{24 \nu_c}{d_b |\mathbf{u}_d - \mathbf{u}_c|} + \frac{6}{1 + \left( \frac{d_h |\mathbf{u}_d - \mathbf{u}_c|}{\nu_c} \right)} \right] \frac{3}{4d_b} |\mathbf{u}_d - \mathbf{u}_c| (\mathbf{u}_d - \mathbf{u}_c).
\]

(6.12)

To handle this non-linearity, Eq. 6.12 is simplified and \(|\mathbf{u}_d - \mathbf{u}_c|\) is set equal to a constant \(a\), since this will ultimately be a scalar value. Performing a Taylor series expansion about \(a\), using only the zero-order and first-order terms, and then setting \(a_0\) equal to the constant dispersed-phase velocity \(u_{d0}\) in the uniform state, yields an expression for the drag force:

\[
F_D = -\alpha_d (1 - \alpha_d) \rho_c \left[ \frac{21 |\mathbf{u}_d - \mathbf{u}_c| (\mathbf{u}_d - \mathbf{u}_c)}{20d_b} + \frac{18 \nu_c (\mathbf{u}_d - \mathbf{u}_c)}{d_b^2} + \frac{9 |\mathbf{u}_d - \mathbf{u}_c| (\mathbf{u}_d - \mathbf{u}_c)}{2d_b \left( 1 + \sqrt{Re_0} \right)} \right]
\]

\[
- \frac{9 |\mathbf{u}_d - \mathbf{u}_c| (\mathbf{u}_d - \mathbf{u}_c)}{4d_b \left( 1 + \sqrt{Re_0} \right)^2} + \frac{9u_{d0} (\mathbf{u}_d - \mathbf{u}_c)}{4d_b \left( 1 + \sqrt{Re_0} \right)^2},
\]

(6.13)

where

\[
Re_0 = \frac{d_b u_{d0}}{\nu_c}.
\]

(6.14)

Finally, through vector manipulation, the sum of the lift and rotation forces can be expressed as
\[ F_L + F_{rot} = -C\alpha_d \alpha_c \left( \alpha_c \rho_c + \alpha_d \rho_d \right) \left[ (\nabla u_c + \nabla u_d) - (\nabla u_c + \nabla u_d)^T \right] \cdot (u_c - u_d), \]  

(6.15)

where \( C = C_L = C_{rot} \) and \( 2C = C_L + C_{rot} \).

### 6.3.2 Uniform State

We next determine the continuous- and dispersed-phase momentum balances (Eqs. 6.3 and 6.4) in the uniform state. In the uniform state for gas-liquid flows, \( \alpha_d = \alpha_{d0} \), \( u_c = 0 \), and \( u_d = u_{d0} \mathbf{i} \), where \( \alpha_{d0} \) and \( u_{d0} \) are constants and \( \mathbf{i} \) is the unit vector in the upward vertical direction (Jackson, 2000). Substituting these values into Eqs. 6.3 and 6.4 (including the closures discussed previously) yields the following expressions for the continuous- and dispersed-phase momentum balances, respectively:

\[ 0 = -\nabla p_0 - \frac{F_{d0}}{1 - \alpha_{d0}} + \rho_c \mathbf{g} \]  

(6.16)

and

\[ 0 = \frac{F_{d0}}{1 - \alpha_{d0}} + \alpha_{d0} \left( \rho_d - \rho_c \right) \mathbf{g}, \]  

(6.17)

where

\[ F_{d0} = -\alpha_{d0} \left( 1 - \alpha_{d0} \right) \rho_c \beta_0 u_{d0} \mathbf{i}, \]  

(6.17a)

with

\[ \beta_0 = \frac{u_{d0}}{d_b} \left[ \frac{21}{20} + \frac{18}{20 \, \text{Re}_0} + \frac{9}{2 \left( 1 + \sqrt{\text{Re}_0} \right)} \right]. \]  

(6.17b)

For a given value of the uniform-flow holdup \( \alpha_{d0} \), it can be seen that Eq. 6.16 determines the uniform-flow pressure drop \( \nabla p_0 \):

\[ \nabla p_0 = \rho_c \mathbf{g} + \alpha_{d0} \rho_c \beta_0 u_{d0} \mathbf{i} \]  

(6.18)

and Eq. 6.17 determines the uniform rise velocity \( u_{d0} \):

\[ -\left( \frac{\rho_d - \rho_c}{\rho_c} \right) \mathbf{g} = \beta_0 u_{d0}. \]  

(6.19)

Note that Eq. 6.19 can be used to eliminate \( u_{d0} \) in Eq. 6.18 so that the uniform-flow pressure drop depends only on the volume-averaged fluid density as expected.
6.3.3 Perturbations to the Uniform State

The uniform state is perturbed using \( \alpha_d = \alpha_{d0} + \alpha_{d1} \), \( p = p_0 + p_1 \), \( u_d = u_{d0} \hat{i} + u_{d1} \), and \( u_c = u_{c0} + u_{c1} \), where \( \alpha_{d0}, p_0, \) and \( u_{d0} \) are constants, \( u_{c0} = 0 \), and \( \hat{i} \) is the unit vector in the upward vertical direction (Jackson, 2000). Additional details for the linearization are in Appendix B. Note that a perturbation value (denoted with a subscript 1) multiplied with another perturbation value is set equal to zero. Perturbing the continuous- and dispersed-phase continuity equations (Eqs. 6.9 and 6.10) yields, respectively:

\[
-\frac{\partial \alpha_{d1}}{\partial t} + (1 - \alpha_{d0}) \nabla \cdot \mathbf{u}_c = 0 ,
\]

and

\[
\frac{\partial \alpha_{d1}}{\partial t} + u_{d0} \frac{\partial \alpha_{d1}}{\partial x} + \alpha_{d0} \nabla \cdot \mathbf{u}_{d1} = 0 ,
\]

where \( x \) represents the vertical direction in this analysis.

The continuous- and dispersed-phase momentum balances are perturbed in the same manner. The linearized continuous-phase momentum balance is given as

\[
\rho_c \frac{\partial \mathbf{u}_c}{\partial t} = -\nabla p_i + \left( \mu_{0,c} + C_{BT} \rho_c d_s \alpha_{d0} u_{d0} \right) \left[ \nabla^2 \mathbf{u}_c + \nabla \left( \nabla \cdot \mathbf{u}_c \right) \right] + \alpha_{d1} \rho_c \beta_1 (\mathbf{u}_{d1} - \mathbf{u}_c) + \alpha_{d0} \rho_v C_v \left( \frac{\partial \mathbf{u}_{d1}}{\partial t} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - \frac{\partial \mathbf{u}_c}{\partial t} \right) - \alpha_{d0} \rho_v \left( u_{d0} \frac{\partial \mathbf{u}_c}{\partial x} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - u_{d0} \mathbf{i} \cdot \nabla \mathbf{u}_{c1} - u_{d0} \mathbf{i} \cdot \nabla \mathbf{u}_{d1} \right) + \alpha_{d0} \rho_v C_s \left( u_{d0} \frac{\partial \mathbf{u}_c}{\partial x} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} + u_{d0} \mathbf{i} \cdot \nabla \mathbf{u}_{c1} + u_{d0} \mathbf{i} \cdot \nabla \mathbf{u}_{d1} \right) ,
\]

where

\[
\rho_{v0} = (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d
\]

and

\[
\beta_1 = \frac{u_{d0}}{d_b} \left[ \frac{21}{10} + \frac{18}{\sqrt{Re_0}} + \frac{9}{\left( 1 + \sqrt{Re_0} \right)} - \frac{9 \sqrt{Re_0}}{4 \left( 1 + \sqrt{Re_0} \right)^2} \right] ,
\]

a term that results from the linearized drag term (Eq. 6.13).
The linearized dispersed-phase momentum balance is expressed as

\[
\alpha_d \rho_d \frac{\partial u_{d1}}{\partial t} + \alpha_d \rho_d u_{d0} \frac{\partial u_{d1}}{\partial x} = \alpha_d \rho_c \frac{\partial u_{c1}}{\partial t} - \left( \alpha_d \mu_{0,c} + C_{BT} \rho_c d_\rho \alpha_d^2 u_{d0} \right) \left[ \nabla^2 u_{c1} + \nabla (\nabla \cdot u_{c1}) \right] + \rho_c C_{BP}^2 \left( \frac{\alpha_d^2}{\alpha_{dp}} - 2 \frac{\alpha_d}{\alpha_{dp}} \right) \nabla \alpha_{dp} + \left( \alpha_d \mu_{0,d} + C_{BT} \rho_c d_\rho \alpha_d^2 u_{d0} \right) \left[ \nabla^2 u_{d1} + \nabla (\nabla \cdot u_{d1}) \right] + \alpha_{d1} (\rho_d - \rho_c) g 
\]
come from including the vector components in the third dimension \((k_3)\). Based on symmetry, the equations for the third dimension \((k_3)\) should have the same form as those for the second dimension \((k_2)\).

The algebraic equations resulting from the linearized continuous- and dispersed-phase continuity equations are, respectively:

\[
-s\hat{\alpha}_{d_1} + (1 - \alpha_{d_0}) i k_1 \hat{u}_{c_{1,1}} + (1 - \alpha_{d_0}) i k_2 \hat{u}_{c_{1,2}} = 0,
\]

and

\[
(s + u_{d_0} i k_1) \hat{\alpha}_{d_1} + \alpha_{d_0} i k_1 \hat{u}_{d_{1,1}} + \alpha_{d_0} i k_2 \hat{u}_{d_{1,2}} = 0.
\]

Solving the partial differential equation arising from the linearized continuous-phase momentum balance results in two algebraic equations, corresponding to the two components (vertical and horizontal) of \(u_{c_1}1\):

\[
\hat{u}_{c_{1,1}} \left[ -\rho_c s - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0} \right) (k^2 + k_1^2) - \alpha_{d_0} \rho_c \beta_1 - \alpha_{d_0} \rho_v c_{vm} s + 2 \alpha_{d_0} \rho_v C_s u_{d_0} i k_1 \right]
\]

\[+ \hat{u}_{c_{1,2}} \left[ - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0} \right) k_2 k_1 \right]
\]

\[+ \hat{u}_{d_{1,1}} \left[ \alpha_{d_0} \rho_c \beta_1 + \alpha_{d_0} \rho_v c_{vm} (s + u_{d_0} i k_1) + 2 \alpha_{d_0} \rho_v C_s u_{d_0} i k_1 \right]
\]

\[+ \hat{u}_{d_{1,2}} (0) + \hat{\alpha}_{d_1} (\rho_c \beta_1 u_{d_0}) + \hat{p}_1 (-i k_1) = 0,
\]

and

\[
\hat{u}_{c_{1,1}} \left[ - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0} \right) k_1 k_2 + \alpha_{d_0} \rho_v \left( C + C_s \right) u_{d_0} i k_2 \right]
\]

\[+ \hat{u}_{c_{1,2}} \left[ - \rho_c s - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0} \right) (k^2 + k_2^2) \right]
\]

\[\quad - \alpha_{d_0} \rho_c \beta_1 - \alpha_{d_0} \rho_v c_{vm} s + \alpha_{d_0} \rho_v \left( C_s - C \right) u_{d_0} i k_1 \]

\[+ \hat{u}_{d_{1,1}} \left[ \alpha_{d_0} \rho_v \left( C + C_s \right) u_{d_0} i k_2 \right]
\]

\[+ \hat{u}_{d_{1,2}} \left[ \alpha_{d_0} \rho_c \beta_1 + \alpha_{d_0} \rho_v c_{vm} s + \alpha_{d_0} \rho_v \left( c_{vm} - C + C_s \right) u_{d_0} i k_1 \right]
\]

\[+ \hat{\alpha}_{d_1} (0) + \hat{p}_1 (-i k_2) = 0.
\]

Solving the partial differential equation arising from the linearized dispersed-phase momentum balance results in two algebraic equations, corresponding to the two components of \(u_{d_1}\):
\[ \hat{u}_{c_{11}} \left\{ \alpha_{d_0} \rho_c s + \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) \left( k_1^2 + k_2^2 \right) + \alpha_{d_0} \rho_c \beta_1 + \alpha_{d_0} \rho_v \alpha_{vm} s \right\} \\
- \alpha_{d_0} \rho_v 2 C_S u_{d_0} i k_1 + \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0}^2 / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i k_1 \right] \\
+ \hat{u}_{c_{12}} \left[ \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) k_2 k_1 \right] \\
+ \hat{u}_{d_{11}} \left\{ - \alpha_{d_0} \rho_c s - \alpha_{d_0} \rho_v u_{d_0} i k_1 - \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0}^2 / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i k_1 \\
- \left( \alpha_{d_0} \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) \left( k_1^2 + k_2^2 \right) - \alpha_{d_0} \rho_c \beta_1 \right\} \\
- \alpha_{d_0} \rho_v C_{vm} s - \alpha_{d_0} \rho_v \left( C_{vm} + 2 C_S \right) u_{d_0} i k_1 \right] \\
+ \hat{u}_{d_{12}} \left[ - \left( \alpha_{d_0} \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) k_2 k_1 \right] \\
+ \hat{\alpha}_{d_{1}} \left[ - \rho_c C_{BP} u_{d_0}^2 \left( \frac{2 \alpha_{d_0}}{\alpha_{d_0}} - \frac{3 \alpha_{d_0}^2}{\alpha_{d_0}^2} \right) i k_1 - \left( \rho_d - \rho_c \right) g - \rho_c \beta_0 u_{d_0} \right] + \hat{p}_1 (0) = 0, \tag{6.29} \]

and

\[ \hat{u}_{c_{11}} \left[ \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) k_1 k_2 - \alpha_{d_0} \rho_v \left( C + C_S \right) u_{d_0} i k_2 \right] \\
+ \hat{u}_{c_{12}} \left\{ \alpha_{d_0} \rho_c s + \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) \left( k_2^2 + k_1^2 \right) \right\} \\
+ \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0}^2 / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i k_1 \\
+ \alpha_{d_0} \rho_c \beta_1 + \alpha_{d_0} \rho_v \alpha_{vm} s + \alpha_{d_0} \rho_v \left( C - C_S \right) u_{d_0} i k_1 \right] \\
+ \hat{u}_{d_{11}} \left[ - \left( \alpha_{d_0} \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) k_1 k_2 - \alpha_{d_0} \rho_v \left( C + C_S \right) u_{d_0} i k_2 \right] \\
+ \hat{u}_{d_{12}} \left\{ - \alpha_{d_0} \rho_d s - \alpha_{d_0} \rho_d u_{d_0} i k_1 - \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0}^2 / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i k_1 \\
- \left( \alpha_{d_0} \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0}^2 u_{d_0} \right) \left( k_2^2 + k_1^2 \right) - \alpha_{d_0} \rho_c \beta_1 \right\} \\
- \alpha_{d_0} \rho_v C_{vm} s + \alpha_{d_0} \rho_v \left( C - C_{vm} - C_S \right) u_{d_0} i k_1 \right] \\
+ \hat{\alpha}_{d_{1}} \left[ - \rho_c C_{BP} u_{d_0}^2 \left( \frac{2 \alpha_{d_0}}{\alpha_{d_0}} - \frac{3 \alpha_{d_0}^2}{\alpha_{d_0}^2} \right) i k_2 \right] + \hat{p}_1 (0) = 0. \tag{6.30} \]
The following sequence is used to reduce the system of six algebraic equations to one equation in terms of $\hat{\alpha}_{d1}$ that is a function of $s$, $k_1$, $k_2$, and the two-fluid model parameters. (The 3D case would follow a reduction sequence similar to that of the 2D case discussed below.) Further details are given in Appendix C.

1. Eq. 6.25 is solved for $\hat{u}_{c1,1}$ in terms of $\hat{\alpha}_{d1}$ and $\hat{u}_{c1,2}$.

2. Eq. 6.26 is solved for $\hat{u}_{d1,1}$ in terms of $\hat{\alpha}_{d1}$ and $\hat{u}_{d1,2}$.

3. The results of steps 1 and 2 replace $\hat{u}_{c1,1}$ and $\hat{u}_{d1,1}$ in Eqs. 6.27-6.30, and then terms are collected according to the remaining four unknowns ($\hat{\alpha}_{d1}$, $\hat{u}_{c1,2}$, $\hat{u}_{d1,2}$, and $\hat{p}_1$).

4. After step 3 is applied to Eq. 6.27, the resulting expression is solved for $\hat{p}_1$ in terms of $\hat{u}_{c1,2}$, $\hat{u}_{d1,2}$, and $\hat{\alpha}_{d1}$.

5. After step 3 is applied to Eq. 6.28, the expression for $\hat{p}_1$ derived in step 4 is then substituted into Eq. 6.28, yielding an expression that depends on $\hat{u}_{c1,2}$, $\hat{u}_{d1,2}$, and $\hat{\alpha}_{d1}$.

6. The expression derived in step 5 is solved for $\hat{u}_{c1,2}$ in terms of $\hat{u}_{d1,2}$ and $\hat{\alpha}_{d1}$.

7. After step 3 is applied to Eqs. 6.29 and 6.30, the expression for $\hat{u}_{c1,2}$ derived in step 6 is then substituted into Eqs. 6.29 and 6.30, yielding expressions that depend only on $\hat{u}_{d1,2}$ and $\hat{\alpha}_{d1}$.

8. There are now two equations and two unknowns ($\hat{u}_{d1,2}$ and $\hat{\alpha}_{d1}$). One equation is solved to find $\hat{u}_{d1,2}$ in terms of $\hat{\alpha}_{d1}$, and the result is substituted into the second equation.

9. $\hat{\alpha}_{d1}$ is factored out of the final expression.

The above sequence ultimately yields

$$Z (AB + \gamma \Psi) + \Omega (\Phi B - \gamma \Xi) - \Gamma (\Phi \Psi + \Lambda \Xi) = 0,$$

where

(6.31)
\[ A(s,k) = A_1 s + A_0, \quad (6.31a) \]
\[ \Psi(s,k) = \Psi_1 s + \Psi_0, \quad (6.31b) \]
\[ \Omega(s,k) = \Omega_2 s^2 + \Omega_1 s + \Omega_0, \quad (6.31c) \]
\[ \Phi(s,k) = \Phi_1 s + \Phi_0, \quad (6.31d) \]
\[ \Xi(s,k) = \Xi_1 s + \Xi_0, \quad (6.31e) \]
\[ Z(s,k) = Z_2 s^2 + Z_1 s + Z_0, \quad (6.31f) \]
\[ \gamma(s,k) = \gamma_1 s + \gamma_0, \quad (6.31g) \]
\[ B(s,k) = B_1 s + B_0, \quad (6.31h) \]
\[ Y(s,k) = Y_1 s + Y_0. \quad (6.31i) \]

All coefficients are defined in Table 6.1.

It may be noted that Eqs. 6.25-6.30 can also be expressed in the form
\[ C(s,k) \mathbf{x} = \mathbf{0}, \]
where
\[ \mathbf{x} = \begin{bmatrix} \hat{u}_{c1,1} \\ \hat{u}_{c1,2} \\ \hat{u}_{d1,1} \\ \hat{u}_{d1,2} \\ \hat{\alpha}_{d1} \\ \hat{p}_1 \end{bmatrix}. \quad (6.32) \]

The matrix \( C(s,k) \) represents the coefficients depending on the two-fluid model parameters. As noted previously, \( \hat{\alpha}_{d1}, \hat{p}_1 \), and the horizontal and vertical components of \( \hat{u}_{c1} \) and \( \hat{u}_{d1} \) are the unknowns. A characteristic polynomial in \( s \) is found by setting the determinant of \( C(s,k) \) equal to zero.
Table 6.1. Coefficients of characteristic polynomial.

<table>
<thead>
<tr>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_0 = (k_1^2 + k_2^2) \left[ i k_c \alpha_{d0} \rho_{v0} (C - C_S) u_{d0} + \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right) (k_1^2 + k_2^2) + \alpha_{d0} \rho_c \beta_1 \right]$</td>
</tr>
<tr>
<td>$A_1 = (k_1^2 + k_2^2) \left( \rho_c + \alpha_{d0} \rho_{v0} C_{vm} \right)$</td>
</tr>
<tr>
<td>$\Psi_0 = (k_1^2 + k_2^2) \left[ \alpha_{d0} \rho_c \beta_1 + k_1 \alpha_{d0} \rho_{v0} (C_{vm} + C_S - C) u_{d0} i \right]$</td>
</tr>
<tr>
<td>$\Psi_1 = (k_1^2 + k_2^2) \alpha_{d0} \rho_{v0} C_{vm}$</td>
</tr>
<tr>
<td>$\Omega_0 = \left[ k_i u_{d0} \rho_{v0} (C_{vm} + C_S - C) i - \rho_c (\beta_0 - \beta_1) \right] u_{d0} k_i k_2$</td>
</tr>
<tr>
<td>$\Omega_1 = \alpha_{d0} \rho_{v0} \left( C - C_S \right) u_{d0} k_i - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right) (k_1^2 + k_2^2) i$</td>
</tr>
<tr>
<td>$\Omega_2 = \left[ i k_2 (- \rho_c - \rho_{v0} C_{vm}) \right] / (1 - \alpha_{d0})$</td>
</tr>
<tr>
<td>$\Phi_0 = k_2 \alpha_{d0} \left{ - \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right) (k_1^2 + k_2^2) - \rho_c \beta_1 \right}$</td>
</tr>
<tr>
<td>$\Phi_1 = (- \rho_c - \rho_{v0} C_{vm}) k_2 \alpha_{d0}$</td>
</tr>
<tr>
<td>$\Xi_0 = k_0 \alpha_{d0} \left{ i k_i \rho_c C_{BP} 2 u_{d0} \left( \alpha_{d0} / \alpha_{dcp} \right) \left[ 1 - \left( \alpha_{d0} / \alpha_{dcp} \right) \right] + i k_i \rho_{v0} 2 C_{S} u_{d0} \right}$</td>
</tr>
<tr>
<td>$\Xi_1 = (\rho_d + \rho_{v0} C_{vm}) k_2 \alpha_{d0}$</td>
</tr>
<tr>
<td>$Z_0 = k \left[ - \rho_c C_{BP} u_{d0}^2 \left( \frac{2 \alpha_{d0}}{\alpha_{dcp}} - \frac{3 \alpha_{d0}^2}{\alpha_{dcp}^2} \right) \right] i k_i - \rho_d - \rho_c - \rho_{v0} \left( \beta_0 - \beta_1 \right)$</td>
</tr>
<tr>
<td>$Z_1 = - \alpha_{d0} \left( \frac{\mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0}}{1 - \alpha_{d0}} \right) \left( \frac{2 k_1^2 + k_2^2}{1 - \alpha_{d0}} \right) + k_i \rho_c C_{BP} 2 u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \right] \left[ \rho_c \beta_1 \right]$</td>
</tr>
<tr>
<td>$Z_2 = \left( \frac{\alpha_{d0}}{1 - \alpha_{d0}} - \frac{\rho_{v0} C_{vm}}{1 - \alpha_{d0}} - \rho_d \right)$</td>
</tr>
</tbody>
</table>
Table 6.1. Coefficients of characteristic polynomial (continued).

\[
\gamma_0 = \alpha_{d_0} \left[ k_1 \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) (k_1^2 + k_2^2) + \rho_c \rho_v \left( C + C_S \right) u_{d_0} i k_2^2 + k_1 \rho_c \beta_1 
+ \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0} \alpha_{d_p} \right) \left[ 1 - \left( \alpha_{d_0} \alpha_{d_p} \right) \right] i k_1^2 + \rho_v \left( C - C_S \right) u_{d_0} i k_1^2 \right]
\]

\[
\gamma_1 = \left( \rho_c + \rho_v C_{vm} \right) k_i \alpha_{d_0}
\]

\[
B_0 = \alpha_{d_0} \left[ -\rho_d u_{d_0} i k_1^2 - \rho_c C_{BP} 2 u_{d_0} \left( \alpha_{d_0} \alpha_{d_p} \right) \left[ 1 - \left( \alpha_{d_0} \alpha_{d_p} \right) \right] i k_1^2 
- k_1 \left( k_1^2 + k_2^2 \right) \left( \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) - k_1 \rho_c \beta_1 
+ \rho_v \left( C - C_{vm} - C_S \right) u_{d_0} i k_1^2 + \rho_v \left( C + C_S \right) u_{d_0} i k_1^2 \right]
\]

\[
B_1 = \left( -\rho_d - \rho_v C_{vm} \right) k_i \alpha_{d_0}
\]

\[
\gamma_0 = u_{d_0} k_1 k_2 \left[ \left( \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) k_i + u_{d_0} \rho_v \left( C + C_S \right) - \rho_c C_{BP} u_{d_0} \left( 2 \alpha_{d_0} \alpha_{d_p} - 3 \alpha_{d_0} \alpha_{d_p} \right) i \right]
\]

\[
\gamma_1 = k_2 \left[ \frac{\rho_v \left( C + C_S \right) u_{d_0} \left( 1 - 2 \alpha_{d_0} \right)}{1 - \alpha_{d_0}} - \left( \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) i k_i 
- \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) i k_i \right]
\]

6.3.5 Dispersion Relations

The dispersion relations allow one to examine the behavior of a small-amplitude disturbance wave having a specified wave vector \( k \) (Jackson, 2000), for which \( |k| = k = \sqrt{k_1^2 + k_2^2 + k_3^2} \). In this study, the growth rate \( \lambda(k) \) and the velocity of propagation \( v(k) \) are found from the roots of the characteristic polynomial in \( s \). We have opted to look at particular cases of (i) vertical modes, where \( k_2 = 0 \) (and \( k_3 = 0 \) if 3D), and (ii) horizontal modes, where \( k_1 = 0 \).

For Case (i) when \( k_2 = 0 \) (and \( k_3 = 0 \) if 3D), \( \Omega(s, k) = \gamma(s, k) = 0 \), leaving \( Z(AB + \gamma \Psi) = 0 \). This characteristic polynomial can be factored as

\[
(a_s^2 + b_s s + c_s) (a_s^2 + b_s s + c_s) = 0,
\]

where the coefficients are defined in Table 6.2.
Table 6.2. Coefficients of characteristic polynomial for Case (i), Eq. 6.33.

<table>
<thead>
<tr>
<th>Term</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>$\alpha_{d_0} (\rho_c - \rho_d) + \rho_{v_0} C_{v_m} + \rho_d$</td>
</tr>
<tr>
<td>$b_1$</td>
<td>$\alpha_{d_0} (\mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0}) + (\mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0}) 2k_1^2 + (1 - \alpha_{d_0}) \rho_{v_0} C_{v_m} u_{d_0} + 2ik_1 \rho_{v_0} C_{v_m} u_{d_0}$</td>
</tr>
<tr>
<td>$c_1$</td>
<td>$k_1 (1 - \alpha_{d_0}) u_{d_0} (\mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0}) 2ik_1^2 - u_{d_0} \rho_{v_0} (C_{v_m} + 2\alpha_c) k_1 - u_{d_0} \rho_d k_1$</td>
</tr>
<tr>
<td>$a_2$</td>
<td>$\rho_c (\rho_d + \rho_{v_0} C_{v_m}) - \alpha_{d_0} \rho_{v_0} C_{v_m} (\rho_c - \rho_d)$</td>
</tr>
<tr>
<td>$b_2$</td>
<td>$\rho_c \mu_{0,c} k_1^2 + \alpha_{d_0} C_{BT} \rho_c d_b \alpha_{d_0} d_d u_{d_0} k_1^2 + \mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d_0} u_{d_0} k_1^2 + (1 - \alpha_{d_0}) \rho_{v_0} C_{v_m} \mu_{0,c} k_1^2 + \rho_d \mu_{0,c} k_1^2 + \alpha_{d_0} \rho_{v_0} C_{v_m} u_{d_0} k_1^2 + \alpha_{d_0} \rho_c \rho_d \beta_i + (1 - \alpha_{d_0}) \rho_c \beta_i$</td>
</tr>
<tr>
<td>$c_2$</td>
<td>$k_1^2 \left[ - \alpha_{d_0} \rho_{v_0} (C - C_S) \rho_d u_{d_0}^2 + k_1^2 \mu_{0,c} (C - C_S) \rho_d u_{d_0}^2 + k_1^2 C_{BT} \rho_c d_b \alpha_{d_0} d_d u_{d_0} \mu_{0,d} k_1^2 \right]$</td>
</tr>
</tbody>
</table>

Note that the pairs of roots from $(a_1 s^2 + b_1 s + c_1) = 0$ and $(a_2 s^2 + b_2 s + c_2) = 0$ take the form:

\[
s = \frac{-(p + iq) \pm \sqrt{(p + iq)^2 - 4(P + iQ)}}{2}
\]

which is equivalent to the form used by Jackson (2000):
\[ s = \frac{-(p + iq) \pm \sqrt{(p^2 - q^2 - 4P) + (2pq - 4Q)i}}{2}. \]  

(6.35)

For the first pair, \((b_i/a_i) = p + iq\) and \((c_i/a_i) = P + iQ\), and for the second pair, \((b_2/a_2) = p + iq\) and \((c_2/a_2) = P + iQ\).

The dispersion relation \(\lambda(k_1)\) arises from the real part of \(s\) (Jackson, 2000):

\[ \lambda = \text{Re}(s) = \frac{1}{2} \left\{ \sqrt{\left(\frac{p^2 - q^2 - 4P}{2}\right)^2 + \left(\frac{2pq - 4Q}{2}\right)} - p \right\}. \]

(6.36)

If \(\lambda(k_1)\) decreases from zero with increasing wavenumber \(k_1\), then the solution is linearly stable. Otherwise, if there are values of \(k_1\) for which \(\lambda\) is positive, then the solution is linearly unstable for those wavenumbers. The dispersion relation \(\nu(k_1)\) arises from the imaginary part of \(s\):

\[ \nu = -\text{Im}(s) \]

\[ = -\frac{1}{2k_1} \left\{ \text{sgn}(2pq - 4Q) \left[ \sqrt{\left(\frac{p^2 - q^2 - 4P}{2}\right)^2 + \left(\frac{2pq - 4Q}{2}\right)} - \left(\frac{2pq - 4Q}{2}\right) \right] - q \right\}. \]

(6.37)

For Case (ii) (horizontal modes), the characteristic polynomial (Eq. 6.31) can be expressed as

\[ a_4s^4 + a_3s^3 + a_2s^2 + a_1s + a_0 = 0, \]

(6.38)

where all coefficients are real-valued and defined as

\[ a_0 = Z_0 (A_0 B_0 + \gamma_0 \Psi_0) + \Omega_0 (\Phi_0 B_0 - \gamma_0 \Xi_0) - (\Phi_0 \Psi_0 + A_0 \Xi_0) Y_0, \]

(6.38a)

\[ a_1 = Z_0 (A_0 B_1 + A_1 B_0 + \gamma_0 \Psi_1 + \gamma_1 \Psi_0) + Z_1 (A_0 B_0 + \gamma_0 \Psi_0) + \Omega_0 (\Phi_0 B_0 - \gamma_0 \Xi_0) + \Omega_1 (\Phi_0 B_0 - \gamma_0 \Xi_0) \]

\[ + \Omega_0 (\Phi_0 B_1 + \Phi_1 B_0 - \gamma_0 \Xi_1 - \gamma_1 \Xi_0) + \Omega_1 (\Phi_0 B_0 - \gamma_0 \Xi_0) \]

\[ - (\Phi_0 \Psi_0 + A_0 \Xi_0) Y_1 - (\Phi_0 \Psi_1 + \Phi_1 \Psi_0 + A_0 \Xi_1 + A_1 \Xi_0) Y_0, \]

(6.38b)
The coefficients $a_0 - a_4$ are defined in terms of the coefficients of the characteristic polynomial (Eq. 6.31). It should be noted that $k_1$ is a factor of Eq. 6.31: when $k_1$ is set equal to zero, the left-hand side of Eq. 6.31 is equal to zero. Therefore, to determine the coefficients for Eq. 6.38, we first divide the characteristic polynomial by $k_1$ and then take the limit as $k_1$ approaches zero. This results in real-valued expressions for $a_0 - a_4$ for the horizontal case. Note that the roots of Eq. 6.38 are highly complicated expressions, and thus their behavior is best studied numerically. They are further discussed in Section 6.4.

6.4 Results and Discussion of Linear Stability Analysis

The following discussion shows how the behavior of a small-amplitude disturbance depends on the wavenumber and direction (i.e., $k_1$, $k_2$, or $k_3$) and on the two-fluid model formulation, including bubble pressure, effective viscosity, force-model coefficients, and gas volume fraction $\alpha_{\infty_0}$. In this study, we focus on bubbles approximately 4 mm in diameter $d_b$, the same size as those observed experimentally by Hartevel (2005). This corresponds to $Re_0 \approx 700$ and $u_{\infty_0} \approx 17.68$ cm/s. We then examine how changing $\alpha_{\infty_0}$ affects the linear stability.

Both 2D and 3D geometries are investigated. However, the majority of the results presented are for 2D geometries and organized into cases of (i) vertical modes, where $k_2 = 0$ (and $k_3 = 0$), and (ii) horizontal modes, where $k_1 = 0$. The wavelengths $l_1$, $l_2$, and $l_3$ and the wavenumbers $k_1$, $k_2$, and $k_3$ can be related by (Jackson, 2000)

$$k_1 = 2\pi/l_1, k_2 = 2\pi/l_2, k_3 = 2\pi/l_3.$$  (6.39a)
The majority of the simulations discussed in Chapters 4 and 5 utilized a 0.25 cm grid resolution. Thus, the largest wavenumbers that are typically resolved on the computational grid are given by

\[ k_{1,\text{max}}, k_{2,\text{max}}, k_{3,\text{max}} = \left( \frac{2\pi}{0.25} \right) \approx 25. \]  

Note that \( k_1, k_2, k_3, \lambda(k_1), \lambda(k_2), \) and \( \lambda(k_3) \) can be made dimensionless by scaling with the characteristic length \( d_b \) and the characteristic time \( d_b / u_{d0} \).

In order to illustrate the changes observed in linear stability, transitions from uniform to non-uniform flow are simulated. This is accomplished by using running-average and plane-average routines in the CFDLib code. The plane-average routine determines the average value of a variable \( X \) on each horizontal plane \( j \), and then sets all values of \( X \) at each calculation node on plane \( j \) equal to the average value of \( X \) determined for plane \( j \). In other words, \( X = \langle X \rangle_j \). This creates rising plane waves, making the flow one-dimensional in the vertical direction. The running-average is defined in terms of plane-averages by the following expression:

\[ \bar{X}_j = \frac{1}{j} \left[ (j-1) \bar{X}_{j-1} + \langle X \rangle_j \right]. \]  

To capture transitions from uniform to non-uniform flow, the simulations are initialized at the uniform state conditions, as described by Eqs. 6.16 and 6.17. Then, the running-average routine is carried out for the interval \( 0 \leq t < T_1 \), where \( T_1 \) is the time necessary for the simulation to reach a uniform state. In other words, a uniform state is reached through averaging. Simulation startup tends to introduce non-uniformities. Thus, if the initial conditions applied correspond to the uniform state, then presumably a shorter time interval would be necessary for the simulation to reach that uniform state, in which the flow is zero-dimensional and stationary. The value of \( T_1 \) is chosen such that all disturbances arising from the simulation startup have been completely damped out. In order to examine transient one-dimensional flow, the plane-average routine may be carried out for the interval \( T_1 \leq t < T_2 \). This routine induces instabilities in the form of plane waves. Neither the plane-average routine nor the running-average routine is applied to examine 2D (or 3D) transient flow, for which random non-uniformities are
observed. 2D (or 3D) flow may be examined for the interval $T_2 \leq t$, after the plane-
average routine has completed, or for the interval $T_1 \leq t$, after the running-average routine
has completed.

The results of the linear stability analysis are presented as follows. First, we
examine the effect of force models (with parameter values consistent with the simulations
in Chapters 4 and 5) on the linear stability of both the vertical and horizontal modes.
Next, we examine the stabilizing effect of the bubble-pressure model for the vertical
modes. Finally, we look at the effect of modes on flow dynamics. There are two types of
vertical modes arising from the two pairs of roots for the characteristic equation of the
linearized model (Eq. 6.33). When one type or the other is kept stable, distinctly
different flow dynamics are observed. We explore the implications of this difference on
the transition from homogeneous to heterogeneous flow.

6.4.1 Effect of Force Models

As noted in the discussion of the dispersion relations for vertical modes, there are
two pairs of roots (Eq. 6.33) to consider for Case (i). The pair obtained from
$a_1 s^2 + b_1 s + c_1 = 0$ corresponds to the definitions obtained via Jackson’s (2000) method,
and thus will be referred to as the Jackson modes. Note that the lift and rotation
parameters $C_L$ and $C_{rot}$ do not appear in this root pair. The second pair obtained from
$a_2 s^2 + b_2 s + c_2 = 0$ will be referred to as the secondary modes in this study. Note that the
Jackson modes can be found with only a one-dimensional model while the secondary
modes require a two-dimensional model.

As noted in the discussion of the dispersion relations for horizontal modes, there
are four roots (Eq. 6.38) to consider for the characteristic polynomial for Case (ii). Recall
that the coefficients $a_0 - a_4$ in Eq. 6.38 are all real; therefore, the four roots should be
either real or complex conjugate pairs. Thus, we conclude that the propagation velocity
of the horizontal modes is zero.

The behavior of the real parts of the four roots in Case (ii) determines whether or
not the solution is linearly stable. The real parts of two of these roots were negative for
all values of $k_2$, indicating stability. Thus, these two roots will not be discussed further.
The third and fourth roots formed a complex conjugate pair for small \( k_2 \), and the behavior varied depending on the model formulation:

1. The real parts of both the third and fourth roots are equal to zero when \( k_2 \) is zero, and then decrease with increasing \( k_2 \) up to a particular value of \( k_2 \) where the imaginary part is zero, after which both roots are real-valued.

2. The real part of the third root is zero when \( k_2 \) is zero, and then decreases with increasing \( k_2 \), while the fourth root is zero for all values of \( k_2 \), indicating marginal stability.

3. The real parts of both the third and fourth roots are zero when \( k_2 \) is equal to zero, and then decrease with increasing \( k_2 \).

Since the behavior of the most positive real part of a root is the most important when comparing the model formulations, only this root is illustrated in detail. It may be noted that there are three model formulations for which \( \lambda \) is equal to zero for all values of \( k_2 \):

- Drag and added-mass forces enabled, with BIT and bubble pressure disabled (\( C_{vm} = 0.5, C_L = 0, C_{rot} = 0, C_S = 0, C_{BT} = 0, C_{BP} = 0 \)).
- Drag and added-mass forces enabled, BIT included, bubble pressure disabled (\( C_{vm} = 0.5, C_L = 0, C_{rot} = 0, C_S = 0, C_{BT} = 0.6, C_{BP} = 0 \)).
- Drag force and BIT enabled, with bubble pressure disabled (\( C_{vm} = 0, C_L = 0, C_{rot} = 0, C_S = 0, C_{BT} = 0.6, C_{BP} = 0 \)).

Thus, in general, a positive bubble-pressure coefficient is required to ensure that the horizontal modes are linearly stable.

It may be noted that the effect of the lift and rotation terms is additive, with the lift term as the contribution from the continuous phase and the rotation term as the contribution from the dispersed phase. (Similarly, the strain term includes contributions from both the continuous and dispersed phases.) Thus, if \( C_L \) is large enough, the behavior observed when \( C_{rot} = 0 \) would be qualitatively similar to the behavior observed when including both the lift and rotation forces. Note that in CFDLib, the lift and rotation forces are calculated as one summed term. Thus, in order to compare the simulations with the linear stability analysis, both \( C_L \) and \( C_{rot} \) are set equal to the parameter \( C \) in the following discussion, where \( 2C = C_L + C_{rot} \).
The numerical studies in Chapters 4 and 5 focused on several model formulations, including all forces enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$ and $C_S = 0.125$, a baseline homogeneous model that applies all force terms; and only the drag force enabled, a “minimal” model applied since the drag force cannot be neglected. Both model formulations used $C_{BP} = 0.2$. We wish to compare these model formulations with two other examples. The first is a “standard” model in which the drag, added-mass, and lift forces are included, but the strain term is not included ($C_S = 0$). The second is a model in which the lift parameter $C_L = C$ takes a negative value as done in the work of Lucas et al. (2005, 2006). Thus, the model formulations compared are

(i) Baseline model including all force terms: $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$, $C_S = 0.125$, $C_{BT} = 0.6$, $C_{BP} = 0.2$.

(ii) Baseline model with strain term disabled: $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 0.2$.

(iii) Drag force only, bubble-pressure model disabled: $C_{vm} = 0$, $C_L = C_{rot} = C = 0$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 0$.

(iv) Drag force only, bubble-pressure model enabled: $C_{vm} = 0$, $C_L = C_{rot} = C = 0$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 0.2$.

(v) Baseline model with negative lift: $C_{vm} = 0.5$, $C_L = C_{rot} = C = -0.375$, $C_S = 0.125$, $C_{BT} = 0.6$, $C_{BP} = 0.2$.

For the model formulations discussed above, Fig. 6.1 shows the dependence of vertical disturbance growth rate on wavenumber $k_1$ for the Jackson modes (upper plots) and horizontal disturbance growth rate on wavenumber $k_2$ (lower plots) for both $\alpha_{d0} = 0.1$ and $\alpha_{d0} = 0.6$. The increase in $\alpha_{d0}$ simply lowers the decay rate by a factor of about 6. Since $C_L$ and $C_{rot}$ (and therefore $C$) do not appear in the Jackson modes, the negative lift curve is not shown in the upper plots in Fig. 6.1. Note that for these model formulations, the secondary modes for the vertical case are stable. Model parameter combinations for which the secondary modes are unstable are discussed in later sections of this chapter.

We first discuss the linear stability for the vertical modes. It can be seen in Fig. 6.1 that the model formulation in which only the drag force is enabled yields lower values
of vertical disturbance growth rate than the baseline model formulation, either with or without the strain term included. In Fig. 6.1, it also can be seen that when only the drag force is enabled but the bubble-pressure model is disabled, the resulting values of $\lambda$ are larger than when both the drag force and the bubble-pressure model are enabled. However, the effect of the bubble-pressure model is lessened for $\alpha_{d0} = 0.6$, in that the values of $\lambda$ when the bubble-pressure model is disabled are only slightly larger than the values of $\lambda$ resulting when the bubble-pressure model is enabled. This would be consistent with the observed turbulent flow for higher $\alpha_{d0}$. Finally, it may be noted that for the model formulations presented in Fig. 6.1, the normalized vertical propagation velocity $\nu/u_{d0}$ is approximately equal to $0.9$ for all $k_1$ when $\alpha_{d0} = 0.1$, and $\nu/u_{d0}$ is approximately equal to $0.4$ for all $k_1$ when $\alpha_{d0} = 0.6$. Thus, $\nu/u_{d0}$ as predicted by the Jackson modes is approximately equal to $(1 - \alpha_{d0})$, which decreases as $\alpha_{d0}$ increases.

We next discuss the linear stability for the horizontal modes. It can be seen in Fig. 6.1 that the formulation including the drag force and the bubble-pressure model is more stable than the formulation that includes the drag force but not the bubble-pressure model. For the model formulations applying the bubble-pressure model, $\lambda$ approaches a negative constant value as $k_2$ increases. The model formulation applied in Chapters 4 and 5, in which all forces are enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$, $C_S = 0.125$, $C_{BT} = 0.6$, and $C_{BP} = 0.2$, is the most stable. With negative lift, instability is observed at lower $k_2$ values. This observation is consistent with previous reports (Lucas et al., 2005, 2006).

The curves in Fig. 6.1 corresponding to model formulations including lift ($C = C_L$) and/or strain ($C_S$) are those for which $\lambda$ decreases from zero with increasing $k_2$, reaches a minimum at a particular value of $k_2$, and then increases with increasing $k_2$, eventually approaching a constant value. However, as $\alpha_{d0}$ increases, the value of $k_2$ for which the minimum $\lambda$ is reached decreases, and the minimum value of $\lambda$ becomes less negative, indicating that the horizontal modes are less stable at higher gas holdup. Thus, the stabilizing effect of the bubble-pressure model decreases with increasing $\alpha_{d0}$, which would be consistent with the observed turbulent flow for higher $\alpha_{d0}$. 
The main observation from Fig. 6.1 is that all the formulations presented are unstable. This is consistent with the simulations presented in Chapters 4 and 5 that were not uniform (although sometimes homogeneous) and always time dependent. We can thus conclude that linear stability analysis cannot tell us why some simulations were homogeneous while others were turbulent. It is therefore of interest to determine whether uniform solutions are possible for other choices of the model parameters, and, if they exist, how such solutions can become unstable.
6.4.2 Effect of Bubble-Pressure Model

In the previous section, the model formulations applying the bubble-pressure model were more stable than the model formulations that did not consider bubble pressure, though the stabilizing effect of the bubble-pressure model lessened as holdup increased. While $C_{BP} = 0.2$ could stabilize the horizontal modes, the vertical modes remained unstable. Thus, we next examine the effect of the bubble-pressure model on the linear stability of the vertical modes. The range of gas holdups ($\alpha_{d0}$) considered is up to 0.6. Four different force-model combinations used in Chapters 4 and 5 are considered:

a: All forces enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$ and $C_S = 0.125$; the baseline homogeneous model that includes all force terms.

b: Only drag force enabled; a “minimal” model applied since the drag force cannot be neglected.

c: Drag and added-mass forces enabled; considers the added-mass term that is known to be important in gas-liquid flow.

d: All forces enabled with $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.75$, and $C_S = 0.25$; considered to examine the effect of the lift and strain coefficients on the stability of the vertical flow.

For each of the parameter sets, we examine the effect of the bubble-pressure model for both laminar model formulations ($C_{BT} = 0$) and formulations applying bubble-induced turbulence ($C_{BT} = 0.6$). It may be noted that the minimum value of the bubble-pressure model constant $C_{BP}$ that can stabilize the vertical modes changes depending on both the gas holdup and the other model parameters applied, as discussed below.

When the BIT model is applied ($C_{BT} = 0.6$), the secondary modes are stable for all values of $C_{BP}$ for all of the parameter sets discussed above. However, as shown in Fig. 6.2, there is a minimum value of $C_{BP}$ that results in a linearly stable solution for the Jackson modes. It can be seen in Fig. 6.2 that for all model formulations considered, the minimum value of $C_{BP}$ increases with increasing $\alpha_{d0}$. However, for $\alpha_{d0} \leq 0.4$, this increase is small and gradual. It is only for the highest values of $\alpha_{d0}$ that noticeably larger values of $C_{BP}$ are needed to stabilize the Jackson modes. This trend is consistent
with the findings discussed in Chapter 5, where an increase in inlet gas flow and, in turn, holdup resulted in the homogeneous flow eventually becoming unstable. It is also worth noting that the model formulation including only the drag force is the most stable, while the model formulation including all forces and having the highest value of $C_S$ is the least stable.

![Graph showing minimum value of $C_{BP}$ for different forces](image)

**Figure 6.2.** Minimum value of $C_{BP}$ that results in a linearly stable solution for the vertical component of the Jackson modes with $C_{BT} = 0.6$. Squares: All forces ($C_{vm} = 0.5, C = 0.375, C_S = 0.125$). Circles: Drag force only ($C_{vm} = 0, C = 0, C_S = 0$). Diamonds: Drag and added-mass forces ($C_{vm} = 0.5, C = 0, C_S = 0$). Triangles: All forces ($C_{vm} = 0.5, C = 0.75, C_S = 0.25$).

For laminar model formulations ($C_{BT} = 0$) the behavior of both the Jackson modes and the secondary modes changes. In general, applying the same minimum values of $C_{BP}$ presented in Fig. 6.2 will yield a linearly stable solution for the Jackson modes, but only...
for wavenumbers resolved on our computational grid (i.e., wavenumbers up to $k_1 = 25$ cm$^{-1}$). Additionally, for $\alpha_{d0} = 0.6$, the minimum value of $C_{BP}$ required is even higher for the laminar flow model formulations than for the formulations applying BIT. However, no realistic value of $C_{BP}$ could stabilize the solutions as $k_1$ approached infinity. For the four force-model combinations used in Fig. 6.2, the only laminar flow model formulations that can be stabilized for $k_1 \to \infty$ are when only the drag force is enabled and $\alpha_{d0} \leq 0.1$. We can thus conclude that suppression of bubble-induced turbulence will eventually result in all model formulations becoming unstable.

The behavior of the secondary modes for the laminar flow models shows that the lift parameter $C_L = C$ can affect the vertical flow stability. For these cases:

- **a:** $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.375$, $C_S = 0.125$, $C_{BT} = 0$
- **b:** $C_{vm} = 0$, $C_L = C_{rot} = C = 0$, $C_S = 0$, $C_{BT} = 0$
- **c:** $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0$, $C_S = 0$, $C_{BT} = 0$

the secondary modes are stable when $C_{BP} > 0$ for all $k_1$. However, for the following case:

- **d:** $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.75$, $C_S = 0.25$, $C_{BT} = 0$,

the secondary modes become unstable for lower values of $k_1$ when $C_{BP}$ is applied. It may be noted for parameter set **d** that $2(C - C_S) > C_{vm}$ (or $(C_L + C_{rot} - 2C_S) > C_{vm}$). For parameter sets **a**, **b**, and **c**, $2(C - C_S) \leq C_{vm}$ (or $(C_L + C_{rot} - 2C_S) < C_{vm}$). In general, it was found that when $C_{BT} = 0$, the secondary-mode instability occurs if the coefficients satisfy $2(C - C_S) > C_{vm}$ (or $(C_L + C_{rot} - 2C_S) > C_{vm}$), and $C > C_S$. This would occur if the (positive) lift coefficient were sufficiently large. For example, in the absence of the rotation and strain forces, a secondary-mode instability will occur when the lift coefficient is larger than the virtual-mass coefficient. We will explore the consequences of unstable secondary modes on the flow dynamics next.

### 6.4.3 Effect of Roots on Flow Dynamics

In order to illustrate changes observed in linear stability between the Jackson modes and the secondary modes, we simulated the following four model formulations for $\alpha_{d0} = 0.1$:

- **A:** All modes stable: $C_{vm} = 0$, $C_L = C_{rot} = C = 0$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 1$. 

B: Only secondary modes unstable: $C_{vm} = 1.5$, $C_L = C_{rot} = C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 4$.

C: Only Jackson modes unstable: $C_{vm} = 0.5$, $C_L = C_{rot} = C = 0.25$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 0$.

D: Both Jackson and secondary modes unstable: $C_{vm} = 1.5$, $C_L = C_{rot} = C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 1$.

The model parameters were selected in order to distinguish between the four stability cases discussed above and emphasize the differences in flow dynamics.

Figure 6.3 shows the dependence of vertical disturbance growth rate (top) and the dependence of vertical propagation velocity (bottom) on wavenumber. As discussed previously, $\lambda$ is positive when modes are unstable and negative when modes are stable. When both modes are stable, the secondary modes exhibit higher stability. When both modes are unstable, the instability due to the Jackson modes has a slightly higher growth rate than the instability due to the secondary modes. When $k_1 = 0$, $\nu^*$ is approximately 0.9 for the Jackson modes and zero for the secondary modes. When the modes are both stable or both unstable, $\nu^*$ does not change significantly as $k_1$ increases. When only the secondary modes are unstable, $\nu^*$ for the secondary modes increases slowly with increasing $k_1$. When only the Jackson modes are unstable, $\nu^*$ for the Jackson modes gradually decreases as $k_1$ increases.

Figure 6.4 shows the flow profiles for 2D simulations for each case. When both the Jackson modes and the secondary modes are stable, the flow profile is uniform. This particular example applies only bubble-induced turbulence, bubble pressure, and the drag force. When only the secondary modes are unstable, the corresponding flow profile shows large-scale instabilities, as observed in heterogeneous flows. When only the Jackson modes are unstable, the flow profile exhibits small flow structures similar to those observed for homogeneous flow (Monahan et al., 2005). When both modes are unstable, the flow profile is similar to that observed when only the secondary modes are unstable. This would suggest that nonlinear interactions with the secondary modes and not the Jackson modes are responsible for transition to heterogeneous flow.
Figure 6.3. Dependence of vertical disturbance growth rate $\lambda$ (top) and propagation velocity $\nu^*$ (bottom) on wavenumber $k_1$ for Jackson modes (closed symbols) and secondary modes (open symbols) at $\alpha_0 = 0.1$. Squares: All modes stable ($C_{vm} = 0$, $C = 0$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 1$). Circles: Only secondary modes unstable ($C_{vm} = 1.5$, $C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 4$). Diamonds: Only Jackson modes unstable ($C_{vm} = 0.5$, $C = 0.25$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 0$). Triangles: Jackson and secondary modes unstable ($C_{vm} = 1.5$, $C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 1$).
Figure 6.4. Water volume fraction for $\alpha_{d0} = 0.1$. A: All modes stable ($C_{vm} = 0$, $C = 0$, $C_S = 0$, $C_{BT} = 0.6$, $C_{BP} = 1$). B: Only secondary modes unstable ($C_{vm} = 1.5$, $C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 4$). C: Only Jackson modes unstable ($C_{vm} = 0.5$, $C = 0.25$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 0$). D: Jackson and secondary modes unstable ($C_{vm} = 1.5$, $C = 2$, $C_S = 0$, $C_{BT} = 0$, $C_{BP} = 1$).

6.4.4 A Scenario for Transition to Heterogeneous Flow

The studies presented in Chapter 5 have shown that bubble-column simulations become turbulent if the gas holdup is large enough. As noted earlier, the BIT model proportionality constant $C_{BT}$ should decrease with increasing gas holdup because bubble wakes will be suppressed by the close presence of other bubbles. While no model for $C_{BT}$ currently exists to describe such behavior, the qualitative effect can be examined by lowering the value of $C_{BT}$. Therefore, a possible scenario for the instability observed in the flow profiles at high volume fraction is that $C_{BT}$ decreases with increasing holdup until the secondary modes become unstable (while the Jackson modes remain stable). To test this scenario, simulations were carried out for which the average holdup is
approximately 0.5, with model parameters $C_{vm} = 0.5$, $C_S = 0$, and $C_{BP} = 2$ in order to keep the Jackson modes stable at low values of $C_{BT}$. The lift parameter $C$ is then set to 1 (recall that the Jackson modes do not depend on $C_L = C_{rot} = C$) and $C_{BT}$ is lowered to 0.1, a value for which the secondary modes are unstable, but the Jackson modes are stable.

Figure 6.5 shows the flow profiles when $\alpha_{d0} = 0.5$. It can be seen that when $C_{BT}$ is 0.1, the secondary modes are unstable and the flow profile is turbulent. However, when $C_{BT}$ is set to the standard value of 0.6, both the Jackson and secondary modes are stable and the flow profile is uniform. Thus, suppressing bubble-induced turbulence results in a
transition from uniform to turbulent flow at high holdup, even for a large positive lift coefficient (e.g., $C = 1$). The flow profiles presented in Fig. 6.6 illustrate how the instabilities in the secondary modes start and propagate. A uniform state is simulated until $t = 20$ seconds, after which the flow is perturbed. It can be seen in Fig. 6.6 that the flow becomes unstable within a few seconds. Vertical plumes gradually form within the column, rise, and break apart into smaller structures. As $t$ approaches 100 seconds, fully developed flow structures such as those presented in Fig. 6.5 are observed.

**Figure 6.6.** Water volume fraction for $\alpha_{d0} = 0.5$, with secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} = 0.1$, $C_{BP} = 2$). Profiles illustrate behavior after the flow becomes unstable at $t = 20$ s.

Figure 6.7 is a neutral stability plot that shows how the critical value of $C_{BT}$ depends on average holdup and the lift parameter $C$, with $C_{vm} = 0.5$, $C_S = 0$, and $C_{BP} = 2$. It can be seen in Fig. 6.7 that for all values of $C$, the $C_{BT}$ vs. $\alpha_{d0}$ curve exhibits an
inverted parabolic shape, in which the maximum value of $C_{BT}$ occurs when $\alpha_{d0}$ is between 0.3 and 0.4. It may be noted that as $\alpha_{d0}$ increases to 0.6, the Jackson modes become unstable, so the stabilizing effect of $C_{BT}$ on the secondary modes may no longer prevent the flow from becoming turbulent. Figure 6.7 also shows that as $C$ increases, the magnitudes of the critical $C_{BT}$ values increase. For a large positive lift coefficient such as $C = 2$, a critical $C_{BT}$ higher than the standard value of 0.6 would be needed to stabilize the secondary modes. These findings are consistent with the observation found previously for laminar flow ($C_{BT} = 0$), where the secondary modes are unstable if the coefficients satisfy $2(C - C_S) > C_{vm}$ and $C > C_S$. Thus, if the lift coefficient is high enough, the secondary modes will be unstable if $C_{BT}$ decreases sufficiently. We have thus identified a mechanism wherein the flow can transition from uniform to turbulent flow at high holdups without invoking negative lift, mean shear, or cooperative/hindered rise.

The coupling that leads to the instability can be described as follows. The stabilizing function of the bubble-pressure model is to drive bubbles from regions of higher $\alpha_d$ to regions of lower $\alpha_d$. For high gas holdup (e.g., $\alpha_{d0} = 0.5$), it is not unreasonable for the bubble-pressure model coefficient $C_{BP}$ to have a large value such as 2 in order to stabilize the flow. Indeed, such a value stabilizes the Jackson modes at $\alpha_{d0} = 0.5$. However, the lift force is driving bubbles from regions of lower $\alpha_d$ to regions of higher $\alpha_d$, which would destabilize the flow. Thus, the effects of the bubble-pressure model and the lift force counteract one another. The BIT model smoothes out the profile since increasing the effective viscosity can dampen flow instabilities, and therefore the BIT model could be said to enhance the stabilizing effect of the bubble-pressure model. When $C_{BT}$ decreases, this decreases the ability of the BIT model to enhance the stabilizing effect of the bubble-pressure model. Thus, if the effect of the lift force becomes greater than the effect of the bubble-pressure model (combined with the BIT model), the flow will become unstable. Similar behavior has been observed by Sankaranarayanan and Sundaresan (2002).
Figure 6.7. Critical value of $C_{BT}$ for the secondary modes with $C_{vm} = 0.5$, $C_{S} = 0$, and $C_{BP} = 2$. Up triangles: $C = 0.375$. Squares: $C = 0.5$. Circles: $C = 1$. Diamonds: $C = 1.5$. Down triangles: $C = 2$. Values of $C_{BT}$ above the critical curves yield stable uniform flow up to the point where the Jackson modes become unstable (see Fig. 6.2). Dashed curves represent the approximate stability criterion in Eq. 6.41.

The instabilities arising from the secondary modes at high holdup and positive lift coefficient are further examined by plotting $\lambda$ versus wavenumber for the secondary modes for $C_{BT}$ values just below the critical value in Fig. 6.8. For $\alpha_{d0} = 0.5$, Table 6.3 shows the critical values of $C_{BT}$ for each $C$ value, and the $C_{BT}$ values (just below the critical value) used to calculate $\lambda$. As in the previous studies, $C_{vm} = 0.5$, $C_{S} = 0$, and $C_{BP} = 2.0$ in order to hold the Jackson modes stable. Figure 6.8 shows $\lambda$ for wavenumbers between 0 and 1. As $C$ increases, an increase in the wavenumber corresponding to the maximum value of $\lambda$ is observed. For $C = 0.5$, maximum $\lambda$ occurs at $k_1 \approx 0.5$. Note that
this critical wavenumber is relatively low (cf. Fig. 6.1) and leads to large-scale flow structures that are easily resolved on our computational grid. For $C = 1$, maximum $\lambda$ occurs at $k_1 \approx 0.6$. For $C = 1.5$ and 2, maximum $\lambda$ occurs at $k_1 \approx 0.65$. Additionally, it should be noted that between wavenumbers 0 and 1, the normalized vertical propagation velocity $\nu/u_{d0}$ increases from zero very slowly as $k_1$ increases.

Table 6.3. Critical $C_{BT}$ values and $C_{BT}$ values used in Fig. 6.8, corresponding to a particular parameter $C = C_L = C_{rot}$.

<table>
<thead>
<tr>
<th>Parameter $C$</th>
<th>$C_{BT}$, critical</th>
<th>$C_{BT}$ in Fig. 6.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.103</td>
<td>0.1</td>
</tr>
<tr>
<td>1.0</td>
<td>0.314</td>
<td>0.3</td>
</tr>
<tr>
<td>1.5</td>
<td>0.525</td>
<td>0.5</td>
</tr>
<tr>
<td>2.0</td>
<td>0.736</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Figure 6.8. Dependence of vertical disturbance growth rate $\lambda$ on wavenumber for $k_1$ between 0 and 1 for the secondary modes at $\alpha_0 = 0.5$, with $C_{vm} = 0.5$, $C_S = 0$, and $C_{BP} = 2$. Squares: $C = 0.5$. Circles: $C = 1$. Diamonds: $C = 1.5$. Down triangles: $C = 2$. 

In order to better understand how the model parameters affect the secondary-mode instability, we have derived an approximate stability condition in the following manner. First we note that the propagation velocity is close to zero at the critical wavenumber. This implies that we can neglect the imaginary parts of the coefficients \( a_2, b_2, \) and \( c_2 \). Next, we consider the case where \( \rho_c \) is much larger than \( \rho_d \) and neglect molecular viscosity relative to the BIT model. In this limit it can easily be shown that \( a_2 \) and \( b_2 \) are always positive; hence, one root will be unstable if and only if \( c_2 \) is negative. Setting \( c_2 \) equal to zero leads to the following expression for the critical value of \( C_{BT} \):

\[
C_{BT,\text{crit}} = \varphi \alpha_{d_0} (1 - \alpha_{d_0}) C_{BP} \left( 2C - 2C_S - C_{vm} \right),
\]

where \( \varphi \) is a constant of order one. This expression is plotted as dashed curves in Fig. 6.7 with \( \varphi \approx 0.725 \) fit to the curve for \( C = 2 \). Note that this approximation is consistent with our previous observation that secondary-mode instabilities are only observed when \( 2(C - C_S) > C_{vm} \). In addition, we can now observe that secondary-mode instabilities also require a nonzero bubble-pressure coefficient. Thus, the secondary-mode instability results from the combined effects of bubble pressure and positive lift, and can be eliminated by setting \( C < C_S + (C_{vm}/2) \). However, in bubble-column flows at high gas holdup we would expect both \( C_{BP} \) and \( C \) to be large enough to produce non-negligible positive values for \( C_{BT,\text{crit}} \). Thus, dampening of BIT due to bubble-bubble interactions and the corresponding decrease in \( C_{BT} \) at high gas holdup should be considered as a plausible scenario for homogeneous-heterogeneous flow transitions in bubble columns.

### 6.4.5 Effect of Wall Boundary Conditions on Flow Behavior

In order to understand the nature of the secondary-mode instability, the eigenvalues and eigenvectors for the unstable vertical modes are determined via the following process. First, a solution with the form of

\[
(u_{c_1}, u_{d_1}, \alpha_{d_1}, p_1) = [u_{c_1}(t), u_{d_1}(t), \alpha_{d_1}(t), p_1(t)] \exp(ik \cdot x)
\]

is substituted into the six linear partial differential equations arising from the linearized continuity equations and momentum balances. Note that this solution differs from the
solution applied previously (Eq. 6.24). This yields a linear system of six algebraic equations that can be expressed in the form of

\[ B(k) \dot{X} = C(k) X, \]  

(6.43)

where

\[ X(t) = \begin{bmatrix} u_{c,11}(t) \\ u_{c,12}(t) \\ u_{d,11}(t) \\ u_{d,12}(t) \\ \alpha_{d1}(t) \\ p_i(t) \end{bmatrix} \]  

(6.44)

and the matrices \( B(k) \) and \( C(k) \) represent the coefficients depending on the two-fluid model parameters. The parameters \( \alpha_{d0}, C_{vm}, C_S, \) and \( C_{BP} \) are selected such that the Jackson modes are held stable while the secondary modes are unstable. For such formulations, each value of \( C \) has a corresponding value of \( C_{BT,\text{crit}} \). The eigenvalues and eigenvectors of \( C(k) \) are determined when \( C_{BT} \) is either below or above \( C_{BT,\text{crit}} \). When \( C_{BT} \) is above \( C_{BT,\text{crit}} \), none of the six eigenvalues contain a positive real part, indicating stable secondary modes. However, when \( C_{BT} \) is below \( C_{BT,\text{crit}} \), one eigenvalue contains a positive real part, indicating unstable secondary modes.

We can then construct a diagonal matrix, \( E(k) \), in which the nonzero elements are the six eigenvalues. We then set all eigenvalues equal to zero except the one containing a positive real part, yielding the diagonal matrix \( E^*(k) \). Using the matrix constructed from the eigenvectors, \( Q(k) \), an amended form of \( C(k) \), designated \( C^*(k) \), can be calculated:

\[ C^*(k) = Q(k) E^*(k) Q^{-1}(k). \]  

(6.45)

From the expression

\[ B(k) \dot{X} = C^*(k) X, \]  

(6.46)

we can determine the origin of the instabilities.
Figure 6.9. Continuous-phase (dashed lines) and dispersed-phase (solid lines) horizontal velocity components at the centerline vs. column height, for $\alpha_d^0 = 0.5$ with secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} = 0.1$, $C_{BP} = 2$). Profiles illustrate behavior after the flow becomes unstable at $t = 20$ s (see Fig. 6.6).

We have tested a model formulation in which $\alpha_d^0 = 0.5$, $C_{vm} = 0.5$, $C_S = 0$, and $C_{BP} = 2$, such that the Jackson modes are held stable while the secondary modes are unstable. For this formulation, we considered the example with $C = 1$, for which $C_{BT,crit}$ is 0.314. The critical eigenvector was determined with $C_{BT}$ set to $C_{BT,crit}$. From the critical eigenvector, it was found that the secondary-mode instability arises from the horizontal components of the continuous- and dispersed-phase velocities, $u_{c,1,2}$ and $u_{d,1,2}$, as shown in Fig. 6.9. When the uniform state is simulated (up to $t = 20$ seconds), the horizontal velocity components along the centerline are zero. After the uniform state is
perturbed (by numerical “noise” in this case), the horizontal velocity components begin to deviate from zero at the centerline and are non-negligible at approximately $t = 21.5$ seconds. By 22.5 seconds the velocity magnitudes near the bottom of the column have increased by about a factor of ten, with the dispersed-phase velocity having the higher magnitude. Because the horizontal velocities at the vertical walls are zero, a non-zero horizontal velocity at the centerline must generate a compression (expansion) wave in the gas holdup in order to satisfy continuity. These vertical structures are clearly observable in Fig. 6.6 starting at 22.5 seconds.

![Figure 6.10. Qualitative sketch of the behavior of the velocity vector fields depending on the boundary conditions applied at the column walls. In the right-hand picture, gray and white bars represent alternating high-holdup and low-holdup columnar structures, analogous to those observed in Fig. 6.6.](image)

In other words, although the secondary-mode instability does not directly involve fluctuations in $\alpha_d$, nor $p_1$, as is the case for previously reported instabilities (Sankaranarayanan and Sundaresan, 2002; Lucas et al., 2005, 2006), it does lead to
columnar structures in the gas holdup due to the vertical walls (which are not explicitly accounted for in the linear stability analysis). Figure 6.10 shows the qualitative behavior of the velocity vector fields depending on the boundary conditions applied at the column walls. When the two-fluid model is simulated with periodic boundary conditions at the vertical walls (which would correspond to the conditions used for the linear stability analysis), banded horizontal velocity fields are observed, even when the volume fraction appeared spatially uniform. Such behavior was reported in Chapter 4, and these banded-flow structures can now be attributed to the instabilities in the secondary modes. When zero-flux boundary conditions are applied at the vertical walls, the secondary-mode instability eventually produces vertical bands in the volume fraction that subsequently lead to other nonlinear instabilities and then turbulent flow. Although the columnar structures in the volume fraction (e.g., Fig. 6.6) are reminiscent of those observed in the cooperative-rise instability (Sankaranarayanan and Sundaresan, 2002), the secondary-mode instability has a completely different origin.

The effect of wall boundary conditions on the secondary-mode instabilities is further examined in Figures 6.11-6.13, in which flow profiles are shown for 2D simulations that apply periodic boundary conditions, zero-flux boundary conditions, or zero-liquid-velocity boundary conditions, respectively, at the column walls. For the flow profiles shown in Figures 6.11-6.13, we examine cases for which $C_{vm} = 0.5$, $C = 1$, $C_S = 0$, and $C_{BP} = 2$, and thus $C_{BT,crit}$ is about 0.31 (see Fig. 6.7). Note that in the simulations presented in Figs. 6.11-6.13, $C_{BT}$ remains constant (i.e., $C_{BT}$ maintains the same value for $0 < t < T_{final}$). If $C_{BT}$ is below $C_{BT,crit}$, the flow should be unstable.

Figure 6.11 shows the flow profiles from simulations applying periodic boundary conditions at the column walls. Large-scale flow structures are observed when $C_{BT} = 0.1$, as seen previously (e.g., Fig. 6.5). Fewer flow structures are observed when $C_{BT} = 0.2$; thus, less suppression of BIT results in a less unstable profile. Meandering plumes are observed in both of these profiles, which is consistent with the 2D simulations discussed in Chapter 4 that applied periodic boundary conditions. When $C_{BT} = 0.3$ (near the critical value), the profile appears uniform. Thus, the periodic boundary condition simulations generally agree with the prediction that setting $C_{BT} < C_{BT,crit}$ yields unstable flow profiles.
Figure 6.11. Comparison of flow profiles when $\alpha_{00} = 0.5$ from 2D simulations applying periodic BC at the column walls. Secondary modes considered ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} < C_{BT,crit}$, $C_{BP} = 2$).

Figure 6.12 shows the flow profiles from simulations applying zero-flux boundary conditions at the column walls. Again as expected, the most segregation is observed when $C_{BT} = 0.1$, and the profile appears slightly less unstable when $C_{BT} = 0.2$. When $C_{BT} = 0.3$ (near $C_{BT,crit}$), only a few structures are observed at the top of the column. Thus, these simulations also demonstrate that less suppression of BIT results in less unstable flow profiles. Additionally, the zero-flux boundary condition simulations generally agree with the prediction that setting $C_{BT} < C_{BT,crit}$ yields unstable flow profiles.
Figure 6.12. Comparison of flow profiles when $\alpha_{d0} = 0.5$ from 2D simulations applying zero-flux BC at the column walls. Secondary modes considered ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} < C_{BT,\text{crit}}$, $C_{BP} = 2$).

Figure 6.13 shows the flow profiles from simulations applying zero-liquid-velocity boundary conditions at the column walls. These profiles differ significantly from those shown in Figs. 6.11 and 6.12. First, the profile appears uniform when $C_{BT} = 0.2$, which is much lower than $C_{BT,\text{crit}}$ (~0.31). Additionally, when $C_{BT} = 0.1$, the flow is unstable, but the profile is not as segregated as those obtained when the other wall boundary conditions are applied. The narrow domain and the zero-liquid-velocity wall boundary condition restrict the motion in the column, and this could create a stabilizing factor that is not accounted for in the linear stability analysis. This may explain the
disagreement between the zero-liquid-velocity boundary condition simulations and the prediction that the flow should be unstable for $C_{BT} < C_{BT,crit}$.

![Flow Profiles Comparison](image)

**Figure 6.13.** Comparison of flow profiles when $\alpha_{d0} = 0.5$ from 2D simulations applying zero-liquid-velocity BC at the column walls. Secondary modes considered ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} < C_{BT,crit}$, $C_{BP} = 2$).

It may be noted that for each of the wall boundary conditions considered (periodic, zero-flux, or zero-liquid-velocity), using a fully-developed unstable flow profile with $C_{BT} = 0.1$ as an initial condition and then gradually increasing $C_{BT}$ to a value slightly above $C_{BT,crit}$ will make the flow become stable again. (For example, $C_{BT} = 0.1$ for the interval $0 < t < T_a$, $C_{BT} = 0.2$ for the interval $T_a < t < T_b$, and $C_{BT} > C_{BT,crit}$ for the
interval $T_b < t < T_{final}$.) However, when the zero-liquid-velocity boundary conditions are applied, increasing $C_{BT}$ from 0.1 to 0.2 (much lower than $C_{BT, crit}$) will suffice in re-stabilizing the flow. Thus, the choice of wall boundary conditions affects the agreement between the simulations and the linear stability analysis predictions.

6.4.6 Linear Stability Analysis for 3D Geometry

The final objective is to compare linear stability analysis predictions for the full 3D model to simulations, and use the simulations to explore the flow structure after the secondary-mode instability occurs. It has been noted that periodic boundary conditions would correspond to the conditions used in the linear stability analysis. In order to determine the effect of wall boundary conditions on the flow behavior in 3D simulations, we again compare the use of periodic boundary conditions, zero-flux boundary conditions, and zero-liquid-velocity boundary conditions at the column walls.

![Figure 6.14. Comparison of flow profiles when $\alpha_{d0} = 0.5$ from 3D simulations applying either periodic BC, zero-flux BC, or zero-liquid-velocity BC at the column walls. Secondary modes unstable ($C_{vm} = 0.5, C = 1, C_S = 0, C_{BT} = 0.1, C_{BP} = 2$).](image-url)
Figure 6.14 shows the 3D water volume fraction profiles when $\alpha_{d0} = 0.5$ and the Jackson modes are held stable while the secondary modes are unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_B = 0.1$, $C_{BP} = 2$). In order to illustrate the bubble swarms expected for high gas holdups, Figure 6.15 shows iso-surfaces where $\alpha_d = \alpha_{d0} = 0.5$ within the corresponding 3D simulations depicted in Figure 6.14. As seen for 2D columns with secondary modes unstable, the flow profiles shown in Figs. 6.14 and 6.15 exhibit large-scale flow structures throughout the column. However, the profile for which zero-liquid-velocity wall boundary conditions are applied shows less segregation and more ordered structures than the other flow profiles. The narrow column width (6 cm) and the zero-liquid-velocity wall boundary condition restrict the overall motion in the column, creating a stabilizing factor that cannot be accounted for in the linear stability analysis.

Figure 6.15. Iso-surfaces showing where $\alpha_d = \alpha_{d0} = 0.5$ within the 3D simulations depicted in Figure 6.14. Secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_B = 0.1$, $C_{BP} = 2$).
In order to “see inside” the 3D columns, Figure 6.16 shows the water volume fraction profiles in cross-sections extracted from the centers of the columns depicted in Figs. 6.14 and 6.15. It can be seen in Fig. 6.16 that each flow profile exhibits large-scale structures. Qualitatively, there is little difference between the flow profiles resulting from the periodic boundary condition simulations and the zero-flux boundary condition simulations. However, when zero-liquid-velocity boundary conditions are applied at the column walls, the flow profile is less segregated than the other two flow profiles. Additionally, as column height increases, the flow structures roughly alternate between bubble-rich and bubble-lean sections. Thus, applying zero-liquid-velocity boundary conditions yields less random flow structures than those observed when the other boundary conditions are applied. As noted previously, the narrow domain and the zero-liquid-velocity wall boundary condition restrict the motion in the column, and keep the flow from becoming as unstable as seen in the other flow profiles.

Figure 6.17 shows the water velocity vector fields in square planes at the midpoint column height. (In other words, for a 50 cm high column, cross-sections are extracted at Y = 25 cm, while directions X and Z vary.) The X- and Z-components of the water velocity vectors are shown. It can be seen in Fig. 6.17 that when zero-flux boundary conditions are applied, the vectors form a boundary at X = 0, X = 6, Z = 0, and Z = 6 (i.e., along the column walls). As expected, such a boundary is not observed in the plane for which periodic boundary conditions are applied. Also as expected, when zero-liquid-velocity boundary conditions are applied, there are no vectors present at X = 0, X = 6, Z = 0, and Z = 6 (i.e., at the column walls). Circulation cells are observed in each vector field shown in Fig. 6.17, and there is little difference in velocity magnitude between the vector fields resulting from the periodic boundary condition simulations and the zero-flux boundary condition simulations. However, the field from the simulations applying zero-liquid-velocity boundary conditions shows much smaller velocity magnitude (represented by shorter vectors) than the other vector fields. This is not unexpected; the zero-liquid-velocity wall boundary condition and the narrow column width restrict the liquid motion, resulting in smaller velocity magnitude within the column.
Figure 6.16. Cross-sections extracted from the centers of the columns depicted in Figs. 6.14 and 6.15 when $\alpha_{d0} = 0.5$. Secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} = 0.1$, $C_{BP} = 2$).

Figure 6.17. Comparison of water velocity vector fields from 3D simulations when $\alpha_{d0} = 0.5$ and either periodic BC, zero-flux BC, or zero-liquid-velocity BC are applied at the column walls. Secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} = 0.1$, $C_{BP} = 2$). Planes extracted from the center of the column.
In Figs. 6.14-6.17, the average water velocity magnitude is 3.57 cm/s when periodic boundary conditions are applied, 3.75 cm/s when zero-flux boundary conditions are applied, and 1.44 cm/s when zero-liquid-velocity boundary conditions are applied. It may also be noted that the maximum water velocity magnitude in the zero-liquid-velocity boundary condition simulation is only about 6 cm/s. This is about 3 times lower than the maximum water velocity magnitude observed when the other wall boundary conditions are used. The iso-surfaces presented in Figure 6.18 illustrate the effect of wall boundary conditions on the water velocity behavior throughout the column for the corresponding 3D simulations depicted in Figure 6.14. A velocity magnitude of 3 cm/s is selected for the iso-surfaces in Fig. 6.18 since this value lies between zero and the maximum velocity magnitude observed in the zero-liquid-velocity boundary condition simulation, and this value is on the order of the average water velocity magnitudes observed when either periodic or zero-flux boundary conditions are applied.

Figure 6.18. Iso-surfaces showing where the water velocity magnitude is 3 cm/s within the 3D simulations depicted in Figure 6.14. Secondary modes unstable ($C_{vm} = 0.5$, $C = 1$, $C_S = 0$, $C_{BT} = 0.1$, $C_{BP} = 2$).
When either the periodic boundary conditions or the zero-flux boundary conditions are applied at the column walls, there is a high degree of fluctuation in the iso-surface profiles in Fig. 6.18. This is consistent with the large, random circulation cells observed in the corresponding velocity vector fields in the planes in Fig. 6.17, as well as the large-scale flow structures in the corresponding flow profiles in Figs. 6.14-6.16. When the zero-liquid-velocity boundary conditions are applied at the column walls, the profile shows small, somewhat ordered iso-surfaces in Fig. 6.18. The ordered behavior and the low degree of fluctuation are consistent with the behavior of the circulation cells observed in the corresponding velocity vector field in the plane in Fig. 6.17, as well as the corresponding flow structures in Figs. 6.14-6.16, which appeared to alternate between bubble-rich and bubble-lean sections.

Figure 6.19. Comparison of 2D and 3D periodic BC simulations. For 3D case, cross-sections extracted from the center of the column. $\alpha_{d0} = 0.5, C_{vm} = 0.5, C = 1, C_S = 0, C_BT = 0.1, C_{BP} = 2$. 
As noted previously, 2D simulations applying periodic boundary conditions at the vertical walls yielded banded horizontal velocity fields, even when the volume fraction appeared spatially uniform. This behavior, first reported in Chapter 4, has been attributed to the secondary-mode instabilities. In order to determine if such structures are observed in a 3D domain, Figure 6.19 compares both the volume fraction profiles and the water velocity vector fields for 2D and 3D periodic boundary condition simulations, when $\alpha_{d0} = 0.5$ and the secondary modes are unstable. It can be seen in Figure 6.19 that meandering plumes are observed in the 2D water volume fraction profile, while random large-scale structures (no meandering) are observed in the 3D water volume fraction profile. Similarly, bands are present in the 2D water velocity vector field, especially in the middle of the column. However, the water velocity vectors do not exhibit a banded pattern in the field resulting from the 3D simulation. We can speculate that in the 3D domain, there is no preference toward the X- or Z-direction due to symmetry.

6.5 Summary and Conclusions

The linear stability analysis shows that the growth rate $\lambda$ and the propagation velocity $\nu$ for disturbances depend on the wavenumber $k$ and the two-fluid model parameters, including gas holdup ($\alpha_{d0}$), effective viscosity ($C_{BT}$), bubble pressure ($C_{BP}$), added-mass ($C_{vm}$), lift ($C = C_L$), and rate-of-strain ($C_S$). A preliminary analysis of the model formulations considered in Chapters 4 and 5 shows that enabling only the drag force yields less unstable vertical modes, while enabling all the interphase forces yields more stable horizontal modes. The latter trend appears consistent with the results presented in Chapter 5, for which the simulations with all forces enabled transitioned to turbulent flow at higher gas holdups than the simulations for which only the drag force or only the drag and added-mass forces were enabled.

For the horizontal modes, enabling the bubble-pressure model enhances linear stability, but the effect of $C_{BP}$ diminishes with increasing $\alpha_{d0}$. The horizontal modes can be strongly stabilized by certain combinations of $C_{BP}$, $C_L = C_{rot} = C$, and $C_S$, which could explain the delayed onset of turbulent flow observed in Chapter 5 for certain model formulations. However, for the vertical modes (either Jackson or secondary), the effect
of the bubble-pressure model depends on which other models are included in the formulation. If the BIT model \(C_{BT} = 0.6\) is applied with either the baseline homogeneous formulation including all forces, the minimal formulation including only drag, the formulation including both drag and added-mass forces, or the formulation including all forces such that \(2(C - C_s) > C_{vm}\) (or \((C_L + C_{rot} - 2C_s) > C_{vm}\)), the secondary modes are stable for all values of \(C_{BP}\). However, stabilizing the Jackson modes requires a minimum value of \(C_{BP}\), and this minimum increases with increasing \(\alpha_0\). If the laminar flow model \(C_{BT} = 0\) is applied, using a minimum value of \(C_{BP}\) will stabilize the Jackson modes for wavenumbers resolved on the computational grid \(k_1 \approx 25\), but in many cases a minimum value of \(C_{BP}\) will not stabilize the Jackson modes as \(k_1\) approaches infinity. In general, the secondary modes are unstable if \(2(C - C_s) > C_{vm}\) (or \((C_L + C_{rot} - 2C_s) > C_{vm}\)) when \(C_{BP} > 0\) and \(C_{BT} = 0\). Note that unlike previously reported instabilities associated with negative lift \((C_L < 0)\), the secondary modes become unstable when the lift coefficient is sufficiently positive.

The Jackson and secondary vertical mode instabilities show distinctly different flow dynamics. When only the Jackson modes are unstable, the flow profile is nonuniform with no large-scale turbulent structures. In contrast, the turbulent flow profile observed when just the secondary modes are unstable is similar to the flow profile observed when both types of vertical modes are unstable, which suggests that nonlinear interactions with the secondary modes may cause the transition to turbulent flow in bubble columns. Additionally, we show that lowering the value of the BIT model constant \(C_{BT}\) until the secondary modes become unstable (while keeping the Jackson modes stable) yields a transition from uniform to turbulent flow at high gas holdup (~0.5), even if a positive lift coefficient (~1) is applied.

Based on these observations, a possible scenario for the instability observed in the Harteveld (2005) experiments can be identified: bubble wakes are suppressed as gas holdup increases, thereby decreasing \(C_{BT}\) enough to cause the secondary modes to become unstable. This scenario is distinctly different than the one proposed by Lucas et al. (2005, 2006), who concluded that a negative lift coefficient was required to attain
turbulent flow. It is also different than the scenario reported by Sankaranarayanan and Sundaresan (2002) for the formation of columnar structures at low gas holdups due to the dependence of the drag coefficient on holdup combined with a positive lift coefficient. In the present work, the form of drag coefficient was chosen such that rise velocity is independent of holdup (as seen in the experiments of Harteveld, 2005) and hence the bubbles are neither in the cooperative- nor hindered-rise regimes. To our knowledge, there are no previous reports in the literature describing either the secondary-mode instability or turbulent profiles at large holdups caused by a large positive lift coefficient relative to added-mass ($C_{vm}$), bubble pressure ($C_{BP}$), and turbulent dispersion ($C_{BT}$).

Extending this work to include 3D domains allows a more complete investigation into the flow behavior resulting from secondary-mode instabilities. The iso-surfaces illustrate the appearance of bubble swarms in columns with high holdup (~0.5) when the secondary modes are unstable. The choice of wall boundary conditions affects the flow behavior observed. When periodic boundary conditions are applied in a 2D column, meandering structures are observed, and horizontal bands occur in the velocity vector fields. Such behavior is not observed in a 3D column, as there should be no preference toward the X- or Z-direction due to symmetry. Both 2D and 3D flow profiles show large-scale structures when BIT is suppressed (e.g., $C_{BT} = 0.1$). The flow profiles from simulations applying periodic or zero-flux wall boundary conditions are qualitatively similar. However, when zero-liquid-velocity wall boundary conditions are applied, with the same model parameters, the flow profile appears less unstable than the profiles obtained when using the other types of wall boundary conditions. The motion in the column is restricted by both wall boundary condition and narrow column width, creating a stabilizing effect. Thus, further study may be needed to account for the effect of domain size and boundary conditions on the agreement between simulations and linear stability analysis predictions.
Chapter 7. Validation Study of Bubble-Column Simulations for Uniform and Non-uniform Aeration Conditions

The numerical studies presented in Chapters 4-6 showed that predictions for flow-regimes and flow-transition regions in air-water bubble columns are highly dependent on the momentum-transfer model formulation, which includes drag, virtual-mass, lift, rotation, and strain forces, and Sato’s bubble-induced turbulence (BIT) model. Applying all interphase force models with a particular set of model parameters agreed qualitatively with the experiments of Harteveld et al. (2004, 2005), who observed homogeneous flow for holdup values up to 0.50 (Harteveld et al., 2004, 2005; Mudde, 2005b).

We now report on a validation study of our results against those of the experimental research group at Delft University of Technology. Specifically, we focus on their rectangular pseudo-two-dimensional column with width 24.3 cm, in which non-homogeneous flow can be obtained by changing the aeration pattern. Experiments for the Delft rectangular column include one uniform aeration pattern and six non-uniform aeration patterns (Harteveld et al., 2004, 2005). CFD simulations of the uniform and non-uniform aeration patterns considered in the Delft rectangular column are carried out on a uniform grid.

This chapter is organized as follows. First, a brief description of the Delft pseudo-2D bubble column experiments is provided. Then, we review the two-fluid model formulation applied in this validation study. Next, both qualitative and quantitative CFD results for the seven different aeration cases are compared with the flow behavior observed in the corresponding experiments. Quantitative analyses examine liquid axial velocity profiles across the column width and gas volume fraction profiles across the column width. Conclusions are drawn in the final section of this chapter.

7.1 Overview of Delft Experiments

The research group at Delft University of Technology studied bubble columns in which the flow was homogeneous for gas holdups from 0.05 – 0.5 (Harteveld et al., 2004, 2005; Mudde, 2005b). These experiments were performed in cylindrical columns, which have limited visual accessibility (Harteveld, 2005). Thus, additional experiments have
been performed in a pseudo-2D column in order to more easily examine the behavior of large-scale structures. The Delft rectangular pseudo-2D column is 24.3 cm wide, 99 cm high, and 4.1 cm deep, with an initial water level of 70 cm. A superficial gas velocity of 2 cm/s was used for all experiments, including one uniform aeration pattern and six non-uniform aeration patterns, all illustrated in Figure 7.1. The aeration system consisted of constant flow-rate air injection needles organized into groups, resulting in a narrow size distribution: bubbles observed ranged between 3.5 to 4.5 mm in diameter. The aeration sections at the bottom of the column could be either enabled or disabled in order to change the aeration pattern, which in turn determined if homogeneous or non-homogeneous flow would appear. Uniform aeration (pattern 1) yielded homogeneous flow, while having non-aerated sections could result in flow instabilities. If the non-aerated sections near the column walls were small (e.g., patterns 2-4, less than 22% total non-aeration), either large-scale structures were not observed, or large-scale structures were present but remained in a fixed position. An increase in total non-aeration to ~30% (e.g., pattern 5) eventually produced dynamic large-scale structures with periodic behavior. Non-aeration in the center of the column (pattern 7) resulted in circulation cells near the sparger (Harteveld et al., 2004, 2005).

Several different techniques were applied to gather the data used to describe the behavior observed in the Delft experiments. Particle Image Velocimetry (PIV) was used to determine the bubble velocity vector fields from sequences of camera-recorded images. Particle Tracking Velocimetry (PTV) for polystyrene tracer particles was used to determine the liquid flow behavior in the column. In order to distinguish between bubbles and tracer particles, the tracers were painted black and were typically smaller (~2.5 mm) than the range of bubble sizes observed. Because of high tracer particle inertia, only the largest flow structures could be determined by the technique, while the effect of smaller structures was filtered out. Five glass fiber probes were used simultaneously to measure the gas volume fraction at individual points along a path extending from the column center to the wall. Laser Doppler Anemometry (LDA) was used to determine the mean liquid velocities. Velocity data was taken at various points along a line extending across the width of the column. Axial and tangential components
were determined with different colored beams, but were never measured in the same time instants. A further description of these techniques and the equipment used can be found in Harteveld et al. (2004, 2005).

Figure 7.1. The seven aeration patterns for the Delft pseudo-2D bubble column. Percentages at the right-hand side denote the amount of aeration.

7.2 Review of Model Formulation

The data from the experiments described above is used to validate the Eulerian two-fluid model used in CFDLib (Kashiwa et al., 1994). The full description of the two-fluid model is in Chapter 3, and a brief review of the notable terms is given below. Subscripts $c$ and $d$ refer to the continuous phase (water) and the dispersed phase (air), respectively, while $\alpha$, $\rho$, and $u$ represent volume fraction, density, and velocity, respectively.

The mass balance equation for phase $k$ ($= c, d$) is expressed as

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \left( \alpha_k \rho_k u_k \right) = 0.$$  \hspace{1cm} (7.1)

The momentum balance equation for phase $k$ is given by
\[\alpha_k \rho_k \frac{\partial \mathbf{u}_k}{\partial t} + \alpha_k \rho_k \mathbf{u}_k \cdot \nabla \mathbf{u}_k = -\alpha_k \nabla p - \nabla P_k + \nabla \cdot \alpha_k \mu_{\text{eff},k} \left[ \nabla \mathbf{u}_k + \left( \nabla \mathbf{u}_k \right)^T \right] + \sum_f F_{jk} + \alpha_k \rho_k \mathbf{g}, \quad (7.2)\]

where the terms on the right-hand side represent, from left to right, the pressure gradient, the bubble-pressure model, the effective stress model, the interphase momentum exchange, and the gravitational force.

The bubble-pressure model, which is applied only in the dispersed-phase momentum balance (i.e., \(P_c = 0\)), is that proposed by Biesheuvel and Gorissen (1990):

\[P_d = \rho_c C_{BP} \alpha_d \left( \mathbf{u}_d - \mathbf{u}_c \right) \cdot \left( \mathbf{u}_d - \mathbf{u}_c \right) H(\alpha_d), \quad (7.3a)\]

where (Batchelor, 1988)

\[H(\alpha_d) = \left( \frac{\alpha_d}{\alpha_{dep}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dep}} \right). \quad (7.3b)\]

In Eqs. 7.3a and 7.3b, \(C_{BP}\) is a proportionality constant and \(\alpha_{dep}\) denotes the gas volume fraction at close packing (set equal to 1.0).

The effective stress term for phase \(k\) is defined as

\[\nabla \cdot \alpha_k \mu_{\text{eff},k} \left[ \nabla \mathbf{u}_k + \left( \nabla \mathbf{u}_k \right)^T \right], \quad (7.4)\]

where \(\mu_{\text{eff},k}\) represents the effective viscosity. In this study, the effective viscosity for the continuous phase is equal to the sum of the molecular viscosity of the continuous phase and a value for turbulent viscosity, or \(\mu_{\text{eff},c} = \mu_{0,c} + \mu_{t,c}\). The effective viscosity for the dispersed phase is equal to the molecular viscosity of the dispersed phase, or \(\mu_{\text{eff},d} = \mu_{0,d}\). Sato’s bubble-induced turbulence (BIT) model (Sato and Sekoguchi, 1975) is used to determine \(\mu_{t,c}\):

\[\mu_{t,c} = C_{BT} \rho_c d_s \alpha_d |\mathbf{u}_d - \mathbf{u}_c|, \quad (7.5)\]

where the model constant \(C_{BT}\) is set equal to 0.6 (Sato et al., 1981).

The interphase momentum exchange is defined as a sum of the drag, virtual-mass, lift, rotation, and strain forces:
\[ \sum_{f} F_{jk} = F_{D,k} + F_{vm,k} + F_{L,k} + F_{rot,k} + F_{S,k}. \]  

(7.6)

The drag force is defined in CFDLib as

\[ F_D = -\alpha_d \alpha_r \rho_c C_D \left( Re \right) \frac{3}{4d_b} \left| u_d - u_c \right| (u_d - u_c), \]

(7.7)

where \( Re \) denotes the bubble Reynolds number:

\[ Re = \frac{d_b \left| u_d - u_c \right|}{\nu_c}. \]

(7.8)

For the drag coefficient, CFDLib uses the following function of the bubble Reynolds number (Kashiwa et al., 1994):

\[ C_D \left( Re \right) = C_{\infty} + \frac{24}{Re} + \frac{6}{1 + \sqrt{Re}}, \]

(7.9)

where \( C_{\infty} \) is set to 0.5 in order to give the correct average volume fraction \( \alpha_d \approx 0.07 \) as a function of superficial gas velocity \( (u_g = 2 \text{ cm/s}) \) for the uniform feed case in the pseudo-2D experiments (Harteveld et al., 2004, 2005).

The virtual-mass force is defined in CFDLib as

\[ F_{vm} = -\alpha_d \alpha_r \rho_c C_{vm} \left[ \left( \frac{\partial \vec{u}}{\partial t} + \vec{u}_d \cdot \nabla \vec{u}_d \right) - \left( \frac{\partial \vec{u}}{\partial t} + \vec{u}_c \cdot \nabla \vec{u}_c \right) \right], \]

(7.10)

where \( \rho_c \) denotes the volume-averaged density, \( \rho_c = \alpha_c \rho_c + \alpha_d \rho_d \). In this study, the virtual-mass coefficient \( C_{vm} \) is set to 0.5.

As discussed in Chapter 3, interaction terms proposed by Kashiwa (1998) give rise to the lift, rotation, and strain forces, which are defined as:

\[ F_L = \alpha_c \alpha_d \rho_c C_L \left( u_d - u_c \right) \times \nabla \times u_c, \]

(7.11)

\[ F_{rot} = \alpha_c \alpha_d \rho_c C_{rot} \left( u_d - u_c \right) \times \nabla \times u_d, \]

(7.12)

where \( C_L = C_{rot} \), and

\[ F_S = \alpha_d \alpha_c \rho_c C_S \left[ (\nabla u_c + \nabla u_d) + (\nabla u_c + \nabla u_d)^T \right] \cdot (u_c - u_d). \]

(7.13)

As shown in Chapters 4-6, we have found that including these interaction terms (with a particular set of model parameters) suppresses flow transitions up to relatively large values (\( \approx 0.5 \)) for the average gas volume fractions.
7.3 Validation Study Results

The validation study comparing our numerical results to the pseudo-2D experiments of Harteveld et al. (2004, 2005) is organized into qualitative and quantitative analyses. We have simulated each of the seven aeration patterns illustrated in Figure 7.1. These fully-resolved simulations were carried out on a grid with 100 cells in the horizontal direction, resulting in cell spacing of 0.243 cm. Using a uniform grid with square cells results in a slightly smaller domain height, 97.2 cm, than that used in the experiments (99 cm). In the experiments, the bubble diameter ranged between 3.5-4.5 mm (Harteveld, 2005); thus an input bubble diameter of 4 mm has been selected. It is reasonable to approximate the bubbles as non-coalescing spheres in the simulations since Harteveld (2005) was able to suppress bubble coalescence by using “aged” or “contaminated” water, and a low gas flow rate ($u_g = 2$ cm/s) was used in the pseudo-2D experiments (Harteveld, 2005). Simulation conditions are listed in Table 7.1.

**Table 7.1. Simulation conditions for the validation study.**

<table>
<thead>
<tr>
<th>Column width</th>
<th>24.3 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column height</td>
<td>97.2 cm</td>
</tr>
<tr>
<td>Cell spacing (horizontal and vertical directions)</td>
<td>0.243 cm</td>
</tr>
<tr>
<td>Initial liquid level</td>
<td>70 cm</td>
</tr>
<tr>
<td>Superficial gas velocity</td>
<td>2 cm/s</td>
</tr>
<tr>
<td>Input bubble diameter</td>
<td>4 mm</td>
</tr>
</tbody>
</table>

In the majority of the simulations discussed in Section 7.3, $C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$. These are the same parameter values used in the full model formulation that best agreed with the Delft experiments at high gas holdup (Harteveld, 2005), as shown in the flow map study in Chapter 5. According to the linear stability analysis in Chapter 6, however, this particular set of parameters would yield stable horizontal modes, stable secondary vertical modes, and yet *unstable* Jackson vertical modes. As shown in Fig. 6.2, for the average gas holdup ($\alpha_d \approx 0.07$) observed in the pseudo-2D experiments (Harteveld et al., 2004, 2005), a value of $C_{BP}$ greater than 0.2 would be required to obtain stable Jackson vertical modes. Thus, we also examine how increasing $C_{BP}$ changes the resulting simulated flow behavior in the pseudo-2D column.
for several cases. Unless stated otherwise, zero-flux boundary conditions are applied at the column walls.

7.3.1 Qualitative Analysis

Examining the behavior of the air velocity vector fields allows for a qualitative comparison between the experiments and simulations for all seven aeration patterns. In Figures 7.2-7.8, the left picture shows the experimentally determined bubble velocity vector field, scanned from Harteveld et al. (2004), and the right picture shows the corresponding simulated air (bubble) velocity vector field.

Figure 7.2. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 1.

Figure 7.2 shows the comparison between the experimentally determined air velocity vector field and the corresponding simulated field for uniform aeration pattern 1. Good agreement between experiment and simulation can be seen in Fig. 7.2. This would
be expected when recalling the numerical studies presented in Chapter 5. The simulations for the flow map study also used uniform aeration and the same column width (24.3 cm). As shown in Figs. 5.4a and 5.4b, including all force models and the bubble-induced turbulence model ($C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, $C_S = 0.125$, $C_{BT} = 0.6$, and $C_{BP} = 0.2$) resulted in uniform flow for low gas flow rates (corresponding to low average gas volume fraction $\overline{\alpha}_d$) for nearly the same bubble diameter ($\sim 4$ mm).

Figure 7.3. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 2.

Figure 7.3 shows the comparison between the experimentally determined and simulated air velocity vector fields for non-uniform aeration pattern 2. The non-aerated sections for pattern 2 are small (see Fig. 7.1), with one row of injection needles disabled next to the left and right walls, resulting in about 93 % aeration (Harteveld et al., 2004). However, the vector fields show disagreement between experiment and simulation for
aeration pattern 2. The experimentally determined velocity vector field shows very small non-uniformities at the non-aerated sections at the bottom of the column, but such non-uniformities are no longer observed as the column height increases. Conversely, the simulated vector field shows the vectors traveling toward the center and then up one side of the column, until a height of approximately 200 mm, after which the velocity vectors change direction and travel up the opposite side of the column. The vectors shift direction again between column heights of 500 to 600 mm.

Figure 7.4. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 3.

The agreement between the experimentally determined air velocity vector field and corresponding simulated vector field is reasonable for non-uniform aeration pattern 3, as seen in Figure 7.4. For this pattern, two rows of injection needles were disabled next to the left and right column walls, resulting in approximately 85 % aeration
The velocity vector field determined experimentally shows the velocity vectors almost immediately curving to the left upon entering the column. At a height of about 200 mm, the velocity vectors change direction and head toward the opposite column wall. The vectors move back toward the left column wall at a height between 450 and 500 mm. Above a height of 550 mm, the air velocity vector field appears uniform. In the simulated field, the air velocity vectors also curve toward the left immediately after entering the column, and then travel toward the opposite wall. However, this change in direction occurs at a slightly lower height (~150 mm) than observed experimentally. The simulated air velocity vectors also move back toward the left wall, but at a greater height (~650 mm) than observed experimentally.

Figure 7.5. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 4.
The air velocity vector fields show some qualitative disagreement between experiment and simulation for non-uniform aeration pattern 4, as seen in Figure 7.5. For this pattern, three rows of injection needles were disabled next to the left and right column walls, resulting in approximately 78 % aeration (Harteveld et al., 2004). In the experimentally determined velocity vector field, air enters the column and travels toward the center, and the vectors exhibit a symmetrical configuration. At approximately 350 mm, the vectors curve toward the left wall, and then the vectors shift direction toward the opposite wall at a height of about 550 mm. In the simulated field, air enters the column and travels toward the left wall instead of toward the center, and thus the vectors exhibit an asymmetrical configuration. At about 150 mm, the velocity vectors shift direction toward the right wall, and the vectors later travel back toward the left wall at a height of about 600 mm. Circulation is observed between column heights of 500 to 600 mm.

Figure 7.6. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 5.
The agreement between experiment and simulation for non-uniform aeration pattern 5 is reasonable, as seen in Figure 7.6. For this pattern, four rows of injection needles were disabled next to the left and right column walls, resulting in approximately 70% aeration (Harteveld et al., 2004). In the experimentally determined vector field, air enters the column and travels toward the center, and the vectors exhibit a symmetrical configuration. As the vectors travel upward, they gradually meander from one side of the column to the other. The corresponding simulated air velocity vector field exhibits similar behavior. According to Harteveld et al. (2004), aeration pattern 5 yielded large-scale flow structures that exhibited periodic behavior. Indeed, if the corresponding simulation is animated, the same type of behavior is observed.

Figure 7.7. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 6.
Figure 7.7 shows the experimentally determined and simulated air velocity vector fields for non-uniform aeration pattern 6. This was the only asymmetric pattern used in the experiments; four rows of injection needles next to the right wall were disabled, resulting in about 85% aeration (Harteveld et al., 2004). The agreement between experiment and simulation is reasonable for aeration pattern 6. In both the experimentally determined and simulated velocity vector fields, air enters and travels toward the left wall, then the vectors shift direction toward the right wall, and finally the vectors travel back toward the left wall. However, the shift in direction from the left wall toward the right wall occurs at a column height of about 125 mm in the experimentally determined field, but at a height of about 250 mm in the simulated field. Similarly, the shift in direction back toward the left wall occurs at a height of about 425 mm in the experimentally determined field, but at a height of about 600 mm in the simulated field.

Figure 7.8. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 7.
Figure 7.8 shows the comparison between the experimentally determined and simulated air velocity vector fields for non-uniform aeration pattern 7. Three rows of injection needles in the center of the column were disabled, resulting in about 89% aeration (Harteveld et al., 2004). The agreement between experiment and simulation for pattern 7 is reasonable. The behavior observed near the column air inlet in the simulated velocity vector field is similar to the behavior observed at the same location in the experimentally determined field. Both fields show the vectors gradually traveling from one wall to the other; the main difference is that the simulated field shows this movement in the opposite direction from that observed in the experimentally determined field.

The qualitative agreement between experiments and simulations is closest for uniform aeration pattern 1 and non-uniform aeration patterns 3, 5, 6, and 7. In the simulations for non-uniform aeration patterns 2 and 4, the bubbles appear to move too quickly to the center and then to one side of the column, where sudden upflow is observed. Recall that all simulations discussed above used the same model formulation \((C_{BT} = 0.6, C_{BP} = 0.2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \text{ and } C_S = 0.125)\) that best agreed with the Delft experiments (Harteveld, 2005), as shown in Chapter 5. While this model formulation yields stable horizontal modes and stable secondary vertical modes (see Chapter 6), a value of \(C_{BP}\) greater than 0.2 would be required for stable Jackson vertical modes. Thus, we will later examine how increasing \(C_{BP}\) changes the simulated flow profiles resulting from aeration patterns 2 and 4.

### 7.3.2 Quantitative Analysis

We next examine gas holdup profiles and liquid axial velocity profiles as a function of column height. Note that due to computational expense, the majority of the simulations were only carried out to 75 seconds, while the experimental data was obtained over a period of 300 seconds (Harteveld et al., 2004). However, qualitatively the simulated flow behavior did not change significantly after about 10-15 seconds. Finally, the full model formulation is again used, with \(C_{BT} = 0.6, C_{BP} = 0.2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \text{ and } C_S = 0.125\).

Table 7.2 compares the average gas holdup values obtained in the experiments with the values obtained in the corresponding simulations. The average gas holdup,
\( \alpha_{\text{height}} \) is determined from the difference between the gassed and ungassed liquid height in the bubble column:

\[
\alpha_{\text{height}} = \frac{h_{\text{gassed}} - h_{\text{ungassed}}}{h_{\text{ungassed}}}.
\]  

(7.14)

Overall, the agreement between experiments and simulations appears reasonable. As seen in Table 7.2, all the values of \( \alpha_{\text{height}} \) calculated from simulation data are within 10% of the corresponding values obtained experimentally.

**Table 7.2. Comparison of average gas volume fractions.**

<table>
<thead>
<tr>
<th>Aeration pattern</th>
<th>( \alpha_{\text{height}}, ) experimental</th>
<th>( \alpha_{\text{height}}, ) simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.073</td>
<td>0.076</td>
</tr>
<tr>
<td>2</td>
<td>0.072</td>
<td>0.071</td>
</tr>
<tr>
<td>3</td>
<td>0.070</td>
<td>0.068</td>
</tr>
<tr>
<td>4</td>
<td>0.068</td>
<td>0.063</td>
</tr>
<tr>
<td>5</td>
<td>0.067</td>
<td>0.058</td>
</tr>
<tr>
<td>6</td>
<td>0.070</td>
<td>0.069</td>
</tr>
<tr>
<td>7</td>
<td>0.071</td>
<td>0.069</td>
</tr>
</tbody>
</table>

Figure 7.9 illustrates the time-averaged gas holdup profiles for aeration patterns 1 and 5 at various column heights, denoted by \( z \). The solid lines represent the experimental data and the dotted lines represent the corresponding simulation data. In the experiments, the time-averaged gas volume fraction was determined using data from glass fiber probes, which were located at several different points along the width of the column (Harteveld, 2005). Data was taken at \( z = 0.70 \) m for aeration pattern 1, and at \( z = 0.05 \) m, 0.10 m, 0.20 m, 0.50 m, and 0.70 m for aeration pattern 5. In general, the two-fluid model predicts gas holdup profile trends similar to those observed experimentally, especially for locations away from the column walls. However, the two-fluid model appears to under-predict the magnitude of the gas holdup. Note that the only way to control the average gas holdup for the uniform feed case was to adjust the drag model coefficient \( C_{\infty} \), as discussed in Section 5.3.1, in order to give the correct value of average gas holdup for a superficial gas velocity of 2 cm/s. Thus, the drag model was fixed to obtain the average gas holdup of 0.073 for uniform aeration pattern 1. It is possible that
fixing the drag model coefficient $C_x$ could affect the local or average volume fraction values, and volume fraction profiles, for the other aeration patterns.

Figure 7.9. Time-averaged air volume fraction profiles for aeration patterns 1 and 5 at selected column heights.
Figure 7.10 shows the time-averaged axial liquid velocity profiles for uniform aeration pattern 1. The solid lines represent the experimental data and the dotted lines represent the corresponding simulation data. Velocity data was taken at column heights $z = 0.05$ m, 0.10 m, 0.20 m, 0.50 m, and 0.70 m. The experimentally determined velocity profiles tend to show little variation in the center of the column, and only show liquid downflow near the walls, which is likely due to a narrow region near the walls where gas holdup decreases (Harteveld, 2005). The simulated velocity profiles are nearly uniform, especially when $z \geq 0.10$ m, but predict lower velocity magnitudes (~ 0 m/s).

Harteveld (2005) notes that the amount of relative wall area is larger near the column ends (i.e., $|x| = 121.5$ mm), which leads to an increase in the local driving force for circulation near the column ends. Thus, when $z \leq 0.10$ m, a higher velocity...
magnitude is observed near the column walls rather than in the center. Harteveld (2005) also notes that the total wall area for the pseudo-2D column is much larger than the total wall area for a cylindrical column, for which the average axial liquid velocity profiles were nearly uniform with low magnitude (~0.01 m/s). Consequently, the overall volume containing a lower gas holdup is larger in the pseudo-2D column than in a cylindrical column. Such behavior could lead to higher circulation in the pseudo-2D column, and therefore greater upward velocity in the pseudo-2D experiments (Harteveld, 2005). These observations may partially explain the disagreements in average axial liquid velocity magnitude between the experimentally determined profiles and the corresponding simulated profiles.

Figure 7.11 shows the time-averaged axial liquid velocity profiles for all seven aeration patterns at a column height of 0.05 m, just above the air inlet. Again, the solid lines represent the experimental data, while the dotted lines represent the corresponding simulation data. It can be seen in Figure 7.11 that the agreement between experiments and simulations at this height is closest for uniform aeration pattern 1 and non-uniform aeration patterns 5, 6, and 7. This is not unexpected, as the qualitative agreement at about the same column height was also closest for these particular aeration patterns (Figs. 7.2, 7.6, 7.7, 7.8). The agreement between experiment and simulation is also reasonable for non-uniform aeration pattern 3, as both the experimentally determined and simulated liquid velocity profiles show the highest time-averaged liquid velocity in the left half of the column. However, the velocity magnitude is higher in the simulated profile for pattern 3.

It should be noted that non-uniform aeration patterns 2 and 4 do not yield dynamic behavior in the experiments (Harteveld, 2005). However, in the simulations for these patterns, the bubbles appear to move too quickly toward the center and then to one side of the column, where sudden upflow is observed. Thus, Figure 7.11 shows some disagreement between experiments and simulations for the axial liquid velocity profiles at a column height of 0.05 m for patterns 2 and 4. The experimentally determined liquid velocity profile for pattern 2 shows a peak in the center of the column, while the simulated liquid velocity profile shows a peak in the left half of the column.
Additionally, the velocity magnitude is higher in the simulated profile than in the experimentally determined profile. Both the experimentally determined and simulated liquid velocity profiles for pattern 4 show about the same velocity magnitude. However, the peak is in the center of the experimentally determined profile and in the left half of the simulated profile.

![Figure 7.11. Axial liquid velocity profiles for all aeration patterns, at column height 0.05 m.](image)

Figure 7.12 shows the time-averaged axial liquid velocity profiles for all seven aeration patterns at a column height of 0.70 m. As seen previously, the solid lines represent the experimental data, while the dotted lines represent the corresponding simulation data. As seen in the qualitative comparisons (Figs. 7.2-7.8) and the axial liquid velocity comparisons at the column height of 0.05 m (Fig. 7.11), the agreement...
between experiments and simulations is reasonable for patterns 1, 3, 5, 6, and 7, while disagreement between experiments and simulations is observed for patterns 2 and 4.

Figure 7.12. Axial liquid velocity profiles for all aeration patterns, at column height 0.70 m.

For patterns 1, 5, and 7, the experimentally determined axial liquid velocity profiles at 0.70 m are overall uniform except near the column walls. The corresponding simulated velocity profiles show reasonable agreement, though the average velocity magnitude is slightly lower. For pattern 3, the experimentally determined axial liquid velocity profile at 0.70 m exhibits upflow in the left half of the column and downflow in the right half, while the simulated profile exhibits the opposite—upflow in the right half of the column and downflow in the left half. Thus, the overall behavior—upflow in one half, downflow in the other half—is similar for both the experiment and corresponding simulation for pattern 3. Both the experimentally determined and simulated axial liquid
velocity profiles at 0.70 m for pattern 6 show upflow in the right half of the column and
downflow in the left half, though the simulated profile shows a larger velocity magnitude.
Recall that the qualitative comparison for pattern 6 (Fig. 7.7) showed the air velocity
vectors in the experimentally determined field shifting direction at different column
heights than in the simulated field. Such behavior may affect the differences in local
liquid velocity magnitude, and consequently time-averaged velocity, between the
experiments and simulations.

For patterns 2 and 4, the experimentally determined axial liquid velocity profiles
at 0.70 m are overall uniform with low magnitude, but the corresponding simulated
profiles show upflow in the right half of the column and downflow in the left half. As
noted previously, in the simulations for patterns 2 and 4, the bubbles appear to move too
quickly toward the center and then to one side of the column, where sudden upflow is
observed. Such behavior would likely affect the local liquid velocity, and hence the time-
averaged velocity, throughout the column, resulting in disagreement between
experiments and simulations. This is consistent with the behavior seen in the qualitative
comparisons for patterns 2 and 4 (Figs. 7.3 and 7.5, respectively). The experimentally
determined air velocity vector fields were overall uniform at 0.70 m, while the simulated
fields showed upflow in the right half of the column above 0.60 m.

7.3.3 Further Examination of Aeration Patterns 2 and 4

As noted previously, the simulations discussed in Sections 7.3.1 and 7.3.2 used
the same model formulation (\( C_{BT} = 0.6 \), \( C_{BP} = 0.2 \), \( C_{vm} = 0.5 \), \( C_L = C_{rot} = 0.375 \), and \( C_S = 0.125 \)) that best agreed with the Delft experiments (Harteveld, 2005), as shown in
Chapter 5. This model formulation yields stable horizontal modes and stable secondary
vertical modes (see Chapter 6), yet a value of \( C_{BP} \) greater than 0.2 would be required for
stable Jackson vertical modes. Since disagreement between experiments and simulations
was observed for aeration patterns 2 and 4, we now examine how selected changes to the
model formulation affect the simulated flow behavior. The following six cases are
compared in both qualitative and quantitative analyses for aeration patterns 2 and 4:

A: The experimentally determined (Harteveld, 2005) bubble (air) velocity vector
fields (qualitative) or time-averaged axial liquid velocity profiles (quantitative).
B: The model formulation applied in the simulations discussed in Sections 7.3.1 and 7.3.2 \( (C_{BT} = 0.6, \ C_{BP} = 0.2, \ C_{vm} = 0.5, \ C_L = C_{rot} = 0.375, \) and \( C_S = 0.125 \)).

C: A model formulation in which \( C_{BP} \) is increased to a value of 2, for which the Jackson vertical modes should be stable \( (C_{BT} = 0.6, \ C_{BP} = 2, \ C_{vm} = 0.5, \ C_L = C_{rot} = 0.375, \) and \( C_S = 0.125 \)).

D: A model formulation in which \( C_{BP} \) is increased to a value of 2, and \( C_S \) is set to zero to determine whether the profiles change in the absence of the strain force, which is not reported in the literature \( (C_{BT} = 0.6, \ C_{BP} = 2, \ C_{vm} = 0.5, \ C_L = C_{rot} = 0.375, \) and \( C_S = 0 \)).

E: A model formulation in which \( C_{BP} \) is increased to a value of 2 \( (C_{BT} = 0.6, \ C_{BP} = 2, \ C_{vm} = 0.5, \ C_L = C_{rot} = 0.375, \) and \( C_S = 0.125 \)). Additionally, zero-liquid-velocity boundary conditions are now applied at the column walls to determine whether a change in wall boundary conditions would improve agreement between experiments and simulations.

F: A model formulation in which \( C_{BP} \) is increased to a value of 2, and \( C_S \) is set to zero \( (C_{BT} = 0.6, \ C_{BP} = 2, \ C_{vm} = 0.5, \ C_L = C_{rot} = 0.375, \) and \( C_S = 0 \)). Additionally, zero-liquid-velocity boundary conditions are now applied at the column walls.

A qualitative analysis for aeration pattern 2 is shown in Figure 7.13, which compares the experimentally determined bubble (air) velocity vector field with simulated air velocity vector fields obtained using the model formulations summarized above. As discussed in Section 7.3.1, the experimentally determined velocity vector field (A) shows very small non-uniformities near the non-aerated sections at the bottom of the column, but is overall uniform elsewhere in the column. However, the original simulated field (B) shows the vectors traveling toward the center and then along the left side of the column until a height of approximately 200 mm, after which the velocity vectors change direction and travel along the right side. The vectors shift direction again toward the left side at about 550 mm. Simply increasing \( C_{BP} \) from 0.2 to 2 (C) does not significantly change the simulated air velocity vector field. A minor change is observed in the simulated vector field (D) resulting from increasing \( C_{BP} \) from 0.2 to 2 and also disabling the strain force
(\(C_S = 0\)). The shift in direction from the right side to the left side, observed previously at about 550 mm (B, C), occurs instead at a slightly lower height, about 450 mm (D).

Figure 7.13. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 2. Effect of model formulation is examined. A: experimentally determined vector field (Harteveld, 2005). B: \(C_{BT} = 0.6, C_{BP} = 0.2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \(C_S = 0.125;\) zero-flux wall BC. C: \(C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \(C_S = 0.125;\) zero-flux wall BC. D: \(C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \(C_S = 0;\) zero-flux wall BC. E: \(C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \(C_S = 0.125;\) zero-liquid-velocity wall BC. F: \(C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \(C_S = 0;\) zero-liquid-velocity wall BC.
As seen in Fig. 7.13, when zero-liquid-velocity boundary conditions are applied at the column walls (E, F), the air velocity vectors initially travel to the right side of the column instead of the left side (B, C, D). Additionally, the vectors shift direction from one side to another more frequently when zero-liquid-velocity wall boundary conditions are applied (E, F) than when zero-flux wall boundary conditions are applied (B, C, D). However, disabling the strain force by lowering $C_S$ from 0.125 (E) to zero (F) does not change the simulated vector field significantly. Finally, as observed in Chapter 6, applying zero-liquid-velocity wall boundary conditions appears to provide a stabilizing effect. Above a height of about 600 mm, simulated vector fields E and F are overall uniform, unlike simulated vector fields B, C, and D, for which zero-flux wall boundary conditions are applied.

A qualitative analysis for aeration pattern 4 is shown in Figure 7.14, which compares the experimentally determined bubble (air) velocity vector field with simulated air velocity vector fields obtained using the model formulations summarized above. As discussed in Section 7.3.1, the experimentally determined velocity vector field (A) shows air entering the column and traveling toward the center, and the vectors exhibit a symmetrical configuration. At approximately 350 mm, the vectors curve toward the left wall, and then shift direction toward the right wall at about 550 mm. In the original simulated field (B), air enters the column and travels toward the left wall instead of toward the center, and thus the vectors exhibit an asymmetrical configuration. At about 150 mm, the velocity vectors shift direction toward the right wall, and then shift back toward the left wall at about 600 mm. Similar vector field behavior is observed when $C_{BP}$ is increased to 2 (C), or when $C_{BP}$ is increased to 2 and the strain force is disabled by setting $C_S = 0$ (D). Thus, these changes to the model formulation do not improve agreement with the experimentally determined field (A).

As seen in Fig. 7.14, when zero-liquid-velocity wall boundary conditions are applied (E, F), the shift in direction from right wall to left wall occurs at about 350 mm instead of about 600 mm (B, C, D). However, disabling the strain force by lowering $C_S$ from 0.125 (E) to zero (F) does not change the simulated air velocity vector field significantly. Finally, as observed in Chapter 6, applying zero-liquid-velocity wall
boundary conditions appears to provide a stabilizing effect. Above a height of about 500 mm, simulated vector fields E and F are overall uniform, unlike simulated vector fields B, C, and D, for which zero-flux wall boundary conditions are applied.

Figure 7.14. Comparison of experimentally determined and simulated air velocity vector fields for aeration pattern 4. Effect of model formulation is examined. A: experimentally determined vector field (Harteved, 2005). B: \( C_{BT} = 0.6, C_{BP} = 0.2, C_{vm} = 0.5, C_{L} = C_{rot} = 0.375, \) and \( C_{S} = 0.125; \) zero-flux wall BC. C: \( C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_{L} = C_{rot} = 0.375, \) and \( C_{S} = 0.125; \) zero-flux wall BC. D: \( C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_{L} = C_{rot} = 0.375, \) and \( C_{S} = 0; \) zero-flux wall BC. E: \( C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_{L} = C_{rot} = 0.375, \) and \( C_{S} = 0.125; \) zero-liquid-velocity wall BC. F: \( C_{BT} = 0.6, C_{BP} = 2, C_{vm} = 0.5, C_{L} = C_{rot} = 0.375, \) and \( C_{S} = 0; \) zero-liquid-velocity wall BC.
Figure 7.15. Axial liquid velocity profiles for aeration pattern 2 (left) and aeration pattern 4 (right), at column height 0.05 m. Effect of model formulation is examined.

Figure 7.15 shows the time-averaged axial liquid velocity profiles for aeration patterns 2 (left plot) and 4 (right plot) at a column height of 0.05 m, just above the air inlet. The experimentally determined liquid velocity profile for pattern 2 shows a peak in the center of the column. The liquid velocity profiles obtained from simulations using zero-flux wall boundary conditions show peaks in the left half of the column. Conversely, the liquid velocity profiles obtained from simulations using zero-liquid-velocity wall boundary conditions show peaks in the right half of the column. This is consistent with the qualitative analysis for pattern 2, where simulations applying zero-flux wall boundary conditions resulted in air velocity vectors traveling to the left initially, and simulations applying zero-liquid-velocity wall boundary conditions resulted in air velocity vectors traveling to the right initially. Additionally, the velocity magnitude is higher in all the simulated profiles for pattern 2 than in the experimentally determined profile. Thus, for pattern 2, increasing $C_{BP}$ does not improve agreement between experiment and simulation at a column height of 0.05 m, and as seen previously, the profiles do not change significantly in the absence of the strain force ($C_S = 0$). Applying zero-liquid-velocity wall boundary conditions moves the peak from the left half of the
column to the right half, but does not improve agreement with the experimentally determined profile for pattern 2 at 0.05 m.

As seen in Fig. 7.15, the experimentally determined liquid velocity profile and all simulated liquid velocity profiles at 0.05 m for pattern 4 show about the same velocity magnitude. However, the peak is in the center of the experimentally determined profile and in the left half of all the simulated profiles. This is consistent with the qualitative analysis for pattern 4, where all simulations resulted in the air velocity vectors traveling to the left initially. Thus, for pattern 4, the selected changes to the model formulation do not improve agreement with the experimentally determined liquid velocity profile at a column height of 0.05 m.

Figure 7.16. Axial liquid velocity profiles for aeration pattern 2 (left) and aeration pattern 4 (right), at column height 0.70 m. Effect of model formulation is examined.

Figure 7.16 shows the time-averaged axial liquid velocity profiles for aeration patterns 2 (left plot) and 4 (right plot) at a column height of 0.70 m. The experimentally determined profile for pattern 2 is overall uniform with low magnitude. However, the profile obtained from the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$) with zero-flux wall boundary conditions shows upflow in
the right half of the column and downflow in the left half. Increasing $C_{BP}$ to 2 does not significantly change the axial liquid velocity profile. Increasing $C_{BP}$ to 2 and also disabling the strain force ($C_S = 0$) results in a change in the axial liquid velocity profile—upflow in the left half of the column and downflow in the right half—but does not improve agreement with the experimentally determined profile for pattern 2. Applying zero-liquid-velocity wall boundary conditions, however, does significantly improve agreement with the experimentally determined profile for pattern 2. As seen in Fig. 7.16, the experimentally determined axial liquid velocity profile at 0.70 m for pattern 4 is overall uniform with low magnitude. The profile obtained from the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$) with zero-flux wall boundary conditions shows upflow in the right half of the column and downflow in the left half. Increasing $C_{BP}$ to 2 does not significantly change the axial liquid velocity profile; however, increasing $C_{BP}$ to 2 and also disabling the strain force ($C_S = 0$) slightly improves agreement with the experimentally determined profile for pattern 4. Agreement with the experimentally determined profile is significantly improved when zero-liquid-velocity boundary conditions are applied at the column walls.

7.4 Conclusions

In the validation study carried out for the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$), simulation results are compared with data from the uniform and non-uniform aeration experiments in the Delft rectangular pseudo-2D column (Harteveld, 2005). The baseline model formulation, with zero-flux wall boundary conditions, is partially validated by the experimental data. Reasonable agreement between the experimental data and corresponding simulation is observed for uniform aeration pattern 1, which would be expected since the baseline model formulation showed the best qualitative agreement with the uniform aeration experiments (Harteveld et al., 2004, 2005) discussed in Chapter 5. The baseline model formulation also shows reasonable agreement between experiments and simulations for non-uniform aeration patterns 3, 5, 6, and 7. However, in the simulations for non-uniform aeration patterns 2 and 4, it appears that the bubbles move too quickly to the center and then to
one side of the column, where sudden upflow is observed. Thus, disagreements between experiments and simulations are observed for aeration patterns 2 and 4.

Accordingly, we have also examined whether selected adjustments to the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$) could improve agreement between experiments and simulations for aeration patterns 2 and 4. Since the baseline model formulation yields stable horizontal modes, stable secondary vertical modes, but unstable Jackson vertical modes (see Chapter 6), we have studied the effect of increasing $C_{BP}$ to 2, which would then stabilize the Jackson vertical modes. Additionally, we have considered the effect of disabling the strain force (setting $C_S = 0$), since it is not a standard term reported in the literature. Finally, we have studied the effect of applying zero-liquid-velocity boundary conditions at the column walls.

Simply adjusting the values of $C_{BP}$ and $C_S$ does not significantly change the simulated flow behavior for patterns 2 and 4. After entering the column, the bubbles continue to move toward one side, where sudden upflow is observed. Thus, the agreement between experiments and simulations is not improved. Applying zero-liquid-velocity wall boundary conditions also results in the entering bubbles initially moving toward one side of the column, where upflow is observed. However, in the upper part of the column, applying zero-liquid-velocity wall boundary conditions appears to provide a stabilizing effect, and in turn improves agreement between experiments and simulations for patterns 2 and 4. Above a height of about 0.60 m, the simulated air velocity vector fields and the corresponding experimentally determined fields appear uniform. At 0.70 m, the simulated liquid velocity profiles and the experimentally determined profiles do not differ extensively in magnitude. As discussed in Chapter 6, applying zero-liquid-velocity wall boundary conditions restricts column motion and thus creates a stabilizing effect. For both patterns 2 and 4, this stabilizing effect is apparent at a column height of 0.70 m (Fig. 7.16), but not at a height of 0.05 m (Fig. 7.15). Note, however, that minor instabilities in the flow would be expected near the air inlet (i.e., near 0.05 m), while greater stability in the flow could be expected at a height of 0.70 m, far from the air inlet.
Chapter 8. Conclusions and Recommendations for Future Work

The numerical studies presented in this work demonstrate that the ability of multiphase CFD models to predict known flow regimes in bubble columns has a strong dependence on grid resolution and model formulation. Sufficient resolution is obtained when cell spacing of 0.25 cm or smaller is used for air-water bubble column simulations. As discussed in Chapter 2, several previous CFD studies reported in the literature used 0.5 cm cell spacing or larger, and it is possible that these results are affected by numerical diffusion. The present work also illustrates that the bubble Reynolds number, the bubble-pressure model, the bubble-induced turbulence model, and the force models (drag, virtual-mass, lift, rotation, and strain) and coefficients have a combined effect on the flow profiles and stability observed in grid-independent CFD simulations of bubble columns.

The fundamental simulation study presented in Chapter 4 shows that using the bubble-induced turbulence model and all force models with \( C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \( C_S = 0.125 \) yields the expected uniform flow predictions for 6-cm, 20-cm, and 40-cm columns operating with low inlet air velocity (e.g., 2 cm/s). It is concluded that the two-fluid model, with these specifications, successfully predicts column scale-up in the homogeneous-flow regime. A reasonable representation of transitions from uniform flow in small (e.g., 6-cm) columns can also be achieved with this model formulation. However, using the BIT model and all force models with \( C_{vm} = 0.5, C_L = C_{rot} = 0.375, \) and \( C_S = 0.125 \) does not result in the expected churn-turbulent flow profile when the column diameter is increased (e.g., 40 cm) for high-flow-rate simulations. This may be due to the absence of a bubble-coalescence model. For high-flow-rate simulations (e.g., 12 cm/s), the flow structures observed in simulations of 6-cm columns have a strong dependence on the bubble Reynolds number. Smaller bubbles \((Re \approx 26)\) yield random structures, while larger bubbles \((Re \approx 880 – 1090)\) yield ordered horizontal plane waves or swarms. Finally, these numerical studies demonstrate that the inlet gas flow rate controls \( \bar{\alpha}_d \) and the bubble diameter controls \( Re. \)

As shown in Chapter 5, flow maps can be used to identify the regions in \( Re-\bar{\alpha}_d \) space where particular flow profiles are observed and to illustrate where flow transitions occur. The dependence of the flow map predictions on the two-fluid model formulation
is examined by enabling all interphase forces, only the drag force, or both the drag and virtual-mass forces. It is concluded that flow-regime predictions for bubble-column simulations must include the full set of force models with $C_{vm} = 0.5$, $C_L = C_{rot} = 0.375$, and $C_S = 0.125$ in order to predict homogeneous flow at high average void fractions as observed in the experiments of Harteveld (2005). Additionally, this model formulation yields homogeneous flow in the same range of inlet flow rates as those used in the Delft experiments (Harteveld et al., 2003, 2004, 2005). The behavior of selected force model components corresponds to the profiles predicted by the flow maps. Examining the behavior of the net vertical drag component shows whether or not the effective drag coefficient for the bubbles is decreasing, yielding an increase in rise velocity. This increase in rise velocity corresponds to the smaller $\bar{\alpha}_d$ value for which transitional or turbulent behavior may be observed for a particular model formulation. It also appears that the role of the strain term is to modulate the instability exhibited by the non-uniform drag components, allowing for a transition from uniform flow to banded structures.

A linear stability analysis of the two-fluid model has been carried out to understand why certain model formulations may yield stable or unstable flow profiles. The analysis in Chapter 6 is primarily organized into vertical and horizontal modes. The horizontal modes appear to be strongly stabilized by certain combinations of $C_{BP}$, $C_L = C_{rot} = C$, and $C_S$, though this effect diminishes with increasing gas holdup. Applying a minimum value of $C_{BP}$ can stabilize the vertical Jackson modes, but this minimum value increases with increasing gas holdup. In general, the vertical secondary modes become unstable if $C_{BP} > 0$ and $2(C - C_S) > C_{vm}$ when bubble-induced turbulence ($C_{BT}$) is suppressed. A non-uniform flow profile with no large-scale turbulent structures is observed when the Jackson modes are unstable, while a turbulent profile is observed when the secondary modes are unstable or when both types of vertical modes are unstable. These observations suggest that nonlinear interactions with the secondary modes may cause transitions to turbulent flow in bubble columns.

It is plausible that at high gas holdups, bubble wakes are suppressed by bubble-bubble interactions, which would dampen bubble-induced turbulence. This would be comparable to modeling $C_{BT}$ as a decreasing function of gas holdup. Indeed, the
numerical studies show that lowering the value of the BIT model constant $C_{BT}$ until the secondary modes become unstable (while keeping the Jackson modes stable) yields a transition from uniform to turbulent flow at high gas holdup ($\sim 0.5$) with a positive lift coefficient. This mechanism differs from previous reports (e.g., Lucas et al., 2005, 2006; Sankaranarayanan and Sundaesan, 2002), in that a transition from uniform to turbulent flow at high holdups occurs without invoking negative lift or cooperative/hindered rise. The column geometry and the choice of wall boundary conditions affect the simulated flow behavior observed after the secondary-mode instability occurs. Applying periodic boundary conditions in a 2D column yields meandering flow structures and banded velocity vector fields. Such behavior is not observed when periodic boundary conditions are applied in a 3D column, as there should be no preference toward the X- or Z-direction due to symmetry. The 3D flow profiles from simulations applying periodic or zero-flux wall boundary conditions are qualitatively similar and exhibit large-scale structures. However, when zero-liquid-velocity wall boundary conditions are applied, the motion in the column is restricted, and thus the flow profile is less unstable than the profiles obtained when using the other types of wall boundary conditions.

The linear stability analysis predictions show consistency with the model formulations that resulted in the homogeneous profiles discussed in Chapters 4 and 5. The baseline model formulation, for which $C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_{L} = C_{rot} = 0.375$, and $C_{S} = 0.125$, yielded the expected homogeneous profiles for the range of bubble $Re$ considered in Chapter 4 for columns operating with low inlet air velocity (e.g., 2 cm/s). In contrast, a nominal model formulation, for which $C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_{L} = C_{rot} = 0.75$, and $C_{S} = 0.25$, did not yield homogeneous profiles for the range of $Re$ considered in Chapter 4. The linear stability analysis shows that both the baseline model formulation and the nominal formulation yield stable horizontal modes, yield stable vertical secondary modes, and can yield stable vertical Jackson modes provided $C_{BP}$ is sufficiently increased. However, the nominal model formulation requires a higher $C_{BP}$ value than that required for the baseline formulation. Thus, the baseline formulation was more likely to yield the desired homogeneous flow profiles. In Chapter 5, simulations using the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_{L} = 0.375$, and $C_{S} = 0.125$) yielded the expected homogeneous profiles for the range of bubble $Re$ considered in Chapter 5.
$C_{\text{rot}} = 0.375$, and $C_{S} = 0.125$) gave the expected homogeneous flow profiles even at high holdup at $Re \approx 700$ as described in Harteveld (2005). This delayed onset of turbulent flow could be attributed to the strongly stabilized horizontal modes, resulting from the particular combination of $C_{BP}$, $C_{L} = C_{\text{rot}}$, and $C_{S}$. In contrast, model formulations including only the drag force ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0$, $C_{L} = C_{\text{rot}} = 0$, and $C_{S} = 0$) or only the drag and virtual-mass forces ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_{L} = C_{\text{rot}} = 0$, and $C_{S} = 0$) did not yield strongly stabilized horizontal modes, and also did not agree qualitatively with the experiments of Harteveld (2005).

Overall, the numerical studies presented in this work demonstrate that the effective viscosity model, the bubble-pressure model, and the full set of interphase force models, with carefully chosen parameters, should be included in order to obtain the flow profiles expected for the operating conditions applied. For example, Chapter 7 shows that the baseline model formulation ($C_{BT} = 0.6$, $C_{BP} = 0.2$, $C_{vm} = 0.5$, $C_{L} = C_{\text{rot}} = 0.375$, and $C_{S} = 0.125$) can predict aspects of flow behavior observed in the experiments of Harteveld (2005) for a uniform aeration case and several non-uniform aeration cases.

Several ideas for future study remain. The present work has been compared to the experiments of Harteveld (2005), for which nearly uniform bubbles are observed and coalescence is suppressed. However, in many practical applications, variations in bubble size and bubble coalescence and breakup would indeed occur. Population balance models could be applied to examine the effect of different bubble sizes in the simulated flow profiles. Coalescence models could perhaps give a more accurate portrayal of column hydrodynamics, especially for high-flow-rate cases. The linear stability analysis focused on disturbances dependent on either vertical or horizontal wavenumbers. Examining the stability at angles in between the vertical and horizontal directions could perhaps provide further insight toward the nature of the instabilities. While linear stability analysis can be used to identify scenarios that might result in flow transitions, it does not account for the wall boundary conditions or domain size. Thus, understanding the nature of flow transitions requires further study regarding the effect of inhomogeneous velocity and volume fraction profiles near the column walls and the effect of the choice of boundary conditions used.
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Appendix A: Expressing the Two-Fluid Model in Dimensionless Form

Recall from Section 3.1 that the continuity equations for the continuous and dispersed phases, respectively, are

$$\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot \left( \alpha_c \rho_c \mathbf{u}_c \right) = 0$$  \hspace{1cm} (A.1)

and

$$\frac{\partial \alpha_d \rho_d}{\partial t} + \nabla \cdot \left( \alpha_d \rho_d \mathbf{u}_d \right) = 0.$$  \hspace{1cm} (A.2)

The momentum balances for the continuous and dispersed phases are

$$\alpha_c \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \alpha_c \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c = -\alpha_c \nabla p + \nabla \cdot \alpha_c \mu_{\text{eff},c} \left[ \nabla \mathbf{u}_c + \left( \nabla \mathbf{u}_c \right)^T \right] + \sum_f F_{fc} + \alpha_c \rho_c g$$  \hspace{1cm} (A.3)

and

$$\alpha_d \rho_d \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = -\alpha_d \nabla p - \nabla P_d + \nabla \cdot \alpha_d \mu_{\text{eff},d} \left[ \nabla \mathbf{u}_d + \left( \nabla \mathbf{u}_d \right)^T \right] + \sum_f F_{fd} + \alpha_d \rho_d g.$$  \hspace{1cm} (A.4)

The terms on the right-hand sides of Eqs. A.3 and A.4 represent, from left to right, the pressure gradient, effective stress, interphase momentum exchange, and the gravitational force. The bubble-pressure model, which is only applied in the dispersed phase (Eq. A.4), is represented by $\nabla P_d$. Finally, recall from Section 3.1.3 that

$$\sum_f F_{jd} = F_{D,d} + F_{vm,d} + F_{L,d} + F_{rot,d} + F_{S,d},$$  \hspace{1cm} (A.5)

and

$$\sum_f F_{jd} = -\sum_f F_{fc}.$$  \hspace{1cm} (A.6)

In the interest of simplicity, the momentum balances can also be expressed in a general form for phase $k$ ($k = c, d$), with the second phase denoted by $l$:

$$\alpha_k \rho_k \frac{\partial \mathbf{u}_k}{\partial t} + \alpha_k \rho_k \mathbf{u}_k \cdot \nabla \mathbf{u}_k = -\alpha_k \nabla p - \nabla P_k + \nabla \cdot \alpha_k \mu_{\text{eff},k} \left[ \nabla \mathbf{u}_k + \left( \nabla \mathbf{u}_k \right)^T \right] + \sum_f F_{fk} + \alpha_k \rho_k g.$$  \hspace{1cm} (A.7)
Expanding Eq. A.7 to show the interphase forces discussed in Section 3.1.3 yields the following expression for the momentum balance for phase $k$:

$$
\alpha_k \rho_k \frac{\partial u_k}{\partial t} + \alpha_k \rho_k u_k \cdot \nabla u_k = -\alpha_k \nabla p - \nabla P_k + \nabla \cdot \alpha_k \mu_{eff,k} \left[ \nabla u_k + \left( \nabla u_k \right)^T \right] + \alpha_k \rho_k g 
$$

$$
-\alpha_k \alpha_i \rho_i C_D \left( Re \right) \frac{3}{4d_b} \left| u_k - u_i \right| \left( u_k - u_i \right) 
$$

$$
-\alpha_k \alpha_i \rho_i C_{vm} \left[ \left( \frac{\partial u_k}{\partial t} + u_k \cdot \nabla u_k \right) - \left( \frac{\partial u_i}{\partial t} + u_i \cdot \nabla u_i \right) \right] 
$$

$$
+\alpha_k \alpha_i \rho_i C_L \left( u_k - u_i \right) \times \nabla \times u_c + \alpha_k \alpha_i \rho_i C_{ro} \left( u_k - u_i \right) \times \nabla \times u_d 
$$

$$
+\alpha_k \alpha_i \rho_i C_S \left[ \left( \nabla u_k + \nabla u_i \right) + \left( \nabla u_k + \nabla u_i \right)^T \right] \cdot \left( u_i - u_k \right) . \quad \text{(A.8)}
$$

The two-fluid model can be scaled using the volume-averaged slip velocity $\bar{U}_S$ for the characteristic velocity, the bubble diameter $d_b$ for the characteristic length, and the continuous-phase molecular viscosity $\mu_{0,c}$ for the characteristic viscosity. The characteristic density is $\rho_c$ and the characteristic time is set to $d_b/\bar{U}_S$. Thus:

$$
x^* = (x/d_b) \Rightarrow x = x^* d_b , \quad \text{(A.9a)}
$$

$$
u^*_k = (u_k/\bar{U}_S) \Rightarrow u_k = u^*_k \bar{U}_S , \quad \text{(A.9b)}
$$

$$
\rho^*_k = (\rho_k/\rho_c) \Rightarrow \rho_k = \rho^*_k \rho_c , \quad \text{(A.9c)}
$$

$$
t^* = \frac{t}{(d_b/\bar{U}_S)} \Rightarrow t = t^* d_b/\bar{U}_S , \quad \text{(A.9d)}
$$

$$
\mu^*_{eff,k} = \left( \mu_{eff,k}/\mu_{0,c} \right) \Rightarrow \mu^*_{eff,k} = \mu^*_{eff,k} \mu_{0,c} , \quad \text{(A.9e)}
$$

$$
p^* = \frac{p}{\rho_c (\bar{U}_S)^2} \Rightarrow p = p^* \rho_c (\bar{U}_S)^2 , \quad \text{(A.9f)}
$$

$$
P^*_k = \frac{P_k}{\rho_c (\bar{U}_S)^2} \Rightarrow P_k = P^*_k \rho_c (\bar{U}_S)^2 , \quad \text{(A.9g)}
$$

and

$$
g^* = g \frac{1}{d_b} \left( \frac{d_b}{\bar{U}_S} \right)^2 = \frac{gd_b}{(\bar{U}_S)^2} \Rightarrow g = g^* \left( \frac{\bar{U}_S}{d_b} \right)^2 . \quad \text{(A.9h)}
$$
Scaling the continuity equation for the continuous phase (Eq. A.1) yields:

\[ \frac{\dot{U}_S}{d_b} \frac{\partial \rho_c \rho_c^*}{\partial t^*} + \frac{1}{d_b} \nabla \cdot \left( \alpha_c \rho_c^* \rho_c^* \mathbf{u}_c^* \dot{U}_S \right) = 0. \]  

(A.10a)

The constants are factored out, resulting in the final expression:

\[ \frac{\rho_c \dot{U}_S}{d_b} \left[ \frac{\partial \rho_c \rho_c^*}{\partial t^*} + \nabla \cdot \left( \alpha_c \rho_c^* \mathbf{u}_c^* \right) \right] = 0 \Rightarrow \frac{\partial \rho_c \rho_c^*}{\partial t^*} + \nabla \cdot \left( \alpha_c \rho_c^* \mathbf{u}_c^* \right) = 0. \]  

(A.10b)

Similarly, for the dispersed phase (Eq. A.2):

\[ \frac{\dot{U}_S}{d_b} \frac{\partial \rho_d \rho_d^*}{\partial t^*} + \frac{1}{d_b} \nabla \cdot \left( \alpha_d \rho_d^* \mathbf{u}_d^* \dot{U}_S \right) = 0 \]  

(A.11a)

\[ \frac{\rho_d \dot{U}_S}{d_b} \left[ \frac{\partial \rho_d \rho_d^*}{\partial t^*} + \nabla \cdot \left( \alpha_d \rho_d^* \mathbf{u}_d^* \right) \right] = 0 \Rightarrow \frac{\partial \rho_d \rho_d^*}{\partial t^*} + \nabla \cdot \left( \alpha_d \rho_d^* \mathbf{u}_d^* \right) = 0. \]  

(A.11b)

Scaling the general form of the momentum balance (Eq. A.8) yields:

\[ \alpha_k \rho_k^* \frac{\dot{U}_S}{d_b} \frac{\partial \mathbf{u}_k^*}{\partial t^*} + \alpha_k \rho_k^* \rho_k^* \mathbf{u}_k^* \dot{U}_S \cdot \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S = -\alpha_k \frac{1}{d_b} \nabla \cdot \rho_k^* \left( \dot{U}_S \right)^2 - \frac{1}{d_b} \nabla \rho_k^* \left( \dot{U}_S \right)^2 \]

\[ \cdots \left[ \frac{\partial \rho_k^*}{\partial t^*} + \nabla \cdot \left( \alpha_k \rho_k^* \mathbf{u}_k^* \right) \right] \]

\[ \left[ \dot{U}_S \frac{\partial \mathbf{u}_k^*}{\partial t^*} + \mathbf{u}_k^* \frac{\partial \dot{U}_S}{\partial t^*} \cdot \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S \right] - \left[ \dot{U}_S \frac{\partial \mathbf{u}_k^*}{\partial t^*} + \mathbf{u}_k^* \frac{\partial \dot{U}_S}{\partial t^*} \cdot \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S \right] \]

\[ + \alpha_k \rho_k^* \rho_k^* \mathbf{C}_{\text{pm}} \left( \mathbf{u}_k^* \dot{U}_S - \mathbf{u}_k^* \dot{U}_S \right) \times \frac{1}{d_b} \nabla \times \mathbf{u}_k^* \dot{U}_S \]

\[ + \alpha_k \rho_k^* \rho_k^* \mathbf{C}_{\text{rot}} \left( \mathbf{u}_k^* \dot{U}_S - \mathbf{u}_k^* \dot{U}_S \right) \times \frac{1}{d_b} \nabla \times \mathbf{u}_k^* \dot{U}_S \]

\[ + \alpha_k \rho_k^* \rho_k^* \mathbf{C}_{\text{Tr}} \left( \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S + \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S \right) + \left( \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S + \frac{1}{d_b} \nabla \mathbf{u}_k^* \dot{U}_S \right)^T \]

\[ \cdots \left( \mathbf{u}_k^* \dot{U}_S - \mathbf{u}_k^* \dot{U}_S \right). \]  

(A.12)
Note that $\rho^*_c$ and $d^*_b$ are both equal to 1. The constants are factored out:

$$\left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \rho^*_k \frac{\partial \mathbf{u}^*_k}{\partial t} + \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \rho^*_k \mathbf{u}^*_k \cdot \nabla \mathbf{u}^*_k$$

$$= -\left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \nabla \mathbf{p}^* - \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \nabla \mathbf{p}^*_k$$

$$+ \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \rho^*_k \mathbf{g}^* + \left( \frac{\mu_{oc}}{d_b} \frac{\bar{U}_S}{d_b} \right) \nabla \cdot \alpha_k \mu^*_{eff,k} \left[ \nabla \mathbf{u}^*_k + \left( \nabla \mathbf{u}^*_k \right)^T \right]$$

$$- \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \alpha_c \rho^*_c C_D \left( \text{Re} \right) \frac{3}{4 d_b} \left[ \mathbf{u}^*_k - \mathbf{u}^*_i \right] \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right)$$

$$- \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \alpha_i \rho^*_i C_m \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \mathbf{C} + \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \cdot \nabla \mathbf{u}^*_i$$

$$+ \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \alpha_i \rho^*_i C_k \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \times \nabla \times \mathbf{u}^*_k$$

$$+ \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \alpha_i \rho^*_i C_{rl} \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \times \nabla \times \mathbf{u}^*_d$$

$$+ \left[ \rho_c \left( \bar{U}_S \right)^2 / d_b \right] \alpha_k \alpha_i \rho^*_i C_S \left( \mathbf{u}^*_k + \mathbf{u}^*_i \right) \cdot \left( \nabla \mathbf{u}^*_k + \left( \nabla \mathbf{u}^*_k \right)^T \right) \cdot \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right).$$

(A.13)

Each term is divided by $\rho_c \left( \bar{U}_S \right)^2 / d_b$, and the Reynolds number appears in the effective viscosity term. Note that the dimensionless numbers now appearing in the two-fluid model are $\text{Re}$ and the force-model coefficients (which may depend on $\text{Re}$).

$$\alpha_k \rho^*_k \frac{\partial \mathbf{u}^*_k}{\partial t} + \alpha_k \rho^*_k \mathbf{u}^*_k \cdot \nabla \mathbf{u}^*_k = -\alpha_k \nabla \mathbf{p}^* - \nabla \mathbf{p}^*_k + \alpha_k \rho^*_k \mathbf{g}^* + \frac{1}{\text{Re}} \nabla \cdot \alpha_k \mu^*_{eff,k} \left[ \nabla \mathbf{u}^*_k + \left( \nabla \mathbf{u}^*_k \right)^T \right]$$

$$- \alpha_k \alpha_i \rho^*_i C_D \left( \text{Re} \right) \frac{3}{4 d_b} \left[ \mathbf{u}^*_k - \mathbf{u}^*_i \right] \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right)$$

$$- \alpha_k \alpha_i \rho^*_i C_m \left[ \left( \frac{\partial \mathbf{u}^*_k}{\partial t} + \mathbf{u}^*_k \cdot \nabla \mathbf{u}^*_k \right) - \left( \frac{\partial \mathbf{u}^*_i}{\partial t} + \mathbf{u}^*_i \cdot \nabla \mathbf{u}^*_i \right) \right]$$

$$+ \alpha_k \alpha_i \rho^*_i C_k \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \times \nabla \times \mathbf{u}^*_k + \alpha_k \alpha_i \rho^*_i C_{rl} \left( \mathbf{u}^*_k - \mathbf{u}^*_i \right) \times \nabla \times \mathbf{u}^*_d$$

$$+ \alpha_k \alpha_i \rho^*_i C_S \left[ \left( \nabla \mathbf{u}^*_k + \nabla \mathbf{u}^*_i \right) + \left( \nabla \mathbf{u}^*_k + \nabla \mathbf{u}^*_i \right)^T \right] \cdot \left( \mathbf{u}^*_i - \mathbf{u}^*_k \right).$$

(A.14)
Appendix B: Perturbations to the Uniform State

A simplified version of the linearization process was given in Chapter 6. Further details can be found in this Appendix.

B.1 Bubbly Flow Equations

The continuity equations for the continuous and dispersed phases are, respectively:

\[
\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c \mathbf{u}_c) = 0 , \tag{B.1}
\]

and

\[
\frac{\partial \alpha_d \rho_d}{\partial t} + \nabla \cdot (\alpha_d \rho_d \mathbf{u}_d) = 0 . \tag{B.2}
\]

Since \( \rho_c \) and \( \rho_d \) are assumed constant, these are divided out of the continuity equations. Also, the substitution \( \alpha_d = 1 - \alpha_c \) is made in Eq. B.1. The continuity equations become:

\[
\frac{\partial (1 - \alpha_d)}{\partial t} + \nabla \cdot [(1 - \alpha_d) \mathbf{u}_c] = 0 , \tag{B.3}
\]

and

\[
\frac{\partial \alpha_c}{\partial t} + \nabla \cdot (\alpha_c \mathbf{u}_d) = 0 . \tag{B.4}
\]

The momentum equations for the continuous and dispersed phases are, respectively:

\[
\alpha_c \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \alpha_c \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c = -\alpha_c \nabla p + \nabla \cdot \alpha_c \mu_{\text{eff},c} \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] + \sum_f F_{fc} + \alpha_c \rho_c \mathbf{g} , \tag{B.5}
\]

and

\[
\alpha_d \rho_d \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = -\alpha_d \nabla p - \nabla \cdot \alpha_d \mu_{\text{eff},d} \left[ \nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T \right] + \sum_f F_{fd} + \alpha_d \rho_d \mathbf{g} . \tag{B.6}
\]

Note that both phases share the pressure \( p \) in \( -\nabla p \), which is unknown. The continuous phase momentum balance (Eq. B.5) can be used to solve for \( -\nabla p \):

\[
-\nabla p = \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c - \frac{1}{\alpha_c} \nabla \cdot \alpha_c \mu_{\text{eff},c} \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] - \frac{1}{\alpha_c} \sum_f F_{fc} - \rho_c \mathbf{g} , \tag{B.7}
\]
and the resulting expression for \(-\nabla p\) derived in Eq. B.7 can be substituted into the dispersed phase momentum balance:

\[
\alpha_d \rho_d \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = \alpha_d \left\{ \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c - \frac{1}{\alpha_c} \nabla \cdot \mathbf{u}_c \mu_{eff,c} \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] - \frac{1}{\alpha_c} \sum_f F_{fc} - \rho_c g \right\} \\
- \nabla P_d + \nabla \cdot \alpha_d \mu_{eff,d} \left[ \nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T \right] + \sum_f F_{fd} + \alpha_d \rho_d g .
\] (B.8)

Noting that \(\sum_f F_{fc} = -\sum_f F_{fd}\) and grouping the like terms allows Eq. B.8 to simplify to

\[
\alpha_d \rho_d \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = \alpha_d \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \alpha_d \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c + \left(1 + \frac{\alpha_d}{1 - \alpha_d}\right) \sum_f F_{fd} - \nabla P_d \\
- \frac{\alpha_d}{1 - \alpha_d} \nabla \cdot (1 - \alpha_d) \mu_{eff,c} \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] + \nabla \cdot \alpha_d \mu_{eff,d} \left[ \nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T \right] + (\rho_d - \rho_c) \alpha_d g .
\] (B.9)

Recall from Section 3.1.1 that

\[
P_d = \rho_c C_{BP} \alpha_d \left( \mathbf{u}_d - \mathbf{u}_c \right) \cdot \left( \mathbf{u}_d - \mathbf{u}_c \right) \left( \frac{\alpha_d}{\alpha_{dp}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dp}} \right).
\] (B.10a)

Additionally, recall from Section 3.1.2 that

\[
\mu_{eff,c} = \mu_{0,c} + C_{bt} \rho_c d_b \alpha_d \left| \mathbf{u}_d - \mathbf{u}_c \right| ,
\] (B.10b)

if the bubble-induced turbulence model is applied in the continuous phase, and

\[
\mu_{eff,d} = \mu_{0,d} + C_{bt} \rho_d d_b \alpha_d \left| \mathbf{u}_d - \mathbf{u}_c \right| ,
\] (B.10c)

if the bubble-induced turbulence model is applied in the dispersed phase. Placing these closures in Eqs. B.5 and B.9 yields the following continuous- and dispersed-phase momentum balances, respectively:

\[
(1 - \alpha_d) \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + (1 - \alpha_d) \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c = - (1 - \alpha_d) \nabla p \\
+ \nabla \cdot (1 - \alpha_d) \left( \mu_{0,c} + C_{bt} \rho_c d_b \alpha_d \left| \mathbf{u}_d - \mathbf{u}_c \right| \right) \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] - \sum_f F_{fd} + (1 - \alpha_d) \rho_c g ,
\] (B.11)
and

\[ \frac{\alpha_d \rho_d}{\partial_t} \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = \alpha_d \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \alpha_d \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c \]

\[ - \frac{\alpha_d}{1 - \alpha_d} \nabla \cdot (1 - \alpha_d) \left( \mu_0 \alpha_c + C_{BT} \rho_c d_b \alpha_d \mathbf{u}_d - \mathbf{u}_c \right) \left[ \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right] \]

\[ + \frac{1}{1 - \alpha_d} \sum_f F_{jd} - \nabla \left[ \rho_c C_{BT} \alpha_d \left( \mathbf{u}_d - \mathbf{u}_c \right) \cdot \left( \mathbf{u}_d - \mathbf{u}_c \right) \left( \frac{\alpha_d}{\alpha_{dp}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dp}} \right) \right] \]

\[ + \nabla \cdot \alpha_d \left( \mu_0 \alpha_d + C_{BT} \rho_c d_b \alpha_d \mathbf{u}_d - \mathbf{u}_c \right) \left[ \nabla \mathbf{u}_d + (\nabla \mathbf{u}_d)^T \right] + \left( \rho_d - \rho_c \right) \alpha_d g, \]

(B.12)

where

\[ \sum_f F_{jd} = F_D + F_m + F_L + F_{rot} + F_S = -\alpha_d \left( 1 - \alpha_d \right) \rho_c C_D \left( Re \right) \frac{3}{4d_b} \mathbf{u}_d - \mathbf{u}_c \left( \mathbf{u}_d - \mathbf{u}_c \right) \]

\[ - \alpha_d \left( 1 - \alpha_d \right) \left[ \left( 1 - \alpha_d \right) \rho_c + \alpha_d \rho_d \right] C_m \left[ \left( \frac{\partial \mathbf{u}_d}{\partial t} + \mathbf{u}_d \cdot \nabla \mathbf{u}_d \right) - \left( \frac{\partial \mathbf{u}_c}{\partial t} + \mathbf{u}_c \cdot \nabla \mathbf{u}_c \right) \right] \]

\[ + \alpha_d \left( 1 - \alpha_d \right) \left[ \left( 1 - \alpha_d \right) \rho_c + \alpha_d \rho_d \right] C_L \left( \mathbf{u}_d - \mathbf{u}_c \right) \times \nabla \times \mathbf{u}_d \]

\[ + \alpha_d \left( 1 - \alpha_d \right) \left[ \left( 1 - \alpha_d \right) \rho_c + \alpha_d \rho_d \right] C_{rot} \left( \mathbf{u}_d - \mathbf{u}_c \right) \times \nabla \times \mathbf{u}_d \]

\[ + \alpha_d \left( 1 - \alpha_d \right) \left[ \left( 1 - \alpha_d \right) \rho_c + \alpha_d \rho_d \right] C_S \left[ \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right) + \left( \nabla \mathbf{u}_c + \nabla \mathbf{u}_d \right)^T \right] \left( \mathbf{u}_c - \mathbf{u}_d \right). \]

(B.13)

The drag coefficient \( C_D \left( Re \right) \) is a function of the Reynolds number. In Chapters 5-6, \( C_\infty \) is set equal to 7/5 in order to agree with the experiments of Harteveld (2005). Thus, the drag force can be expressed as

\[ F_D = -\alpha_d \left( 1 - \alpha_d \right) \rho_c \left[ \frac{7}{5} + \frac{24v_c}{d_b \left| \mathbf{u}_d - \mathbf{u}_c \right|} + \frac{6}{1 + \left( \frac{d_b \left| \mathbf{u}_d - \mathbf{u}_c \right|}{v_c} \right)^{1/2}} \right] \frac{3}{4d_b} \left| \mathbf{u}_d - \mathbf{u}_c \right| \left( \mathbf{u}_d - \mathbf{u}_c \right). \]

(B.14a)
In order to handle the non-linearity in the drag term, Eq. B.14a is simplified and \( |u_d - u_c| \) is set equal to a scalar variable \( a \):

\[
F_d = -\alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21a (u_d - u_c)}{20d_b} + \frac{18\nu_c (u_d - u_c)}{d_b^2} + \frac{9a (u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a}{\nu_c} \right)^\frac{1}{2} \right]^{-1} \right\}.
\]

(B.14b)

Then, a Taylor series expansion about \( a = a_0 \) is performed for Eq. B.14b. Only the zero-order and first-order terms are included (i.e., \( f'(a) = f'(a_0) (a - a_0) \)):

\[
F_d = -\alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21a_0 (u_d - u_c)}{20d_b} + \frac{18\nu_c (u_d - u_c)}{d_b^2} + \frac{9a_0 (u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-1} \right\}
- (a - a_0) \alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21(u_d - u_c)}{20d_b} + \frac{9(u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-1} \right\}
- \frac{9a_0 (u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-2} \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \frac{d_b}{\nu_c} \right\}

(B.15a)

\[
= -\alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21a_0 (u_d - u_c)}{20d_b} + \frac{18\nu_c (u_d - u_c)}{d_b^2} + \frac{9a_0 (u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-1} \right\}
- \alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21(a - a_0)(u_d - u_c)}{20d_b} + \frac{9(a - a_0)(u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-1} \right\}
- \frac{9(a - a_0)(u_d - u_c)}{4d_b} \left[ 1 + \left( \frac{d_b a_0}{\nu_c} \right)^\frac{1}{2} \right]^{-2} \frac{d_b a_0}{\nu_c} \right\}

(B.15b)
Recall that $\alpha$ is equal to $|u_d - u_c|$, and set $a_0$ equal to $u_{d0}$, the constant dispersed-phase velocity in the uniform state. Subsequently, let

$$Re_0 = \frac{d_b u_{d0}}{v_c},$$

the bubble Reynolds number for the uniform state. This yields

$$F_b = -\alpha_d (1 - \alpha_d) \rho_c \left\{ \frac{21a (u_d - u_c) + 18v_c (u_d - u_c)}{20d_b} + \frac{9a (u_d - u_c)}{2d_b} \left[ 1 + \left( \frac{d_b a_0}{v_c} \right)^2 \right]^{-1} \right\},$$

(B.15c)

Finally, recall from Chapter 3 that, through vector manipulation, the lift and rotation forces may also be expressed as:

$$F_L + F_{rot} = \left[ \alpha_c \rho_c C_L (u_d - u_c) \times \nabla \times u_c \right] + \left[ \alpha_c \alpha_d \rho_c C_{rot} (u_d - u_c) \times \nabla \times u_d \right]$$

$$= \alpha_d (1 - \alpha_d) \left[ (1 - \alpha_d) \rho_c + \alpha_d \rho_d \right] (-C) \left[ (\nabla u_c + \nabla u_d) - (\nabla u_c + \nabla u_d)^T \right] (u_c - u_d),$$

(B.16)

where $C_L = C_{rot} = C$.

**B.2 Uniform State**

In order to represent the uniform state for gas-liquid flows, we set $\alpha_d = \alpha_{d0}$, $u_c = 0$, and $u_d = u_{d0} i$, where $\alpha_{d0}$ and $u_{d0}$ are constants and $i$ is the unit vector in the upward vertical direction (Jackson, 2000). The continuous- and dispersed-phase momentum balances from Eqs. B.11 and B.12, respectively, become:
\[(1 - \alpha_{d0}) \rho_c \frac{\partial \mathbf{0}}{\partial t} + (1 - \alpha_{d0}) \rho_c \mathbf{0} \cdot \nabla \mathbf{0} = -(1 - \alpha_{d0}) \nabla \rho_0 \]
\[+ \nabla \cdot (1 - \alpha_{d0}) \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} |u_{d0} i - 0| \right) \left[ \nabla \mathbf{0} + (\nabla \mathbf{0})^T \right] - \sum_f F_{f_{d0}} + (1 - \alpha_{d0}) \rho_c \mathbf{g}, \quad (B.17) \]

and
\[\alpha_{d0} \rho_d \frac{\partial u_{d0} i}{\partial t} + \alpha_{d0} \rho_d u_{d0} i \cdot \nabla u_{d0} i = \alpha_{d0} \rho_c \frac{\partial \mathbf{0}}{\partial t} + \alpha_{d0} \rho_c \mathbf{0} \cdot \nabla \mathbf{0} \]
\[- \frac{\alpha_{d0}}{1 - \alpha_{d0}} \nabla \cdot (1 - \alpha_{d0}) \left( \mu_{0,c} + C_{BT} \rho_c d_b \alpha_{d0} |u_{d0} i - 0| \right) \left[ \nabla \mathbf{0} + (\nabla \mathbf{0})^T \right] \]
\[+ \frac{1}{1 - \alpha_{d0}} \sum_f F_{f_{d0}} - \nabla \left[ \rho_c C_{BT} \alpha_{d0} (u_{d0} i - 0) \cdot (u_{d0} i - 0) \left( \frac{\alpha_{d0}}{\alpha_{dp}} \right) \left( \frac{1 - \alpha_{d0}}{\alpha_{dp}} \right) \right] \]
\[+ \nabla \cdot \alpha_{d0} \left( \mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d0} |u_{d0} i - 0| \right) \left[ \nabla u_{d0} i + (\nabla u_{d0} i)^T \right] + (\rho_d - \rho_c) \alpha_{d0} \mathbf{g}, \quad (B.18) \]

where
\[\sum_f F_{f_{d0}} = F_{D0} + F_{vm,0} + F_{L0} + F_{rot,0} + F_{S0} \]
\[= -\alpha_{d0} (1 - \alpha_{d0}) \rho_c \left[ \frac{21 |u_{d0} i - 0| (u_{d0} i - 0)}{20 d_b} + \frac{18 \nu_u (u_{d0} i - 0) \sqrt{Re_0}}{d_b^2} + \frac{9 |u_{d0} i - 0| (u_{d0} i - 0)}{2 d_b (1 + \sqrt{Re_0})} \right] \]
\[- \frac{9 |u_{d0} i - 0| (u_{d0} i - 0) \sqrt{Re_0}}{4 d_b (1 + \sqrt{Re_0})^2} + \frac{9 u_{d0} (u_{d0} i - 0) \sqrt{Re_0}}{4 d_b (1 + \sqrt{Re_0})^2} \]
\[- \alpha_{d0} (1 - \alpha_{d0}) \left[ (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \right] C_{vm} \left[ \left( \frac{\partial u_{d0} i}{\partial t} + u_{d0} i \cdot \nabla u_{d0} i \right) - \left( \frac{\partial \mathbf{0}}{\partial t} + \mathbf{0} \cdot \nabla \mathbf{0} \right) \right] \]
\[+ \alpha_{d0} (1 - \alpha_{d0}) \left[ (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \right] C_L (u_{d0} i - 0) \times \nabla \times \mathbf{0} \]
\[+ \alpha_{d0} (1 - \alpha_{d0}) \left[ (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \right] C_L (u_{d0} i - 0) \times \nabla \times u_{d0} i \]
\[+ \alpha_{d0} (1 - \alpha_{d0}) \left[ (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \right] C_S \left[ (\nabla \mathbf{0} + \nabla u_{d0} i) + (\nabla \mathbf{0} + \nabla u_{d0} i)^T \right] : (\mathbf{0} - u_{d0} i). \quad (B.19) \]

Eqs. B.17 and B.18 simplify to
\[ 0 = -\nabla p_0 - \frac{F_{d0}}{1 - \alpha_{d0}} + \rho_c g, \quad (B.20) \]

and
\[ 0 = \frac{F_{d0}}{1 - \alpha_{d0}} + \alpha_{d0} (\rho_d - \rho_c) g, \quad (B.21) \]

respectively, where
\[ F_{d0} = -\alpha_{d0} (1 - \alpha_{d0}) \rho_c \beta_0 u_{d0} i, \quad (B.22a) \]

and
\[ \beta_0 = \frac{21u_{d0}}{20d_b} + \frac{18v_c}{d_b^2} + \frac{9u_{d0}}{2d_b (1 + \sqrt{Re_0})}. \quad (B.22b) \]

The sum of Eqs. B.20 and B.21 determines the following hydrostatic equation:
\[ 0 = -\nabla p_0 + \rho_c g + \alpha_{d0} \rho_d g - \alpha_{d0} \rho_c g \Rightarrow \nabla p_0 = \left[ \alpha_{d0} \rho_d + (1 - \alpha_{d0}) \rho_c \right] g. \quad (B.23) \]

Eq. B.20 also determines \( \nabla p_0 \):
\[ 0 = -\nabla p_0 - \left[ \frac{-\alpha_{d0} (1 - \alpha_{d0}) \rho_c \beta_0 u_{d0} i}{1 - \alpha_{d0}} \right] + \rho_c g \Rightarrow \nabla p_0 = \rho_c g + \alpha_{d0} \rho_c \beta_0 u_{d0} i. \quad (B.24) \]

Eq. B.21 determines \( u_{d0} \):
\[ 0 = \frac{-\alpha_{d0} (1 - \alpha_{d0}) \rho_c \beta_0 u_{d0} i}{1 - \alpha_{d0}} + \alpha_{d0} (\rho_d - \rho_c) g, \quad (B.25a) \]
\[ \Rightarrow 0 = \frac{(\rho_d - \rho_c) g}{\rho_c \beta_0} - u_{d0} i \Rightarrow 0 = -\frac{(\rho_d - \rho_c) g}{\rho_c \beta_0} - u_{d0} \Rightarrow -\frac{(\rho_d - \rho_c) g}{\rho_c \beta_0} = u_{d0} \quad (B.25b) \]

If there is no liquid coflow, once \( u_{d0} \) is known, \( \alpha_{d0} \) can be determined from \( u_{d0} \alpha_{d0} = u_g \), where \( u_g \) is the magnitude of the inlet gas velocity.

**B.3 Linear Stability: Perturbations to the Uniform State**

The uniform state is perturbed by setting \( \alpha_d = \alpha_{d0} + \alpha_{d1} \), \( p = p_0 + p_1 \), \( u_d = u_{d0} i + u_{d1} \), and \( u_c = u_{c0} + u_{c1} \), where \( \alpha_{d0} \), \( p_0 \), and \( u_{d0} \) are all constants, \( u_{c0} = 0 \), and \( i \) is the unit vector in the upward vertical direction (Jackson, 2000). Note that a perturbation value (denoted with a subscript 1) multiplied by another perturbation value...
is equal to zero (e.g., $\alpha_d \mathbf{u}_{d1} = 0$). Finally, when necessary we set $\left| \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c1} \right|$ equal to $\left| \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c1} \right|$, and assume the higher order terms are negligible.

Perturbing the continuity equation for the continuous phase (Eq. B.3) yields:

\[
\frac{\partial}{\partial t} \left( 1 - \alpha_{d0} - \alpha_{d1} \right) + \nabla \cdot \left[ (1 - \alpha_{d0} - \alpha_{d1}) \left( \mathbf{u}_{c0} + \mathbf{u}_{c1} \right) \right] = 0 \tag{B.26a}
\]

\[
\rightarrow \frac{\partial}{\partial t} (-\alpha_{d1}) + \nabla \cdot \left[ (1 - \alpha_{d0}) \left( \mathbf{u}_{c1} \right) \right] = 0 \tag{B.26b}
\]

\[
\rightarrow -\frac{\partial \alpha_{d1}}{\partial t} + (1 - \alpha_{d0}) \nabla \cdot \mathbf{u}_{c1} = 0 . \tag{B.26c}
\]

Perturbing the continuity equation for the dispersed phase (Eq. B.4) yields:

\[
\frac{\partial}{\partial t} \left( \alpha_{d0} + \alpha_{d1} \right) + \nabla \cdot \left[ \left( \alpha_{d0} + \alpha_{d1} \right) \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} \right) \right] = 0 \tag{B.27a}
\]

\[
\rightarrow \frac{\partial}{\partial t} \left( \alpha_{d0} + \alpha_{d1} \right) + \nabla \cdot \left( \alpha_{d0} \mathbf{u}_{d0} \mathbf{i} + \alpha_{d1} \mathbf{u}_{d1} \right) + \alpha_{d0} \mathbf{u}_{d1} + \alpha_{d1} \mathbf{u}_{d1} = 0 \tag{B.27b}
\]

\[
\rightarrow \frac{\partial \alpha_{d1}}{\partial t} + \mathbf{u}_{d0} \frac{\partial \alpha_{d1}}{\partial x} + \alpha_{d0} \nabla \cdot \mathbf{u}_{d1} = 0 , \tag{B.27c}
\]

where $x$ represents the vertical direction.

Treating the interphase drag force includes additional assumptions, as discussed below. First, the perturbations are applied:

\[
\mathbf{F}_D = \left[ -\alpha_{d0} (1 - \alpha_{d0}) \rho_c - \alpha_{d1} (1 - 2 \alpha_{d0}) \rho_c \right]
\]

\[
\star \left[ \frac{21}{20 d_b} \left| \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right| \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) + \frac{18 \nu_c}{d_b^2} \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \frac{1}{\left( 1 + \sqrt{Re_0} \right)} \right]
\]

\[
+ \frac{9}{2 d_b} \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \frac{1}{\left( 1 + \sqrt{Re_0} \right)} \right]
\]

\[
- \frac{9}{4 d_b} \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \frac{1}{\left( 1 + \sqrt{Re_0} \right)} \right]
\]

\[
+ \frac{9 u_{d0} \left( \mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1} \right) \sqrt{Re_0}}{4 d_b \left( 1 + \sqrt{Re_0} \right)^2}
\]  

\[
+ \frac{9 u_{d0} (\mathbf{u}_{d0} \mathbf{i} + \mathbf{u}_{d1} - \mathbf{u}_{c0} - \mathbf{u}_{c1}) \sqrt{Re_0}}{4 d_b \left( 1 + \sqrt{Re_0} \right)^2} \tag{B.28a}
\]
\[ \rightarrow \mathbf{F}_D = \left[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c - \alpha_{d_1} (1 - 2 \alpha_{d_0}) \rho_c \right] \left[ \frac{21(u_{d_0} u_{d_0})^2 + u_{d_0} u_{d_1} - u_{d_0} u_{c_1} + |u_{d_1} - u_{c_1}| u_{d_0} i}{20d_b} + \frac{18\nu_c (u_{d_0} i + u_{d_1} - u_{c_1})}{d_b^2} \right] \]

\[ + \frac{9(u_{d_0} u_{d_0} i + u_{d_0} u_{d_1} - u_{d_0} u_{c_1} + |u_{d_1} - u_{c_1}| u_{d_0} i)}{2d_b \left( 1 + \sqrt{Re_0} \right)} - \frac{9\sqrt{Re_0} |u_{d_1} - u_{c_1}| u_{d_0} i}{4d_b \left( 1 + \sqrt{Re_0} \right)^2} \]  

(B.28b)

\[ \rightarrow \mathbf{F}_D = \left[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c - \alpha_{d_1} (1 - 2 \alpha_{d_0}) \rho_c \right] \left[ \frac{21u_{d_0} + 18\nu_c}{d_b^2} + \frac{9u_{d_0}}{2d_b \left( 1 + \sqrt{Re_0} \right)} \right] (u_{d_1} - u_{c_1}) \]

\[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c \left[ \frac{21u_{d_0} + 9u_{d_0}}{20d_b} \right] \left[ \frac{u_{d_0}}{2d_b \left( 1 + \sqrt{Re_0} \right)} \right] \left( u_{d_1} - u_{c_1} \right) \]  

(B.28c)

Assume \(|u_{d_1} - u_{c_1}| i \approx (u_{d_1} - u_{c_1})\) since the vertical component is significantly higher in magnitude than the other components:

\[ \mathbf{F}_D = \left[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c - \alpha_{d_1} (1 - 2 \alpha_{d_0}) \rho_c \right] \left[ \frac{21u_{d_0} + 18\nu_c}{2d_b \left( 1 + \sqrt{Re_0} \right)} \right] u_{d_0} i \]

\[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c \left[ \frac{21u_{d_0} + 18\nu_c}{10d_b} \right] \left[ \frac{u_{d_0}}{d_b \left( 1 + \sqrt{Re_0} \right)} \right] \left( u_{d_1} - u_{c_1} \right) \]

(B.28d)

which simplifies to

\[ \mathbf{F}_D = \left[ -\alpha_{d_0} \left( 1 - \alpha_{d_0} \right) \rho_c - \alpha_{d_1} (1 - 2 \alpha_{d_0}) \rho_c \right] \beta_i u_{d_0} i - \alpha_{d_0} (1 - \alpha_{d_0}) \rho_c \beta_i (u_{d_1} - u_{c_1}) \]

(B.28e)

where

\[ \beta_i = \frac{21u_{d_0} + 18\nu_c}{10d_b} \left[ \frac{u_{d_0}}{d_b \left( 1 + \sqrt{Re_0} \right)} \right] - \frac{9u_{d_0} \sqrt{Re_0}}{4d_b \left( 1 + \sqrt{Re_0} \right)^2} \]  

(B.28f)
Next, recall the continuous-phase momentum balance (Eq. B.11):

\[
(1 - \alpha_d) \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + (1 - \alpha_d) \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c = -(1 - \alpha_d) \nabla \rho
\]

\[+ \nabla \cdot (1 - \alpha_d) \left( \mu_{0c} + C_{BT} \rho_c d \alpha_d \mathbf{u}_d - \mathbf{u}_c \right) \left[ \mathbf{\nabla} \mathbf{u}_c + (\mathbf{\nabla} \mathbf{u}_c)^T \right] - \sum_f F_{fd} + (1 - \alpha_d) \rho_c \mathbf{g}, \]

and divide each term by \((1 - \alpha_d)\):

\[
\rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c = -\nabla \rho + \frac{1}{1 - \alpha_d} \nabla \cdot (1 - \alpha_d) \left( \mu_{0c} + C_{BT} \rho_c d \alpha_d \mathbf{u}_d - \mathbf{u}_c \right) \left[ \mathbf{\nabla} \mathbf{u}_c + (\mathbf{\nabla} \mathbf{u}_c)^T \right]
\]

\[- \frac{1}{1 - \alpha_d} \sum_f F_{fd} + \rho_c \mathbf{g}. \]

The perturbations are applied to the individual terms and the sum of the interphase forces \(\sum F_{fd}\) in Eq. B.29. Recall that a perturbation value multiplied by another perturbation value is equal to zero (e.g., \(\mathbf{u}_{c1} \cdot \nabla \mathbf{u}_{c1} = 0\)), and thus such product terms drop out of the equations. The resulting linearized continuous-phase momentum balance is:

\[
\rho_c \frac{\partial \mathbf{u}_{c1}}{\partial t} = -\nabla p_0 - \nabla p_1 + \left( \mu_{0c} + C_{BT} \rho_c d \alpha_d \mathbf{u}_d \right) \left[ \nabla^2 \mathbf{u}_{c1} + \nabla (\nabla \cdot \mathbf{u}_{c1}) \right] + \rho_c \mathbf{g}
\]

\[- \left[ \frac{1}{1 - \alpha_d} + \frac{\alpha_{d1}}{(1 - \alpha_d)^2} \right] \left[ (1 - \alpha_d) (1 - \alpha_d) \rho_c - \alpha_{d1} (1 - 2\alpha_d) \rho_c \right] \beta_0 \mathbf{u}_d \mathbf{i} \]

\[+ \left[ - \alpha_{d0} (1 - \alpha_d) \rho_c \right] \beta_1 \left( \mathbf{u}_d - \mathbf{u}_{c1} \right) \]

\[- \left[ \frac{1}{1 - \alpha_d} + \frac{\alpha_{d1}}{(1 - \alpha_d)^2} \right] \left[ (1 - \alpha_d) (1 - \alpha_d) \rho_c + \alpha_{d0} \rho_d \right] \]

\[\* C \left( \frac{\partial \mathbf{u}_{d1}}{\partial t} + \mathbf{u}_d \frac{\partial \mathbf{u}_{d1}}{\partial x} - \frac{\partial \mathbf{u}_{c1}}{\partial t} \right) \]

\[- \left[ \frac{1}{1 - \alpha_d} + \frac{\alpha_{d1}}{(1 - \alpha_d)^2} \right] \alpha_{d0} (1 - \alpha_d) \left[ (1 - \alpha_d) \rho_c + \alpha_{d0} \rho_d \right] \]

\[\* C \left[ \mathbf{u}_d \frac{\partial \mathbf{u}_{c1}}{\partial x} + \mathbf{u}_d \frac{\partial \mathbf{u}_{d1}}{\partial x} - \mathbf{u}_d \mathbf{i} \cdot (\nabla \mathbf{u}_{c1})^T \mathbf{u}_d \mathbf{i} \cdot (\nabla \mathbf{u}_{d1})^T \right] \]
\[
- \left[ \frac{1}{1 - \alpha_{d0}} + \frac{\alpha_{d1}}{(1 - \alpha_{d0})^2} \right] \alpha_{d0} (1 - \alpha_{d0}) \left[ (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \right]
\]

\[
\times C_s \left[ -u_{d0} \frac{\partial u_{c1}}{\partial \chi} - u_{d0} \frac{\partial u_{d1}}{\partial \chi} - u_{d0} i \cdot (\nabla u_{c1})^T - u_{d0} i \cdot (\nabla u_{d1})^T \right].
\]

(B.30a)

Let \( \rho_{vo} = (1 - \alpha_{d0}) \rho_c + \alpha_{d0} \rho_d \) and perform further simplification:

\[
\rho_c \frac{\partial u_{c1}}{\partial t} = -\nabla p_0 - \nabla p_1 + (\mu_{o,c} + C_{BT} \rho_c d_o \alpha_{d0} u_{d0}) \left[ \nabla^2 u_{c1} + \nabla \left( \nabla \cdot u_{c1} \right) \right] + \rho_c \mathbf{g}
\]

\[
+ \beta_0 u_{d0} i \left[ \frac{\alpha_{d0} (1 - \alpha_{d0}) \rho_c}{1 - \alpha_{d0}} + \frac{\alpha_{d1} (1 - 2 \alpha_{d0}) \rho_c}{1 - \alpha_{d0}} + \frac{\alpha_{d0} \alpha_{d0} (1 - \alpha_{d0}) \rho_c}{(1 - \alpha_{d0})^2} + \frac{\alpha_{d1} (1 - 2 \alpha_{d0}) \rho_c}{(1 - \alpha_{d0})^2} \right]
\]

\[
+ \frac{\alpha_{d0} (1 - \alpha_{d0}) \rho_c \beta_1 (u_{d1} - u_{c1})}{1 - \alpha_{d0}} + \frac{\alpha_{d0} (1 - \alpha_{d0}) \rho_c \rho_{vo} C_{sm}}{1 - \alpha_{d0}} \left( \frac{\partial u_{d1}}{\partial t} + u_{d0} \frac{\partial u_{d1}}{\partial \chi} - \frac{\partial u_{c1}}{\partial t} \right)
\]

\[
- \frac{\alpha_{d0} (1 - \alpha_{d0}) \rho_c \rho_{vo} C_{s}}{1 - \alpha_{d0}} \left[ -u_{d0} \frac{\partial u_{c1}}{\partial \chi} - u_{d0} \frac{\partial u_{d1}}{\partial \chi} - u_{d0} i \cdot (\nabla u_{c1})^T - u_{d0} i \cdot (\nabla u_{d1})^T \right].
\]

(B.30b)

Recall from Eq. B.20 that

\[
0 = -\nabla p_0 + \rho_c \mathbf{g} + \frac{\alpha_{d0} (1 - \alpha_{d0}) \rho_c \beta_0 u_{d0} i}{1 - \alpha_{d0}};
\]

thus, these terms can be subtracted out of the momentum balance. Finally, the linearized continuous-phase momentum balance equation is given as:

\[
\rho_c \frac{\partial u_{c1}}{\partial t} = -\nabla p_1 + (\mu_{o,c} + C_{BT} \rho_c d_o \alpha_{d0} u_{d0}) \left[ \nabla^2 u_{c1} + \nabla \left( \nabla \cdot u_{c1} \right) \right]
\]

\[
+ \alpha_{d1} \rho_c \beta_0 u_{d0} i + \alpha_{d0} \rho_c \beta_1 (u_{d1} - u_{c1}) + \alpha_{d0} \rho_c \rho_{vo} C_{sm} \left( \frac{\partial u_{d1}}{\partial t} + u_{d0} \frac{\partial u_{d1}}{\partial \chi} - \frac{\partial u_{c1}}{\partial t} \right)
\]

\[
- \alpha_{d0} \rho_c \rho_{vo} C_{s} \left[ -u_{d0} \frac{\partial u_{c1}}{\partial \chi} - u_{d0} \frac{\partial u_{d1}}{\partial \chi} - u_{d0} i \cdot (\nabla u_{c1})^T - u_{d0} i \cdot (\nabla u_{d1})^T \right]
\]

\[
+ \alpha_{d0} \rho_c \rho_{vo} C_{s} \left[ u_{d0} \frac{\partial u_{c1}}{\partial \chi} + u_{d0} \frac{\partial u_{d1}}{\partial \chi} + u_{d0} i \cdot (\nabla u_{c1})^T + u_{d0} i \cdot (\nabla u_{d1})^T \right].
\]

(B.30c)
Finally, recall the dispersed-phase momentum balance (Eq. B.12):
\[
\alpha_d \rho_d \frac{\partial \mathbf{u}_d}{\partial t} + \alpha_d \rho_d \mathbf{u}_d \cdot \nabla \mathbf{u}_d = \alpha_d \rho_c \frac{\partial \mathbf{u}_c}{\partial t} + \alpha_d \rho_c \mathbf{u}_c \cdot \nabla \mathbf{u}_c \\
- \frac{\alpha_d}{1 - \alpha_d} \nabla \cdot \left( (1 - \alpha_d) \left[ \mu_{0,c} + C_B \rho_c d_i \alpha_d |\mathbf{u}_d - \mathbf{u}_c| \right] \nabla \mathbf{u}_c + \left( \nabla \mathbf{u}_c \right)^T \right) \\
+ \frac{1}{1 - \alpha_d} \sum_f F_{fd} - \nabla \left[ \rho_c C_B \alpha_d \left( \mathbf{u}_d - \mathbf{u}_c \right) \cdot \left( \mathbf{u}_d - \mathbf{u}_c \right) \left( \frac{\alpha_d}{\alpha_{dp}} \right) \left( 1 - \frac{\alpha_d}{\alpha_{dp}} \right) \right] \\
+ \nabla \cdot \alpha_d \left( \mu_{0,d} + C_B \rho_c d_i \alpha_d |\mathbf{u}_d - \mathbf{u}_c| \right) \left( \nabla \mathbf{u}_d + \left( \nabla \mathbf{u}_d \right)^T \right) + \left( \rho_d - \rho_c \right) \alpha_d \mathbf{g}.
\] (B.12)

The perturbations are applied to the individual terms and the sum of the interphase forces \( \sum_f F_{fd} \) in Eq. B.12. Recall that a perturbation value multiplied by another perturbation value is equal to zero (e.g., \( \mathbf{u}_{c_1} \cdot \nabla \mathbf{u}_{c_1} = 0 \)), and thus such product terms drop out of the equations. The resulting linearized dispersed-phase momentum balance is:
\[
\alpha_{d0} \rho_d \frac{\partial \mathbf{u}_{d1}}{\partial t} + \alpha_{d0} \rho_d \mathbf{u}_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} = \left[ \alpha_{d0} \mu_{0,c} + C_B \rho_c d_i \alpha_{d0}^2 u_{d0} \right] \left( \nabla^2 \mathbf{u}_{c1} + \nabla \left( \nabla \cdot \mathbf{u}_{c1} \right) \right) \\
- \rho_c C_B \alpha_{d0}^2 \left( \frac{\alpha_{d0}}{\alpha_{dp}} \right) \left( 1 - \frac{\alpha_{d0}}{\alpha_{dp}} \right) \left( \rho_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - u_{d0} \frac{\partial \mathbf{u}_{c1}}{\partial x} \right) - \rho_c C_B u_{d0}^2 \left( 2 \frac{\alpha_{d0}}{\alpha_{dp}} - \frac{3 \alpha_{d0}^2}{\alpha_{dp}^2} \right) \nabla \mathbf{u}_{c1} \\
+ \left( \alpha_{d0} \mu_{0,d} + C_B \rho_c d_i \alpha_{d0}^2 u_{d0} \right) \left( \nabla^2 \mathbf{u}_{d1} + \nabla \left( \nabla \cdot \mathbf{u}_{d1} \right) \right) + \left( \alpha_{d0} + \alpha_{d1} \right) \left( \rho_d - \rho_c \right) \mathbf{g} \\
+ \left[ \frac{1}{1 - \alpha_{d0}} + \frac{\alpha_{d1}}{(1 - \alpha_{d0})^2} \right] \left[ -\alpha_{d0} \left( 1 - \alpha_{d0} \right) \rho_c - \alpha_{d1} \left( 1 - 2 \alpha_{d0} \right) \rho_c \right] \beta_0 u_{d0} \mathbf{i} \\
+ \left[ -\alpha_{d0} \left( 1 - \alpha_{d0} \right) \rho_c \right] \beta_1 \left( \mathbf{u}_{d1} - \mathbf{u}_{c1} \right) \\
+ \left[ \frac{1}{1 - \alpha_{d0}} + \frac{\alpha_{d1}}{(1 - \alpha_{d0})^2} \right] \left[ -\alpha_{d0} \left( 1 - \alpha_{d0} \right) \rho_c + \alpha_{d0} \rho_d \right] \\
* C_{v_m} \left( \frac{\partial \mathbf{u}_{d1}}{\partial t} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - \frac{\partial \mathbf{u}_{c1}}{\partial t} \right)
\]
\[
\left[ \frac{1}{1 - \alpha_{d_0}} + \frac{\alpha_{d_1}}{(1 - \alpha_{d_0})^2} \right] \alpha_{d_0} (1 - \alpha_{d_0}) \left[ (1 - \alpha_{d_0}) \rho_c + \alpha_{d_0} \rho_d \right] \\
* C \left[ u_{d_0} \frac{\partial u_{c_1}}{\partial x} + u_{d_0} \frac{\partial u_{d_1}}{\partial x} - u_{d_0} i \cdot (\nabla u_{c_1})^T - u_{d_0} i \cdot (\nabla u_{d_1})^T \right] \\
\left[ \frac{1}{1 - \alpha_{d_0}} + \frac{\alpha_{d_1}}{(1 - \alpha_{d_0})^2} \right] \alpha_{d_0} (1 - \alpha_{d_0}) \left[ (1 - \alpha_{d_0}) \rho_c + \alpha_{d_0} \rho_d \right] \\
\left[ \frac{1}{1 - \alpha_{d_0}} + \frac{\alpha_{d_1}}{(1 - \alpha_{d_0})^2} \right] \alpha_{d_0} (1 - \alpha_{d_0}) \left[ (1 - \alpha_{d_0}) \rho_c + \alpha_{d_0} \rho_d \right] \\
* C_s \left[ -u_{d_0} \frac{\partial u_{c_1}}{\partial x} - u_{d_0} \frac{\partial u_{d_1}}{\partial x} - u_{d_0} i \cdot (\nabla u_{c_1})^T - u_{d_0} i \cdot (\nabla u_{d_1})^T \right].
\]  

(B.31a)

Let \( \rho_{v_0} = (1 - \alpha_{d_0}) \rho_c + \alpha_{d_0} \rho_d \) and perform further simplification:

\[
\begin{align*}
\alpha_{d_0} \rho_d \frac{\partial u_{d_1}}{\partial t} + \alpha_{d_0} \rho_d u_{d_0} \frac{\partial u_{d_1}}{\partial x} \\
= \alpha_{d_0} \rho_c \frac{\partial u_{c_1}}{\partial t} - \left( \alpha_{d_0} \mu_{o_x} + C_{BT} \rho_c \alpha_{d_0} \alpha_{d_0} \alpha_{d_0} u_{d_0} \right) \left[ \nabla^2 u_{c_1} + \nabla (\nabla \cdot u_{c_1}) \right] \\
- \rho_c C_B \beta_2 \left( \frac{\alpha_{d_0}^2}{\alpha_{d_p}} \right) \left( 1 - \frac{\alpha_{d_0}}{\alpha_{d_p}} \right) \left( u_{d_0} \frac{\partial u_{d_1}}{\partial x} - u_{d_0} \frac{\partial u_{c_1}}{\partial x} \right) - \rho_c C_B \beta_2 \frac{\alpha_{d_0}^2}{\alpha_{d_p}} \frac{3 \alpha_{d_0}^2}{\alpha_{d_p}^2} \nabla \alpha_{d_1} \\
+ \left( \alpha_{d_0} \mu_{o_d} + C_{BT} \rho_c \alpha_{d_0} \alpha_{d_0} \alpha_{d_0} u_{d_0} \right) \left[ \nabla^2 u_{d_1} + \nabla (\nabla \cdot u_{d_1}) \right] + \left( \alpha_{d_0} + \alpha_{d_1} \right) \left( \rho_d - \rho_c \right) g \\
+ \beta_0 u_{d_0} i \left[ \frac{- \frac{\alpha_{d_0} \rho_c}{1 - \alpha_{d_0}} - \frac{\alpha_{d_1} \rho_c}{1 - \alpha_{d_0}} - \frac{\alpha_{d_0} \rho_c}{1 - \alpha_{d_0}} - \frac{\alpha_{d_1} \rho_c}{1 - \alpha_{d_0}}}{1 - \alpha_{d_0}} \right] \\
- \frac{\alpha_{d_0} \rho_c}{1 - \alpha_{d_0}} \beta_1 \left( u_{d_1} - u_{c_1} \right) - \frac{\alpha_{d_0} \rho_c}{1 - \alpha_{d_0}} \frac{\rho_{v_0} C_{W_m}}{1 - \alpha_{d_0}} \left( \frac{\partial u_{d_1}}{\partial t} + u_{d_0} \frac{\partial u_{d_1}}{\partial x} - \frac{\partial u_{c_1}}{\partial t} \right) \\
+ \frac{\alpha_{d_0} \rho_{v_0} C_s}{1 - \alpha_{d_0}} \left[ u_{d_0} \frac{\partial u_{c_1}}{\partial x} + u_{d_0} \frac{\partial u_{d_1}}{\partial x} - u_{d_0} i \cdot (\nabla u_{c_1})^T - u_{d_0} i \cdot (\nabla u_{d_1})^T \right] \\
+ \frac{\alpha_{d_0} \rho_{v_0} C_s}{1 - \alpha_{d_0}} \left[ -u_{d_0} \frac{\partial u_{c_1}}{\partial x} - u_{d_0} \frac{\partial u_{d_1}}{\partial x} - u_{d_0} i \cdot (\nabla u_{c_1})^T - u_{d_0} i \cdot (\nabla u_{d_1})^T \right].
\end{align*}
\]  

(B.31b)

Recall from Eq. B.21 that

\[
0 = - \frac{\alpha_{d_0} \rho_{v_0} u_{d_0} i}{1 - \alpha_{d_0}} + \alpha_{d_0} \left( \rho_d - \rho_c \right) g;
\]
thus, these terms can be subtracted out of the momentum balance. Finally, the linearized dispersed-phase momentum balance equation is given as:

\[ \alpha_{d0} \rho_d \frac{\partial \hat{u}_{d1}}{\partial t} + \alpha_{d0} \rho_d u_{d0} \frac{\partial \hat{u}_{d1}}{\partial x} = \alpha_{d0} \rho_c \frac{\partial \hat{u}_{c1}}{\partial t} - \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho_c \alpha_{d0}^2 u_{d0} \right) \left[ \nabla^2 u_{c1} + \nabla \left( \nabla \cdot u_{c1} \right) \right] \]

\[-\rho_c C_{bp} 2 \left( \frac{\alpha_{d0}^2}{\alpha_{dep}} \right) \left( 1 - \frac{\alpha_{d0}^2}{\alpha_{dep}} \right) \left( u_{d0} \frac{\partial u_{d1}}{\partial x} - u_{d0} \frac{\partial u_{c1}}{\partial x} \right) - \alpha_{d1} C_{bp} \rho_{d0}^2 \left( \frac{2 \alpha_{d0}}{\alpha_{dep}} - \frac{3 \alpha_{d0}^2}{\alpha_{dep}^2} \right) \nabla \alpha_{d1} \]

\[+ \left( \alpha_{d0} \mu_{0,d} + C_{BT} \rho_c \alpha_{d0}^2 u_{d0} \right) \left[ \nabla^2 u_{d1} + \nabla \left( \nabla \cdot u_{d1} \right) \right] + \alpha_{d1} (\rho_d - \rho_c) g \]

\[-\alpha_{d1} \rho_c \beta_0 u_{d0} i - \alpha_{d0} \rho_c \beta_1 \left( u_{d1} - u_{c1} \right) - \alpha_{d0} \rho_{v0} C_{vm} \left( \frac{\partial u_{d1}}{\partial t} + u_{d0} \frac{\partial u_{d1}}{\partial x} - \frac{\partial u_{c1}}{\partial t} \right) \]

\[+ \alpha_{d0} \rho_{v0} C_s \left[ u_{d0} \frac{\partial u_{c1}}{\partial x} + u_{d0} \frac{\partial u_{d1}}{\partial x} - u_{d0} i \cdot (\nabla u_{c1})^\top - u_{d0} i \cdot (\nabla u_{d1})^\top \right] \]

\[-\alpha_{d0} \rho_{v0} C_s \left[ u_{d0} \frac{\partial u_{c1}}{\partial x} + u_{d0} \frac{\partial u_{d1}}{\partial x} + u_{d0} i \cdot (\nabla u_{c1})^\top + u_{d0} i \cdot (\nabla u_{d1})^\top \right]. \quad (B.31c) \]

According to Jackson (2000), the perturbed continuity equations and momentum balance equations comprise a set of linear partial differential equations in the components of \( u_{c1} \), the components of \( u_{d1} \), and the scalar variables \( \alpha_{d1} \) and \( p_1 \). Solutions take the form

\[ \left( u_{c1}, u_{d1}, \alpha_{d1}, p_1 \right) = \left( \hat{u}_{c1}, \hat{u}_{d1}, \hat{\alpha}_{d1}, \hat{p}_1 \right) \exp( st ) \exp( ik \cdot x ), \quad (B.32) \]

where \( \hat{\alpha}_{d1}, \hat{p}_1 \), and the components of \( \hat{u}_{c1} \) and \( \hat{u}_{d1} \) are constants. Appendix C presents the solution of the set of linear partial differential equations and the derivation of the dispersion relations for the two-fluid model.
Appendix C: Derivation of Dispersion Relations

The set of linear partial differential equations derived in Appendix B is solved using (Jackson, 2000):

\[
\left( u_{c1}, u_{d1}, \alpha_{d1}, p_{i} \right) = (\hat{u}_{c1}, \hat{u}_{d1}, \hat{\alpha}_{d1}, \hat{p}_{i}) \exp(st) \exp(ik \cdot x). \quad (B.32)
\]

This yields a set of algebraic equations with \( \hat{\alpha}_{d1}, \hat{p}_{i} \), and the components of \( \hat{u}_{c1} \) and \( \hat{u}_{d1} \) as the unknowns. For simplicity, the derivation presented here is for a 2D case—only the vertical \( (k_{1}) \) and horizontal \( (k_{2}) \) velocity components for \( \hat{u}_{c1} \) and \( \hat{u}_{d1} \) are included. The 3D case would include two additional equations arising from the velocity components in the third dimension. Based on symmetry, the equations for the third dimension \( (k_{3}) \) would have the same form as those for the second dimension \( (k_{2}) \). Finally, note that \( i \) is a unit vector in the upward vertical direction, and that direction 1 is vertical. Also, \( x \) denotes a vector, while \( x \) denotes the vertical component (i.e., \( x_{1} \)).

C.1 Solving System of Equations

The continuity equation for the continuous phase is solved first:

\[
- \frac{\partial \alpha_{d1}}{\partial t} + (1 - \alpha_{d0}) \nabla \cdot u_{c1} = 0
\]

\[
\rightarrow - \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) \frac{\partial}{\partial t} + (1 - \alpha_{d0}) \nabla \cdot \left[ \hat{u}_{c1} \exp(st) \exp(ik \cdot x) \right] = 0 \quad (C.1a)
\]

\[
\rightarrow -s \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) + (1 - \alpha_{d0}) (\hat{u}_{c1} \cdot ik) \exp(st) \exp(ik \cdot x) = 0 \quad (C.1b)
\]

\[
\rightarrow -s \hat{\alpha}_{d1} + (1 - \alpha_{d0}) ik_{1} \hat{u}_{c1,1} + (1 - \alpha_{d0}) ik_{2} \hat{u}_{c1,2} = 0. \quad (C.1c)
\]

The continuity equation for the dispersed phase is solved next:

\[
\frac{\partial \alpha_{d1}}{\partial t} + u_{d0} \frac{\partial \alpha_{d1}}{\partial x} + \alpha_{d0} \nabla \cdot u_{d1} = 0
\]

\[
\rightarrow \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) \frac{\partial}{\partial t} + u_{d0} \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) \frac{\partial}{\partial x} + \alpha_{d0} \nabla \cdot \left[ \hat{u}_{d1} \exp(st) \exp(ik \cdot x) \right] = 0 \quad (C.2a)
\]

\[
\rightarrow s \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) + u_{d0} \hat{\alpha}_{d1} ik_{1} \exp(st) \exp(ik \cdot x) + \alpha_{d0} (\hat{u}_{d1} \cdot ik) \exp(st) \exp(ik \cdot x) = 0 \quad (C.2b)
\]

\[
\rightarrow (s + u_{d0} ik_{1}) \hat{\alpha}_{d1} + \alpha_{d0} ik_{1} \hat{u}_{d1,1} + \alpha_{d0} ik_{2} \hat{u}_{d1,2} = 0. \quad (C.2c)
\]
Recall that the linearized continuous-phase momentum equation is defined as:

\[
\rho_c \frac{\partial \mathbf{u}_c}{\partial t} = -\nabla p + \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left[ \nabla^2 \mathbf{u}_c + \nabla (\nabla \cdot \mathbf{u}_c) \right] \\
+ \alpha_{d1} \rho_c \beta_0 u_{d0} \mathbf{i} + \alpha_{d0} \rho_c \beta_1 (\mathbf{u}_{d1} - \mathbf{u}_c) + \alpha_{d0} \rho_c \gamma_0 C_{sm} \left( \frac{\partial \mathbf{u}_{d1}}{\partial t} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - \frac{\partial \mathbf{u}_c}{\partial t} \right) \\
- \alpha_{d0} \rho_c \gamma_0 C_s \left[ u_{d0} \frac{\partial \mathbf{u}_c}{\partial x} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} - u_{d0} \mathbf{i} \cdot (\nabla \mathbf{u}_c)^T - u_{d0} \mathbf{i} \cdot (\nabla \mathbf{u}_{d1})^T \right] \\
+ \alpha_{d0} \rho_c \gamma_0 C_s \left[ u_{d0} \frac{\partial \mathbf{u}_c}{\partial x} + u_{d0} \frac{\partial \mathbf{u}_{d1}}{\partial x} + u_{d0} \mathbf{i} \cdot (\nabla \mathbf{u}_c)^T + u_{d0} \mathbf{i} \cdot (\nabla \mathbf{u}_{d1})^T \right]. 
\]

(C.3)

Applying the solution to the linearized continuous-phase momentum balance yields:

\[
\rho_c \mathbf{s} \hat{\mathbf{u}}_c \exp(st) \exp(ik \cdot x) = -\hat{\mathbf{p}}_i \exp(st) ik \exp(ik \cdot x) \\
+ \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left[ -k^2 \hat{\mathbf{u}}_c \exp(st) \exp(ik \cdot x) + \left( \hat{\mathbf{u}}_c + ik \hat{\mathbf{u}}_{d1} \right) \exp(st) \right] \\
+ \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) \rho_c \beta_0 u_{d0} \mathbf{i} + \alpha_{d0} \rho_c \beta_1 \exp(st) \exp(ik \cdot x) \left( \hat{\mathbf{u}}_{d1} - \hat{\mathbf{u}}_c \right) \\
+ \alpha_{d0} \rho_c \gamma_0 C_{sm} \left[ \mathbf{s} \hat{\mathbf{u}}_{d1} \exp(st) \exp(ik \cdot x) + u_{d0} \hat{\mathbf{u}}_{d1} \exp(st) \right] ik \exp(ik \cdot x) \\
- \mathbf{s} \hat{\mathbf{u}}_{c1} \exp(st) \exp(ik \cdot x) \\
- \alpha_{d0} \rho_c \gamma_0 \mathbf{C}_{ud0} \left( ik \hat{\mathbf{u}}_c \exp(st) \exp(ik \cdot x) + ik \mathbf{u}_{d1} \exp(st) \exp(ik \cdot x) \right) \\
- \left[ \hat{\mathbf{u}}_c \exp(st) \cdot \mathbf{i} \right] ik \exp(ik \cdot x) - \left[ \hat{\mathbf{u}}_{d1} \exp(st) \cdot \mathbf{i} \right] ik \exp(ik \cdot x) \\
+ \alpha_{d0} \rho_c \gamma_0 \mathbf{C}_{ud0} \left( ik \hat{\mathbf{u}}_c \exp(st) \exp(ik \cdot x) + ik \mathbf{u}_{d1} \exp(st) \exp(ik \cdot x) \right) \\
+ \left[ \hat{\mathbf{u}}_c \exp(st) \cdot \mathbf{i} \right] ik \exp(ik \cdot x) + \left[ \hat{\mathbf{u}}_{d1} \exp(st) \cdot \mathbf{i} \right] ik \exp(ik \cdot x) \right]. 
\]

(C.4)

Place each term in Eq. C.4 on the same side and divide by \( \exp(st) \exp(ik \cdot x) \):

\[
-\rho_c \mathbf{s} \hat{\mathbf{u}}_c - \hat{\mathbf{p}}_i \mathbf{k} + \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left[ -k^2 \hat{\mathbf{u}}_c + (\hat{\mathbf{u}}_c + ik \hat{\mathbf{u}}_{d1}) \mathbf{k} \right] \\
+ \hat{\alpha}_{d1} \rho_c \beta_0 u_{d0} \mathbf{i} + \alpha_{d0} \rho_c \beta_1 \left( \mathbf{u}_{d1} - \mathbf{u}_c \right) + \alpha_{d0} \rho_c \gamma_0 C_{sm} \left( \mathbf{s} \hat{\mathbf{u}}_{d1} + u_{d0} \hat{\mathbf{u}}_{d1} \mathbf{k} - \mathbf{s} \hat{\mathbf{u}}_c \right) \\
- \alpha_{d0} \rho_c \gamma_0 \mathbf{C}_{ud0} \left[ ik \hat{\mathbf{u}}_c + ik \hat{\mathbf{u}}_{d1} - (\hat{\mathbf{u}}_c \cdot \mathbf{i}) \mathbf{k} - (\hat{\mathbf{u}}_{d1} \cdot \mathbf{i}) \mathbf{k} \right] \\
+ \alpha_{d0} \rho_c \gamma_0 \mathbf{C}_{ud0} \left[ ik \hat{\mathbf{u}}_c + ik \hat{\mathbf{u}}_{d1} + (\hat{\mathbf{u}}_c \cdot \mathbf{i}) \mathbf{k} + (\hat{\mathbf{u}}_{d1} \cdot \mathbf{i}) \mathbf{k} \right] = 0. 
\]

(C.5)
Eq. C.5 is now expressed in terms of vector components:

\[
-\rho_S \begin{bmatrix} \dot{u}_{c_{11}} \\ \dot{u}_{c_{12}} \end{bmatrix} - \tilde{p}_i \begin{bmatrix} k_1 \\ k_2 \end{bmatrix} + \left( \mu_{0,c} + C_{BT} \rho_c d_\alpha \alpha_{d0} u_{d0} \right) \begin{bmatrix} -k_1^2 \begin{bmatrix} \ddot{u}_{c_{11}} \\ \ddot{u}_{c_{12}} \end{bmatrix} + \begin{bmatrix} \dot{u}_{c_{11}} i k_1 + \dot{u}_{c_{12}} i k_2 \end{bmatrix} i k_3 \\ \ddot{u}_{c_{12}} \end{bmatrix} \\
+ \rho_c \beta_0 u_{d0} \begin{bmatrix} \tilde{a}_{d_{11}} \\ \tilde{a}_{d_{12}} \end{bmatrix} \cdot \alpha_{d0} \rho_c \beta_1 \begin{bmatrix} \ddot{u}_{d_{11},1} - \ddot{u}_{c_{11}} \\ \ddot{u}_{d_{12},1} - \ddot{u}_{c_{12}} \end{bmatrix} + \alpha_{d0} \rho_v C_{sm} \begin{bmatrix} s \begin{bmatrix} \ddot{u}_{d_{11},1} \\ \ddot{u}_{d_{12},1} \end{bmatrix} + u_{d0} i k_1 \begin{bmatrix} \dot{u}_{d_{11},1} \\ \dot{u}_{d_{12},1} \end{bmatrix} - s \ddot{u}_{c_{11}} \end{bmatrix} \\
- \alpha_{d0} \rho_v C_{d0} \begin{bmatrix} i k_1 \dot{u}_{c_{11}} \\ i k_1 \dot{u}_{c_{12}} \end{bmatrix} + i k_1 \begin{bmatrix} \ddot{u}_{c_{11}} \\ \ddot{u}_{c_{12}} \end{bmatrix} - \dddot{u}_{c_{11}} i k_1 - \dddot{u}_{c_{12}} i k_2 \end{bmatrix} = 0.
\]

(C.6)

Eq. C.6 is simplified:

\[
-\rho_S \begin{bmatrix} \dot{u}_{c_{11}} \\ \dot{u}_{c_{12}} \end{bmatrix} - \tilde{p}_i \begin{bmatrix} k_1 \\ k_2 \end{bmatrix} + \left( \mu_{0,c} + C_{BT} \rho_c d_\alpha \alpha_{d0} u_{d0} \right) \begin{bmatrix} -k_1^2 \begin{bmatrix} \ddot{u}_{c_{11}} \\ \ddot{u}_{c_{12}} \end{bmatrix} + \begin{bmatrix} \dot{u}_{c_{11}} i k_1 + \dot{u}_{c_{12}} i k_2 \end{bmatrix} i k_3 \\ \ddot{u}_{c_{12}} \end{bmatrix} \\
+ \rho_c \beta_0 u_{d0} \begin{bmatrix} \tilde{a}_{d_{11}} \\ 0 \end{bmatrix} + \alpha_{d0} \rho_c \beta_1 \begin{bmatrix} \ddot{u}_{d_{11},1} - \ddot{u}_{c_{11}} \\ \ddot{u}_{d_{12},1} - \ddot{u}_{c_{12}} \end{bmatrix} + \alpha_{d0} \rho_v C_{sm} \begin{bmatrix} s \begin{bmatrix} \ddot{u}_{d_{11},1} \\ \ddot{u}_{d_{12},1} \end{bmatrix} + u_{d0} i k_1 \begin{bmatrix} \dot{u}_{d_{11},1} \\ \dot{u}_{d_{12},1} \end{bmatrix} - s \ddot{u}_{c_{11}} \end{bmatrix} \\
- \alpha_{d0} \rho_v C_{d0} \begin{bmatrix} i k_1 \dot{u}_{c_{11}} \\ i k_1 \dot{u}_{c_{12}} \end{bmatrix} + i k_1 \begin{bmatrix} \ddot{u}_{c_{11}} \\ \ddot{u}_{c_{12}} \end{bmatrix} - \dddot{u}_{c_{11}} i k_1 - \dddot{u}_{c_{12}} i k_2 \end{bmatrix} = 0.
\]

(C.7)

Two equations can be obtained from the matrix expressions in Eq. C.7. These are:

\[
-\rho_v \dot{u}_{c_{11}} - \tilde{p}_i k_1 + \left( \mu_{0,c} + C_{BT} \rho_c d_\beta \alpha_{d0} u_{d0} \right) \begin{bmatrix} -k_1^2 \dddot{u}_{c_{11}} + \begin{bmatrix} \dot{u}_{c_{11}} i k_1 + \dot{u}_{c_{12}} i k_2 \end{bmatrix} i k_3 \\ \ddot{u}_{c_{12}} \end{bmatrix} \\
+ \rho_c \beta_0 u_{d0} \tilde{a}_{d_{11}} + \alpha_{d0} \rho_c \beta_1 \begin{bmatrix} \ddot{u}_{d_{11},1} - \ddot{u}_{c_{11}} \\ \ddot{u}_{d_{12},1} - \ddot{u}_{c_{12}} \end{bmatrix} + \alpha_{d0} \rho_v C_{sm} \begin{bmatrix} s \ddot{u}_{d_{11},1} + u_{d0} i k_1 \ddot{u}_{d_{11},1} - s \ddot{u}_{c_{11}} \\ s \ddot{u}_{d_{12},1} + u_{d0} i k_1 \ddot{u}_{d_{12},1} - s \ddot{u}_{c_{12}} \end{bmatrix} \\
- \alpha_{d0} \rho_v C_{d0} \begin{bmatrix} i k_1 \ddot{u}_{c_{11}} + i k_1 \ddot{u}_{c_{12}} \end{bmatrix} - \dddot{u}_{c_{11}} i k_1 + \dddot{u}_{c_{12}} i k_2 \end{bmatrix} = 0,
\]

(C.8)
Expanding the terms in Eq. C.8 yields

\[-\rho_c \hat{u}_{c_{11}} - \hat{p}_1 k_1 - \left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \left( k^2 \hat{u}_{c_{11}} - \left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \hat{u}_{c_{11}} k_1^2 \right) \]

\[-\left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \hat{u}_{c_{11}} k_1^2 + \rho_c \beta_0 u_{d_0} \hat{\alpha}_d + \alpha_d \rho_c \beta_1 \hat{u}_{d_{11}} - \rho_c \beta_1 \hat{u}_{c_{11}} + \alpha_d \rho_c \beta_0 \hat{u}_{d_{11}} \]

\[+\alpha_d \rho_c \beta_1 \left( \hat{u}_{d_{11}} \right) - \alpha_d \rho_c \beta_1 \hat{u}_{d_{11}} + \alpha_d \rho_c \beta_0 \hat{u}_{c_{11}} k_1 \]

\[+\alpha_d \rho_c \beta_0 \hat{u}_{c_{11}} k_1 + \alpha_d \rho_c \beta_0 \hat{u}_{d_{11}} k_1 \]

Grouping the like terms in Eq. C.10 yields

\[\hat{u}_{c_{11}} \left[ -\rho_c s - \left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \left( k^2 + k_1^2 \right) - \alpha_d \rho_c \beta_1 - \alpha_d \rho_c \beta_0 C_{vm} s + 2\alpha_d \rho_c \beta_0 C_{vm} u_{d_0} k_1 \right] \]

\[+\hat{u}_{c_{12}} \left[ -\left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) k_1 k_2 \right] \]

\[+\hat{u}_{d_{11}} \left[ \alpha_d \rho_c \beta_1 + \alpha_d \rho_c \beta_0 C_{vm} \left( s + u_{d_0} k_1 \right) + 2\alpha_d \rho_c \beta_0 C_{vm} u_{d_0} k_1 \right] \]

\[+\hat{u}_{d_{12}} \left( 0 + \hat{\alpha}_d \left( \rho_c \beta_0 u_{d_0} \right) + \hat{p}_1 \left( -k_1 \right) \right) = 0. \]

Similarly, expanding the terms in Eq. C.9 yields

\[-\rho_c \hat{u}_{c_{12}} - \hat{p}_1 k_2 - \left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \left( k^2 \hat{u}_{c_{12}} - \left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \hat{u}_{c_{12}} k_2 \right) \]

\[-\left( \mu_{0,c} + C_{BT} \rho_c d, \alpha_d u_{d_0} \right) \hat{u}_{c_{12}} k_2^2 + \rho_c \beta_0 u_{d_0} \hat{\alpha}_d + \alpha_d \rho_c \beta_1 \hat{u}_{d_{12}} - \rho_c \beta_1 \hat{u}_{c_{12}} + \alpha_d \rho_c \beta_0 \hat{u}_{d_{12}} \]

\[+\alpha_d \rho_c \beta_1 \left( \hat{u}_{d_{12}} \right) - \alpha_d \rho_c \beta_1 \hat{u}_{d_{12}} + \alpha_d \rho_c \beta_0 \hat{u}_{c_{12}} k_2 \]

\[+\alpha_d \rho_c \beta_0 \hat{u}_{c_{12}} k_2 + \alpha_d \rho_c \beta_0 \hat{u}_{d_{12}} k_2 + \alpha_d \rho_c \beta_0 C_{vm} u_{d_0} k_2 \]

\[+\alpha_d \rho_c \beta_0 C_{vm} u_{d_0} k_2 = 0, \]

and grouping the like terms in Eq. C.12 yields
Recall that the linearized dispersed-phase momentum equation is expressed as:

\[
\alpha_d \rho_u \frac{\partial \hat{u}_{d1}}{\partial t} + \alpha_d \rho_u u_{d1} \frac{\partial \hat{u}_{d1}}{\partial x} = \alpha_d \rho_c \frac{\partial \hat{u}_{c1}}{\partial t} - \left( \alpha_d \rho_{0x} + C_{BT} \rho_c \alpha_0 \alpha^2_d u_0 \right) \left[ \nabla^2 \hat{u}_{c1} + \nabla (\hat{\nabla} \cdot \hat{u}_{c1}) \right] \\
- \rho_c C_{bp} 2 \left( \frac{\alpha_{d,0}}{\alpha_{d,p}} \right) \left( u_{d0} \frac{\partial \hat{u}_{d1}}{\partial x} - u_{d0} \frac{\partial \hat{u}_{c1}}{\partial x} \right) - \rho_c C_{bp} u_{d0} \left( \frac{2 \alpha_{d,0}}{\alpha_{d,p}} - \frac{3 \alpha_{d,0}^2}{\alpha_{d,p}^2} \right) \nabla \alpha_{d1} \\
+ \left( \alpha_d \rho_{0,0} + C_{BT} \rho_c \alpha_0 \alpha^2_d u_0 \right) \left[ \nabla^2 u_{d1} + \nabla (\hat{\nabla} \cdot u_{d1}) \right] + \alpha_{d1} (\rho_d - \rho_c) g \\
- \alpha_{d1} \rho_c \beta_0 u_{d0} i - \alpha_d \rho_c \beta_1 (u_{d1} - u_{c1}) - \alpha_d \rho_v \left( \alpha_{d,0} \frac{\partial \hat{u}_{d1}}{\partial t} + u_{d0} \frac{\partial \hat{u}_{d1}}{\partial x} - u_{d0} \frac{\partial \hat{u}_{c1}}{\partial x} \right) \\
+ \alpha_d \rho_v C \left[ u_{d0} \frac{\partial \hat{u}_{c1}}{\partial x} + u_{d0} \frac{\partial \hat{u}_{d1}}{\partial x} - u_{d0} i \cdot (\hat{\nabla} \hat{u}_{c1})^T - u_{d0} i \cdot (\hat{\nabla} \hat{u}_{d1})^T \right] \\
- \alpha_d \rho_v C \left[ u_{d0} \frac{\partial \hat{u}_{c1}}{\partial x} + u_{d0} \frac{\partial \hat{u}_{d1}}{\partial x} + u_{d0} i \cdot (\hat{\nabla} \hat{u}_{c1})^T + u_{d0} i \cdot (\hat{\nabla} \hat{u}_{d1})^T \right]. \quad (C.14)
\]

Applying the solution to the linearized dispersed-phase momentum balance yields:

\[
\alpha_d \rho_s \hat{s} \hat{u}_{d1} \exp(st) \exp(ik \cdot x) + \alpha_d \rho_d u_{d1} \hat{u}_{d1} \exp(st) \exp(ik \cdot x) \\
= \alpha_d \rho_c \hat{s} \hat{u}_{c1} \exp(st) \exp(ik \cdot x) \\
- \left( \alpha_d \rho_{0x} + C_{BT} \rho_c \alpha_0 \alpha^2_d u_0 \right) \left[ -k^2 \hat{u}_{c1} \exp(st) \exp(ik \cdot x) + (\hat{u}_{c1} \cdot i) \exp(st) i \exp(ik \cdot x) \right] \\
- \rho_c C_{bp} 2 u_{d0} \left( \frac{\alpha_{d,0}^2}{\alpha_{d,p}} \right) \left( 1 - \frac{\alpha_{d,0}}{\alpha_{d,p}} \right) \exp(st) \exp(ik \cdot x) ik_i (\hat{u}_{d1} - \hat{u}_{c1})
\]
Place each term in Eq. C.15 on the same side and divide by \(\exp(st)\exp(ik \cdot x)\):

\[
-\rho_c C_{bp} u_{d0}^2 \left( \frac{2\alpha_{d0}}{\alpha_{dep}} - \frac{3\alpha_{d0}^2}{\alpha_{dep}^2} \right) \hat{\alpha}_{d1} \exp(st) i k \exp(ik \cdot x)
\]

\[
+ \left( \alpha_{d0} \mu_{0,d} + C_{BT} \rho_c d_0^2 \alpha_{d0}^2 u_{d0} \right) [-k^2 \hat{u}_{d1} \exp(st) \exp(ik \cdot x) + (\hat{u}_{d1} \cdot ik) \exp(st) i k \exp(ik \cdot x)]
\]

\[
- \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) (\rho_d - \rho_c) gi - \hat{\alpha}_{d1} \exp(st) \exp(ik \cdot x) \rho_c \beta_0 u_{d0} i
\]

\[
- \alpha_{d0} \beta_c \exp(st) \exp(ik \cdot x) (\hat{u}_{d1} - \hat{u}_{c1})
\]

\[
- \alpha_{d0} \rho_c \rho_v C_{vm} \left[ s \hat{u}_{d1} \exp(st) \exp(ik \cdot x) + u_{d0} \hat{u}_{d1} \exp(st) i k \exp(ik \cdot x) \right]
\]

\[
- s \hat{u}_{c1} \exp(st) \exp(ik \cdot x)]
\]

\[
+ \alpha_{d0} \rho v C_{u0} \{ ik \hat{u}_{c1} \exp(st) \exp(ik \cdot x) + ik \hat{u}_{d1} \exp(st) \exp(ik \cdot x) \}
\]

\[
- \left[ \hat{u}_{c1} \exp(st) \cdot i \right] i k \exp(ik \cdot x) - \left[ \hat{u}_{d1} \exp(st) \cdot i \right] i k \exp(ik \cdot x) \}
\]

\[
- \alpha_{d0} \rho v C_{u0} \left( s \hat{u}_{d1} \exp(st) \exp(ik \cdot x) + u_{d0} \hat{u}_{d1} \exp(st) \exp(ik \cdot x) \right)
\]

\[
+ \left[ \hat{u}_{c1} \exp(st) \cdot i \right] i k \exp(ik \cdot x) + \left[ \hat{u}_{d1} \exp(st) \cdot i \right] i k \exp(ik \cdot x) \}.
\]

(C.15)

Eq. C.16 is now expressed in terms of vector components:
\[-\alpha_d \rho_s \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} - \alpha_d \rho_s u_d i k_1 \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \alpha_d \rho_s \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-(\alpha_d \mu_{0,c} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-(\rho_c \mu_{0,d} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-\rho_c C_{bp} 2 u_d \left( \frac{\alpha_d}{\alpha_{dep}} \right) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} - \rho_c C_{bp} u_d \left( 2 \frac{\alpha_d}{\alpha_{dep}} \right) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} \]
\[+ (\rho_c \mu_{0,d} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[= 0 \quad \text{(C.17)} \]

Eq. C.17 is simplified:
\[-\alpha_d \rho_s \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} - \alpha_d \rho_s u_d i k_1 \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \alpha_d \rho_s \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-(\alpha_d \mu_{0,c} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-(\rho_c \mu_{0,d} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[-\rho_c C_{bp} 2 u_d \left( \frac{\alpha_d}{\alpha_{dep}} \right) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} - \rho_c C_{bp} u_d \left( 2 \frac{\alpha_d}{\alpha_{dep}} \right) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} \]
\[+ (\rho_c \mu_{0,d} + C_{BT} \rho_d \alpha_d^2 u_d) \begin{bmatrix} \hat{u}_{d,1,1} \\ \hat{u}_{d,1,2} \end{bmatrix} + \begin{bmatrix} \hat{u}_{c,1,1} \\ \hat{u}_{c,1,2} \end{bmatrix} \]
\[= 0 \]
\[-(\rho_d - \rho_c) g \begin{bmatrix} \hat{\alpha}_{d1} \\ 0 \end{bmatrix} - \rho_c \beta_0 u_{d0} \begin{bmatrix} \hat{\alpha}_{d1} \\ 0 \end{bmatrix} - \alpha_{d0} \rho_c \beta_1 \begin{bmatrix} \hat{u}_{d1,1} - \hat{u}_{c1,1} \\ \hat{u}_{d1,2} - \hat{u}_{c1,2} \end{bmatrix} \]

\[-\alpha_{d0} \rho_v \rho_C \begin{bmatrix} s \begin{bmatrix} \tilde{u}_{d1,1} \\ \tilde{u}_{d1,2} \end{bmatrix} + u_{d0} i k_1 \begin{bmatrix} \tilde{u}_{d1,1} \\ \tilde{u}_{d1,2} \end{bmatrix} - s \begin{bmatrix} \tilde{u}_{c1,1} \\ \tilde{u}_{c1,2} \end{bmatrix} \end{bmatrix} \]

\[+ \alpha_{d0} \rho_v C u_{d0} \begin{bmatrix} ik_1 \begin{bmatrix} \hat{u}_{c1,1} \\ \hat{u}_{c1,2} \end{bmatrix} + ik_1 \begin{bmatrix} \hat{u}_{d1,1} \\ \hat{u}_{d1,2} \end{bmatrix} + \hat{u}_{c1,1,ik1} \\ \hat{u}_{c1,1,ik2} \end{bmatrix} + \hat{u}_{d1,1,ik1} \]

\[-\alpha_{d0} \rho_v C s u_{d0} \begin{bmatrix} ik_1 \begin{bmatrix} \hat{u}_{c1,1} \\ \hat{u}_{c1,2} \end{bmatrix} + ik_1 \begin{bmatrix} \hat{u}_{d1,1} \\ \hat{u}_{d1,2} \end{bmatrix} + \hat{u}_{c1,1,ik1} \\ \hat{u}_{c1,1,ik2} \end{bmatrix} + \hat{u}_{d1,1,ik1} \]}

\[= 0. \quad (\text{C.18})\]

Out of the above matrix equation (Eq. C.18), we can get two equations. These are

\[-\alpha_{d0} \rho_c s \hat{u}_{d1,1} - \alpha_{d0} \rho_d u_{d0} i k_i \hat{u}_{d1,1} + \alpha_{d0} \rho_c s \hat{u}_{c1,1} \]

\[-\left( \alpha_{d0} \mu_{ac} + C_{Br} \rho_c d_{0} \alpha_{d0}^2 u_{d0} \right) \left[ -k^2 \hat{u}_{c1,1} + \left( \hat{u}_{c1,1,ik1} + \hat{u}_{c1,1,ik2} \right) ik_i \right] \]

\[-\rho_c C_{Br} 2 u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dc}} \right) \left( 1 - \frac{\alpha_{d0}}{\alpha_{dc}} \right) ik_i \left( \hat{u}_{d1,1} - \hat{u}_{c1,1} \right) - \rho_c C_{Br} u_{d0}^2 \left( \frac{2 \alpha_{d0}}{\alpha_{dc}} - \frac{3 \alpha_{d0}^2}{\alpha_{dc}^2} \right) \hat{u}_{d1,ik1} \]

\[+ \left( \alpha_{d0} \mu_{ac} + C_{Br} \rho_c d_{0} \alpha_{d0}^2 u_{d0} \right) \left[ -k^2 \hat{u}_{d1,1} + \left( \hat{u}_{d1,1,ik1} + \hat{u}_{d1,1,ik2} \right) ik_i \right] - \left( \rho_d - \rho_c \right) g \hat{\alpha}_{d1} \]

\[-\rho_c \beta_0 u_{d0} \hat{\theta}_{d1} - \alpha_{d0} \rho_c \beta_1 \left( \hat{u}_{d1,1} - \hat{u}_{c1,1} \right) - \alpha_{d0} \rho_v \rho_C \left( s \hat{u}_{d1,1} + u_{d0} i k_i \hat{u}_{d1,1} - s \hat{u}_{c1,1} \right) \]

\[+ \alpha_{d0} \rho_v C u_{d0} \left( ik_i \hat{u}_{c1,1} + ik_i \hat{u}_{d1,1} - \hat{u}_{c1,1,ik1} - \hat{u}_{d1,1,ik1} \right) \]

\[-\alpha_{d0} \rho_v C s u_{d0} \left( ik_i \hat{u}_{c1,1} + ik_i \hat{u}_{d1,1} + \hat{u}_{c1,1,ik1} + \hat{u}_{d1,1,ik1} \right) = 0, \quad (\text{C.19})\]

and

\[-\alpha_{d0} \rho_c s \hat{u}_{d1,2} - \alpha_{d0} \rho_d u_{d0} i k_i \hat{u}_{d1,2} + \alpha_{d0} \rho_c s \hat{u}_{c1,2} \]

\[-\left( \alpha_{d0} \mu_{ac} + C_{Br} \rho_c d_{0} \alpha_{d0}^2 u_{d0} \right) \left[ -k^2 \hat{u}_{c1,2} + \left( \hat{u}_{c1,1,ik1} + \hat{u}_{c1,2,ik2} \right) ik_i \right] \]

\[-\rho_c C_{Br} 2 u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dc}} \right) \left( 1 - \frac{\alpha_{d0}}{\alpha_{dc}} \right) ik_i \left( \hat{u}_{d1,2} - \hat{u}_{c1,2} \right) - \rho_c C_{Br} u_{d0}^2 \left( \frac{2 \alpha_{d0}}{\alpha_{dc}} - \frac{3 \alpha_{d0}^2}{\alpha_{dc}^2} \right) \hat{u}_{d1,ik2} \]

\[+ \left( \alpha_{d0} \mu_{ac} + C_{Br} \rho_c d_{0} \alpha_{d0}^2 u_{d0} \right) \left[ -k^2 \hat{u}_{d1,2} + \left( \hat{u}_{d1,1,ik1} + \hat{u}_{d1,2,ik2} \right) ik_i \right] - \alpha_{d0} \rho_c \beta_1 \left( \hat{u}_{d1,2} - \hat{u}_{c1,2} \right) \]

\[-\alpha_{d0} \rho_v \rho_C \left( s \hat{u}_{d1,2} + u_{d0} i k_i \hat{u}_{d1,2} - s \hat{u}_{c1,2} \right) + \alpha_{d0} \rho_v C u_{d0} \left( ik_i \hat{u}_{c1,2} + ik_i \hat{u}_{d1,2} - \hat{u}_{c1,1,ik2} - \hat{u}_{d1,1,ik2} \right) \]

\[-\alpha_{d0} \rho_v C s u_{d0} \left( ik_i \hat{u}_{c1,2} + ik_i \hat{u}_{d1,2} + \hat{u}_{c1,2,ik2} + \hat{u}_{d1,2,ik2} \right) = 0. \quad (\text{C.20})\]
Expanding the terms in Eq. C.19 yields

\[-\alpha_{d0} \rho c \hat{u}_{t1,1} - \alpha_{d0} \rho c u_{d0} \hat{k}_1 \hat{u}_{t1,1} + \alpha_{d0} \rho c \hat{u}_{c1,1} + \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) k^2 \hat{u}_{c1,1} + \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) k^2 \hat{u}_{c1,2} k_2 k_1 \]

\[-\rho c C_{BP} 2u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right] \hat{k}_1 \hat{u}_{t1,1} + \rho c C_{BP} 2u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right] \hat{k}_1 \hat{u}_{c1,1} \]

\[-\rho c C_{BP} u_{d0}^2 \left( \frac{2\alpha_{d0}}{\alpha_{dcp}} - \frac{3\alpha_{d0}^2}{\alpha_{dcp}^2} \right) \hat{k}_1 \hat{a}_{d1} - \left( \alpha_{d0} \mu_{0,d} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) k^2 \hat{u}_{d1,1} \]

\[-\left( \rho_d - \rho c \right) g \hat{a}_{d1} - \rho c \beta_0 u_{d0} \hat{a}_{d1} - \alpha_{d0} \rho c \beta_1 \hat{u}_{c1,1} + \alpha_{d0} \rho c \beta_1 \hat{u}_{c1,1} \]

Grouping the like terms in Eq. C.21 yields

\[\hat{u}_{c1,1} \left\{ \alpha_{d0} \rho c s + \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) \left( k_1^2 + k^2 \right) + \alpha_{d0} \rho c \beta_1 + \alpha_{d0} \rho c v_0 C_{sm} s \right\} \]

\[-\alpha_{d0} \rho c v_0 C_{sm} s u_{d0} \hat{k}_1 + \rho c C_{BP} 2u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right] \hat{k}_1 \]

\[+ \hat{u}_{c1,2} \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) k_2 k_1 \]

\[+ \hat{u}_{d1,1} \left\{ -\alpha_{d0} \rho_d s - \alpha_{d0} \rho_d u_{d0} \hat{k}_1 - \rho c C_{BP} 2u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right] \hat{k}_1 \right. \]

\[-\left( \alpha_{d0} \mu_{0,d} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) \left( k_1^2 + k^2 \right) - \alpha_{d0} \rho c \beta_1 \]

\[-\alpha_{d0} \rho v_0 C_{sm} s - \alpha_{d0} \rho v_0 \left( C_{sm} + 2C_s \right) u_{d0} \hat{k}_1 \}

\[+ \hat{u}_{d1,2} \left[ -\left( \alpha_{d0} \mu_{0,d} + C_{BT} \rho c d_b \alpha_{d0}^2 u_{d0} \right) k_2 k_1 \right] \]

\[+ \hat{a}_{d1} \left[ -\rho c C_{BP} u_{d0}^2 \left( \frac{2\alpha_{d0}}{\alpha_{dcp}} - \frac{3\alpha_{d0}^2}{\alpha_{dcp}^2} \right) \hat{k}_1 - \left( \rho_d - \rho c \right) g - \rho c \beta_0 u_{d0} \right] + \hat{p}_1 \left( 0 \right) = 0 . \]
Similarly, expanding the terms in Eq. C.20 yields

\[
-\alpha_{d_0} \rho_{c} s \hat{u}_{d_{1,2}} - \alpha_{d_0} \rho_{d} u_{d_0} d_0 k_1 \hat{u}_{d_{1,2}} + \alpha_{d_0} \rho_{c} s \hat{u}_{c_{1,2}} + \left(\alpha_{d_0} \mu_{0,c} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) k^2 \hat{u}_{c_{1,2}} \\
+ \left(\alpha_{d_0} \mu_{0,c} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) \hat{u}_{c_{1,2}} k_1 k_2 + \left(\alpha_{d_0} \mu_{0,c} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) \hat{u}_{c_{1,2}} k_2^2 \\
- \rho_c C_{BP} 2 u_{d_0} \left(\frac{\alpha_{d_0}^2}{\alpha_{d_{0,0}}^2}\right) i k_1 \hat{u}_{d_{1,2}} + \rho_c C_{BP} 2 u_{d_0} \left(\frac{\alpha_{d_0}^2}{\alpha_{d_{0,0}}^2}\right) i k_2 \hat{u}_{d_{1,2}} \\
- \rho_c C_{BP} u_{d_0}^2 \left(\frac{2 \alpha_{d_0} \alpha_{d_{0,0}}}{\alpha_{d_{0,0}}^2} - \frac{3 \alpha_{d_0} \alpha_{d_{0,0}}}{\alpha_{d_{0,0}}^2}\right) i k_2 \hat{d}_{1} - \left(\alpha_{d_0} \mu_{0,d} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) k^2 \hat{d}_{1,2} \\
- \alpha_{d_0} \rho_{c} \beta_1 \hat{d}_{1,2} + \alpha_{d_0} \rho_{c} \beta_1 \hat{u}_{d_{1,2}} \\
- \alpha_{d_0} \rho_{v_0} C_{sym} s \hat{u}_{d_{1,2}} - \alpha_{d_0} \rho_{v_0} C_{sym} u_{d_0} i k_1 \hat{u}_{d_{1,2}} + \alpha_{d_0} \rho_{v_0} C_{sym} s \hat{u}_{c_{1,2}} \\
+ \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_1 \hat{u}_{c_{1,2}} + \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_1 \hat{u}_{c_{1,2}} - \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_2 \\
- \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_2 - \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_2 \\
- \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_2 - \alpha_{d_0} \rho_{v_0} C_{u_0} u_{d_0} i k_2 = 0. \\
\text{(C.23)}
\]

Grouping the like terms in Eq. C.23 yields

\[
\hat{u}_{c_{1,2}} \left[\left(\alpha_{d_0} \mu_{0,c} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) k_1 k_2 - \alpha_{d_0} \rho_{v_0} \left(C + C_S\right) u_{d_0} i k_2\right] \\
+ \hat{u}_{c_{1,2}} \left[\alpha_{d_0} \rho_{c} s + \left(\alpha_{d_0} \mu_{0,c} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) \left(k^2 + k_2^2\right)\right] \\
+ \rho_c C_{BP} 2 u_{d_0} \left(\alpha_{d_0}^2 / \alpha_{d_{0,0}}^2\right) i k_1 \left[\left(\alpha_{d_0} / \alpha_{d_{0,0}}\right) - \left(\alpha_{d_0} / \alpha_{d_{0,0}}\right)\right] i k_1 \\
+ \alpha_{d_0} \rho_{c} \beta_1 \left[\alpha_{d_0} \rho_{v_0} C_{sym} s + \alpha_{d_0} \rho_{v_0} \left(C + C_S\right) u_{d_0} i k_1\right] \\
+ \hat{u}_{d_{1,1}} \left[-\left(\alpha_{d_0} \mu_{0,d} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) k_1 k_2 - \alpha_{d_0} \rho_{v_0} \left(C + C_S\right) u_{d_0} i k_2\right] \\
+ \hat{u}_{d_{1,2}} \left[-\alpha_{d_0} \rho_{c} s - \alpha_{d_0} \rho_{d} u_{d_0} i k_1 - \rho_c C_{BP} 2 u_{d_0} \left(\alpha_{d_0}^2 / \alpha_{d_{0,0}}^2\right) \left[\left(\alpha_{d_0} / \alpha_{d_{0,0}}\right) - \left(\alpha_{d_0} / \alpha_{d_{0,0}}\right)\right] i k_1\right] \\
- \left(\alpha_{d_0} \mu_{0,d} + C_{BT} \rho_{c} d_0 \alpha_{d_0} u_{d_0}\right) \left(k^2 + k_2^2\right) - \alpha_{d_0} \rho_{c} \beta_1 \\
- \alpha_{d_0} \rho_{v_0} C_{sym} s + \alpha_{d_0} \rho_{v_0} \left(C - C_S\right) u_{d_0} i k_1\right] \\
+ \hat{d}_1 \left[-\rho_c C_{BP} u_{d_0}^2 \left(\frac{2 \alpha_{d_0} \alpha_{d_{0,0}}}{\alpha_{d_{0,0}}^2} - \frac{3 \alpha_{d_0} \alpha_{d_{0,0}}}{\alpha_{d_{0,0}}^2}\right) i k_2\right] + \hat{p}_1 \left(0 = 0\right). \\
\text{(C.24)}
\]


\section*{C.2 Reducing the System of Equations}

The dispersion relations are found from the roots of the characteristic polynomial for the linear system of six algebraic equations. Eqs. C.1c and C.2c result from the continuous- and dispersed-phase continuity equations. Eqs. C.11 and C.13 correspond to the two components (vertical and horizontal) of \( \mathbf{u}_c \). Eqs. C.22 and C.24 correspond to the two components of \( \mathbf{u}_d \). In order to determine the characteristic polynomial, the system of six equations is reduced to one equation. (The 3D case would include two additional algebraic equations arising from the velocity components in the third dimension \((k_3)\), giving a system of eight equations. This system would be reduced in a similar sequence to that of the 2D case.) The reduction sequence is as follows.

Eq. C.1c is solved for \( \hat{u}_{c,1} \) in terms of \( \hat{\alpha}_{d,1} \) and \( \hat{u}_{c,1,2} \):

\[
\hat{u}_{c,1} = \left[ s\hat{\alpha}_{d,1} - (1 - \alpha_{d,0})ik_2\hat{u}_{c,1,2} \right] / (1 - \alpha_{d,0})ik_1. \tag{C.25}
\]

Eq. C.2c is solved for \( \hat{u}_{d,1} \) in terms of \( \hat{\alpha}_{d,1} \) and \( \hat{u}_{d,1,2} \):

\[
\hat{u}_{d,1} = \left[ -(s + u_{d,0}ik_1)\hat{\alpha}_{d,1} - \alpha_{d,0}ik_2\hat{u}_{d,1,2} \right] / \alpha_{d,0}ik_1. \tag{C.26}
\]

The expressions from Eqs. C.25 and C.26 are placed in Eqs. C.11, C.13, C.22, and C.24. Terms are collected according to the remaining unknowns \( (\hat{\alpha}_{d,1}, \hat{u}_{c,1,2}, \hat{u}_{d,1,2}, \text{and} \hat{p}_1) \):

\[
\hat{u}_{c,1,2} \left[ \frac{k_2\rho_c s}{k_1} + \frac{k_2(\mu_{0,c} + C_{BT}\rho_c d_c\alpha_{d,0}u_{d,0})k^2}{k_1} + \frac{k_2\alpha_{d,0}\rho_c \beta_1}{k_1} + \frac{k_2\alpha_{d,0}\rho_v C_{vm}s}{k_1} - 2\alpha_{d,0}\rho_v C_S u_{d,0}ik_2 \right] \\
+ \hat{u}_{d,1,2} \left[ -\frac{\alpha_{d,0}k_2\rho_c \beta_1}{k_1} - \frac{\alpha_{d,0}k_2\rho_v C_{vm}s}{k_1} - \alpha_{d,0}ik_2\rho_v (C_{vm} + 2C_S)u_{d,0} \right] \\
+ \hat{\alpha}_{d,1} \left[ \rho_c (\beta_0 - \beta_1)u_{d,0} + \frac{s^2\rho_c i}{(1 - \alpha_{d,0})k_1} + \frac{s(\mu_{0,c} + C_{BT}\rho_c d_c\alpha_{d,0}u_{d,0})ik^2}{(1 - \alpha_{d,0})k_1} \right. \\
-2s\rho_v (C_{vm} + C_S)u_{d,0} - u_{d,0}^2\rho_v (C_{vm} + 2C_S) \\
\left. + s(\mu_{0,c} + C_{BT}\rho_c d_c\alpha_{d,0}u_{d,0})ik_1 \right] \\
+ s\rho_c \beta_1 (1 - \alpha_{d,0})k_1 + \frac{s^2\rho_v C_{vm} i}{(1 - \alpha_{d,0})k_1} + \frac{2s\alpha_{d,0}\rho_v C_S u_{d,0}}{1 - \alpha_{d,0}} \right] \\
+ \hat{p}_1 (-ik_1) = 0, \tag{C.27}
\]
(from C.11)
\[
\hat{u}_{c_{1,2}} \left\{ -\rho_c s - (\mu_0 + C_{BT} \rho_c d \alpha_{d0} u_{d0}) k^2 - \alpha_{d0} \rho_c \beta_1 - \alpha_{d0} \rho_v C_{vm} s \right. \\
+ \alpha_{d0} \rho_v (C_S - C) u_{d0} i k_1 - \left[ \frac{i k_2^2 \alpha_{d0} \rho_v (C + C_S) u_{d0}}{k_1} \right] \\
+ \hat{u}_{d_{1,2}} \left\{ \alpha_{d0} \rho_c \beta_1 + \alpha_{d0} \rho_v C_{vm} s + \alpha_{d0} \rho_v (C_{vm} - C + C_S) u_{d0} i k_1 - \left[ \frac{i k_2^2 \alpha_{d0} \rho_v (C + C_S) u_{d0}}{k_1} \right] \\
+ \hat{a}_d \left[ s \left( \mu_0 + C_{BT} \rho_c d \alpha_{d0} u_{d0} \right) i k_2 - s \left( 1 - 2 \alpha_{d0} \right) \rho_v (C + C_S) u_{d0} k_2 - \left( 1 - \alpha_{d0} \right) k_1 \right] \\
+ \hat{\rho}_i (i k_2) = 0, \quad \text{ (C.28)}
\]

\[
\hat{u}_{c_{1,2}} \left[ - \frac{k_2 \alpha_{d0} \rho_c s}{k_1} - \frac{k_2 \left( \alpha_{d0} \mu_0 + C_{BT} \rho_c d_b \alpha_{d0}^2 u_{d0} \right)}{k_1} k^2 - \frac{i k_2 \rho_c C_{BP} 2 u_{d0} \left( \frac{\alpha_{d0}^2}{\alpha_{d0} - \alpha_{d0}} \right)}{k_1} - \frac{k_2 \alpha_{d0} \rho_c \beta_1}{k_1} - \frac{k_2 \alpha_{d0} \rho_v C_{vm} s}{k_1} + \frac{i k_2 \alpha_{d0} \rho_v 2 C_S u_{d0}}{k_1} \right] \\
+ \hat{u}_{d_{1,2}} \left[ - \frac{k_2 \alpha_{d0} \rho_d s}{k_1} + \frac{i k_2 \alpha_{d0} \rho_d u_{d0}}{k_1} + \frac{i k_2 \rho_c C_{BP} 2 u_{d0} \left( \frac{\alpha_{d0}^2}{\alpha_{d0} - \alpha_{d0}} \right)}{k_1} + \frac{i k_2 \alpha_{d0} \rho_v (C_{vm} + 2 C_S) u_{d0}}{k_1} \right] \\
+ \hat{a}_d \left[ - \rho_c C_{BP} u_{d0}^2 \left( \frac{2 \alpha_{d0}^2}{\alpha_{d0} - \alpha_{d0}} - \frac{3 \alpha_{d0}^2}{\alpha_{d0} - \alpha_{d0}} \right) i k_1 \left( \rho_c - \rho_c \right) g - \rho_c u_{d0} \left( \beta_0 - \beta_1 \right) - \frac{s^2 \alpha_{d0} \rho_d i}{\left( 1 - \alpha_{d0} \right) k_1} \right] \\
- \frac{s \alpha_{d0} \left( \mu_0 + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right)}{\left( 1 - \alpha_{d0} \right) k_1} i k_1 \left( k_1^2 + k^2 \right) + \frac{2 s \rho_c C_{BP} 2 u_{d0} \left( \alpha_{d0} \right)}{1 - \alpha_{d0}} \left( \frac{\alpha_{d0}}{\alpha_{d0} - \alpha_{d0}} \right) \left( 1 - \alpha_{d0} \right) k_1 \left( k_1^2 + k^2 \right) \\
- \frac{s \rho_c \beta_1}{\left( 1 - \alpha_{d0} \right) k_1} - \frac{s^2 \rho_v C_{vm} i}{\left( 1 - \alpha_{d0} \right) k_1} - \frac{s \alpha_{d0} \rho_v 2 C_S u_{d0}}{1 - \alpha_{d0}} \frac{s \rho_v i}{k_1} - \frac{2 u_{d0} \rho_d s}{\left( 1 - \alpha_{d0} \right) k_1} + u_{d0} \left( \mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right) \left( k_1^2 + k^2 \right) + 2 s \rho_v \left( C_{vm} + C_S \right) u_{d0} + \frac{2 s \rho_v u_{d0} \left( C_{vm} + 2 C_S \right) i k_1}{k_1} \right] \\
+ u_{d0} i k_1 \rho_c C_{BP} 2 u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{d0} - \alpha_{d0}} \right) \left( 1 - \frac{\alpha_{d0}}{\alpha_{d0}} \right) - s \left( \mu_{0,d} + C_{BT} \rho_c d_b \alpha_{d0} u_{d0} \right) i k_1 \left( k_1^2 + k^2 \right) \right] \\
= 0, \quad \text{ (C.29)}
\]

(from C.22)
and

\[ \hat{u}_{c_{1,2}} \left\{ \alpha_{d_0} \rho_c s + \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha^2_{d_0} u_{d_0} \right) k^2 + \rho_c C_{BP} 2u_{d_0} \left( \alpha^2_{d_0} / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i_{k_{1}} \right. \]

\[ + \alpha_{d_0} \rho_c \beta_i + \alpha_{d_0} \rho_{v_0} C_{sm}s + \alpha_{d_0} \rho_{v_0} \left( C - C_S \right) u_{d_0} i_{k_{1}} + \left[ \alpha_{d_0} \rho_{v_0} \left( C + C_S \right) u_{d_0} i_{k_{2}} \right] / k_1 \left\} \right. \]

\[ + \hat{u}_{d_{1,2}} \left\{ - \alpha_{d_0} \rho_d s - \alpha_{d_0} \rho_d u_{d_0} i_{k_{1}} - \rho_c C_{BP} 2u_{d_0} \left( \alpha^2_{d_0} / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right] i_{k_{1}} \right. \]

\[ - k^2 \left( \alpha_{d_0} \mu_{0,d} + C_{BT} \rho_c d_0 \alpha^2_{d_0} u_{d_0} \right) - \alpha_{d_0} \rho_c \beta_i - \alpha_{d_0} \rho_{v_0} C_{sm}s \]

\[ + \alpha_{d_0} \rho_{v_0} \left( C - C_{sm} - C_S \right) u_{d_0} i_{k_{1}} + \left[ \alpha_{d_0} \rho_{v_0} \left( C + C_S \right) u_{d_0} i_{k_{2}} \right] / k_1 \left\} \right. \]

\[ + \hat{a}_{d_{1}} \left[ - \rho_c C_{BP} u_{d_0}^2 \left( 2 \alpha_{d_0} / \alpha_{d_0} - 3 \alpha^2_{d_0} / \alpha_{d_0} \right) i_{k_{2}} - s \left( \alpha_{d_0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha^2_{d_0} u_{d_0} \right) i_{k_{2}} / \left( 1 - \alpha_{d_0} \right) \right. \]

\[ - s \left( \mu_{0,d} + C_{BT} \rho_c d_0 \alpha^2_{d_0} u_{d_0} \right) i_{k_{2}} + u_{d_0} \left( \mu_{0,d} + C_{BT} \rho_c C_{sm} \alpha_{d_0} u_{d_0} \right) k_{1} k_{2} \]

\[ + s \left( 1 - 2 \alpha_{d_0} \right) \rho_{v_0} \left( C + C_S \right) u_{d_0} k_{2} / \left( 1 - \alpha_{d_0} \right) k_{1} + \rho_{v_0} \left( C + C_S \right) i_{k_{2}} \right] \]

\[ = 0. \quad \text{(C.30)} \]

(from \( \text{C.24} \))

Eq. C.27 is solved for \( \hat{p}_1 \) in terms of \( \hat{u}_{c_{1,2}}, \hat{u}_{d_{1,2}}, \) and \( \hat{a}_{d_{1}} \):

\[ \hat{p}_1 = \hat{u}_{c_{1,2}} \left[ - \frac{i_{k_{2}} \rho_c s}{k_{1}^2} - \frac{i_{k_{2}} \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha^2_{d_0} u_{d_0} \right) k^2}{k_{1}^2} \right. \]

\[ + \frac{i_{k_{2}} \alpha_{d_0} \beta_i + \alpha_{d_0} k_{2} \rho_{v_0} C_{sm}s}{k_{1}^2} - \frac{\alpha_{d_0} k_{2} \rho_{v_0} \left( C_{sm} + 2 C_S \right) u_{d_0}}{k_{1}} \right] \]

\[ + \hat{u}_{d_{1,2}} \left[ - \frac{\rho_c \left( \beta_0 - \beta_i \right) u_{d_0} i_{k_{1}}}{k_{1}} + \frac{s \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) k^2}{k_{1}^2} / \left( 1 - \alpha_{d_0} \right) k_{1} \right. \]

\[ + \frac{s \left( \mu_{0,d} + C_{BT} \rho_c d_0 \alpha_{d_0} u_{d_0} \right) k_{2}^2}{k_{1}^2} / \left( 1 - \alpha_{d_0} \right) k_{1} \right. \]

\[ + \frac{s \rho_{v_0} C_{sm}}{k_{1}} + \frac{s \rho_{v_0} \left( C_{sm} + C_S \right) u_{d_0} i_{k_{1}}}{k_{1}} - \frac{s \rho_{v_0} \left( C_{sm} + 2 C_S \right) u_{d_0} i_{k_{1}}}{k_{1}} \right] \]

\[ \quad \text{(C.31)} \]
The expression for $\hat{p}_i$ is substituted in Eq. C.28 to yield an expression that now depends on $\hat{u}_{c1,2}$, $\hat{u}_{d1,2}$, and $\hat{\alpha}_d$:

$$
\hat{u}_{c1,2} \left[ \frac{ik_2^2 \alpha_{d0} \rho_{\nu_0} (C_S - C) u_{d0}}{k_1} - \frac{k_2^2 \rho_s}{k_1^2} - \rho_c s - (\mu_{0,x} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0}) k^2 - \alpha_{d0} \rho_c \beta_i \\
- \alpha_{d0} \rho_s C_{vm} s - \alpha_{d0} \rho_{\nu_0} (C_S - C) u_{d0} i k_1 \\
- \frac{k_2^2 (\mu_{0,x} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0}) k^2}{k_1^2} - \frac{k_2^2 \alpha_{d0} \rho_c \beta_i}{k_1^2} - \frac{k_2^2 \alpha_{d0} \rho_{\nu_0} C_{vm} s}{k_1^2} \right]
$$

$$
+ \hat{u}_{d1,2} \left[ \alpha_{d0} \rho_c \beta_i + \alpha_{d0} \rho_{\nu_0} C_{vm} s + \alpha_{d0} \rho_{\nu_0} (C_{vm} - C) u_{d0} i k_1 + \frac{\alpha_{d0} k_2^2 \rho_c \beta_i}{k_1^2} \\
+ \frac{ik_2^2 \alpha_{d0} \rho_{\nu_0} (C_{vm} + C_{S} - C) u_{d0} k_2}{k_1} + \frac{\alpha_{d0} k_2^2 \rho_{\nu_0} C_{vm} s}{k_1^2} \right]
$$

$$
+ \hat{\alpha}_d \left[ \frac{s \alpha_{d0} \rho_{\nu_0} (C - C_S) u_{d0} k_2}{(1 - \alpha_{d0}) k_1} + \frac{s \rho_{\nu_0} (2 C_{vm} + C_{S} - C) u_{d0} k_2}{k_1^2} - \frac{\rho_c (\beta_0 - \beta_i) u_{d0} k_2}{k_1} \\
- \frac{s^2 \rho_{\nu_0} i k_2}{(1 - \alpha_{d0}) k_1^2} - \frac{s \left( \mu_{0,x} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) k^2 i k_2}{k_1^2 (1 - \alpha_{d0})} \\
- \frac{s \rho_{\nu_0} i k_2}{(1 - \alpha_{d0}) k_1^2} - \frac{s^2 \rho_{\nu_0} C_{vm} i k_2}{k_1^2 (1 - \alpha_{d0})} + u_{d0} \rho_{\nu_0} (C_{vm} + C_{S} - C) i k_2 \right]
$$

$$= 0. \quad \text{(C.32)}$$

Eq. C.32 is solved for $\hat{u}_{c1,2}$ in terms of $\hat{u}_{d1,2}$ and $\hat{\alpha}_d$:

$$
\hat{u}_{c1,2} \left[ \frac{ik_2^2 \alpha_{d0} \rho_{\nu_0} (C - C_S) u_{d0}}{k_1} + \frac{k_2^2 \rho_s}{k_1^2} + \rho_c s + (\mu_{0,x} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0}) k^2 + \alpha_{d0} \rho_c \beta_i \\
+ \alpha_{d0} \rho_{\nu_0} C_{vm} s - \alpha_{d0} \rho_{\nu_0} (C_S - C) u_{d0} i k_1 \\
+ \frac{k_2^2 (\mu_{0,x} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0}) k^2}{k_1^2} + \frac{k_2^2 \alpha_{d0} \rho_c \beta_i}{k_1^2} + \frac{k_2^2 \alpha_{d0} \rho_{\nu_0} C_{vm} s}{k_1^2} \right]
$$
\[ \hat{u}_{d,1,2} \left[ \alpha_{d,0} \rho_c \beta_1 + \alpha_{d,0} \rho_v \gamma \left( C_{vm} - C + C_s \right) u_{d,0} k_1 + \frac{\alpha_{d,0} k_2^2 \rho_c \beta_1}{k_1^2} \right] 
\]

\[ + \hat{\alpha}_d \left[ \frac{s \alpha_{d,0} \rho_v \left( C - C_s \right) u_{d,0} k_2}{(1 - \alpha_{d,0}) k_1} + \frac{s \rho_v \left( 2C_{vm} + C_s - C \right) u_{d,0} k_2}{k_1} - \frac{\rho_c \left( \beta_0 - \beta_1 \right) u_{d,0} k_2}{k_1} \right] \]

\[ - \frac{s^2 \rho_v i k_2}{(1 - \alpha_{d,0}) k_1} - \frac{\left( \mu_{0,0} + C_{BT} \rho_c d \alpha_{d,0} u_{d,0} \right) k^2 i k_2}{k_1^2} \]

\[ - \frac{s \rho_c \beta_1 i k_2}{(1 - \alpha_{d,0}) k_2} + \frac{s \rho_v C_{vm} i k_2}{k_1^2 (1 - \alpha_{d,0})} \]

\[ + \frac{u_{d,0} \rho_v \left( C_{vm} + C_s - C \right) i k_2}{k_1} \]. \quad \text{(C.33)}

The expression for \( \hat{u}_{c,1,2} \) (Eq. C.33) is substituted into Eqs. C.29 and C.30 to obtain two equations in terms of two unknowns, \( \hat{u}_{d,1,2} \) and \( \hat{\alpha}_d \). To avoid division by a polynomial expression, the following process is applied. Consider an equation like

\[ A \hat{u}_{c,1,2} = B \hat{u}_{d,1,2} + C \hat{\alpha}_d, \quad \text{(C.34a)} \]

where \( A, B, \) and \( C \) represent sets of terms with polynomials in \( s \). Next, consider a similar second equation,

\[ D \hat{u}_{c,1,2} = E \hat{u}_{d,1,2} + F \hat{\alpha}_d. \quad \text{(C.34b)} \]

\( D, E, \) and \( F \) are also sets of terms with polynomials in \( s \). To eliminate \( \hat{u}_{c,1,2} \), multiply Eq. C.34a by \( D \) and Eq. C.34b by \( A \):

\[ DA \hat{u}_{c,1,2} = DB \hat{u}_{d,1,2} + DC \hat{\alpha}_d; \quad \text{(C.35a)} \]

\[ AD \hat{u}_{c,1,2} = AE \hat{u}_{d,1,2} + AF \hat{\alpha}_d. \quad \text{(C.35b)} \]

Finally, subtract Eq. C.35b from Eq. C.35a to yield an expression in \( \hat{u}_{d,1,2} \) and \( \hat{\alpha}_d \):

\[ 0 = (DB - AE) \hat{u}_{d,1,2} + (DC - AF) \hat{\alpha}_d \quad \text{(C.36)} \]

The expressions resulting from substituting Eq. C.33 into Eqs. C.29 and C.30 are:

\[ \hat{u}_{d,1,2} (\Phi \Psi + A \Xi) + \hat{\alpha}_{d,1} (\Phi \Omega + A \Xi) = 0 \quad \text{(C.37)} \]

and
\[ \hat{u}_{d1,2} \left( \gamma \Psi + AB \right) + \hat{\alpha}_{d1} \left( \gamma \Omega + AY \right) = 0, \quad (C.38) \]

where

\[
A = \left( k_1^2 + k_2^2 \right) \rho \sigma s + \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( k_1^2 + k_2^2 \right)^2 + \left( k_1^2 + k_2^2 \right) \alpha_{d0} \rho_c \beta_i \\
+ \left( k_1^2 + k_2^2 \right) \alpha_{d0} \rho_c v_{C_m} s - k_1^2 \alpha_{d0} \rho_c \left( C_s - C \right) u_{d0} i + ik_2^2 \alpha_{d0} \rho_c v_{C_m} \left( C - C_s \right) u_{d0},
\]

\[ \Psi = \left( k_1^2 + k_2^2 \right) \alpha_{d0} \rho_c \beta_i + \left( k_1^2 + k_2^2 \right) \alpha_{d0} \rho_c v_{C_m} s + k_1^2 \alpha_{d0} \rho_c v_{C_m} \left( C_{vm} - C + C_s \right) u_{d0} i \\
+ ik_2^2 \alpha_{d0} \rho_c v_{C_m} \left( C_{vm} + C_s - C \right) u_{d0}, \quad (C.39a) \]

\[
\Omega = \frac{s \alpha_{d0} \rho_c v_{C_m} \left( C - C_s \right) u_{d0} k_1 k_2}{1 - \alpha_{d0}} - k_1 \rho_c \left( \beta_0 - \beta_i \right) u_{d0} k_2 - \frac{s^2 \rho_c i k_2}{1 - \alpha_{d0}} \\
- \frac{s \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( k_1^2 + k_2^2 \right) i k_2}{1 - \alpha_{d0}} - \frac{s \rho_c \beta_i k_2}{1 - \alpha_{d0}} - \frac{s^2 \rho_c v_{C_m} i k_2}{1 - \alpha_{d0}} \\
+ s \rho_c v_{C_m} \left( 2 C_{vm} + C_s - C \right) u_{d0} k_1^2 + k_1^2 u_{d0} v_{C_m} \left( C_{vm} + C_s - C \right) i k_2, \quad (C.39b) \]

\[
\Phi = -k_2 \alpha_{d0} \rho_c s - k_2 \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( k_1^2 + k_2^2 \right) - k_2 \alpha_{d0} \rho_c \beta_i - k_2 \alpha_{d0} \rho_c v_{C_m} s \\
- ik_2 \rho_c \left( \alpha_{d0} / \alpha_{dcp} \right) 2 u_{d0} \left( \alpha_{d0} / \alpha_{dcp} \right) \left[ 1 - \left( \alpha_{d0} / \alpha_{dcp} \right) \right] + ik_2 \alpha_{d0} \rho_c v_{C_m} \left( C_{vm} + C_s - C \right) u_{d0}, \quad (C.39c) \]

\[
\Xi = k_2 \alpha_{d0} \rho_c s + ik_2 \rho_c \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( k_1^2 + k_2^2 \right) + k_2 \alpha_{d0} \rho_c \beta_i \\
+ ik_2 \alpha_{d0} \rho_c v_{C_m} \left( C_{vm} + 2 C_s \right) u_{d0} + ik_2 \alpha_{d0} \rho_c v_{d0}, \quad (C.39d) \]

\[
Z = -\rho_c C_{BP} u_{d0}^2 \left( \frac{2 \alpha_{d0}}{\alpha_{dcp}} - \frac{3 \alpha_{d0}^2}{\alpha_{dcp}^2} \right) ik_1^2 - k_1 (\rho_d - \rho_c) g - k_1 \rho_c u_{d0} (\beta_0 - \beta_i) - \frac{s^2 \rho_c i}{1 - \alpha_{d0}} \\
- \frac{s \alpha_{d0} \left( \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) i (2 k_1^2 + k_2^2)}{1 - \alpha_{d0}} + k_s \rho_c C_{BP} 2 u_{d0} \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right] \left( 1 - \frac{\alpha_{d0}}{\alpha_{dcp}} \right), \quad (C.39e) \]
\[ -s \rho_c \beta i - \frac{s^2 \rho_v C_m i}{1 - \alpha_{d0}} \left[ k_i^2 + 2s \rho_d i + k_i^2 \rho_d \kappa_1^2 \right] \]
\[ + ik^2 \rho_c C_{BP} 2u_{d0} \frac{\alpha_{d0}}{\alpha_{d0}} \left[ \left( \frac{\alpha_{d0}}{\alpha_{d0}} \right) - s \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \right] \]
\[ + k_i u_{d0} \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( 2k^2 + k_2^2 \right) + k_i 2s \rho_v \left( C_{vm} + C_S \right) u_{d0} \]
\[ + u_{d0} \rho_v \left( C_{vm} + 2C_S \right) ik^2, \quad (C.39f) \]

\[ \gamma = k_i \alpha_{d0} \rho_S + k_i \left( \alpha_{d0} \mu_{0,c} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \left( k_1^2 + k_2^2 \right) \]
\[ + \rho_c C_{BP} 2u_{d0} \frac{\alpha_{d0}}{\alpha_{d0}} \left[ \left( \frac{\alpha_{d0}}{\alpha_{d0}} \right) - s \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \right] \]
\[ + k_i \alpha_{d0} \rho_c \beta_1 + k_i \alpha_{d0} \rho_v \left( C_{vm} + C_S \right) u_{d0} ik_1^2, \quad (C.39g) \]

\[ B = -k_i \alpha_{d0} \rho_S - \alpha_{d0} \rho_u d_0 ik_1^2 - \rho_c C_{BP} 2u_{d0} \frac{\alpha_{d0}}{\alpha_{d0}} \left[ \left( \frac{\alpha_{d0}}{\alpha_{d0}} \right) - s \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) \right] \]
\[ - k_i \left( k_1^2 + k_2^2 \right) \left( \alpha_{d0} \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) - k_i \alpha_{d0} \rho_c \beta_1 - k_i \alpha_{d0} \rho_v \left( C_{vm} + C_S \right) u_{d0} \]
\[ + \alpha_{d0} \rho_v \left( C - C_{vm} - C_S \right) u_{d0} ik_1^2 + \alpha_{d0} \rho_v \left( C + C_S \right) u_{d0} ik_2^2, \quad (C.39h) \]

and

\[ Y = -\rho_c C_{BP} u_{d0}^2 \left( \frac{2\alpha_{d0}}{\alpha_{d0}} - \frac{3\alpha_{d0}^2}{\alpha_{d0}^2} \right) ik_1 k_2 \]
\[ - s \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) ik_1 k_2 + u_{d0} \left( \mu_{o,d} + C_{BT} \rho_c d_0 \alpha_{d0} u_{d0} \right) k_1^2 k_2 \]
\[ + \frac{s \rho_v \left( C + C_S \right) u_{d0}^2 \left( 1 - 2\alpha_{d0} \right)}{1 - \alpha_{d0}} + u_{d0} \rho_v \left( C + C_S \right) ik_1 k_2. \quad (C.39i) \]

### C.3 Determining the Dispersion Relations

In order to eliminate \( \hat{u}_{d1,2} \) and obtain an expression in \( \hat{d}_{d1} \), Eqs. C.37 and C.38 are treated in a manner similar to that described by Eqs. C.34-C.36. This yields

\[ \hat{d}_{d1} \left[ \left( \gamma \Psi + AB \right) \left( \Phi \Omega + AZ \right) - \left( \gamma \Omega + A \xi \right) \left( \Phi \Psi + A \Xi \right) \right] = 0. \quad (C.40) \]

Eq. C.40 is simplified to obtain a function of \( s, k_1, k_2, \) and the two-fluid model parameters:
\[
A \left[ Z(AB + \gamma\Psi) + \Omega (\Phi B - \gamma \Xi) - Y (\Phi \Psi + A \Xi) \right] = 0. \tag{C.41}
\]

We examine particular cases of (i) vertical waves, where \( k_2 = 0 \), and (ii) horizontal waves, where \( k_1 = 0 \). For Case (i), \( \Omega = Y = 0 \) in Eq. C.41, leaving

\[
AZ(AB + \gamma\Psi) = 0. \tag{C.42}
\]

There are five roots for Eq. C.42. The first root corresponds to \( A = 0 \):

\[
s = \frac{-k_1^2 \mu_{0,c} - \alpha_{d_0} \beta \rho_c - \alpha_{d_0} C_{B,T} d_b k_1^2 \rho_c u_{d_0} + i \alpha_{d_0} (C_S - C) k_1 \rho_{v_0} u_{d_0}}{\rho_c + \alpha_{d_0} C_{v,m} \rho_{v_0}}. \tag{C.43}
\]

It may be noted that the root corresponding to \( A(s, k) = 0 \) is always stable, so it can be factored out of the characteristic polynomial in Eq. C.42. The resulting characteristic polynomial, \( Z(AB + \gamma\Psi) = 0 \), can be factored as

\[
(a_1 s^2 + b_1 s + c_1)(a_2 s^2 + b_2 s + c_2) = 0, \tag{C.44}
\]

where \( a_1 s^2 + b_1 s + c_1 = 0 \) corresponds to \( Z = 0 \) and \( a_2 s^2 + b_2 s + c_2 = 0 \) corresponds to \( (AB + \gamma\Psi) = 0 \). The complex-valued coefficients are defined below:

\[
a_1 = \alpha_{d_0} (\rho_c - \rho_d) + \rho_{v_0} C_{v,m} + \rho_d, \tag{C.44a}
\]

\[
b_1 = \alpha_{d_0} \left( \mu_{0,c} + C_{B,T} \rho_c d_b \alpha_{d_0} u_{d_0} \right) 2 k_1^2 + \left( \mu_{0,d} + C_{B,T} \rho_c d_b \alpha_{d_0} u_{d_0} \right) 2 k_1^2 \left( 1 - \alpha_{d_0} \right)
+ ik_1 \rho_c C_{B,T} 2 u_{d_0} \left( \alpha_{d_0} / \alpha_{d_0} \right) \left[ 1 - \left( \alpha_{d_0} / \alpha_{d_0} \right) \right]
- ik_1 \alpha_{d_0} \rho_{v_0} 2 C_S u_{d_0}
+ 2 ik_1 u_{d_0} \rho_d \left( 1 - \alpha_{d_0} \right) + 2 ik_1 \rho_{v_0} \left( C_{v,m} + C_S \right) u_{d_0} \left( 1 - \alpha_{d_0} \right) + \rho_c \beta_1, \tag{C.44b}
\]

\[
c_1 = k_1 \left( 1 - \alpha_{d_0} \right) \left[ u_{d_0} \left( \mu_{0,d} + C_{B,T} \rho_c d_b \alpha_{d_0} u_{d_0} \right) 2 k_1^2 - u_{d_0}^2 \rho_{v_0} \left( C_{v,m} + 2 C_S \right) k_1 - u_{d_0}^2 \rho_d k_1
+ \rho_c C_{B,T} u_{d_0}^2 \left( \frac{2 \alpha_{d_0}}{\alpha_{d_0}} - \frac{3 \alpha_{d_0}^2}{2 \alpha_{d_0}} \right) k_1
- k_1 \rho_c C_{B,T} 2 u_{d_0}^2 \left( \frac{\alpha_{d_0}}{\alpha_{d_0}} \right) \left( 1 - \alpha_{d_0} \right)
- \rho_d \rho_c \left( \beta_0 - \beta_1 \right), \tag{C.44c}
\]

\[
a_2 = \rho_c \left( \rho_d + \rho_{v_0} C_{v,m} \right) - \alpha_{d_0} \rho_{v_0} C_{v,m} \left( \rho_c - \rho_d \right), \tag{C.44d}
\]
\[ b_2 = \rho_d \mu_{0,c} k_1^2 + \alpha_{d0} C_{BT} \rho_c \rho_d \mu_{u_0} k_1^2 + \alpha_{d0} \rho_c C_{vm} C_{BT} \rho_c \mu_{d} u_0 k_1^2 + (1 - \alpha_{d0}) \rho_{v0} C_{vm} \mu_{0,c} k_1^2 \]
\[ + \alpha_{d0} \rho_{v0} C_{vm} \mu_{0,d} k_1^2 + \alpha_{d0} \rho_c \mu_{u_0} k_1^2 + \alpha_{d0} \rho_{c} C_{BT} \rho_c \mu_{d} u_0 k_1^2 + \alpha_{d0} \rho_c \mu_{d} \beta_1 + (1 - \alpha_{d0}) \rho_{c} \beta_1 \]
\[ + i k_1 \{ \rho_c \rho_d u_0 + \alpha_{d0} \rho_d \rho_{v0} (C_{vm} + C - C_S) u_0 + \rho_{c}^2 C_{BP} 2u_0 \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \right] \]
\[ + (1 - \alpha_{d0}) \rho_c \rho_{v0} \left( C_{vm} + C_S - C \right) u_0 \}, \quad (C.44e) \]

and

\[ c_2 = k_1^2 \left\{ -\alpha_{d0} \rho_{v0} (C - C_S) \rho_d u_0^2 + k_1^2 \mu_{0,c} \mu_{0,d} + k_1^2 C_{BT} \rho_c \mu_{d} u_0 (\mu_{0,d} + \mu_{0,c}) \right. \]
\[ + k_1^2 (C_{BT} \rho_c \mu_{d} u_0) + \alpha_{d0} \rho_c \beta_1 \mu_{0,c} + (1 - \alpha_{d0}) \rho_c \beta_1 \mu_{0,c} + \alpha_{d0} \rho_{c}^2 \beta_1 C_{BT} \mu_{d} u_0 \]
\[ - \alpha_{d0} \rho_{v0} (2C - 2C_S - C_{vm}) \rho_c C_{BP} 2u_0^2 \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \right] \]
\[ + i k_1 u_0 \left\{ \alpha_{d0} \rho_c \beta_1 \mu_{d} + \rho_c C_{BP} 2 \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \right] \right\} k_1^2 \mu_{0,c} \]
\[ + \alpha_{d0} \rho_{c}^2 C_{BP} C_{BT} \mu_{d} u_0 \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \left[ 1 - \left( \frac{\alpha_{d0}}{\alpha_{dcp}} \right) \right] k_1^2 + \rho_2 k_1^2 \mu_{0,c} \]
\[ + \alpha_{d0} \rho_{d}^2 k_1^2 C_{BT} \rho_c \mu_{d} u_0 + (1 - \alpha_{d0}) \rho_{v0} (C_{vm} + C_S - C) k_1^2 \mu_{0,c} \]
\[ + \alpha_{d0} \rho_{d}^2 k_1^2 C_{BT} \rho_c \mu_{d} u_0 + \alpha_{d0} \rho_{v0} (C_S - C) k_1^2 C_{BT} \rho_c \mu_{d} u_0 \]
\[ + \alpha_{d0} \rho_{v0} (C - C_S) k_1^2 \mu_{0,c} + \alpha_{d0}^2 \rho_{v0} (C - C_S) k_1^2 C_{BT} \rho_c \mu_{d} u_0 \} \]. \quad (C.44f) \]

Note that the two pairs of roots from \( a_i s^2 + b_i s + c_i = 0 \) and \( a_2 s^2 + b_2 s + c_2 = 0 \) take the form
\[ s = \frac{- (p + i q) \pm \sqrt{(p + i q)^2 - 4 (P + i Q)}}{2}, \quad (C.45a) \]
which is equivalent to the form used by Jackson (2000):
\[ s = \frac{- (p + i q) \pm \sqrt{(p^2 - q^2 - 4P) + (2pq - 4Q)i}}{2}, \quad (C.45b) \]
where, for the first pair, \( (b_1/a_1) = p + i q \) and \( (c_1/a_1) = P + i Q \), and for the second pair, \( (b_2/a_2) = p + i q \) and \( (c_2/a_2) = P + i Q \).

For the roots discussed above (Eqs. C.44a-f), the dispersion relations \( \lambda (k_1) \) and \( \nu (k_1) \) are defined as (Jackson, 2000):
\[ \lambda = \text{Re}(s) = \frac{1}{2}(M - p), \]  
(C.46a)

and

\[ \nu = -\text{Im}(s) = \frac{-(N - q)}{k_1}, \]  
(C.46b)

where

\[ M = \left[ \frac{\sqrt{(p^2 - q^2 - 4P)^2 + (2pq - 4Q)^2 + (p^2 - q^2 - 4P)^2}}{2} \right]^{\frac{1}{2}}, \]  
(C.47a)

and

\[ N = \text{sgn}(2pq - 4Q) \left[ \frac{\sqrt{(p^2 - q^2 - 4P)^2 + (2pq - 4Q)^2 - (p^2 - q^2 - 4P)^2}}{2} \right]^{\frac{1}{2}}. \]  
(C.47b)

Note that the dispersion relations can be made dimensionless by scaling with the characteristic length \(d_b\) and the characteristic time \((d_b/u_{d_0})\).

For Case (ii), \(k_1 = 0\). Unlike for Case (i), however, no terms reduce to zero. The expression given in Eq. C.41 can also be expressed as:

\[ A\left[ \gamma (\Psi Z - \Omega \Xi) + \Phi (B\Omega - \Gamma \Psi) + A (BZ - \Gamma \Xi) \right] = 0. \]  
(C.48)

There are five roots for Case (ii). One root is obtained when \(A = 0\) and is always stable:

\[ s = \frac{-k_2^2 \mu_{0,c} - \alpha_{d_0} \beta_c \rho_s - \alpha_{d_0} C_{\theta t} d_b k_2^2 \rho_s u_{d_0}}{\rho_c + \alpha_{d_0} C_{\text{vm}} \rho_c}. \]  
(C.49)

Four roots are obtained from

\[ \gamma (\Psi Z - \Omega \Xi) + \Phi (B\Omega - \Gamma \Psi) + A (BZ - \Gamma \Xi) = 0. \]  
(C.50)

It may be noted that \(k_1\) is a factor of Eq. C.50. Thus when \(k_1\) is set equal to zero, Eq. C.50 is also equal to zero. This means that Eq. C.50 must be divided by \(k_1\) first before setting \(k_1\) equal to zero. However, the four roots resulting from Eq. C.50 are highly complicated, and their behavior is best studied numerically, as shown in Chapter 6.