One-dimensional CFD model of a multiphase loop polymerization reactor

Michael Christopher Baker

Iowa State University

Follow this and additional works at: http://lib.dr.iastate.edu/etd

Part of the Chemical Engineering Commons

Recommended Citation

One-dimensional CFD model of a multiphase loop polymerization reactor

by

Michael Christopher Baker

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

MASTER OF SCIENCE

Major: Chemical Engineering

Program of Study Committee:
Rodney O. Fox, Major Professor
Alberto Passalacqua
Dennis Vigil

Iowa State University
Ames, Iowa
2015

Copyright © Michael Christopher Baker, 2015. All rights reserved.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF TABLES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>xv</td>
</tr>
<tr>
<td>CHAPTER 1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Liquid-phase polypropylene polymerization in tubular loop reactors</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Thesis outline</td>
<td>2</td>
</tr>
<tr>
<td>CHAPTER 2. REVIEW OF LITERATURE</td>
<td>5</td>
</tr>
<tr>
<td>2.1 Industrial scale tubular loop reactor modeling</td>
<td>5</td>
</tr>
<tr>
<td>2.2 Pilot scale tubular loop reactor CFD studies</td>
<td>10</td>
</tr>
<tr>
<td>2.3 Process control in industrial loop polymerization reactors</td>
<td>14</td>
</tr>
<tr>
<td>2.4 One-dimensional fluid dynamics modeling of tubular polymerization reactors</td>
<td>15</td>
</tr>
<tr>
<td>CHAPTER 3. THEORY</td>
<td>16</td>
</tr>
<tr>
<td>3.1 Model introduction</td>
<td>16</td>
</tr>
<tr>
<td>3.2 WENO scheme</td>
<td>17</td>
</tr>
<tr>
<td>3.2.1 Solution methodology</td>
<td>18</td>
</tr>
<tr>
<td>3.3 Continuity equation</td>
<td>21</td>
</tr>
<tr>
<td>3.3.1 Solution methodology</td>
<td>22</td>
</tr>
<tr>
<td>3.3.2 Constitutive relations: Growth and harvesting/injection</td>
<td>23</td>
</tr>
<tr>
<td>3.4 Momentum equation</td>
<td>26</td>
</tr>
<tr>
<td>3.4.1 Solution methodology</td>
<td>26</td>
</tr>
<tr>
<td>3.4.2 Constitutive relation: Effective solid viscosity</td>
<td>28</td>
</tr>
<tr>
<td>3.4.3 Constitutive relation: Granular Pressure</td>
<td>29</td>
</tr>
</tbody>
</table>
5.2.1 Analysis ................................................................. 59

5.3 Uniform trial parameter study ........................................... 59
  5.3.1 Particle diameter ................................................. 59
  5.3.2 Liquid phase laminar viscosity ................................ 61
  5.3.3 Maximum solid fraction ......................................... 62
  5.3.4 Restitution coefficient ......................................... 63
  5.3.5 Analysis .............................................................. 64

5.4 Settled restart parameter study ....................................... 64
  5.4.1 Particle diameter ................................................. 64
  5.4.2 Liquid phase laminar viscosity ................................ 66
  5.4.3 Maximum solid fraction ......................................... 68
  5.4.4 Restitution coefficient ......................................... 69
  5.4.5 Analysis .............................................................. 69

5.5 Harvest, growth, and injection trials with constant circulation . 70
  5.5.1 Uniform .............................................................. 71
  5.5.2 Settled restart ..................................................... 76
  5.5.3 Half-plug loading ................................................ 79
  5.5.4 Quarter-plug loading ............................................. 82
  5.5.5 Plug Length Comparison ........................................ 85
  5.5.6 Analysis .............................................................. 87

5.6 Harvest, growth, and injection trials with pump circulation .......... 87
  5.6.1 Uniform .............................................................. 88
  5.6.2 Settled restart ..................................................... 92
  5.6.3 Half-plug loading ................................................ 95
  5.6.4 Quarter-plug loading ............................................. 98
  5.6.5 Plug Length Comparison ........................................ 101
  5.6.6 Analysis .............................................................. 103

5.7 Operational modifications ............................................... 103
  5.7.1 Solid fraction loading .......................................... 104
5.7.2 Slow harvesting response ........................................... 107
5.7.3 Delay time .......................................................... 113
5.7.4 Multiple harvest points .......................................... 119
5.7.5 Analysis ............................................................. 125

CHAPTER 6. CONCLUSIONS AND RECOMMENDATIONS ............. 126

BIBLIOGRAPHY .......................................................... 130

APPENDIX A. NOMENCLATURE ....................................... 136

APPENDIX B. MATLAB CODE AND SUBROUTINES .............. 138
**LIST OF TABLES**

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 4.1</td>
<td>Reactor geometric parameters</td>
<td>46</td>
</tr>
<tr>
<td>Table 4.2</td>
<td>Phase Parameters</td>
<td>49</td>
</tr>
<tr>
<td>Table A.1</td>
<td>Subscripts and superscripts</td>
<td>136</td>
</tr>
<tr>
<td>Table A.2</td>
<td>Nomenclature table</td>
<td>137</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 2.1</td>
<td>Representation of the reactor from Zacca and Ray [52]</td>
<td>6</td>
</tr>
<tr>
<td>Figure 3.1</td>
<td>Graphical representation of the 5th-order method as applied in this model to calculate the face values. Based on a picture in Shu and Qiu [42]</td>
<td>18</td>
</tr>
<tr>
<td>Figure 3.2</td>
<td>Introduction of harvesting harmonics and representation of harvesting in-phase and out-of-phase over four space times</td>
<td>43</td>
</tr>
<tr>
<td>Figure 3.3</td>
<td>Harvesting slightly out-of-phase example</td>
<td>44</td>
</tr>
<tr>
<td>Figure 4.1</td>
<td>Geometric representation of the reactor modeled in this study including boundary conditions</td>
<td>46</td>
</tr>
<tr>
<td>Figure 5.1</td>
<td>Liquid and solid phase velocity profiles over time using a uniform initial condition</td>
<td>51</td>
</tr>
<tr>
<td>Figure 5.2</td>
<td>Periodic behavior of the solid fraction profile over the first two reactor space times using a uniform initial condition.</td>
<td>52</td>
</tr>
<tr>
<td>Figure 5.3</td>
<td>Solid fraction profile over time using a uniform initial condition. The time increment was chosen such that the transient wave is in-phase in each plot</td>
<td>53</td>
</tr>
<tr>
<td>Figure 5.4</td>
<td>Pressure drop and pressure oscillation standard deviation over time using a uniform initial condition. Each standard deviation was taken over a single reactor space time</td>
<td>53</td>
</tr>
<tr>
<td>Figure 5.5</td>
<td>Liquid and solid phase velocity profiles over time using a settled initial condition</td>
<td>55</td>
</tr>
<tr>
<td>Figure 5.6</td>
<td>Solid fraction profile and extrema over time using a settled initial condition. The spatial axis of the plug profile is in a plug-static reference frame based on the overall circulation velocity.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.7</td>
<td>Pressure drop and pressure oscillation standard deviation over time using a settled initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.8</td>
<td>The effect of the plug position on the pressure drop.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.9</td>
<td>The effect of the plug position on the pressure drop (cont.).</td>
<td></td>
</tr>
<tr>
<td>Figure 5.10</td>
<td>Velocity profile and pressure drop oscillation standard deviation over time varying the average particle diameter and using a uniform initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.11</td>
<td>Velocity profile and pressure drop oscillation standard deviation over time varying the laminar fluid viscosity and using a uniform initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.12</td>
<td>Velocity profile and pressure drop oscillation standard deviation over time varying the maximum solid fraction and using a uniform initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.13</td>
<td>Velocity profile and pressure drop oscillation standard deviation over time varying the restitution coefficient and using a uniform initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.14</td>
<td>The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the average particle diameter and using a settled plug initial condition.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.15</td>
<td>Solid fraction profile over time using a settled plug initial condition and an average particle diameter ten times the magnitude of the control case.</td>
<td></td>
</tr>
<tr>
<td>Figure 5.16</td>
<td>The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying fluid laminar viscosity and using a settled plug initial condition.</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5.17 Solid fraction profile over time using a settled plug initial condition and a liquid phase laminar viscosity one-tenth the magnitude of the control case .......................................................... 67

Figure 5.18 The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the solid fraction at maximum packing and using a settled plug initial condition ....... 69

Figure 5.19 The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the particle restitution coefficient and using a settled plug initial condition ................. 70

Figure 5.20 Solid fraction profile and extrema over time with growth, harvesting, and injection using a uniform initial condition .................. 72

Figure 5.21 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a uniform initial condition .... 72

Figure 5.22 In-phase harvesting over time using a uniform initial condition ...... 73

Figure 5.23 In-phase harvesting over time using a uniform initial condition (cont.) 74

Figure 5.24 In-phase harvesting over time using a uniform initial condition (cont.) 75

Figure 5.25 Solid fraction profile and extrema over time with growth, harvesting, and injection using a settled initial condition .................. 77

Figure 5.26 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a settled initial condition .... 77

Figure 5.27 Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a settled initial condition .......................... 78

Figure 5.28 Solid fraction profile and extrema over time with growth, harvesting, and injection using a half-plug initial condition .................. 80

Figure 5.29 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a half-plug initial condition .. 80
Figure 5.30  Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a half-plug initial condition ......................... 81

Figure 5.31  Solid fraction profile and extrema over time with growth, harvesting, and injection using a quarter-plug initial condition ......................... 83

Figure 5.32  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a quarter-plug initial condition 83

Figure 5.33  Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a quarter-plug initial condition ......................... 84

Figure 5.34  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the harvest, growth, and injection trials .............................. 86

Figure 5.35  Application of the pump performance curve to the circulation velocity of the reactor using a uniform initial condition. Adjusted units for pressure and velocity using respective reference values are used ...................... 88

Figure 5.36  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition ......................... 89

Figure 5.37  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition ......................... 90

Figure 5.38  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the uniform initial condition trials with and without the pump curve applied ...................... 91

Figure 5.39  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a settled initial condition .............................. 93
Figure 5.40  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a settled initial condition ............... 93

Figure 5.41  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the settled initial condition trials with and without the pump curve applied ............... 94

Figure 5.42  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition ............... 96

Figure 5.43  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition ............... 96

Figure 5.44  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the half-plug initial condition trials with and without the pump curve applied ............... 97

Figure 5.45  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a quarter-plug initial condition ............... 99

Figure 5.46  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a quarter-plug initial condition ............... 99

Figure 5.47  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the quarter-plug initial condition trials with and without the pump curve applied ............... 100

Figure 5.48  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the harvest, growth, and injection trials ............... 102
Figure 5.49 Comparison of the pressure drop oscillation standard deviation, adjusted circulation velocity, overall reactor solid fraction, and maximum solid fraction using a uniform initial condition at overall solid fraction loading of 0.13, 0.29, and 0.45 .......................... 106

Figure 5.50 Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor .... 108

Figure 5.51 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor ........................................ 108

Figure 5.52 Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor .... 110

Figure 5.53 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor ........................................ 110

Figure 5.54 Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction using a uniform and half-plug initial conditions with and without a slow response interval . 112

Figure 5.55 Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control response is delayed by 6 seconds ......................... 114
Figure 5.56 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control response is delayed by 6 seconds .......................... 114

Figure 5.57 Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control response is delayed by 6 seconds .......................... 116

Figure 5.58 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control response is delayed by 6 seconds .......................... 116

Figure 5.59 Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction using a uniform and half-plug initial conditions with and without delaying the harvesting control response .......................... 118

Figure 5.60 Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one .......................... 120

Figure 5.61 Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one .......................... 120
Figure 5.62  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one. 122

Figure 5.63  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one. 122

Figure 5.64  Comparison of the harvest and injection coefficient with one and two harvest outlets. 123

Figure 5.65  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum and minimum solid fraction using a uniform and half-plug initial conditions with one and two harvesting locations. 124
ACKNOWLEDGEMENTS

I will like to take this opportunity to show my appreciation and thanks for the significant contributions others have made to the development of this model. I would like to first thank my adviser, Prof. Rodney Fox, who provided the theoretical bedrock everything in this model is based upon and indispensable guidance at every stage of its creation. I would also like to thank Prof. Alberto Passalacqua for his early work in simulating this system in OpenFOAM and guidance in all the later stages. I give special thanks to Dr. Bo Kong for his critical work and help at the late stages of this project. I owe thanks to all of the Prof. Rodney Fox and Prof. Alberto Passalacqua research group members who have helped me in a plethora of ways over the years, with special mention to David Williams who offered invaluable 11th-hour computational resources. Finally, I would like to thank the people at Chevron Phillips Chemical for their generous support of this research.
CHAPTER 1. INTRODUCTION

1.1 Liquid-phase polypropylene polymerization in tubular loop reactors

There are a wide range of choices for producing olefins on the industrial scale depending on economics, feedstock availability, and type and quality of the product desired [51]. Metallic solid catalyzed reactions have been successfully applied in both the gas and liquid phases. For reactions in the gas phase, reactor types are most often of the stirred or fluidized bed variety. Gas phase reactors are known for producing high yields without the need for liquid inventory [51]. Reactions in the liquid phase involve suspending small solid catalyst particles with diameter on the order of 10-200 microns in a liquid medium composed of monomer feedstock and inert solvents [51]. The feedstock permeates the particles and begin to polymerize due to contact with the catalytic surface. The polymer grows, breaking apart the catalyst and eventually becoming a polymer particle as large as 5 mm in diameter [51]. Liquid phase polymerization reactors generally have two distinct forms: stirred tank reactors and tubular reactors. For the purposes of this research, a particular type of the latter is focused on: tubular loop reactors.

Tubular loop polymerization reactors have a very simple design of a single continuous pipe loop with circulation driven by a pump or a series of pumps. Connections at particular points feed the reaction components into the reactor and harvest the products from it. Initial work on tubular reactors in the production of ethylene at high pressure began in the 1930s and 1940s at ICI, BASF, DuPont, and Union Carbide and has since expanded to a wide spectrum of olefins [32] [44]. With the development of Ziegler-Natta catalysts in the 1960s came the ability to produce stereospecific polypropylene at the industrial scale and thus the ability to produce polypropylene in these tubular reactors [26] [30].
Tubular reactors are attractive due to how they offer increased control of how the polymer is produced relative to tank reactors [44] [52]. When faced with high concentrations of solid polymer particles, tank reactors often experience difficulties related to thermal transport and mixing [52]. This is specifically a problem in reactors producing polypropylene due to the highly exothermic and temperature-dependent nature of the reaction [50]. The increased surface area of tubular reactors offers the opportunity for better temperature control and thus better reaction control [38]. Uniformly turbulent flow within the tubes offers superior mixing of reaction components throughout the reactor [4]. This is especially important given that olefins like polypropylene often are generated with a specified molecular mass grade in mind [17] [43]. Better mixing and reaction control ensures that the distribution of molecular weights in the final product is narrower and has an average closer to the desired molecular mass grade.

Major challenges in the operation of tubular polymerization reactors include clogging of the tubes and fouling of the tube surface [33]. Clogging not only inhibits flow and mixing, it also puts pressure on the pump driving circulation. Fouling of the tube surface can impede the thermal control of the system. Ouzened et al [33] details several varied methods that have had success in individual cases in preventing this behavior in the operation of reactors including heavy mixing of the reactor feed, changing the material of the interior tube wall, and pulsing the recirculation velocities. Although those methods worked in those particular cases, generating a model of the system is desirable in order to find the specific conditions which cause these behaviors.

1.2 Thesis outline

The purpose of this study is to develop a one-dimensional solid-liquid computational fluid dynamics model to examine axial variation in an industrial-scale tubular loop polypropylene reactor to gain insight into its behavior during operation. The primary focus of these models is on how detrimental effects such as plugging or wild swings of the overall pressure drop can develop in the reactor and what particular methods can be employed to deal with them or prevent them from happening in the first place. After the history of modeling tubular loop reactors is introduced in chapter 2, the theory behind the model is presented in chapter 3. The
geometry of the generic 8-leg polypropylene loop polymerization reactor and the parameters of the solid and liquid phases flowing through it are introduced in chapter 4. The first study in section 5.1 examines two-phase flow around the repeat unit of the reactor starting from a uniform solid phase profile. Section 5.2 duplicates the trial in section 5.1 while starting from an initial condition simulating the state a reactor would be in if circulation were stopped and the solid phase settled to the bottom. The purpose of this study is to observe how the reactor responds to a preexisting region of highly concentrated solid phase. Section 5.3 and 5.4 are parameter studies varying the average particle size, the liquid phase laminar viscosity, the solid fraction at maximum packing, and the restitution coefficient using both uniform and settled plug initial conditions to explore how those changes cause the results to differ from those in section 5.1 and 5.2. Section 5.5 applies solid phase growth and harvesting effects controlled by a pressure drop-based PI control system on a complete 8-leg reactor. Furthermore, the control system is tested by examining its response to different sizes of plugs introduced by the initial condition. Section 5.6 shows the implementation of a pump performance curve which drives the circulation rate through the overall pressure drop. The trials involving initial plug size variation are repeated using pump performance curve driven flow. Lastly, a series of changes in the operation of the reactor are done in section 5.7 using the results gathered from previous trials designed to correct or prevent particular issues detrimental to the operation of the reactor. This includes decreasing or increasing the solid phase loading in the reactor, slowing down the harvesting response, delaying the harvest response, and adding an additional harvesting outlet.
From all of these trials, conclusions on the following are made:

- How several parameters varied uniformly within the reactor impact the results

- How undesirable behavior such as plugging and wild pressure oscillation can be developed or sustained over time

- What role the control system plays related to that behavior

- How the pump performance curve affects the control system

- The effectiveness of the modifications to the model designed to address undesirable behavior
CHAPTER 2. REVIEW OF LITERATURE

2.1 Industrial scale tubular loop reactor modeling

There is a significant dearth of CFD modeling of tubular polymerization reactors in the literature, especially at the industrial scale. In most modeling studies of these reactors, the fluid dynamics typically are either highly simplified or avoided entirely, with the preference to model the system as plug flow or as an ideal CSTR [38] [41]. The reasoning behind this can primarily be found in the landmark study Zacca and Ray [52], which demonstrated that under a large amount of recirculation a tubular polymerization reactor will act like a series of interconnected plug flow reactors or an ideal CSTR. With this justification, studies focusing on thermal and reaction effects or macro process design-scale studies which make up the bulk of the literature are able to significantly reduce the complexity of their particular model despite its limitations [41]. Later work based on Zacca and Ray [52] further explored its implications in ways that both validate it and cast into question some of the assumptions made in its development [4] [30] [36] [50].

The earliest work in the literature focused on industrial scale modeling of tubular polymerization reactors focused on continuous tubular polymerization reactors [38] [19] [18] [20]. While extremely similar in intention to a loop polymerization reactor, continuous tubular reactors are not fully recirculated systems; catalyst and monomer are combined towards the beginning of a tube and a stream yielding the polymerized product exits the other [20]. Due to the lack of recirculation, these reactors often are longer or operate at slower velocities than tubular loop reactors [44] [20] [11]. Although early analysis of these reactors such as Reimschuessel and Nagasubramanian [37] assumed simplified plug flow, others such as Sala et al [38] and Klein-streuer and Agarwal [19] used the full steady state continuity, momentum, and energy balances
to obtain the axial and radial profiles of short single phase continuous tubular polymerization reactors. Hamer and Ray [11] even developed a similar dynamic model of a continuous polymerization reactor 1 km in length. Despite those particular developments, they were not fully carried over to the development of loop polymerization reactors and other methods of modeling the reactors took precedence.

Zacca and Ray [52] is a milestone study in modeling the behavior of a loop polymerization reactor at the industrial scale that had a significant impact on the field. It modeled an industrial-scale olefin loop polymerization reactor with a total length of 178 meters. The geometry of the reactor in the model is two one-dimensional sections connected together in a loop, with the inlet and outlet of the reactor at the different connection points on either side of each section. A representation of this reactor is displayed in Figure 2.1 A recycle ratio controls how much of the stream is harvested while the inlet flowrate remains constant. Consequently, the recycle ratio controls the circulation velocity of the reactor, speeding up or slowing down the circulation to maintain a constant reactor volume if the recycle ratio is smaller or larger. Not only did it include generalized olefin reaction kinetics in the model, it also included thermal and basic transport models. The equations were solved using a mean weighted residual method. One key assumption in the development of the model was that the flowrate was necessarily quick enough such that there is no significant difference in the velocities of the solid phase and the liquid phase and thus only the liquid phase transport was considered. Only the axial
distribution of the reactor was considered; it was assumed that the flowrate was sufficiently turbulent to eliminate any significant radial variation. Axial concentration of the various species in the reactor was calculated in material balance equations including an axial dispersion model for diffusion. The axial velocity of the profile was calculated to vary through maintaining a constant volume in the reactor with the growth of the solid phase from the polymerization reaction consuming the less-dense liquid monomer. Effects such as gravity, turbulence, and wall friction did not have an effect on the magnitude of the axial circulation velocity profile, although wall friction was included in the calculation of the reactor pressure drop. The thermal profile was calculated using an energy balance and considered the presence of a cooling jacket throughout the entire length of the reactor.

Zacca and Ray [52] evaluated the reactor at various recycling ratios and compared the results of the average monomer concentration and the degree of polymerization to that predicted by a simple ideal CSTR model. As the recycling ratio increased, the more the reactor behaved like the ideal CSTR model. In particular, it concluded that recycling ratios above 30 behaved like the ideal CSTR model. It also showed that larger recycling ratio resulted in an increasingly uniform axial distribution of monomer in the reactor. The results were also compared to the results predicted by solving the conversion of the system as a pair of plug flow reactors in series. Only at the largest recycling ratios did the solution match the solution for a pair of interconnected plug for reactors. The critical settling velocities were also computed at a spectrum of recycle ratios. It predicted that settling becomes significant at recycle ratios equal to or less than 1.

The thermal profile results in Zacca and Ray [52] had a significant feature to them: the sustained oscillation of temperature throughout the reactor over time. The period of these oscillations matches that of the residence time of the reactor. These oscillations are a result of the periodic imbalance between the heat generated by the polymer throughout the reactor, the uniform cooling by the cooling jacket, and input of cool feed at the reactor inlet. These oscillations are significant enough as to have an effect on the molecular weight of the polymer harvested at the outlet.
Further analysis of these type of oscillations was done in Melo et al [30] in a simulation of a smaller 3.17 meter long reactor. The flow was modeled using a slightly modified version of the Zacca and Ray [52] model which neglected the velocity gradients from particle growth and included a thermal dissipation model with the external thermal capacitance of the reactor taken into account. Although the results primarily focused on extremely low recirculation velocities where the significant thermal oscillations first begin to develop rather than the turbulent operating conditions of Zacca and Ray [52], it demonstrated that sufficient cooling throughout the reactor is able to maintain thermal stability. If the cooling system becomes inadequate for the cooling needs of the reactor due to deficient design or failure, thermal oscillation will result. If any solvent or reaction component present in the reactor has a low bubble point, these thermal spikes may cause the formation of gas and corresponding damage to the reactor equipment.

One element missing in the presentation of the model in Zacca and Ray [52] is any sort of comparison of its results with data measured from an actual reactor. De Lucca et al [4] helps to fix this through modeling a particular tubular loop polymerization reactor with confidential geometry and operating parameters using a modified version of the model in Zacca and Ray [52] similar to Melo et al [30]. Results for the melt flow index and xylene solubles fraction of the outflow indicated by the model were compared to measured data from the reactor. The data measurements of the reactor included instances where the feed of the reactor was changed such that the grade of polymer produced was modified and the feed parameters of the model were similarly changed at those points to reflect this. Even through these changes the results of the model were extremely close to the measurements over time, consistently remaining within the range of measurement accuracy.

Following-up to Zacca and Ray [52], Reginato et al [36] noted that a potential problem in modeling the reactor as an ideal CSTR was that the output for the solid product removed might not be always consistent with the average reactor polymer concentration due to segregation of the solid and liquid phases within the reactor. To address this, Reginato et al [36] developed a non-ideal CSTR model introducing a discharge factor to an ideal CSTR model. The discharge factor was developed as a parameter to indirectly define a ratio between the harvested solid concentration and the average reactor solid concentration. This was applied to slurry density
data from a particular industrial loop polymerization reactor collected over a week-long run that indicated a significantly lighter slurry density in the output than that predicted by the ideal CSTR model. Using the non-ideal CSTR model, the value for the discharge factor was tuned to successfully force the CSTR model to fit the reactor data.

Yang et al [50] revisited Zacca and Ray [52] and added key changes to the model related to how it is solved and how the recirculation velocity varies throughout the system. Rather than using a mean weighted residuals method, Yang et al [50] discretized the partial differential equations using the Crank-Nicholson method and solved them implicitly at each time step. More importantly, Yang et al [50] included the Tait equation of state linking pressure to the local temperature and slurry density in the reactor. This in turn allowed the pressure drop calculation originally presented in Zacca and Ray [52] to be used to solve for the recirculation velocity profile of the reactor. With these changes, an interesting deviation emerged: At larger and larger recycle ratios, Zacca and Ray [52] predicted an increasingly uniform profile down the length of the reactor, converging to a result predicted by an ideal CSTR model. The results of Yang et al [50] show even at large recycle ratios this uniformity is not complete; there is a consistent difference in the composition and temperature profile before and after the location of the recycling output. It is at that location where a part of the stream depending on the recycle ratio is diverted to the output and thus the second half of the reactor is flowing at a slower flowrate. Although the model results still can approximate an ideal CSTR at large recycling ratios due to this difference being very small, it demonstrates that the axial profile changes due to the change in velocity. These results were validated through successfully matching the range of temperature, pressure, velocity, and composition data with the operating conditions of a particular industrial reactor.

Zacca and Ray [52] and the papers that proceeded it have demonstrated that the ideal CSTR and plug flow models are able to provide a reasonable approximation of the thermal and compositional behavior of loop polymerization reactors, albeit not without some caveats. Melo et al [30] further investigated the thermal oscillations seen in Zacca and Ray [52], confirming that they are the product of a deficient reactor cooling system. De Lucca et al [4] confirmed that the model from Zacca and Ray [52] to able to successfully model elements of the outflow
composition of a real industrial reactor. Reginato et al [36] developed a workaround parameter in a non-ideal CSTR model to predict the density of the outflow given a situation where there is a non-uniform distribution of polymer solid phase in the reactor. Although the non-ideal CSTR model was able to be successfully simulate a real industrial reactor with a significantly lighter slurry density than what the ideal CSTR model predicted, the need for a tuning procedure to match each particular reactor potentially limits its use in general application. Improvement made in Yang et al [50] to the solution method and calculation of the recirculation velocity demonstrated that internal velocity variations in the reactor will have an impact on the reactor profile. Finally, it is important to note that Zacca and Ray [52] and the research based on its conclusions neglect solid phase maldistribution in the reactor and thus have little to say when examining the underlying reasons for radial accumulation along bends or axial clogging.

2.2 Pilot scale tubular loop reactor CFD studies

Despite the absence of significant CFD research on industrial scale reactors, more recently there has been significant work in modeling a tubular polypropylene loop reactor using CFD on the pilot scale. In particular, Shi et al [41], Gao et al [7], Yan et al [47], and Yan et al, all focused on the same loop reactor with slightly different approaches and intentions. The particular loop reactor modeled is a single rectangular loop with a total length of 11.3 meters that matches the geometry of a pilot reactor in China [41]. Flow is driven in this reactor by an impeller pump located at the corner of the reactor. In Shi et al [41], Gao et al [7], and Yan et al [48], the impeller movement modeled through a separate rotating reference frame was used to circulate the slurry through the reactor. In Yan et al [47] the impeller is not included in the model and instead circulation was maintained using a pressure jump discontinuity estimating the overall pressure drop of the loop at the location of the pump.

Shi et al [41] is the foundation of all of the proceeding papers on the pilot reactor. It uses the two phase Euler-Euler model equations including the standard k-epsilon model for turbulence and the kinetic theory of granular flow closures for the solid phase parameters. A steady state solution of the full three-dimensional geometry of the reactor is found using the SIMPLE algorithm. The model used a Johnson and Jackson partial slip wall drag model.
In a series of runs Shi et al [41] varied the average particle size and the impeller pump rotational velocity parameters to examine their respective effects on the cross sectional solid fraction profile of the pipe at various points in the reactor. As the average particle size was increased, the solid fraction profile became less uniform. This was especially apparent in the bend cross sections where the solid phase accumulated along the outer rim at the expense of the solid phase at the inner rim. Although increasing the circulation velocity increased the uniformity of the profile in the straight legs of the pipe, significant non-uniformity was maintained along the bends at all velocities. This is due to how the non-uniformity at the bends is primarily a product of particle inertia.

Shi et al [41] was validated by comparing the overall pressure drop of the loop at a series of velocities to that predicted by the Newitt correlation. Overall, the pressure drops predicted by the model has good numerical correspondence with the Newitt correlation. This was significantly helped along by how the specularity factor parameter in the wall drag was specifically tuned at one velocity to produce an identical pressure drop to that predicted by the Newitt correlation. Given this, this validation only confirms that this model was able to produce a pressure drop that scales with velocity in a similar way to the Newitt correlation.

Gao et al [7] expands the model in Shi et al [41] through solving the temperature profile of the reactor alongside the fluid dynamics. The temperature profile at the locations of solid fraction accumulation is of interest in regard to the management of the exothermic polymerization reaction. The reaction rate drives the thermal production and in Gao et al [7] it was dependent on the local concentration of the solid phase. For the thermal boundary conditions, the upward and horizontal legs included a water-cooled jacket while the bends were assumed to be adiabatic. Gao et al [7] had an identical validation procedure to Shi et al [41].

The temperature profiles from the upward flowing leg and the bend leading to the downward flowing leg were the primary focus areas of measurement. Similar to Shi et al [41], both circulation velocity and particle size was varied in a series of runs along with the overall reactor solid fraction. As the concentration of solid fraction increased in the reactor, so did the magnitude of the temperature profile in the leg portion of the reactor. The profile of the bend saw an even greater increase in the temperature magnitude at larger solid fractions. There was
also a corresponding asymmetry in the profile due to the accumulation of heat-producing solid phase along the outer rim. The magnitude of the temperature profile significantly decreased in both the leg and bend portions with increasing recirculation velocities. Smaller particle sizes resulted in larger temperature magnitudes in both the bend and the leg.

Yan et al [48] duplicates the conditions of Shi et al while examining how the addition of a guiding vane to the impeller pump affects the cross sectional solid phase distribution. The guiding vane reduces the rotating angular velocity of the solid phase exiting from the impeller and results in a more uniform solid phase distribution. An important addition first seen in Yan et al [48] is that the validation process now includes the pressure drop data from the plant itself which agrees well with both the pressure drop predicted by the Newitt correlation and the model data.

In a departure from the other studies, Yan et al [47] uses equations from the mixture model solved dynamically in time. Unlike the two equation Euler-Euler model, the mixture model considers the flow as a unified liquid and solid phase. Although only the slurry velocity is solved for, the velocities of the respective phases are tracked using a correlation for interphase drag. The mixture model generally is not well-suited for systems with Stokes numbers significantly more than one where there are large differences between the solid phase and liquid phase response times [1]. The geometry of the solution is also simplified into a two-dimensional cross section cut vertically.

The key addition featured in Yan et al [47] is the application of a population balance model allowing particle size effects related to growth, aggregation, and breakage to be incorporated into the solution. The changes in the particle size distribution from the population balance model are applied to the CFD model equations through the corresponding changes in the mean particle size. The run permutations included considering growth, aggregation, and breakage separately and all three of them combined. Although Yan et al [47] was solved dynamically, all of the results still retain the features of the steady state solutions of the other studies, including accumulation of solid phase along the outer rims of the bends. Beyond the differences between the bends and the legs of the system, no significant axial variations were developed in the model over time. The aggregation run involved a steady increase in the average size of the solid phase.
over time and resulted in a correspondingly steady increase in solid phase concentration along the outer rim of the bends. Breakage precipitously decreased the solid phase size from the initial condition to a consistent smaller mean particle size. The solid fraction distribution correspondingly remained unchanging after the initial drop. The growth-only run resulted in a significant increase in the particle size over time. This also resulted in a corresponding increase in the magnitude of the Stokes number, reaching values as large as 100 at the largest sizes. Similar to the aggregation run, the increase in average particle size resulted in an increased accumulation of solid phase along the outer rim of the bends. When all three effects were combined, growth was enormously dominant and all the results strongly resembled the growth-only trial, although the particle size was consistently slightly smaller over time due to breakage.

Similar to the other studies, Yan et al [47] was validated using the Newitt correlation. When compared to the other studies, the pressure drops predicted by this model show significantly less clear agreement with the Newitt correlation. A significant factor in this may be due to how the validation curve data was developed using varying solid fractions due to the population balance model changing it over time. Because the specularity factor used for wall drag was tuned at a specific solid fraction, this may be an indicator that the factor may need to be varied with the changing solid fraction.

Overall, this series of studies demonstrated that a CFD model can be applied to obtain a better idea of the solid phase distribution in the reactor not present in the previous literature, particularly at examining the radial cross section of the reactor while varying key operating parameters as in Shi et al [41]. Gao et al [7] not only demonstrated that accumulation of solid phase resulted in areas of the reactor with significantly higher temperatures, it also showed that having a greater overall reactor solid fraction exacerbates this accumulation, particularly in the bends. Yan et al [48] showed that rotational velocity supplied by the impeller pump can have a significant effect on the radial solid fraction profile of the reactor. Finally, Yan et al [47] was able to model the reactor dynamically through the simplifications of using the mixture model instead of the two-equation Euler-Euler model and reducing the geometry to two dimensions. It was also able to include how particle aggregation, breakage, and growth over time can affect the solid phase distribution in the model.
2.3 Process control in industrial loop polymerization reactors

Although studies such as Melo et al [30] highlight the development of temperature oscillations caused by poor thermal control, study on process control is another facet of operating industrial loop polymerization reactors that only has sparse precedent in the literature. The primary focus in the existing literature focuses on the grade control of the product [25]. Cheng and Liu [3] describes the main challenge of a control system for polymer grade in that it requires a two hour long analytical laboratory procedure to accurately measure. It later devises a method for a slurry tank polymerization reactor correlating easy-to-measure reactor conditions with the slurry melt index of the reactor output. Using its particular method, it was able to achieve good predictive accuracy of the output of a particular industrial tank reactor.

In a distinctive study focusing on polymer loop reactors, Vega et al [45] applied a hybrid-neural network control system for the temperature for a particular reactor. Although it was based on only an extremely simplistic CSTR model that ignored any sort of axial or radial non-uniformity in regard to both transport and temperature, it was able to successfully exercise control of the conversion and average molecular weight through controlling the temperature and feed concentration. Despite its success, the process of teaching the neural network was arduous and the resultant control system is exclusive to the reactor it was applied to.

Luo et al [24] was another isolated paper that focused on modeling the pressure of a complete multi-loop reactor polypropylene polymerization system in the context of emergency accidents where pressure-relief systems would need to be employed. The fluid dynamics were significantly simplified in this model, with the individual loop reactors being modeled as CSTRs and the flow in the pipes between reactors modeled using the Bernoulli equation for incompressible flow. The particular incidents in the reactor simulated included the fluctuations in the input catalyst and feedstock and heat removal failure related to the cooling system and fouling of the reactor walls. They found that increases in the feed flowrates for both feedstock and catalyst resulted in a surprising decrease in the system pressure. Failure of the heat removal system resulted in a significant pressure increase and a corresponding increased chance of hotspots in the reactor.
2.4 One-dimensional fluid dynamics modeling of tubular polymerization reactors

Although one-dimensional simplifications have been around for as long as there have been complex multi-dimensional systems, there is some history of applying them to CFD modeling of tubular polymerization reactors. In Kolhapure and Fox [21], a simple constant velocity model in a single dimension was applied to a continuous tubular low-density polyethylene reactor in order to examine the effects of micromixing on polymerization. Mummudi Boopathy [32] took this a few steps further and developed a comprehensive one-dimensional model including fluid dynamics, the thermal profile including cooling, and reaction effects for high-pressure low-density polyethylene production in continuous industrial-scale polymerization reactors. It includes a one-dimensional turbulence model and enforces a constant overall flowrate. The equations are solved using a 5th-order WENO method for the advective fluxes and a 3rd-order Runge-Kutta method for advancement in time. In the results it was observed that the reactor has a stable profile for temperature. When the reactor is disturbed by pressure pulses through the periodic opening and closing of a kick-valve at the end of the reactor, it was observed that the temperature decreases as the pressure also decreases as the valve is opened and the temperature increases as the pressure increases as the valve is closed. However, the magnitude of the temperature increase through closing is greater than that of the temperature decrease through opening, resulting in a net increase in temperature each cycle. It was also observed that the response of the cooling system to temperature increases was slow and concluded that heat transfer alone cannot effectively control the reaction temperature.
CHAPTER 3. THEORY

3.1 Model introduction

This model is designed to calculate the composition and the respective phase velocities and pressure fields involved in the axial flow of a solid-liquid slurry within a tubular medium. The framework for this model is based on the two-phase Euler-Euler model solved dynamically in time with the application of the kinetic theory of granular flow and additional constraints. The major general fluid dynamic assumptions in the development of the model are:

- One-dimensional incompressible flow
- Respective velocity fields for the solid and liquid phases [1]
- Uniform overall volumetric circulation rate
- Uniformly turbulent flow in one-dimension where axial turbulent velocity fluctuations are approximately 10% of the mean velocity [32]
- Turbulent kinetic energy and dissipation are independent of position [32]

The fundamental equations solved in this model are based on the conservation of mass,

$$\frac{\partial}{\partial t}(\alpha_s) + \frac{\partial}{\partial z}(\alpha_s U_s) = S_{cont,s}(\alpha_s, U_s, \Theta_s, t, z) \quad (3.1)$$

solid phase momentum,

$$\frac{\partial}{\partial t}(\alpha_s U_s) + \frac{\partial}{\partial z} \left(\alpha_s U_s U_s + \frac{p_s}{\rho_s} - \nu_{eff,s} \frac{\partial}{\partial z} U_s\right) = S_{mom,s}(\alpha_s, U_s, \Theta_s, t, z) \quad (3.2)$$

and granular energy,

$$\frac{3}{2} \left[ \frac{\partial}{\partial t}(\alpha_s \Theta_s) + \frac{\partial}{\partial z} \left(\alpha_s U_s \Theta_s - \rho_s \frac{\partial}{\partial z} \Theta_s\right) \right] = S_{gran}(\alpha_s, U_s, \Theta_s) \quad (3.3)$$
where \( \alpha_s \) is the volumetric solid fraction, \( U_s \) is the velocity field for the solid phase, \( \Theta_s \) is the granular temperature, \( p_s \) is the granular pressure, \( \rho_s \) is the solid phase bulk density, \( v_{eff,s} \) is the effective solid viscosity, \( \kappa_s \) is the fluctuating energy conductivity, and \( S \) are the respective source and sink terms for each equation. From the solution of these equations, the corresponding volume fraction and velocity for the liquid phase, \( \alpha_l \) and \( U_l \), are calculated through the sum of all volume fractions,

\[
\alpha_s + \alpha_l = 1 \quad (3.4)
\]

and the assumption that a uniform volumetric velocity, \( U_c \), is maintained within the reactor,

\[
\alpha_s U_s + \alpha_l U_l = U_c \quad (3.5)
\]

The liquid phase pressure field is calculated through applying those two assumptions to the sum of the momentum equations for each phase and then solving for the liquid phase pressure, \( p_l \):

\[
p_l(z) = -\rho_l \left( \alpha_s U_s U_s + \frac{p_s}{\rho_s} - v_{eff,s} \frac{\partial}{\partial z} U_s + \alpha_l U_l U_l - v_{eff,l} \frac{\partial}{\partial z} U_l \right) \bigg|_0^z + \rho_l \int_0^z S_{mom,total}(\alpha_s, U_s) \, dz' \quad (3.6)
\]

where \( \rho_l \) is the liquid phase bulk density, \( v_{eff,l} \) is the liquid phase effective viscosity, and \( S_{mom,total} \) is the summed total of the source and sink terms from the liquid and solid momentum equations.

Limiting the model to a single dimensions makes certain physical phenomena difficult to resolve. Although the solid phase shear interaction with the wall and the change in the direction of gravity relative to the direction of flow corresponding to the geometry of the reactor are considered through source terms, inertial effects are not. Because of this, results such as the redistribution of the solid phase along bends in the reactor as seen in the Shi et al [41] series of studies cannot be seen using this model.

### 3.2 WENO scheme

The WENO (Weighted Essentially No Oscillation) scheme is a procedure for reconstructing face side values in the context of a finite volume or a finite difference approach initially intro-
Figure 3.1 Graphical representation of the 5th-order method as applied in this model to calculate the face values. Based on a picture in Shu and Qiu [42].

The following focuses on the precise details of the WENO methodology as applied in this model. It is based on the generalized procedure presented in Shu and Qiu [42] for any $2o + 1$-ordered WENO method, where $o$ is a positive integer. A 5th-order WENO method was applied...
in this model to calculate the face side values for the solid volume fraction, solid phase velocity, and granular temperature. Because this is a 5th-order method, for each series of interior face values of a given cell, it involves using all adjacent cell-averaged values within two cells for a total set of five cells centered at the particular cell. Within this set of five cells, each cell-averaged value can be described using a 5th-order interpolating polynomial $Q$

$$\left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+l}}^n = C_{pm} \int Q(z) \, dz, \ l = -2, -1, 0, 1, 2$$  \hfill (3.7)

where the integration is done within the space of the given individual constituent cell, $C_{i+l}$. This polynomial is defined as the large stencil. These set of five cells can be broken down into three sets of three adjacent cells, each with a corresponding 3rd-order polynomial, $p_j$, defined as

$$\left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+l}}^n = C_{pm} \int p_0(z) \, dz, \ l = -2, -1, 0$$  \hfill (3.8)

$$\left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+l}}^n = C_{pm} \int p_1(z) \, dz, \ l = -1, 0, 1$$  \hfill (3.9)

$$\left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+l}}^n = C_{pm} \int p_2(z) \, dz, \ l = 0, 1, 2$$  \hfill (3.10)

These smaller polynomials are the sub-stencils.

The output of the polynomials can be applied to the location of the cell faces. In explicit form the value of large stencil at the left and right face of a cell are

$$\left[ Q \right]_{L_i}^n = -\frac{1}{20} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-2}}^n + \frac{9}{20} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-1}}^n + \frac{47}{60} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i}}^n - \frac{13}{60} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+1}}^n + \frac{1}{30} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+2}}^n$$  \hfill (3.11)

$$\left[ Q \right]_{R_i}^n = -\frac{1}{30} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-2}}^n - \frac{13}{60} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-1}}^n + \frac{47}{60} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i}}^n + \frac{9}{20} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+1}}^n - \frac{1}{20} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+2}}^n$$  \hfill (3.12)

The value at the left and right face of a cell according to the explicit form of sub-stencils are

$$\left[ p_0 \right]_{L_i}^n = \frac{1}{3} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i}}^n + \frac{5}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-1}}^n - \frac{1}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-2}}^n$$  \hfill (3.13)

$$\left[ p_1 \right]_{L_i}^n = -\frac{1}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i}}^n + \frac{5}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+1}}^n + \frac{1}{3} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i-1}}^n$$  \hfill (3.14)

$$\left[ p_2 \right]_{L_i}^n = -\frac{1}{3} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+2}}^n - \frac{7}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i+1}}^n + \frac{11}{6} \left[ \alpha_s, U_s, \Theta_s \right]_{C_{i}}^n$$  \hfill (3.15)
These linear weights are constant in this model and equal to

\[ [p_0]^n_{R_i} = \left( \frac{1}{3} [\alpha_s, U_s, \Theta_s]_{C_{i-2}}^n - \frac{7}{6} [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n + \frac{11}{6} [\alpha_s, U_s, \Theta_s]_{C_i}^n \right) \] (3.16)

\[ [p_1]^n_{R_i} = \left( -\frac{1}{6} [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n + \frac{5}{6} [\alpha_s, U_s, \Theta_s]_{C_i}^n + \frac{1}{3} [\alpha_s, U_s, \Theta_s]_{C_{i+1}}^n \right) \] (3.17)

\[ [p_2]^n_{R_i} = \left( \frac{1}{3} [\alpha_s, U_s, \Theta_s]_{C_i}^n + \frac{5}{6} [\alpha_s, U_s, \Theta_s]_{C_{i+1}}^n - \frac{1}{6} [\alpha_s, U_s, \Theta_s]_{C_{i+2}}^n \right) \] (3.18)

The face values indicated by the small stencil polynomials can be related to that of the large stencil through a series of linear weights, \( \gamma_j \):

\[ [Q]^n_{L_i} = \sum_{j=0}^{2} [\gamma_j]^n_{L_i} [p_j]^n_{L_i} \] (3.19)

\[ [Q]^n_{R_i} = \sum_{j=0}^{2} [\gamma_j]^n_{R_i} [p_j]^n_{R_i} \] (3.20)

These linear weights are constant in this model and equal to

\[ [\gamma_0]^n_{L_i} = [\gamma_2]^n_{R_i} = \frac{3}{10} \] (3.21)

\[ [\gamma_1]^n_{L_i} = [\gamma_1]^n_{R_i} = \frac{6}{10} \] (3.22)

\[ [\gamma_2]^n_{L_i} = [\gamma_0]^n_{R_i} = \frac{1}{10} \] (3.23)

These linear weights can be immediately used to directly reconstruct the interior face values for each cell but the key part of the WENO scheme involves factoring in smoothness into this reconstruction. This is done through computing the smoothness indicator, \( \beta_j \), for each sub-stencil.

\[ \beta_j = \int C_{pm}^{-1} \left( \frac{\partial}{\partial z} p_j \right)^2 dx + \int C_{pm}^{-3} \left( \frac{\partial^2}{\partial z^2} p_j \right)^2 dx, \quad j = 0, 1, 2 \] (3.24)

In the 5\textsuperscript{th}-order method, both 2\textsuperscript{nd}-order and 1\textsuperscript{st}-order smoothness is considered. The explicit form of the smoothness indicator as applied in this model are

\[ [\beta_0]^n_{L_i} = [\beta_0]^n_{R_i} = \frac{13}{12} \left( [\alpha_s, U_s, \Theta_s]_{C_{i-2}}^n - 2[\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n + [\alpha_s, U_s, \Theta_s]_{C_i}^n \right)^2 \] (3.25)

\[ + \frac{1}{4} \left( [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n - 4[\alpha_s, U_s, \Theta_s]_{C_{i-2}}^n + 3[\alpha_s, U_s, \Theta_s]_{C_i}^n \right)^2 \]

\[ [\beta_1]^n_{L_i} = [\beta_1]^n_{R_i} = \frac{13}{12} \left( [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n - 2[\alpha_s, U_s, \Theta_s]_{C_{i-2}}^n + [\alpha_s, U_s, \Theta_s]_{C_i}^n \right)^2 \] (3.26)

\[ + \frac{1}{4} \left( -[\alpha_s, U_s, \Theta_s]_{C_{i+1}}^n + [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n \right)^2 \]
\[ [\beta_2^n]_{L_i} = [\beta_2^n]_{R_i} = \frac{13}{12} \left( [\alpha_s, U_s, \Theta_s]_{C_i}^n - 2 [\alpha_s, U_s, \Theta_s]_{C_{i+1}}^n + [\alpha_s, U_s, \Theta_s]_{C_{i+2}}^n \right)^2 + \frac{1}{4} \left( [\alpha_s, U_s, \Theta_s]_{C_i}^n - 4 [\alpha_s, U_s, \Theta_s]_{C_{i-1}}^n + 3 [\alpha_s, U_s, \Theta_s]_{C_{i+2}}^n \right)^2 \]  

(3.27)

These smoothness indicators are used to weight the linear weights to generate the unnormalized non-linear weights, \( \omega'_j \):

\[ [\omega'_j]_{L_i}^n = \frac{[\omega_j]_{L_i}^n}{\sum_{j=0}^{2} (e_{nz} + [\beta_0]_{L_i}^n)} \]  

(3.28)

\[ [\omega'_j]_{R_i}^n = \frac{[\omega_j]_{R_i}^n}{\sum_{j=0}^{2} (e_{nz} + [\beta_0]_{R_i}^n)} \]  

(3.29)

where \( e_{nz} \) is small value to ensure that there are no infinite or near-infinite weights in the event of a zero or near-zero smoothness factor summation. The nonlinear weights are normalized to determine the normalized non-linear weights, \( \omega_j \):

\[ [\omega_j]_{L_i}^n = \frac{[\omega'_j]_{L_i}^n}{\sum_{j=0}^{2} [\omega'_j]_{L_i}^n} \]  

(3.30)

\[ [\omega_j]_{R_i}^n = \frac{[\omega'_j]_{R_i}^n}{\sum_{j=0}^{2} [\omega'_j]_{R_i}^n} \]  

(3.31)

Finally, these non-linear weights are applied to the sub-stencils for each cell to reconstruct the approximate interior face values for each cell:

\[ [\alpha_s, U_s, \Theta_s]_{L_i}^n \approx \sum_{j=0}^{2} [\omega_j]_{L_i}^n [p_j]_{L_i}^n \]  

(3.32)

\[ [\alpha_s, U_s, \Theta_s]_{R_i}^n \approx \sum_{j=0}^{2} [\omega_j]_{R_i}^n [p_j]_{R_i}^n \]  

(3.33)

The corresponding exterior face values for each cell are the corresponding interior face values of the adjacent cells:

\[ [\alpha_s, U_s, \Theta_s]_{L_i}^n = [\alpha_s, U_s, \Theta_s]_{R_{i-1}}^n \]  

(3.34)

\[ [\alpha_s, U_s, \Theta_s]_{R_i}^n = [\alpha_s, U_s, \Theta_s]_{L_{i+1}}^n \]  

(3.35)

### 3.3 Continuity equation

The continuity equation is developed from the application of the Reynolds Transport Theorem to a Lagrangian moving mass balance:

\[ \frac{\partial}{\partial t} (\alpha_s) + \frac{\partial}{\partial z} (\alpha_s U_s) = S_{cont,s}(\alpha_s, U_s, \Theta_s, t, z) \]  

(3.36)
Its purpose within the model is to solve for the evolution of the solid fraction profile in time through being subjected to advective flux seen on the left side of the equation along with solid phase growth and harvest stream outflow and replacement liquid phase inflow in the source and sink terms:

$$S_{cont,s} (\alpha_s, U_s, \Theta_s, t, z) = S_{cont,growth,s} (\alpha_s) + S_{cont,harvest/injection,s} (\alpha_s, U_s, \Theta_s, t, z) \tag{3.37}$$

### 3.3.1 Solution methodology

Operator splitting is utilized to separate the advective flux and source terms. This separation simplifies the solution into a simple sourceless advection equation followed up by a reaction-like step in time including the source and sink terms [46]. The advection part of the equation is discretized and solved for the advection-only partial step advancement of the solid fraction, $$a'_s$$, in accordance with the finite volume method:

$$\frac{([a'_s]_C^{n+1} - [a_s]_C^n)}{\Delta t} + C_{pm} (AF ([a_s U_s]_R^n) - AF ([a_s U_s]_L^n)) = 0 \tag{3.38}$$

where $$C_{pm}$$ is the number of cells per meter and $$\Delta t$$ is the time-step [49] [53]. The methodology prescribed here assumes that a uniform mesh with a constant number of cells per meter is used throughout although non-uniform meshes can be applied with appropriate modifications. The fluxes on the left and right sides of each cell are computed as follows:

$$AF ([a_s U_s]_L^n) = \frac{1}{2} \left( [a_s U_s]_L^n + [a_s U_s]_{L+}^n \right) - D_L \tag{3.39}$$

$$AF ([a_s U_s]_R^n) = \frac{1}{2} \left( [a_s U_s]_{R-}^n + [a_s U_s]_{R+}^n \right) - D_R \tag{3.40}$$

The face-side values, $$[a_s U_s]_{L-}^n$$, $$[a_s U_s]_{L+}^n$$, $$[a_s U_s]_{R-}^n$$, and $$[a_s U_s]_{R+}^n$$, are computed using a fifth-order WENO method (see –insert relevant chapter- for details). A global Lax-Friedrichs flux splitting scheme was chosen for the flux dissipation terms in line with work done in Zhang et al [53]:

$$D_L = \frac{1}{2} \max \left| \frac{\partial}{\partial \alpha_s} (a_s U_s) \right| \left( [a_s]_{L+}^n - [a_s]_{L-}^n \right) \tag{3.41}$$

$$D_R = \frac{1}{2} \max \left| \frac{\partial}{\partial \alpha_s} (a_s U_s) \right| \left( [a_s]_{R+}^n - [a_s]_{R-}^n \right) \tag{3.42}$$
For parallel processing, the global Lax-Friedrich scheme becomes a local Lax-Friedrich scheme localized such that the maximum was computed within each processor partition rather than globally down the profile of the reactor. This was done to prevent the need for a large degree of interprocessor communication whenever face-side values would be computed. The absolute value of the derivative of $\alpha_s U_s$ with respect to $\alpha_s$ is calculated locally within each cell using the interior face values:

$$\left| \frac{\partial}{\partial \alpha_s} (\alpha_s U_s) \right| = \frac{\left[ (\alpha_s U_s)_R^n - (\alpha_s U_s)_L^n \right]}{\left[ (\alpha_s)_R^n - (\alpha_s)_L^n \right]}$$

(3.43)

Once the resultant solid fraction from the advective half of the equation is computed, it is then inserted into the source and sink terms for the continuity equation which are applied explicitly to step the solution forward:

$$\frac{([\alpha_s]_{C}^{n+1} - [a'_s]_{C}^{n+1})}{\Delta t} = S_{\text{cont.growth},s} \left( [a'_s]_{C}^{n+1} \right)$$

$$+ S_{\text{cont.harvest/injection},s} \left( [a'_s]_{C}^{n+1}, [U_s]_{C}^n, [\Theta_s]_{C}^n, t, z \right)$$

(3.44)

### 3.3.2 Constitutive relations: Growth and harvesting/injection

Although this model does not directly model the reaction effects, it does model a major consequence of the reaction: the growth of the solid fraction over time. This growth is modeled through the volume fraction of the solid phase increasing through the consumption of the liquid phase. Furthermore, it also includes terms that act as the harvesting process creating the reactor product output stream and the injection process for adding a mixture of fresh feedstock and solvent to maintain the reaction. The harvest and injection processes take place within a specified area within the reactor. These are significant simplifications which involve the following assumptions:

- The growth process is a one-to-one volume exchange from the liquid phase to the solid phase
- The volumetric growth rate of the solid phase is linear in respect to the local volumetric solid fraction; there is ideal control of the feedstock to solvent ratio, catalyst concentration, and reaction conditions such that the growth rate coefficient is constant throughout the reactor
• The harvesting and injection processes are synchronized; as a volume of the reactor in
the harvesting region is removed by the product stream an equal volume of liquid phase
enters the reactor through injection

• The harvest and injection processes are localized within the same region in the reactor

• The composition of the product stream is equivalent to the local compositions in the
harvest and injection region

• The harvesting rate is directly proportional to the flow rate of the liquid phase leaving
the reactor

• The solid fraction of catalyst in the injection stream is negligible

• The average particle size is maintained constant and uniform throughout the reactor
through a combination of growth, harvesting, injection, aggregation, and breakage.

Given these assumptions, the growth, harvest, and injection process are as follows in terms
of volumetric flowrate, $\dot{Q}$:

$$\dot{Q}_{\text{growth},s} + \dot{Q}_{\text{consumption},l} = 0 \quad (3.45)$$

$$\dot{Q}_{\text{growth},s} = K_{\text{growth}} \alpha_s \quad (3.46)$$

$$\dot{Q}_{\text{injection},l} = K_{\text{harvest}} (1 + \frac{\alpha_s}{\alpha_l}) \quad (3.47)$$

$$\dot{Q}_{\text{injection},s} = 0 \quad (3.48)$$

$$\dot{Q}_{\text{harvest},l} = K_{\text{harvest}} \quad (3.49)$$

$$\dot{Q}_{\text{harvest},s} = K_{\text{harvest}} \frac{\alpha_s}{\alpha_l} \quad (3.50)$$

where $K_{\text{growth}}$ is the volumetric growth rate coefficient in respect to the solid fraction and
$K_{\text{harvest}}$ is the volumetric harvesting rate coefficient set equal to the volumetric flowrate of
liquid phase being harvested from the reactor. These growth, harvest, and injection effects are
applied to the continuity equation through the source and sink terms:

$$S_{\text{cont},s}(\alpha, U_s, \Theta_s, t, z) = S_{\text{cont,growth},s}(\alpha_s) + S_{\text{cont,harvest/injection},s}(\alpha_s, U_s, \Theta_s, t, z)$$

$$= k_g \alpha_s - k_{hi}(\alpha_s, U_s, \Theta_s, t) \delta_{hir}(z) \frac{\alpha_s}{1 - \alpha_s} \quad (3.51)$$
where \( k_g \) is the solid fraction growth rate coefficient, \( k_{hi} \) is the solid fraction harvesting rate coefficient, and \( \delta_{hir} \) is an indicator function of the distance down the reactor set equal to one in the designated area where injection and harvesting exists and zero outside of it. \( k_g \) and \( k_{hi} \) respectively correspond to \( K_{growth} \) and \( K_{harvest} \) divided by cell volume.

The harvesting rate coefficient depends on the desired control methodology for the reactor. This can be set to a constant value or depend on a specific timetable or set of reactor conditions. The control system applied in this particular model is based on the one described in U.S. patent 8,816,024 [12] and involves applying a mixture of proportional and integral control response, \( k_{hi,p} \) and \( k_{hi,i} \), in regard to a desired overall pressure drop, \( p_{drop,set,l} \):

\[
\begin{align*}
    k_{hi}(\alpha_s, U_s, \Theta_s, T_{s,p} + \phi_d) &= k_{hi,p}(\alpha_s, U_s, \Theta_s, t_s) + k_{hi,i}(\alpha_s, U_s, \Theta_s, t_s) \quad (3.52) \\
    k_{hi,p}(\alpha_s, U_s, \Theta_s, t_s) &= k_{c,p} \max(p_{drop,l}(\alpha_s, U_s, \Theta_s, t_s) - p_{drop,set,l}, 0) \quad (3.53) \\
    k_{hi,i}(\alpha_s, U_s, \Theta_s, t_s) &= k_{c,i} \max(p_{drop,l}(\alpha_s, U_s, \Theta_s, t_s) - p_{drop,set,l}, 0) + k_{c,j} \max(p_{drop,l}(\alpha_s, U_s, \Theta_s, t_s) - p_{drop,set,l}, 0) \quad (3.54) \\
    T_{s,p} &\in [t_s, t_s + t_{s,i}] \quad (3.55)
\end{align*}
\]

where \( k_{c,p} \) and \( k_{c,i} \) are the proportional and integral control coefficients. This control is applied at specific regular sampling times, \( t_s \), with interval \( t_{s,i} \) where the overall pressure drop of the reactor, \( p_{drop,l} \), is measured and the harvesting coefficient is adjusted accordingly to be constant over the proceeding sampling period, \( T_{s,p} \). A constant delay in control response, \( \phi_d \), can also be specified. The maximum function ensures that the harvesting and liquid-phase injection process cannot reverse and directly cause an increase in the solid fraction in the event that the pressure drop in the system goes below the set point. At those times this control system ensures that the harvesting valve is closed to allow for solid phase growth to increase the pressure drop again. The integral control response is reset to zero as the harvesting valve is closed.
### 3.4 Momentum equation

The solid phase momentum balance,

\[
\frac{\partial}{\partial t} (\alpha_s U_s) + \frac{\partial}{\partial z} \left( \alpha_s U_s U_s + \frac{p_s}{\rho_s} - \nu_{eff,s} \frac{\partial}{\partial z} U_s \right) = S_{mom,s}(\alpha_s, U_s, \Theta_s, t, z)
\]  \hspace{1cm} (3.56)

originates from the application of the divergence theorem, the Reynolds transport theorem, and the continuity equation to a force balance of surface stress forces, external forces, and interphase forces related to interactions and transference [8]. The left side of the equation include the advective and diffusive terms along with the effect of the granular pressure gradient. The momentum sources and sinks on the right side of the equation include the influence of hydrostatic force, \( S_{mom,hydrostatic,s} \); interphase drag, \( S_{mom,interphase,s} \); the liquid phase pressure gradient, \( S_{mom,pressure,s} \); wall shear, \( S_{mom,wall,s} \); growth, \( S_{mom,growth,s} \); and harvesting and injection, \( S_{mom,harvest/injection,s} \):

\[
S_{mom,s}(\alpha_s, U_s, \Theta_s, t, z) = S_{mom,hydrostatic,s}(\alpha_s) + S_{mom,interphase,s}(\alpha_s, U_s) \]
\[
+ S_{mom,pressure,s}(\alpha_s, U_s, \Theta_s) + S_{mom,wall,s}(\alpha_s, U_s) \]
\[
+ S_{mom,growth,s}(\alpha_s, U_s) \]
\[
+ S_{mom,harvest/injection,s}(\alpha_s, U_s, \Theta_s, t, z)
\]  \hspace{1cm} (3.57)

#### 3.4.1 Solution methodology

As in the continuity equation, operator splitting is used to separate the spatial derivative terms and the source terms [46]. The finite volume method is used to evaluate the advective, granular pressure, and diffusive flux terms to obtain the solid phase velocity partial step, \( U'_s \):

\[
\frac{([\alpha_s]^n_C [U_s]^n_C - [\alpha_s]^n_C [U_s]^n_C)}{\Delta t} + \frac{C_{pm}}{\rho_s} \left( AF ([\alpha_s]^n [U_s]^n_R) - AF ([\alpha_s]^n [U_s]^n_L) \right) \]
\[
+ \frac{C_{pm}}{\rho_s} \left( PF (p_s ([\alpha_s]^n_R; [T]^n_R)) - PF (p_s ([\alpha_s]^n_L; [T]^n_L)) \right) \]
\[
- C_{pm} \nu_{eff,s} \left( DF \left( \left[ \frac{\partial}{\partial z} U_s \right]^n_R \right) - DF \left( \left[ \frac{\partial}{\partial z} U_s \right]^n_L \right) \right) = 0
\]  \hspace{1cm} (3.58-3.60)
The advective flux term in the momentum equation is computed in a way identical to that used in the continuity equation, including using the global Lax-Friedrichs flux limiter [53]:

\[
AF ([\alpha_s]_L^n [U_s^2]_L^n) = \frac{1}{2} ( [\alpha_s]_L^n - [U_s^2]_L^n + [\alpha_s]_L^n [U_s^2]_L^n) - D_L 
\] (3.61)

\[
AF ([\alpha_s]_R^n [U_s^2]_R^n) = \frac{1}{2} ( [\alpha_s]_R^n - [U_s^2]_R^n + [\alpha_s]_R^n [U_s^2]_R^n) - D_R 
\] (3.62)

\[
D_L = \frac{1}{2} \max \left| \frac{\partial}{\partial (a_s U_s)} (\alpha_s U_s^2) \right| ([\alpha_s]_L^n [U_s^n]_L^n - [\alpha_s]_L^n [U_s^n]_L^n) 
\] (3.63)

\[
D_R = \frac{1}{2} \max \left| \frac{\partial}{\partial (a_s U_s)} (\alpha_s U_s^2) \right| ([\alpha_s]_R^n [U_s^n]_R^n - [\alpha_s]_R^n [U_s^n]_R^n) 
\] (3.64)

\[
\left| \frac{\partial}{\partial (a_s U_s)} (\alpha_s U_s^2) \right| = \left( \frac{[\alpha_s]_R^n - [U_s^n]_R^n - [\alpha_s]_R^n [U_s^n]_R^n}{[\alpha_s]_L^n [U_s^n]_R^n - [\alpha_s]_L^n [U_s^n]_L^n} \right) 
\] (3.65)

The granular pressure flux is similarly calculated using the values at the faces [8]:

\[
PF (\alpha_s)_L^n, [T]_L^n) = \frac{1}{2} \left( p_s ([\alpha_s]_{L-}, [T]_{L-}) + p_s ([\alpha_s]_{L+}, [T]_{L+}) \right) - D_L 
\] (3.66)

\[
PF (\alpha_s)_R^n, [T]_R^n) = \frac{1}{2} \left( p_s ([\alpha_s]_{R-}, [T]_{R-}) + p_s ([\alpha_s]_{R+}, [T]_{R+}) \right) - D_R 
\] (3.67)

\[
D_L = \frac{1}{2} \max \left| \frac{\partial}{\partial (a_s U_s)} (p_s (\alpha_s, \Theta_s)) \right| ([\alpha_s]_L^n [U_s^n]_L^n - [\alpha_s]_L^n [U_s^n]_L^n) 
\] (3.68)

\[
D_R = \frac{1}{2} \max \left| \frac{\partial}{\partial (a_s U_s)} (p_s (\alpha_s, \Theta_s)) \right| ([\alpha_s]_R^n [U_s^n]_R^n - [\alpha_s]_R^n [U_s^n]_R^n) 
\] (3.69)

\[
\left| \frac{\partial}{\partial (a_s U_s)} (p_s (\alpha_s, \Theta_s)) \right| = \left( \frac{p_s ([\alpha_s]_{R-}, [T]_{R-}) - p_s ([\alpha_s]_{R+}, [T]_{R+})}{[\alpha_s]_R^n [U_s^n]_R^n - [\alpha_s]_R^n [U_s^n]_L^n} \right) 
\] (3.70)

The diffusion equation fluxes use a fourth-order central difference reconstruction as seen in Zhang et al [53]. This particular method of reconstruction was attractive due to it originally being successfully implemented alongside a fifth-order WENO scheme for advection:

\[
DF \left( \left[ \frac{\partial}{\partial z} U_s^n \right]_{Li} \right) = C_{pm} \left( \frac{1}{2} [U_s^n]_{Ci+1} - \frac{15}{12} [U_s^n]_{Ci} + \frac{15}{12} [U_s^n]_{Ci-1} - \frac{1}{12} [U_s^n]_{Ci-2} \right) 
\] (3.71)

\[
DF \left( \left[ \frac{\partial}{\partial z} U_s^n \right]_{Ri} \right) = C_{pm} \left( \frac{1}{2} [U_s^n]_{Ci-1} - \frac{15}{12} [U_s^n]_{Ci} + \frac{15}{12} [U_s^n]_{Ci+1} - \frac{1}{12} [U_s^n]_{Ci+2} \right) 
\] (3.72)

As in the continuity equation, the source terms use the computed solid phase velocity from the advection, diffusion, and granular pressure gradient terms in the momentum source terms.
and step the solution forward in time explicitly:

$$\frac{([\alpha_s]^n_C [U_s]^n_C - [\alpha_s]^n_C C [U_s]^n+1_C)}{\Delta t} = S_{mom,hydrostatic,s} ([\alpha_s]^n_C)$$

$$+ S_{mom,interphase,s} ([\alpha_s]^n_C, [U_s]^n+1_C)$$

$$+ S_{mom,pressure,s} ([\alpha_s]^n_C, [U_s]^n+1_C, [\Theta_s]^n_C)$$

$$+ S_{mom,wall,s} ([\alpha_s]^n_C, [U_s]^n+1_C)$$

$$+ S_{mom,growth,s} ([\alpha_s]^n_C, [U_s]^n+1_C, [\Theta_s]^n_C, t, z)$$

$$+ S_{mom,harvest/injection,s} ([\alpha_s]^n_C, [U_s]^n+1_C, [\Theta_s]^n_C)$$

(3.73)

### 3.4.2 Constitutive relation: Effective solid viscosity

The diffusion term uses an effective solid phase viscosity composed of the solid phase shear viscosity, $\nu_{shear,s}$; shear dilute viscosity, $\nu_{dilute,s}$; bulk viscosity, $\nu_{bulk,s}$; k-epsilon turbulent viscosity, $\nu_{ket,s}$; and bubble-induced turbulent viscosity, $\nu_{bit,s}$:

$$\nu_{eff,s} = \nu_{shear,s} + \nu_{dilute,s} + \nu_{bulk,s} + \nu_{ket,s} + \nu_{bit,s}$$

(3.74)

The shear, dilute, and bulk viscosities of the solid phase are computed in accordance with the Gidaspow granular temperature model [8]:

$$\nu_{shear,s} = \frac{16}{15} \alpha_s d_{part} g_0(\alpha_s)(1 + e_{rest})(\frac{\Theta_s}{p})^{\frac{1}{2}}$$

(3.75)

$$\nu_{dilute,s} = \frac{5}{36} \frac{g_0(\alpha_s) (1 + e_{rest})}{g_0(\alpha_s)(1 + e_{rest})\alpha_s} \frac{d_{part} (p \Theta_s)^{\frac{1}{2}}}{\alpha_s}$$

(3.76)

$$\nu_{bulk,s} = \frac{4}{3} \alpha_s^2 \frac{d_{part} g_0(\alpha_s)(1 + e_{rest})(\frac{\Theta_s}{p})^{\frac{1}{2}}}{\alpha_s}$$

(3.77)

where $d_{part}$ is the particle diameter and $e_{rest}$ is the particle collision restitution coefficient.

$g_0(\alpha_s)$ is defined as the radial distribution function,

$$g_0 (\alpha_s) = \left(1 - \left(\frac{\alpha_s}{\alpha_{s,\max}}\right)^\frac{1}{3}\right)^{-1}$$

(3.78)

where $\alpha_{s,\max}$ is the solid fraction at maximum particle packing [8]. The k-epsilon turbulent viscosity is computed using the assumptions from Mummudi Boopathy [32] that turbulent
kinetic energy, $k_{turb,s}$, and turbulent dissipation, $\rho_s$, is independent of position and that the turbulent velocity in one dimension is equal to one-tenth of the mixture velocity:

$$k_{turb,s} = \frac{3}{2} \left( \frac{1}{10} \rho_s \alpha_s U_s + \rho_l \left( 1 - \alpha_s \right) U_l \right)^2$$

(3.79)

$$\epsilon_{turb,s} = \frac{k_{turb,s}^{3/2}}{d_{pipe}}$$

(3.80)

$$v_{kst,s} = C_\mu \frac{k_{turb,s}^2}{\rho_s}$$

(3.81)

where $d_{pipe}$ is the pipe diameter and $C_\mu$ is the turbulent viscosity coefficient. The bubble-induced turbulence from Sato and Sekoguchi [39] is applied according to Marchisio and Fox [27]:

$$v_{bit,s} = C d_{part} \alpha_s |U_r|$$

(3.82)

where $U_r$ is the interphase relative velocity of the solid phase in respect to the liquid phase.

### 3.4.3 Constitutive relation: Granular Pressure

The granular pressure is evaluated using the values for the solid fraction and granular temperature as outlined in Gidaspow [8]:

$$p_s(\alpha_s, \Theta_s) = \rho_s \Theta_s \left( 1 + 2 \left( 1 + e_{rest} \right) g_0(\alpha_s) \alpha_s \right)$$

(3.83)

### 3.4.4 Constitutive relation: Hydrostatic force

The hydrostatic force term is the gravitational acceleration in relation to the direction of flow, $g$, multiplied by the solid volume fraction [8]:

$$S_{mom,hydrostatic,s}(\alpha_s) = g \alpha_s$$

(3.84)
3.4.5 Constitutive relation: Interphase drag

The Gidaspow Ergun Wen-Yu method was used for interphase drag in the interphase source term [8]:

\[ S_{mom,interphase,s} (\alpha_s, U_s) = \frac{\beta (\alpha_s, U_s)}{\rho_s} U_r \] (3.85)

where \( \beta \) is the overall interphase drag coefficient.

Obtaining the overall interphase drag coefficient first involves the computation of the interphase Reynolds number, \( Re_i \)

\[ Re_i (\alpha_s, U_s) = \frac{d_{part} \alpha_s |U_r|}{\nu_{laminar, l}} \] (3.86)

where \( \nu_{laminar, l} \) is the fluid phase laminar viscosity, and then selects the most appropriate method for computing the particle drag coefficient, \( C_D \),

\[ C_D (\alpha_s, U_s) = \begin{cases} \frac{24}{Re_i (\alpha_s, U_s)} \left[ 1 + 0.15 Re_i (\alpha_s, U_s)^{0.687} \right], & Re_i > 1000 \\ 0.44, & Re_i \leq 1000 \end{cases} \] (3.87)

The drag coefficient is applied to the overall interphase drag coefficient in the Wen and Yu-based dilute flow case

\[ \beta (\alpha_s, U_s) = \frac{3}{4} C_D (\alpha_s, U_s) \left[ a_s^{-1.65}] \right] \frac{p_l |U_r|}{d_{part}}, \alpha_s < .2 \] (3.88)

but it is not used in the Ergun-equation-based dense flow case

\[ \beta (\alpha_s, U_s') = 150 \frac{\nu_{laminar, l} \rho_l \alpha_s^2}{(1 - \alpha_s)^2 d_{part}^2} + \frac{7}{4} \frac{\rho_l \alpha_s U_r}{(1 - \alpha_s) d_{part}}, \alpha_s \geq .2 \] (3.89)

3.4.6 Constitutive relation: Pressure gradient

The pressure gradient, \( \frac{\partial}{\partial z} p_l \), computed in section 3.6.1 using the face values of the pressure for each cell, is applied to the momentum balance as its own source term:

\[ S_{mom,pressure,s} (\alpha_s, U_s, T) = \alpha_s \frac{\partial}{\partial z} p_l (\alpha_s, U_s, T) \] (3.90)
3.4.7 Constitutive relation: Solid phase wall shear

The solid phase contribution to the wall shear,

\[ S_{mom,wall,s}(\alpha_s, U_s) = -0.0214 \frac{4}{d_{pipe}} Re_p(\alpha_s, U_s)^{36} \left( \frac{d_{part}}{d_{pipe}} \right)^{0.99} (g_0(\alpha_s) - 1)^{1.31} \]  

(3.91)

where \( Re_p \) is the particle Reynolds number equal to

\[ Re_p = \frac{d_{part}|U_s|}{\nu_{laminar,l}} \]  

(3.92)

is calculated using a correlation developed by Ferre and Shook [5] for solid-liquid flow in upward legs. The wall shear contribution of the solid phase was calculated through measuring the pressure drop of a vertical flowing slurry in a tubular leg and comparing the result to that predicted by the commonly-used Darcy-Weisbach correlation for a pure liquid. The correlation for momentum losses due to solid phase interactions with the wall was designed to make up for the difference in pressure drop between the pure liquid correlation and experimental data for the slurry case.

3.4.8 Constitutive relations: Growth and harvesting/injection

The impact of growth, harvesting, and injection on the momentum balance is based on the same principles and assumptions from section 3.3.2 and has a similar form:

\[ S_{mom,growth,s}(\alpha_s, U_s) + S_{mom,harvest/injection,s}(\alpha_s, U_s, T, t, z) = k_g \alpha_s U_l - k_{hi}(\alpha_s, U_s, \Theta_s, t) \delta_{hir}(z) \alpha_s U_s \]  

(3.93)

The growth term represents the solid phase momentum gained from the liquid phase transferring to the solid phase due to the reaction and the harvesting and injection term represents the change of solid phase momentum due to it being removed and replaced with a liquid phase of different density.
3.5 Granular temperature equation

The granular energy balance from Gidaspow’s kinetic theory of granular flow

\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} (\alpha_s \Theta_s) + \frac{\partial}{\partial z} \left( \alpha_s U_s \Theta_s - \rho_s \frac{\partial}{\partial z} \Theta_s \right) \right] = S_{\text{gran}}(\alpha_s, U_s, \Theta_s)
\]  

(3.94)
is applied in this model to obtain key closures for the solid phase that affect terms in the momentum equation of the model [8]. The kinetic theory of granular flow is based upon describing the small-scale behavior of particles in a medium in a way analogous to how the movement of molecules are described in the kinetic theory of gases. Granular temperature represents the mean squared fluctuating velocity of particles in a single dimension as they vibrate and collide with each other [8]. Granular pressure from section 3.4.3 is the resultant force per unit area of this movement. Granular temperature is also used to compute the shear, dilute, and bulk viscosity for the effective viscosity as seen in section 3.4.2.

Like the momentum equation, the granular temperature equation is split between the spatial gradient terms and the source and sink terms. The spatial gradient terms include advective and thermal conductive flux terms. The granular energy sources and sinks include granular energy gains and losses from shess, \( S_{\text{gran,shear}}(\alpha_s, U_s, \Theta_s) \); interphase dampening, \( S_{\text{gran,interphase}}(\alpha_s, U_s, \Theta_s) \); interparticle collisions, \( S_{\text{gran,collision}}(\alpha_s, U_s, \Theta_s) \); and turbulent effects, \( S_{\text{gran,turbulence}}(\alpha_s, U_s) \).

\[
S_{\text{gran}}(\alpha_s, U_s, \Theta_s) = S_{\text{gran,stress}}(\alpha_s, U_s, \Theta_s) + S_{\text{gran,interphase}}(\alpha_s, U_s, \Theta_s)
+ S_{\text{gran,collision}}(\alpha_s, U_s, \Theta_s) + S_{\text{gran,turbulence}}(\alpha_s, U_s)
\]

(3.95)

3.5.1 Solution methodology

Once again, following operator splitting, the finite volume method is used to solve the advective and diffusive flux terms for the partial step for the granular temperature, \( \Theta_s' \) [46]:

\[
\frac{([\alpha_s]^n_R, [\Theta_s]^n_R) - [\alpha_s]^n_L, [\Theta_s]^n_L)}{\Delta t} + C_{pm} \left( \frac{\partial}{\partial z} [\Theta_s]^n_R - \frac{\partial}{\partial z} [\Theta_s]^n_L \right) - C_{pm} \kappa_s \left( DF \left( \left[ \frac{\partial}{\partial z} \Theta_s \right]^n_R \right) - DF \left( \left[ \frac{\partial}{\partial z} \Theta_s \right]^n_L \right) \right) = 0
\]  

(3.96)
The advective term for the granular temperature equation is computed in a way identical to that of the continuity and momentum equations [53]:

\[
AF \left([\alpha_s U_s]^n\right)_{L} = \frac{1}{2} \left(([\alpha_s U_s]^n_{L+} [\Theta_s]^n_{L-} + [\alpha_s U_s]^n_{L-} [\Theta_s]^n_{L+}) - D_L \right) \tag{3.98}
\]

\[
AF \left([\alpha_s U_s]^n\right)_{R} = \frac{1}{2} \left(([\alpha_s U_s]^n_{R-} [\Theta_s]^n_{R+} + [\alpha_s U_s]^n_{R+} [\Theta_s]^n_{R-}) - D_R \right) \tag{3.99}
\]

The global Lax-Friedrichs flux limiter is similarly used [53]:

\[
D_L = \frac{1}{2} \max \left|\frac{\partial}{\partial (\alpha_s \Theta_s)} (\alpha_s U_s \Theta_s) \right| \left(\left|\alpha_s U_s \Theta_s \right|_{L+} \left|\alpha_s U_s \Theta_s \right|_{L-} \right) \tag{3.100}
\]

\[
D_R = \frac{1}{2} \max \left|\frac{\partial}{\partial (\alpha_s \Theta_s)} (\alpha_s U_s \Theta_s) \right| \left(\left|\alpha_s U_s \Theta_s \right|_{R+} \left|\alpha_s U_s \Theta_s \right|_{R-} \right) \tag{3.101}
\]

\[
\left|\frac{\partial}{\partial (\alpha_s \Theta_s)} (\alpha_s U_s \Theta_s) \right| = \left(\frac{[\alpha_s U_s]^n_{R-} [\Theta_s]^n_{R+} - [\alpha_s U_s]^n_{R+} [\Theta_s]^n_{R-}}{[\alpha_s U_s]^n_{R-} [\Theta_s]^n_{R+} - [\alpha_s U_s]^n_{R+} [\Theta_s]^n_{R-}} \right) \tag{3.102}
\]

Like the viscous diffusive flux term in the momentum equation, a fourth order central difference method is applied to the thermal conductivity diffusive flux term in the granular temperature balance [53]:

\[
DF \left(\left[\frac{\partial}{\partial z} \Theta_s \right]^n \right)_{L} = C_{pm} \left(\frac{1}{2} \left|\Theta_s \right|_{C+1}^{n} - \frac{15}{12} \left|\Theta_s \right|_{C}^{n} + \frac{15}{12} \left|\Theta_s \right|_{C-1}^{n} - \frac{1}{12} \left|\Theta_s \right|_{C-2}^{n} \right) \tag{3.103}
\]

\[
DF \left(\left[\frac{\partial}{\partial z} \Theta_s \right]^n \right)_{R} = C_{pm} \left(\frac{1}{2} \left|\Theta_s \right|_{C-1}^{n} - \frac{15}{12} \left|\Theta_s \right|_{C}^{n} + \frac{15}{12} \left|\Theta_s \right|_{C+1}^{n} - \frac{1}{12} \left|\Theta_s \right|_{C+2}^{n} \right) \tag{3.104}
\]

As is done in the continuity and momentum equations, the source and sink terms are applied explicitly in the second partial step.

\[
\frac{1}{\Delta t} \frac{[\alpha_s]^n_C [\Theta_s]^n_{C+1} - [\alpha_s]^n_C [\Theta_s]^n_{C}}{[\Theta_s]^n_{C+1}} = \frac{2}{3} \left( S_{gran, stress} \left([\alpha_s]^n_C, [U_s]^n_C, [\Theta_s]^n_{C+1} \right) + S_{gran, interphase} \left([\alpha_s]^n_C, [U_s]^n_C, [\Theta_s]^n_{C+1} \right) + S_{gran, collision} \left([\alpha_s]^n_C, [U_s]^n_C, [\Theta_s]^n_{C+1} \right) + S_{gran, turbulence} \left([\alpha_s]^n_C, [U_s]^n_C \right) \right) \tag{3.105}
\]

Several of the source terms require the computation of the solid phase velocity gradient. This is computed through calculating the linear gradient within each cell using the interior face values:

\[
\left[\frac{\partial}{\partial z} U_s \right]^n_C = C_{pm} \left(U_s|^n_{L+} + U_s|^n_{R-} \right) \tag{3.106}
\]
3.5.2 Constitutive relation: Fluctuating energy conductivity

The fluctuating energy conductivity coefficient,

$$\kappa_s = \frac{150 d_{\text{part}} g_0 \sqrt{\Theta_s}}{384 g_0 (\alpha_s)(1 + \epsilon_{\text{rest}})} \left[ 1 + \frac{6}{5} g_0 (\alpha_s) (1 + \epsilon_{\text{rest}}) \right]^2 +$$

$$+ 2 a_s^2 \rho_s d_{\text{part}} g_0 (\alpha_s)(1 + \epsilon_{\text{rest}}) \left( \frac{\Theta_s}{p} \right)^{\frac{1}{2}}$$

(3.107)

is applied to the granular energy balance through a term based on Fourier’s law of heat conduction [8].

3.5.3 Constitutive relation: Granular shear

The stress term in the granular pressure equation is the result of the double dyad of the solid phase stress tensor, $\sigma_s$, and the solid phase velocity gradient [8]:

$$S_{\text{gran,shear}} = \sigma_s : \frac{\partial}{\partial x_i} U_s$$

(3.108)

In a single dimension this reduces to

$$S_{\text{gran,shear}} (\alpha_s, U_s, \Theta_s) = \left( -\frac{p_s (\alpha_s, \Theta_s)}{\rho_s} + v_{\text{eff},s} \frac{\partial}{\partial z} U_s \right) \frac{\partial}{\partial z} U_s$$

(3.109)

The granular pressure is computed as in section 3.4.3 and the effective viscosity is computed as in section 3.4.2. As previously mentioned in the solution methodology in section 3.5.1, the spatial gradient of the velocity is computed using the linear gradient between the interior face values within each cell.

3.5.4 Constitutive relation: Interphase dampening

The dampening of the oscillating motion of particles in a medium through the medium itself is handled by the interphase dampening term [8]:

$$S_{\text{gran,interphase}} (\alpha_s, U_s, \Theta_s) = -\frac{3}{\rho_s} \beta (\alpha_s, U_s) \Theta_s$$

(3.110)

The $\beta$ variable is the same interphase drag coefficient used in section 3.4.5 for the momentum equation.
3.5.5 Constitutive relation: Interparticle collisions

The loss of granular energy from inelastic particle collisions is applied in the granular collision term [8]:

\[ S_{\text{gran,collision}}(\alpha_s, U_s, \Theta_s) = -3\alpha_s g_0(\alpha_s) \Theta_s (1 - e_{\text{rest}}) \left[ 4 \left( \frac{\Theta_s}{p} \right)^\frac{1}{2} - \frac{\partial}{\partial z} U_s \right] \] (3.111)

The velocity gradient in the term is applied using the linear cell gradient of the interior face values as mentioned in the solution methodology.

3.5.6 Constitutive relation: Turbulence

The influence of turbulence on granular energy is applied using the one-dimensional version of the solid-liquid turbulence model introduced in Fox [6]:

\[ S_{\text{gran,turbulence}}(\alpha_s, U_s) = \alpha_s \epsilon_{\text{turb,s}} \] (3.112)

The solid phase turbulence dissipation is computed as in section 3.4.2 for the k-epsilon turbulent viscosity.

3.6 Pressure calculation

The liquid phase pressure field is calculated by first summing the momentum equations for the liquid and solid phases

\[ \frac{\partial}{\partial t} (\alpha_s U_s + \alpha_l U_l) + \frac{\partial}{\partial z} \left( \alpha_s U_s U_s + \alpha_l U_l U_l + \frac{p_s}{\rho_s} + \frac{p_l}{\rho_l} - \nu_{\text{eff,s}} \frac{\partial}{\partial z} U_s - \nu_{\text{eff,l}} \frac{\partial}{\partial z} U_l \right) = S_{\text{mom,total}}(\alpha_s, U_s) \] (3.113)

Due to the assumption that a uniform constant circulation velocity is maintained in the reactor,

\[ \alpha_s U_s + \alpha_l U_l = U_c \] (3.114)

The equation becomes

\[ \frac{\partial}{\partial z} \left( \alpha_s U_s U_s + \alpha_l U_l U_l + \frac{p_s}{\rho_s} + \frac{p_l}{\rho_l} - \nu_{\text{eff,s}} \frac{\partial}{\partial z} U_s - \nu_{\text{eff,l}} \frac{\partial}{\partial z} U_l \right) = S_{\text{mom,total}}(\alpha_s, U_s) \] (3.115)
With this equation, the liquid phase pressure gradient can be directly solved for

$$\frac{\partial}{\partial z} p_l = - \rho_l \left( \alpha_s U_s U_s + \frac{p_s}{\rho_s} - \nu_{eff,s} \frac{\partial}{\partial z} U_s + \alpha_l U_l U_l - \nu_{eff,l} \frac{\partial}{\partial z} U_l \right)$$

(3.116)

and the corresponding pressure at any point in the reactor can be determined through integration

$$p_l(z) = - \rho_l \left( \alpha_s U_s U_s + \frac{p_s}{\rho_s} - \nu_{eff,s} \frac{\partial}{\partial z} U_s + \alpha_l U_l U_l - \nu_{eff,l} \frac{\partial}{\partial z} U_l \right) \bigg|_0^z + \rho_l \int_0^z S_{mom,total}(\alpha_s, U_s) dz'$$

(3.117)

Through the extraction of the liquid phase pressure term and the summation of the source and sink terms, the growth, injection, and harvesting terms disappear, leaving behind the total hydrostatic force contribution, $S_{mom,hydrostatic,total}$; the total interfacial interaction forces, $S_{mom,interphase,total}$; and the total wall shear, $S_{mom,wall,total}$:

$$S_{mom,total}(\alpha_s, U_s) = S_{mom,hydrostatic,total} + S_{mom,interphase,total}(\alpha_s, U_s) + S_{mom,wall,total}(\alpha_s, U_s)$$

(3.118)

### 3.6.1 Solution methodology

The liquid phase pressure field is computed on the faces of the cells. The pressure field calculated is a gauge pressure with a reference pressure of zero at the first face of the solution mesh. The values on the faces for all of the variables are computed through averaging the face values on either side of each face. For the solid fraction, for example, the face values are computed like this:

$$\alpha_s(z) = \frac{1}{2} \left( [\alpha_s]^n_{L_i+} + [\alpha_s]^n_{R_j-} \right)$$

(3.119)

$$i = C_{pm} z + 1, j = C_{pm} z$$

(3.120)

The effective viscosities for the solid and liquid phases are calculated using these face values using the methodology from section 3.4.2 and 3.6.2 respectively. The granular pressure is similarly calculated using the face values for solid fraction and granular temperature as in
section 3.4.3. The velocity pressure gradients at the faces are calculated using a simple central difference of the face values directly extrapolated to the cell center:

$$\frac{\partial}{\partial z}U_k(z) = C_{pm} \left( [U_k]^n_{L_{i+}} + [U_k]^n_{R_{j-}} \right)$$

$$i = C_{pm}z + 1, j = C_{pm}z$$

(3.121)

(3.122)

Riemann sum integration over the source terms containing the cell-averaged values is used to compute the source term integral at each face:

$$\int_0^z S_{mom,total}(\alpha_s, U_s)dz' \approx C_{pm}^{-1} \sum_{i=1}^m S_{mom,total}([\alpha_s]^n_{C_i}, [U_s]^n_{C_i})$$

$$m = C_{pm}z$$

(3.123)

(3.124)

The fluid pressure gradient within each cell that is applied to the momentum balance is calculated using linear interpolation between the pressure face values.

$$[\frac{\partial}{\partial z}p]^n_{C_m} = C_{pm}(p_l(z) + p_l(z - C_{pm}^{-1}))$$

$$m = C_{pm}z$$

(3.125)

(3.126)

The solved pressure field is slightly modified for the purpose of accommodating parallel processing. To limit the need for interprocessor communication, the first edge in the domain of every processor partition is set at a reference pressure of zero rather than having a global reference point at the first edge. The pressure equation correspondingly becomes

$$p_{par, l}(z) = -p_l \left( \alpha_s U_s U_s + \frac{p_s}{\rho_s} - \nu_{eff,s} \frac{\partial}{\partial z}U_s + \alpha_l U_l U_l - \nu_{eff,l} \frac{\partial}{\partial z}U_l \right) \bigg|_{z_{ref}} + p_l \int_{z_{ref}}^z S_{mom,total}(\alpha_s, U_s) \ dz'$$

where the source term integral is computed as

$$\int_{z_{ref}}^z S_{mom,total}(\alpha_s, U_s)dz' \approx C_{pm}^{-1} \sum_{i=C_{pm}z_{ref}+1}^m S_{mom,total}([\alpha_s]^n_{C_i}, [U_s]^n_{C_i})$$

$$m = C_{pm}z$$

(3.127)

(3.128)

(3.129)

Given that only the pressure gradient affects the rest of the equations of the model and is left unchanged by using processor-local reference pressures instead of a global reference pressure,
this modification does not impact the model result. The overall liquid pressure field of the entire reactor can be reconstructed through resetting the reference pressure for each processor to the corresponding value for pressure calculated at the linked final edge in the adjacent processor.

3.6.2 Constitutive relation: Effective liquid viscosity

While the effective solid viscosity is calculated using the sum of viscosities seen in section 3.6.2, the effective liquid viscosity is composed of the liquid phase laminar viscosity, \( \nu_{laminar,l} \); bulk viscosity, \( \nu_{bulk,l} \); k-epsilon turbulent viscosity, \( \nu_{ket,l} \); and bubble-induced turbulence viscosity, \( \nu_{bit,l} \).

\[
\nu_{eff,l} = \nu_{laminar,l} + \nu_{bulk,l} + \nu_{ket,l} + \nu_{bit,l}
\]

(3.130)

The liquid phase laminar viscosity is specified by the material properties of the fluid used. The liquid phase bulk viscosity in a slurry is calculated through the relative interphase velocity [34]:

\[
\nu_{bulk,l} = \frac{1}{2} \left( \frac{\alpha_s \rho_s + \alpha_l \rho_l}{\rho_l} \right) \frac{d_{part}}{|U_r|}
\]

(3.131)

The liquid phase k-epsilon viscosity is computed identically to that of the solid phase [32]:

\[
k_{turb,l} = \frac{3}{2} \left( \frac{1}{10} \frac{\rho_s \alpha_s U_s + \rho_l (1 - \alpha_s) U_s}{\rho_s \alpha_s + \rho_l (1 - \alpha_s)} \right)^2
\]

(3.132)

\[
\nu_{ket,l} = \frac{k_{turb,l}^{3/2}}{d_{pipe}}
\]

(3.133)

\[
\epsilon_{ket,l} = \frac{C k_{turb,l}^2}{\rho_l}
\]

(3.134)

The same is true for the bubble-induced turbulent viscosity [27]:

\[
\nu_{bit,l} = C d_{part} \alpha_s |U_r|
\]

(3.135)

3.6.3 Constitutive relation: Total hydrostatic force

The total hydrostatic force term is simply the acceleration of gravity in respect to the direction of flow [8]:

\[
S_{mom,hydrostatic,total} = g
\]

(3.136)
3.6.4 Constitutive relation: Total interfacial force

The total interfacial force is the sum of the liquid and solid phase interphase interactions [8]:

\[ S_{\text{mom,interphase,total}}(\alpha_s, U_s) = (\frac{1}{\rho_s} - \frac{1}{\rho_l}) \beta (\alpha_s, U_s) (U_l - U_s) \]  

(3.137)

The interphase drag coefficient is calculated in the same way as section 3.4.5.

3.6.5 Constitutive relation: Total wall shear

The total wall drag term uses a mixture of a correlation for slurry wall drag and the solid phase wall drag calculated in section 3.4.7:

\[ S_{\text{mom,wall,total}} = \max(S_{\text{mom,wall,slurry}}, S_{\text{mom,wall,s}}) \]  

(3.138)

This is done due to how the slurry correlation has limited ability to approximate the behavior of the slurry as the solid fraction approaches maximum packing due to not considering the volume fraction at maximum packing. As the solid fraction approaches the maximum solid fraction, the radial distribution term in the solid phase wall shear will approach infinity and thus dominate the wall shear. A consequence of this in the model is that at maximum packing the solid phase will clog the reactor and stop entirely while the liquid phase continues to move through the voids.

Otherwise, at lesser solid phase volume fractions, the contribution of the solid phase to the wall drag is assumed to be contained within the slurry correlation for wall shear which includes both solid and liquid contributions [2]:

\[ S_{\text{mom,wall,slurry}}(\alpha_s, U_s) = -\frac{1}{2} \left( \frac{1 + \alpha_s \rho_s}{1 - \alpha_s} f_l \frac{U_l^2}{\nu_l} \right) \]  

(3.139)

where \( f_l \) is the Darcy friction factor. The friction factor is calculated using an explicit form of the Colebrook equation [54]:

\[ f_l = \left( -2 \log \left( \frac{\varepsilon_{\text{wall}}}{3.7} - \frac{5.02}{Re_l} \log \left( \frac{\varepsilon_{\text{wall}}}{3.7} - \frac{5.02}{Re_l} \log \left( \frac{\varepsilon_{\text{wall}}}{3.7} + 13 \frac{Re_l}{3.7} \right) \right) \right) \right)^{-2} \]  

(3.140)

where \( \varepsilon_{\text{wall}} \) is the wall roughness parameter and \( Re_l \) is the liquid phase Reynolds number,

\[ Re_l = \frac{d_{\text{pipe}}|U_l|}{\nu_{laminar,l}} \]  

(3.141)
3.7 Pump performance

A special opportunity this model offers through having a specifiable and uniform circulation velocity is the ability to adjust it during operation. In particular, this circulation velocity can be set to a specific value given a particular overall pressure drop through the implementation of the head versus velocity performance curve of the pump driving the reactor. Given the amount of existing inertia in the system traveling at the current velocity, any change in the circulation velocity in response to a changing pressure drop can only be realistically applied incrementally rather than instantaneously. This is done through Newton’s second law relating the acceleration or deceleration of circulation in the reactor, \( A_{\text{pump}} \), to the difference in the pressure drop between what is calculated by the model and what is predicted by the performance curve, \( \Delta P_{\text{pump}} \), via the total inertial mass of the reactor, \( m_{\text{reactor}} \), divided by the cross sectional area, \( a_{\text{cross}} \):

\[
A_{\text{pump}} = \frac{F_{\text{pump}}}{m_{\text{reactor}}} = \frac{F_{\text{pump}}}{m_{\text{reactor}}} = \frac{\Delta P_{\text{pump}}}{m_{\text{reactor}} a_{\text{cross}}} \tag{3.142}
\]

where \( F_{\text{pump}} \) is the additional force applied by the pump to force the circulation velocity to follow the pump performance curve. The equation applied in the model is

\[
\frac{\partial}{\partial t} U_c = -p_{\text{drop,l}}(\alpha_s, U_s, \Theta_s, t_s) - p_{\text{drop,curve,l}}(U_c) - p_{\text{drop,curve,l}}(U_c) - l_{\text{total}}(\alpha_{\text{overall,s}} \rho_s + (1 - \alpha_{\text{overall,s}}) \rho_l) \tag{3.143}
\]

where \( p_{\text{drop,curve,l}} \) is a function representing the performance curve, \( l_{\text{total}} \) is the total length of the reactor, and \( \alpha_{\text{overall,s}} \) is the overall solid fraction in the reactor. It is important to note that the pressure drop variables are defined as the magnitude of the pressure at the last edge of the solution space given the first edge of the solution is used as the reference pressure of zero. The discretized form of this equation is

\[
[U_c]_n^{n+1} = [U_c]_n^n - \Delta t \frac{p_{\text{drop,l}}([a_s]^n_C, [U_s]^n_C, [\Theta_s]^n_C, t) - p_{\text{drop,curve,l}}([U_c]^n_{global})}{l_{\text{total}}([\alpha_{\text{overall,s}}]^n_{global} \rho_s + (1 - [\alpha_{\text{overall,s}}]^n_{global}) \rho_l]} \tag{3.144}
\]

A consequence of this is while the circulation velocity corresponding to the current pressure drop may not always match the pump performance curve, it will try to follow it.
The force applied by the pump affects the solution for the pressure field such that the unsteady term no longer drops out of the summed momentum equations:

\[
\frac{\partial}{\partial t} U_c + \frac{\partial}{\partial z} \left( a_s U_s U_s + a_l U_l U_l + \frac{p_s}{\rho_s} + \frac{p_l}{\rho_l} - \nu_{eff,s} \frac{\partial}{\partial z} U_s - \nu_{eff,l} \frac{\partial}{\partial z} U_l \right) = S_{mom,total}(a_s, U_s, \Theta_s, t, z)
\]  

(3.145)

This change first requires an adjusted solution, \(p_{\text{adjusted},l}\), for the overall pressure drop

\[
p_{\text{drop,adj},l}(a_s, U_s, \Theta_s, t_s) = \frac{p_{\text{drop},l}(a_s, U_s, \Theta_s, t_s) + \zeta_{adj} p_{\text{drop,curve},l}(U_c)}{1 + \zeta_{adj}}
\]

(3.146)

where \(\zeta_{adj}\) is a coefficient equal to

\[
\zeta_{adj} = \frac{p_l}{(\alpha_{\text{overall},s} \rho_s + (1 - \alpha_{\text{overall},s}) \rho_l)}
\]

(3.147)

This adjusted overall pressure drop is then applied to the solution of the entire reactor profile

\[
p_{\text{adj},l}(z) = (p_{\text{drop,adj},l}(a_s, U_s, \Theta_s, t_s) - p_{\text{drop,curve},l}(U_c))(\frac{\zeta_{adj} z}{l_{total}}) + p_l(z)
\]

(3.148)

In regard to the pressure drop calculation, in the current version of the model the applied acceleration or deceleration by the pump is not directly considered in the calculation for the pressure profile or gradient. The primary consequence of this is there a lesser response to any deviations from the pump curve, making the model including the adjusted pressure term follow the pump curve with greater success, although the difference in practice is marginal. This is due to how in both cases the term is designed to minimize itself to be as small as possible.

### 3.8 Harvesting harmonics

One of the primary interests of this model is observing the operation of the harvesting valve-based control system as it responds to the current conditions of the continuously cycling loop reactor. The concept of “harvesting harmonics” is introduced in this study to try to characterize different instances of this behavior into specific identifiable modes. For example, if a binary open-closed harvesting valve were set on a specific time-table to change from open-to-closed or closed-to-open each reactor space time cycle, \(\tau_{\text{space}}\), it was be described as “harvesting out-of-phase” due to the entire length of the reactor being exposed at one time or another to
harvesting every two space-time cycles. If that same valve were set to change every half reactor space time, only half of the reactor would get exposed to the open harvesting valve. This is called “harvesting in-phase” and it has significant repercussions in the operation of the reactor when growth of the solid phase is present. If only half of the total volume of a reactor is consistently exposed to harvesting, the solid phase in the other half of the reactor will grow almost uninterrupted. Only the diffusion of the solid phase into the harvested half of the reactor will limit its accumulation in the unharvested half. Such accumulation is a precursor to the solid phase clogging the reactor. Although one of the simplifications assumed for this model assumes that a uniform particle diameter is maintained throughout the reaction, another potential impact of in-phase harvesting in a real reactor is a maldistribution of particle sizes in the reactor where there are some partitions of mostly small particles that are being consistently harvested and other partitions with large particles which are not. Figure 3.2 shows examples of in-phase and out-of-phase modes.

As can be seen in by Figure 3.3, one potential challenge for systems with slightly out-of-phase harvesting is that the timescale where harvesting eventually reaches a particular partition is significantly longer than the growth timescale, making the harvesting system ineffective at maintaining a uniform solid fraction throughout the reactor.

The simple solution to avoid harvesting in-phase when the harvesting is based on a timetable is to choose a control response period that is not an even fraction or multiple of the reactor space time. When the control system for the harvesting on the state of the reactor rather than time, this is not so simple. If the quantity being measured and controlled by the control system such as the overall pressure drop fluctuates in a periodic fashion consistently over each space time, it will fall into an in-phase harvesting state. This could be exacerbated especially if the control response such as opening the harvest value ends up directly or indirectly reinforcing the fluctuation, making the in-phase harvesting self-sustaining or even generating a positive feedback loop that constantly increases the fluctuations.
Figure 3.2 Introduction of harvesting harmonics and representation of harvesting in-phase and out-of-phase over four space times.
Figure 3.3  Harvesting slightly out-of-phase example
CHAPTER 4. INDUSTRIAL TUBULAR LOOP REACTOR
GEOMETRY AND PARAMETERS

4.1 Reactor geometry

Publicly available information on the specifics of the design of industrially-relevant tubular loop polymerization reactors is primarily limited to the patent literature. One basic design that appears often in the patent literature is a vertical switchback setup where the loop reactor is a series of tall vertical tube legs connected by hemisymmetric bends alternating on the top and bottom of the tubes [40] [28] [22] [15]. The flow of polymerizing slurry is cycled through this closed-looped system through a single pump or a series of pumps located along the bottom bends [15]. The injection of the feedstock, catalyst, and any inert diluents also is typically featured along the lower bends as is the point where the product stream is harvested [15].

The earliest patent literature details reactors of this type with as few as two vertical leg sections [40]. Over time, the design of the reactors has expanded to examples with four, six, or more legs [28] [22] [13]. With the increased number of legs comes more volume within the reactor and thus the ability to produce more polymerized product over the same timeframe [13]. With this in mind, an eight leg reactor was chosen for the design of the primary hypothetical industrial reactor modeled in this study. A graphical representation of this reactor is seen in Figure 4.1. This design is featured in a series of recent patents detailing various technology related to the liquid-phase production of polypropylene. Patents connected to this design include those concerned with the pumping apparatus and the harvesting process [14] [12].

The geometry of the model itself is a simple line of square prisms of uniform length corresponding to the cells of a one-dimensional finite volume model. Because this is a loop reactor, the boundary conditions are fully cyclic in regard to the solid fraction, phase velocities, and
the granular temperature; the first and last faces of the geometry in regard to those variables are one and the same without any modification, duplication, or mapping. Although the pressure profile cannot be handled cyclically, only the pressure gradient is considered in the model equations and thus a reference pressure of zero at the first face is used. This is extended in the parallel processing of this model where the first face of each processor domain is set to a reference pressure of zero. The choices for the lengths of the straight legs and bends and the tubular diameter were chosen to represent the dimensions of a generic industrial tubular loop polymerization reactor rather than a particular one. The dimensions chosen are summarized in Table 4.1. These dimensions are comparable to publically available press release information and photography of various industrial-scale loop reactors [10] [35] [9].

Table 4.1 Reactor geometric parameters

<table>
<thead>
<tr>
<th>Leg Length (m)</th>
<th>Bend Length (m)</th>
<th>Tubular Diameter (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>6</td>
<td>0.56</td>
</tr>
</tbody>
</table>

Although many details of the geometry are necessarily lost in a one-dimensional model, a few major aspects are still preserved. The changing direction of gravity relative to the direction of axial flow in the reactor, for instance, is naturally a consequence of the geometry. This behavior
is applied in the hydrostatic force term where gravity becomes a piecewise function of the axial distance down the reactor, varying relative to the direction of flow in the pipe.

The regions where locations where injection and harvesting occur are designated using the indicator function from Equation 3.51. For this model, the harvesting system is modeled after U.S. patent 8,816,024 [12] where the harvesting and injection location is at the bottom of the first lower bend of the geometry where a small cylindrical continuous takeoff tube leading to the product line is attached perpendicularly to the reactor. Other reactor designs in the literature use larger settling legs to retrieve the polymerized product at those locations [13]. The patents for the injection and control system describe a three valve system to continuously remove product over time [12]. The first valve is a ram valve in the takeoff tube which can be used as an emergency shutoff and to move obstructions from the tube. The second valve down the line is a block value which can be integrated with the programmed control system to shutdown harvesting entirely under certain conditions such as the pressure drop falling below the set point. The third valve is the one most directly linked to the control system and adjusts the flowrate of the harvesting stream according to whatever is chosen as the controlled variable. In this case, the controlled variable is the pressure drop. Care must be taken when choosing the range of harvesting flowrates due to the potential of too slow harvesting velocities resulting in clogging of the harvesting line and too quick velocities overwhelming the downstream processes. Following the third valve, the harvested stream is flashed in a two-stage system designed to remove and recycle the liquid phase diluent so that it can be used again in the injection stream.

Several of the patents feature the harvesting and injection process happening at the bottom of separate bends or even injection occurring at multiple points throughout the reactor [13] [12]. These instances are not included in this model due to the complications that would result in regard to circulation; there would be a different circulation velocity between the harvest and injection regions that would depend on the magnitude of the harvesting outflow. The most potentially interesting physical phenomena that would result from this separation such as the maldistribution of feedstock relative to the partitions of particles where the solid phase is harvested is already lost due to the simplifications made for the reaction system in the model.
Details on the pumping apparatus for the reactor vary in the literature. While some designs only include one pump, other designs have multiple pumps in series [13] [14]. One in particular has two impellers in the same lower bend rotating in opposite directions to encourage mixing [14]. The main attraction of adding more pumps in series is the addition of pump capacity to the reactor system, allowing for higher concentrations of solid phase to be loaded into the system through the increase in the circulation velocity. Faster circulation velocities helps offset problems related to high solid loading including hot spots and fouling of the reactor wall through turbulent mixing promoting more uniform thermal and particle transport [14]. In the context of this model, while local physical effects of a pump at a particular location such as radial mixing from the pump rotation are not included, the influence of the entire pumping system on the axial flow is achieved through the pump performance control as seen in section 3.7. With multiple pumps in series the total effective performance curve of any number of pumps present in the system can be applied to the model. The pump performance curve uses a modified industrial slurry pump performance curve adjusted such that the initial condition in regards to the circulation velocity and pressure drop exists on the curve and approximately within the high-efficiency region.

4.2 Phase physical parameters

Many of the physical parameters for the solid and liquid phases are taken from or influenced by the Shi et al [41] series of papers. The standard parameters used in all of the trials, unless noted otherwise, are summarized in Table 4.2. The magnitude of the growth rate coefficient, \( k_{growth,s} \), used in the growth term in the continuity equation 3.51 will not be specified due to its origin in proprietary data.
Table 4.2  Phase Parameters

<table>
<thead>
<tr>
<th>Solid Phase</th>
<th>Units</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$kg/m^3$</td>
<td>$\rho_s$</td>
<td>903</td>
</tr>
<tr>
<td>Average Particle Diameter</td>
<td>$\mu m$</td>
<td>$d_{part}$</td>
<td>765</td>
</tr>
<tr>
<td>Solid Fraction at Maximum Packing</td>
<td>-</td>
<td>$\alpha_{s,max}$</td>
<td>0.5</td>
</tr>
<tr>
<td>Restitution Coefficient</td>
<td>-</td>
<td>$e_{rest}$</td>
<td>0.8</td>
</tr>
<tr>
<td>Solid Phase Growth</td>
<td>1/s</td>
<td>$k_g$</td>
<td>-</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Liquid Phase</th>
<th>Units</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$kg/m^3$</td>
<td>$\rho_l$</td>
<td>408</td>
</tr>
<tr>
<td>Laminar Viscosity</td>
<td>$m^2/s$</td>
<td>$\nu_{l,laminar}$</td>
<td>1.30E-07</td>
</tr>
<tr>
<td>Relative Surface Roughness</td>
<td>-</td>
<td>$\varepsilon_{wall}$</td>
<td>0.000286</td>
</tr>
</tbody>
</table>
CHAPTER 5. RESULTS

5.1 Uniform trial

This first trial is designed to observe the behavior of the system when there is initially a uniform solid fraction throughout the reactor. Both growth and harvesting is turned off. Because there is no harvesting region to distinguish a particular lower bend from another, the length of the eight leg reactor is reduced to the repeat unit of the reactor. A circulation velocity of $11.5 \text{ m/s}$ ensures uniformly turbulent axial flow throughout the reactor. A uniform solid volume fraction of 0.29 was chosen for this trial. The total trial is 40 minutes of reactor time.

The phase velocity profiles of the reactor settle into a steady profile dependent on the geometry of the reactor seen in Figure 5.1. In the upward-flowing leg, the solid phase velocity travels slower than the liquid phase. But in the downward-flowing leg, the solid phase travels quicker than the liquid phase. This is due to the application of hydrostatic force from the solid phase being denser than the liquid phase. The velocity profiles do not vary significantly in time for the uniform case.
Figure 5.1  Liquid and solid phase velocity profiles over time using a uniform initial condition

This velocity profile has an interesting effect on the initially uniform solid phase profile. In the initial reactor space time increments, the solid fraction profile is in a periodic state where, as seen in Figure 5.2, the profile fluctuates between the initial uniform state and a state where there is a uniformly greater solid fraction in the upward leg than in a downward leg. There are only subtle differences between the reactor profiles at each 11.47 second space time increment.

Over the longer time increments displayed in Figure 5.3, this fluctuation diffuses into a wave-like behavior and it no longer returns to the initial uniform state. The time increments in this case where chosen such that they were a multiple of the overall space time of the reactor in order to ensure that the location of the center of the fluctuation traveling around the reactor would approximately be in the same place at each time and thus be in-phase with each other. This wave continues to decline over time to a state where there is a uniformly larger solid fraction in the upward-flowing leg than in the downward flowing leg.

This wave-like behavior corresponds with the periodic behavior of the overall liquid phase pressure drop over time in Figure 5.4. As seen in the zoomed window, the pressure drop has oscillations with period equal to the space time of the reactor. The amplitudes of these oscillations decline significantly in time. This matches that of the decline of the wave fluctuation in the solid fraction profile. As a clear way of presenting pressure fluctuation such as this and also as a means of comparing the behavior of the pressure oscillations over time between different trials, the standard deviation of the pressure drop over each space time can be used. This is
Figure 5.2  Periodic behavior of the solid fraction profile over the first two reactor space times using a uniform initial condition.
Figure 5.3  Solid fraction profile over time using a uniform initial condition. The time increment was chosen such that the transient wave is in-phase in each plot.

Figure 5.4  Pressure drop and pressure oscillation standard deviation over time using a uniform initial condition. Each standard deviation was taken over a single reactor space time.
able to single out a measure linked to the amplitude of the oscillations such that they can be used in comparisons of trials with differing or changing average pressure drops over each space time. Larger standard deviations indicate greater amplitudes of oscillation.

5.1.1 Analysis

Overall, this trial indicates that the solid phase settles to a particular solid fraction value that is uniform within each leg and is larger or smaller than the average solid fraction depending on whether the direction of flow is opposing the direction of gravitational force or parallel to it. This corresponds with the phase velocities where the solid phase travels quicker going downward than upward due to hydrostatic force. This complements the results in Yang et al [50] which observed a difference in the concentration profile depending on the velocity, although in that case the change in velocity was due to the location of the recycle outlet rather than hydrostatic force. Despite this difference, this variation in the solid fraction profile due to the geometry of the reactor is very small, as are the transient wave-like fluctuations in the solid fraction profile and the corresponding amplitude of the pressure drop fluctuations. There is no evidence that either on their own can cause the formation of plugs in the reactor starting from a uniform initial condition.

5.2 Settled restart trial

This trial is designed to observe how the system responds to including a pre-existing high solid fraction region in the initial condition. Specifically, this initial condition is designed to mimic a restart of the reactor where circulation has been halted and the solid phase has settled to the bottom, creating a solid-rich region on the bottom of the reactor and a dilute region at the top of the reactor. Although the overall solid fraction of the reactor is identical to the uniform case, 0.29, the entire lower half of the reactor is initially set to a volume fraction of 0.45 and the upper half of the reactor is set to 0.13. Like the uniform trial, the trial time is 40 minutes.

One difference in the velocity trials using the plug initial condition is that, at least initially, the large solid fraction gradients caused by the plugs have a significant effect on the solid phase
Figure 5.5 Liquid and solid phase velocity profiles over time using a settled initial condition.

Figure 5.6 Solid fraction profile and extrema over time using a settled initial condition. The spatial axis of the plug profile is in a plug-static reference frame based on the overall circulation velocity.

velocity. As seen in Figure 5.5, there is initially a pair of spikes in the velocity profiles of both phases located on the anterior and posterior locations on the plug that for the most part flatten out after 400 seconds. The solid phase velocity profile also initially clearly shows the location of the plug through a decrease in the velocity in the upward leg and an increase in velocity in the downward leg. This is due to the amplification of the hydrostatic force difference between the solid and liquid phases when there is a greater concentration of solid phase.

The process of the velocity converging is concurrent with the diffusive smoothing of the plug over time seen in Figure 5.6. One difference is that although the velocity profile becomes nearly uniform after 800 seconds, there still is a non-insignificant plug present at that time. The
spatial profile of the solid fraction is adjusted to a reference frame such that the plug remains static over time. This helps to examine the changing shape of the plug, which is almost entirely eliminated by the end of this run. Given this behavior, it can be extrapolated that given more time the plug case will reach the same final state as the uniform initial condition.

Similar to the uniform initial condition case, the plug initial condition case has a steady decline in the pressure drop oscillations as seen in Figure 5.7. The pressure oscillations in the plug case are of significantly larger magnitude than that seen in the uniform case, with initial oscillations approaching 400,000 Pa in amplitude compared to the few hundred Pascal in the uniform case.

As seen in Figures 5.8 and 5.9, these oscillations vary within each space time according to where in the loop the plug is located at. When the plug is split almost evenly between traveling upwards and downwards at time 12, 17, and 24 seconds, the pressure drop is at an average. When the bulk of the plug is traveling upwards at 14 seconds, the pressure drop reaches a local maximum. When most of the plug is contained within the downward-flowing leg at 20 seconds, the pressure drop is at a local minimum. Similar to the transient oscillations seen with the uniform initial condition, because the plug is not sustained over time, these oscillations continuously decline over time.
Figure 5.8 The effect of the plug position on the pressure drop
Figure 5.9  The effect of the plug position on the pressure drop (cont.)
5.2.1 Analysis

This run demonstrated that the axial reactor flow inherently resists the existence of non-uniformities in the solid fraction profile such as plugs under these standard conditions, even if a fully-formed one is introduced as an initial condition. It also demonstrated that the presence of a plug results in significant pressure oscillations over time depending on the location of the plug in the reactor. This has major implications related to the behavior of the recirculating pump and any pressure drop-based control system for harvesting.

5.3 Uniform trial parameter study

The purpose of these series of trials is to change a series of physical parameters to observe their effect on the axial properties of the reactor using the uniform start condition. These trials are done such that the uniform study from section is used as the control while each parameter is individually varied. The parameters that are varied for these studies include average particle diameter, fluid laminar viscosity, the maximum solid fraction, and restitution coefficient. The primary focus of the uniform parameter study trials is to examine the effect of modifying the parameter on the phase velocities. Determination of whether these trials also show a steady decline in the pressure oscillations from the corresponding decline in the wave-like transient solid phase wave in section 5.1 is also important to see if varying any of these behaviors results in a reversal of that behavior.

5.3.1 Particle diameter

The average particle diameter in the reactor can significantly vary due to influences such as the composition of the feed, reaction conditions, and harvesting methodology. In a real reactor, the average particle size is likely to vary axially, although as mentioned in section, for simplicity's sake this is ignored in this model and the average diameter is assumed to be uniform across the reactor profile. The range of particle sizes tested in this model are varied over an order of magnitude smaller and larger than the control particle size.
Figure 5.10 shows that smaller particle sizes result in a more uniform flow profile that is closer to the circulation velocity in the upward and downward legs. A corollary to this is that the liquid phase velocity is also closer to the circulation velocity and thus there is less of a difference between the liquid and solid velocity. This produces the expected effect when the Stokes number is reduced through the decreased particle size in that the solid phase follows the behavior of the liquid phase more closely. In terms of the equations used in this model, this is primarily a consequence of the drag coefficient in the momentum equation seen in section 3.4.5 becoming larger at smaller particle diameters enforcing the difference in the phase velocity between the solid and liquid phases to be smaller.

Figure 5.10 also shows that with increased particle diameters comes an increase in the magnitude of the pressure oscillations corresponding to a larger transient solid fraction wave circulating around the reactor. The major factor behind this is the weakened interphase drag at those diameters allowing for a greater degree of uncoupling between the solid and liquid phases due to hydrostatic forces. There is no evidence of any reversal of the control case where the transient wave increases rather than decreases over time, corresponding with a steadily increasing pressure oscillation. Interestingly, at the largest diameter, there is a visible increase in the rate of decline, also likely due to the increased decoupling encouraging more axial diffusion.
5.3.2 Liquid phase laminar viscosity

The liquid phase viscosity in a polymerization reaction is significantly linked to the thermodynamics and progression of the reaction. Higher temperatures are expected to cause a decrease in liquid viscosity while an increase in viscosity may be observed at higher degrees of polymerization, although in the latter case for this particular reaction this increase will significantly depend on the concentration of diluent in the liquid phase [29] [31]. The liquid phase laminar viscosity is changed over a range of an order of magnitude smaller and larger.

Figure 5.11 demonstrates that increasing the fluid laminar viscosity has a similar effect on the phase velocities as decreasing the particle size; the solid phase follows the liquid phase closer. This is again primarily due to the magnitude of the interphase drag coefficient which increases with increasing fluid viscosity. In terms of relative impact, increasing or decreasing the fluid viscosity by an order of magnitude from the control resulted in less of a change in the phase velocities than that seen by decreasing or increasing the particle size respectively. In much the same way, with the increased decoupling of the phase velocities due to decreased fluid laminar viscosities comes an increased magnitude of the pressure drop oscillations. All of the pressure oscillations show a clear decline over time, although unlike when varying the particle diameter there is no significant increase or decrease in the rate of decline with increased or decreased decoupling in any of the particular trials.
5.3.3 Maximum solid fraction

The maximum solid fraction is primarily a product of the ability of the solid phase particles to pack. If all of the particles are perfectly spherical, the maximum solid fraction is expected to be around 0.63, the approximated maximum volume fraction for spherical particles packed randomly. If the particles are irregular or varied in shape, this volume fraction can be significantly smaller. A range of 0.46 to 0.63 maximum volume fractions are used in this study.

Changing the solid fraction at maximum packing did not result in any significant change to the velocity profile using a uniform initial condition as seen in Figure 5.12. Similarly, there is only a very small change in the magnitude of the pressure oscillations over time from the control case. This is due to how the terms which include the maximum packing factor, particularly the particle radial distribution introduced in section 3.4.2, only become significant when the solid fraction is close to maximum packing. One oddity in these results is that there is no clear progression over this time period in these trials precisely identifying if varying the maximum packing solid fraction increases or decreases the solid fraction oscillations over time. Although loner runs might clarify this, a result like this indicates a complex albeit subtle relationship between the maximum solid fraction and the pressure drop between the kinetic theory closures and solid phase wall drag term that may work in different direction in regard to the pressure drop.

Figure 5.12  Velocity profile and pressure drop oscillation standard deviation over time varying the maximum solid fraction and using a uniform initial condition
5.3.4 Restitution coefficient

The restitution coefficient represents how the solid phase particles collide with one another and is highly relevant to the kinetic theory of granular flow closures as seen in sections 3.4.2 and 3.4.3. At a restitution coefficient of one, particles collide elastically and the speed of the particles before and after the collision are the same. At zero, both particles are halted completely with each collision. The full range of restitution coefficients are applied in this study.

As with the maximum solid fraction, Figure 5.13 shows varying the restitution coefficient did not result in any significant change in the velocity profile. It resulted in even less change in the pressure drop over time, with only a slight divergence of the perfectly elastic case towards the end of the trial. Given how the restitution coefficient interacts with the rest of the model through the kinetic theory closures whose magnitude is strongly dependent on how close the solid fraction is to the maximum, this lack of change is not surprising when considering a uniform initial solid fraction 0.29 which is significantly smaller than the maximum packing solid fraction of 0.50.
5.3.5 Analysis

Varying these parameters starting from an initial condition did not show any evident reversal in the decline of the pressure oscillation over time and corresponding decrease in magnitude of the transient solid fraction wave over time. It did show that these parameters can have an effect on the velocity profile and the magnitude of the oscillation caused by the transient wave, particularly when changing the average particle size and the liquid phase laminar viscosity. The case of the largest particle diameter showed the largest increase in the magnitude of the pressure oscillation yet it also has an increased rate of decline over time. Varying the solid fraction at maximum packing and the restitution coefficient did not have a substantial effect on the behavior of the reactor. This is due to how both parameters are linked to how close the solid fraction in the reactor is to maximum packing which in this case is not significant due to using a uniform initial solid phase volume fraction of 0.29.

5.4 Settled restart parameter study

These set of trials mirror that of the uniform parameter study except that the initial condition is the settled restart initial condition from section 5.2. The primary purpose behind these trials is to determine whether a change in any of these parameters will result in a change in how the plugs smooth out over time as previously observed. Unlike the uniform study, parameters such as the maximum solid fraction and restitution coefficient will have more relevance due to potions of the reactor being closer to the maximum solid fraction. As indicated in equation 3.78, the magnitude of the radial distribution that relates the kinetic theory closures to properties in the momentum equation is dependent on how close the solid fraction is to the maximum.

5.4.1 Particle diameter

Like the uniform case, the plot of the maximum of the solid fraction profile in Figure 5.14 demonstrates that the increased solid fraction results in an increase in the size of the transient wave. Additionally, it affirms that increasing the particle size results in an increased rate of
Figure 5.14  The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the average particle diameter and using a settled plug initial condition
decline of non-uniformities in the solid fraction profile over time. Interestingly, at the smallest diameter, there is almost no transient variation in the solid profile over time. Figure 5.15 shows that in this case the plug from the initial condition is only being affected by diffusion very slowly; there is no indication that the plug is self-sustaining. This suggests strongly that phase coupling plays a complex role in the reactor system in that while decoupling can cause certain kinds of non-uniformities to develop in the solid fraction profile while at the same time working against other kinds of non-uniformities.
Figure 5.15 Solid fraction profile over time using a settled plug initial condition and an average particle diameter ten times the magnitude of the control case

5.4.2 Liquid phase laminar viscosity

As with varying the particle size, Figure 5.16 shows that decreasing the decoupling of the phases in the reactor also results in the decreased ability to smooth out a plug initially applied to the system. While all of cases showed a steady decline in the pressure oscillation, less viscous trials declined at a faster rate. The most significant change to this decline happened when the laminar fluid viscosity was increased by an order of magnitude where, similar to the trial with the largest particle diameter, there was no significant decline in the maximum profile solid fraction or pressure drop oscillation. Figure 5.17 shows that although the change in the plug might show even a slight increase in the maximum solid fraction of the profile, the overall diffusion of the plug ensures that this slight increase is not sustainable.
Figure 5.16  The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying fluid laminar viscosity and using a settled plug initial condition

Figure 5.17  Solid fraction profile over time using a settled plug initial condition and a liquid phase laminar viscosity one-tenth the magnitude of the control case
5.4.3 Maximum solid fraction

Changing the solid fraction at maximum packing as seen in Figure 5.18 only resulted in a significant change from the control case at the lowest value for the maximum packing fraction. In that case, it both demonstrated an increased transient oscillation and a faster rate of decline for the applied initial plug. This primarily due to the pushback from the granular pressure term as the solid fraction most closely approached the maximum solid fraction in the plug region. Interestingly, although the plug was smoothing out quicker over time for this case than the cases with larger maximum solid fractions, the magnitude of the pressure drop oscillations are constantly larger. Despite this, the gap between them was consistently getting smaller over time and it is expected that the oscillation magnitude will eventually drop below the other cases over time. Paradoxically, the other trials indicate that larger maximum solid fraction correspond with smaller pressure drop oscillation. This reaffirms the complexity of varying the maximum packing fraction on the behavior of the reactor.
Figure 5.18  The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the solid fraction at maximum packing and using a settled plug initial condition

5.4.4 Restitution coefficient

Figure 5.19 indicates that the restitution coefficient caused no significant change in the maximum of the solid fraction profile over time as it was varied, although the pressure drop oscillations slightly decreased as the restitution coefficient was increased. The lack of any significant variation in these trials is likely linked to the similar lack of change seen in the solid fraction at maximum packing variation trials where the value was increased from the control. Even starting with a plug with a solid fraction of 0.45, it still isn’t close enough to the solid fraction at maximum packing of 0.50 to be a major influence on the model. Either increasing the solid fraction of the plug or decreasing the maximum packing solid fraction would likely make the variation of the restitution coefficient more significant.

5.4.5 Analysis

The key takeaway in the results from these parameter studies with a plug initial condition is that even with significant variation of the given parameters, none of the trials showed any sign of increasing or sustaining the plug over time. All of the trials appear to be on the path of matching the corresponding asymptotic solution of the uniform initial condition over time. Changing the parameters primarily influenced the rate at which the plug from the initial condition declined. Increased viscosity and decreased particle size resulted in plugs that decay
Figure 5.19 The maximum of the solid fraction profile and pressure drop oscillation standard deviation over time varying the particle restitution coefficient and using a settled plug initial condition.

much slower than in decreased viscosity and increased particle size trials. Trial with the solid fraction at maximum packing closest to the solid fraction of the plug showed an increased rate of decline of the initial plug. The other maximum packing trials along with all of the restitution coefficient trials only showed insignificant variation from the control case.

5.5 Harvest, growth, and injection trials with constant circulation

These trials include the application of growth, harvesting, and injection at the full eight-leg length of the reactor. Harvesting and injection happens within a 0.4 meter zone at the bottom of the first lower bend and is controlled through the set pressure drop as described in section 3.51. The set pressure drop is the time-averaged value for the pressure drop from the previous uniform trial in section 5.1 and is equal to $4.92 \times 10^5 Pa$. Integral control is emphasized in the harvest valve response with a control coefficient of $5 \times 10^{-6} \frac{1}{Pa \ s}$ and a pressure drop sampling time of 1 second. The circulation velocity of the reaction is set a constant value of $11.5 \frac{m}{s}$. This condition is comparable to a reactor where the pumps are oversized such that any increase in pump head does not change the circulation rate by any measurable degree. The overall reactor solid fraction for all of these trials is 0.29 and the primary aspect varied between these them is the length of a plug-like concentrated solid region at the initial condition. Within these regions, the solid faction is initially 0.45. In the dilute regions, the solid fraction is equal to 0.13. A
uniform trial along with a trio of trials with plug length equal to one-eighth, one-fourth, and one-half of the reactor are done under these conditions. The total trial time for all of these trials is 20 minutes.

5.5.1 Uniform

This trial starts from the same uniform solid fraction profile from section 5.1. Figure 5.20 indicates the formation of significant non-uniform features in the solid fraction profile of the reactor under the growth, harvest, and injection scheme applied to this model. Over time, the profile redistributes itself into a series of four peaks of higher solid fraction hereafter anomalously referred to as plugs evenly spaced between valleys containing local minima. As in section 5.2, the axis of the solid fraction profile in Figure 5.20 uses the constant circulation velocity to generate a spatial reference frame such that the plug is static. By the end of the trial, it appears that the maximum height of the plugs has hit its apex and the local minima have almost stopped decreasing further.

Corresponding with the growth of the plugs is the increase in the amplitude of the pressure oscillations as seen in Figure 5.21. Interestingly, even after the plug has hit its maximum solid fraction the oscillations continue to grow. This is due to how the harvesting process is increasing the solid fraction gradients through harvesting in the valleys rather than at the plugs. These solid fraction gradients drive the pressure oscillations which in turn drive the frequency of harvesting. This harvesting frequency is consistent and sustained and thus can be classified as in-phase harvesting as introduced in section 3.8. Figures 5.22, 5.23, and 5.24 show how this occurs. At 1012 and 1014 seconds, the pressure drop is near its peak while the harvesting and injection coefficient dependent on the difference between the pressure drop set point and measurement is still ramping up. As developed in section 3.3.2 the harvesting and injection coefficient corresponds with the valve controlling the flowrate out of the reactor. The solid fraction passing through the harvesting zone at these times is on the upward gradient of the solid fraction peak. At this time the bulk of the plugs in the reactor are traveling up the upward leg. At 1016 seconds, the harvesting coefficient reaches its peak right as the local minima for the solid fraction passes through the harvesting region. As the bulk of the plug
begins traveling down the downward leg, the pressure hits a minimum and the harvesting valve
shuts at 1018 seconds. At 1021 seconds, the peak of the plug is traveling through the harvesting
area and the pressure drop is beginning to rise above the set point, opening the harvesting valve
again. At 1024 seconds, the system returns to a state similar to what it was approximately 12
seconds ago.

From these figures, it is apparent that the major portion of the harvesting only happens
when the bulk of the solid fraction is traveling up the upward leg. This causes the harvesting
system to necessarily miss that bulk of particles because the harvesting outlet is at the bottom
Figure 5.22  In-phase harvesting over time using a uniform initial condition
Figure 5.23  In-phase harvesting over time using a uniform initial condition (cont.)
Figure 5.24 In-phase harvesting over time using a uniform initial condition (cont.)
of the reactor leg. Over time, missing this bulk consistently resulted in in-phase harvesting causing the formation of sustained plugs. The reason why the concentration of the plugs doesn’t grow up to the maximum packing solid fraction is due to the diffusion of the plugs over time. This diffusion was highlighted in the settled plug trial in section 5.2 and the subsequent parameter studies in section 5.4 where the initially introduced plug would decay over time. As the solid fraction gradient decreased, so did the rate of the decay. The key factor which differentiates this case from those previous trials is the presence of growth increasing the solid fraction along the entire profile of the reactor that can counteract this diffusion over time. The end result is that the combination of in-phase harvesting, spatial diffusion, and growth have effects which balance each other out in a state where plugs of a certain concentration and length are not only generated but are also self-sustaining. Although in this case the plugs are limited in concentration by diffusion, they do still generate significant pressure oscillations over time that may pose a danger to the operational integrity of the system components.

5.5.2 Settled restart

As in the plug trials in section 5.2 and 5.4, the settled restart initial condition involves the lower half of the reactor initially having a solid fraction significantly denser than the upper half. In this case, the result is a series of four plugs with length each equal to one-eighth of the total reactor length. Figure 5.25 shows that these plugs decay and almost disappear over time, not unlike the plug trials without any growth, injection, or harvesting. Although there are still small remnants of the plug present, they have a concentration significantly less than the concentration of the final plugs in the uniform trial. The pressure oscillation amplitude shows a steady decay in Figure 5.26 parallel to the decline in the plugs. Although at first glance that given these observations it might appear that the settled plug managed to somehow avoid getting locked into in-phase harvesting, this apparent stability is based on the fact that the harvesting system is completely turned off for the second half of the run as seen in Figure 5.27. Due to the large initial pressure oscillations, there is a correspondingly large response by the harvesting system which harvests a significant portion of the solid phase. When the diffusion of the large solid fraction gradients is added on top of this response, the result is that the pressure
Figure 5.25  Solid fraction profile and extrema over time with growth, harvesting, and injection using a settled initial condition

Figure 5.26  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a settled initial condition

drop ends up stabilizing at a value where even the peaks of the oscillations do not rise above the pressure drop set point. But it will not be below the set point forever due to the growth of solid phase. When that happens, the harvesting cycles will begin anew and likely result in the same final state as was seen in the uniform initial condition.
Figure 5.27  Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a settled initial condition
5.5.3 Half-plug loading

A half-plug loading initial condition represents a particularly dire case in reactor operation where the solid fraction is concentrated in a single plug that takes up half of the length of the reactor. Such a case could develop from a significant maldistribution of catalyst or feedstock, a pileup from a clog that was eventually dissipated by the pump, or other phenomena related to reaction or thermal effects not covered in the physics of this model.

The dire nature of the half-plug initial condition is entirely apparent in Figure 5.28 where it shows a portion of the plug growing close to the maximum packing solid fraction. At that point, the plug becomes more of a clog or packed bed than a dispersed phase and has significant ramifications for the operation of the reactor. Figure 5.29 shows that the pressure oscillations eventually stabilize. When cross-referencing Figure 5.28 and 5.29, this initial period involves the front half of the initial half-plug being harvested while leaving the back half largely untouched. Figure 5.30 demonstrates that the presence of a clog isn’t a temporary feature from the same overcorrection by the control system as seen in the settled restart case causing the harvesting system to close. The harvesting system is operating in-phase and it is sustaining the clog through controlling the pressure by sacrificially harvesting only the front of the plug as it grows. Because of this, the only limitation to the height of the plug is the amount of spatial diffusion. In the settled restart and the uniform cases, the lengths of the plugs were short enough such that diffusion was able to limit their height. In this case, the plug is long enough to allow the growth of the solid phase to countermand this diffusion limitation, and thus it forms a sustainable clog that grows unbound as it dodges the harvesting system.
Figure 5.28  Solid fraction profile and extrema over time with growth, harvesting, and injection using a half-plug initial condition

Figure 5.29  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a half-plug initial condition
Figure 5.30  Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a half-plug initial condition
5.5.4 Quarter-plug loading

Although no precise premise for the formation of a pair of equally-sized plugs with length equal to one-quarter of the reactor comes immediately to mind, it does provide an interpolating point in terms of plug length between the restart trial and the front loading trail. One point of interest in regard to the latter involves the observation that half of the plug was sacrificially used to regulate the overall pressure drop while the rest of the plug was maintained. In this case where there are two separate plugs, determination of whether one of the plugs similarly turned out to be the primary focus of the control system while the other one consistently slips by it seemed to be worth investigating.

The quarter plug trial demonstrates once again in Figure 5.31 that a plug of sufficient size is capable of forming a sustainable clog in the reactor. As in the half-plug initial condition case, Figure 5.32 shows that an initial drop in the pressure drop to the set point. In this case, that drop corresponds to the significant harvesting of one of the plugs of the initial condition but not the other. In this case the clogging plug has a slightly smaller sustained solid fraction that the one seen in the half-plug case. This is likely due to the half-plug having a longer base on the anterior side which reduces the rate of diffusion over time. Another factor is how as the solid fraction approaches the maximum solid fraction, the granular pressure from section 3.4.3 goes to infinity, creating a strong dissipative force in the granular pressure gradient term. Figure 5.33 verifies that the solid fraction profile is being maintained by in-phase harvesting.
Figure 5.31  Solid fraction profile and extrema over time with growth, harvesting, and injection using a quarter-plug initial condition

Figure 5.32  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection using a quarter-plug initial condition
Figure 5.33  Pressure drop, overall reactor solid fraction, and harvesting and injection coefficient over time with growth, harvesting, and injection using a quarter-plug initial condition
5.5.5 Plug Length Comparison

Figure 5.34 compares the pressure oscillation standard deviation, the overall reactor solid fraction, and maximum solid fraction between all of the trials with a constant circulation velocity. Interestingly, the uniform case is the one that has the worst pressure drop oscillations at its final state. This is due to how the plugs that are formed in the uniform case are spaced out such that all of plugs will be flowing in the same kind of geometry of the reactor at the same time. For example, at the maximum of the pressure oscillation, all of the plugs are traveling through the upward leg. This is why the settled restart initial condition initially had the largest pressure drop oscillations. Longer plugs will have portions of the plug traveling downwards that will partially offset some of the pressure increase while the bulk of the plug is traveling upwards. The quarter-plug case having a slightly larger pressure oscillation than the half-plug case demonstrates this in that the shorter plug will have less ability to offset its pressure drop in other parts of the geometry as it is traveling upwards. All of the cases show a decline from the initial solid fraction of 0.29. This is important because a reduction of the loading is highly undesirable from an operational stand point. Less solid fraction in the reactor means a slower rate of production of polymerized product. Non-uniform features such as the plugs generated in all of these trials use up more valuable pressure drop capital and thus with a control system designed to maintain the system at a particular pressure drop, more non-uniform features means less solid fraction can be present in the reactor. An over reactive control response such as that seen in the settled restart case is also undesirable given that there is a significant period of reduced solid fraction as the system recovers from the response. The maximum solid fraction plot showcases the two different types of asymptotic states depending on the initial length of a plug. Smaller plugs like the settled restart condition will eventually decay and end up in a state like the uniform initial condition. Longer plugs will stick around close to the solid fraction at maximum packing.
Figure 5.34  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the harvest, growth, and injection trials.
5.5.6 Analysis

From these results, it is apparent that there is a critical plug length in this system where a combination of the diffusive dissipation and harvesting of the plug become equal to the growth of the plug from polymerization. Below this critical length, the plug will decay and the reactor will look like the uniform and settled cases. These cases involve the formation of a series of small plugs causing significant pressure oscillation in the reactor. Above this length, the plug will grow until it approaches the maximum packing solid fraction as in the half and quarter plug cases. These cases can be characterized as having a single clogging plug and less severe pressure oscillations. From these trials, it is evident that this critical length of a plug is a value between one-eighth of the reactor length and one-fourth of it. In all of these cases, the overall solid fraction of the reactor is reduced from the desired control amount because of the non-uniform features that generate due to in-phase harvesting which is an inevitable result of directly using the pressure drop as the controlled variable. Because the pressure drop local maxima in time only exist as the plug is traveling up the upward leg, the plug will always be out of reach of the harvest point located at the bottom of the reactor bend.

5.6 Harvest, growth, and injection trials with pump circulation

These trials mirror that seen in section 5.5 except that the pump performance curve is applied to the circulation velocity as introduced in section 3.7. The pump performance curve used is from an industrial slurry pump modified such that the time-averaged pressure drop from the trial in section 5.1 and corresponding circulation velocity of 11.5 \( \frac{m}{s} \) was located on the curve in the high-efficiency region. As previously mentioned, while the acceleration and deceleration from the pump curve are applied to the circulation velocity, they are not applied to the pressure for these results. A consequence of this is that the velocity change only indirectly impacts the pressure drop and thus the pump curve is not followed as precisely, although as seen in Figure 5.35, the pump curve is still followed quite well despite this limitation. It also shows that the changes in the pressure drop reflect inversely on the circulation velocity as is expected through the application of the pump curve. Because propriety data on an actual industrial
Figure 5.35 Application of the pump performance curve to the circulation velocity of the reactor using a uniform initial condition. Adjusted units for pressure and velocity using respective reference values are used.

The pump performance curve is implemented in this model, the velocity data in Figure 5.35 and in all cases where it is implemented will use adjusted units for velocity using an arbitrary reference velocity. While the restart and quarter loading cases ran for 20 minutes each, the uniform case was done over 60 minutes to determine if the overall solid fraction fully stabilizes over that time. Similarly, the front loading case was done over a period of 40 minutes.

5.6.1 Uniform

It can be seen in Figure 5.36 that the solid fraction profile has the same general structure as that seen in the constant circulation case upon the application of the pump performance curve controlling the circulation velocity. The uniform initial condition becomes a series of self-
Figure 5.36 Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition sustaining plugs leading to significant pressure oscillations as seen in Figure 5.37. One readily apparent difference is that while the constant circulation run was showing signs of stabilization by the end of 1200 seconds, a similar state is not achieved until after 2500 seconds in this case.

Figure 5.38 shows that the pressure oscillation with constant circulation is significantly greater than the trial when the pump performance curve control the circulation velocity. This is because the pump curve applies a dampening response to the pressure drop oscillations. As the pressure drop increases, the pump curve causes the circulation velocity to decrease. This first directly impacts the liquid phase velocity in Equation 3.5 which in turn slows down the solid phase velocity using the interphase drag term in section 3.4.5. Slowing down the phase velocities pushes against the increase in pressure drop. The end result is that the pressure oscillations when the pump performance curve is applied are reduced in amplitude. Interestingly, the overall solid fraction of the reactor does not get significantly reduced over time as was seen in the constant circulation trial. In that case, the harvesting system removed more of the solid phase to offset the increase in the pressure drop from the non-uniform features in the solid fraction profile. The applied force from the application of the pump performance curve responds to the increased pressure drop from the non-uniform features by decreasing the circulation velocity faster than the response of the harvest control system to remove the solid phase. This decline in the circulation velocity is also evident in Figure 5.36 through how the profiles of
the plugs over time are not in the same location in the now-misnomer plug-static reference frame which is adjusted from the standard spatial reference frame using the initial circulation velocity. Although the harvest control system still plays a significant role in the regulation of the pressure drop, it is in competition with the pump performance curve. The decreased magnitude of the pressure oscillations caused by the pump performance curve dampens the harvesting control response and is the most likely candidate for the reason why this run took longer to fully stabilize. Despite this difference in the overall solid fraction, the heights of the plugs with and without the pump curve applied nearly match.
Figure 5.38  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the uniform initial condition trials with and without the pump curve applied
5.6.2 Settled restart

An in the uniform initial condition, the application of the pump curve does not change the general shape and structure of the results for the settled restart initial condition, such as in the solid fraction profile in Figure 5.39. The plugs still decay over time and the likely asymptotic behavior is likely to be that of the uniform case. Likewise in the behavior of the pressure drop over time in Figure 5.40, the pressure drop still begins with large oscillations which decay with the height of the plugs.

The details revealed by the comparison with the corresponding constant circulation trial in Figure 5.41 reveal some differences caused by the application of the pump curve. For one, as in the uniform case comparison, the application of the pump curve significantly dampened the pressure drop oscillations. This in turn caused the harvest overshoot of the solid fraction seen in the constant circulation case to be reduced through the decrease in the circulation velocity, to the point where pressure drop oscillations never fully make it completely under the control threshold as was seen in the constant circulation case. Despite this, the control system did initially take away a significant amount of the reactor solid fraction which it is still recovering from by the end of the trial. One sign of this recovery can be seen in how the circulation velocity peaks above the constant circulation trial. The pump accelerated the circulation velocity in response to the decline in pressure from the compounded diffusion following the initial control response.
Figure 5.39  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a settled initial condition

Figure 5.40  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a settled initial condition
Figure 5.41 Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the settled initial condition trials with and without the pump curve applied.
5.6.3 Half-plug loading

The solid fraction profile of the half-plug initial condition with an applied pump performance curve in Figure 5.42 deviates significantly from the constant circulation case in that a clog approaching the maximum packing solid fraction is not generated. Instead, the entire height of the plug declines with a pair of peaks with approximately equal height acting as maximums. The anterior side of the plug in this case is not sacrificially used to maintain the clog. This is due to the dampening effect of the pump curve on the pressure oscillations seen in Figure 5.43 causing the harvesting response to also dampen. Thus the removal of solid phase on the anterior side of the plug isn't enough to control the pressure drop and the response on the posterior side of the plug is greater. The pump curve effectively acts as an equalizer of the harvesting response across the profile of the reactor. Along with showing the standard reduction of both the magnitude of the pressure oscillations and the decline of the solid fraction from the initial value, the comparison in Figure 5.44 shows that the circulation velocity for this case is consistently slower when the pump curve is applied. Furthermore, the circulation velocity is in steady decline in the latter half of the run. This may be linked to how the maximum height of the profile is still increasing over time by the end of the trial, albeit at an extremely slow rate. With growth over time this may provoke a greater response by the control system, halting the increase in the height of the plug and stabilizing the circulation velocity, but in the meantime the plug is self-sustaining even if it does not quite have the concentration to be characterized as a clog.
Figure 5.42  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition.

Figure 5.43  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition.
Figure 5.44 Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the half-plug initial condition trials with and without the pump curve applied
5.6.4 Quarter-plug loading

The quarter-plug initial condition trial results seen in Figure 5.45 and 5.46 have many of the changes from the corresponding constant circulation case seen in the half-plug initial condition. The solid fraction profile shows a slight decay from the initial condition that is stabilized in both of the plugs. Unlike the half-plug case, there is greater variation between the heights of the plugs, although not nearly to the extent seen without the application of the pump performance curve. This is because the adjacency of the plugs in the half-plug case shields one side of each plug from diffusive effects. Correspondingly, the sustained plug height seen in Figure 5.47 is less in the quarter-plug case due to this reduction of diffusion.
Figure 5.45  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a quarter-plug initial condition

Figure 5.46  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a quarter-plug initial condition
Figure 5.47  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the quarter-plug initial condition trials with and without the pump curve applied
5.6.5 Plug Length Comparison

The comparison of the different plug lengths in Figure 5.48 are for the most part very similar to what was seen in the constant circulation case with a few minor differences. One caveat is that some of the differences observed in this figure may be attributed to how applying the pump performance curve significantly slows down the path to full stabilization and thus some of these differences will not be maintained over time. The uniform initial condition having the smallest pressure oscillation, for example, can primarily be attributed how the pressure oscillation doesn’t stabilize until after 2500 seconds. Additionally, the pressure oscillation for both the settled restart and half-plug initial conditions are clearly declining at 1200 seconds. For the quarter-plug initial condition, its trajectory is less sure. The overall reactor solid fraction is remaining steady in the case of the uniform case but is slowly increasing in the quarter and half plug cases while significantly increasing in the settled restart case as it recovers from the initial response. The continued presence of the sustained plugs in the quarter and half plug cases is why the overall reactor solid fraction is increasing only by a small amount. The plugs in those cases both have a nearly identical height.
Figure 5.48  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction for the harvest, growth, and injection trials
5.6.6 Analysis

The general shape and structure of the profiles with pump performance curve-driven circulation did not differ significantly from the constant circulation trials in section 5.5 and the conclusions from those trials still hold. The primary effect of applying the pump curve is a distinct dampening of the amplitude of the oscillations through the variation of the circulation velocity. This has repercussions in regards to the control of the overall solid fraction through the pressure drop in the model such that the magnitude of the control response is lessened. In the uniform case, although there was the same generation of self-sustaining plugs as in the constant circulation case, the overall solid fraction was not reduced to accommodate the non-uniform features in regard to controlling the overall pressure drop. Instead, the reactor circulation velocity was slowed down to reduce the pressure drop faster than the control system could respond by removing the solid phase. The stabilization of the profile also took significantly longer due to this dampened harvest response. In the case of the settled restart initial condition, the dampened control response prevented the pressure drop from overshooting the set point to a degree that the control response needed to turn off to recover the reactor solid fraction. When the pump performance curve was applied to the initially formed half and quarter-length plugs, the reduced response in those cases is applied more equally across the entire profile, reducing the effect seen in the constant circulation case where the control response would be focused on a particular area of the reactor while ignoring the formation of a plug in another.

5.7 Operational modifications

These series of trials involve making a series of modifications in the operation methodology of the reactor that would be available to an industrial operator. These changes were done with the prevention of sustained plugs and pressure oscillations in mind in a reactor with pump circulation and growth, injection, and harvesting as applied previously in section 5.6. One way a reactor operator could respond to sustained pressure oscillations that may take the pressure drop above acceptable bounds is to decrease the overall solid fraction loading in the reactor, albeit this would be done at the detriment of production. Slowing down the harvesting response...
would prevent in-phase harvesting through making the periodicity of the harvesting equal to that of the circulation, although that would make it less able to respond to plugs that could form in other ways. Applying a delay in the control response offered promise in preventing the sustained oscillations in solid fraction. Finally, adding more injection and harvesting points has the potential in better enforcement of the uniformity in the reactor, especially when dealing with long plugs.

5.7.1 Solid fraction loading

These trials change the overall loading of solid fraction within the reactor to observe the corresponding effect on the magnitudes of the pressure oscillations. The pressure drop set point for each overall reactor solid fraction is determined through the time averaging of the pressure drop in a separate run at the respective reactor solid fraction with no harvesting or growth similar to the trial in section 5.1. Figure 5.49 shows a comparison between the uniform initial condition trials at loadings of 0.13, 0.29, and 0.45. The 0.13 trial clearly shows that reducing the solid fraction loading significantly reduces the magnitude of the pressure oscillations. Additionally the oscillations are decreasing over the trial time rather than increasing as is the case in the 0.29 and 0.45 trials. One possibility that was considered in the creation of this trial was that lower fraction pressure drop set point corresponding to a uniform profile of 0.13 is on a more vertical point of the pressure performance curve. At that point, the circulation velocity will not change as much as the pressure drop changes and thus the trial has the potential to have oscillations of greater magnitude like the constant circulation trials than the dampened ones seen in the other pump performance curve trials. This result shows that with this particular pump curve and an overall solid fraction of 0.13, this effect is not seen. Although running a reactor with a set point designed to maintain an overall solid fraction of 0.45 is highly counterintuitive due to the almost inevitable chance of clogging, it still is something of interest to see how the pressure oscillations respond as the plugs approach the maximum packing solid fraction closely. In this case there is less dissipative force on the growing plugs from diffusion due to the initial uniformity of the solid fraction profile. The pushback from the closures including the radial distribution term introduced in section 3.4.2 ends up dampening the oscillations
such that they are not too much different in magnitude from the 0.29 case. Even with a large
pressure drop set point corresponding to a uniform 0.45 solid fraction profile, the circulation
velocity is not radically smaller than the other trials. One issue foreseen in cases involving large
pressure drops is that the pump performance curve flattens out. This causes small changes in
the pressure drop to result in drastic changes in the circulation velocity, possibly causing axial
circulation to slow down or even stop. Given that neither this scenario nor the one involving
smaller pressure drops causing results similar to the constant circulation cases came to pass in
this trials, it is evident that the pump curve applied to the model is sized well enough for this
particular reactor to handle a wide spectrum of overall solid fraction without falling into either
extremes.
Figure 5.49 Comparison of the pressure drop oscillation standard deviation, adjusted circulation velocity, overall reactor solid fraction, and maximum solid fraction using a uniform initial condition at overall solid fraction loading of 0.13, 0.29, and 0.45
5.7.2 Slow harvesting response

The change in operation for these trials involves increasing the sampling time period for the pressure drop for the control response such that it is equal to the space-time of a reactor traveling around 11.5 $\frac{m}{s}$. The harvesting integral response coefficient is increased proportionally to the delay in the sampling time, with a value of $2.5 \times 10^{-4} \frac{1}{Pa \ s}$. The intention behind this approach is that the full space time profile of the reactor will be exposed to the same harvest outflow rate between the time increments where the outflow rate is changed in response to the changing pressure drop. This is designed to prevent the formation of any non-uniform features in the solid fraction profile over time.

5.7.2.1 Uniform

Starting with a uniform solid fraction profile, Figure 5.50 shows that this control methodology was able to maintain a reasonably uniform solid fraction profile over time, with no significant plugs growing in the profile over time. Consequently, the pressure drop oscillations seen in Figure 5.51 are extremely minor and show no sign of sustained growth over time.
Figure 5.50  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor.

Figure 5.51  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor.
5.7.2.2 Half-Plug loading

The effect of a slower frequency of harvesting control when a half-plug initial condition is applied to the model is seen in Figures 5.52 and 5.53 where the initially applied plug is reduced significantly by the first few harvesting responses. Following this response, the pressure drop completely falls below the set point of $4.92 \times 10^5 Pa$ and the control system shuts off for the remainder of the trial, similar to the settled restart case under constant circulation in section 5.5.2. Because of this, the plug continues to persist and grow in the reactor, revealing the primary weakness of this control scheme.
Figure 5.52  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor.

Figure 5.53  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half–plug initial condition. In this trial the harvesting control sampling and response interval is slowed to the space time of the reactor.
5.7.2.3  Comparison

Figure 5.54 displays the trade-offs involved with the slower response rate. When starting from a uniform profile it does an excellent job of preventing the formation of any plugs and subsequent pressure oscillations. When responding to any non-uniform feature in the reactor, on the other hand, the response is clumsy due to the control system not being able to recognize or target any specific axial variation in the profile for its response. In the half-plug case the control system over-reacted to the presence of the plug and removed a significant portion of the solid fraction from the reactor. A reduction in the control coefficient may have prevented such an over-reaction but that runs the risk of not being powerful enough to prevent further growth of the plug. Even in this case, the plug as a feature remained intact and was growing as the harvest value was shut off.
Figure 5.54 Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction using a uniform and half-plug initial conditions with and without a slow response interval.
5.7.3 Delay time

These trials are designed to determine if applying a constant delay time to the control response for the harvest valve will result in avoiding the generation of sustained axial variation seen in the other trials. The delay time applied is approximately equal to one eighth of the total reactor space time or the approximate time it takes for a particle to traverse from the apex upper bend to the bottom of the lower bend when the circulation velocity is around 11.5 \( \frac{m}{s} \). Through this, the harvesting response will wait for a plug that caused a local maximum in the pressure drop as it traveled up the upward leg to go down to the downward bend where the harvesting region is. Cases involving uniform and half-plug initial conditions were both observed to see if a delay like this either prevented plugs from forming or handled existing plugs better.

5.7.3.1 Uniform

With the uniform initial condition, the delayed control methodology maintained almost complete stability in the solid fraction profile in Figure 5.55 and the pressure drop profile in Figure 5.56. No generation of any sort of plugs in the solid fraction profile or significant oscillations in the pressure drop were seen in this case.
Figure 5.55  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control response is delayed by 6 seconds.

Figure 5.56  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial the harvesting control response is delayed by 6 seconds.
5.7.3.2 Half-plug loading

The half-plug initial condition case, on the other hand, showed only minor differences in the solid fraction profile from the case in section 5.6.3 and still maintained a plug in the reactor over time as seen in Figure 5.57. The pressure drop in Figure 5.58 is still oscillating due to the persistent presence of this plug. One physical difference is that the plug is much smoother and has its maximum solid fraction closer to the beginning of the plug than from the end.
Figure 5.57  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control response is delayed by 6 seconds.

Figure 5.58  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial the harvesting control response is delayed by 6 seconds.
5.7.3.3 Comparison

As was highly evident by the solid fraction profile and pressure drop, the uniform case with delay has minimal pressure oscillations as seen in Figure 5.59. The overall solid fraction in that case is also keeping very steady. Despite the continued presence of the plug, the plug case with the delay had significantly reduced pressure oscillations. This is likely due to the smoother profile of the long plug that is more able to offset oscillations while the bulk of the plug is traveling upwards. Otherwise the half-plug case had very similar behavior compared to the case without the delay, with a nearly identical solid fraction and only a slightly lower maximum plug solid fraction.
Figure 5.59  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum solid fraction using a uniform and half-plug initial conditions with and without delaying the harvesting control response
5.7.4 Multiple harvest points

The purpose of these trials is to observe whether the addition of a harvesting region halfway down the reactor from the existing harvesting region is able to enforce a more uniform reactor solid fraction. This is a simple expansion of the harvesting region, none of the other control parameters are modified in this case. Both a front loading case and a uniform case initial condition are applied with this modification.

5.7.4.1 Uniform

For the uniform initial condition, no notable change is immediately apparent in the solid fraction profile in Figure 5.60 and the pressure drop in Figure 5.61.
Figure 5.60  Solid fraction profile and extrema over time over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one.

Figure 5.61  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a uniform initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one.
5.7.4.2 Half-plug loading

As in the uniform case, the general behavior of the pressure drop seen in Figure 5.63 using a half-plug initial condition is not significantly different for when using just a single harvest outlet on Figure 5.43, but the solid fraction profile does have a couple subtle differences. The posterior of the plug in Figure 5.62 has a less steep solid fraction gradient and there is a greater difference between the peaks in the plug. A reasonable prediction would be that the source of this variance is the product of having two concurrent harvest outlets with a harvest coefficient equal to half of that seen with a single outlet but the comparison of the harvesting coefficient in Figure 5.64 reveals the exact opposite: a second harvesting outlet results in a greater harvesting response. Even more interesting is how although the oscillations of both have the same frequency, the two harvest outlet case is slightly offset in time from the single one.
Figure 5.62  Solid fraction profile and extrema over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one.

Figure 5.63  Pressure drop and pressure oscillation standard deviation over time with growth, harvesting, and injection and an applied pump performance curve using a half-plug initial condition. In this trial there are two harvest and injection locations at 129 and 393 meters from the beginning of the reactor profile rather than one.
Figure 5.64 Comparison of the harvest and injection coefficient with one and two harvest outlets

5.7.4.3 Comparison

This increase in the harvesting response with an additional outlet becomes especially clear when comparing the uniform trials in Figure 5.65. The pressure oscillations of the two harvest outlet trial grow significantly faster than the single harvest outlet. Examining the maximum and minimum of the two harvesting outlet trial shows that this increase in the oscillation isn’t being driven by more concentrated plug but rather plugs that are being formed faster over time. This comes down to a fundamental truth about the harvesting response for all trials in that it is able to sustain itself because it feeds back into itself through in-phase harvesting. The harvesting response creates non-uniform behavior in the profile which in turn generates the pressure oscillations which drive the harvesting response. An additional outlet allows for this cycle to accelerate at a faster rate through having another location that can generate gradients in the solid fraction profile. It is not unreasonable to assume that the two harvest outlet trials stabilize at similar outcomes that the single harvesting outlet trials eventually achieve.
Figure 5.65  Comparison of the pressure drop oscillation standard deviation, overall reactor solid fraction, and maximum and minimum solid fraction using a uniform and half-plug initial conditions with one and two harvesting locations.
5.7.5 Analysis

These trials helped to clarify the effect of several operational changes that could be made to the reactor to provide better control of the pressure drop and overall reactor solid fraction. Reducing the loading resulted in a corresponding reduction in the pressure drop oscillations but is undesirable from an operation point of view because there will be less product produced in the reactor. Slowing down the harvesting response was able to significantly reduce the pressure oscillations when starting with a uniform initial condition, but when starting with a half-plug the control system overharvested the solid phase. Such overharvesting also slows down the production of solid phase in the reactor. Slowing down the harvesting system makes control of the overall solid fraction of the reactor much clumsier, especially in a situation when a plug develops from physics external to this model. Using information on the harvesting harmonics from previous trials to implement a delay time in the response resulted in almost perfect control of the pressure drop when starting from a uniform initial condition. It also significantly reduced but did not get rid of entirely the pressure oscillations when starting with a half-plug. Finally, adding an additional harvesting outlet halfway down the reactor starting from a uniform profile resulted in the pressure oscillations growing towards stabilization at a much faster rate and did nothing to prevent them. In all cases starting with the half-plug, modifying the operation of the reactor did not prevent the remains of the initial conditions from becoming a permanent self-sustaining feature of the solid profile.
CHAPTER 6. CONCLUSIONS AND RECOMMENDATIONS

The uniform profile trial in section 5.1 demonstrated that hydrostatic force causes the velocity of each respective phase to be different depending on the direction of flow. In the portions of the reactor where there is upward flow, the less dense liquid phase is traveling faster than the solid phase. Where there is downward flow, the solid phase travels faster. This simple observation is the source of almost all of the phenomena that is of interest in this study. Within the uniform profile, this difference in velocities causes the formation of a transient wave of marginally more concentrated solid fraction passing through the reactor. This small wave cycles through the reactor, decaying over time towards a steady solution where the solid phase is more concentrated in the upward flow regions than the downward flow ones. As it does so, it causes tiny oscillations with the same period as the reactor space time in the overall pressure drop depending on whether the bulk of the wave is traveling upward or downward. These tiny oscillations in the pressure drop continue to decline with the transient plug. When there is a large plug initially taking up half of the reactor repeat unit geometry as in section 5.2, there are similar but with much more intense pressure drop oscillations from that plug traveling around the loop. The pressure oscillations in this case are highly significant and from an operators point of view would be highly undesirable given the potential wear on the reactor components. Fortunately, the plug decays over time, moving towards the steady state solution from the uniform case. With the decay in the plugs comes a similar decline in the pressure oscillations. All the same, this trial indicates that caution should be taken when starting the reactor from this state due to the large initial pressure fluctuations. The parameter studies in section 5.3 using the uniform initial condition showed that the velocity profile can vary significantly with the average size of the particles and the fluid viscosity such that difference between the solid and liquid phase velocities decreases at higher fluid viscosities and smaller
average particle sizes and increases at lower fluid viscosities and larger average particle sizes. This in turn affects the transient small scale pressure oscillations associated with the uniform initial conditions. When the oscillation magnitude increases with introduction of a plug initial condition in section 5.4, this difference in velocity becomes a major factor in how it dissipates. When there is a greater difference between the solid and liquid phase velocities, the decoupling of the solid and liquid phases causes the plug to decay faster. This is in spite of how the trials with the greatest amount of decoupling in the uniform initial condition cases have the worst transient pressure oscillations. Between varying the restitution coefficient and the solid fraction at maximum packing, only the trial with the lowest possible maximum solid fraction showed any significant difference from the standard parameters. This is due to how the closures related to both parameters only become significant at solid fractions extremely close to the maximum. The asymptotical state for all cases done with the uniform and settled plug initial condition in the repeat unit of the reactor is of the same type as the uniform case, changing the viscosity or the particle size only appears to change the time it takes to reach it. If there is any plugging or sustained significant pressure oscillation observed by the operators in this kind of reactor, these results indicate that it comes from a source outside of the scope of the physics modeled in these initial cases.

When growth, harvesting, and injection were applied to the model in section 5.5 using constant circulation, both plugging close to the maximum solid fraction and large sustained pressure oscillations were observed depending on the length of the plug initially applied to the system. For shorter plugs and the uniform initial condition, the solid fraction profile converges to a series of four small plugs. Although these plugs are limited in concentration by spatial diffusion and thus cannot reach anywhere near the maximum solid fraction, they do cause large sustained pressure oscillations. For longer plugs with length equal to a quarter of the reactor or longer, a sustained plug close to the maximum solid fraction forms and is largely left untouched by the harvesting control system. For all these cases, these sustained non-uniform regions contribute more to the overall pressure drop, causing the overall reactor solid fraction to decrease through the pressure drop setpoint in the harvesting control system. The reason these distinctly undesirable states form is because of in-phase harvesting caused by
the control system using pressure drop as the controlled variable. The pressure drop maxima occurring when the majority of the plugs is flowing up the upward legs due to hydrostatic effects ensures a positive feedback loop such that the harvest system will continually remove solid phase at locations in the solid fraction profile that are disadvantageous for maintaining uniformity or a stable pressure drop. Application of the pressure performance curve in section 5.6 resulted in a dampening of the pressure drop oscillations and a corresponding dampening of the harvest control system. This is due to how the performance curve pushed the circulation velocity in a direction such that it tries to offset increases and decreases in the pressure drop with decreases and increases in velocity respectively. Although none of the general behaviors in the pressure drop seen in constant circulation cases from section 5.5 were changed, there was a reduction in the maximum sustained plug solid fraction for the plug cases and also one for the pressure oscillations in all cases. Furthermore, this case also reduced the significant losses from the solid fraction getting overharvested. Instead, the circulation velocity of the entire profile decreased. Although a large decrease in velocity could result in an unwanted reduction of mixing efficiency, with this particular pump curve the decline was only minor. In an attempt to prevent in inevitable oscillation and clogging seen in sections 5.5 and 5.6, the first step done in section 5.7.1 was to reduce the overall solid fraction in the reactor. As expected, the pressure oscillations significantly decreased but at the same time this comes at a significant cost to production efficiency. Similarly, in section 5.7.2 although slowing down the harvesting response to eliminate the formation of plugs did stabilize the uniform initial condition, applying to a half-plug initial condition resulted in significant overharvesting of the solid phase. Delaying the harvesting time by a value equal to half of the space time of the repeat unit in the reactor in 5.7.3 also demonstrated a significant improvement in maintaining a uniform solid fraction without any significant pressure oscillations but still failed to do the same when a plug was applied. Finally, adding another harvest point in section 5.7.4 resulted in the positive feedback loop of in-phase harvesting accelerating faster, causing quicker generation and stabilization of pressure oscillations over time. The first and foremost recommendation is the need for validation of this model with actual data from industrial reactors. Parameters in the model such as the relative wall roughness can be adjusted to fit the pressure drop of the
model with experimental data. Beyond that, the most interesting area in the development of the model is in improving the reaction effects and how they relate to the other constitutive relations. While varying the average particle size and fluid viscosity did show some clear trends in how they would generally affect the entire reactor, more exciting is the prospect of those parameters varying in space due to them being tied to the reaction effects. In-phase harvesting would take on a new dimension with varied particle diameter given that the plugs which it avoids would primarily include particles that grow to larger and larger sizes while areas which it constantly harvests would only have smaller particles, potentially significantly affecting the yield from this reactor. Finally, one point that can be made from these trials is that the pressure drop on its own does not seem to do an ideal job of maintaining a uniform solid fraction of the magnitude desired by the set point. Although the control system itself can certainly be modified and improved such as the trial when the control response was delayed, it still only is a single value that has no ability to spatially define the solid fraction profile to be able to adequately control any non-uniform features. Despite these disadvantages, due to the scale of this system the pressure drop still is the most available way to obtain information on the solid fraction profile. One potential improvement may be to add more pressure sensors down the length of the reactor to get a better idea of where exactly a plug might be forming at. A more complex harvesting control system developed in hand with a model like this then could use this information accordingly to pinpoint plugs as they emerge and prevent them from becoming a problem.
BIBLIOGRAPHY


APPENDIX A. NOMENCLATURE

Table A.1  Subscripts and superscripts

<table>
<thead>
<tr>
<th>Subscript/Superscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>Solid phase</td>
</tr>
<tr>
<td>l</td>
<td>Liquid phase</td>
</tr>
<tr>
<td>n</td>
<td>Time step</td>
</tr>
<tr>
<td>i</td>
<td>Spatial step</td>
</tr>
<tr>
<td>C</td>
<td>Cell-averaged variable</td>
</tr>
<tr>
<td>L</td>
<td>Left face value</td>
</tr>
<tr>
<td>R</td>
<td>Right face value</td>
</tr>
<tr>
<td>L+</td>
<td>Left face value approached from the right side</td>
</tr>
<tr>
<td>L-</td>
<td>Left face value approached from the left side</td>
</tr>
<tr>
<td>R+</td>
<td>Right face value approached from the right side</td>
</tr>
<tr>
<td>R-</td>
<td>Right face value approached from the left side</td>
</tr>
</tbody>
</table>
Table A.2  Nomenclature table

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega_j$</td>
<td>Weights</td>
</tr>
<tr>
<td>$\delta_{hi}$</td>
<td>Harvest spatial region switch</td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>$C_{pm}$</td>
<td>Cells per meter</td>
</tr>
<tr>
<td>$C_\mu$</td>
<td>Turbulent viscosity coefficient</td>
</tr>
<tr>
<td>$k_c$</td>
<td>Control coefficient</td>
</tr>
<tr>
<td>$k_g$</td>
<td>Growth coefficient</td>
</tr>
<tr>
<td>$k_{hi}$</td>
<td>Harvest and injection coefficient</td>
</tr>
<tr>
<td>$k_t$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$K_i$</td>
<td>Growth or harvest coefficient</td>
</tr>
<tr>
<td>$p_i$</td>
<td>Phase pressure</td>
</tr>
<tr>
<td>$Q$</td>
<td>Large WENO stencil polynomial</td>
</tr>
<tr>
<td>$S_i$</td>
<td>Source or sink term</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$U_i$</td>
<td>Phase velocity</td>
</tr>
<tr>
<td>$\dot{Q}$</td>
<td>Volumetric flowrate</td>
</tr>
<tr>
<td>$U_r$</td>
<td>Interphase velocity</td>
</tr>
<tr>
<td>$d_{part}$</td>
<td>Particle diameter</td>
</tr>
<tr>
<td>$d_{pipe}$</td>
<td>Pipe diameter</td>
</tr>
<tr>
<td>$\epsilon_{rest}$</td>
<td>Restitution coefficient</td>
</tr>
<tr>
<td>$f_l$</td>
<td>Liquid phase friction factor</td>
</tr>
<tr>
<td>$\epsilon_{wall}$</td>
<td>Wall frictional roughness</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>$g_0$</td>
<td>Particle radial distribution function</td>
</tr>
<tr>
<td>$\epsilon_t$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$p_j$</td>
<td>Sub-stencil polynomial linearization</td>
</tr>
<tr>
<td>$\alpha_i$</td>
<td>Phase volume fraction</td>
</tr>
<tr>
<td>$\beta_j$</td>
<td>Smoothness indicator</td>
</tr>
<tr>
<td>$\gamma_j$</td>
<td>Linear weight</td>
</tr>
<tr>
<td>$\gamma_s$</td>
<td>Collisonal energy dissipation</td>
</tr>
<tr>
<td>$\kappa_s$</td>
<td>Fluctuating energy conductivity</td>
</tr>
<tr>
<td>$\tau_{space}, \tau_{st}$</td>
<td>Reactor space time</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>Phase density</td>
</tr>
<tr>
<td>$\nu_i$</td>
<td>Phase kinematic viscosity</td>
</tr>
<tr>
<td>$p_i$</td>
<td>Normalized weights</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Turbulent dissipation</td>
</tr>
<tr>
<td>$\Theta_s$</td>
<td>Granular temperature</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time-step</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Interphase momentum transfer coefficient</td>
</tr>
<tr>
<td>$e_{n,z}$</td>
<td>Corrector for zero smoothness</td>
</tr>
</tbody>
</table>
APPENDIX B. MATLAB CODE AND SUBROUTINES

Master code with growth, harvesting, and pump curve

```matlab
clear;
mpiInit();
tic;

%-------------------Geometric Parameters-------------------

% reactor properties

dPipe=0.5603875; % m
lTotal=132*4; % m
lS=60;
lb1=6;
lb2=6;
cpm=50; % cells per meter;

% Build Mesh

zSides=0:1/(cpm):lTotal;

meshLength=length(zSides);
```
22 \texttt{zLeft=\texttt{zSides\ (1,1:\texttt{meshLength}-1));}
23 \texttt{zRight=\texttt{zSides\ (1,2:\texttt{meshLength});}
24 \texttt{zCenter=(1/2)\ast(\texttt{zLeft+\texttt{zRight});}
25
26 \%---------Time\ Step----------
27
28 \texttt{TOTALTIME}=300;
29 \texttt{ts}=4e^{-5};
30 \texttt{t init}=0;
31 \% \texttt{tcMax}=2500000+\texttt{t init}+2/\texttt{ts};
32 \texttt{tcMax}=\texttt{t init}+\texttt{TOTALTIME}/\texttt{ts};
33 \texttt{t Max}=\texttt{tcMax}\ast\texttt{ts};
34 \% \texttt{t Mat}=0:\texttt{ts}:\texttt{t Max};
35
36 \%---------Phase\ Parameters---------
37
38 \% phase A properties
39
40 \texttt{rhoA}=\texttt{903.441334291};\ % \texttt{kg/m}^3
41 \texttt{nua}=\texttt{1e-06};\ % \texttt{m}^2/\texttt{s} \hspace{1cm} \text{PLACEHOLDER}
42 \texttt{da}=\texttt{765e-6};
43 \%765 e-6;\ % \texttt{m}
44
45 \% phase b properties
46
47 \texttt{rhoB}=\texttt{408.470816036};\ % \texttt{kg/m}^3
48 \texttt{nub}=\texttt{1.29752E-007};\ % \texttt{m}^2/\texttt{s}
49 \texttt{db}=\texttt{1};\ % \texttt{m} \hspace{1cm} \text{PLACEHOLDER}
% Liquid Wall Friction

eRoughness = 0.015/dPipe*10^-3;

% Solid Phase Growth

% kg=0; % s^-1
kg=0;

% Solid Phase Harvesting Coefficient

deltikh=0*ones(1,meshLength-1); % piecewise coefficient to designate harvest area
khSet=-0; % s^-1 harvesting rate
kh=khSet;
khperiod=132/11.5;

% kihpulsetime=khperiod*6;
%
% kihpulsetimes=0:kihpulsetime:tMax;

% kih=0;

zhargvFront=ls*2+lb1+3.2;
zhargvBack=ls*2+lb1+2.8;
for harvc =1:length(zCenter)
    if zCenter(1,harvc)<zharvFront&&zCenter(1,harvc)>zharvBack
        deltikh(1,harvc)=1;
    end
end

% Overall Growth and Harvest Coefficient

kihInit=(deltikh);

% Maximum Solid Fraction

alphaMax=0.50;

% Gravity

g = -9.81; % m/s^2

% gMatInit=g*ones(1,meshLength-1);
gMatInit = gravreactorFN(zCenter,g,ls,lb1,lb2);

% Turbulent Response Time

Ct=1/2;

Cmu=0.09;

% Restitution Coefficient

eRest = .8;
% Square Root of Pi

sqrtPi = sqrt(pi);

%---------Initial Conditions---------

alphaSet = .29;
p PressureDropSet = 4.9147e+05;

% alphaInit = .29*ones(1, meshLength - 1);
uInit = uCirculation * ones(1, meshLength - 1);
thetaInit = 10^-3 * ones(1, meshLength - 1);
pInit = (zSides) * g * rhob;

Circulation Velocity

uCirculation = 11.5;

zplugFront = lTotal / 2;
zplugBack = 0;

for plugc = 1:length(zCenter)
    if zCenter(1, plugc) < ls / 2
        alphaInit(1, plugc) = .45;
    end

    if zCenter(1, plugc) > (ls * 3/2 + lb1) && zCenter(1, plugc) < (ls * 5/2 + lb1 * 2)
alphaInit(1, plugc) = .45;

end

if zCenter(1, plugc) > (ls * 7/2 + 3 * lb1) && zCenter(1, plugc) < (ls * 9/2 + lb1 * 4)
    alphaInit(1, plugc) = .45;
end

if zCenter(1, plugc) > (ls * 11/2 + 5 * lb1) && zCenter(1, plugc) < (ls * 13/2 + lb1 * 6)
    alphaInit(1, plugc) = .45;
end

if zCenter(1, plugc) > (ls * 15/2 + 7 * lb1)
    alphaInit(1, plugc) = .45;
end

alphaInit = smooth(alphaInit, 'moving');
alphaInit = smooth(alphaInit, 'moving');
alphaInit = smooth(alphaInit, 'moving');
alphaInit = smooth(alphaInit, 'moving');
alphaInit = smooth(alphaInit, 'moving');

%———Prep Graphing Variables———
graphc = 0;

graphHarvestc = 1;

graphHarvest = round(((tcMax - t c i n i t ) / TOTALTIME));

%——— Prep Gathering Variables ———

gatherSamplec = 0;

% gatherPressurec = 1;

gatherSampleTime = round (1 / ts);

gatherPressureTime = round (1);

massReactor = lTotal * pi * (dPipe / 2)^2 * (mean(alphaInit) * rhoa + (1 - mean(alphaInit)) * rhob);

%——— Parallel Decomposition ———

parMax = 12; % number of processors

meshLengthPar = (meshLength - 1) / parMax;

alphaPar = cell(1, parMax);
uPar = cell(1, parMax);
thetaPar = cell(1, parMax);
pPar = cell(1, parMax);

alphaNextPar = cell(1, parMax);
uNextPar = cell(1, parMax);
thetaNextPar = cell(1, parMax);
gMatPar = cell(1, parMax);
kihPar = cell(1, parMax);
alphaSum = cell(1, parMax);

alphaParEdge = cell(1, parMax);
uaParEdge = cell(1, parMax);
thetaParEdge = cell(1, parMax);

alphaStor = cell(round((tMax/ ts - tcinit)/ graphHarvest) - 1, parMax);
uaStor = cell(round((tMax/ ts - tcinit)/ graphHarvest) - 1, parMax);
thetaStor = cell(round((tMax/ ts - tcinit)/ graphHarvest) - 1, parMax);
pStor = cell(round((tMax/ ts - tcinit)/ graphHarvest) - 1, parMax);
uCircStor = cell(round((tMax/ ts - tcinit)/ graphHarvest) - 1, 1);

indLeft3 = circshift(1: (meshLength - 1), [0, 3]);
indRight3 = circshift(1: (meshLength - 1), [0, -3]);

ALPHA = zeros(1, (meshLength - 1));
UA = zeros(1, (meshLength - 1));
THETA = zeros(1, (meshLength - 1));

ALPHAMAT = zeros(round((tMax/ ts - tcinit)/ graphHarvest), (meshLength - 1));
UAMAT = zeros(round((tMax/ ts - tcinit)/ graphHarvest), (meshLength - 1));
THETAMAT = zeros(round((tMax/ ts - tcinit)/ graphHarvest), (meshLength - 1));
PRESSUREMAT = zeros(round((tMax/ ts - tcinit)/ graphHarvest), meshLength);

for pdec = 1:(parMax)
    alphaPar{1, pdec} = alphaInit(1, ((pdec - 1)*(meshLengthPar) + 1): (pdec*
meshLengthPar ) );

uaPar{1,pdec} = uaInit (1,((pdec -1)*(meshLengthPar)+1):(pdec*
    meshLengthPar ));

thetaPar{1,pdec} = thetaInit (1,((pdec -1)*(meshLengthPar)+1):(pdec*
    meshLengthPar ));

gMatPar{1,pdec} = gMatInit (1,((pdec -1)*(meshLengthPar)+1):(pdec*
    meshLengthPar ));

kihPar{1,pdec} = kihInit (1,((pdec -1)*(meshLengthPar)+1):(pdec*
    meshLengthPar ));

alphaParEdge{1,pdec} = horzcat ( . . .
    alphaInit (1,indLeft3 (1,((pdec -1)*meshLengthPar+1):((pdec -1)*
        meshLengthPar+3))) , . . .

alphaPar{1,pdec} , . . .

alphaInit (1,indRight3 (1,((pdec)*meshLengthPar -2):((pdec)*
    meshLengthPar ))) . . .
)

uaParEdge{1,pdec} = horzcat ( . . .
    uaInit (1,indLeft3 (1,((pdec -1)*meshLengthPar+1):((pdec -1)*
        meshLengthPar+3))) , . . .

uaPar{1,pdec} , . . .

uaInit (1,indRight3 (1,((pdec)*meshLengthPar -2):((pdec)*
    meshLengthPar ))) . . .
)

thetaParEdge{1,pdec} = horzcat ( . . .
    thetaInit (1,indLeft3 (1,((pdec -1)*meshLengthPar+1):((pdec -1)*
        meshLengthPar+3))) , . . .

thetaPar{1,pdec} , . . .
\[
\theta_{\text{Init}}(1, \text{indRight3}(1, ((\text{pdec})*\text{meshLengthPar}-2):( (\text{pdec})*\text{meshLengthPar} ))) \ldots
\]

\)

end

spmd (parMax)

\[\text{indParLeft} = \text{circshift}(1:\text{parMax}, [0, 1]);\]

\[\text{indParRight} = \text{circshift}(1:\text{parMax}, [0, -1]);\]

for tc=tcinit:(tcMax+1)

\[\{\alpha_{\text{NextPar}}\{1, \text{labindex}\}, u_{\text{NextPar}}\{1, \text{labindex}\}, \theta_{\text{NextPar}}\{1, \text{labindex}\}, p_{\text{Par}}\{1, \text{labindex}\}\} = \]

masterexplicitfunctionNEWHARVEST(\ldots

\[\alpha_{\text{Par}}\{1, \text{labindex}\}, \alpha_{\text{ParEdge}}\{1, \text{labindex}\}, \ldots\]

\[u_{\text{Par}}\{1, \text{labindex}\}, u_{\text{ParEdge}}\{1, \text{labindex}\}, \ldots\]

\[\theta_{\text{Par}}\{1, \text{labindex}\}, \theta_{\text{ParEdge}}\{1, \text{labindex}\}, \ldots\]

\[g_{\text{MatPar}}\{1, \text{labindex}\}, k_{\text{ihPar}}\{1, \text{labindex}\}, \ldots\]

\[\text{meshLengthPar}, \text{cpm}, \text{uCirculation}, \alpha_{\text{Max}}, e_{\text{Rest}}, \text{da}, C_{\mu},\]

\[d_{\text{Pipe}}, \rho_{a}, \rho_{b}, n_{\mu}, e_{\text{Roughness}}, \sqrt{\pi}, t_{s}, k_{g}, \ldots\]

\[k_{\text{ih}}\];

\]

% Update and Store Variables

\[\alpha_{\text{Par}}\{1, \text{labindex}\} = \alpha_{\text{NextPar}}\{1, \text{labindex}\};\]

\[u_{\text{Par}}\{1, \text{labindex}\} = u_{\text{NextPar}}\{1, \text{labindex}\};\]

\[\theta_{\text{Par}}\{1, \text{labindex}\} = \theta_{\text{NextPar}}\{1, \text{labindex}\};\]

\[\alpha_{\text{ParEdgeLeftSen}} = \alpha_{\text{NextPar}}\{1, \text{labindex}\}(1, 1:3);\]
alphaParEdgeRightSen=alphaNextPar{1,labindex}(1, (meshLengthPar−2):meshLengthPar);

uaParEdgeLeftSen=uaNextPar{1,labindex}(1,1:3);

uaParEdgeRightSen=uaNextPar{1,labindex}(1,(meshLengthPar−2):meshLengthPar);

thetaParEdgeLeftSen=thetaNextPar{1,labindex}(1,1:3);

thetaParEdgeRightSen=thetaNextPar{1,labindex}(1,(meshLengthPar−2):meshLengthPar);

labBarrier; % this sets a point each timestep such that all the processors can 'catch-up' if any one is running slow/fast

alphaParEdgeLeftRec = labSendReceive(indParRight(labindex),
                                   indParLeft(labindex),alphaParEdgeRightSen);

labBarrier;

alphaParEdgeRightRec = labSendReceive(indParLeft(labindex),
                                   indParRight(labindex),alphaParEdgeLeftSen);

labBarrier;

uaParEdgeLeftRec = labSendReceive(indParRight(labindex),
                                   indParLeft(labindex),uaParEdgeRightSen);

labBarrier;

uaParEdgeRightRec = labSendReceive(indParLeft(labindex),
                                   indParRight(labindex),uaParEdgeLeftSen);

labBarrier;

thetaParEdgeLeftRec = labSendReceive(indParRight(labindex),
                                   indParLeft(labindex),thetaParEdgeRightSen);
labBarrier;

thetaParEdgeRightRec = labSendReceive(indParLeft(labindex),
   indParRight(labindex), thetaParEdgeLeftSen);

alphaParEdge{1, labindex} = horzcat(...
   alphaParEdgeLeftRec, ...,
   alphaPar{1, labindex}, ...,
   alphaParEdgeRightRec ...);

uaParEdge{1, labindex} = horzcat(...
   uaParEdgeLeftRec, ...,
   uaPar{1, labindex}, ...,
   uaParEdgeRightRec ...);

thetaParEdge{1, labindex} = horzcat(...
   thetaParEdgeLeftRec, ...,
   thetaPar{1, labindex}, ...,
   thetaParEdgeRightRec ...);

if graphc==graphHarvest
   alphaStor{graphHarvestc, labindex} = alphaPar{1, labindex};
   uaStor{graphHarvestc, labindex} = uaPar{1, labindex};
   thetaStor{graphHarvestc, labindex} = thetaPar{1, labindex};
   pStor{graphHarvestc, labindex} = pPar{1, labindex};
   uCircStor{graphHarvestc, labindex} = uCirculation(1,1);
   graphHarvestc = graphHarvestc + 1;
   graphc = 0;
display(tc)
end

if gatherSamplec==gatherSampleTime
    pressureInt=pPar{1,labindex};
    pressureDropPar=pressureInt(1,meshLengthPar);

    labBarrier;
    pressureDrop=-gop(@plus,pressureDropPar);

    kih=min(kih+5e-6*(pressureDropSet-pressureDrop),0);

    if (pressureDropSet-pressureDrop)>0
        kih=0;
    end

    gatherSamplec=0;
end

pressureInt=pPar{1,labindex};
alphaInt=alphaPar{1,labindex};
pressureDropPar=pressureInt(1,meshLengthPar);
alphaAvePar=mean(mean(alphaInt));

labBarrier;
pressureDrop=-gop(@plus,pressureDropPar);
labBarrier;
alphaTotal = gop (@plus, alphaAvePar) / parMax;

massReactor = lTotal * pi * (dPipe / 2)^2 * (alphaTotal * rhoa + (1 - alphaTotal) * rhob);

uCirculationMinMax = min(max(uCirculation, 4), 15.65);

pressureDropPumpCurve = REDACTED;

uCirculation = uCirculation - (pressureDrop - pressureDropPumpCurve) / massReactor * ts;

gatherSamplec = gatherSamplec + 1;

graphc = graphc + 1;

end
end

% Reconstruct Variables

[ALPHAMAT, UMAT, THETAMAT, PRESSUREMAT] = reconstructParNextFN(ALPHAMAT, UMAT, THETAMAT, PRESSUREMAT, ...)

alphaStor, uaStor, thetaStor, pStor, ...
tMax, ts, parMax, graphHarvest, meshLengthPar);

UCIRCMAT = uCircStor {1,1};

RUNTIME = toc;

Explicit stepping function

function [alphaNext, uaNext, thetaNext, p] = 
masterexplicitfunctionNEWHARVEST( ...)

alpha, alphaEdge, ...
ua, uaEdge, ...
theta, thetaEdge, ...
gMat, kihdelta, ...
meshLengthPar, cpm, uCirculation, alphaMax, eRest, da, Cmu, dPipe, rhoa, rhob, nub, eRoughness, sqrtPi, ts, kg, ...
kih

% Calculate the Values on the Sides of the Faces
[ alphaFaceLeftRight, alphaFaceRightLeft, alphaFaceRightRight] = wenok2FacesLITEPAR(alphaEdge, meshLengthPar); % 5th order weno finite volume method
[ uaFaceLeftRight, uaFaceRightLeft, uaFaceRightRight, uaDiffFluxLeft, uaDiffFluxRight] = wenok2FacesLITEPARwDiff(uaEdge, meshLengthPar, cpm);
[ thetaFaceLeftRight, thetaFaceRightLeft, thetaFaceRightRight, thetaDiffFluxLeft, thetaDiffFluxRight] = wenok2FacesLITEPARwDiff(thetaEdge, meshLengthPar, cpm);

% % % % % % % % % % % % % % % % % % PRESSURE CALCULATION % % % % % % % % % % % % % % % % % % % % % % % %

% Apply Physical Constraints
beta = 1 - alpha;
ur = (uCirculation - ua) ./ (1 - alpha);
ub = ur + ua;

% Calculate Radial Distribution Function
\( g_0 = g_0\text{FN}(\alpha, \alpha\text{Max}) \);

\% Calculate Solid Phase Viscosity (Gidaspow)

\( \text{nuaEff} = \text{gidaspowViscREV2}(\alpha, u_a, u_b, \theta, \rho_a, \rho_b, d\text{Pipe}, g_0, e\text{Rest}, d_a, C\text{mu}) \);

\% Calculate Liquid Phase Viscosity (Launder and Spaulding)

\% \( \text{nubEff} = \text{liquidViscFN}(\alpha, u_a, u_b, \rho_a, \rho_b, d\text{Pipe}, C\mu, d_a, u\text{Circulation}, nub) \);

\% Fluid Wall Drag Coefficient (Used in Pressure Calculation)

\( \text{reMix} = |u\text{Circulation}| \cdot d\text{Pipe} \cdot (\alpha \cdot \rho_a + \beta \cdot \rho_b) / (nub \cdot \rho_b \cdot (1 + (5/2) \cdot \alpha)) \);

\% \( \text{reMix} = |u\text{Circulation}| \cdot d\text{Pipe} / (nub \cdot (1 + (5/2) \cdot \alpha)) \);

\( f\text{Friction} = (-2 \cdot \log_{10}(e\text{Roughness} / 3.7...) - (5.02 / \text{reMix}) \cdot \log_{10}(e\text{Roughness}...) - (5.02 / \text{reMix}) \cdot \log_{10}(e\text{Roughness} / 3.7...) + 13 / \text{reMix}))) . \)^{(-2)} ;

\( \text{kpwallcontCoeff} = -0.5 \cdot f\text{Friction} \cdot \beta \cdot |u\text{Circulation}| / d\text{Pipe} \cdot ((1 + \alpha \cdot \rho_a / \rho_b) / \beta \cdot 2) \);

\% \( \text{kpwallcontCoeff} = -0.5 \cdot f\text{Friction} \cdot \beta \cdot |u\text{Circulation}| / d\text{Pipe} \);

\% Bagnold Wall Drag Coefficient


```
reParticle = abs(ua) * da / (nub);
linC = g0 - 1;
kpwallpartCoeff = -0.0214 * 4 / dPipe * reParticle ^ -36 * (da / dPipe) ^ 0.99 *
      linC ^ 1.31;

% Interphase Drag Coefficient (Ergun Wen and Yu)
kpinterphaseCoeff = gidaspowInterphase(alpha, ur, rhob, nub, da);

% Gravity Coefficient
kgravityCoeff = gMat;

% Granular Pressure Calculation
granPGrad = granPGradFN(alphaFaceLeftRight, alphaFaceRightLeft,
                         thetaFaceLeftRight, thetaFaceRightLeft, alphaMax, eRest, rhoa, cpm);

% Fluid Pressure Calculation
alphaFaceRight = (1/2) * (alphaFaceRightLeft + alphaFaceRightRight);
betaFaceRight = 1 - alphaFaceRight;

uaFaceRight = (1/2) * (uaFaceRightLeft + uaFaceRightRight);
ubFaceRight = circcontFN(alphaFaceRight, uaFaceRight, uCirculation);
uaGradFaceRight = cpm * (uaFaceRightRight - uaFaceRightLeft);
ubGradFaceRight = cpm * (circcontFN(alphaFaceRightRight,
```
uaFaceRightRight, uCirculation)...  
−circcontFN(alphaFaceRightLeft, uaFaceRightLeft, uCirculation));  

thetaFaceRight = (1/2) * (thetaFaceRightLeft + thetaFaceRightRight);  

granPGradFaceRight = granPGradFN(alphaFaceRightLeft, alphaFaceRightRight, thetaFaceRightLeft, thetaFaceRightRight, alphaMax, eRest, rhoa, cpm);  

nuaEffFaceRight = gidaspowViscREV(alphaFaceRight, uaFaceRight, ubFaceRight, thetaFaceRight, rhoa, rhob, dPipe, alphaMax, eRest, da, Cmu);  

nubEffFaceRight = liquidViscFN(alphaFaceRight, uaFaceRight, ubFaceRight, rhoa, rhob, dPipe, Cmu, da, uCirculation, nub);  

pressnonIntFaceRight = −rhob * ( 
  alphaFaceRight .* uaFaceRight.^2 − alphaFaceRight (1,1).* uaFaceRight (1,1).^2 ...  
  + betaFaceRight .* ubFaceRight.^2 − betaFaceRight (1,1).* ubFaceRight (1,1).^2 ...  
  − nuaEffFaceRight .* uaGradFaceRight+nuaEffFaceRight (1,1).* uaGradFaceRight (1,1)...  
  − nubEffFaceRight .* ubGradFaceRight+nubEffFaceRight (1,1).* ubGradFaceRight (1,1)...  
  + granPGradFaceRight/rhoa−granPGradFaceRight (1,1)/rhoa...  
); % nonintegrated pressure terms  

pressInt = rhob/cpm * (...
\[ kp_{\text{interphaseCoeff}} \cdot u_r \cdot \left( \frac{1}{\rho_a} - \frac{1}{\rho_b} \right) \ldots \]

\[ + \min \left( \left[ kp_{\text{wallpartCoeff}}, u_a \cdot \hat{u}_2 \right], kp_{\text{wallcontCoeff}} \cdot u_{\text{Circulation}} \right), 2) \ldots \]

\[ + k_{\text{gravityCoeff}} \ldots \]

); % integrated pressure Terms evaluated cell by cell

\[ \text{pressIntsum} = \text{cumsum}(\text{pressInt}); \]

\[ \text{pNextRight} = \text{pressnonIntFaceRight}(1,2 : (\text{meshLengthPar}+1)) + \text{pressIntsum}; \]

\[ \text{p} = \text{horzcat}(0, \text{pNextRight}); \]

\[ \% \text{pNextLeft}(1,1 : (\text{meshLength} - 1)) = \text{pNextRight}(1, \text{horzcat}(\text{meshLength} - 1, 1: (\text{meshLength} - 2))); \]

\[ \text{pNextLeft} = \text{circshift}(\text{pNextRight}, [0, 1]); \]

\[ \text{pNextLeft}(1,1) = 0; \]

\[ \text{pressureGrad} = \text{cpm} \cdot (\text{pNextRight} - \text{pNextLeft}); \]

% % % % % % % % % % % % % % % CONTINUITY EQUATION % % % % % % % % % % % % % % % % % % % % % % %

% Continuity Advection FV

\[ \text{globalLFCoeffCont} = \text{globalLFREV} (\text{alphaFaceLeftRight}, \text{alphaFaceRightLeft}, \ldots \]

\[ \text{alphaFaceLeftRight} \cdot u_{\text{FaceLeftRight}}, \text{alphaFaceRightLeft} \cdot \ldots \]
uaFaceRightLeft);

contMaxDervRight = max (globalLFCoeffCont, isnan(globalLFCoeffCont)) *
(alphafaceRightRight - alphafaceRightLeft) / 2;

contfluxRightInt = (1/2) * (alphafaceRightLeft * alphafaceRightLeft +
alphafaceRightRight * alphafaceRightRight) ...
- contMaxDervRight;

contfluxRight = contfluxRightInt (1,2:(meshLengthPar+1));
contfluxLeft = contfluxRightInt (1,1:(meshLengthPar));

% contfluxLeft (1,1:(meshLength - 1)) = contfluxRight (1, horzcat(
meshLength - 1,1:(meshLength - 2)));

% contfluxLeft = circshift (contfluxRight,[0,1]);

alphastardt = -cpm * (contfluxRight - contfluxLeft);

alphaStar = alpha + ts * alphastardt;

% Continuity Reaction

% kihvary = kih * sign(1 - sign(sin(tc*ts/kihfreq*pi))); % square Wave

% kihvary = kih * pulstran(tc*ts,kihpulsetimes,rectpuls,kihperiod);

% alphaNext = alphaStar * exp(ts*(kg+kih)); % analytical solution for
reaction equation

sourceContInt = (... kg.*alpha...
+ kih*kihDelta.*(alpha)/(1-alpha));

alphaNext = alphaStar+ts*sourceContInt;

%%%%%%%%%%%%%%%% END CONTINUITY EQUATION %%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%% MOMENTUM EQUATION %%%%%%%%%%%%%%%%%%%%

% NOTE: Calculated Explicitly at ua[n] and alpha[n]

% Solid Phase Viscosity is calculated in the previous step

% Momentum Advection–Diffusion FV

globalLFCoeffMom= (globalLFREV( alphaFaceLeftRight.*uaFaceLeftRight,
alphaFaceRightLeft.*uaFaceRightLeft,...
alphaFaceLeftRight.*uaFaceLeftRight.^2, alphaFaceRightLeft.*
uaFaceRightLeft.^2));

globalLFCoeffMom=max( globalLFCoeffMom, isnan( globalLFCoeffMom));

momfluxRightInt = (1/2)*(uaFaceRightLeft.^2.*alphaFaceRightLeft+
uaFaceRightRight.^2.*alphaFaceRightRight)...
- globalLFCoeffMom/2.*(alphaFaceRightRight.*uaFaceRightRight-
\[ \text{alphaFaceRightLeft} \times \text{uaFaceRightLeft} ; \]

\[ \text{momfluxRight} = \text{momfluxRightInt} \left( 1, 2 : (\text{meshLengthPar}+1) \right) ; \]

\[ \text{momfluxLeft} = \text{momfluxRightInt} \left( 1, 1 : (\text{meshLengthPar}) \right) ; \]

\[ \% \text{momfluxLeft} \left( 1, 1 : (\text{meshLength} - 1) \right) = \text{momfluxRight} \left( 1, \text{horzcat} \left( \text{meshLength} - 1, 1 : (\text{meshLength} - 2) \right) \right) ; \]

\[ \% \text{momfluxLeft} = \text{circshift} \left( \text{momfluxRight} , [0, 1] \right) ; \]

\[ q = \text{alpha} \times \text{ua} ; \]

\[ q_{\text{StardtAdv}} = -\text{cpm} \times (\text{momfluxRight} - \text{momfluxLeft}) ; \]

\[ q_{\text{StardtDiff}} = \text{cpm} \times (\text{nuaEff} \times \text{uaDiffFluxRight} - \text{nuaEff} \times \text{uaDiffFluxLeft}) ; \]

\[ q_{\text{Star}} = q + ts \times (q_{\text{StardtAdv}} + q_{\text{StardtDiff}}) ; \]

\[ \text{uaStar} = q_{\text{Star}} / \text{alpha} ; \]

\[ \% \text{Momentum Source} \]

\[ \% \text{Build variables at uastar and alpha} \]

\[ \text{urStar} = (u\text{Circulation} - \text{uaStar}) / (1 - \text{alpha}) ; \]

\[ \text{ubStar} = \text{urStar} + \text{uaStar} ; \]

\[ \% \text{Interphase Drag Coefficient (Ergun Wen and Yu)} \]
kinterphaseCoeff = gidaspowInterphase(alpha, urStar, rhob, nub, da);

% Bagnold Wall Drag Coefficient

reParticle=abs(uaStar)*da/(nub);

kwallpartCoeff=−0.0214*4/dPipe*reParticle.^−.36*(da/dPipe).^−.99*linC.^1.31;

% Growth Coefficient

growthCoeff=kg;

% Harvest Coefficient

kharvestCoeff=−kih*kih delta;

% Granular Pressure Gradient

kgranP=granPGrad(1,2:(meshLengthPar+1))/rhoa;

% Apply Source Terms

sourceInt = (... 

      kinterphaseCoeff.*urStar/rhoa... 
      −alpha.*pressureGrad/rhoa... 
      +kwallpartCoeff.*uaStar.^2 ...
+kg\text{gravityCoeff} \times \alpha \ldots
+k\text{growthCoeff} \times \alpha \times \text{ubStar} \ldots
-k\text{harvestCoeff} \times \alpha \times \text{uaStar} \ldots
-k\text{granP}) ;

q_{\text{Next}} = q_{\text{Star}} + t_s \times \text{sourceInt} ;
\text{uaNext} = q_{\text{Next}} / \alpha ;

% % % % % % % % % % END MOMENTUM EQUATION % % % % % % % % % %

% % % % % % % % % % KINETIC THEORY EQUATION % % % % % % % % %

% Conductivity

kappa_{\text{dil}} = (75/384) \times \sqrt{\pi} \times \rho_a \times d_a \times \sqrt{\theta} ;

kappa = 2 ./ ( (1 + e_{\text{Rest}}) \times g_0 \times (1 + (6/5) \times e_{\text{Rest}} \times g_0 \times \alpha) ^ 2 \times kappa_{\text{dil}} \ldots
+ 2 \times \alpha ^ 2 \times \rho_a \times d_a \times g_0 \times (1 + e_{\text{Rest}}) \times (\theta) ^ {(1/2)} / \sqrt{\pi} ;

% Kinetic Theory Advection–Diffusion FV

\text{globalLFCoeffKT} = \text{globalLFREV}(\alpha_{\text{FaceLeftRight}} \times \theta_{\text{FaceLeftRight}} ,
\alpha_{\text{FaceRightLeft}} \times \theta_{\text{FaceRightLeft}} , \ldots
\alpha_{\text{FaceLeftRight}} \times \text{uaFaceLeftRight} \times \theta_{\text{FaceLeftRight}} ,
\alpha_{\text{FaceRightLeft}} \times \text{uaFaceRightLeft} \times \theta_{\text{FaceRightLeft}} ) ;

\text{globalLFCoeffKT} = \max(\text{globalLFCoeffKT} , \text{isnan}(\text{globalLFCoeffKT})) ;
ktfluxRightInt = (1/2) * (uaFaceRightLeft * alphaFaceRightLeft * 
thetaFaceRightLeft . . . 
+ uaFaceRightRight * alphaFaceRightRight * thetaFaceRightRight) . . . 
- globalLFCoeffKT . / (2) * (alphaFaceRightRight * 
thetaFaceRightRight . . . 
- alphaFaceRightLeft * thetaFaceRightLeft);

ktfluxRight = ktfluxRightInt (1, 2: (meshLengthPar + 1));
ktfluxLeft = ktfluxRightInt (1, 1: (meshLengthPar));

% ktfluxLeft = circshift (ktfluxRight, [0, 1]);

% ktfluxLeft (1, 1: (meshLength - 1)) = ktfluxRight (1, horzcat (meshLength 
- 1, 1: (meshLength - 2)));

r = alpha * theta;

rStardtAdv = - cpm * (ktfluxRight - ktfluxLeft);

rStardtDiff = cpm * (kappa * thetaDiffFluxRight - kappa * thetaDiffFluxLeft);

rStar = r + ts * (rStardtAdv + rStardtDiff);

thetaStar = rStar / alpha;

thetaStar = max (thetaStar, 10^(-8));
% Kinetic Theory Source Terms

uaGrad = cpm*(uaFaceRightLeft(1,2:(meshLengthPar+1))-uaFaceLeftRight(1,2:(meshLengthPar+1)))

% Interphase Drag Coefficient (Ergun Wen and Yu)

% ktinterphaseCoeff = gidaspowInterphase(alpha, ur, rhob, nub, da);
% identical to the value calculated for the previous iteration pressure

% Collisional Dissipation

ktgammaCol = 3*(1-eRest^2)*rhoa*alpha.*g0.*(4/da*sqrt(thetaStar)/sqrtPi-uaGrad); % m^2/s^3

% Surface Force Double Diad

granPStar = rhoa.*alpha.*thetaStar.*(1+2*(1+eRest)*g0.*alpha); %
granular pressure \Pa

[nuaEff, eaT] = gidaspowViscREVwE2(alpha, ua, ub, thetaStar, rhoa, rhob, dPipe, g0, eRest, da, Cmu);

ktSurfaceDD = (-granPStar./rhoa+nuaEff.*uaGrad).*uaGrad;

% Apply Source Terms
sourcekInt = (2/3) * (...
    kpterphaseCoeff * thetaStar/rhoa ...
    -ktgammaCol * thetaStar/rhoa ...
    +ktSurfaceDD ...
    +eaT * alpha);

rNext = r + ts * sourcekInt;
thetaNext = rNext / alpha;
thetaNext = max(thetaNext, 10^{-8});

function [ variableFaceLeftRight, variableFaceRightLeft, 
    variableFaceRightRight ] = wenok2FacesLITEPAR( variableInput, 
    meshLengthPar)
meshLengthParMod = meshLengthPar + 2;

variableLeft2(1,1:(meshLengthParMod)) = variableInput(1,1: 
    meshLengthParMod);
variableLeft(1,1:(meshLengthParMod)) = variableInput(1,2: 
    meshLengthParMod+1));
variable(1,1:(meshLengthParMod)) = variableInput(1,3:( 
    meshLengthParMod+2));
variableRight(1,1:(meshLengthParMod)) = variableInput(1,4: 
    meshLengthParMod+3));

WENO functions
variableRight2(1,1:(meshLengthParMod)) = variableInput(1,5:(meshLengthParMod+4));

pl0 = (11/6) * variable + (-7/6) * variableRight + (1/3) * variableRight2;
pl1 = (1/3) * variableLeft + (5/6) * variable + (-1/6) * variableRight;
pl2 = (-1/6) * variableLeft2 + (5/6) * variableLeft + (1/3) * variable;

pr0 = (1/3) * variable + (5/6) * variableRight + (-1/6) * variableRight2;
pr1 = (-1/6) * variableLeft + (5/6) * variable + (1/3) * variableRight;
pr2 = (1/3) * variableLeft2 + (-7/6) * variableLeft + (11/6) * variable;

gaml0 = (1/10);
gaml1 = (6/10);
gaml2 = (3/10);

gamr0 = (3/10);
gamr1 = (6/10);
gamr2 = (1/10);

beta0 = (13/12) * (variableLeft2 - 2 * variableLeft + variable) .^ 2 + (1/4) * (3 * variableLeft2 - 4 * variableLeft + variable) .^ 2;

beta1 = (13/12) * (variableLeft - 2 * variable + variableRight) .^ 2 + (1/4) * (3 * variableLeft - variableRight) .^ 2;

betar0 = (13/12) * (variable - 2 * variableRight + variableRight2) .^ 2 + (1/4) * (variable - 4 * variableRight + variableRight2) .^ 2;

beta0 = (13/12) * (variable - 2 * variableRight + variableRight2) .^ 2 + (1/4) * (3 * variable - 4 * variableRight + variableRight2) .^ 2;
beta1 = \( (13/12) \times (\text{variableLeft} - 2 \times \text{variable} + \text{variableRight})^2 + (1/4) \times (\text{variableLeft} - \text{variableRight})^2 \);

beta2 = \( (13/12) \times (\text{variableLeft}^2 - 2 \times \text{variableLeft} + \text{variable})^2 + (1/4) \times (\text{variableLeft}^2 - 4 \times \text{variableLeft} + 3 \times \text{variable})^2 \);

e = 10^{-6};

wl0 = \( \text{gaml0} / (e + \text{beta0})^2 \);
wl1 = \( \text{gaml1} / (e + \text{beta1})^2 \);
wl2 = \( \text{gaml2} / (e + \text{beta2})^2 \);

wnl0 = \( \text{wl0} / (\text{wl0} + \text{wl1} + \text{wl2}) \);
wnl1 = \( \text{wl1} / (\text{wl0} + \text{wl1} + \text{wl2}) \);
wnl2 = \( \text{wl2} / (\text{wl0} + \text{wl1} + \text{wl2}) \);

wr0 = \( \text{gamr0} / (e + \text{beta0})^2 \);
wr1 = \( \text{gamr1} / (e + \text{beta1})^2 \);
wr2 = \( \text{gamr2} / (e + \text{beta2})^2 \);

wnr0 = \( \text{wr0} / (\text{wr0} + \text{wr1} + \text{wr2}) \);
wnr1 = \( \text{wr1} / (\text{wr0} + \text{wr1} + \text{wr2}) \);
wnr2 = \( \text{wr2} / (\text{wr0} + \text{wr1} + \text{wr2}) \);

variableFaceLeftRightInt = \( \text{wnl0} \times \text{pl0} + \text{wnl1} \times \text{pl1} + \text{wnl2} \times \text{pl2} \);
variableFaceRightLeftInt = \( \text{wnr0} \times \text{pr0} + \text{wnr1} \times \text{pr1} + \text{wnr2} \times \text{pr2} \);

variableFaceLeftRight (1, 1: (meshLengthPar+1)) =
variableFaceLeftRightInt (1, 1: (meshLengthPar+1));
variableFaceRightLeft (1,1:(meshLengthPar+1)) =
    variableFaceRightLeftInt (1,1:(meshLengthPar+1));

variableFaceRightRight (1,1:(meshLengthPar+1)) =
    variableFaceLeftRightInt (1,2:meshLengthParMod);

end

function [variableFaceLeftRight, variableFaceRightLeft, variableFaceRightRight, variableDiffFluxLeft, variableDiffFluxRight] = wenok2FacesLITEPARwDiff(variableInput, meshLengthPar, cpm)

meshLengthParMod = meshLengthPar + 2;

variableLeft2 (1,1:(meshLengthParMod)) = variableInput (1,1:
    meshLengthParMod);

variableLeft (1,1:(meshLengthParMod)) = variableInput (1,2:
    (meshLengthParMod+1));

variable (1,1:(meshLengthParMod)) = variableInput (1,3:
    (meshLengthParMod+2));

variableRight (1,1:(meshLengthParMod)) = variableInput (1,4:
    (meshLengthParMod+3));

variableRight2 (1,1:(meshLengthParMod)) = variableInput (1,5:
    (meshLengthParMod+4));

pl0 = (11/6) * variable + (-7/6) * variableRight + (1/3) * variableRight2;

pl1 = (1/3) * variableLeft + (5/6) * variable + (-1/6) * variableRight;

pl2 = (-1/6) * variableLeft2 + (5/6) * variableLeft + (1/3) * variable;

pr0 = (1/3) * variable + (5/6) * variableRight + (-1/6) * variableRight2;
pr1 = (-1/6) * variableLeft + (5/6) * variable + (1/3) * variableRight;

pr2 = (1/3) * variableLeft2 + (-7/6) * variableLeft + (11/6) * variable;

gaml0 = (1/10);
gaml1 = (6/10);
gaml2 = (3/10);

gamr0 = (3/10);
gamr1 = (6/10);
gamr2 = (1/10);

beta0 = (13/12) * (variableLeft2 - 2 * variableLeft + variable) ^ 2 + (1/4) * (3 * variableLeft2 - 4 * variableLeft + variable)^2;

beta1 = (13/12) * (variableLeft - 2 * variable + variableRight) ^ 2 + (1/4) * (3 * variableLeft - variableRight)^2;

beta2 = (13/12) * (variable - 2 * variableRight + variableRight2) ^ 2 + (1/4) * (variable - 4 * variableRight + variableRight2)^2;

beta0 = (13/12) * (variable - 2 * variableRight + variableRight2) ^ 2 + (1/4) * (variable - 4 * variableRight + variableRight2)^2;

beta1 = (13/12) * (variableLeft - 2 * variable + variableRight) ^ 2 + (1/4) * (variableLeft - variableRight)^2;

beta2 = (13/12) * (variableLeft2 - 2 * variableLeft + variable) ^ 2 + (1/4) * (variableLeft2 - 4 * variableLeft + 3 * variable)^2;

e = 10^-6;

wl0 = gaml0 / (e + beta0)^2;
\begin{verbatim}
wl1 = gaml1 / (e + beta1) * 2;
wl2 = gaml2 / (e + beta2) * 2;

wnl0 = wl0 / (wl0 + wl1 + wl2);
wnl1 = wl1 / (wl0 + wl1 + wl2);
wnl2 = wl2 / (wl0 + wl1 + wl2);

wr0 = gamr0 / (e + beta0) * 2;
wr1 = gamr1 / (e + beta1) * 2;
wr2 = gamr2 / (e + beta2) * 2;

wnr0 = wr0 / (wr0 + wr1 + wr2);
wnr1 = wr1 / (wr0 + wr1 + wr2);
wnr2 = wr2 / (wr0 + wr1 + wr2);

variable Face Left Right Int = wnl0 * pl0 + wnl1 * pl1 + wnl2 * pl2;
variable Face Right Left Int = wnr0 * pr0 + wnr1 * pr1 + wnr2 * pr2;

variable Face Left Right (1, 1: (meshLengthPar + 1)) =
    variable Face Left Right Int (1, 1: (meshLengthPar + 1));
variable Face Right Left (1, 1: (meshLengthPar + 1)) =
    variable Face Right Left Int (1, 1: (meshLengthPar + 1));

variable Face Right Right (1, 1: (meshLengthPar + 1)) =
    variable Face Left Right Int (1, 2: meshLengthParMod);

variable Diff Flux Right Int = cpm * (1/2 * variable Left - 15/12 * variable + 15/12 *
    variable Right - 1/12 * variable Right2);
\end{verbatim}
variableDiffFluxLeftInt=cpm*(1/2*variableRight -15/12*variable +15/12*variableLeft -1/12*variableLeft^2);

variableDiffFluxRight (1,1:(meshLengthPar))=variableDiffFluxRightInt (1,2:(meshLengthPar+1));

variableDiffFluxLeft (1,1:(meshLengthPar))=variableDiffFluxLeftInt (1,2:(meshLengthPar+1));

end

Global Lax-Friedrichs function

function [localLFCoeff ] = globalLFREV (variableLeft,variableRight,
                            fovLeft,fovRight)

localLFCoeff=max( sign(abs(variableRight−variableLeft)).*abs((
                            fovRight−fovLeft)).*max(abs(variableRight−variableLeft)).^−1);

end

Solid phase viscosity functions

function [nuaEff] = gidaspowViscREV (alpha , ua , ub , theta , rhoa , rhob ,
                             dPipe , alphaMax , eRest , da , Cmu)

beta=1−alpha;
g0=(1−(alpha./alphaMax).^(.3)).^−1;
nuaTBulk=(4/3)*da*(1+eRest)*alpha.*g0.*( theta/pi ).*(1/2); %Bulk

Turbulent Viscosity
7  nuaDil=(5/96)*da*(pi*theta).^(1/2);
8  nua=2/(1+eRest)*(nuaDil./g0).*(1+4/5*(1+eRest)*g0.*alpha).^2 ...
9  +(4/5)*da*(1+eRest)*g0.*alpha.^2.*(theta/pi).^((1/2));

10  uMean=(alpha.*rhoa.*abs(ua)+beta.*rhob.*abs(ub)).*(alpha*rhoa+beta*rhob).^(-1);

12  kaT=(3/2)*((5/100)*uMean).^2;
13  eaT=kaT.^((3/2)/dPipe);
15  nuaTLS=Cmu*kaT.^2./eaT;
17  nuaEff=4/3*nua+nuaTBulk+nuaTLS;
19  end

1  function [nuaEff] = gidaspowViscREV2(alpha, ua, ub, theta, rhoa, rhob, dPipe, g0, eRest, da, Cmu)
2  beta=1-alpha;
4  %g0=(1-(alpha./alphaMax).^(.3)).^(-1);
5  nuaTBulk=(4/3)*da*(1+eRest)*alpha.*g0.*(theta/pi).^(1/2); %Bulk Turbulent Viscosity
9  nuaDil=(5/96)*da*(pi*theta).^(1/2);
8  nua=2/(1+eRest)*(nuaDil./g0).*(1+4/5*(1+eRest)*g0.*alpha).^2 ...
9  +(4/5)*da*(1+eRest)*g0.*alpha.^2.*(theta/pi).^((1/2));
10  uMean=(alpha.*rhoa.*abs(ua)+beta.*rhob.*abs(ub)).*(alpha*rhoa+beta*rhob).^(-1);
function [nuaEff,eaT] = gidaspowViscREVwE2(alpha, ua, ub, theta, rhoa, rhob, dPipe, g0, eRest, da, Cmu)

beta=1-alpha;
%g0=(1-(alpha./alphaMax).^(.3)).^-1;
nuaTBulk=(4/3)*da*(1+eRest)*alpha.*g0.*(theta/pi).^((1/2)); %Bulk Turbulent Viscosity

nuaDil=(5/96)*da*(pi*theta).^((1/2));
nua=2/(1+eRest)*((nuaDil./g0).*(1+4/5*(1+eRest)*g0.*alpha).^2...
+(4/5)*da*(1+eRest)*g0.*alpha.^2.*(theta/pi).^((1/2));

uMean=(alpha.*rhoa.*abs(ua)+beta.*rhob.*abs(ub)).*(alpha*rhoa+beta*rhob).^^-1;

kaT=(3/2)*((5/100)*uMean).^2;
eaT=kaT.^(3/2)/dPipe;
nuaTLS=Cmu*kaT.^2./eaT;
nuaEff=4/3*nua+nuaTBulk+nuaTLS;
Liquid phase viscosity function

```matlab
function [nubEff] = liquidViscFN(alpha, ua, ub, rhoa, rhob, dPipe,
                                  Cmu, da, uCirculation, nub)

beta=1-alpha;
ur=(uCirculation-ua)./(1-alpha);

uMean=(alpha.*rhoa.*abs(ua)+beta.*rhob.*abs(ub)).*(alpha*rhoa+beta*rhob).^(-1);

kbT=(3/2)*((1/10)*uMean).^2;

ebT=kbT.^((3/2)/dPipe);
nubT=Cmu*kbT.^2./ebT;

rhoMix=alpha*rhoa+beta*rhob;
nubTBulk=(1/2)*da*rhoMix.*abs(ur)/rhob;

nubEff=nubT+nub+nubTBulk;
end
```

Interphase coefficient function

```matlab
function kinterphaseCoeff = gidaspowInterphase(alpha, ur, rhob, nub, da)

beta=1-alpha;
```
\texttt{Constant circulation liquid phase velocity function}

\begin{verbatim}
function [ub] = circcontFN(alpha, ua, uCirculation)
  ur=(uCirculation-ua)/(1-alpha);
  ub=ur+ua;
end
\end{verbatim}

\texttt{Granular pressure gradient function}

\begin{verbatim}
function [granPGrad] = granPGradFN(alphaFaceLeftRight, alphaFaceRightLeft, thetaFaceLeftRight, thetaFaceRightLeft, alphaMax, eRest, rhoa, cpm)
\end{verbatim}
Radial distribution function

function \([g_0]\) = g0FN(alpha, alphaMax)

\[
g_0 = ((\alphaMax / \alpha)^{0.3} - 1)^{-1} - 1 + 1;
\]

end

Reactors gravity piecewise function

function \([nubEff]\) = liquidViscFN(alpha, ua, ub, rhoa, rhob, dPipe, 
                           Cmu, da, uCirculation, nub)

beta = 1 - alpha;

ur = (uCirculation - ua) / (1 - alpha);

uMean = (alpha * rhoa * abs(ua) + beta * rhob * abs(ub)) * (alpha * rhoa + beta * rhob)^(-1);
\[ kbT = \left( \frac{3}{2} \right) \times \left( \frac{1}{10} \right) \times \text{uMean} \times 2; \]
\[ ebT = kbT \times \left( \frac{3}{2} \right) / \text{dPipe}; \]
\[ nubT = Cmu \times kbT \times 2 / ebT; \]
\[ nubMix = alpha \times \rhoa + beta \times \rhob; \]
\[ nubTBulk = \left( \frac{1}{2} \right) \times da \times \rhoMix \times abs(\text{ur}) / \rhob; \]
\[ nubEff = nubT + nub + nubTBulk; \]

Positive and negative functions

function [output] = negativeFN (input)
output = sign(abs(sign(input)) \times (1 - sign(input)));
end

function [output] = positiveFN (input)
output = sign(abs(sign(input)) \times (1 + sign(input))));
end

Parallel reconstruction function

function [ALPHAMAT, UAMAT, THETAMAT, PRESSUREMAT] = reconstructParNextFN(
ALPHAMAT, UAMAT, THETAMAT, PRESSUREMAT, ...
alphaStor, uaStor,thetaStor, pStor, ...
tMax, ts, parMax, graphHarvest, meshLengthPar)
for parreconc=1:parMax
    alphaParInt1=alphaStor(1, parreconc);
    alphaParInt2=alphaParInt1{1,1};

    uaParInt1=uaStor(1, parreconc);
    uaParInt2=uaParInt1{1,1};

    thetaParInt1=thetaStor(1, parreconc);
    thetaParInt2=thetaParInt1{1,1};

    for treoncc=1:size(ALPHAMAT,1)
        alphaParInt3=alphaParInt2{treoncc, parreconc};
        uaParInt3=uaParInt2{treoncc, parreconc};
        thetaParInt3=thetaParInt2{treoncc, parreconc};
        ALPHAMAT(treoncc,((parreconc-1)*meshLengthPar+1):((parreconc)*meshLengthPar))=...
            alphaParInt3;
        UAMAT(treoncc,((parreconc-1)*meshLengthPar+1):((parreconc)*
            meshLengthPar))=...
            uaParInt3;
        THETAMAT(treoncc,((parreconc-1)*meshLengthPar+1):((parreconc)*meshLengthPar))=...
            thetaParInt3;
    end
end

pParInt1=pStor(1,1);
pParInt2=pParInt1{1,1};
for treoncc = 1: (size(ALPHAMAT, 1))
    pParInt3 = pParInt2{treoncc, 1};
    PRESSUREMAT(treoncc, 1: (meshLengthPar+1)) = pParInt3;
end

for parreconc = 2: parMax
    pParInt1 = pStor(1, parreconc);
    pParInt2 = pParInt1{1, 1};
    for treoncc = 1: (size(ALPHAMAT, 1))
        pParInt3 = pParInt2{treoncc, parreconc};
        PRESSUREMAT(treoncc, ((parreconc - 1) * meshLengthPar + 2): ((parreconc) * meshLengthPar + 1)) = ...
        PRESSUREMAT(treoncc, (parreconc - 1) * meshLengthPar) +
        pParInt3(2: (meshLengthPar + 1));
    end
end