Excitation temperature and electron number density distributions experienced by analyte species in an inductively coupled argon plasma

Dennis James Kalnicky
Iowa State University

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Excitation temperature and electron number density distributions experienced by analyte species in an inductively coupled argon plasma

by

Dennis James Kalnicky

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CHAPTER I: INTRODUCTION

Inductively coupled, argon-supported plasmas (ICP's) possess properties that make them useful atomization-ionization-excitation sources for analytical atomic emission spectroscopy (1). Among the several fundamental ICP properties that have not been adequately characterized are the excitation temperature distributions and the electron number densities (hereafter denoted by $n_e$) that are experienced by the analyte species and the argon support gas. Most measurements reported to date have primarily characterized the temperature and $n_e$ environment of the support gas in plasmas that have not been extensively used for analytical purposes (2-14). Recently, several experimental studies of the excitation temperature and $n_e$ distributions experienced by analyte species have been reported (15-20) and theoretical treatments of these and other relevant ICP properties have been discussed (21-23). Despite these efforts significant discrepancies and inconsistencies still exist among the reported results. The following typical examples may be cited. First, effective (spatially integrated) temperatures and number densities were reported by Boumans and de Boer (19) who concluded that their data could not be used for explaining interelement effects because it was useless to "speculate on what precisely happens without detailed knowledge of the complex changes in the spatial structure of
the ICP." Second, some preliminary radial (spatially resolved) temperatures reported by Kornblum and de Galan (16) exhibited large scatter and peculiarly steep off-axis peak behavior. Third, the $n_e$ values determined by Jaroz et al. (2b) and Mermet (17a) from Stark broadening measurements were two orders of magnitude greater than those obtained from Saha ionization equilibrium calculations based on Mg atom/ion emission line intensity ratios. Fourth, Kalnicky et al. (18) recently reported spatially resolved, radial excitation temperatures experienced by the Fe I thermometric species that were essentially in agreement with the values reported by Mermet and Robin (2a) and Alder and Mermet (15) and with the Doppler temperatures reported by Human and Scott (20) but disagreed significantly with excitation temperatures reported by Kornblum and de Galan (16), who cautioned that "only the overall shapes of the distributions and the order of magnitude of the quantities" could be concluded from their data. Fifth, recognized differences still exist between computer simulation and experimental studies of ICP's used for spectrochemical analysis (21,22). Finally, even the temperature measurements themselves are rendered inconsistent by the lack of accuracy and agreement in published transition probability data (15,17,18).

The large discrepancies between the $n_e$ values calculated by line broadening methods and those obtained from Saha
ionization calculations, which were reported by Jaroz et al. (2b) and Mermet (17a) led these investigators to question the validity of the local thermodynamic equilibrium (LTE) assumption for the operating conditions of their plasma. Clearly, more investigations on temperature and $n_e$ distributions are required to interpret discrepancies in reported values and to lead to a more definitive understanding of the atomization, ionization, and excitation processes occurring in analytically useful ICP's. The purpose of this investigation is, therefore, to examine the spatially resolved, radial excitation temperatures and radial $n_e$ distributions experienced by the analyte species. These examinations include observations at several sites in the plasma and, with and without the presence of an easily ionized element (EIE).
CHAPTER II. DIAGNOSTIC TECHNIQUES

LTE in Analytical Inductively Coupled Plasmas

In a rigorous sense, temperature is a physically meaningful concept only when a system is in complete thermodynamic equilibrium (TE). In such a system a unique value of temperature describes: (1) a Maxwellian velocity distribution for all particles; (2) excitation according to Boltzmann's distribution law; (3) ionization according to the Saha-Eggert relationship; (4) dissociation-recombination according to the Guldberg-Waage mass action law; and (5) the distribution of the electromagnetic radiation according to Planck's law (24-31). However, the strong temperature and density gradients which exist in almost all laboratory plasmas prevent the establishment of TE and it follows that the radiation collected from these plasmas strongly deviates from the Planck function distribution (29). Despite these deviations from TE, conditions may exist for which the useful concept of local thermodynamic equilibrium can be employed in these plasmas. The latter applies when radiation equilibrium is not established but all other TE relationships remain valid and are governed by the "local temperature" even though different temperatures are allowed at different points in the plasma. The LTE state is reached when the local rate of equipartition of energy over the different degrees of freedom
is much faster than the net rate of transport of heat, mass, and radiation through the plasma.

When the various degrees of freedom are not equilibrated it is useful to designate "temperatures" which are named after the special process to which they apply, e.g., translation temperature, excitation temperature, etc. The better the agreement between these temperatures, the closer the approach to equilibrium, and the more physically meaningful the temperature concept. The conditions necessary to assure the validity of the LTE assumption for common laboratory plasmas have been discussed in detail elsewhere (29,31) and will not be reiterated here. Likewise, many excellent theoretical treatments related to plasma diagnostics are available (3,11,24,29,32-48). Therefore, the following discussions will be limited to those techniques relevant to temperature and \( n_e \) measurements.

Spectroscopic methods of temperature measurement are generally considered superior to probe techniques because the former do not disturb the microscopic system and, in fact, may be the only feasible approach for high temperature sources or for those sources which are inaccessible to probes (3b,47,48).

The LTE state is generally assumed to exist in the central portions of argon-supported, inductively coupled plasmas sustained at atmospheric pressure (18). If this
assumption is accepted, spectroscopic techniques may be combined with the Boltzmann energy distribution and the Saha-Eggert ionization equilibrium relationships to yield temperature and $n_e$ distributions. The limitations and physical significance of the temperature values so obtained have been adequately reviewed (30,36,40). In particular, caution must be exercised in interpreting the physical significance of the temperatures and $n_e$ values determined unless appropriate mathematical treatments, such as Abel inversion techniques (49-58), are used to transform the experimentally measured lateral (average) distributions of spectral line radiances to their corresponding spatially resolved radial (local) distributions. The requirements of the Abel inversion techniques employed in this investigation are discussed in a later section of this Chapter.

The observations of Jaroz et al. (2b) and Mermet (17) and the results of this investigation suggest that the LTE assumption may be invalid for some operating conditions employed in the spectrochemical applications of these plasmas. Indeed, the assumption of LTE has been questioned for other plasmas as well (45,59-63).

Temperature Calculations, Thermometric Species, and Transition Probabilities

The relative lateral intensity of an emission line radiating from a source in LTE with negligible self-absorption
and homogeneous analyte distribution is given by (29,30,40)

\[ I_{qp}(X) = \frac{d}{4\pi} A_{qp} h \nu_{qp} n_q(X) \]  

(1)

where,  
- \( d \) = optical depth of the plasma within the viewing field of the spectrometer,
- \( A_{qp} \) = relative transition probability of spontaneous emission for the transition \( q \rightarrow p \),
- \( h \) = Planck's constant,
- \( \nu_{qp} \) = frequency of the emission transition,
- \( n_q(X) \) = number density of the emitting level at lateral displacement \( X \).

This equation describes the space-integrated (averaged) emission over the depth of the plasma and, accordingly, represents the power radiated per unit solid angle per unit area, which is collected within the viewing field of the spectrometer (29,40). Equation 1 may be combined with the Boltzmann expression for \( n_q \) to yield

\[ I_{qp}(X) = \frac{d}{4\pi} A_{qp} h \nu_{qp} g_q \frac{g_q}{E_o} n_o(X) \exp \left\{ -\frac{E_q}{kT(X)} \right\} \]  

(2)

where,  
- \( g_q, g_o \) = statistical weights of the emitting and ground level, respectively,
- \( n_o(X) \) = number density of the ground level at lateral displacement \( X \),
- \( E_q \) = energy of the emitting level,
k = Boltzmann's constant,  
\[ T(X) = \text{temperature at lateral displacement } X. \]

The desired relative radial (local) intensities \( J_{qp} \) are obtained from Abel inversion of the measured lateral (averaged) intensity profiles and represent spatially resolved, per-unit-volume quantities.

With consideration of radial quantities and by rearrangement of Equation 2, the radial "slope" temperature is given by (29,33,36,40)

\[
\ln \left( \frac{g^A_{q} J_{qp} v_{qp}}{J_{qp}(R)} \right) = \frac{E_q}{kT(R)} + \ln \left( \frac{4\pi g_o}{h n_o(R)} \right)
\]

(3)

where \( R \) denotes the radial position in the plasma. For emission lines originating from the same ionization stage a plot of \( \ln \left( \frac{E^A_{q+p}}{J_{qp}} \right) \) vs. \( E_q \) should yield a straight line with slope equal to \( 1/kT(R) \) where, \( T(R) \) is the "slope" temperature at radius \( R \). Equation (3) may be solved simultaneously for two spectral emission lines \( (q+p \text{ and } t+s) \) to yield the radial "two-line" temperature defined by the following expression:

\[
T(R) = 0.6247(E_q - E_t) \sqrt{\log_{10} \left( \frac{g^A_{q} v_{qp} J_{ts}(R)}{g^A_{t} v_{ts} J_{qp}(R)} \right)}
\]

(4)

when \( E_q \) and \( E_t \) are expressed in reciprocal centimeters (cm\(^{-1}\)).
Certain conditions must be satisfied before Equations 3 and 4 may be used for temperature determinations, namely, relative radial emission intensities must be directly proportional to integrated line radiances and they must not be affected by self-absorption (30). The importance of employing quantities strictly proportional to integrated line radiances for calculations based on spectroscopic measurements where slit effects are important has been extensively treated for molecular (64) as well as atomic lines (24,30,65), therefore, only a brief summary will be presented here.

When emission from a spectral transition is monitored by a spectrometer, the true profile is distorted by the instrument with the distortion being proportional to the reciprocal of the resolving power of the monochromator. These distortions are of electrical and optical origin and it is convenient to treat them separately. Accurate intensities can be obtained only if instrumental distortions are properly accounted in the measurement. When a spectrometer is set at a single value, a discrete wavelength is not transmitted but, rather, a range of wavelengths are collected each of which contributes to the recorded line profile. This wavelength interval is referred to as the bandpass of the instrument. The weight of each contribution can be expressed as a function of displacement from the line center and determines a curve called the slit function. Accurate intensity measurements are made only when the bandpass of the instrument is
negligible in comparison to the halfwidth of the line intensity profile. The exit slit distribution is predominantly determined by diffraction effects for slits narrow in comparison to the wavelength of the impinging radiation. When the slits are sufficiently wide, the contributions to the geometrical image from diffraction and optical distortions are rendered negligible. Thus, if the width of the exit slit is much wider than the entrance slit, the geometrical image of the latter falls entirely within the band pass of the spectrometer and the measured intensity is proportional to integrated line radiance (30). A trapezoidal line shape should be obtained. Aberration and diffraction effects tend to round off the top and base of the profile.

The lateral emission intensities obtained here were measured with the entrance and exit slits of the monochromator set at the same width (15 \( \mu \)m). Time integrated intensities were obtained at the maximum of the respective emission line profiles when the monochromator was "peaked" on a line. Under these conditions, the measurements did not represent the integrated area (radiance) under the line profiles. However, the peak intensities for Fe I thermometric lines were proportional to integrated radiances when the latter were obtained with the exit slit much wider than the entrance slit (30). Consequently, peak intensities were employed in this study because: (1) these intensities were
proportional to integrated line radiances, (2) the resolution of the monochromator deteriorated rapidly as the exit slit was opened wider than the entrance slit, and (3) more elaborate measurement procedures were required to obtain the integrated radiances.

Neutral iron was selected as the thermometric species because its emission lines possess desirable characteristics for spectroscopic temperature determinations (30,110). Among the factors considered in the line selection process were: (a) maximal spread in excitation potentials to minimize relative error in calculated temperatures, (b) freedom of spectral interference from plasma components, (c) availability of accurate transition probabilities, and (d) wavelength proximity precluding the necessity of calibrating the detector response with respect to wavelength. So that the measurements and Abel inversion operations would not be too unwieldy, the number of lines initially employed was restricted to four.

A number of Fe I transition probability tabulations were examined for these lines (30,66-73a); of the most recent compilations, only the Reif (30), and the Banfield and Huber (66) collections provided transition probability data on all of the four lines, and Huber and Parkinson (67) on only two of the lines. These lines, their wavelengths, excitation energies and the statistical weights of the emitting levels (74), and relevant transition probability
data are summarized in Table I. The relative transition probabilities for the useful sets of data were normalized to the Fe I 371.994 nm line because the lifetime of this transition is well known \((66,67)\). It is evident that there is good agreement among the Fe 382.043, 382.444, and 382.588 nm lines for the Reif and Banfield and Huber data. Thus, a priori, good agreement in the temperature profiles should be obtained for calculations based on these lines, but a lack of consistency should be evident if the Fe 381.584 line were included. Indeed, temperatures obtained with various combinations of transition probabilities involving the Fe I 381.584 nm line showed this lack of consistency particularly for those calculated from two-line combinations \((18)\).

Because virtually identical temperature profiles resulted from three-line slope temperature calculations \((18)\) for transition probability data from references 30 and 66, the three-line set excluding the Fe I 381.584 nm line was considered acceptable for inclusion in studies for this dissertation research.

\[^{1}\text{After this dissertation research was completed an additional transition probability tabulation (73b) was found which provided data on three of the four lines in Table I. Consideration of these values revealed good agreement with the Fe I 382.043 nm and 382.588 nm line data but not for the 381.584 nm line. Inclusion of these data would neither change the conclusions drawn about these lines nor affect the temperature results obtained with the lines employed from this table.}\]
Table I. Fe I emission line data (four-line set)

<table>
<thead>
<tr>
<th>( \lambda (\text{nm}) )^a</th>
<th>( E_q (\text{cm}^{-1}) )^b</th>
<th>( g_q )^c</th>
<th>Relative Transition Probabilities(^d)</th>
<th>R</th>
<th>BH</th>
<th>HP</th>
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<td>38175</td>
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<td>382.043</td>
<td>33096</td>
<td>9</td>
<td>0.638</td>
<td>0.656</td>
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<tr>
<td>382.444</td>
<td>26140</td>
<td>7</td>
<td>0.0283</td>
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<tr>
<td>382.588</td>
<td>33507</td>
<td>7</td>
<td>0.567</td>
<td>0.610</td>
<td>---</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\lambda = \text{wavelength of the transition } q \rightarrow p, \text{ and for subsequent tables.}\)

\(^bE_q = \text{excitation energy of the emitting level, and for subsequent tables.}\)

\(^c g_q = \text{statistical weight of the emitting level, and for subsequent tables.}\)

\(^d\text{Relative transition probabilities normalized to the Fe I } 371.994 \text{ nm line by } A_{371.994} = 0.163:\ R = \text{Reif (30); BH = Banfield and Huber (66); HP = Huber and Parkinson (67).}\)
An additional Fe I ten-line set was selected for temperature measurements; the relevant data for these lines are summarized in Table II.\(^1\) In selecting these lines, the criteria discussed previously as well as consistency among the transition probability data were emphasized. An Ar I eight-line set was also selected for determination of the excitation temperature environment experienced by the support gas. The relevant data for these lines are given in Table III (74-80).

The operation of the temperature and Abel inversion computer program for slope temperature calculations employed in this dissertation research is discussed in Appendix A. A listing of the source statements of this program is also included in this appendix.

Abel Inversion Calculations and Source Symmetry

Excellent discussions of the basic principles of the Abel inversion calculation and the various methods of solution are found in references 49 and 50. Preliminary

\(^1\)The Bridges and Kornblith tabulation (73b) also provided transition probability data on these lines which were in excellent agreement with the values listed in Table II. As before, inclusion of these data would neither significantly change the conclusions drawn about these lines nor the temperatures obtained with them.
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<thead>
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<th>(\lambda) (nm)</th>
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<th>(g_q)</th>
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<td>26875</td>
<td>11</td>
<td>0.163</td>
<td>0.163</td>
<td>0.163</td>
</tr>
<tr>
<td>372.256</td>
<td>27560</td>
<td>5</td>
<td>0.0505</td>
<td>0.0531</td>
<td>0.0580</td>
</tr>
<tr>
<td>373.487</td>
<td>33695</td>
<td>11</td>
<td>0.886</td>
<td>0.776</td>
<td>0.867</td>
</tr>
<tr>
<td>373.713</td>
<td>27167</td>
<td>9</td>
<td>0.143</td>
<td>0.140</td>
<td>0.143</td>
</tr>
<tr>
<td>374.826</td>
<td>27560</td>
<td>5</td>
<td>0.0904</td>
<td>0.0870</td>
<td>0.0994</td>
</tr>
<tr>
<td>374.949</td>
<td>34040</td>
<td>9</td>
<td>0.744</td>
<td>0.681</td>
<td>0.798</td>
</tr>
<tr>
<td>375.824</td>
<td>34329</td>
<td>7</td>
<td>0.611</td>
<td>0.611</td>
<td>0.674</td>
</tr>
<tr>
<td>376.379</td>
<td>34547</td>
<td>5</td>
<td>0.523</td>
<td>0.610</td>
<td>0.622</td>
</tr>
</tbody>
</table>
Table III. Ar I emission line data

<table>
<thead>
<tr>
<th>λ(nm)</th>
<th>$E_q$(cm$^{-1}$)</th>
<th>$E_q$</th>
<th>$A_{qp} \times 10^{-7}$ (sec$^{-1}$)</th>
<th>AP</th>
<th>MC</th>
<th>CS</th>
<th>BTW</th>
<th>G</th>
<th>BW</th>
</tr>
</thead>
<tbody>
<tr>
<td>425.118</td>
<td>116,660</td>
<td>3</td>
<td>0.0085</td>
<td>0.0089</td>
<td>0.0132</td>
<td>0.0075</td>
<td>0.0079</td>
<td>0.0076</td>
<td></td>
</tr>
<tr>
<td>425.936</td>
<td>118,871</td>
<td>1</td>
<td>0.360</td>
<td>0.3665</td>
<td>0.450</td>
<td>0.3643</td>
<td>0.360</td>
<td>0.320</td>
<td></td>
</tr>
<tr>
<td>426.629</td>
<td>117,184</td>
<td>5</td>
<td>0.028</td>
<td>0.0265</td>
<td>0.036</td>
<td>0.0294</td>
<td>0.028</td>
<td>0.023</td>
<td></td>
</tr>
<tr>
<td>427.217</td>
<td>117,151</td>
<td>3</td>
<td>0.071</td>
<td>0.0688</td>
<td>0.090</td>
<td>0.0769</td>
<td>0.071</td>
<td>0.063</td>
<td></td>
</tr>
<tr>
<td>430.010</td>
<td>116,999</td>
<td>5</td>
<td>0.034</td>
<td>0.0318</td>
<td>0.042</td>
<td>0.0366</td>
<td>0.034</td>
<td>0.031</td>
<td></td>
</tr>
<tr>
<td>433.356</td>
<td>118,469</td>
<td>5</td>
<td>0.049</td>
<td>0.0506</td>
<td>0.074</td>
<td>0.0551</td>
<td>0.049</td>
<td>0.048</td>
<td></td>
</tr>
<tr>
<td>433.535</td>
<td>118,459</td>
<td>3</td>
<td>0.0333</td>
<td>0.0308</td>
<td>0.044</td>
<td>0.0385</td>
<td>0.040</td>
<td>0.029</td>
<td></td>
</tr>
<tr>
<td>434.545</td>
<td>118,408</td>
<td>3</td>
<td>0.028</td>
<td>0.0273</td>
<td>0.041</td>
<td>0.0273</td>
<td>0.028</td>
<td>0.022</td>
<td></td>
</tr>
</tbody>
</table>

$^a$Absolute transition probabilities: AP = Adcock and Plume (75); MC = Malone and Corcoran (76); CS = Corliss and Shumaker (77); BTW = B. T. Wujec (78); G = Gericke (79); BW = B. Wende (80).
calculations indicated that the Cremers and Birkebak data approximation method (50) was superior to the numerical method of Nestor and Olsen (49). The Cremers and Birkebak method provided: (a) better agreement of calculated radial coefficients with known values ($\pm 1-2\%$) when integrable test functions were employed (53) and, (b) less scatter in calculated radial intensities when real data were employed. The computational procedures and error analyses for these methods are discussed in Appendix B. An F-test for best fit (81) from the linear to the maximum allowed 4-th degree fit and polynomials of the type of Equations B20 and B36 in Appendix B were applied to smoothed lateral intensity profiles when the Cremers and Birkebak method was employed. Second degree polynomials with $\sim 20$ points per profile were generally found to provide adequate fits for bell-type lateral profiles but higher degree fits were required for toroidal distributions.

The optical system employed and the emission symmetry of the radiating source must meet several requirements if lateral emission profiles are to be reliably transformed by Abel inversion techniques. Figure B-1 (Appendix B) illustrates the spatial relationship between the measured lateral intensity, $I(X)$, at displacement $X$; and, the radial intensity, $J(R)$, at radius $R$ from the center of a circularly symmetric source when normal side-on observation is employed. Examination of
this diagram reveals that the following conditions are necessary prerequisites for reliable radial intensity calculations:

1) The depth-of-field (DOF) of the optical transfer system (OTS) must extend beyond the source boundaries.

2) The analyte emission intensity distribution must be circularly symmetric about the plasma axis.

In addition to these requirements, the plasma source must be optically thin, i.e., there must be negligible self-absorption of the emission lines of interest.

For the ideal case the OTS would have infinite DOF so that all emission points within the source volume along the optical axis would be transferred with exactly the same efficiency. However, the DOF of any real OTS is not infinite so that defocussing along the optical axis is an important consideration (82) when relative intensity measurements are made. For radial intensity calculations a DOF extending beyond the plasma boundaries is sufficient. This is accomplished with a low aperture optical system (f/40 to f/50) in which the lens and monochromator entrance slit are stopped to a diameter so that the plasma volume observed is essentially cylindrical. When the latter condition prevails the observed solid angle is chosen so that any two lines \( Y_1 = X \) and \( Y_2 = X + AX \) (Figure B-1) defining the lateral
sampling zone for an I(X) value can be considered parallel. For the wavelength range employed in the present investigation, the focal length of the lens was about 150 mm so that a 3 mm diaphragm produced an approximate f/50 system. Hence, at a plasma radius of 10 mm, the f/50 system sampled radiation over a cross section of 0.2 mm diameter. With the above conditions the DOF extended beyond the plasma boundaries and, defocussing problems were minimized. The large aperture optical systems normally employed in analytical investigations cannot be used if precise lateral intensities are to be measured. The enlarged acceptance cone of such systems introduces defocussing problems into lateral intensity measurements, leading to distorted lateral intensity profiles, and, subsequently, erroneous radial intensity and temperature distributions.

The second condition necessary for reliable radial intensity determination was verified when profiles across the entire emission zone showed circular symmetry about the plasma axis. Experimental verification of this symmetry criterion is presented later in the RESULTS section (Chapter V) of this thesis. The requirement of negligible self-absorption was verified for the analyte thermometric lines of interest when plots of log I(X) vs. log C showed linearity over several orders of magnitude in concentration.
Electron Number Density Measurements

Saha-Eggert's ionization equilibria methods

The theory and application of $n_e$ determinations from Saha-Eggert ionization equilibrium calculations has been discussed elsewhere (29,36,40,83). This method requires the measurement of relative emission line intensities from successive ionization stages, generally for the neutral atom and singly ionized species. When these intensities are combined with the known equilibrium relationships between spectral emission and temperature and with the Saha-Eggert's expression, the $n_e$ may be calculated. The $n_e$ values so obtained are dependent upon the assumption that the plasma is in the LTE state, which may not be the case.

Five elements with neutral atom ionization potentials ranging from 6.11 eV (Ca I) to 9.39 eV (Zn I) were selected for atom/ion emission line intensity measurements. The factors considered in the selection process were: (a) availability of sufficiently intense atom/ion line pairs; (b) availability of transition probability data for the atom and ion lines; (c) closely matched excitation energies for the atom and ion lines so that the exponential temperature effect would be minimized; (d) freedom from spectral interferences; and (e) wavelength proximity precluding the necessity of calibrating the detector response with respect to wavelength. The line wavelengths, their excitation
energies, statistical weights of emitting levels (74,84) and transition probability data (66,85-92) for the species selected are given in Table IV. The last column of this table gives the averages and ± limits of the $g\lambda$ ratios listed. The relative ± limits range from about ±2% for Ca to ±12% for Cd.

For the emission lines of the neutral atom and first ionized species the radial $n_e$ is given by (29,36,40)

$$n_e(R) = 4.83 \times 10^{15} \frac{J^O(R)}{J^+(R)} \frac{g^+A^+\lambda^O}{g^O A^O \lambda^+} T(R)^{3/2}$$

where, (O), (+) denote the neutral atom and singly ionized species, respectively,

\begin{align*}
\lambda &= \text{wavelength of the emission transition,} \\
E_1^O &= \text{ionization energy of the neutral atom species,} \\
\Delta E_1^O &= \text{lowering of the ionization energy.}
\end{align*}

A $\Delta E_1^O$ correction was applied to the ionization energy to account for the interaction of free atom states with the electric microfield, which is produced by the charged plasma particles (31,36). A number of methods for calculating $\Delta E_1^O$ have been reported (31,36,59). When the Unsöld formula (31) was applied, a value of $\Delta E_1^O = 403 \text{ cm}^{-1} (0.05 \text{ eV})$ was found.
Table IV. Emission line data for Saha-Eggert's electron number density calculations

<table>
<thead>
<tr>
<th>Species</th>
<th>λ (nm)</th>
<th>E&lt;sub&gt;q&lt;/sub&gt; (cm&lt;sup&gt;-1&lt;/sup&gt;)</th>
<th>g&lt;sub&gt;q&lt;/sub&gt;</th>
<th>( \frac{g^o A^o \lambda^+}{g^+ A^+ \lambda^0} ) Ratios&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Average Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca I</td>
<td>422.673</td>
<td>23652</td>
<td>3</td>
<td>2.173 (SL), 2.0488 (SG), 2.1029 (NBS)&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2.0911 ± 0.0379</td>
</tr>
<tr>
<td>Ca II</td>
<td>396.847</td>
<td>25192</td>
<td>2</td>
<td>2.173 (SL), 2.0488 (SG), 2.1029 (NBS)&lt;sup&gt;b&lt;/sup&gt;</td>
<td>1.4066 ± 0.0773</td>
</tr>
<tr>
<td>Mg I</td>
<td>285.213</td>
<td>35087</td>
<td>3</td>
<td>1.431 (SL), 1.504 (ADJS), 1.333 (SG), 1.3578 (NBS)</td>
<td>2.8708 (SL), 3.0161 (ADJS), 2.6649 (SG), 2.8273 ± 0.154</td>
</tr>
<tr>
<td>Mg II</td>
<td>279.583</td>
<td>35732</td>
<td>4</td>
<td>2.6575 (AS 2), 3.3949 (BS)</td>
<td>2.7747 ± 0.254</td>
</tr>
<tr>
<td>Mg II</td>
<td>280.270</td>
<td>35652</td>
<td>2</td>
<td>3.0290 (AS 2), 2.5203 (BS)</td>
<td>3.1502 ± 0.270</td>
</tr>
<tr>
<td>Fe I</td>
<td>252.285</td>
<td>39626</td>
<td>9</td>
<td>3.4050 (AS 1), 2.8658 (BH/H)</td>
<td>3.1502 ± 0.270</td>
</tr>
<tr>
<td>Fe II</td>
<td>258.588</td>
<td>38660</td>
<td>8</td>
<td>3.4050 (AS 1), 2.8658 (BH/H)</td>
<td>3.0262 ± 0.369</td>
</tr>
<tr>
<td>Cd I</td>
<td>228.802</td>
<td>43692</td>
<td>3</td>
<td>2.6575 (AS 2), 3.3949 (BS)</td>
<td>3.0262 ± 0.369</td>
</tr>
<tr>
<td>Cd II</td>
<td>226.502</td>
<td>44136</td>
<td>2</td>
<td>2.6575 (AS 2), 3.3949 (BS)</td>
<td>3.0262 ± 0.369</td>
</tr>
<tr>
<td>Zn I</td>
<td>213.86</td>
<td>46745</td>
<td>3</td>
<td>3.0290 (AS 2), 2.5203 (BS)</td>
<td>2.7747 ± 0.254</td>
</tr>
<tr>
<td>Zn II</td>
<td>206.19</td>
<td>48481</td>
<td>2</td>
<td>3.0290 (AS 2), 2.5203 (BS)</td>
<td>2.7747 ± 0.254</td>
</tr>
</tbody>
</table>

<sup>a</sup>Numerals I, II and superscripts (°), (+) denote neutral atom and first ion species, respectively.

<sup>b</sup>Transition probability sources: ADJS = Andersen, et al. (85); AS 1 = Assousa and Smith (86); AS 2 = Andersen and Sorensen (87); BH/H = Banfield and Huber (66) and Huber (88); BS = Bauman and Smith (89); NBS = National Bureau of Standards (90); SG = Smith and Gallagher (91); SL = Smith and Liszt (92).
to be compatible with the temperatures and densities considered in this study.

The ratio of the ion number density to that of the neutral atoms is given by (40)

\[
\frac{n_{A^+}(R)}{n_{A^0}(R)} = \frac{j^+(R)}{j^0(R)} g_0^{A^0} \lambda^+ \cdot \frac{Z^+[T(R)]}{Z^0[T(R)]} \cdot \exp \left( \frac{E^+ - E^0}{kT(R)} \right)
\]  

where, \( Z[T(R)] \) is the partition function for the radial temperature \( T(R) \). Partition functions for neutral atom and singly ionized species were calculated from the method suggested by Griem (36), which included a correction for the lowering of the ionization energy. The details of the partition function calculations and the Saha \( n_e \) computer program employed in this investigation are discussed in Appendix C.

**Stark broadening methods**

The theory and application of Stark broadening methods for the determination of \( n_e \) in plasmas has been discussed extensively (36,93-98). Atomic hydrogen lines are most frequently employed for these calculations because of the availability of extensive tabulations of Stark broadening parameters for the complete line profiles (36,96,98) and because the theory is somewhat simpler to apply and more accurate than that for multielectron atomic species. Griem (36,96) has also tabulated Stark broadening parameters for
the emission lines of a number of other neutral atom and singly ionized species.

\[ H_\beta \text{ line} \]

The \( H_\beta \) line (486.13 nm) was selected for \( n_e \) calculations because: (a) it is free from spectral interference by plasma components; (b) the range of half-widths anticipated (\( \sim 1.0 \) to 5.0 Å) and the relative intensities observed were of sufficient magnitude to allow accurate measurement at various observation heights in the plasma; (c) extensive Stark data were available for the complete line profile (96,98) encompassing a broad range of \( n_e \) values and temperatures; and (d) greater accuracy is generally associated with Stark calculations for the \( H_\beta \) line than for other atomic hydrogen lines. The theory developed by Griem (36), Kepple and Griem (95) and Griem (96) and the tabulated Stark parameters from Videl et al. (98) were employed in these calculations.

The Stark width for the \( H_\beta \) line is related to \( n_e \) by (94-96,98)

\[
n_e(R) = \left( \frac{\Delta \lambda^S_{1/2}(R)}{2 \alpha_{1/2}(2.61 e)} \right)^{3/2}
\]

where \( \Delta \lambda^S_{1/2}(R) \) = Stark half-width at radius \( R \),

\( \alpha_{1/2} \) = reduced Stark profile half-width parameter,

\( e \) = electrostatic unit of charge.

Equation 7 cannot be used directly unless experimental line
profiles have been deconvoluted to account for Doppler and instrument broadening. This correction, on a half-width basis, is not a straightforward procedure. A simpler alternative is to use pure Stark reduced profiles, $S(\alpha)$, at various $n_e$ and temperature combinations (98) as base values and then apply convolution calculations to account for other broadening contributions. These calculations were accomplished as follows: (a) Doppler profiles were convoluted with the $S(\alpha)$ profiles (98) to yield Doppler corrected profiles, $S^D(\alpha)$ and (b) the instrument profile was measured (99) and then convoluted with the $S^D(\alpha)$ profiles to yield the desired instrument and Doppler corrected Stark profiles, $S(\alpha^*)$. This convolution procedure yielded a set of reduced half-widths, $\alpha^*_\frac{2}{3}$, which could be compared directly with experimentally observed $H_\beta$ half-widths, $\Delta \lambda^O_\frac{2}{3}(R)$. When these quantities were substituted for $\Delta \lambda^S_\frac{2}{3}(R)$ and $\alpha^*_\frac{2}{3}$ in Equation 7 and the constants were evaluated, the radial $n_e$ was given by

$$n_e(R) = 7.9658 \times 10^{12} \left( \frac{\Delta \lambda^O_\frac{2}{3}(R)}{\alpha^*_\frac{2}{3}} \right)^{3/2}$$  \hspace{1cm} (8)$$

A discussion of the details and accuracy of the convolution procedure and of the $H_\beta$ $n_e$ computer program employed in this study is given in Appendix D.

**Ar I lines** The Ar I 542.135 and 549.588 nm lines were also employed for effective $n_e$ determinations; the Stark parameters given by Griem (36,96) were used in these
calculations. The parameters for $n_e$ values and temperatures not listed were obtained by using the scaling procedure indicated in the description of these parameters (36,96).

For neutral atom emitters the Stark half-widths are given approximately by (36,96)

$$\Delta \lambda_k^S \approx 2w[1 + 1.75 A (1 - 0.75 R')]$$

where $w =$ electron impact width, proportional to $n_e$, $A =$ ion broadening parameter, proportional to $(n_e)^{1/2}$, $R' =$ ratio of the mean distance between ions, $r_1$, to the Debye radius $\rho_D$.

The $R'$ term in Equation 9, which is a measure of ion-ion correlations and Debye shielding, is given by (36,96)

$$R' = \frac{r_1}{\rho_D} = 1.82 \left(\frac{\pi^{1/6} \frac{e}{(kT)^{1/2}}}{n_e^{1/6}}\right)$$

where, $k$ is the Boltzmann constant and other symbols have their usual meaning. Values of $w$ and $A$ are tabulated for Ar I lines by Griem (36,96) for $n_e = 10^{16}$ cm$^{-3}$ and temperatures of 2,500; 5,000; 10,000; 20,000; and 40,000 K. Stark half-widths were calculated from the $w$ and $A$ parameters given for the Ar I 542.135 nm line and for the 549.588 nm line in references 36 and 96, respectively. These $\Delta \lambda_k^S$ values were obtained for each line at the temperatures listed and for
from $10^{13.5}$ to $10^{16}$ cm$^{-3}$ in half-order steps by appropriate scaling of the tabulated $w$ and $A$ values (36,96). The Gaussian contribution to Ar I line half-widths, $\Delta \lambda_G^{\frac{1}{2}}$, was calculated from the Doppler and instrument profile contributions (99); a value of $\Delta \lambda_G^{\frac{1}{2}} = 0.22$ Å was employed for temperatures of $T = 2,500$ K to 10,000 K.
CHAPTER III: FACILITIES

Experimental Facilities

The experimental facilities, except as modified for this study, were adapted from those previously described by Scott et al. (100). The principal components of the equipment employed here are outlined in Table V and the modifications incorporated for this study are described below.

The mechanism for positioning the impedance matching network was altered to provide for adjustment along the optical axis as well as providing the capability of precise horizontal and vertical positioning of the plasma torch. To achieve the latter the impedance matching network and plasma torch were mounted on a stand which allowed movement of the torch vertically, horizontally (laterally), and parallel to the monochromator optical axis. The vertical and horizontal movements could be read to ± 0.05 mm on a vernier scale. The parallel torch movement and lens positioning along the optical axis were accurate to ± 0.5 mm. A He-Ne laser (λ = 632.8 nm, C. W. Radiation Inc., Mountain View, CA) was employed for optical alignment and to check the validity of the horizontal and parallel movements of the torch. The lens aperture and the monochromator entrance slit were limited to 3 mm openings to achieve compliance with the criteria necessary for Abel inversion calculations.
<table>
<thead>
<tr>
<th><strong>Plasma Generation</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Radiofrequency generator</strong></td>
</tr>
<tr>
<td><strong>Impedence matching network</strong></td>
</tr>
<tr>
<td><strong>Plasma torch</strong></td>
</tr>
<tr>
<td><strong>coolant tube</strong></td>
</tr>
<tr>
<td><strong>plasma tube</strong></td>
</tr>
</tbody>
</table>
### Table V. (Continued)

<table>
<thead>
<tr>
<th>Aerosol Generation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>aerosol tube</strong></td>
<td>Clear fused quartz, 6 mm o.d., 4 mm i.d., tapered orifice, 1.5 mm i.d.</td>
</tr>
</tbody>
</table>
| **Argon flow rates** | Coolant; 12.5 l/min.  
Plasma; Optional, used when igniting the plasma to prevent "burning" the plasma and aerosol tubes.  
Aerosol; 1.0 l/min and 1.3 l/min. |
| **Ignition**        | Tesla coil ignition with no aerosol flow and coolant-plasma flow of approximately 15 l/min.  
After the plasma was formed the tesla coil was shut off and flow rates were adjusted to operating values. |

**Nebulizer**
Right-angle pneumatic, uptake approximately 2.5 ml/min at 1.0 l/min aerosol flow, construction details given in reference 102.

**Aerosol chamber**
Dual tube aerosol chamber (100) and (later) a simpler Teflon and glass chamber (103). The simpler chamber reduced the clear-out time between sample-background readings.
Table V. (Continued)

**Spectroscopic Equipment**

<table>
<thead>
<tr>
<th>Spectrometer</th>
<th>0.5 meter, Ebert mount, scanning monochromator (Jarrell-Ash Division, Fisher Scientific Co., Waltham, MA, Model No. 82000).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grating</td>
<td>1180 rulings/mm, blazed at 2500 Å, first order.</td>
</tr>
<tr>
<td>Slits</td>
<td>Fixed, 15 μm entrance and exit, entrance slit height masked to 3 mm.</td>
</tr>
<tr>
<td>Reciprocal linear dispersion</td>
<td>16 Å/mm, first order.</td>
</tr>
<tr>
<td>Detector</td>
<td>EMI 6256B photomultiplier, S-13 response (Gencom Division, Emitronics, Inc., Plainview, NY)</td>
</tr>
<tr>
<td>Optical transfer system</td>
<td>Plasma emission focussed by 16 cm focal length x 5 cm diameter plano-convex, fused quartz lens with aperture limited to 3 mm by adjustable iris diaphragm concentrically mounted on the lens holder. Lens positioned at twice the focal length (2f) from the entrance slit and plasma central axis for each wavelength region studied.</td>
</tr>
<tr>
<td>Amplifier</td>
<td>Linear picommeter with zero suppression (Keithly Instruments, Cleveland, OH, Model 417)</td>
</tr>
<tr>
<td>Integrator</td>
<td>Digital readout system, hard copy only (Infotronics, Houston, TX, Model CRS-80).</td>
</tr>
<tr>
<td>Recorder</td>
<td>X-Y recorder (Moseley Division, Hewlett-Packard, Pasadena, CA, Model 7001-A).</td>
</tr>
</tbody>
</table>
The power supply to the filament of the RF generator power tube was modified to accommodate time-independent relative intensity measurements. With reference to this modification it is worth noting that many high frequency generators produce a sinusoidal 60 Hz modulation on the forward power high voltage envelope; this was found to be true for the radio-frequency (RF) generator employed in this investigation. Consequently, emission from analyte and Ar I lines observed in the plasma displayed similar 60 Hz modulations; the peak-to-peak magnitudes of these modulations were a sensitive function of the excitation energies. Subsequently, the relative intensities obtained represented time-averages over the integration period employed for the intensity measurements; these intensities yielded erroneous time-averaged excitation temperature values.

Experimental verification of this effect is provided by the oscilloscope tracings shown in Figure 1 for the Fe I 381.584 nm and 382.444 nm lines; these neutral atom lines possessed excitation energies of 38,175 cm$^{-1}$ and 26,140 cm$^{-1}$, respectively. The tracings shown in Figure 1 were obtained by filtering the signal current taken directly from the photomultiplier tube output. Trace C for the higher excitation potential line clearly displays greater intensity sensitivity to forward power modulation than does the lower excitation potential line shown in trace B. Consequently,
Figure 1. Oscilloscope tracings showing emission intensity modulation with a 60 Hz ripple on the forward power to the plasma: (A) dark current, (B) Fe I 382.444 nm, (C) Fe I 381.584 nm
the intensity ratio of the two lines was significantly different in the peak and valley regions of the oscilloscope tracings. The peak and valley relative intensities (above dark current), intensity ratios, and the corresponding two-line temperatures calculated from these ratios with two sets of transition probabilities are summarized in Table VI. Because peak values were clearly \( \approx 15\% \) higher than the valley temperatures, erroneous time-averaged excitation temperatures were obtained under these conditions. These temperatures were biased by the excitation energy range of the lines employed. The actual time-independent temperatures were obtained when the 60 Hz ripple was eliminated from the generator power tube filament. This was accomplished with the DC power supply which by-passed the generator ac supply, the source of the 60 Hz modulation. With the elimination of the 60 Hz ripple on the RF forward power, a smaller 120 Hz sawtooth ripple of \( \approx 9\% \) peak-to-peak magnitude, remained. The 120 Hz ripple was reduced to \( \approx 3\% \) near maximum power and to \( <1\% \) at 900 W by increasing the generator high voltage filtering network capacitance from 4\( \mu \)F to 12\( \mu \)F. For the latter the reflected power was reduced from \( \approx 10 \) W to \( \approx 1 \) W when the 60 Hz ripple was eliminated.

Computer Facilities

Off-line computer calculations were handled by PLL and FORTRAN IV programs which were processed on the IBM 370/158.
Table VI. Intensities, intensity ratios, and two-line temperatures for Fe I lines in peak and valley regions with 60 Hz modulation on the forward power.

<table>
<thead>
<tr>
<th>Region</th>
<th>Relative Intensity</th>
<th>Ratio(^a)</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe I 381.584</td>
<td>Fe I 382.444</td>
<td>Fe I 381.584</td>
<td>Fe I 382.444</td>
</tr>
<tr>
<td>peak</td>
<td>3.3</td>
<td>1.4</td>
<td>0.42</td>
</tr>
<tr>
<td>valley</td>
<td>1.3</td>
<td>0.85</td>
<td>0.65</td>
</tr>
</tbody>
</table>

\(^a\)Intensity ratio, \(I_{382.444}/I_{381.584}\).

\(^b\)Transition probability data: BH = Banfield and Huber (66); R = Reif (30).
and M/65 facilities at the Iowa State University Computations Center. Remote processing was accomplished with the facilities located at the Ames Laboratory Computer Garage. The expert assistance provided by the staff of the Ames Laboratory Computer Service Group was invaluable during the writing and debugging of a number of the programs employed in this investigation. The ASR 35 teletype in B28 Spedding Hall was employed to process CPS/PL1 jobs which were mainly used for disk data file management. A Digital Equipment Corporation (DEC) PDP 8/e minicomputer with 8K of core was employed for some preliminary on-line profiling experiments on a different plasma facility than the one used in this study. The characteristics and potential of this DEC PDP 8/e plasma system will be briefly discussed in a later chapter of this thesis.
CHAPTER IV: EXPERIMENTAL PROCEDURES

Intensity Measurements, Lateral Profiling, and Abel Inversions

The analyte thermometric species (Fe I) was nebulized into the plasma (100,102,103) as a 150 µg Fe/ml solution. The relative intensities of the Fe I emission lines listed in Table II and those for the three-line set from Table I were measured at increasing lateral displacements (0.4-1.0 mm intervals) from the axial channel of the plasma until the signals could no longer be detected. Three to four data points on the opposite side of center were also collected to assure accurate location of the vertical symmetry axis of the plasma. The latter was taken at the position of the peak of the symmetric bell-type lateral distributions after a smooth curve was drawn through the original data points. Spectral backgrounds at each emission line of interest were measured while deionized water was aspirated into the plasma. The signals and spectral backgrounds were integrated over an 8-second period. The net relative intensities used in the final calculations were the averages of three to five background corrected values. These relative intensities were plotted vs. displacement to construct a lateral profile for each Fe I line of interest. Relative intensity measurements were taken for all lines at a given displacement before proceeding to the next lateral observation zone.
Complete lateral profiles from one edge of the plasma through the geometric center to the opposite edge were obtained in a similar fashion for the neutral atom and first ion lines listed in Table IV. The center of the bell-type profiles so obtained was taken at the peak of the distribution. Complete lateral profiles with water nebulized into the plasma at an aerosol carrier gas flow of 1.0 l/min were also obtained for the Ar I spectral lines listed in Table III. The spectral backgrounds for these Ar I lines were obtained from the continuum emission adjacent to the lines. The center of the toroidally-shaped lateral distributions obtained for these Ar I lines was taken as the midpoint between the off-axis peaks.

The Cremers and Birkebak Abel inversion method described previously was used to obtain spatially resolved radial intensity distributions from the corresponding lateral profiles. The right and left portions of the complete lateral intensity profiles discussed above were inverted separately for comparative purposes.

Temperature Calculations

The slope method described previously (Equation 3) was used to calculate radial excitation temperature distributions from the corresponding radial intensity profiles. The temperature profiles so obtained for the different thermometric
species, Fe I and Ar I, and for different Fe I line sets and transition probabilities are compared later in Chapter V of this thesis.

Electron Number Density from Saha-Eggert's Ionization Calculations

Equation 5 was used to calculate radial $n_e$ values from the corresponding radial intensities for the atom/ion line combinations and average $(g^OA^0\lambda^+/g^+A^+\lambda^0)$ ratios given in Table IV. Radial number density ratios ($n_{x+}(R)/n_{x0}(R)$) were obtained from Equation 6 for the atom/ion line combinations listed in this table. A listing of the source statements of the computer program employed in these calculations is given in Appendix C.

Electron Number Density from Stark Broadening Calculations

$H_\beta$ line

Wavelength scans over the $H_\beta$ line profile were obtained at successive lateral displacements across the plasma discharge. First, each scan was divided into $\approx25$ constituent wavelengths spanning the entire interval of the $H_\beta$ line profile. Second, lateral profiles were constructed for each constituent wavelength and the spectral background was interpolated from the continuum emission beyond the $H_\beta$ line.
wings. Third, radial intensity profiles were obtained from the corresponding lateral profiles for each constituent wavelength by employing the Abel inversion method described previously. Finally, the Hβ profile at each radial position was reconstructed from the radial intensity data; the radial half-widths, $\Delta \lambda^0(R)$, were measured from these Hβ profiles.

A FORTRAN IV computer program was written to perform the $n_e$ calculations. The details of this program are discussed and a listing of the source statements is given in Appendix D. The computer calculations were performed as follows. First, a matrix of $a_\frac{1}{2}^\prime$ vs. $\log_{10} T$ values was constructed from the instrument and Doppler corrected reduced Stark half-width data (98) for $n_e$ from $10^{12}$ to $10^{16}$ cm$^{-3}$ in half-order steps, and for temperatures of 2,500; 5,000; 10,000; 20,000; and 40,000 K. The values obtained are shown in Figure 2. Second, the value of $\Delta \lambda^0(R)$ obtained as described above was inserted into Equation 8 to evaluate the $[\Delta \lambda^0(R)]^{3/2}$ term. Third, $[a_\frac{1}{2}^\prime, n_e(R)]$ pairs were calculated by appropriate interpolation methods (98) for the Fe I excitation temperature, $T(R)$, at radius R. Fourth, an approximate $[a_\frac{1}{2}^\prime]_0$ was selected and inserted into Equation 8 to calculate a zero-order approximation to the electron density, $[n_e(R)]_0$. Fifth, a first-order $[a_\frac{1}{2}^\prime]_1$ value was interpolated from the $a_\frac{1}{2}^\prime$ vs. $n_e(R)$ relationship and from the value of $[n_e(R)]_0$. This value for $[a_\frac{1}{2}^\prime]_1$ was used in Equation 8 to give a
Figure 2. Reduced Stark profile half-widths, $\alpha^*_H$, corrected for Doppler and instrument broadening plotted vs. $\log_{10} T$ for electron densities from $10^{12}$ to $10^{16} \text{ cm}^{-3}$ for the H$_3$ 486.13 nm line
first-order electron density, \([n_e(R)]_1\). Finally, this procedure was repeated iteratively until a self-consistent pair of \([\alpha^R, n_e(R)]\) values was obtained to the desired accuracy.

**Ar I lines**

Wavelength scans over the lateral (effective) Ar I line profiles were obtained at the central axis of the plasma discharge. The Ar I lines were assumed to have Voigt profiles so that the tabulated half-width ratios (93); i.e., \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) and \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\), could be used to calculate the expected experimental half-width, \(\Delta \lambda \frac{\lambda}{G}\), at the appropriate \(n_e\) and temperature combinations. The \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) ratios were plotted as a function of the \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) ratios for the values given in reference 93. Equation 9 was used to calculate the \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) values and the \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) ratio was obtained from the Stark half-width and the known value for \(\Delta \alpha^G \frac{G}{\lambda}\). The corresponding \(\Delta \alpha^S \frac{S}{\Delta \alpha^G \frac{G}{\lambda}}\) ratio was interpolated from the plot and the \(\Delta \lambda \frac{\lambda}{G}\) value was calculated from this ratio. This procedure was used to obtain \(\Delta \lambda \frac{\lambda}{G}\) values for each Ar I line at each \(n_e\) and temperature combination considered. The semi-log plots of \(\Delta \lambda \frac{\lambda}{G}\) vs. \(\log_{10} T\) which were constructed for each line in half-order steps for \(n_e\) from \(10^{13.5}\) to \(10^{16}\) cm\(^{-3}\) are shown in Figure 3. The \(n_e\) corresponding to an experimentally measured Ar I line half-width was then obtained by linear interpolation between
Figure 3. Doppler and instrument profile corrected Stark half-widths for Ar I lines, \( \Delta \lambda_4 \) vs. \( \log_{10} T \) for electron density from \( 10^{13.5} \) to \( 10^{16} \) cm\(^{-3}\).
The graph shows the relationship between temperature and the half width of a specific line. The graph includes data for different temperatures and concentrations, with lines representing different concentrations of Ar I 542.135 and Ar I 549.588. The x-axis represents temperature in units of $10^{-3}$ K, and the y-axis represents the half width of the line in Å.

- Ar I 542.135
  - Line: $1 \times 10^{16}$
  - Symbol: ○
- Ar I 549.588
  - Line: $3.162 \times 10^{15}$
  - Symbol: △
- Ar I 542.135
  - Line: $3.162 \times 10^{14}$
  - Symbol: ●
- Ar I 549.588
  - Line: $3.162 \times 10^{13}$
  - Symbol: ★
the values plotted in this figure. Effective temperatures were estimated for observation heights at which no measurements were obtained, i.e., below 15 mm.
CHAPTER V: RESULTS AND DISCUSSION

Symmetry

The bell-type lateral intensity distributions which were obtained for Fe I thermometric emission lines complied well with the circular symmetry requirement discussed in Chapter II. The bell-type profiles of the emission lines given in Table IV for Saha-Eggert's \( n_e \) calculations were also in compliance with this symmetry criterion. In contrast, the toroidally shaped Ar I lateral intensity distributions for the thermometric lines given in Table III showed deviations from symmetry primarily in the off-axis regions. The lateral intensity distributions for the wavelength constituents of the H\( _\beta \) line profile displayed similar toroidal shapes and similar deviations from circular symmetry. The different lateral distributions are discussed in the following sections.

Intensity Distributions of Analyte Lines

Figure 4 shows typical lateral intensity profiles for the Zn, Fe, and Ca atomic and ionic emission lines listed in Table IV. It is seen that bell-type intensity distributions were obtained for the wide range of excitation and ionization energies represented by the spectral lines of these species. Similar profiles were obtained for the Mg and Cd atomic and
Figure 4. Lateral profiles for Saha species at 15 mm, 1000 W and 1.0 l/min aerosol carrier gas flow

<table>
<thead>
<tr>
<th>Species</th>
<th>Without Na</th>
<th>With 6900 μg Na/mL</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 μg Zn/mL:</td>
<td>Zn II 206.19 nm (---O---) (---□---)</td>
<td>Zn I 213.88 nm (---X---) (---+---)</td>
</tr>
<tr>
<td>150 μg Fe/mL:</td>
<td>Fe II 258.588 nm (---O---) (---□---)</td>
<td>Fe I 252.285 nm (---X---) (---+---)</td>
</tr>
<tr>
<td>10 μg Ca/mL:</td>
<td>Ca II 396.847 nm (---O---) (---□---)</td>
<td>Ca I 422.673 nm (---X---) (---+---)</td>
</tr>
</tbody>
</table>
ionic lines from Table IV. The corresponding Abel inverted radial intensity profiles showed similar bell-type behavior.

The addition of a large excess of an EIE should, under equilibrium conditions, suppress ionization of the analyte species. The trends of the Ca profiles in Figure 4 tend to support this interpretation, i.e., the atomic line is slightly enhanced while the ionic line is relatively more depressed. However, the axial depressions in the atomic line profiles of Fe and Zn suggest ionization suppression is not the dominating process. This suggestion is supported by the data in Table VII which lists ion/atom lateral or "averaged" intensity ratios at the plasma central axis for the line profiles shown in Figure 4 and for the Mg and Cd lines listed in Table IV. Again, the existence of some analyte ionization suppression is indicated by the decrease in these ratios upon the addition of Na to the plasma but, in comparison to flames, the suppression is surprisingly small (104). These unusually small interference effects were first reported by Larson et al. (103) and confirmed later by Mermet and associates (105) and by Boumans and de Boer (11c).

Further evidence that ionization suppression plays only a minor role at least under some combinations of experimental conditions is found in the radial relative intensity profiles shown in Figure 5 for the Fe I 382.043 nm emission line. These profiles clearly show that Fe I radial intensity
Table VII. Ion to neutral atom lateral intensity ratios for lines of Zn, Cd, Fe, Mg and Ca with and without added Na

<table>
<thead>
<tr>
<th>Species</th>
<th>$I^+ / I^0$ Ratios$^a$</th>
<th>(I$^+ / I^0$)$_{Na}$</th>
<th>(I$^+ / I^0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Without Na</td>
<td>With 6900 µg Na/ml</td>
<td>(I$^+ / I^0$)$_{Na}$</td>
</tr>
<tr>
<td>Zn</td>
<td>0.22</td>
<td>0.18</td>
<td>0.82</td>
</tr>
<tr>
<td>Cd</td>
<td>0.88</td>
<td>0.67</td>
<td>0.76</td>
</tr>
<tr>
<td>Fe</td>
<td>4.6</td>
<td>3.8</td>
<td>0.83</td>
</tr>
<tr>
<td>Mg$^b$</td>
<td>10.4</td>
<td>9.9</td>
<td>0.95</td>
</tr>
<tr>
<td>Mg$^c$</td>
<td>5.3</td>
<td>5.1</td>
<td>0.96</td>
</tr>
<tr>
<td>Ca</td>
<td>85</td>
<td>70</td>
<td>0.82</td>
</tr>
</tbody>
</table>

$^a$Relative intensity ratio, ion line intensity/atom line intensity.

$^b$Ion line, Mg II 279.553 nm.

$^c$Ion line, Mg II 280.270 nm.
Figure 5. Radial intensity distributions for the Fe I 382.043 nm line at 1000W for three observation heights and two aerosol carrier gas flows; 150 µg Fe/ml (—O—) and 150 µg Fe/ml + 6900 µg Na/ml (—Δ—)
distributions are essentially unchanged upon addition of Na as an EIE at the lower aerosol carrier gas flow but, are enhanced about two-fold at the higher flow.

These observations imply that greater interferences due to the presence of an EIE would be expected to occur at higher aerosol carrier gas flows when lateral intensities are measured under analytical experimental conditions. Indeed, Larson et al. (103) and Boumans and de Boer (1c) have established that this is so. It is important to note that the combination of argon carrier gas flow of ~1.0 l/min and an observation height of ~15-20 mm corresponds to the values of these parameters that lead to excellent powers of detection and a low degree of ionization and other interelement interactions (1b,1c,103).

Intensity Distributions of Ar Lines

The typical toroidal lateral and radial relative intensity distributions for the Ar I 425.936 nm line reproduced in Figure 6 clearly show that both the lateral and radial profiles are asymmetric, as evidenced by the larger left side peak in the lateral profile and by the disagreement between right and left side intensities in the central region of the radial profile. These observations are typical for Ar I profiles, even though elaborate precautions were taken in order to assure symmetry in the construction of the plasma
Figure 6. Toroidal lateral and radial relative intensity distributions for the Ar I 425.936 nm line at 15 mm, 1000W and 1.0 l/min aerosol carrier gas flow.
torch. Evidently very critical adjustments beyond present fabrication technology are required for precise control of Ar flow patterns. Asymmetry in the magnetic and electric fields induced by the load coil and in the interaction of these fields with the Ar plasma support gas may also contribute to asymmetry in the Ar I lateral profiles. The toroidal lateral and radial relative intensity distributions which were obtained for the constituents of the $H_\beta$ line profile displayed similar asymmetric characteristics. Other investigators have also reported similar problems with asymmetric toroidal lateral intensity distributions when Abel inversion methods have been applied to these profiles (2a,15,16,45). These results suggest that further refinements in torch and coil design should be explored ultimately; these studies were not considered important enough to justify their inclusion in the present context.

Temperature Profiles

The excitation temperatures obtained from Equation 3 for analyte (Fe I) and support gas (Ar I) thermometric lines are plotted in Figure 7. It is seen that the excitation temperatures calculated from different sets of transition probabilities (30,66,67) for the Fe I three-line set (From Table I) and for the expanded ten-line set (given in Table II) agree to within ~3% in the axial channel region and within ± 10%
Figure 7. Radial excitation temperatures at 15 mm, 1000W and 1.0 l/min aerosol carrier gas flow. Ar I eight-line with Corliss and Shumaker (77) transition probability data (—○—); Fe I ten-line with Huber and Parkinson (67) data (—X—) and with Reif (30) and Banfield and Huber (66) data (—○—); Fe I three-line with Reif data (—△—) and with Banfield and Huber data (—□—)
in the wings. The temperature data obtained from the Ar I eight-line set (listed in Table IV) are not that encouraging, even though the temperatures obtained with the transition probability data given in references 75-77, and 80 agreed to within ± 3%. The uncertainty in the Ar I data as represented by the scatter of the points in the radial temperature profile, and the disagreement with the Fe I temperatures, are reconcilable. First, the asymmetric character of the toroidal Ar I lateral intensity distributions (see Figure 6) introduces large uncertainties into Abel inversion calculations, especially for the axial region (2a,15,16,18,45). Second, errors in relative intensity measurements are amplified considerably when the selected lines possess a limited range of excitation energies, as shown by the data plotted in Figure 8. These plots, which were calculated by methods discussed elsewhere (2a,81,106), clearly show that the Ar I temperature calculations are subject to an approximate five-fold larger uncertainty than the Fe I values for the same ΔI/I measurement error.

In view of the good agreement between the Fe I temperatures and the large uncertainties associated with the Ar I temperatures henceforth, only the temperatures calculated for the Fe I three-line set from Table I will be considered. These temperatures, which were obtained at two aerosol carrier gas flows and with and without the presence of relatively high concentrations of an EIE, are shown in Figure 9.
Figure 8. Percent uncertainty in temperature as a function of percent uncertainty of intensity for typical Fe I and Ar I lines employed in temperature calculations.
Figure 9. Radial Fe I excitation temperatures at 1000W for three observation heights and two aerosol carrier gas flows; 150 µg Fe/ml (---○---), 150 µg Fe/ml + 6900 µg Na/ml (---●---)
Examination of this figure reveals several important features. First, the excitation temperature distributions obtained at the respective aerosol carrier gas flows and observation heights are not significantly changed upon addition of Na as an EIE. Second, the temperatures for the higher flow are significantly lower (400 to 1400 K) than the corresponding temperatures for the lower flow. Third, for the higher carrier-gas flow, the central zone temperatures at 15 mm are relatively low and the off-axis peak is much more pronounced than for the lower flow. Finally, central zone temperatures at the lower flow are essentially unchanged from 15 to 20 mm but decrease by about 10% at 25 mm. These results correlate well with the empirical observations of others at this laboratory (103,107) namely, that the "compromise" experimental conditions which yield excellent powers of detection and also yield a high degree of freedom from interelement effects are \(1.0 \ell/\text{min}\) aerosol carrier gas flow and \(15-20 \text{ mm}\) observation height. Figure 9 clearly shows that there is essentially no decrease in temperature from 15 to 20 mm yet additional residence time is gained for desolvation, atomization, and excitation of the analyte. These profiles also reveal the drastic temperature drop at the higher flow which is undesirable from excited state population and residence time considerations. The substantial temperature drop between 20 and 25 mm for the lower flow is also undesirable from the excited state population standpoint for most species.
Boumans and de Boer (1c) have reported different "compromise" operating conditions which were based on their observations of interelement effects and detection limits obtained for their plasma system. These authors suggested experimental conditions of 1.3 to 1.5 l/min carrier gas flow and 15 mm observation height at 700 W power input and, 1.5 to 1.7 l/min carrier gas flow at 20 mm height for a power input of 850 W. It is worth noting that the relative intensity data in Figure 5 and the temperature data in Figure 9 combined with the observations of Larson et al. (103) suggest that an aerosol carrier gas flow of 1.3 l/min is undesirable for plasma operating conditions at this laboratory because greater interelement effects are observed at this flow.

Electron Number Density Profiles

Because the temperature profiles shown in Figure 9 exhibited definite off-axis or toroidal peaks, it was of particular interest to determine whether the $n_e$ profiles at this observation height reflected these temperature distributions. The profiles shown in Figure 10 indeed show similar off-axis peaks, but they reveal several other features worthy of comment. First, the $H_\beta$ Stark broadening $n_e$ profiles are a factor of 30- to 50-fold greater than the Saha-Eggert's ionization profiles. Second, the $n_e$ profiles were not significantly changed upon addition of Na as an EIE. Finally,
Figure 10. Radial electron density distributions at 1000W, 15 mm and 1.0 l/min aerosol carrier gas flow for H\(\text{g}\) Stark broadening (—X—) and Saha calculations; 10 µg Ca/ml (—○—), 150 µg Fe/ml (—□—), 10 µg Mg/ml (—△—), 10 µg Cd/ml (—×—), 10 µg Zn/ml (—●—)
ELECTRON DENSITY (cm$^{-3}$)

WITHOUT Na

6900$\mu$g Na/ml

RADIAL POSITION FROM PLASMA CENTER (mm)
for the central axial region the Saha $n_e$ profiles agree to within a factor of three for the five different analyte species. Considering first the disagreement among the Saha $n_e$ values, the range of values obtained is not particularly surprising in view of the magnitude of potential errors involved. This range may reflect inherent errors in the published transition probability data for the lines employed or varying degrees of $n_e$ contribution by the analytes because of their different degrees of ionization in the plasma. These uncertainties plus those accumulated in the lateral intensity measurements and Abel inversion calculations may account for up to a factor of two error in the Saha-Eggert's $n_e$ values. A 10% uncertainty is generally associated with theoretical Stark data for the $H_β$ line (36,93-96,98,99). Accumulated uncertainties from convolution calculations, instrument profile measurements, and Abel inversions account for ~30% error in the radial $H_β$ half-width determinations. These considerations suggest that ~40% error may be associated with the $n_e$ values determined by $H_β$ Stark broadening calculations. Although the errors in both sets of measurements are substantial, they are clearly inadequate in accounting for the factor of 30- to 50-fold difference between the $n_e$ values determined by the Saha and Stark methods. These large differences suggest that LTE may not prevail for the plasma operating conditions employed in this work, a subject that is discussed later in this chapter.
It is worth noting that the Stark broadening $n_e$ values shown in Figure 10 are about a factor of five-fold smaller than the similar measurements reported by Mermet (17a) and are about two-fold smaller than the continuum calculations reported by Kornblum and de Galan (16). However, Kornblum and de Galan reported Saha $n_e$ values obtained with Mg atom/ion lines that were two to three orders of magnitude greater than those obtained here and those reported by Mermet (17a). The effective Saha $n_e$ values reported by Mermet were essentially identical to the similar values obtained here and reported later in this chapter.

Because the Saha $n_e$ values obtained from the Mg atom/ion line pairs (Table IV) represented a value near the average obtained for all the species plotted in Figure 10, Mg was selected for additional $n_e$ measurements at different observation heights. These line combinations possessed several other desirable advantages; namely, (a) four sets of transition probability data which were in good agreement, were available for both Mg atom/ion line combinations, (b) the lines were free from spectral interference, (c) the excitation energies of the atomic and ionic lines were well matched, and (d) the lines were in close wavelength proximity so that the instrument response with wavelength could be assumed constant. The results of $n_e$ measurements on the Mg atom/ion line combinations are shown in Figure 11. Surprisingly, the $n_e$
Figure 11. Radial Saha-Eggert's electron density distributions at 15, 20, and 25 mm for Mg atom/ion line combinations; 10 μg Mg/ml (---O---, ---□---, ---△---), 10 μg Mg/ml + 6900 μg Na/ml (---○---, ---■---, ---▲---)
profiles at 15 and 20 mm observation heights show little change upon the addition of an EIE to the plasma. The primary change in the 25 mm height profile is in the wing region, where there is an enhancement significantly greater than the experimental error. It is also evident that the toroidal $n_e$ distribution at 15 mm disappears at 20 and 25 mm, being replaced at the latter heights by bell-type profiles which are relatively uniform for the central 4 mm of the plasma. The change in $n_e$ in this central axial zone upon the addition of Na is insignificant. The surprisingly small changes in $n_e$ and temperature profiles at 15 and 20 mm upon the addition of Na as an EIE suggest that changes in the total composition of the sample do not affect the radial excitation temperature nor degree of ionization of analyte species in a dominant manner. The significant increase in $n_e$ in the wings of the 25 mm profile upon addition of Na as an EIE suggests that ionization suppression may play a role, if a significant fraction of the analyte diffuses into this region. These results are in harmony with empirical observations reported by Larson et al. (103) and by Boumans and de Boer (1c) which indicated low levels of interelement effects at low observation heights (15 to 20 mm) and increased effects higher in the plasma.

The radial $n_{Mg^+/Mg^0}$ profiles obtained from Equation 6 for the Mg atomic and ionic lines listed in Table IV are given in Figure 12. With consideration of potential errors, the
Figure 12. Radial number density ratios, $n_{Mg^+}/n_{Na}$, at 1000W and 1.0 l/min aerosol carrier gas flow for Mg lines employed in electron density calculations; 10 µg Mg/ml at 15 mm (—○—), 20 mm (—□—), and 25 mm (—△—); 10 µg Mg/ml + 6900 µg Na/ml at 15 mm (—●—), 20 mm (—X—), and 25 mm (—△—)
ratios are essentially unchanged upon addition of Na as an EIE. These profiles also clearly show that Mg is more than 90% ionized in the central axial zone of the plasma at all observation heights. The radial $n_{X^+}/n_{X^0}$ ratios which were obtained for the other species given in Table IV are listed in Table VIII. The decrease in these ratios upon addition of Na to the plasma indicates the existence of some analyte ionization suppression but the degree of this suppression is much smaller than that commonly observed in flames (104). The data in this table also clearly show the high degree of ionization of analyte species in the central axial region of the plasma. In particular, Ca is more than 99% ionized and Zn more than 50% ionized even when a high concentration of an EIE is present in the plasma. These results correlate well with recent empirical observations at this laboratory which have been made on a direct-reading polychromator plasma system that has been in daily use for three years. The experience with this instrument (107) has indicated that superior powers of detection may be obtained with the ionic lines of many analytes particularly those elements with low ionization energy. Indeed, the fact that many of the most sensitive lines of these elements originated from singly ionized species was recorded by Dickinson and Fassel (108) in 1969 and later by Souillart and Robin (109). In view of these observations it is curious that Boumans and de Boer (1c)
Table VIII. Radial ion to atom number density ratios, \( n_{X^+}(R)/n_{X^0}(R) \), for Zn, Cd, Fe and Ca with and without added Na at 1000W, 1.0 l/min, and 15 mm height

<table>
<thead>
<tr>
<th>Radius (mm)</th>
<th>Zn</th>
<th>Cd</th>
<th>Fe</th>
<th>Ca</th>
<th>Without Na</th>
<th>Zn</th>
<th>Cd</th>
<th>Fe</th>
<th>Ca</th>
<th>With 6900 μg Na/ml</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>2.1</td>
<td>6.2</td>
<td>18</td>
<td>610</td>
<td>1.5</td>
<td>4.4</td>
<td>15</td>
<td>300</td>
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<td>4.3</td>
<td>4.5</td>
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were surprised to rediscover this fact; namely, that the ion lines of the alkaline earth elements yielded far better detection limits than the neutral atom lines for their "compromise" plasma operating conditions.

Additional documentation that $n_e$ do not change upon addition of an EIE is found in the effective (noninverted) half-widths of the $H_β$ and Ar I line profiles shown in Table IX. This observation was confirmed by the effective $n_e$ values obtained from these Stark broadening measurements and those obtained from Saha-Eggert's calculations for Mg lines which are plotted in Figure 13. The Stark broadening $n_e$ values for the $H_β$ and the two Ar I lines are essentially identical at the various observation heights and, in harmony with the Saha $n_e$ values, did not change significantly when the EIE was added to the plasma. In agreement with the radial measurements plotted in Figure 10, the effective Saha values are 30- to 50-fold smaller than the Stark broadening $n_e$ values.

Analyte Excitation

The large differences between $n_e$ values calculated from Stark broadening methods and those obtained from Saha-Eggert's ionization considerations (Figures 10 and 13) may be interpreted to support the earlier stated conclusion that LTE does not exist for the plasma operating conditions employed in this investigation. From observations quite similar to
Table IX. Effective half-widths\textsuperscript{a} of $\text{H}_\beta$ and Ar I lines measured at the plasma axis for 1000W forward power and 1.0 l/min aerosol carrier gas flow

<table>
<thead>
<tr>
<th>Observation Height (mm)</th>
<th>Ar I 542.135 nm Without Na</th>
<th>Ar I 549.588 nm Without Na</th>
<th>H\textsubscript{\beta} 486.13 nm Without Na</th>
<th>Ar I 542.135 nm With Na\textsuperscript{b}</th>
<th>Ar I 549.588 nm With Na</th>
<th>H\textsubscript{\beta} 486.13 nm With Na</th>
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<td>2.36</td>
<td>1.79</td>
<td>5.47</td>
<td>2.49</td>
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<td>1.88</td>
<td>1.40</td>
<td>4.49</td>
<td>2.01</td>
<td>1.40</td>
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<td>0.851</td>
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<td>2.08</td>
<td>0.656</td>
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<td>0.522</td>
<td>0.434</td>
<td>1.53</td>
<td>0.487</td>
<td>0.435</td>
<td>1.59</td>
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<td>25</td>
<td>0.432</td>
<td>0.346</td>
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<td>0.443</td>
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\textsuperscript{a}Half-widths expressed in units of Angstroms (Å), 10 Å = 1 nm.

\textsuperscript{b}6900 \mu g Na/ml added to the plasma.
Figure 13. Effective electron density at 1000W and 1.0 l/min aerosol carrier gas flow for several observation heights. Stark broadening with deionized water nebulized; H$_2$ 486.13 nm (—O—), Ar I 542.14 nm (—□—), Ar I 549.59 nm (—△—). Stark broadening with 5900 μg Na/ml nebulized; H$_2$ 486.13 nm (—●—), Ar I 542.14 nm (—*—), Ar I 549.59 nm (—+—). Saha-Eggert's ionization; 10 μg Mg/ml (—◇—), 10 μg Mg/ml + 5900 μg Na/ml (—◆—).
EFFECTIVE ELECTRON DENSITY (cm$^{-3}$)

HEIGHT ABOVE LOAD COIL (mm)
those reported in this dissertation, Jaroz et al. (2b) and Mermet (17) have in fact concluded that LTE does not exist for their plasma operating conditions. Mermet (17b) has suggested that Ar I metastables are involved in analyte excitation through Penning ionization reactions, and that Ar II levels may also be involved through a similar process. Robin and Trassy (110) observed stimulated emission for resonance lines of Al and Ti below a critical concentration while above this concentration atomic absorption prevailed. These authors suggested that the observation of this phenomenon indicated the absence of LTE in their 40 MHz discharge. The calculations of Hey (111) and Cillars et al. (112) on the n_e criteria necessary to ensure LTE suggest that low lying metastable levels play a role in population of excited states for the species considered. Indeed, energy transfer mechanisms involving rare gas metastables are well known and are observed in many classes of low pressure discharges (113-115). However, experimental observations at atmospheric pressure are not readily obtained because the metastable level lifetimes are much shorter due to collisional deactivation. It should be noted that Hey's calculations are for homogeneous nonhydrogenic plasmas and hence, may not apply to plasmas used for spectrochemical purposes which generally possess relatively large spatial gradients in temperature and analyte number densities.
The \( n_e \) differences may alternately be interpreted to indicate the presence of significant electric and/or magnetic fields induced in the plasma region by the load coil that are not accounted for by particle field considerations in the Stark broadening theory. An approximate calculation of Stark splitting of the \( H_\beta \) line in a static electric field (96,116, 117) reveals that \( \approx20,000 \) volts/cm would account for the increased broadening. Magnetic fields of \( \approx10,000 \) gauss would be required to produce splitting equivalent to that produced by the particle field (96). Calculations for typical atmospheric pressure argon induction discharges assumed to be in LTE (6,118) indicate that axial magnetic fields and azimuthal electric fields should be on the order of a few hundred gauss and a few hundred volt/cm, respectively. For a pure induction discharge in LTE the axial electric field is zero (118). Field strength calculations for nonequilibrium plasmas are generally not available because the theory is not well understood. Although the nonparticle field strengths calculated by the models mentioned above are very much smaller than necessary to produce significant line splittings, the unknown nature of possible nonequilibrium fields precludes a definitive interpretation of their effects on line broadening in the present context.

The present inability to interpret \( n_e \) differences in a more definitive manner should not detract from the fact that the results of this dissertation research correlate very well
with empirical observations (lc,103) which indicate low levels of interelement effects at low observation heights and increased effects higher in the plasma. The surprisingly low sensitivity of \( n_e \) and temperature distributions at 15 and 20 mm to the addition of an EIE (see Figures 9 and 11) suggests that changes in the total composition of the sample should not affect radial excitation temperatures nor degree of ionization of analytes in a dominant manner. The significant increase in \( n_e \) in the wings of the 25 mm profile when Na is added as an EIE suggests that ionization suppression may play a role if a significant fraction of the analyte diffuses into these regions. Indeed, some evidence of this type of diffusion is provided by the Ca I 422.7 nm line profile data reported by Larson et al. (103), which showed a peculiar off-axis "hump" when Na was added to the plasma for an observation height of 20 mm. These results provide additional evidence that careful consideration of the region sampled by the viewing field of the spectrometer is an important factor when plasma performance is analyzed (18). This is especially true when the enlarged acceptance cone of the wide aperture optical systems commonly employed for the analytical applications of these plasmas samples a significant portion of the off-axis regions.
CHAPTER VI: SUGGESTIONS FOR FUTURE WORK

Although this investigation has aided in the understanding of several important aspects of analyte excitation in ICP's employed for spectrochemical analysis, a number of avenues of research remain open.

Certainly, the validity of the LTE assumption for different ICP operating conditions should be ascertained because the absolute interpretations of the results of many diagnostic methods (e.g., excitation temperature and Saha $n_e$ measurements) are critically dependent upon LTE conditions prevailing in the plasma. The role of support gas and sample metastable levels should be elucidated because this may provide useful information about analyte excitation mechanisms and may help resolve the LTE question.

Studies concerning the effects on lateral intensity profiles and, subsequently Abel inversion calculations from asymmetries in the plasma torch, in the induced magnetic and electric fields, and in the gas flow patterns should be pursued. Improvements in the Abel inversion procedure should help to avert some of the problems encountered when toroidal lateral intensity distributions are inverted.

Investigations on the applications of other diagnostic techniques such as laser techniques (119-121) and interferometric (122, 123) methods should be initiated because these techniques could provide powerful alternative approaches for
probing spatial particle density and temperature distributions in the plasma. The work proceeding in this laboratory on coupling a mass analyzer to an ICP (124) may also provide a valuable diagnostic tool.

Work on the spectroscopic probing of the spatially resolved radial excitation temperatures and $n_e$ distributions experienced by analytes should continue because even though the results of these studies may lack absolute interpretation from lack of LTE in the plasma, valuable information will still be obtained on relative excitation trends (e.g., increased interelement effects may be partially or completely explained by a drastic change in the $n_e$ distribution at 1.3 L/min aerosol carrier gas flow when an EIE is added to the plasma). Studies of the effects on excitation temperature and $n_e$ distributions when ultrasonic nebulization of the sample solution is employed, with and without desolvation, may provide some insight into the reasons why better than order of magnitude improvements in ICP detection limits have been noted when this method was compared to pneumatic nebulization (1c,125).

Near the end of this dissertation research, work was begun on adaptation of a modular computer-controlled plasma facility (126) to perform automated lateral intensity profiling experiments. Progress in this area and suggestions for further modifications were summarized in several recent
research reports (127). An assembly language program to perform these experiments was written for the DEC PDP 8/e minicomputer on this system (127). This program was designed for the existing facilities but may easily be modified as the equipment is updated. The work on this system should be continued to facilitate profiling experiments by the efficient utilization of the minicomputer capability for on-line control of these experiments.
1. For recent reviews on inductively-coupled plasma, analytical emission spectroscopy the reader is referred to:


107. R. K. Winge, unpublished data, Ames Laboratory, USERDA, Iowa State University, Ames, IA.


124. R. S. Houk, unpublished dissertation research, Department of Chemistry, Iowa State University, Ames, IA.


127. D. J. Kalnicky, Quarterly Research Reports, Ames Laboratory, USERDA, Iowa State University, Ames, IA.


132. (a) H. Hormann, Z. Physik, 97, 539 (1935).


ACKNOWLEDGEMENTS

More individuals have contributed to the events over the past twenty-seven and one-half years preceding this point in time than I can properly acknowledge; to them my deepest appreciation.

Without the expertise and many long hours contributed by George Holland of the Ames Laboratory Instrument Service Group, the stabilization of the RF generator necessary for the successful completion of this project could not have been accomplished. The unsurpassed skills and superb craftsmanship of the master machinists and glass blowers must also be acknowledged. Gary Wells, Harry Amenson, Tom Johnson, Eldon Ness, and Harold Hall were major contributors to the success of my experiments.

The guidance and critical review of this work by Dr. Velmer A. Fassel and Dr. Richard N. Kniseley is greatly appreciated. The financial support granted me by the National Science Foundation and the Shell Companies Foundation is gratefully acknowledged.

Above all, I am thankful for the loving guidance and encouragement of my parents, Frank and Bess Kalnicky, for had they made another decision some twenty-eight and one-quarter years ago, I would not have been able to begin this project.
APPENDIX A: ABEL INVERSION AND TEMPERATURE PROGRAM

The Abel inversion and radial temperature calculations were performed in a single FORTRAN IV computer program. A complete listing of the source statements of the most recent version of this program is included as C337TEM2. [A Cal-Comp Digital Incremental Plotter could be (optionally) employed off-line to plot the radial intensity and temperature data obtained from this program.] In conjunction with the plotting subroutines (RADPL, TEMP, and SLOPET) in this program, two ISU library programs, GRAPH and GRAPHS, were utilized. These routines were part of the SIMPLOTTER (128) library, which was available for graph production. For an installation without SIMPLOTTER, the RADPL subroutine and the CALL RADPL statement in the main program should be removed. The CALL GRAPH and CALL GRAPHS statements in subroutines TEMP and SLOPET should also be removed. In this manner the program size will be reduced and the plotting capability will be lost. The data card input variable requirements are outlined in Table A-1 and these variables are defined in the beginning of the program listing.

An earlier version of this program (C337TEM1) was also employed for some inversions of the lateral relative intensity profiles obtained for Fe I lines. This earlier program incorporated a different polynomial fitting method in the Abel
inversion subroutine (CBABEL) than the one used in the C337TEM2 subroutine, DKABEL (see Appendix B). An F-test for goodness to fit (81) was incorporated into the latter program; this test sometimes yielded fits of artificially high degree to the bell-type Fe I relative intensity data. Subsequently, erroneous radial temperature profiles were calculated from the resulting intensities, particularly for the observation height of 15 mm. These profiles were recognized by: (1) very large calculation uncertainties for the radial intensities and temperatures obtained (cf., Equation B36, Appendix B), and (2) the peculiar shaped radial intensity and temperature profiles that resulted from these inversions especially at 15 mm. For the latter, unrealistically steep off-axis peaks were sometimes obtained in the toroidal temperature profiles typical for this observation height. These situations were corrected by: (1) employing DKABEL in C337TEM2 but, restricting the fits to be a maximum of 2-nd degree, or (2) employing CBABEL in C337TEM1, which incorporated fixed 2-nd degree fits to all profile zones (cf., Figure B-3, Appendix B) but was more restrictive with respect to data input. For the latter, the lateral relative intensity profiles were required to consist of equally spaced data points in multiples of 5n+1 where, n≥2. It was sometimes difficult to obtain lateral relative intensity data that complied with these criteria. However, in most cases employing the
restricted 2-nd degree (maximum) fits with C337TEM2 remedied the problem, precluding the necessity of resorting to the C337TEM1 method.
Table A-1. Data card requirements for C337TEM2

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<tr>
<td>46-50</td>
<td>LSHIFT</td>
<td>I5</td>
<td>Option to zero correct lateral displacements</td>
<td></td>
<td></td>
</tr>
<tr>
<td>51-60</td>
<td>XZERO</td>
<td>F10.0</td>
<td>Zero position for lateral displacement array (used when LSHIFT = 1 specified)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Type #</td>
<td># Cards</td>
<td>Columns</td>
<td>Variable Name</td>
<td>Format</td>
<td>Remarks</td>
</tr>
<tr>
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</tr>
<tr>
<td>61-65</td>
<td>NFACTR</td>
<td>I5</td>
<td>Weight factor selection for endpoints of spline fits</td>
<td></td>
<td></td>
</tr>
<tr>
<td>66-7C</td>
<td>KWT</td>
<td>I5</td>
<td>Option to select reading uncertainty array for lateral intensities from cards</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9a-2</td>
<td>NPTS/line 1-10</td>
<td>XDIST</td>
<td>F10.0</td>
<td>Smoothed lateral displacement array</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>YINT</td>
<td>F10.0</td>
<td>Corresponding lateral intensity array</td>
<td></td>
</tr>
<tr>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>SIGMAY</td>
<td>F10.0</td>
<td>Corresponding uncertainty array</td>
<td></td>
</tr>
<tr>
<td>9b-1</td>
<td>1/line 1-5</td>
<td>IMA</td>
<td>I5</td>
<td>Number of points in lateral intensity array</td>
<td></td>
</tr>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>6-10</td>
<td>NS1</td>
<td>I5</td>
<td>Defines number of zones for Abel inversion poly fit (same as 9a-1 NS1)</td>
<td></td>
</tr>
<tr>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>XPNT</td>
<td>F10.0</td>
<td>Distance between successive radial intensity calculations (same as 9a-1 ZNPT)</td>
<td></td>
</tr>
<tr>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>XBIG</td>
<td>F10.4</td>
<td>Lateral position of profile maximum</td>
<td></td>
</tr>
</tbody>
</table>

NOTE: Types 9a-1 and 9b-1 are mutually exclusive; 9a-1 is used only with subroutine SPLINE (L2 = 0) and 9b-1 only with subroutine XYCALC (L2 = 1)
<table>
<thead>
<tr>
<th>Type #</th>
<th># Cards</th>
<th>Columns</th>
<th>Variable Name</th>
<th>Format</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>10a</td>
<td>1/set</td>
<td>1-40</td>
<td>GA</td>
<td>4F10.0</td>
<td>OPTIONAL: ( g_{q^*}^{A} ) array for Ar I lines listed in comment card section, used when LKODE = 2 and IARTP &gt; 6</td>
</tr>
<tr>
<td>10b-1</td>
<td>1/set</td>
<td>1-40</td>
<td>EQ</td>
<td>4F10.0</td>
<td>OPTIONAL: Excitation energy of ELNAME lines employed, used when LKODE = 3</td>
</tr>
<tr>
<td>10b-2</td>
<td>1/set</td>
<td>1-40</td>
<td>GA</td>
<td>4F10.0</td>
<td>OPTIONAL: ( g_{q^*}^{A} ) array for ELNAME lines, used when LKODE = 3</td>
</tr>
</tbody>
</table>
*** DEFINITION OF IMPORTANT VARIABLES AND INDEXES USED ***

** CONTROL SWITCHES **

L1 = 0, NO LATERAL OR RADIAL INTENSITY PLOTS
L1 = 1, SUPERIMPOSED PLOTS OF LATERAL AND RADIAL INTENSITY
L2 = 0, MEASURED INTENSITY FIT BY SEGMENTED SPLINE AND ZERO CORRECTED IF NECESSARY (LSHIFT=1)
L2 = 1, SPLINE FIT NOT NECESSARY; SMOOTHED LATERAL PROFILE (ZERO CORRECTED) SUPPLIED AND SUBROUTINE XYCALC USED
L3 = 0, AVERAGE LINE PAIR TEMPERATURE AND PLOT
L3 = 1, TEMPERATURES OF INDIVIDUAL LINE PAIRS AND PLOT
L5 = 0, TEMPERATURES CALCULATED FROM I(X) & I(R) DATA
L5 = 1, ONLY RADIAL INTENSITIES CALCULATED---TEMP BY-PASSED

F - TEST FOR 0.5 TO 50.0 PERCENT PROBABILITY OF EXCEEDING THE F-VALUE; NL DEFINES THE LOWER LIMIT, NH DEFINES UPPER LIMIT
MAX NH=7, MIN NL=1

PERCENT  NL  ALLOWED NH VALUES
0.5      1  1,2,3,4,5,6,7
1.0      2  2,3,4,5,6,7
2.5      3  3,4,5,6,7
5.0      4  4,5,6,7
10.0     5  5,6,7
25.0     6  6,7
50.0     7  7

Lkode = 1, FE LINES USED
Lkode = 2, AR LINES USED
Kplot1 = 7, ALL 2-LINE T'S NOT PLOTTED
Kplot2 = 1, AVE. 2-LINE T'S NOT PLOTTED
Kplot3 = 1, SLOPE T NOT PLOTTED
Kline1 < 2, ALL 2-LINE T'S PLOTTED
    = 2, 1ST 2-LINE T NOT PLOTTED
    = 3, 1ST, 2ND 2-LINE T'S NOT PLOTTED
    = 4, 1ST, ....3RD 2-LINE T'S NOT PLOTTED
    = 5, 1ST, ....4TH " " " "
    = 6, 1ST, ....5TH " " " "
    = 7, ALL NOT PLOTTED
Kline2 > 7, ALL NOT PLOTTED

Kline2 = 0, ALL 2-LINE T'S PLOTTED
    = 1, 1ST LP T NOT PLOTTED
    = 2, 2ND " " "
    = 3, 3RD " " "

0 = 5
1 = 0
2 = 3, 4, 5, 6, 7
3 = 2, 4, 5, 6, 7
4 = 2, 4, 5, 6, 7
5 = 2, 4, 5, 6, 7
6 = 2, 4, 5, 6, 7
7 = 2, 4, 5, 6, 7
8 = 2, 4, 5, 6, 7
9 = 2, 4, 5, 6, 7
10 = 2, 4, 5, 6, 7

11 = 2, 4, 5, 6, 7
12 = 2, 4, 5, 6, 7
13 = 2, 4, 5, 6, 7
14 = 2, 4, 5, 6, 7
15 = 2, 4, 5, 6, 7
16 = 2, 4, 5, 6, 7
17 = 2, 4, 5, 6, 7
18 = 2, 4, 5, 6, 7
19 = 2, 4, 5, 6, 7
20 = 2, 4, 5, 6, 7
21 = 2, 4, 5, 6, 7
22 = 2, 4, 5, 6, 7
23 = 2, 4, 5, 6, 7
24 = 2, 4, 5, 6, 7
25 = 2, 4, 5, 6, 7
26 = 2, 4, 5, 6, 7
27 = 2, 4, 5, 6, 7
28 = 2, 4, 5, 6, 7
29 = 2, 4, 5, 6, 7
30 = 2, 4, 5, 6, 7
31 = 2, 4, 5, 6, 7
32 = 2, 4, 5, 6, 7
33 = 2, 4, 5, 6, 7
34 = 2, 4, 5, 6, 7
35 = 2, 4, 5, 6, 7
36 = 2, 4, 5, 6, 7
37 = 2, 4, 5, 6, 7
38 = 2, 4, 5, 6, 7
39 = 2, 4, 5, 6, 7
40 = 2, 4, 5, 6, 7
41 = 2, 4, 5, 6, 7
42 = 2, 4, 5, 6, 7
43 = 2, 4, 5, 6, 7
44 = 2, 4, 5, 6, 7
45 = 2, 4, 5, 6, 7
46 = 2, 4, 5, 6, 7
47 = 2, 4, 5, 6, 7
48 = 2, 4, 5, 6, 7
49 = 2, 4, 5, 6, 7
50 = 2, 4, 5, 6, 7
$C = 4$, 4TH "" ""
$C = 5$, 5TH "" ""
$C = 6$, 6TH "" ""

> 6, ALL 2-LINE T'S PLOTTED

$\text{KPNED}1 = 1$, LATERAL SLOPE T'S PUNCH ON CARDS FOR USE IN
THE ELECTRON DENSITY PROGRAM ($\text{C337EDEN}$).

$\text{KPNED}2 = 1$, RADIAL SLOPE T'S PUNCH ON CARDS FOR USE IN
THE ELECTRON DENSITY PROGRAM ($\text{C337EDEN}$).

$\text{IARTP} = 1$, MALONE AND CORCORAN GA VALUES: ARGON LINES
$\text{IARTP} = 2$, WUJEC GA
$\text{IARTP} = 3$, ADDOCK AND PLUMTREE GA
$\text{IARTP} = 4$, CORLISS AND SHUMAKER GA
$\text{IARTP} = 5$, WENDE GA
$\text{IARTP} = 6$, GERICKE GA

> 6, READ IN GA DATA CARD AT END OF DATA DECK.

4F10.0 FORMAT
ARGON LINES USED: 4251.2, 4259.4, 4266.3, 4272.2 ANGS

$\text{LKODE} = 1$, IARTP=9, BANFIELD AND HUBER (1973) GA VALUES
USED FOR FE I LINES

$\text{LKODE} = 99$, INPUT SPECIES IDENTIFIER AS ELNAME AND READ IN
GA,EQ VALUES FOR SLOPE TEMP CALCULATION
(TEMP CALCN OPTIONAL, SEE LS SPECIFICATION)

**ARRAYS**

$\text{RBP}$ = EXPERIMENTALLY MEASURED LATERAL DISTANCE ARRAY
$\text{ARI}$ = "" PEAK INTENSITY ARRAY
$\text{N}$ = NUMBER OF ELEMENTS IN 'RBP' OR 'ARI' ARRAY (NOT MORE
$\text{XDIST} =$ MEASURED AND SMOOTHED LATERAL DISTANCE ARRAY,
ORIGIN ZERO SHIFT CORRECTED WITH RESPECT TO
EXPT MEASURED RBP ARRAY SO THAT XDIST=0
CORRESPONDS TO GEOMETRIC CENTER
$\text{YINT} =$ CORRESPONDING MEASURED AND SMOOTHED LATERAL INTENS
$\text{SIGMAY} =$ CORRESPONDING ARRAY OF SIGMA VALUES FOR YINT
$\text{RAD} =$ INTERMEDIATE RADIAL INTENSITY ARRAY
$\text{RDI} =$ "" DISTANCE "" CORRESPONDING TO 'RAD' ARRAY
$\text{RADINT} =$ FINAL RADIAL DISTANCE ARRAY CONTAINING ELEMENTS
CORRESPONDING TO 'RADINT' ARRAY

**INDEXES**

$\text{KT} =$ NUMBER OF ELEMENTS IN 'RAD' OR 'ARI' ARRAY
NSETS = NUMBER OF SETS OF PROFILE DATA TO BE PROCESSED
INDEX FOR PRIMARY DO LOOP
NLZ = NUMBER OF LINES USED (NOT MORE THAN 4)
LAM = DATA ARRAY INDEX FOR PRIMARY DO LOOP
LZ = SPECTRAL LINE INDEX FOR PRIMARY DO LOOP
NOTE:
  LZ = 1, CORRESPONDS TO Fe-I- 3815.84 ANGSTROMS
  LZ = 2 " " 3820.43 "
  LZ = 3 " " 3824.44 "
  LZ = 4 " " 3825.88 "
  THIS LABELLING MUST BE RIGOROUSLY FOLLOWED IN ORDER
  THAT THIS PROGRAM FUNCTION PROPERLY

** INPUT CONSTRAINTS AND VARIABLES **

IMA = NUMBER OF SMOOTHED DATA POINTS IN ARRAY 'XDIST' OR
      (NOT MORE THAN 51)
NS1=3, 3 ZONE POLY FIT
NS1=4, 4 ZONE POLY FIT
NS1=5, 5 ZONE POLY FIT
IWT=0, NO WEIGHTING ON POLY FIT
=1, YINT VALUES WEIGHTED WITH SIGMA Y ARRAY
XPNT = RADIAL DISTANCE (MM) BETWEEN TWO SUCCESSIVELY CALC
      RADIAL INTENSITIES = R(N+1) - R(N)
WAVE = WAVELENGTHS OF SPECTRAL LINES (ANGSTROMS)
XBIG=POSITION OF INT MAX IN LATERAL DIST ARRAY (SUPPLIED
      AS INPUT WHEN SPLINE NOT USED IE., XVCALC USED)
      FOLLOWING INPUT CODES NECESSARY ONLY WHEN SUBROUTINE SPLINE US
      KWT=1, INPUT ARRAY OF INTEN SIGMAS FOR POLY FIT
      0, SIGMAS SET =1.0 IN POLY FIT
      NFACTR=1, SPLINE FIT ENDPONITS X 0.825
      NFACTR=2, " " X 0.850
      NFACTR=3, " " X 0.875
      NFACTR=4, " " X 0.900
      NFACTR=5, " " X 0.925
      NFACTR=6, " " X 0.950
      LSHIFT=1, LATERAL INTENSITIES ZERO CORRECTED BY XZERO
      XZERO=POSITION OF GEOMETRIC CENTER ON ORIGINAL LATERAL
      DISPLACEMENT SCALE
      NPTS=NUMBER OF POINTS FOR SEGMENTED SPLINE FIT
      **** NPTS MUST BE GREATER THAN OR EQUAL TO 10

DIMENSION OLAB(5),TITLE(15),WAVE(4),XDTR(51),RBP(15,4),ARI(15,4),
1 SIGMAY(51),DI(51),INT(51),RAD( 51),RADINT( 51,4,7)
2,RADIST( 51,4,7),ILZ(4,7),XBIG(4),DELA(4),DELIR(51),DELINT(51,4,7)
3),FNUM(7),ELNAME(5)
DATA FNUM/0.5,1.0,2.5,5.0,10.0,25.0,50.0/
READ (5,100) NSETS
103 FORMAT (15)
DO 10 NUM=1,NSETS
READ (5,100) TITLE,DLAB
100 FORMAT (15A4,5A4)
WRITE (6,101) TITLE,DLAB
101 FORMAT (1H1,10X,15A4,5A4///)
READ (5,100) NLZ,IVT
1000 FORMAT (2IS)
1001 FORMAT (2I5,S4)
READ( 5.1001) LKODE.IARTPoELNAME
READ(5.100) NLZ.IWT
iOOO FORMAT(2IS) 161
nOOl FORMAT(2I5,SAA) 162
READ (5.102) ( KAVE( I ) , 1 =
356 1
362 .NL.Î ) . (OELA< J) . J=1 ,NLZ ) 163
102 FORMAT (4F7.2"2X.4F1O .O)
CALL LINDEX ( I. 1 ,L2 ,L3 . L4 » L5 . HL , NH . KPLOT1 . KPLaT2 .KPLOT3 . KLINE1 ,
1KLNE2. KPNE01. KPNE02)
READ (5.106) N
106 FORMAT (12)
DO 1 J=1,NLZ
107 FORMAT (2F10.0)
DO 1 I=1,NLZ
1 DO I=1,N
107 FORMAT (2F10.0)
1 READ (5.107) RBP(I,J),ARI(I,J)
1 DO 8 LZ=1,NLZ
LAM=1
CALL PNTORG(LZ,KM,WAVE,RBP,ARI,N,LKODE,ELNAME)
GO TO (2,3),L2
2 CALL SPLINE (IMA,NS1.XDIV.XDIST.YINT,LAM,XPNT,LZ,XDTR,XD.XBIG.SIGM
1AY,WAVE,IVT)
GO TO 4
3 CALL XYCALC (IMA,NS1.XDIV.XDIST.YINT,LAM,XPNT,LZ,XDTR,XD.XBIG.SIGM
1AY)
4 DO 8 NZ=NL,NH
CALL DKABEL (XDTR,YINT,IMA,NS1,NZ,XPNT,RAD,LDI,KM,XD.XBIG,LZ,DELIR
1SIGMAY.L1.IWT)
IF(KPNE02.NE.1) GO TO 5
DO 199 IPUNCH=1,KT
2001 FORMAT(3F10.4,2X,'LINE*','L1.3X,'FTEST PROB*','F5.2,I X,5A4)
199 WRITE(7,2001) RAD(IPUNCH),RD1(IPUNCH),DEL1(IPUNCH),LZ,FNUM(NZ),DL
1AB
5 GO TO (7*6),L
6 CALL RADPL (IMA,XDIST,YINT,N,RBP,ARI, LZ,RAD,LDI,LAM, DLA
18,KT,NZ)
7 CALL PNTMAP (LZ,KT,RAD,LDI,KM,ILZ,RADINT,RADIST,DELIR,DELINT)
8 CONTINUE
11 GO TO (9,10),L5
9 CALL TEMP (N,KT,RBP,ARI,RADIST,RADINT,NLZ.DLAB,L3,KM,NL,NH,LKODE,
1KPL0T1.KPL0T2,KLINE1,KLINE2,DEL1,DELINT,IARTP)
13 CALL SLOPET (N,KT,RBP,ARI,RADIST,RADINT,NLZ.DLAB,WAVE,KM,NL,NH,LK0
10E,KPL0T3,KPNE01,KPNE02,DEL1,DELINT,IARTP)
10 CONTINUE
STOP
END

SUBROUTINE LINDEX (L1,L2,L3,L4,L5,NL,NH,KPLOT1,KPLOT2,KPLOT3,
  KLINE1,KLINE2,KPNE11,KPNE2)

READ (5,101) L1,L2,L3,L4,L5,NL,NH,KPLOT1,KPLOT2,KPLOT3,KLINE1,
  KLINE2,KPNE11,KPNE2

101 FORMAT(145)

L4=1
1 IF (NL) 4,3,1
2 IF (NH-NL) 4,2,2
3 IF (NH) 4,5,4
5 NL=1
6 NH=1
2 IF (L4) 6,6,7
7 IF (L1) 8,10,10
10 IF (L3) 8,11,11
L1=L1+1
L2=L2+1
L3=L3+1
L5=L5+1
RETURN

4 WRITE (6,102)
GO TO 12
6 WRITE (6,103)
GO TO 12
8 WRITE (6,104)
12 STOP

102 FORMAT (//10X'INPUT ERROR IN SWITCH NL OR NH'
)

104 FORMAT (//10X'INPUT ERROR IN SWITCH L1 OR L3'
)

END

SUBROUTINE PNTORG(LZ,KM,WAVE,RBP,ARI,N,LKODE,ELNAME)

DIMENSION ELNAME(5)
DIMENSION WAVE(1),RBP(15,4),ARI(15,4)
KM=0

1 WRITE (6,100)
GO TO 12
2 WRITE (6,101) LZ,WAVE(LZ)
GO TO 6
3 WRITE (6,102) LZ,WAVE(LZ)
GO TO 6
4 WRITE (6,103) LZ,ELNAME,WAVE(LZ)
GO TO 6
5 WRITE (6,104) LZ,ELNAME,WAVE(LZ)
GO TO 6
6 WRITE (6,105) LZ,ELNAME,WAVE(LZ)

100 FORMAT (5X,'LINE',I3,5X,5A4,F7.2,'/14X','EXPERIMENTALLY MEASURED LATERAL INTENSITY DATA'/21X,'CORRECTED FOR SPECTRAL RESPONSE'/26X,'X
2*11X,'I(X3'//) 210 FORMAT (145)
SUBROUTINE XVCALC (IMA, NS1, XDI V, XDI ST, Y INT, LAM, XPNT, LZ, XBIG, SIGMAY)

DIMENSION XDI ST(1), YINT(1), XBIG(4), XDTR(1)
READ (5, 100) IMA, NS1, XPNT, XBIG(LZ)

IF (XBIG(LZ) .LT. 0.0) GO TO 8
IF (LAM - 1) .LT. 2, 2, 1
WRITE (6, 101)
WRITE (6, 102) IMA
102 FORMAT (2F10.4)
WRITE (6, 103) XDI ST(I), YINT(I), SIGMAY(I)
WRITE (6, 104) XDTR(I) = XDTR(C2) - XDTR(C1)
XPNT = XPNT / XDTR(I)
RETURN
8 WRITE (6, 105)
105 FORMAT (10X 'ERROR IN XBIG INPUT')
STOP
END

SUBROUTINE PNTMAP (LZ, KT, RAD, RDI, KM, ILZ, RADINT, RADIST, DELIR, DELINT)

DIMENSION RAD(1), RDI(1), RADINT(51, 4, 7), RADIST(51, 4, 7), ILZ(4, 7)
KTHOLD = KT
KM = KM + 1
WRITE (6, 100) LZ, KT
DO 4 I = 1, 5
IF (KT - 30*I) .GT. 1
J = KT / I
IF (J .GT. 3) I = 3
RETURN
4 WRITE (6, 101)
101 FORMAT (10X 'ERROR IN KT')
STOP
END
2 J = J + 1
3 GO TO (5, 6, 7, 8, 9), I
4 CONTINUE
5 WRITE (6, 101)
6 GO TO 10
7 WRITE (6, 102)
8 WRITE (6, 103)
9 WRITE (6, 104)
10 DO 16 L = 1, J
   11 L1 = L + J
   12 L2 = L + 2 * J
   13 L3 = L + 3 * J
   14 L4 = L + 4 * J
15 GO TO (11, 12, 13, 14, 15), I
16 CONTINUE
20 INZERO = 0
21 DO 20 IN = 1, KT
22 RDI(IN) = XHOLD(IN)
INZERO = INZERO + 1
YHOLD(INZERO) = RAD(IN)
23 CONTINUE
24 IF (RDI(IN) .LT. 0.) GO TO 22
25 DO 21 IOUT = 1, INZERO
26 RAD(IOUT) = YHOLD(IOUT)
27 RDI(IOUT) = XHOLD(IOUT)
28 KT = INZERO
29 I1Z(LZ, KM) = KT
30 GO TO (5, 6, 7, 8, 9), I
31 CONTINUE
32 WRITE (6, 1000)
33 FORMAT (1H1)
34 WRITE (6, 1001)
35 FORMAT (20X, 'J', 8X, 'LZ', 8X, 'KM', 8X, 'RADIST(J, LZ, KM)', 6X, 'RADINT(J, LZ, KM)', 6X, 'DELINT(J, LZ, KM)')
36 IF (RDI(1) .GE. 0.) GO TO 22
37 INZERO = 0
38 DO 20 IN = 1, KT
39 IF (RDI(IN) .LT. 0.) GO TO 20
40 INZERO = INZERO + 1
41 XHOLD(INZERO) = RDI(IN)
42 YHOLD(INZERO) = RAD(IN)
43 CONTINUE
44 DO 21 IOUT = 1, INZERO
45 RAD(IOUT) = YHOLD(IOUT)
46 RDI(IOUT) = XHOLD(IOUT)
47 KT = INZERO
48 11Z(LZ, KM) = KT
49 STOP
DO 17 I=1,KT
J=KT-I+1
RADIST(J+LZ+KM)=RDI(I)
RADINT(J+LZ+KM)=RAD(I)
DELINT(J+LZ+KM)=DELI(1)
WRITE (6,1002) J,LZ,KM,RADIST(J,LZ,KM),RADINT(J+LZ+KM),DELINT(J+LZ+KM)
1002 FORMAT (20X,3(I3,8X),3(E11.4,10X))
RAD(I)=0.0
KT=KTHOLO
RETURN
17 RDI(I)=0.0
RETURN
END

SUBROUTINE SPLINE (IMA,NS1,ZDIX,ZDIST,ZINT,LAM,ZPNT,LZ,ZDIST,ZBI
I,ZSIG,ZWAVE,INT)
IMPLICIT REAL*8(B-H,O-Y)
DIMENSION ZDIST(1),ZINT(1),ELEMNT(5),ZSIG(1),ZWAVE(1),FACTOR(6),YO
IUT=(10I+3),YINT(51),XDIST(51),SIGMA(51),YMD(50,3),SIGMAS(50),ZDTR
WAVECLZ)=ZWAVE(LZ)
I=LZ
CALL READS(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)
IUT=KWT
CALL INTERP(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)

EXECUTE SPLINE: FIT AND VARIANCE ESTIMATE FOR MIDPTS FOR EACH LINE:
TOT SIGMA = SQRT(FIT SIGMA**2+DATA SIGMA**2) DATA SIGMA IS TAKEN AS AVERAGE OF SIGMA OF FOUR HIGH BORING DATA POINTS EXCEPT FOR THE ENDPOINTS WHERE IT IS TAKEN AS THE AVERAGE OF THE ENDPOINT SIGMA AND THE TWO ADJACENT INTERIOR POINT SIGMA VALUES
WAVE(LZ)=ZWAVE(LZ)
I=LZ
CALL READS(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)
IUT=KWT
CALL INTERP(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)

DATA FACTOR/D,82500,0.8500,0.87500,0.90000,0.92500,0.95000/

EXECUTE SPLINE: FIT AND VARIANCE ESTIMATE FOR MIDPTS FOR EACH LINE:
TOT SIGMA = SQRT(FIT SIGMA**2+DATA SIGMA**2) DATA SIGMA IS TAKEN AS AVERAGE OF SIGMA OF FOUR HIGH BORING DATA POINTS EXCEPT FOR THE ENDPOINTS WHERE IT IS TAKEN AS THE AVERAGE OF THE ENDPOINT SIGMA AND THE TWO ADJACENT INTERIOR POINT SIGMA VALUES
WAVE(LZ)=ZWAVE(LZ)
I=LZ
CALL READS(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)
IUT=KWT
CALL INTERP(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)

DATA FACTOR/D,82500,0.8500,0.87500,0.90000,0.92500,0.95000/

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WAVE(LZ)=ZWAVE(LZ)
I=LZ
CALL READS(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)
IUT=KWT
CALL INTERP(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMA,YL,NS1,ZPNT,KW)
DO 10 N=3,NPTSS
J=N-1
JJ=N-2
NN=N+1
SIGMAS(J)=YMI(D(J,3)
SIG=(SIGMAY(J)+SIGMAY(J)+SIGMAY(N)+SIGMAY(NN))/4.DO
10 YMI(D(J,3)=DSQRT(SIGMAS(J)**2+SIG**2)
N=NPTSS-1
SIGMAS(NPTSS)=YMI(D(NPTSS,3)
SIG=(SIGMAY(N)+SIGMAY(NPTSS)+SIGMAY(NPTSS))/3.DO
YMI(D(NPTSS,3)=DSQRT(SIG**2+SIGMAS(NPTSS)**2)
NUP=NPTS+NPTS-1
DO 30 N=1,NUP
NN=(N/2)*2
IF(NN.NE.N) GO TO 25
LL=N/2
DO 24 L=1,3
24 YOUT(N,L)=YMI(D(LL,L)
GO TO 30
25 LLL=(N+1)/2
YOUT(N,1)=XDIST(LLL)
YOUT(N,2)=YINT(LLL)
YOUT(N,3)=SIGMAY(LLL)
30 CONTINUE

CORRECT YOUT FOR ZERO SHIFT
ITAG=0
IF(LSHIFT.NE.1) GO TO 41
JSTART=1
DO 40 J=1,NUP
YOUT(J,1)=YOUT(J,1)-XZERO
IF(YOUT(J,1).GE.0.0) GO TO 40
JSTART=J+1
40 CONTINUE
41 IF(LSHIFT.NE.1) JSTART=1
DO 45 J=JSTART,NUP
ITAG=ITAG+1
ZDIST(ITAG)=YOUT(J,1)
ZINT(ITAG)=YOUT(J,2)
45 ZSIG(ITAG)=YOUT(J,3)
IMA=ITAG

DETERMINE POSITION OF MAX IN LATERAL INTENSITY ARRAY
ZBIG(LZ)=ZDIST(3)
DO 60 J=4,IMA
JJJ=J-1
IF(ZINT(J).GE.ZINT(JJJ)) ZBIG(LZ)=ZDIST(J)
60 CONTINUE
IF(LAM-1) 65,65,64
64 WRITE(6,1000)
1000 FORMAT(1HI)
65 WRITE(6,1001) IMA
1001 FORMAT(/,1AX,'LATERAL INTENSITY DISTRN HAS BEEN FIT BY SEGMENTED 14X,'RESU
LING LATERAL DATA HAS BEEN ZERO CORRECTED FOR',13,2X,'POINTS',/)
DO 66 J=1,IMA
325,*X',T38,*U(X)',*T60,'SIGMA/U(X)'//
66 WRITE(6,1002) ZDIST(J),ZINT(J),ZSIG(J)
67 ZDIST(J)=ZDIST(J)/ZD
DO 67 J=1,IMA
68 ZPNT=ZPNT/ZD
RETURN
END
SUBROUTINE READS (NPTS,YEND,XDIST,ELEMNT,WAVE,XZERO,LSHIF
IT,SCHK,NFACTR,KWT)
IMPLICIT REAL*8(A-H,O-Y)
DIMENSION VINT(1),XDIST(1),ELEMNT(5),WAVE(1),SIGMAY(1)
READ INPUT X,Y PAIRS FOR LINE I
READ(5,100) NPTS,NS1,ELEMNT,YINT,LSHIFT,XZERO,NFACTR,KWT
100 FORMAT(2IS5,5X,5A4,F10.0,15,F10.0,215)
DO 10 J=1,NPTS
10 READ (5,101) KDIST(J),YINT(J),SIGMAY(J)
SCHK=XDIST(NPTS)
RETURN
END
SUBROUTINE INTERP (NPTS,YINT,XDIST,I,SCHK,YMID,NFACTR.FACTOR)
IMPLICIT REAL*8(A-H,O-Y)
DIMENSION YINT(1),XDIST(1),YMID,YPNT(5),SIGMA(5)
DO 5 J=1,35
YAVE(J)=0.DO
5 SIGMA(J)=0.DO
KOUNT=0
DO 999 J=1,NPTS
999 CONTINUE
IF(JT>NPTS) GO TO 9999
WRITE (6,888)
DO 10 J=1,35
YAVE(J)=0.DO
KOUNT=0
DO 999 J=1,NPTS
999 CONTINUE
IF(JT>NPTS) GO TO 9999
WRITE (6,888)
888 FORMAT (//(T25,*********** TRANSFER ERROR IN XDIST(NPTS) TO INTERP
1. END RUN **********)
STOP
6 KOUNT=KOUNT+1
HSIZE=1.0D0/3.0D0
K=J+1
YMID(KOUNT,1)=(XDIST(J)+XDIST(K))/2.0
XNORM(1)=-HSIZE
DO 10 L=2,6
XL=L-2
10 XNORM(L)=XL*HSIZE
YNORM(1)=FACTR(NFACTR)*YINT(KOUNT)
11 L=KOUNT
DO 20 LL=2,6
L=L+1
20 YNORM(LL)=YINT(L)
YNORM(6)=FACTR(NFACTR)*YNORM(6)
CALL MATRIX INVERSION ROUTINE TO SOLVE FOR SPLINE COEFFICIENTS AND
CALCULATE MIDPOINT X VALUES AND SPLINE FIT INTENSITY VALUES
29 CALL XMATRIX(6,YNORM,COEF,I,HSIZE,KOUNT)
DO 30 LL=2,6
L=LL-1
30 XMID(LL)=(XNORM(LL)+XNORM(L))/2.0
CALL CALCY(I,6,COEF,XMID,HSIZE,YHOLD,KOUNT)
XINC=XDIST(2)-XDIST(1)
DO 40 JJ=1,4
JJJ=KOUNT+JJ
XJJ=JJ
40 YMID(JJJ,1)=YMID(KOUNT,1)+(XJJ*XINC)
DO 50 L=1,5
L=LL-KOUNT+L-1
50 YAVE(LL)=YAVE(LL)+YHOLD(LL)
50 YAVE(LL)=YAVE(LL)+YHOLD(LL)
CALL DEFINE STORAGE ARRAY 'YSTOR' FOR SIGMA CALCULATION
85 IF(KOUNT*LT=5) GO TO 100
DO 90 N1=1,5
N2=N1-1
N3=KOUNT-N2
YSTOR(KOUNT,N1)=YHOLD(N3,N1)
90 CONTINUE
KN=NPTS-5
IF(KOUNT*LT*KN) GO TO 999
DO 91 N1=1,4
N2=KOUNT+N1
N3=N1+1
91 CONTINUE
DO 91 NNN=NN,5
  N3=NNN-N1
  N4=KOUNT+1-N3
  91 YSTOR(N2,N3)=YHOLD(N4,NNN)
  GO TO 999
100 IF(KOUNT.GT.1) GO TO 101
  YSTOR(1,1)=YHOLD(1,1)
  GO TO 999
101 DO 102 NI=1,KOUNT
  N2=NI-1
  N3=KOUNT-N2
  102 YSTOR(KOUNT,N1)=YHOLD(N3,N1)
999 CONTINUE
C
CALCULATE SIGMA AND STORE 'YAVE' AND 'SIGMA' IN 'YMIJ' AS
C
YMIJ(J,2) AND YMIJ(J,3), RESPECTIVELY
C
9999 J=NPTS-1
  DO 70 JJ=1,J
    IF(JJ.LT.5) GO TO 57
    KK=NPTS-5
    IF(JJ.GT.KK) GO TO 65
    YMIJ(JJ,2)=YAVE(JJ)/5.DO
    DO 56 II=1,5
      SIGMA(JJ)=(YSTOR(JJ,II)-YMIJ(JJ,2))**2
      SIGMA(JJ)=DSQRT(SIGMA(JJ)/4.DO)
      YMIJ(JJ,3)=SIGMA(JJ)
      GO TO 70
  57 XJJ=JJ
  YMIJ(JJ,2)=YAVE(JJ)/XJJ
  IF(JJ.LT.1) GO TO 58
  YMIJ(JJ,3)=0.DO
  GO TO 70
58 DO 59 II=1,JJ
  SIGMA(JJ)=YSTOR(JJ,II)-YMIJ(JJ,2))**2
  XII=XJJ-1.DO
  SIGMA(JJ)=DSQRT(SIGMA(JJ)/XII)
  YMIJ(JJ,3)=SIGMA(JJ)
  GO TO 70
59 XXK=NPTS-JJ
  YMIJ(JJ,2)=YAVE(JJ)/XXK
  IF(JJ.LT.J) GO TO 66
  YMIJ(JJ,3)=0.DO
  GO TO 70
65 III=NPTS-JJ
  DO 67 II=1,III
    SIGMA(JJ)=(YSTOR(JJ,II)-YMIJ(JJ,2))**2
    XII=III-II
    SIGMA(JJ)=DSQRT(SIGMA(JJ)/XII)
    YMIJ(JJ,3)=SIGMA(JJ)
  67 CONTINUE
SUBROUTINE KMATRX(NPTS, YINT, COEF, I, HSIZE, KOUNT)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION YINT(6), S(6,6), COEF(6,4), SCALC(6,6), SOUT(36), YCAL(6)

DETERMINE COEFS OF SPLINE FIT WITH FORTRAN SSP ROUTINE 'DGELG' AND RETURN TO INTERP AS 'COEF.'

DO 10 M=1,NPTS
   DO 10 L=1,NPTS
      K=M-L
      J=L-M
      IF(K.EQ.1) GO TO 8
      IF(J.EQ.1) GO TO 8
      IF(L.EQ.M) GO TO 9
      S(M,L)=0.0
      GO TO 10
8   S(M,L)=0.25D0
     GO TO 10
9   S(M,L)=1.0
10 CONTINUE
   DO 15 J=1,NPTS
      DO 15 K=1,NPTS
         SCALC(J,K)=S(J,K)
   DO 16 J=1,NPTS
      YCALC(J)=YINT(J)
   IF(NPTS.EQ.6) GO TO 25
      IX=0
      DO 17 L=1,NPTS
         DO 17 K=1,NPTS
            IX=IX+1
   17 SOUT(IX)=SCALC(K,L)
      GO TO 26
25 CALL DGELG (YCAL,SCALC,6,1,1,0.E-16,IER)
      GO TO 27
26 CALL DGELG (YCAL,SOUT,NPTS,1,1,0.E-16,IER)
27 CONTINUE
   DO 30 K=1,NPTS
      COEF(K,I)=YCAL(K)
      IF(IER.NE.0) GO TO 99999
   RETURN
99999 WRITE(6,2000) IER,KOUNT
2000 FORMAT(///,15,****IER = '',I3.2X,'KOUNT = '',I4)
RETURN
END

SUBROUTINE CALCGY (I,NPTS, COEF, XMID, HSIZE, YHOLD, KOUNT)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION X(5), F(5), COEF(6,4), XMID(5), YHOLD(50,5)
CALCULATE MIDPOINT INTERPOLATED VALUES AND RETURN TO 'INTERP' AS
ARRAY 'YHOLD'

DO 10 J=1,5
10 X(J)=XMD(J)
DO 20 J=1,5
F(J)=0.D0
DO 15 K=1,NPTS
XK=K
X1=X(J)-((XK-2.D0)*HSIZE)
HL=-2.D0*HSIZE
HU=2.D0*HSIZE
IF(X1.GE.HL) GO TO 11
F(J)=F(J)+0.D0
GO TO 15
11 H=-HSIZE
IF(X1.GT.H) GO TO 12
F(J)=F(J)*((X1+(2.D0*HSIZE)***3.D0)/(4.D0*(HSIZE**3.D0)))*COEF(K,I)
GO TO 15
12 IF(X1.GT.0.D0) GO TO 13
TERM=((X1+HSIZE)**3.D0)+((3.D0*(HSIZE**2.D0))*(X1+HSIZE))+(3.D0*HSIZE)
1=((X1+HSIZE)**3.D0)-(3.D0*(X1+HSIZE)**3.D0))
TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)
F(J)=F(J)+TERM
GO TO 15
13 IF(X1.GT.HSIZE) GO TO 14
TERM=(HSIZE**3.D0)+((3.D0*(HSIZE**2.D0))*(HSIZE-X1))+(3.D0*HSIZE)
1=((HSIZE-X1)**3.D0)-(3.D0*(HSIZE-X1)**3.D0))
TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)
F(J)=F(J)+TERM
GO TO 15
14 IF(X1.GT.H) GO TO 16
TERM=((2.D0*HSIZE)-X1)**3.D0
TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)
F(J)=F(J)+TERM
GO TO 15
16 F(J)=F(J)+0.D0
15 CONTINUE
20 CONTINUE
DO 40 N=1,5
40 YHOLD(KOUNT,N)=F(N)
RETURN
END
3) ROST(5)
DATA NTAG/1.0,0.0,0.0,
DATA ROST/1.0,0.1,0.1,0.1,0.1/)
WRITE (6,1000)
1000 FORMAT (///.,'INPUT DATA TRANSFERRED TO DKABEL')
WRITE (6,1001)
DO 100 IDEX=1,IMA
100 FORMAT (///.,I20,T20,E11.4,T50,E11.4)
100 WRITE (6,1002) IDEX,XDTR,IDEX,T50,YINT(IDEX)
DO 5 J=1,5
SEGEND(J)=0.0
DO 5 I=1,5
COEF(I,J)=0.0
5 DELCOF(I,J)=0.0
C
C SET UP ZONE SEGMENTS FOR POLY FIT (3 TO 5 ZONES)
C
NSEGS=NS1
XBIG(LZ)=XBIG(LZ)/XD
IF(NSEGS<4) 10,25,29
10 CHECK=XBIG(LZ)-0.3333333
CHECK=ABS(CHECK)
IF(CHECK<0.100) GO TO 12
IF(XBIG(LZ)-0.3333333)<11.1,11
11 SEGEND(1)=0.450
SEGEND(2)=0.750
SEGEND(3)=1.000
NSEGS=3
GO TO 30
12 CHECK=XBIG(LZ)-0.6666667
CHECK=ABS(CHECK)
IF(CHECK<0.100) GO TO 14
IF(XBIG(LZ)-0.6666667)<13.1,14
13 SEGEND(1)=0.350
SEGEND(2)=0.750
SEGEND(3)=1.000
NSEGS=3
GO TO 30
14 IF(XBIG(LZ)-0.2333333)<15.1,15
15 SEGEND(1)=0.3333333
SEGEND(2)=0.6666667
SEGEND(3)=1.000
NSEGS=3
GO TO 30
16 IF(XBIG(LZ)-0.6666667)<17.1,17
17 IF(XBIG(LZ)-0.4333333)<18.1,19
18 SEGEND(1)=0.250
SEGEND(2)=0.650
SEGEND(3)=1.000
CALL ROUTINE SEGMENT FOR ZONE COEFS AND SIGMA VALUES
CALL SEGMENT (XDR,TINT,IMA,N51,NSEG,NZ,COEF,DELCOF,SEGEND,SIGMAY,
INTAG,IWT)
DO 35 I=1,IMA
XAI(I)=XDR(I)
35 YAI(I)=YINT(I)

COMPARE CALCULATED TO INPUT Y VALUES FOR EACH ZONE
WRITE (6,2000)
2000 FORMAT (///,T10,'REGION',T22,'DIST',T33,'CALCY',T45,'REALY',T56,
'I*DIFF',T73,'PERCENT',T88,'AVE PERCENT',T102,'WEIGHTED STD DEV')
IMSI=INTAG(I)
NSEGS=NSEG
IZONE=1
SUMCT=0.0
SUNERR=0.0
AVEDEV=0.0
YSUM=0.0
DO 75 I=1,IMA
XCHEC2=XA(I)*XAI(I)
XCHEC4=XCHEC2*XCHEC2
XCHEC6=XCHEC4*XCHEC2
XCHEC8=XCHEC6*XCHEC2
YCHECK(I,1)=COEFT(I,1)+(COEFT(2,1)*XCHEC2)+(COEFT(3,1)*XCHEC4)+(COEFT(14,1)*XCHEC6)+(COEFT(5,1)*XCHEC8)
DIFY(I)=YA(I)-YCHECK(I,1)
PERCNT(I)=DIFY(I)*100./YA(I)
PERCNT(I)=ABS(PERCNT(I))
SUMPC1=SUMPC1+PERCNT(I)
SUMERR=SUMERR+(DIFY(I)*DIFY(I)/YA(I))
AVEDEV=AVEDEV+(DIFY(I)*DIFY(I))

IF(I.NE.IMS1) GO TO 74

XI=I
AVEPCT(I)=SUMPC1/XI
STDDEV(I)=SQRT(SUMERR/(XI-1.0))
DEVAVEC(I)=SQRT(AVEDEV/(XI-1.0))/(YSUM/XI)
WRITE(6,3000) IZONE,XA(I),YCHECK(I,1),YA(I),DIFY(I),PERCNT(I),AVE
PCT(I),STDDEV(I),DEVAVEC(I)

3000 FORMAT (T12,T12,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20)

74 WRITE(6,2001) IZONE,XA(I),YCHECK(I,1),YA(I),DIFY(I),PERCNT(I)

2001 FORMAT (T12,T12,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20,T20)

CONTINUE

DO 80 J=2,NSEG
NHOI_D = 0
JJ=J-1
N1=NTAG(JJ)+1
N2=NTAG(J)
SUMPC1=0.0
SUMERR=0.0
AVEDEV=0.0
YSUM=0.0

IF(J.NE.NSEG) GO TO 78

N2=IMA

78 DO 79 K=N1,N2
79 XCHEC1=XA(K)
XCHEC2=XA(K)*XA(K)
XCHEC3=XCHEC2*XA(K)
XCHEC4=XCHEC3*XA(K)

YCHECK(K,J)=COEFT(I,J)+COEFT(2,J)*XCHEC1+COEFT(3,J)*XCHEC2+COEFT(14,J)*XCHEC3+COEFT(5,J)*XCHEC4
DIFY(K)=YA(K)-YCHECK(K,J)

IF(YA(K).EQ.0.0) GO TO 200
PERCNT(K)=ABS((DIFY(K)*100.)/YA(K))
DIF2=DIFY(K)+DIFY(K)/YA(K)
GO TO 201

200 PERCENT(K)=0.0
DIF2=DIFY(K)+DIFY(K)
NHOLD=NHOLD+1
SUMPCT=SUMPCT+PERCNT(K)
AVEDEV=AVEDEV+DIFFY
YSUM=YSUM+YA(K)
SUMERR=SUMERR+DIFF2
IF(K.NE.N2) GO TO 202
XK=N2-N1+1-NHOLD
AVEPCT(J)=SUMPCT/XK
XFREE=N2-N1
IF(XFREE.LE.0.0) XFREE=1.0
STDEV(J)=SORT(SUMERR/XFREE)
DEVAVE(J)=SQRT(AVEDEV/XFREE)/(YSUM/(XFREE+1.0))
WRITE (6,3001) J,XA(K),YCHECK(K,J),YA(K),DIFFY(K),PERCNT(K),AVEPCT(J)
1J,STDEV(J),DEVAVE(J)
3001 FORMAT (II, I12, I12, I20, F8.4, I32, E11.4, I47, E11.4)
GO TO 79
202 WRITE (6,2002) J,XA(K),YCHECK(K,J),YA(K),DIFFY(K),PERCNT(K)
2002 FORMAT (II, I12, I12, I20, D8.4, I32, E11.4, I47, E11.4)
79 CONTINUE
80 CONTINUE
3999 FORMAT (I12, I12, I20, E11.4, I47, E11.4)
WRITE (6,3999)
4000 FORMAT (I12, I12, I20, E11.4, I47, E11.4)
DO 49 I=2,IMS
J=I-1
XAVE=(XA(I)+XA(J))/2.
XC2=XAVE*XAVE
XC4=XC2*XC2
XC6=XC4*XC2
XC8=XC6*XC2
YC(J,1)=COEF(1,1)+(COEF(2,1)*XC2)+(COEF(3,1)*XC4)+(COEF(4,1)*XC6)+
1(COEF(5,1)*XC8)
WRITE (6,4001) I,Z,XAVE,YC(J,1)
4001 FORMAT (II, I12, I12, E8.4, I32, E11.4)
CONTINUE
DO 48 J=2,NSEG
JJ=J-1
N1=NTAG(JJ)+2
N2=NTAG(J) IF(J.NE.NSEG) GO TO 46
N2=NMA
46 DO 47 K=N1,N2
K2=K-1
XAVE=(XA(K)+XA(K2))/2.
XC1=XAVE
CONTINUE
DO 48 J=2,NSEG
JJ=J-1
N1=NTAG(JJ)+2
N2=NTAG(J) IF(J.NE.NSEG) GO TO 46
N2=NMA
46 DO 47 K=N1,N2
K2=K-1
XAVE=(XA(K)+XA(K2))/2.
XC1=XAVE
XC2 = XAVE * XAVE
XC3 = XC2 * XAVE
XC4 = XC3 * XAVE
YC(K2, J) = COEF(1, J) + (COEF(2, J) * XC1) + (COEF(3, J) * XC2) + (COEF(4, J) * XC3) + (COEF(5, J) * XC4)
WRITE (6, 4002) J, XAVE, YC(K2, J)
4002 FORMAT (I12, I2, T20E6, 4, T32E8)
47 CONTINUE
48 CONTINUE

CALCULATE RADIAL INTENSITY VALUES BASED ON POLY FIT

RM = 0.0
X = SEGEND(1)
X3 = X**3
X5 = X**5
X7 = X**7
RA2 = -2. * RA1 / 3.141593
DO 521 J = 2, NSEGS
   XLC = SEGEND(J)
   GO TO (519, 520), I
519 I = 2
   XLC = SEGEND(J - 1)
   GO TO 518
520 RM1 = -(RA(1) - RA(2)) / 3.141593
   RM = RM1 + RM
   GO TO (519, 520), I
521 CONTINUE
   RAD(1) = RA2 + RM
   RDI(1) = 0.0
   KT = 1
   R = 0.0
   LC = 1
   R = R * XPTN
   IF(R.GT.SEQEND(NSEGS)) GO TO 600
   IF(R.GT.SEQEND(LC)) LC = LC + 1
   KT = KT + 1
   RDI(KT) = R
   RM = 0.0
   R2 = R * R
   JC = COEF(1, LC) + (COEF(2, LC) * X2) + (COEF(3, LC) * X2^2) + (COEF(4, LC) * X2^3) + (COEF(5, LC) * X2^4) + (COEF(6, LC) * X2^5) + (COEF(7, LC) * X2^6) + (COEF(8, LC) * X2^7) + (COEF(9, LC) * X2^8) + (COEF(10, LC) * X2^9) + (COEF(11, LC) * X2^10)
1 + R2 * ALOG((X + B)/R)) + 4 * COEF(5, LC)*(B3/3 + R2*B)
RA2 = -RA1/3 * 141593
IF(LC.LT.NSEGS) GO TO 557
RAD(KT) = RA2 + RM
GO TO 550
557 LCUP = LC + 1
RM = 0.0
DO 565 J = LCUP, NSEGS
I = 1
XLC = SEGEND(J)
558 X2LC = XLC * XLC
A = SQRT(X2LC - R2)
A3 = A * A * A
RA1 = COEF(2, J) * ALOG(XLC + A) + 2 * COEF(3, J) * A + 3.0 / 2.0 * COEF(4, J) * (XLC + A) +
     1 * R2 * ALOG((XLC + A)) + 4.0 * COEF(5, J) * (A3 / 3.0 + R2*A)
GO TO (559, 557)
559 I = 2
XLC = SEGEND(J - 1)
GO TO 558
560 RM1 = -(RA1 - RA(2))/3 * 141593
RM = RM1 + RM
565 CONTINUE
RAD(KT) = RA2 + RM
GO TO 550
575 X = SEGEND(1)
X2 = X * X
B = SQRT(X2 - R2)
R4 = R2 * R2
R6 = R2 * R4
B2 = B * B
B3 = B2 * B
B5 = B2 * B3
B7 = B2 * B5
RA1 = 2.0 * COEF(2, 1) * B + 4.0 * COEF(3, 1) * (B3/3 + R2*B) + 6.0 * COEF(4, 1) * (R4 + B2)
   + 1 * R2*B3/3 + B5/5 + 8.0 * COEF(5, 1) * (R5 + B*R4*B3 + 3.0 * R2*B5/5 + B7/7)
RA2 = -RA1/3 * 141593
GO TO 557
600 DO 610 I = 1, KT
610 RDI(I) = RDI(I) * XD
WRITE (6, 5002) NSEGS, NSEGS, (SEGEND(I), I = 1, NSEGS)
5002 FORMAT (///, 'ZONE DIVISIONS FOR', '132X, 'SEGMENTS', '//' T5, 'REGION'
       1(I) ---- REGION('11', '1') '5(E11.4,5X))
CALCULATE SIGMA VALUES FOR RADIAL INTENSITIES
DO 66 I = 1, NSEGS
66 RDST(I) = SEGEND(I)
DO 67 I = 1, KT
67 RDI(I) = RDI(I) / XD
DO 90 I = 1, KT
900
IF(RDI(I) GT ROST(I)) GO TO 82
G=SQRT(RDST(I)**3.-RD(I)**2.)
DEL1=(2.*ABS(G)*DELCOF(2.1)+(4.*ABS(((G**3.)/3.))+(RDI(I)**2.)*G))
1)*DELCOF(3.1)+(6.*ABS((RDST(I)**4.)*G)+(2./3.)*RDST(I)**2.*G))
3.1)**4.)*G))+(G**3.))+(3./*5.)*RDST(I)**2.))+(G**5.))+(1./7.)*G))
4)*DELCOF(5.1))
DEL2=0.0
DO 89 J=2,NSEGS
K=J-1
GJ=SQRT(RDST(J)**2.-RDST(K)**2.)
D2(K)=D2(J)+ADD
DEHRI1)=(OEL1+DEL2)/3.141593)*100.0
DIFF=ABS(DIFRNC)
IF(A8DIF.LT.0.0000001) GO TO 90
DEL1IR(I)=DELIIR(I)/RAD(I)
GO TO 90
85 IF(RDI(I) LE RST(2) ) L=2
IF(RDI(I) LE RST(3) ) L=3
IF(RDI(I) LE RST(4) ) L=4
IF(RDI(I) LE RST(5) ) L=5
IF(RDI(I) GT RST(5) ) GO TO 92
G=SQRT(RDST(I)**2.-RDST(I)**2.)
RD2=RDI(I)*RDI(I)
XTMLOG=ALOG((RDST(1)+GM)/(RDST(1)+GM))
D11=(ABS(ALOG((RDST(1)+GM)/(RDST(1)+GM)))
1)*DELCOF(2.1)+(2.*ABS(G)*DELCOF(3.1)+(1.5*ABS((RDST(1)+GM)-(RDST(1)+GM)+((RDST(1)**2.)*G))
2 ALLOG((RDST(1)+GM)/(RDST(1)+GM)))
DEL1=(2.*ABS(G)*DELCOF(2.1)+(4.*ABS(((G**3.)/3.))+(RDI(I)**2.)*G))
1)*DELCOF(3.1)+(6.*ABS((RDST(I)**4.)*G)+(2./3.)*RDST(I)**2.*G))
3.1)**4.)*G))+(G**3.))+(3./*5.)*RDST(I)**2.))+(G**5.))+(1./7.)*G))
4)*DELCOF(5.1))
DEL2=DEL2+ADD
DEHRI1)=(DEL1+DEL2)/3.141593)*100.0
DIFF=ABS(DIFRNC)
IF(A8DIF.LT.0.0000001) GO TO 90
DEL1IR(I)=DELIIR(I)/RAD(I)
GO TO 90
87 N1=L+1
DEL2=0.0
DO 88 M=N1,NSEGS
N=M-1
GN=SQRT(RDST(M)**3.-RDST(K)**2.)
GN=SQRT(RDST(N)**3.-RDST(N)**2.)
ADD=ABS(ALLOG((RDST(M)+GM)/(RDST(M)+GM))
1)*DELCOF(3.1)+(1.5*ABS((RDST(M)+GM)-(RDST(M)+GM)+((RDST(1)**2.)*G))
2 ALLOG((RDST(M)+GM)/(RDST(M)+GM)))
DEL1=(2.*ABS(G)*DELCOF(2.1)+(4.*ABS(((G**3.)/3.))+(RDI(I)**2.)*G))
3.1)**4.)*G))+(G**3.))+(3./*5.)*RDST(I)**2.))+(G**5.))+(1./7.)*G))
4)*DELCOF(5.1))
DEL2=DEL2+ADD
DEHRI1)=(DEL1+DEL2)/3.141593)*100.0

DELIR(I) = DELIR(I) / RAD(I)
90 CONTINUE
IF(I.EQ.KT) GO TO 93
92 KT = I - 1
93 DO 91 I2 = I, KT
91 ROI(I2) = ROI(I2) * XD
SUMR = 0.
WRITE (6, 6000)
6000 FORMAT (/////,T29,'I'*,T45,'ROI(I)',T67,'RAD(I)',T83,'DELTA RAD IN
PERCENT*')
DO 23 K = 1, KT
101 FORMAT (27X,I3,2(12X,E11.4),T90,E11.4)
SUMR = SUMR + RAD(K)
23 WRITE (6, 101) K, ROI(K), RAD(K), DELIR(K)
WRITE (6, 102) SUMR
102 FORMAT (///,TaO,'SUM R = ',2X,E11.4)
DO 28 J = 1, NSEG
DO 28 I = 2, 5
101 FORMAT (3X,2(I2,E11.4),I2,T30,E11.4)
28 WRITE (6, 101) J, I, DELCOF(I, J)
IF(I.EQ.2) GO TO 300
DO 299 NABS = 1, KT
299 RAD(NABS) = ABS(:RAD(NABS))
300 RETURN
END
SUBROUTINE SEGMNT (XA,YA,IMA,NSEG,NZ,COEF,DELCOF,SEG,SIGA,NTA
1G, IMF)
DIMENSION RELCOF(5,5), RELC(5,5), FTEST5(5), FTEST6(5), FTEST7(5)
DIMENSION XA(1), YA(1), COEF(5,5), DELCOF(5,5), SEG(1), SIGA(1), PERCT(7)
1,FTEST1(5), FTEST2(5), FTEST3(5), FTEST4(5), NTAG(5), STOR(1,5), YSTO
2R(1,5), STOR(1,5), XFIT(35), YFIT(35), SFIT(35), FTEST(5), YCALC(35),
3REAL_C(5), SIGMAC(5), RELC(5), SGMAR(5), CHISQR(5)
DATA FTEST1/16200.0,198.0,55,98.5,34.1,121,16,3/,FTEST2/4050.0,98.5,34.1,1
21,16,3/,FTEST3/4050,0,98.5,34.1,121,16,3/,FTEST4/161,0,18.5,10
21,7,71,6,61/,PERCT/0,5,10,0,2,5,5,0,10,0,25,0,50,0/
DATA FTEST5/399,8,53,5,54,4,54,4,06/,FTEST6/5,83,2,57,2,02,1,81,1
1,69,7,FTEST7/1.00,0,667,0,585,0,549,0,528/
GO TO (1,3,5,7,11,21,31), NZ
1 DO 2 I = 5
2 FTEST(I) = FTEST(I)
GO TO 9
3 DO 4 I = 1, 5
4 FTEST(I) = FTEST2(I)
GO TO 9
5 DO 6 I = 1, 5
6 FTEST(I) = FTEST3(I)
GO TO 9
7 DO 8 I = 1, 5
8 FTEST(I)=FTEST4(I)
11 DO 12 I=1,5
12 FTEST(I)=FTEST5(I)
21 DO 22 I=1,5
22 FTEST(I)=FTEST6(I)
31 DO 32 I=1,5
32 FTEST(I)=FTEST7(I)
9 WRITE (6,1000) PERCENT(Z),NSEGS
1000 FORMAT (1H1,T15,'RADIAl INTENSITY DISTRIBUTION CALCULATION',T15)
11 'ABEL INVERSION UTILIZING WEIGHTED LEAST-SQUARES POLYNOMIAL FITTING'
12 'NG OF THE LATernal INTENSITY DISTRIBUTION',T20,'F-TEST FOR SIGNIFICANCE OF ADDED COEFFICIENT'
13 'PERCENT PROBABILITY OF EXCEEDING THE F-VALUE',T25,'THe LATERAL I(x) PROFILE HAS BEEN DIVIDED INTO 13,2X,ZONES'
14 WRITE (6,1001)
1001 FORMAT (1H1,T15,'ZONE DIVISIONS ON REDUCED RADIUS SCALE',T15)
15 DO 10 I=1,NSEG
1002 FORMAT (10,T15,1S10,E14.7)
10 WRITE (6,1002) I,SEG(I)
1003 FORMAT (10,T15,FTEST(1)---FTEST(5)=,5(2X,E13.6))
1004 FORMAT (10,T15,FTEST(1))
10 WRITE (6,1004) I,FTEST(I)
1005 FORMAT (1H1,T15,'REGION',2X,DEG',19X,A)
13 CONTINUE
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810 CONTINUE
812 CONTINUE
DO 999 LC=1,NSEGS
IF(NSEGS-4)100,200,300
100 GO TO (110,120,130),LC
110 N=NTAG(1)
   DO 115 I=1,N
   XFIT(I)=XSTOR(I,1)**2
   YFIT(I)=YSTOR(I,1)
   SFIT(I)=SSTOR(I,1)
115 SFIT(I)=SSTOR(I,1)
   N=N-1
   DO 116 J=1,3
   I=I+1
   XFIT(I)=XSTOR(J,2)**2
   YFIT(I)=YSTOR(J,2)
   SFIT(I)=SSTOR(J,2)
   NFIT=N+3
   GO TO 500
120 N1=NTAG(1)-2
   N2=NTAG(1)
   N3=NTAG(2)
   I=0
   DO 125 J=N1,N2
   I=I+1
   XFIT(I)=XSTOR(J,1)
   YFIT(I)=YSTOR(J,1)
   SFit(I)=SSTOR(J,1)
   NN=N3-N2
   DO 126 J=1,NN
   I=I+1
   XFIT(I)=XSTOR(J,2)
   YFIT(I)=YSTOR(J,2)
   SFIT(I)=SSTOR(J,2)
126 SFit(I)=SSTOR(J,2)
   DO 127 J=1,3
   I=I+1
   XFIT(I)=XSTOR(J,3)
   YFIT(I)=YSTOR(J,3)
   SFIT(I)=SSTOR(J,3)
127 SFIT(I)=SSTOR(J,3)
   NFIT=1
   GO TO 500
130 N1=(NTAG(2)-NTAG(1))-2
   N2=NTAG(2)-NTAG(1)
   N3=NTAG(3)-NTAG(2)
   I=0
   DO 135 J=N1,N2
   I=I+1
   XFIT(I)=XSTOR(J,2)
   YFIT(I)=YSTOR(J,2)
   SFIT(I)=SSTOR(J,2)
135 SFIT(I)=SSTOR(J,2)
   DO 136 J=1,N3
   I=I+1
   XFIT(I)=XSTOR(J,3)
YFIT(I) = YSTOR(J,3)

SFIT(I) = SSTOR(J,3)
NFIT = I
GO TO 500

200 GO TO (210, 220, 230, 240, LC

210 N1 = NTAG(1)
N2 = NTAG(2) - NTAG(1)
I = 0
DO 215 J = 1, N1
I = I + 1
XFIT(I) = XSTOR(J,1)**2
YFIT(I) = YSTOR(J,1)

215 SFIT(I) = SSTOR(J,1)
DO 216 J = 1, N2
I = I + 1
XFIT(I) = XSTOR(J,2)**2
YFIT(I) = YSTOR(J,2)

216 SFIT(I) = SSTOR(J,2)
NFIT = I
GO TO 500

220 N1 = NTAG(1) * 3/4
N2 = NTAG(1) - N1 + 1
N3 = NTAG(1)
N4 = NTAG(2) - NTAG(1)
N5 = (NTAG(3) - NTAG(2)) * 3/4
I = 0
DO 225 J = N2, N3
I = I + 1
XFIT(I) = XSTOR(J,1)
YFIT(I) = YSTOR(J,1)

225 SFIT(I) = SSTOR(J,1)
DO 226 J = 1, N4
I = I + 1
XFIT(I) = XSTOR(J,2)
YFIT(I) = YSTOR(J,2)

226 SFIT(I) = SSTOR(J,2)
DO 227 J = 1, N5
I = I + 1
XFIT(I) = XSTOR(J,3)
YFIT(I) = YSTOR(J,3)

227 SFIT(I) = SSTOR(J,3)
NFIT = I
GO TO 500

230 N1 = (NTAG(2) - NTAG(1)) * 3/4
N2 = (NTAG(2) - NTAG(1)) - N1 + 1
N3 = NTAG(2) - NTAG(1)
N4 = NTAG(3) - NTAG(2)
N5 = (NTAG(4) - NTAG(3)) * 3/4
I = 0
DO 235 J = N2, N3
I = I + 1
XFIT(I) = XSTOR(J, 2)
YFIT(I) = YSTOR(J, 2)
SFIT(I) = SSTOR(J, 2)
DO 236 J = 1, N4
I = I + 1
XFIT(I) = XSTOR(J, 3)
YFIT(I) = YSTOR(J, 3)
SFIT(I) = SSTOR(J, 3)
DO 237 J = 1, N5
I = I + 1
XFIT(I) = XSTOR(J, 4)
YFIT(I) = YSTOR(J, 4)
SFIT(I) = SSTOR(J, 4)
NFIT = I
GO TO 500
240 N1 = NTAG(3) - NTAG(2)
N2 = NTAG(4) - NTAG(3)
I = 0
DO 245 J = 1, N1
I = I + 1
XFIT(I) = XSTOR(J, 3)
YFIT(I) = YSTOR(J, 3)
SFIT(I) = SSTOR(J, 3)
DO 246 J = 1, N2
I = I + 1
XFIT(I) = XSTOR(J, 4)
YFIT(I) = YSTOR(J, 4)
SFIT(I) = SSTOR(J, 4)
NFIT = I
GO TO 500
300 GO TO (310, 320, 320, 320, 330), L.C
310 N1 = NTAG(1)
N2 = NTAG(2) - NTAG(1)
I = 0
DO 315 J = 1, N1
I = I + 1
XFIT(I) = XSTOR(J, 1)**2
YFIT(I) = YSTOR(J, 1)
SFIT(I) = SSTOR(J, 1)
DO 316 J = 1, N2
I = I + 1
XFIT(I) = XSTOR(J, 2)**2
YFIT(I) = YSTOR(J, 2)
SFIT(I) = SSTOR(J, 2)
NFIT = I
GO TO 500
320 IF(LC .NE. 2) GO TO 321
N1 = NTAG(1)
N2 = NTAG(2) - NTAG(1)
N3 = NTAG(3) - NTAG(2)
GO TO 324

321 LCL1 = LC - 1
LCL2 = LC - 2
LCU = LC + 1
N1 = NTAG(LCL1) - NTAG(LCL2)
N2 = NTAG(LC) - NTAG(LCL1)
N3 = NTAG(LCU) - NTAG(LC)

324 I = 0
DO 325 J = 1, N1
   I = I + 1
   XFIT(I) = XSTOR(J, LC - 1)
   YFIT(I) = YSTOR(J, LC - 1)
   SFIT(I) = SSTOR(J, LC - 1)
DO 326 J = 1, N2
   I = I + 1
   XFIT(I) = XSTOR(J, LC)
   YFIT(I) = YSTOR(J, LC)
   SFIT(I) = YSTOR(J, LC)
DO 327 J = 1, N3
   I = I + 1
   XFIT(I) = XSTOR(J, LC + 1)
   YFIT(I) = YSTOR(J, LC + 1)
   SFIT(I) = SSTOR(J, LC + 1)
NFIT = I
GO TO 500

330 N1 = NTAG(4) - NTAG(3)
N2 = NTAG(5) - NTAG(4)
I = 0
DO 335 J = 1, N1
   I = I + 1
   XFIT(I) = XSTOR(J, 4)
   YFIT(I) = YSTOR(J, 4)
   SFIT(I) = SSTOR(J, 4)
DO 336 J = 1, N2
   I = I + 1
   XFIT(I) = XSTOR(J, 5)
   YFIT(I) = YSTOR(J, 5)
   SFIT(I) = SSTOR(J, 5)
NFIT = I
GO TO 500

500 SUMS = 0.0
DO 510 I = 1, IMA
   SUMS = SUMS + SIGA(I)
   IF(SUMS .GT. 0.0) GO TO 520
   IWT = 0
   NEVEN = 0
   NORDER = 4
   MODE = IWT
   NUMCOF = 0
   MFIT = NFIT - 1

520
IF((MFIT-NORDER).GT.0) GO TO 524
NORDER=3
IF((MFIT-NORDER).GT.0) GO TO 524
NORDER=2
IF((MFIT-NORDER).GT.0) GO TO 524
NORDER=1
524 CALL FITPOL(XFIT, YFIT, SFIT, NFIT, NORDER, NEVEN, MODE, FTEST, YCALC, REAL
1, SIGMAC, RELC, SIGMAR, CHI, NUMCOF)
CHISQR(LC)=CHI
DO 525 I=1, NUMCOF
COEF(I,LC)=REALC(I)
RELCOF(I,LC)=RELC(I)
DELCOF(I,LC)=SIGMAC(I)
525 SRELC(I,LC)=SIGMAR(I)
NPLUS=NUMCOF+1
IF(NPLUS.GT.5) GO TO 527
DO 526 I=NPLUS,5
PEALC(I)=0.0
RELCOF(I,LC)=0.0
526 SRELC(I,LC)=0.0
527 DO 530 I=1,5
TEST=ABS(COEF(I,LC))
IF(TEST.GT.0.0) GO TO 530
NPOLY=I-2
GO TO 532
530 IF(I.EQ.5) NPOLY=4
532 WRITE(6,1004) LC, NPOLY, (REALC(I), I=1,5)
WRITE(6,1008) (RELC(I,LC), I=1,5)
1004 FORMAT(T22- II, 6X, 11, 14X, E13.6, 4(2X, E13.6))
1008 FORMAT(T22.'RELATIVE COEFS = *', 3X, 5(2X, E13.6))
WRITE(6,1005) LC, CHISQR(LC), INT, NUMCOF
1005 FORMAT(T40.'REDUCED CHI-SQUARE FOR REGION', I2, ' = *', E13.6, 2X, 'WEIGHT CODE='
  *I2, '2X, *NO. COEFS=', I2, '/*)
999 CONTINUE
RETURN
END
SUBROUTINE FITPOL(X, Y, SIGMAY, NPTS, NORDER, NEVEN, MODE, FTEST, YFIT, A, S
1, SIGMAA, B, SIGMAE, CHISQR, NTERMS)
DOUBLE PRECISION P, ALPHA, BETA, CHISR, DSQR
DIMENSION X(1), Y(1), SIGMAY(1), FTEST(1), YFIT(1), A(1), SIGMAA(1), B(1)
1, SIGMAE(1)
DIMENSION WEIGHT(S1), P(S1), BETA(5), ALPHA(5,5)
ACCUMULATE WEIGHTS AND POWER SERIES TERMS
11 NTERMS=1
NCOEFF=1
JMAX=NORDER+1
20 DO 40 I=1, NPTS
21 IF(MODE) 22, 27, 29
22 IF(Y(I)) 25,27,23
23 WEIGHT(I)=1.0/Y(I)
   GO TO 31
25 WEIGHT(I)=1.0/(-Y(I))
   GO TO 31
27 WEIGHT(I)=1.0
   GO TO 31
29 WEIGHT(I)=1.0/(SIGMA(Y(I)**2))
31 P(I,1)=1.0
   DO 36 L=1,NORDER
   P(I,L+1)=X(I)**L
   CONTINUE
36
40 CONTINUE

ACCUMULATE MATRICES ALPHA AND BETA

51 DO 54 J=1,NTERMS
   BETA(J)=0.0
   DO 54 K=1,NTERMS
   ALPHA(J,K)=0.0
54
61 DO 66 I=1,NPTS
   ALPHA(J,K)=ALPHA(J,K)+P(I,J)*Y(I)*WEIGHT(I)
   DO 66 K=J,NTERMS
   ALPHA(K,J)=ALPHA(J,K)
66
70 IF(NEVEN) 71,91,81
71 DO 76 J=3,NTERMS,2
   BETA(J)=0.0
   DO 76 K=1,NTERMS
   ALPHA(J,K)=0.0
75 ALPHAK(J,K)=0.0
76 ALPHAJ(J,K)=1.0
   GO TO 91
81 DO 86 J=2,NTERMS,2
   BETA(J)=0.0
   DO 86 K=1,NTERMS
   ALPHA(J,K)=0.0
85 ALPHAK(J,K)=0.0
86 ALPHAJ(J,K)=1.0
91 INVERT CURVATURE MATRIX ALPHA.

91 DO 95 J=1,JMAX
   A(J)=0.0
   SIGMAA(J)=0.0
   SIGMAB(J)=0.0
95
DO 97 I=1,NPTS
  YFIT(I)=0.0
CALL MATINV(ALPHA, NTERMS, DET)
  IF(DET) 111, 103, 111
  CHISQR=0.0
  GO TO 170
C
C  CALCULATE COEFFICIENTS, FIT, AND CHI SQUARE
C
  111 DO 115 J=1, NTERMS
  DO 113 K = 1, NTERMS
  A(J)=A(J)+BETA(K)*ALPHA(J,K)
  DO 115 I=1, NPTS
  YFIT(I)=YFIT(I)+A(J)*P(I, J)
  111 CHISQR=0.0
  DO 123 I=1, NPTS
  CHISQ=CHISQ+(Y(I)-YFIT(I))**2*WEIGHT(I)
  FREE=NPTS-NCOEFF
  CHISQR=CHISQ/FREE
C
C  TEST FOR END OF FIT
C
  131 IF(NTERMS=NMAX) 132, 151, 151
  132 IF(NCOEFF=2) 133, 134, 141
  133 IF(NEVEN) 137, 137, 135
  134 IF(NEVEN) 135, 137, 135
  135 NTERMS= NTERMS+2
  GO TO 138
  137 NTERMS=NTERMS+1
  138 NCOEFF=NCOEFF+1
  CHISQ1=CHISQ
  GO TO 51
  141 FVALUE=(CHISQ1-CHISQ)/CHISQR
  IF(FTEST(NTERMS)=FVALUE) 134, 143, 143
  143 IF(NEVEN) 144, 146, 144
  144 NTERMS= NTERMS-2
  GO TO 147
  146 NTERMS=NTERMS-1
  147 NCOEFF=NCOEFF-1
  JMAX=NTERMS
  GO TO 51
C
C  CALCULATE REMAINDER OF OUTPUT
C
  151 IF(CMODE) 152, 154, 152
  152 VARNCE=1.0
  GO TO 155
  154 VARNCE=CHISQR
  155 DO 156 J=1, NTERMS
  156 SIGMA(J)=DSQRT(VARNCE*ALPHA(J,J))
161 IF(A(1)) 162,170,162
162 DO 166 J=2,NTERMS
163 IF(A(J)) 164,166,164
164 B(J)=A(J)/A(1)
165 SIGMA(B(J))=B(J)*DSQRT((SIGMA(A(J)/A(1)))**2+(SIGMA(A(1)/A(1)))**2-2.0*YARNE*ALPHA(J,1)/(A(J)*A(1)))
166 CONTINUE
170 RETURN
END
SUBROUTINE MATINV(ARRAY,NORDER,DET)
DOUBLE PRECISION ARRAY*AMAX,S;SAVE,DABS
DIMENSION ARRAY(5,5),IK(5),JK(5)
10 DET=1.0
11 DO 100 K=1,NORDER
20 FIND LARGEST ELEMENT ARRAY(I, J) IN REST OF MATRIX
21 AMAX=0.0
22 DO 30 I=K,NORDER
23 DO 30 J=K,NORDER
24 IF(DABS(AMAX)-DABS(ARRAY(I, J))) 24,24,30
25 AMAX=ARRAY(I, J)
26 IK(K)=I
27 JK(K)=J
28 30 CONTINUE
30 INTERCHANGE ROWS AND COLUMNS TO PUT AMAX IN ARRAY(K, K)
31 IF(AMAX) 41,32,41
32 DET=0.0
33 GO TO 140
40 I=IK(K)
41 IF(I=K) 21,5,43
42 DO 50 J=1,NORDER
43 SAVE=ARRAY(K, J)
44 ARRAY(K, J)=ARRAY(I, J)
45 ARRAY(I, J)=SAVE
46 50 CONTINUE
50 IF(J=K) 21,6,53
51 J=JK(K)
52 DO 60 I=1,NORDER
53 SAVE=ARRAY(I, K)
54 ARRAY(I, K)=ARRAY(I, J)
55 ARRAY(I, J)=SAVE
56 60 CONTINUE
60 ACCUMULATE ELEMENTS OF INVERSE MATRIX
61 DO 70 I=1,NORDER
62 IF(I=K) 63,70,63
63 ARRAY(I, K)=-ARRAY(I, K)/AMAX
1551
70 CONTINUE
71 DO 80 I=1,NORDER
72 DO 80 J=1,NORDER
73 IF(I-K) 74,80,74
74 IF(J-K) 75,80,75
75 ARRAY(I,J)=ARRAY(I,J)*ARRAY(I,K)*ARRAY(K,J)
76 CONTINUE
77 DO 90 J=1,NORDER
78 IF(J-K) 83,90,83
79 ARRAY(K,J)=ARRAY(K,J)/AMAX
80 CONTINUE
81 DO 100 J=1,NORDER
82 IF(J-K) 83,100,83
83 ARRAY(K,J)=ARRAY(K,J)/AMAX
84 CONTINUE
85 DET=DET*AMAX
86 RESTORE ORDERING OF MATRIX
87 DO 101 L=1,NORDER
88 K=NORDER-L+1
89 IF(J-K) 111,111,105
90 CONTINUE
91 DO 110 J=1,NORDER
92 IF(J-K) 111,111,113
93 ARRAY(K,J)=SAVE
94 CONTINUE
95 RETURN
END

SUBROUTINE RADPL (IMA,XDIST,YINT,N,RBP,ARI,
LZ,RAD,RLAM,
1 DLB,K,TNZ,
DIMENSION XDIST(N),YINT(N),RBP(15,4),ARI(15,4),
2 RAD(15,4),DL1(1),XX(51),YY(51),DLA(15),DLB(15),DL(15),
3 DL(15),DL1(15),DL1(15),DL(15),DL(15),DL1(15),DL(15),
4 DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),
5 DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),DL1(15),
6 DATA XL1,'X ANS','D R '","(MM)'",","
7 YL1,'(X)'",","
8 21GL,'I PRonomic,','E',","E,",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",",","...

1E0
DATA DL9/*10.0*,'PERC','ENT','PROB','FOR'/ 1601
DATA DL10/*15.0*, 'PERC', 'ENT', 'PROB', 'FOR'/ 1602
DATA DL11/*50.0*, 'PERC', 'ENT', 'PROB', 'FOR'/ 1603
IZEOR=0 1604
DO 1 I=1,IMA 4 1605
IF (XDIST(I) .LT. 0.) GO TO 1 1606
IZEOR=IZEOR+1 1607
X(IZEOR)=XDIST(I) 1608
Y(IZEOR)=YINT(I) 1609
1 CONTINUE 1610
IZE=IMA 1611
IMA=IZEOR 1612
NZERO=0 1613
DO 4 IJ=1,N 1614
IF (RBP(IJ,LZ) .LT. 0.) GO TO 4 1615
NZERO=NZERO+1 1616
XACNZERO)=RBP(IJ,LZ) 1617
YACNZERO)=ARI(IJ,LZ) 1618
4 CONTINUE 1619
N=1620
N=NZERO 1621
IGL(5)=IGL(5)-H_Z 1622
CALL GRAPH(IMA.X.Y.2.7.00.9.00.10.0.0.XL1.YL1.IGL,DLA) 1623
CALL GRAPH (IMA.X.Y.4.107.DL1) 1624
CALL GRAPH (N.XA.YA.1.107.DL2) 1625
IGL(5)=IGL(5)-LZ 1626
LZERO=0 1627
DO 6 LDEX=1,KT 1628
IF (RD(LD) .LT. 0.) GO TO 6 1629
LZERO=LZERO+1 1630
XX(LZERO)=RD(LD) 1631
YY(LZERO)=RAD(LD) 1632
6 CONTINUE 1633
KTHOLD=KT 1634
KT=LZERO 1635
GO TO (9,10,11,15,16,16.16) 1636
9 CALL GRAPH(KT.XX.YY.2.111.DL3) 1637
CALL GRAPH(KT.XX.YY.0.107.DL4) 1638
CALL GRAPH(KT.XX.YY.0.107.DL5) 1639
GO TO 10 1640
10 CALL GRAPH(KT.XX.YY.2.111.DL3) 1641
CALL GRAPH(KT.XX.YY.0.107.DL4) 1642
CALL GRAPH(KT.XX.YY.0.107.DL5) 1643
GO TO 11 1644
11 CALL GRAPH(KT.XX.YY.2.111.DL3) 1645
CALL GRAPH(KT.XX.YY.0.107.DL4) 1646
CALL GRAPH(KT.XX.YY.0.107.DL5) 1647
GO TO 12 1648
15 CALL GRAPH(KT.XX.YY.2.111.DL3) 1649
CALL GRAPH(KT.XX.YY.0.107.DL7) 1650
CALL GRAPHS(KT, XX, YY, 0, 107, DL8)
GO TO 12
16 CALL GRAPHS(KT, XX, YY, 2, 111, DL3)
17 NN=NN-4
GO TO (17, 18, 19), NN
18 CALL GRAPHS(KT, XX, YY, 0, 107, DL10)
GO TO 20
19 CALL GRAPHS(KT, XX, YY, 0, 107, DL11)
20 CALL GRAPHS(KT, XX, YY, 0, 107, DL8)
12 KT=KTHOLD
IMA=IZE
N=NHOLD
DO 13 IPOS=1, KT
13 RAD(IPOS)=ABSCRAD(IPOS))
RETURN
END
SUBROUTINE TEWP(NT, IMAT, RT, RBP, ARI, RADIST, RADINT, NLZT, DLAB, KM, NL, NK, KODE, KJOIN, KLINE1, KLINE2, DELA, DELINT, IARTP)
DIMENSION FNUM(7)
DIMENSION RBP(15, 4), ARI(15, 4), RADIST(51, 4, 7), RADINT(51, 4, 7), TLAB(51), TRAD5(51), TRAD4(51), TRAD3(51), TRAD2(51), TRAD1(51), TRAD0(51), TRAD(-51), TRAD0(51), TRAD(51)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
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DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
DIMENSION NLZT, DLAB(5, 4, 7), IXL(5)
NL = NL - 1
IF (L(KODE*EQ.1)) GO TO 97
RETURN
97 IF (NLZT .GE. 2) GO TO 1
WRITE (6,1000)
1000 FORMAT ('/T',10X,'TEMPS. CANNOT BE CALCULATED; ONLY ONE LINE')
RETURN
1 DO 96 NPOLY = 1, KM
NL = NL + 1
WRITE (6,1001)
1001 FORMAT (1H1)
WRITE (6,3000) NT, KODEN
3000 FORMAT (110X,'TEMP CONTROL PARAMETERS',/,'T15', 'NT = ', I2,5X,
      2* KODEN = ', I2)
IF (KM .EQ. 2) GO TO 5
WRITE (6,100) FNUM(NL)
100 FORMAT (10X,'DKABEL MULTIPLE F-TEST POLYNOMIAL TEMPERATURE CALCULA-
      TIONS FOR', 'T15, F5.2,' PERCENT PROBABILITY OF EXCEEDING THE F-VALU
      2E')
5 WRITE (6,1002)
1002 FORMAT (10X,CALCULATION OF LATERAL AND RADIAL TEMPERATURES FOR 2-LIN
      1E METHOD',/)
WRITE (6,1003)
1003 FORMAT (10X,'SYMBOL KEY')
WRITE (6,1004)
1004 FORMAT (5X,'SYMBOL LINE1 LINE2 EQ1 EQ2 INTEN. 1USED')
WRITE (6,1005)
1005 FORMAT (10X,'TLAT1 3815.84 3820.43 38175 33096 LAT
      IERAL')
WRITE (6,1006)
1006 FORMAT (10X,'TLAT2 ' 3824.44 26140 ') 1
WRITE (6,1007)
1007 FORMAT (10X,'TLAT3 3820.43 ' 33096 ') 1
WRITE (6,1008)
1008 FORMAT (10X,'TLAT4 3815.84 3825.88 38175 33507 ') 1
WRITE (6,1009)
1009 FORMAT (10X,'TLAT5 3824.44 ' 26140 ') 1
WRITE (6,4000)
4000 FORMAT (10X,'TLAT6 3820.43 ' 33096 ') 1
WRITE (6,1010)
1010 FORMAT ('/T',5X,'TRAD1 THRU TRAD6 SIMILAR EXCEPT RADIAL INTEN. USED',
      1//')
WRITE (6,5000) (DELA(I), I = 1, NLZT)
5000 FORMAT (T10X,'DELA(1) = ', FS.2,10X,'DELA(2) = ', FS.2,10X,'DELA(3) = ',
      1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750
IF(S2,10X,DEL)(A)= S5.2
IF(IARTP.EQ.9) WRITE(6,5001)
5001 FORMAT('****T10,****BANFIELD AND HUBER (1973) GA VALUES****')
WRITE (6,1011) NT
1011 FORMAT (40X,*LATERAL TEMPERATURES FOR*,I4,*2X,*EXPERIMENTAL LATERAL
1 POSITIONS IN EMIS, SOURCE*,T20,X,TLAT(X),TLAT2(X),
2 TLAT3(X),TLAT4(X),TLAT5(X),TLAT6(X),*/
DO 10 I=1,NT
TLAT1(I)=3173./ALOG10(1.1605*(ARI(I,2)/ARI(I,1)))
IF(IARTP.EQ.9) TLAT1(I)=TLAT1(I)/(1.0+6.218E-5*TLAT1(I))
IF(NLZT.EQ.2) GO TO 10
TLAT2(I)=7518./ALOG10(33.937*(ARI(I,3)/ARI(I,1)))
IF(IARTP.EQ.9) TLAT2(I)=TLAT2(I)/(1.0+2.559E-5*TLAT2(I))
TLAT3(I)=6345./ALOG10(29.244*(ARI(I,3)/ARI(I,2)))
IF(IARTP.EQ.9) TLAT3(I)=TLAT3(I)/(1.0-1.031E-6*TLAT3(I))
IF(NLZT.EQ.3) GO TO 10
TLAT4(I)=2916./ALOG10(1.676*(ARI(I,4)/ARI(I,1)))
IF(IARTP.EQ.9) TLAT4(I)=TLAT4(I)/(1.0+6.144E-5*TLAT4(I))
TLAT5(I)=4608./ALOG10(0.0494*(ARI(I,4)/ARI(I,3)))
IF(IARTP.EQ.9) TLAT5(I)=TLAT5(I)/(1.0+2.906E-6*TLAT5(I))
TLAT6(I)=2569./ALOG10(1.444*(ARI(I,4)/ARI(I,2)))
IF(IARTP.EQ.9) TLAT6(I)=TLAT6(I)/(1.0+6.894E-5*TLAT6(I))
10 WRITE (6,1012) RBP(I,1),TLAT1(I),TLAT2(I),TLAT3(I),TLAT4(I),TLAT5(I),
11,TLAT6(I)
WRITE (6,1013) IMAT
1013 FORMAT ('***/****/40X,*RADIAL TEMPERATURES FOR*,I4,*2X,*RADIAL POS
1 IITIONS IN THE EMISION SOURCE*,T20,R,TRAD1(R),TRAD2(R),
2 TRAD3(R),TRAD4(R),TRAD5(R),TRAD6(R),*/
DO 20 J=1,IMAT
K=(IMAT-J)+2
TRAD1(J)=3173./ALOG10(1.1605*(RADINT(K,2,NPOLY)/RADINT(K,1,NPOLY)))
1)
IF(IARTP.EQ.9) TRAD1(J)=TRAD1(J)/(1.0+6.218E-5*TRAD1(J))
DELTR1(J)=(TRAD1(J)/(1.439+5079.))*(DEL1+DELINT(K,1,NPOLY)+DELINT(K,2,NPOLY))
IF(NLZT.EQ.2) GO TO 20
TRAD2(J)=7518./ALOG10(33.937*(RADINT(K,3,NPOLY)/RADINT(K,1,NPOLY)))
1)
IF(IARTP.EQ.9) TRAD2(J)=TRAD2(J)/(1.0+2.559E-5*TRAD2(J))
DELTR2(J)=(TRAD2(J)/(1.439+12035.))*(DEL2+DELINT(K,1,NPOLY)+DELINT(K,3,NPOLY))
TRAD3(J)=4608./ALOG10(0.0494*(RADINT(K,4,NPOLY)/RADINT(K,1,NPOLY)))
1)
IF(IARTP.EQ.9) TRAD3(J)=TRAD3(J)/(1.0-1.031E-6*TRAD3(J))
DELTR3(J)=(TRAD3(J)/(1.439+6956.))*(DEL3+DELINT(K,2,NPOLY)+DELINT(K,3,NPOLY))
IF(NLZT.EQ.3) GO TO 20
TRAD4(J)=2916./ALOG10(1.676*(RADINT(K,5,NPOLY)/RADINT(K,1,NPOLY)))
IF(IARTP.EQ.9) TRAD4(J)=TRAD4(J)/(1.0+6.144E-5*TRAD4(J))
1800
DELTR(4,J) = (TRAD4(J)/(1.439*5668.))*(DELA(1)+DELA(4)+DELINT(K,1,NP10LY)+DELINT(K,4,NPOLY))
TRAD5(J) = -4684./ALOG10(1.0496*906E-6*TRAD5(J))

104
IF(IARTP.EQ.9) TRAD5(J)=TRAD5(J)/(1.0+2.906E-6*TRAD5(J))

105
DELTR5(J) = (TRAD5(J)/(1.439*367.))*(DELA(3)+DELA(4)+DELINT(K,3,NP10LY)+DELINT(K,4,NPOLY))
TRAD6(J) = -256.9./ALOG10(1.444*906E-6*TRAD6(J))

106
IF(IARTP.EQ.9) TRAD6(J)=TRAD6(J)/(1.0+6.948E-6*TRAD6(J))

107
DELTR6(J) = (TRAD6(J)/(1.439*411.))*(DELA(2)+DELA(4)+DELINT(K,2,NPOLY)+DELINT(K,4,NPOLY))

108
WRITE (6,1014) RADIST(K,1,NPOLY),TRAD1(J),TRAD2(J),TRAD3(J),TRAD4(J),TRAD5(J),TRAD6(J)

109
WRITE (6,2999) WRITE (6,1014)

2999 FORMAT (15X,F8.3,6X,F8.3)

110
WRITE (6,3001) RADIST(J,1,NPOLY),(DELTR(K,1),K=1,6)

3001 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

111
WRITE (6,3001) RADIST(J,1,NPOLY),(DELTR(K,1),K=1,6)

3001 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

112
DO 29 IMAT=1,1MAT

29 FORMAT (T8,E11.4,T26.5(E11.4,6X),E11.4)

113
WRITE (6,3001) RADIST(J,1,NPOLY),(DELTR(K,1),K=1,6)

3001 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

114
DO 30 J=1,IMAT

30 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

115
RDIST(L)=RADIST(KK,1,NPOLY)

30 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

116
DO 40 M=1,NT

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

117
X(M)=RBP(M,1)

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

118
NN=IMAT

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

119
IF (KPLDT.EQ.1) GO TO 65

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

120
IF (NLZT.EQ.2) GO TO 15

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

121
IF (NLZT.EQ.3) GO TO 21

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

122
IF (NLZT.EQ.4) GO TO 21

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

123
RETURN

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

124
CALL GRAPH (NT,X,TLAT1,0.0,2.7,0.9,0.0,0.2500,E11.4,T,X MM), R(X MM), T(X MM), T(R MM)

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

125
CALL GRAPHS (NT,X,TLAT1,4.107,LATERAL TEMPS.,)

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

126
CALL GRAPHS (NN,RDIST,TRAD1,1,111,RADIAL TEMPS.,)

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

127
GO TO 12

40 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

128
DO 22 N=1,NT

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

129
LA(I,N)=TLAT1(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

130
IF (NLZT.EQ.2) GO TO 22

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

131
LA(2,N)=TLAT2(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

132
LA(3,N)=TLAT3(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

133
IF (NLZT.EQ.3) GO TO 22

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

134
LA(4,N)=TLAT4(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

135
LA(5,N)=TLAT5(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

136
LA(6,N)=TLAT6(N)

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

137
CONTINUE

22 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)

138
DO 23 II=1,IMAT

23 FORMAT (15X,F8.3,6X,E11.4,6X,E11.4)
RA(1,II) = TRAD1(II)
IF (NLZT.EQ.2) GO TO 23
RA(2,II) = TRAD2(II)
RA(3,II) = TRAD3(II)
IF (NLZT.EQ.3) GO TO 23
RA(4,II) = TRAD4(II)
RA(5,II) = TRAD5(II)
RA(6,II) = TRAD6(II)
23 CONTINUE
IF (NLZT.EQ.4) GO TO 50
DO 35 JJ = 1,3
IF (JJ.LE.0) GO TO 34
IF (JJ.EQ.3) GO TO 34
DO 24 KK = 1,NT
24 Y1(KK) = LAC(JJ,KK)
DO 25 LL = 1,IMAT
25 Y2(LL) = RA(JJ,LL)
IXL(1) = IXL(1) + 1
IXR(1) = IXR(1) + 1
CALL GRAPH (NT,X,Y1,0.27.0.0.0.0.2500.0.X AND R (MM); T(X) A
IND T(R); TEMPERATURE PROFILE: DLAB)
CALL GRAPH (NT,X,Y2,4,107,IXL)
CALL GRAPH (NN,RDIST,Y2,1,IXL,IXR)
GO TO 35
34 IXL(1) = IXL(1) + 1
IXR(1) = IXR(1) + 1
35 CONTINUE
IXL(1) = IXL(1) - 3
IXR(1) = IXR(1) - 3
GO TO 12
50 DO 60 JK = 1,6
IF (JK.LE.0) GO TO 59
IF (JK.EQ.6) GO TO 59
DO 51 KL = 1,NT
51 Y1(KL) = LAC(JK,KL)
DO 52 LM = 1,IMAT
52 Y2(LM) = RA(JK,LM)
IXL(1) = IXL(1) + 1
IXR(1) = IXR(1) + 1
CALL GRAPH (NT,X,Y1,0.27.0.0.0.0.2500.0.X AND R (MM); T(X) A
IND T(R); TEMPERATURE PROFILE: DLAB)
CALL GRAPH (NT,X,Y2,4,107,IXL)
CALL GRAPH (NN,RDIST,Y2,1,IXL,IXR)
GO TO 60
59 IXL(1) = IXL(1) + 1
IXR(1) = IXR(1) + 1
60 CONTINUE
IXL(1) = IXL(1) - 6
IXR(1) = IXR(1) - 6
12 IF (L3.EQ.1) GO TO 65
IF (NPOLY<LT.KM) GO TO 96
RETURN

DO 75 IJK=1,NT
SUMLAT(IJK)=0.0
SUMLAT(IJK)=SUMLAT(IJK)+TLAT1(IJK)
IF (NLZT.EQ.0) GO TO 66
SUMLAT(IJK)=SUMLAT(IJK)+TLAT2(IJK)+TLAT3(IJK)
IF (NLZT.EQ.1) GO TO 67
SUMLAT(IJK)=SUMLAT(IJK)+TLAT4(IJK)+TLAT5(IJK)+TLAT6(IJK)
AVELAT(IJK)=SUMLAT(IJK)/6.
GO TO 75

AVELAT(IJK)=SUMLAT(IJK)
GO TO 75

AVELAT(IJK)=SUMLAT(IJK)/3.
CONTINUE

DO 85 LMN=1,IMAT
SUMRAD(LMN)=0.0
SUMRAD(LMN)=SUMRAD(LMN)+TRAD1(LMN)
IF (NLZT.EQ.1) GO TO 76
SUMRAD(LMN)=SUMRAD(LMN)+TRAD2(LMN)+TRAD3(LMN)
IF (NLZT.EQ.2) GO TO 77
SUMRAD(LMN)=SUMRAD(LMN)+TRAD4(LMN)+TRAD5(LMN)+TRAD6(LMN)
AVERAD(LMN)=SUMRAD(LMN)/6.
GO TO 85

AVERAD(LMN)=SUMRAD(LMN)
GO TO 85

AVERAD(LMN)=SUMRAD(LMN)/3.
CONTINUE

WRITE (6,2000)
FORMAT(10X,'DISTANCE AVE. RADIAL T')
DO 90 NNN=1,IMAT
FORMAT(10X,4E11.4)
WRITE (6,2001) RDIST(NNN),AVERAD(NNN)
WRITE (6,2002)
FORMAT(10X,4E11.4)
WRITE (6,2003) X(MMM),AVELAT(MMM)
IF (KPLOT2.EQ.1) GO TO 96
CALL GRAPH (NT,X,AVELAT,0.2709,0.00.25000.'X AND R (MM)';',',AV
IE+ LINE PAIR TEMP*','AVE+ LP TEMP PROFILE','DLAB)
CALL GRAPH (NT,X,AVELAT,4.107,'AVE+ LATERAL TEMPS.';')
CALL GRAPH (IMAT,RDIST,AVERAD,1.111,'AVE+ RADIAL TEMPS.';')
CONTINUE

END

SUBROUTINE SLOPET (NT,IMAT,RTP,ARI,RADIST,RADINT,NLZT,DLAB,WAVE,KM
1,NL,NN,OKODE,KPL03,KPNE01,KPNE02,DELA,DELINT,IARTP)

C LEAST SQUARES SLOPE METHOD OF TEMPERATURE CALCULATION
DIMENSION FNUM(7)
DIMENSION YCALCN(51,4), YINLA(51), TS(5), TLA(51), DLAB(5), RBP(15,4),
IAR(15,4), RADINT(51,4,7), RADIST(51,4,7), SLOPEL(51), ERRPR(51),
2RAYIN(51), WAVE(4), EQ(4), GA(4), RAT(51), RSL(51), RERROR(51),
3X(15), D(51,4),
4CALYLA(51,4), YLA(51,4), YLADIF(51,4), CALYRA(51,4), YRA(51,4),
5YRADIF(51,4), DELTA(4), DELINT(51,4,7), DELTRS(51), COEF(4),
DATA FNUM/0.5, 0.2, 0.5, 5.0, 10.0, 25.0, 50.0/
DATA TS/0.1, 12.7, 0.4, 3.0, 3.3, 4.3, 2.2, 2.7, 7.6/
IF (LKODE.EQ.2) GO TO 30
IF (LKODE.EQ.3) GO TO 1999
TAEQ/3.8175, 7.49, 6.5, 1.6, 2.7, 7.5, 3.8, 2.6, 3.7 /
GA/7.49, 6.5, 1.6, 2.7, 7.5, 3.8, 2.6, 3.7 /
IF (IARTP.NE.9) GO TO 35
1999 FORMAT (///, T10, '* BAINFIELD AND HUBER GA VALUES USED****')
GA(1)=10.25
GA(2)=5.61
GA(3)=0.19
GA(4)=4.05
GO TO 35
30 CONTINUE
EO(1)=116634
EO(2)=118893
EO(3)=117199
EO(4)=117118
GO TO (100, 101, 102, 103, 104, 105), IARTP
READ (5, 2000) (GA(JJJ), JJJ=1, NLZT)
2000 FORMAT (4F10.0)
GO TO 35
1999 READ(5,2000) (EQ(III), III=1, NLZT)
READ(5,2000) (GA(JJJ), JJJ=1, NLZT)
GO TO 35
100 CONTINUE
GA(1)=2.67
GA(2)=36.65
GA(3)=13.25
GA(4)=20.04
GO TO 35
101 CONTINUE
GA(1)=2.25
GA(2)=36.43
GA(3)=14.7
GA(4)=23.07
GO TO 35
102 CONTINUE
GA(1)=2.55
GA(2)=36.0
GA(3)=14.0
GA(4)=21.3
GO TO 35
103 CONTINUE
  GA(1)=3.96
  GA(2)=45.0
  GA(3)=18.0
  GA(4)=27.0
  GO TO 35
104 CONTINUE
  GA(1)=2.28
  GA(2)=32.0
  GA(3)=11.5
  GA(4)=18.9
  GO TO 35
105 CONTINUE
  GA(1)=2.37
  GA(2)=36.0
  GA(3)=14.0
  GA(4)=21.3
35 IF (NLNZT.GE.3) GO TO 1
  WRITE (6,99)
99 FORMAT (15X,'INSUFFICIENT NUMBER OF DATA POINTS TO CALCULATE SLOPE
  1 TEMP. *)
  RETURN
1 DO 25 NPOLY=1,KM
NL=NL+1
WRITE (6,1005)
1005 FORMAT (15X,16X,'DO POLYNOMIAL TEMPERATURE CALCULATIONS FOR',15X,1E11.4,2X,'PERCENT PROBABILITY OF EXCEEDING THE F-VALUE?')
1006 FORMAT (10X,'DKABEL MULTIPLE F-TEST POLYNOMIAL TEMPERATURE CALCULATIONS FOR',15X,1E11.4,2X,'PERCENT PROBABILITY OF EXCEEDING THE F-VALUE?')
15 WRITE (6,1000)
1000 FORMAT (15X,'CALCULATION OF TEMPERATURE BY THE LEAST-SQUARES SLOPE METHOD *')
  DO 2 II=1,NLZT
  DO 2 IJ=1,NT
2 YCALCN(IJ)=ARI(IJ,II)
  CALL LSQ (NT,YCALCN,NLZT,TS,GA,EQ,YINLA,TLA,SLOPEL,ERRORL,WAVE,1CALYLA,YLA,YLADIF)
  WRITE (6,1001)
1001 FORMAT (15X,'X T(X) SLOPE(X) 95 CL
  1 Y-INTERCEPT *')
  DO 3 I=1,NT
3 WRITE (6,1002)
1002 FORMAT (15X,'LATERAL SLOPE DATA FOR ',15X,1E11.4,2X,'RUN')
  DO 29 I2=1,NT
29 WRITE (7,7000) DLAB
7000 FORMAT (15X,'LATERAL SLOPE DATA FOR ',15X,1E11.4,2X,'RUN')
  DO 29 I2=1,NT
29 WRITE (7,7001)
7001 FORMAT (15X,2F10.3)
WRITE (7,7001) TLA(I2),RBP(I2,1)
WRITE (6,7002) DLAB

7002 FORMAT ('/10.1', 'LATERAL SLOPE TEMP DATA HAS BEEN PUNCHED FOR USE'
1 IN THE ELECTRON', '/10.1', 'DENSITY PROGRAM FOR THE DATA RUN', '5X, 5A4)

28 DO 4 KK=1,NLZT
      DO 4 KL=1,IMAT
      K=(IMAT-KL)+2
      YCALCN(KL,KK)=RADINT(K, KK, NPOLY)
      CALL LSQ(IMAT, YCALCN, NLZT, TS, GA, EQ, RAYIN, RAT, RSLOPE, RERRDR, WAVE,
1 CALYR, YRA, YRADIF)
      DO 40 I=1,NLZT
          DO 40 J=1,IMAT
            K=(IMAT-J)+2
            AYCALCN(KL,KK)=RADINT(K, KK, NPOLY)
          CALL LSQ(IMAT, AYCALCN, NLZT, TS, GA, EQ, RAYIN, RAT, RSLOPE, RERRDR, WAVE,
1 CALYR, YRA, YRADIF)
        DO 40 J=1,IMAT
          DO 40 I=1,NLZT

40 DO(J,1)=DELINT(K,1, NPOLY)
     SUMEQ=0.0
     SUMEQ2=0.0
     DO 39 L=1,NLZT
       SUMEQ=SUMEQ+EQ(L)
       SUMEQ2=SUMEQ2+(EQ(L)*EQ(L))
     SUMEQ2=SUMEQ2+(EQ(L)*EQ(L))
     DENOMT=ABS((NLZT*SUMEQ2)-(SUMEQ*SUMEQ))
     DO 38 M=1,NLZT
       COEFT(M)=ABS((NLZT*EQ(M)-SUMEQ)
     DO 37 N=1,IMAT
       XMULT=RAT(N)/(1.439*DENOMT)
       TERM=0.0
       DO 36 M=1,NLZT
         TERM=TERM+CCOEFT(M)*(DELA(M)*D(N,M))
       DELTRS(N)=XMULT*TERM
     WRITE (6,1003) 
1003 FORMAT ('R', 'SLOPE(R) 95 CL', 6X, 'INTERCEPT', 6X, 'DELTA T(R) IN PERCENT')
     DO 5 J=1,IMAT
       KJ=(IMAT-J)+2
     DO 104 FORMAT ('T2, E1, 4, 1X, E11, 4, 2X, E11, 4, 2D(E4, E11, 4), 12D(E11, 4)
5 WRITE (6,1004) RADIST(K1, 1, NPOLY), RAT(J), RSLOPE(J), RERRDR(J), RAYIN
1(J), DELTRS(J)
     IF (KPNED2=4KJ) GO TO 33
8000 FORMAT (10X, 'RADIAL SLOPE TEMP DATA FOR', '5X, 5A4, 5X, 'RUN')
     DO 34 J2=1,IMAT
       K2=(IMAT-J2)+2
     DO 8001 FORMAT (2F10.3, 15X, 'DEGREE', 15, 5A4)
34 WRITE (7,8001) RAT(J2), RADIST(K2, 1, NPOLY), NL, DLAB
8002 FORMAT ('/10.1', 'RADIAL SLOPE TEMP DATA HAS BEEN PUNCHED FOR USE'
1 IN THE ELECTRON', '/10.1', 'DENSITY PROGRAM FOR THE DATA RUN', '5X, 5A4)
33 WRITE (6,3000)
3000 FORMAT ('/10.1')
3001 FORMAT (T25, 'LATERAL INTENSITY DATA, Y=LOG(GA/WAVE*I(X))')
2051
DO 6 N1 = 1, NT
   WRITE (6, 3002) RBP(N1,1), TLA(N1)
3002 FORMAT ('LATERAL DISTANCE = ','E11.4', 'T(X) = ','E11.4')
   WRITE (6, 3003)
3003 FORMAT ('WAVELENGTH CALC Y EXPT Y DEL Y EXC. POT*')
   DO 6 N2 = 1, NLZT
6 WRITE (6, 3004) WAVE(N2), CALYLA(N1,N2), YLA(N1,N2), YLADIF(N1,N2), EQ(N2)
3004 FORMAT ('WAVE(N2)')
   WRITE (6, 3005)
3005 FORMAT ('RADIANT INTENSITY DATA, Y=LOG(GA/WAVE*I(R)))
   DO 7 N3 = 1, IMAT
    KKK = (IMAT - N3) + 2
7 WRITE (6, 3006) RADIUS(KKK,1,NPOLY), RAT(N3)
3006 FORMAT ('RADIAL DISTANCE = ','E11.4', 'T(R) = ','E11.4')
   WRITE (6, 3007)
3007 FORMAT ('WAVELENGTH CALC Y EXPT Y DEL Y EXC. POT*')
   DO 7 N4 = 1, NLZT
7 WRITE (6, 3008) WAVE(N4), CALYPA(N3,N4), YRA(N3,N4), YRAD IF(N3,N4), EQ(N4)
3008 FORMAT ('WAVE(N4)')
   IF (KPLOT3.EQ.1) GO TO 25
   DO 10 M = 1, NT
10 X1(M) = RBP(M,1)
   DO 20 N = 1, IMAT
20 X2(N) = RADIST(K2,1,NPOLY)
   CALL GRAPH (NT,X1,TLA,0,2.7,0.9,0.0,0.25,0.0,'X AND R (MM) ; ''SLOPE TEMP. AND PROFILE; ' 'DLAB')
   CALL GRAPH (IMAT,X2,RAT,1,11,'RADIAL SLOPE TEMP. ; ' )
   CALL GRAPH (IMAT,X2,RAT,1,11,'RADIAL SLOPE TEMP. ; ' )
25 CONTINUE
RETURN
END

SUBROUTINE LSQ (INDEX,YCALCN,NLZT,TS,GA,EQ,YIN,TEMP,SLOPE,ERRORM,
1 WAVE,CALCY,Y,YDIF)
DIMENSION YCALCN(51,4),TS(5),GA(4),EQ(4),YIN(51),TEMP(51),SLOPE(51),
1 ERRORM(51),SUMX(51),SUMY(51),SUMXX(51),SUMXY(51),SOMX(51),SOMXY(51),WAVE(4),DENOM(S
21),SSE(51),SEX(51),XBAR(51),YBAR(51),DIFFX(4),DIFFY(4),
3 CALCY(51,4),Y(51,4),YDIF(51,4)

8 DO 50 I = 1, INDEX
50 SUMX(I) = 0.0
      SUMY(I) = 0.0
      SUMXX(I) = 0.0
      SUMXY(I) = 0.0
      DO 2 J = 1, NLZT
2      SUMX(I) = SUMX(I) + EQ(J)
SUMY(I)=SUMY(I)+ALOG10(GA(J)/(WAVE(J)*YCALCN(I,J)))
SUMX(I)=SUMX(I)+(EQ(J)*EQ(J))
2 SUMXY(I)=SUMXY(I)+(EQ(J)*ALOG10(GA(J)/(WAVE(J)*YCALCN(I,J))))
D=NLZT
DENOM(I)=(D*SUMXX(I))-SUMX(I)*SUMX(I))
SLOPE(I)=((D*SUMXY(I))-SUMX(I)*SUMXY(I))/DENOM(I)
YIN(I)=((SUMXX(I)*SUMY(I))-SUMXY(I)*SUMX(I))/DENOM(I)
SSE(I)=0.0
SSEX(I)=0.0
DO 3 L=1,NLZT
CALCY(I,L)=SLOPE(I)*EQ(L)+YIN(I)
Y(I,L)=ALOG10(GA(L)/(WAVE(L)*YCALCN(I,L)))
YDIF(I,L)=Y(I,L)-CALCY(I,L)
DIFY(L)=YDIF(I,L)*YDIF(I,L)
SSE(I)=SSE(I)+DIFY(L)
XDIFF(EQ(L)-XBAR(I))
DIFX(L)=XDIFF*XDIF
3 SSEX(I)=SSEX(I)+DIFX(L)
SSEX(I)=SQRT(SSEX(I))
S=SQRT(SSE(I)/(D-2.))
ERRORM(I)=(TS(NLZT)*S)/SSEX(I)
TEMP(I)=1./(1.60013*SLOPE(I))
50 CONTINUE
RETURN
END
APPENDIX B:
ABEL INVERSION CALCULATIONS

General Considerations and the
Abel Integral Equation

We consider a cross-section of the plasma which is circularly symmetric with respect to the Z-axis as illustrated in Figure B-1. The experimentally measured lateral intensity, \( I(X) \), at displacement \( X \), is given by the integral of the radial intensity distribution function \( J(R) \), which is collected in the monochromator viewing field over the depth of the source from a horizontal section parallel to the Y-axis,\(^1\)

\[
I(X) = 2 \int_0^{Y(X)} J(R) \, dY
\]  

(Bl)

The factor of 2 in Equation Bl arises from the fact that the integral limits apply to only half of the source and the radial distribution function has been assumed to be symmetric about the X-axis. When the transformation of variables defined by

---

\(^1\) It is important to realize that Equation Bl expresses the geometrical relationship between the spatially resolved emission, which is projected from unit volume of a horizontal section of the source parallel to the Y-axis, i.e., \( J(R) \) and, the space integrated intensity radiated over the depth of that section, i.e., \( I(X) \).
Figure B-1. Spatial relationship between the measured lateral intensity, $I(X)$, at displacement $X$; and, the radial intensity, $J(R)$, at radius $R$ from the center of a circularly symmetric source employing side-on observation. $R_B$ is the boundary radius at which no lateral intensity is detected.
is performed, Equation B1 becomes

\[ I(X) = 2 \int_X^{R_B} R J(R) (R^2 - X^2)^{-1/2} \, dR \]  \hspace{1cm} (B3)

where, \( R \) is the radial distance from the center of the source, \( R_B \) is the radius at the outer boundary, \( X \) is the lateral displacement from the center (Figure B-1) and, the change in limits is given by

\[ R = X \quad \text{at} \quad Y = 0 \]

and,

\[ R = R_B \quad \text{at} \quad Y = Y(X) \]  \hspace{1cm} (B4)

Equation B3 is the Abel integral equation and is a special case of the Volterra equation of the first kind (129). To solve for the unknown \( J(R) \) function, Equation B3 may be analytically inverted to yield \((36,46,129)\).

\[ J(R) = -\frac{1}{\pi} \int_R^{R_B} \frac{I'(X)}{(X^2 - R^2)^{1/2}} \, dX \]  \hspace{1cm} (B5)

provided \( J(R) = 0 \) for all \( R > R_B \). \( I'(X) \) is the first derivative of the radiance function with respect to the lateral coordinate \( X \), i.e.,

\[ I'(X) = \frac{d(I(X))}{dX} \]
Various methods for solving Equation B5 have been devised; these methods can be broken into three general categories (49, 50): (1) graphical, (2) numerical, and (3) data approximation schemes. The latter two approaches utilize curve fitting or other mathematical approximations. A number of graphical or semigraphical methods for solving Equation B3 or B5 have appeared in the literature (52,130-132). Friederish (52) made the assumption that the ratio, I(X)/X, was constant in a given increment interval to simplify evaluation of the Abel integral over that interval; a graphical method was employed to obtain the I(X)/X values. Normann (132a) transformed the variables in Equation B5 to obtain an integral which he evaluated by graphical techniques. Despite some successful applications of these graphical methods, all are time consuming and have been outmoded by faster computer methods. We shall focus our attention on these rapid analysis methods in the following sections.

Numerical Methods

In 1935, Hormann (132a) and more recently in 1950, Gooderum and Wood (131) suggested methods for numerical integration of Equation B5. Both methods could be applied when the spectrometric measurement of lateral intensities was accomplished with a low aperture optical transfer system similar to that described in this work. Nestor and Olsen (49)
simplified these procedures to yield a significantly improved method, especially when a large number of observed functions were to be inverted. This method was also compatible with computer analysis.

For the Nestor and Olsen method, the numerical integration of Equation B5 was performed by dividing the X-axis into N zones of equal width a, as shown in Figure B-2; the n-th zone was defined by the relationships, \( X_n \leq X \leq X_{n+1} \) and \( X_n = na \). With the transformation

\[
v = R^2 \text{ and } u = X^2
\]  

(B6)

Equation B5 became

\[
J(R(v)) = -\frac{1}{\pi} \int_{v}^{R^2} I'(u) (u - v)^{-1/2} \, du
\]  

(B7)

where, the following relationships were employed

\[
dX = \frac{1}{2} u^{-1/2} \, du
\]

\[
(X^2 - R^2)^{1/2} = (u - v)^{1/2}
\]  

(B8)

\[
d(I(u))/du = (d(I(X))/dX)(d(g(u))/du)
\]

and,

\[
g(u) = X = u^{1/2}
\]

\[
I'(X) = 2 \, u^{1/2} \, I'(u)
\]  

(B9)

When the integral in Equation B7 was divided into sub-integrals for each zone and I(u) was assumed to be a linear function of u in each zone, the following form was obtained
Figure B-2. Two-dimensional representation of a circularly symmetric source divided into $N$ zones of equal width, $a$
for any zone, $k$

$$J_k = J(ak) = (-1/\pi) \sum_{n=k}^{N-1} I'_n(u) \int \frac{(a(n+1))^2}{(an)^2} \left( u - \frac{1}{ak} \right)^2 du$$

(B10)

where, the integral limits and the $v$ variable were replaced by the appropriate zone constants. $I'_n(u)$ was approximated within each zone by

$$I'_n(u) = \frac{(I_{n+1}(u) - I_n(u))}{a^2((n+1)^2 - n^2)}$$

(B11)

Substitution of Equation B11 into B10 and subsequent integration yielded

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N-1} (I_{n+1}(u) - I_n(u)) \frac{((n+1)^2 - k^2)^{1/2} - (n^2 - k^2)^{1/2}}{(2n + 1)}$$

(B12)

A transformation to the original coordinate system yielded

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N-1} A_{kn} (I_{n+1}(X) - I_n(X))$$

(B13)

where,

$$A_{kn} = \frac{((n+1)^2 - k^2)^{1/2} - (n^2 - k^2)^{1/2}}{(2n + 1)}$$

(B14)
Equation B14 was further simplified to yield

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N} B_{kn} I_n$$

(B15)

where,

$$B_{kn} = -A_{kn} \text{ for } n = k$$

and

$$B_{kn} = A_{k,n-1} - A_{kn} \text{ for } n > k+1$$

(B16)

Other methods for numerical solution of Equation B5 are also available. Pearce (132b) suggested a procedure similar to the Nestor and Olsen method. Maldonado, et al. (53) described a method which yielded more reliable radial emission coefficients when the measured lateral intensity distribution showed irregular fluctuations, especially in regions where $I(X)$ changed gradually with lateral position $X$. However, this procedure was computationally more complex than the Nestor and Olsen method described above. Maldonado and Olsen (54) generalized the method of reference 53 to include asymmetric sources and applied it to those which possessed a mirror plane of symmetry. Olsen, et al. (55) later extended this application to optically thin plasma cross-sectional geometries of arbitrary shape.

Discussions on the errors associated with numerical methods may be found elsewhere (133,134) and will not be reiterated here. It is worth noting, however, that these
methods generally suffer when the error level on the measured
I(X) profile values is significant because the numerical
solution procedure for obtaining J(R) values greatly magnifies
these errors.

Data Approximation Methods

In 1966, Cremers and Birkebak (50) described a data
approximation scheme for solution of Equation B3 or B5 which
was faster than conventional numerical techniques and could
readily be adapted to computer analysis. The basic assumption
of this method was that the lateral intensity distribution
function could be approximated by an n-th degree polynomial of
the form

\[ I(X) = C_0 + C_1 X + C_2 X^2 + \cdots + C_n X^n \]  \hspace{1cm} (B17)

with the corresponding derivative function

\[ I'(X) = C_1 + 2C_2 X + 3C_3 X^2 + \cdots + nC_n X^{n-1} \]  \hspace{1cm} (B18)

When Equation B18 was substituted into Equation B5 the
following expression for the radial distribution function was
obtained

\[ J(R) = -\frac{1}{\pi} \int_{R}^{R_B} \frac{(C_1 + 2C_2 X + \cdots + nC_n X^{n-1})}{(X^2 - R^2)^{1/2}} \, dX \]  \hspace{1cm} (B19)
An analytical solution of Equation B19 was possible when the polynomial coefficients were determined by least-squares techniques and the equation was separated into "n" component integrals.

Cremers and Birkebak cautioned that fitting the entire curve to a single polynomial resulted in peculiar radial profiles which precluded this approach because of the many poor fits that resulted. Consequently, they suggested subdividing the profiles into m zones and fitting an n-th degree polynomial to the form

\[ I_k(X) = C_0 + \sum_{i=1}^{n} C_i X^i, \text{ for } k = 1, 2, \ldots, m \]  

(B20)
to each zone. To assure smooth transitions from zone to zone, the polynomial fits overlapped into the adjacent zones. When the differential form of Equation B20 was substituted into Equation B5 an integrable expression was obtained.

If the integrant of Equation B5 is defined as

\[ S_k = - \frac{I_k'(X)}{(X^2 - R^2)^{1/2}} \]  

(B21)
a closer examination of the actual integrations indicated by this equation may be carried out. For I(X) divided into m zones and for a given R contained within a zone k such that

\[ R_{k-1} \leq R \leq R_k \]  

(B22)
the radial intensity is given by
\[ J(R) = F_0(R) + F_1(R) \]  
\[ \text{(B23)} \]

where, \( F_0(R) \) and \( F_1(R) \) are defined by

\[ F_0(R) = \int_R^{R_k} S_k \, dX \]  
\[ \text{(B24)} \]

and

\[ F_1(R) = \sum_{i=k+1}^{m} \int_{R_{i-1}}^{R_i} S_i \, dX \quad \text{for} \quad k < m \]  
\[ = 0 \quad \text{for} \quad k = m \]  
\[ \text{(B25)} \]

The subdivision of the \( I(X) \) profile employed in these calculations is schematically represented in Figure B-3.

It should be noted that the zones were counted from the center where \( R_0 = 0 \) to the outer radius of the source where \( R_m = R_B \).

Cremers and Birkebak made an additional refinement on the form of the assumed polynomial in Equation B20 because of the nature of the slope at \( K = 0 \). When Equation B20 was differentiated the following form was obtained

\[ I'_k(X) = k C_1 + \sum_{i=2}^{n} (k C_1) i X^{i-1} \]  
\[ \text{(B26)} \]

and it was noted that \( I'_k(X) \neq 0 \) at \( X = 0 \). Consequently, the profile did not possess the desired zero slope at the
Figure B-3. Schematic representation of five zone subdivision of the I(X) profile (bell-type curve case)
center that a circularly symmetric distribution should have. To avert this problem, Cremers and Birkebak (50) suggested that a polynomial in $X^2$ which possesses the desired zero slope at $X = 0$, be employed for the inner-most zone, i.e.,

$$I_1(X) = C_0 + \sum_{i=1}^{n} C_i X^{2i}$$  \hspace{1cm} (B27)

Therefore, solutions of Equation B5 which utilize the zone dependency of Equations B20 or B27 were considered in this dissertation research.

Cremers and Birkebak also suggested that (1) subdivision of the $I(X)$ profile into five zones and (2) 4-th degree polynomial least-squares fitting of the data, were sufficient for most cases encountered in physical systems. The following discussions of the actual integration procedures employed here have been restricted to these suggestions.

**Method of integration for zones 2-5**

Examination of Equation B23 revealed that it was necessary to evaluate the integrals $\int_{k}^{F_0(R)}$ and $F_1(R)$. Substitution of the 4-th degrees polynomial of the form given by Equation B20 into Equation B24 yielded

$$k F_0(R) = - \frac{1}{\pi} \left( \int_{R_k}^{R_k} \frac{k C_1}{G(X,R)} dX + 2 \int_{R_k}^{R_k} \frac{k C_2 X}{G(X,R)} dX ight) + 3 \int_{R_k}^{R_k} \frac{k C_3 X^2}{G(X,R)} dX + 4 \int_{R_k}^{R_k} \frac{k C_4 X^3}{G(X,R)} dX \right) \hspace{1cm} (B28)$$
where, \( n = 4 \) and

\[
G(X,R) = (X^2 - R^2)^{1/2}
\]  

(B29)

Solutions for the integrals in Equation B28 may be found in most integral tables, e.g., (135). Upon integration of Equation B28 the following form was obtained

\[
k^{F_0}(R) = -\frac{1}{\pi} \left[ k^3 C_1 \ln(X + G(X,R)) + 2 k^2 C_2 G(X,R) + \frac{3}{2} k^3 C_3 (X G(X,R) + R^2 \ln(X + G(X,R))) + 4 k^4 C_4 (G^3(X,R)/3 + R^2 G(X,R)) \right]_{R}^{R_k} \]  

(B30)

Evaluation of Equation B30 at the limits \((R\ to\ R_k)\) and combining terms yielded

\[
k^{F_0}(R) = -\frac{1}{\pi} \left[ k^3 C_1 \ln\left(\frac{R_k + G(R_k,R)}{R}\right) + 2 k^2 C_2 G(R_k,R) + \frac{3}{2} k^3 C_3 (R_k G(R_k,R) + R^2 \ln\left(\frac{R_k + G(R_k,R)}{R}\right)) + 4 k^4 C_4 (G^3(R_k,R)/3 + R^2 G(R_k,R)) \right] \]  

(B31)

where, the following relations were used

\[
(R_k^2 - R^2)^{1/2} = G(R_k,R)
\]

\[
\ln(X + G(X,R)) = \ln(R_k + G(R_k,R)) \quad \text{for} \quad X = R_k
\]
\[(R^2 - R^2)^{1/2} = 0 = G(R,R)\]

and
\[\ln(X + G(X,R)) = \ln(R) \quad \text{for} \quad X = R\]

For a given \(R\) such that \(R_4 \leq R \leq R_5\), \(F_0(R)\) was the only integral that required evaluation. However, when \(k\) was less than \(m\), Equation B25 indicated that \(F_1(R)\) also had to be evaluated. This set of summed integrals possessed solutions identical to those of Equation B30 except that the limits were replaced by the appropriate values from B25, i.e.,

\[
F_1(R) = \sum_{i=k+1}^{5} \left( -\frac{1}{i} \right) \left( C_1 \ln(R_i + G(R_i,R)) + \frac{3}{2} C_2 \ln(R_i G(R_i,R)) + \ln(R_i + G(R_i,R)) \right)
\]

It should be noted that when the integrals were summed from zone to zone, the predetermined least-squares polynomial
coefficients changed smoothly to the zone under consideration because of the overlapping of the fits into adjacent zones.

Method of integration for zone 1

From the previous discussion of the desired behavior of \( I(X) \) in the neighborhood of \( X = 0 \) (\( I'(X=0) = 0 \)) it was apparent that a polynomial of the form of Equation B27 was required for values of \( R \) when \( 0 \leq R < R_1 \), i.e., \( R \) was confined to zone 1. Differentiation, expansion, and substitution of Equation B27 into B24 yielded

\[
1 F_0(R) = \left( -\frac{2}{\pi} \right) \left( \int_R^{R_1} \frac{1}{G(X,R)} \frac{C_1 X}{G(X,R)} \, dX + 2 \int_R^{R_1} \frac{1}{C_2} \frac{X^3}{X^3} \, dX \right) + 3 \int_R^{R_1} \frac{1}{C_3} \frac{X^5}{G(X,R)} \, dX + 4 \int_R^{R_1} \frac{1}{C_4} \frac{X^7}{G(X,R)} \, dX \)  

(B33)

where, \( n = 4 \) and the notation of Equation B29 was used. When the integration was performed and the limits were evaluated, \( 1 F_0(R) \) was given by

\[
1 F_0(R) = \left( -\frac{2}{\pi} \right) \left( C_1 G(R_1,R) + 2 C_2 \frac{G^3(R_1,R)}{3} \right) + R^2 G(R_1,R) \right)
+ 3 C_3 \left( \frac{R^4}{4} G(R_1,R) \right) + \frac{2}{3} R^2 \frac{G^3(R_1,R)}{3} + \frac{1}{5} G^5(R_1,R) \right)
+ 4 C_4 \left( \frac{R^6}{6} G(R_1,R) + \frac{R^4}{4} G^3(R_1,R) \right)
+ \frac{3}{2} R^2 \frac{G^5(R_1,R)}{5} + \frac{1}{7} G^7(R_1,R) \right) \)  

(B34)
Because the other zones (2-5) were not affected by the change in the zone 1 equation for $I(X)$, $F_1(R)$ was evaluated in precisely the same manner established in Equation B32.

Other data approximation methods are also available for solution of the Abel integral equation (B3) or its inverted form (B5). Freeman and Katz (56) suggested a curve-fitting procedure in which a single polynomial was fitted to the $I(X)$ profile data. However, Cremers and Birkebak (50) cautioned that this method yielded peculiar line profiles when it was applied to arc data. Barr (57) suggested a method similar to that of Cremers and Birkebak which employed polynomials determined by least-squares techniques that yielded the best fit of the data over five-point intervals centered about each data point.

**Error analysis**

When Equation B3 was solved for the lateral displacement $X = 0$, the following form was obtained

$$I(X=0) = 2 \int_0^R J(R) \, dR$$

(B35)

Therefore, the area under the radial intensity profile was predicted to equal the lateral intensity at zero displacement from the plasma axis. When test data were employed (50,53), the agreement was better than 1\% while for experimental data
it was $\approx 1$ to 5% for bell-type profiles and $\approx 5$ to 15% for toroidal curves.

Equations B31, B32, and B34 were readily amenable to differential error treatments (81) so that the computational uncertainties in the radial intensities obtained could be calculated. The radial intensity defined by these equations was a function of the polynomial coefficients, $\mathbf{C}_j$, and the radial position $R$. When the uncertainty in $R$ was assumed to be negligible, a maximum differential error treatment yielded

$$
\Delta J(R)_k \approx \sum_{j=1}^{4} \left\{ \left| \frac{\partial \mathbf{F}_1(R)}{\partial \mathbf{C}_j} \right| \Delta \mathbf{C}_j + \sum_{i=k+1}^{5} \left| \frac{\partial \mathbf{F}_1(R)}{\partial \mathbf{C}_j} \right| \Delta \mathbf{C}_j \right\}
$$

(B36)

where, the subscript $k$ denoted the profile zone. For zone 1 the uncertainty, $\Delta J(R)_1$ was obtained by combining Equation B36 with the expressions for $\mathbf{F}_1(R)$ and $\mathbf{F}_1(R)$, Equations B34 and B32, respectively. For the other zones ($2 \leq k \leq 5$) Equation B36 was combined with Equations B31 and B32 to yield the appropriate $\Delta J(R)_k$ values. The $\Delta J(R)_k$ values so obtained represented approximations to the maximum random calculation error in the corresponding $J(R)$ values for each zone. Systematic errors such as those encountered when measuring lateral intensities were accounted for by other means, e.g., added to the random error estimates.
The uncertainties in the coefficients ($\Delta_1 C_j$) were obtained from the error analysis techniques incorporated within the polynomial fitting method employed (reference 81, Chapter 3).
APPENDIX C:

ATOMIC PARTITION FUNCTION AND SAHA-EGGERT'S ELECTRON DENSITY CALCULATIONS

To a first approximation, partition functions appear to be easily calculated by summing over all energy levels of the element of interest which are below the ionization limit; this would be accomplished with the expression (36)

\[ Z_{z-1}^\text{(T)} = \sum_n g_n \exp\left(-\frac{E_n}{kT}\right) \]  

where, \( z-1 \) is the ionization stage and \( g_n \) is the statistical weight of the level, \( n \), with energy \( E_n \) at temperature \( T \). An immediate problem is encountered when attempts are made to apply the above procedure to the calculation of atomic partition functions namely, even the most complete listing of atomic energy levels (136) contains only a fraction of those predicted for a given element. If the missing levels are reasonably high in energy, few problems will be experienced for temperatures below 7000 K. However, the calculated values may be seriously in error at higher temperatures or, for elements for which the missing levels are at relatively low energies. Also, when the ionization limit (\( E_{z-1}^1 \)) of the species is approached, the sum in Equation Cl diverges because the number of discrete levels is unbounded while the
corresponding energies (except for levels which autoionize; 36, p. 140) are restricted to values less than $E_i^{z-1}$.

Several methods for overcoming these difficulties have been reported (31, pp. 231-258). All these theories share the premise that there exists a finite maximum principal quantum number $n^*$ (sometimes referred to as the "effective" quantum number) and, accurate partition function values are obtained only when all energy levels for values of $n$ below $n^*$ are considered in the calculation. The effective quantum number ($n^*$) and the corresponding energy ($E_{n^*}$) are functions of temperature, electron number density, ion densities, and the effective nuclear charge of the species. Therefore, the summation in Equation C1 must be truncated at the reduced ionization limit (RIL), $E_i^{z-1} - \Delta E_i^{z-1}$ where, $\Delta E_i^{z-1}$ is the ionization lowering for the species in question (36). In this manner, only those energy levels less than or equal to the RIL value are counted. This truncation precludes the possibility of counting a single level twice, once in a bound state and once in a free state.

The energies of the levels near the ionization limit which are sufficiently hydrogen-like, are given by the Rydberg formula (36)

$$E_i^{z-1} - E_n^{z-1} = \frac{Z^2 E_H}{n^2} \quad (C2)$$

where, $E_H$ is the ionization energy of atomic hydrogen (109,679 cm$^{-1}$) and $n \geq 4$. The statistical weight of the level
$E_n^{z-1}$, is given by $g_n = 2n^2$. When the term value, $-E_h/(n^*)^2$, is combined with Equation C2, the effective principal quantum number is given by

$$n^* = \left(\frac{z^2 E_h}{\Delta \epsilon}\right)^{1/2} \quad (C3)$$

where, $\Delta \epsilon = E_1^{z-1} - E_n^{z-1}$. The Ritz formula (117) may then be written as

$$n^* = n - \alpha - \frac{z^2}{n^2} \beta \quad (C4)$$

where, $z = 1$ for neutral atoms, $z = 2$ for singly charged ions, $z = 3$ for doubly charged ions, etc., and $\alpha, \beta$ are series parameters. Drawin and Felenbok (31) suggested that Equation C4 be used to complete each spectral series that was considered in the partition function calculation. Generally, the last two members observed in the series were used to evaluate $\alpha$ and $\beta$, which were subsequently employed with Equation C4 to calculate the remaining members of the series. In the case where a spectral series was predicted but for which no members were observed, an alternate series as closely related as possible was substituted and its degeneracy approximately increased to account for the unobserved terms. This method is reasonably accurate for elements with simple energy level schemes, however, its application to complex systems is overly elaborate. An alternate approach was reported by Griem (36)
and was applied to plasma simulation calculations by Barnett (137). This method for calculating atomic partition functions employed only those levels from reasonably complete configurations for which all states with principal quantum numbers less than a maximum value were observed. In this approach, the effective quantum number was defined by

\[ n^* = n_{\text{max}} + \left( \frac{z^2 E_H}{E_i} \right)^{1/2} \]  

where, hydrogen-like character was assumed. Only those levels \( E_n \) with \( n \leq n_{\text{max}} \) contributed to the partition function calculation. The procedure involved two steps: (1) selection of \( n' \), the highest usable principal quantum number for the species, and (2) addition of a correction factor (from \( n' \) to \( n_{\text{max}} \)) with hydrogen-like character assumed but still accounting for multiplicity differences. The complete partition function was then approximately given by (36)

\[
z^{z-1}(T) \approx \sum_{n=1}^{n'} g_n \exp\left(- \frac{E_n}{kT}\right) + (2S_1 + 1)(2L_1 + 1)
\]

\[
x \sum_{n=n'+1}^{n_{\text{max}}} 2n^2 \exp\left(- \frac{E_{2L} - (z^2 E_H/n^2)}{kT}\right) \]

where, the first summation was made over those levels which were included in the complete or nearly complete configurations and, the second summation was the correction term. In
the second summation, \( S_1 \) and \( L_1 \) were the spin and orbital quantum numbers of the parent configuration, i.e., the ground state of the next higher ionization stage \( z \). The degeneracies in the first summation were given by \( g_n = 2J_n + 1 \) where, \( J_n \) was the orbital angular momentum quantum number for the (discrete) level \( E_n \) and, the index \( n \) referred to all relevant quantum numbers (36).

Barnett (137) demonstrated that the Ritz completion method and Griem's method yielded parallel trends in partition function calculations for reasonable temperatures (below 15,000 K). Therefore, because Griem's method was computationally simpler, Equation C6 was employed to calculate the neutral atom (\( z = 1 \)) partition functions of several elements for subsequent use in Saha-Eggert's electron density studies for this dissertation research. The correction term was generally not needed for singly charged and higher ionization stages because the missing levels were high in energy for the elements considered. The value of \( n' \) for each element was determined in the following manner: (1) all observed spectral series were tabulated (136) with the corresponding maximum observed \( n \) values (\( n_{\text{max}} \)); (2) a weighted maximum principal quantum number, \( n_w' \), was calculated according to the total degeneracy of each series term (\( n_w' = (2S+1)(2L+1)(n_{\text{max}}) \)); (3) a weighted average maximum principal quantum number was defined by
where, \( N_d \) = sum of the degeneracies of the observed spectral terms,

\[
N_d = \sum_{j=1}^{N} (n_{\text{max}})^j
\]  

(8)

and, \( N \) = number of observed spectral terms; (4) \( n' \) was taken as the largest integer satisfying the inequality \( n' \leq n_{\text{wa}} \); and (5) the correction was begun at \( n'' = (n'+1) \) where, \( n'' \) was the smallest integer which satisfied the condition, \( n_{\text{wa}} \leq n'' \). Griem (36) concluded that the best procedure for selecting \( n' \) was neither clearly established nor extremely critical because the last terms of the correction sum tend to dominate its contribution to the partition function calculation. The approach outlined here was reasonable because the maximum principal quantum numbers of the observed levels were weighted according to the degeneracy of the spectral term of the series to which they belonged \( (n_{\text{max}} \text{ values}) \) and, the correction for missing levels was begun above a weighted average of these \( n_{\text{max}} \) values. The partition function values calculated by this procedure were in reasonable agreement with those reported by Drawin and Felenbok (31) and those calculated by Barnett (137) for temperatures below 10,000 K.
Use of the Saha-Eggert's Electron Density Program

A FORTRAN IV computer program was written to perform the radial Saha-Eggert's electron density calculations and a complete listing of the source statements is included as C337EDNS. This program employed the partition function values which were calculated by the procedure discussed above. The data card requirements for this program are listed in Table C-1.
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<td>F10.0</td>
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<td>Partition function array for neutral atom species</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>QTEST(2,1)</td>
<td>F10.0</td>
<td></td>
<td>Partition function array for first ion species</td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>QTEST(3,1)</td>
<td>F10.0</td>
<td></td>
<td>Partition function array for second ion species</td>
</tr>
<tr>
<td>3</td>
<td>1/set</td>
<td>1-5</td>
<td>NRUNS</td>
<td>I5</td>
<td>Number of runs in a given data set</td>
</tr>
<tr>
<td>4</td>
<td>1/run</td>
<td>1-73</td>
<td>XIDENT</td>
<td>35A2</td>
<td>Data set identification label</td>
</tr>
<tr>
<td></td>
<td>71-75</td>
<td>NUMAQP</td>
<td>I5</td>
<td></td>
<td>Number of transition probability sources (5 max)</td>
</tr>
<tr>
<td>5</td>
<td>1/run</td>
<td>1-10</td>
<td>WAVEA</td>
<td>F10.0</td>
<td>Wavelength of atomic line (Angstrom units)</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>WAVEI</td>
<td>F10.0</td>
<td></td>
<td>Wavelength of ionic line (Angstrom units)</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>GATOM</td>
<td>F10.0</td>
<td></td>
<td>Degeneracy of atomic line emitting level</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>GION</td>
<td>F10.0</td>
<td></td>
<td>Degeneracy of ionic line emitting level</td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>EQATOM</td>
<td>F10.0</td>
<td></td>
<td>Excitation energy of atomic line (cm$^{-1}$ units)</td>
</tr>
<tr>
<td>Type #</td>
<td># Cards</td>
<td>Columns</td>
<td>Variable Name</td>
<td>Format</td>
<td>Remarks</td>
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<td>---------</td>
<td>---------</td>
<td>--------------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>51-60</td>
<td>EQION</td>
<td>F10.0</td>
<td></td>
<td></td>
<td>Excitation energy of ionic line (cm(^{-1}) units)</td>
</tr>
<tr>
<td>6a</td>
<td>1/run</td>
<td>1-50</td>
<td>A(1,J)</td>
<td>5F10.0</td>
<td>Transition probability array for atomic line (5 max)</td>
</tr>
<tr>
<td>6b</td>
<td>1/run</td>
<td></td>
<td>A(2,J)</td>
<td></td>
<td>Same as 6a except for ionic line</td>
</tr>
<tr>
<td>7</td>
<td>1/run</td>
<td>1-10</td>
<td>XIP</td>
<td>F10.0</td>
<td>Ionization energy of atomic species (cm(^{-1}) units)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11-20</td>
<td>DELXIP</td>
<td>F10.0</td>
<td>Ionization energy lowering</td>
</tr>
<tr>
<td>8</td>
<td>1/run</td>
<td>1-5</td>
<td>NR</td>
<td>I5</td>
<td>Number of radial positions</td>
</tr>
<tr>
<td>9</td>
<td>NR/run</td>
<td>1-10</td>
<td>TR</td>
<td>F10.0</td>
<td>Radial temperature array</td>
</tr>
<tr>
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<td></td>
<td>11-20</td>
<td>R</td>
<td>F10.0</td>
<td>Corresponding radial position array</td>
</tr>
<tr>
<td>10a</td>
<td>NR/run</td>
<td>1-10</td>
<td>XI(1,1)</td>
<td>F10.0</td>
<td>Radial intensity array for atomic line</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21-30</td>
<td>DELIR(1,1)</td>
<td>F10.4</td>
<td>Corresponding relative uncertainty array (%)</td>
</tr>
<tr>
<td>10b</td>
<td>NR/run</td>
<td>XI(1,2)</td>
<td>DELIR(1,2)</td>
<td></td>
<td>Same as 10a except for ionic line</td>
</tr>
</tbody>
</table>

The table continues with additional entries that are not fully visible in the image.
********** C337EDNS **********

PROGRAM TO CALCULATE ELECTRON DENSITIES FROM RADIAL TEMPERATURE AND ATOM, ION LINE INTENSITIES

NUMAOIP = NUMBER OF TRANSITION PROBABILITY PAIRS (5 MAX)
NSETS = NUMBER OF DATA SETS
TSYM = ELEMENT IDENTIFIER FOR QTEST ARRAY ALSO STEPS TTEST READ
TTEST = TEMP ARRAY FOR INPUT PARTITION FUNCTIONS
QTEST(1, I) = PARTITION FUNCTION ARRAY FOR ATOM
QTEST(2, I) = " " " " 1ST ION
QTEST(3, I) = " " " " 2ND ION
NRUNS = NUMBER OF RUNS PER DATA SET
XIDENT = IDENTIFICATION OF DATA SET
WAVEA = ATOM LINE WAVELENGTH (ANGSTROM UNITS)
WAVEI = ION " " " "
GATOM = UPPER LEVEL DEGENERACY FOR ATOM LINE
GION = " " " " ION " "
EQATOM = EXCITATION POTENTIAL OF ATOM LINE (RECIPIROCAL CM UNITS)
EQION = " " " " ION " "
A(1, J) = TRANS PROB ARRAY FOR ATOM LINE (5 MAX)
A(2, J) = " " " " ION " "
XIP = IONIZATION POTENTIAL OFATOM SPECIES (RECIPIROCAL CM UNITS)
NR = NUMBER OF RADIAL POSITIONS
TR(I) = RADIAL TEMP ARRAY
R(I) = " " DIST
XI(I, 1) = RADIAL INTENSITY ARRAY FOR ATOM LINE
XI(I, 2) = " " ION " "
DELIR(I, 1) = RADIAL ERROR ARRAY (PERCENT) FOR ATOM LINE
DELIR(I, 2) = RADIAL ERROR ARRAY (PERCENT) FOR ION LINE

DIMENSION SUMDEN(SI), SUMRAT(SI), SUMS(SI), DELIR(SI, 2)
DIMENSION TTEST(500), S(SI)
DIMENSION TSYM(2), QTEST(3, 500), QZERO(SI), QPLUS(SI), RATION(SI)
DIMENSION XIDENT(35), TR(SI), R(SI), XI(SI, 2), EDENS(SI), A(2, 5)
DATA CHECKT/E0NT/
READ(5, 100) NSETS
100 FORMAT(I5)
DO 999 INDEX = 1, NSETS
DO 5 I = 1, 500
4 FORMAT(2A4, 2X, F10.0, 3F10.4)
READ(5, 4) TSYM, TTEST(I), QTEST(1, I), QTEST(2, I), QTEST(3, I)
M*fu
EIP = EIP/0.69505
EXPIP = 2.71828*(EIP/TR(I))
SSTAR = 4.8296E15*rTERM*ZRATIO*EXPIP
RATION(I) = EXPN*ZRATIO/RATIO
EDENS(I) = 4.8296E15*ZRATIO/RATION
ERR = 200*(DELIR(1,1)**2) + (DELIR(1,2)**2) + ERRFAC
S(I) = SORT(ERR)*EDENS(I)*EDENS(I)
SUMDEN(I) = SUMDEN(I)+EDENS(I)
SUMRAT(I) = SUMRAT(I)+RATION(I)
SUMS(I) = SUMS(I)+S(I)
WRITE(6,1000) XIDENT
1000 FORMAT(/**/,10, 'ELECTRON DENSITY CALCULATION; IDENT= ' ,35A2)
WRITE(6,1001) WAVEA,GATOM,EQATOM,AATOM
1001 FORMAT(/**/,T15,'ATOMIC LINE DATA; WAVELENGTH = ',F10.4,'EQ = ',F10.4,'AQP = ',F10.4)
WRITE(6,1002) WAVEG1ON,EQICN,AION
1002 FORMAT(/**/,T15,'ION LINE DATA; WAVELENGTH = ',F10.4,'EQ = ',F10.4,'AQP = ',F10.4)
WRITE(6,1003) XIP,DXIP
1003 FORMAT(/**/,T15,'IONIZATION POTENTIAL = ',F10.4,'LOWERING OF IONIZATION POTENTIAL = ',F10.4)
WRITE(6,1004)
1004 FORMAT(/**/,T10,'RADIUS',T20,'TEMPERATURE',T35,'ION LINE INT',T55,'ION ATOM RATIO',T110,'DELTA NE PERCENT')
DO 40 N=1, NR
40 WRITE(6,1005) R(N),TR(N),XI(N,2),XI(N,1),EDENS(N),RATION(N),S(N)
998 CONTINUE
WRITE(6,1006)
1006 FORMAT(/**/,T10,'AVERAGE VALUES')
WRITE(6,1004)
DO 50 N=1, NR
50 WRITE(6,1007) R(N),TR(N),XI(N,2),XI(N,1),SUMDEN(N),SUMRAT(N),SUMS(N)
999 CONTINUE
STOP
END
We consider the convolution integral for the "folding" of lorentzian and gaussian line profiles (61,93)

\[ I^F(\Delta \lambda^*) = \int_{-\infty}^{+\infty} I^G(\Delta \lambda) I^L(\Delta \lambda^* - \Delta \lambda) \, d(\Delta \lambda) \quad (D1) \]

where, \( I^G(\Delta \lambda) \) = gaussian profile, \( I^L(\Delta \lambda) \) = lorentzian profile, and \( I^F(\Delta \lambda) \) = folded line profile. Equation D1 mathematically expresses the effect of superimposition of the "smearing" function \( I^L \) on the gaussian line profile \( I^G \). Each gaussian intensity contribution \( I^G(\Delta \lambda) \) at displacement \( \Delta \lambda \) from the unperturbed line center is smeared out over all other positions of the profile by the lorentzian broadening function centered at \( \Delta \lambda \). The contribution of this smeared intensity to the \( I^F \) profile at a distance \( \Delta \lambda^* \) from the unperturbed line center is given by the product of the gaussian at \( \Delta \lambda \), \( I^G(\Delta \lambda) \), with the lorentzian centered at \( \Delta \lambda \), \( I^L(\Delta \lambda^* - \Delta \lambda) \). The resulting folded intensity at the point \( \Delta \lambda^* \) from the unperturbed line center is obtained by integration over all intensities contributing at \( \Delta \lambda^* \).

The total area under the line envelope remains constant so it is convenient to normalize
\[
\int_{-\infty}^{+\infty} I^G(\Delta \lambda) \, d(\Delta \lambda) = \int_{-\infty}^{+\infty} I^L(\Delta \lambda) \, d(\Delta \lambda) = 1 \quad (D2)
\]

and, consequently
\[
\int_{-\infty}^{+\infty} \bar{I}^F(\Delta \lambda) \, d(\Delta \lambda) = 1 \quad (D3)
\]

Because convolution is commutative, either the gaussian or the lorentzian profile may be considered to be the smearing function; this is shown as follows. First, we define

\[
\Delta \lambda' = \Delta \lambda^* - \Delta \lambda \quad (D4)
\]

then,

\[
\Delta \lambda = \Delta \lambda^* - \Delta \lambda'
\]

and

\[
d(\Delta \lambda') = d(\Delta \lambda^*) - d(\Delta \lambda)
\]

but,

\[
d(\Delta \lambda^*) = 0 \quad (D6)
\]

thus,

\[
d(\Delta \lambda') = -d(\Delta \lambda) \quad (D7)
\]

The change in the integration limits is given by
\[
\Delta \lambda = -\infty \implies \Delta \lambda' = +\infty
\]

and
\[
\Delta \lambda = +\infty \implies \Delta \lambda' = -\infty
\]

(D8)
Combining Equation D1 with the variable transformations given by Equations D5, D7, and D8 yields

$$I^F(\Delta \lambda^*) = -\int_{-\infty}^{+\infty} I^G(\Delta \lambda^* - \Delta \lambda') I^L(\Delta \lambda') \, d(\Delta \lambda')$$  \hspace{1cm} (D9)

but, the $\Delta \lambda'$ variable is only an integration dummy so this equation may be written

$$I^F(\Delta \lambda^*) = \int_{-\infty}^{+\infty} I^L(\Delta \lambda) I^G(\Delta \lambda^* - \Delta \lambda) \, d(\Delta \lambda)$$  \hspace{1cm} (D10)

where the relationship

$$\int_{-\infty}^{+\infty} = \int_{-\infty}^{+\infty}$$

has been used.

A FORTRAN IV computer program was written to perform the convolution calculations described in Chapter II of this dissertation and a complete listing of the source statements is included as C337CONV. The Cal-Comp plotting facility described in Appendix A was (optionally) employed to produce plots of the $H_\beta$ Stark profiles folded with Doppler and instrument contributions, which were obtained from this program. This was accomplished in the PLOT subroutine, which made use of the SIMPLOTTER program library described in Appendix A. The PLOT subroutine and the CALL PLOT
statement in the main program should be removed for installations where SIMPLOTTER is not available; the plotting capability will be lost if this is done.

The user input variables for this program are defined at the beginning of the C337CONV listing. The card input of Stark profile data was designed to accommodate the format employed in the Stark profile tabulations of Vidal et al. (98). Either the instrument broadening profiles which were read from data cards (ICONV = 1) or, internally generated Doppler profiles for the temperatures employed in the calculations of reference 98 (ICONV = 0) could be employed as smearing functions. The broadening profile could be symmetric (ISYMBP = 0) for which only intensities at positive displacements from the center were required or, it could be asymmetric (ISYMBP = 1) for which complete profile data were required.

Because the comment cards included in the C337CONV listing are generally self-explanatory, only a brief description of the program operation will be presented here. First, the number of data sets (NSETS) was read where one data set was associated with each instrument broadening profile employed. The value of the primary DO loop variable (NUMSET) ranged from 1 to NSETS. Second, the appropriate number of runs (NRUNS) was read for the NUMSET value where NRUNS corresponded to the number of different electron density \(n_e\) values associated with the data set. Third, the relevant
instrument profile variables and the profile itself were read from data cards. Fourth, the variables associated with the run were input from data cards. Fifth, the reduced wavelength scaling factor defined by (98)

\[ \text{DENOM} = 1.25 \times 10^{-9} n_e^{2/3} \]  

was calculated for the electron density run. The wavelength displacements and half-widths of the instrument profile were divided by this scaling factor to yield reduced values and the instrument profile was area normalized. Sixth, the appropriate area normalized reduced Stark profile data (98) for positive displacements were read from data cards for the electron density run. Seventh, the convolution integration calculations were performed and the resulting folded profiles were area normalized. Finally, the half-widths of the folded profiles were determined by appropriate interpolation methods (98).

Within the convolution calculation section of the program, the ratio of the reduced instrument profile half-width to that of the appropriate reduced Stark profile, i.e., \( \frac{\Delta \lambda^G}{\Delta \lambda^S} \) was calculated to determine the "narrowest" of the two profiles. When this ratio was 1.5 or greater, the convolution was integrated with respect to the "narrow" Stark profile (see Equation D10) but, for values less than 1.5 it was performed with respect to the gaussian-like instrument
profile (Equation D1). The instrument profile displacement axis was divided into 100 parts for the integration calculations and the corresponding intensity values were obtained by interpolation between the original data points.

Before the empirical "narrowness" test was devised the convolution integration had been carried out exclusively over the reduced Stark profile displacement variable and very serious errors in calculated \( I^F(\Delta\lambda^*) \) values were subsequently obtained, because integration over the wide reduced Stark profiles often obscured the effect of the narrower reduced instrument broadening profile. When this test was incorporated into the program the fine structure of these profiles was not lost and, consequently, the accuracy of the convolution calculation was significantly improved.

The convolution calculation was carried out over successive four-point segments from the negative to the positive integral limits; these limits were determined from the Stark and instrument broadening profiles employed in these calculations. The appropriate \( I^G \cdot I^S \) products from Equation D1 or D10 were calculated for each segment and the area of that segment was determined which the DCSIQU function or the RLFOTh and RLDOpM subroutines. These routines were obtained from the International Mathematical and Statistical Libraries (IMSL) subroutine library (138) which was available at the ISU Computations Center.
The half-widths, profile maximum intensity values, and profile center intensities obtained here agreed within 1-3\% with the corresponding values from Vidal et al. (98) when these Hβ Stark and Doppler profile data were used to test the convolution method developed in this dissertation research. The accuracy of this method was better than 0.1\% for pure Doppler-Doppler test convolutions; the folded profile half-widths and intensity values could be directly calculated for these data (93).

The contents of the data cards required for operation of the C337CONV program are listed in Table D-1.

Hβ Electron Density Program

The FORTRAN IV computer program which was written to perform the electron density calculations from Stark broadening measurements on the Hβ line (C337BROD) is listed after the convolution program. Electron densities were calculated in this program with the iterative approximation procedure outlined in Chapter II of this dissertation. The comment cards at the beginning of the listing of C337BROD define all input variables necessary for the operation of this program. The ALFA array in lines 33 to 38 of this program contained the reduced half-widths (α'β), which were calculated for the Hβ line with the spectroscopic equipment employed in this investigation. These values were obtained with the convolution
program discussed above (C337CONV) and are shown in Figure 2 (Chapter IV) of this dissertation. Table D-2 outlines the contents of the data cards required for operation of C337BROD.
<table>
<thead>
<tr>
<th>Type #</th>
<th># Cards</th>
<th>Columns</th>
<th>Variable Name</th>
<th>Format</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1-5</td>
<td>NSETS</td>
<td>I5</td>
<td>Number of data sets</td>
</tr>
<tr>
<td>2</td>
<td>1/set</td>
<td>1-5</td>
<td>NRUNS</td>
<td>I5</td>
<td>Number of runs for a given data set</td>
</tr>
<tr>
<td>3</td>
<td>1/set</td>
<td>1-5</td>
<td>NPOINT</td>
<td>I5</td>
<td>Number of points in the instrument profile array</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6-10</td>
<td>ICONV</td>
<td>I5</td>
<td>Doppler/instrument profile convolution selection</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11-15</td>
<td>ISYMBP</td>
<td>I5</td>
<td>Symmetric/asymmetric instrument profile switch</td>
</tr>
<tr>
<td></td>
<td></td>
<td>16-20</td>
<td>IFLOT</td>
<td>I5</td>
<td>Plot option switch</td>
</tr>
<tr>
<td>4</td>
<td>NPOINT</td>
<td>1-10</td>
<td>WAVE</td>
<td>F10.0</td>
<td>Wavelength displacement array of instrument profile (Angstrom units)</td>
</tr>
<tr>
<td></td>
<td>/set</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td></td>
<td>11-22</td>
<td>PRFINT</td>
<td>E12.5</td>
<td>Corresponding instrument profile intensity array</td>
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<td>5</td>
<td>1/run</td>
<td>1-60</td>
<td>TITLE</td>
<td>15A4</td>
<td>Experiment label for run calculations</td>
</tr>
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<td></td>
<td>61-68</td>
<td>HLINE</td>
<td>2A4</td>
<td>Name of hydrogen line corresponding to ILINE value</td>
</tr>
<tr>
<td>6</td>
<td>1/run</td>
<td>1-5</td>
<td>ISKIP</td>
<td>I5</td>
<td>Option to print calculation iterations (normally 0, i.e., not printed)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6-10</td>
<td>ILINE</td>
<td>I5</td>
<td>Number corresponding to H\textsubscript{8}, H\textsubscript{Y}, or H\textsubscript{6} convolution</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11-15</td>
<td>NTLOW</td>
<td>I5</td>
<td>Beginning NT value for convolutions (see comment cards and reference 98)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>16-20</td>
<td>NTUP</td>
<td>I5</td>
<td>Ending NT value</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21-32</td>
<td>DENS</td>
<td>E12.5</td>
<td>Electron density for the run</td>
</tr>
<tr>
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<td></td>
<td>36-55</td>
<td>LDENS</td>
<td>5A4</td>
<td>Graph label for plot identification</td>
</tr>
<tr>
<td>Type #</td>
<td># Cards</td>
<td>Columns</td>
<td>Variable Name</td>
<td>Format</td>
<td>Remarks</td>
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<td>---------</td>
<td>---------------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>7</td>
<td>1/run</td>
<td>1-5</td>
<td>NALPHA</td>
<td>I5</td>
<td>Number of Stark profile data points</td>
</tr>
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<td></td>
<td>6-10</td>
<td>NCONV</td>
<td>I5</td>
<td>Number of convolutions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11-15</td>
<td>ISYMCP</td>
<td>I5</td>
<td>Symmetric/asymmetric Stark profiles to be convoluted with instrument broadening profile</td>
</tr>
<tr>
<td></td>
<td></td>
<td>15-20</td>
<td>IPUNCH</td>
<td>I5</td>
<td>Option to punch convoluted (folded) profiles</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21-25</td>
<td>IREAD</td>
<td>I5</td>
<td>Option to input profile data from disk file (see comment cards)</td>
</tr>
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<td></td>
<td>26-30</td>
<td>IPROFL</td>
<td>I5</td>
<td>Option to apply asymptotic wing formula in convolution calculation (see comment cards)</td>
</tr>
<tr>
<td>8</td>
<td>NAPHA</td>
<td>1-10</td>
<td>ALPHA</td>
<td>F10.0</td>
<td>Reduced displacement array for Stark profiles</td>
</tr>
<tr>
<td></td>
<td>/run</td>
<td>11-70</td>
<td>STARK</td>
<td>5E12.5</td>
<td>Stark profile intensity arrays for temperatures from NTLOW to NTUP (see comment cards and reference 98)</td>
</tr>
</tbody>
</table>
**C337CONV**

PROGRAM TO CALCULATE CONVOLUTION INTEGRAL OF UNEQUALLY SPACED NUMERICAL DATA

NSETS = NUMBER OF DISTINCT DATA SETS; ONE SET PER GIVEN INSTRUMENT BROADENING PROFILE

NRUNS = NUMBER OF RUNS TO BE MADE WITHIN A GIVEN BROADENING PROFILE SET

TITLE = LABEL FOR CALCULATION FOR A GIVEN RUN

ILINE = 1, H-BETA CONVOLUTION CALCULATION

   = 2, H-GAMMA " "

   = 3, H-DELTA " "

   NT = 1, TEMPERATURE = 2500 K

   = 2, " = 5000 K

   = 3, " = 10000 K

   = 4, " = 20000 K

   = 5, " = 40000 K

HLINE = LABEL FOR LINE CORRESPONDING TO ILINE

DENs = ELECTRON DENSITY FOR A GIVEN RUN

LDENS = GRAPH LABEL TO IDENTIFY PLOTS (IF IPLOT = 1 SPECIFIED)

NALPHA = NUMBER OF REDUCED DISPLACEMENTS FOR WHICH THERE ARE STARK PROFILE POINTS TABULATED

NCONV = NUMBER OF CONVOLUTIONS TO BE DONE WITHIN GIVEN RUN (SET EQUAL TO NALPHA)

ISYMCP = 0, SYMMETRIC PROFILE TO BE CONVOLVED WITH THE BROADENING PROFILE: READ IN RIGHT HALF (POS DISPLACEMENT)

   = 1, NOT SYMMETRIC; READ IN COMPLETE PROFILES

ISKIP = 0, SKIP PRINTING ITERATIVE VALUES

NE 0, PRINT INTERMEDIATE VALUES

IPunch = 0, CONVOLVED PROFILES NOT PUNCHED

   = 1, CONVOLVED PROFILES PUNCHED ON CARDS

IPROF = 0, PURE STARK OR STARK/DOPPLER PROFILES TO BE CONVOLVED WITH THE BROADENING PROFILE --- ASYMPTOTIC WING FORMULAS NOT APPLIED

   = 1, ASYMPTOTIC STARK/DOPPLER WING FORMULAS NOT APPLIED

NTLOW = STARTING NT VALUE FOR CONVOLUTION CALCULATION

NTUP = ENDING NT

STARK(I, NT) = TABULATED BROADENING INPUT DATA ARRAY AT TEMPERATURE CORRESPONDING TO NT; 5E12.5, COLUMNS 11-70

ALPHA(I) = PROFILE REDUCED DISPLACEMENT ARRAY CORRESPONDING TO STARK(I, NT) DATA; COLUMNS 1-10

NPOINT = NO. POINTS IN THE INSTRUMENT PROFILE ARRAY

ICONV = 0, DOPPLER CONVOLUTION

   = 1, INSTRUMENT CONVOLUTION
ISYM3P=0. SYMMETRIC BROADENING PROFILE; READ IN FROM ZERO
DISPLACEMENT TO PRFINT(NPOINT); PROGRAM GENERATES
LEFT (NEGATIVE DISPLACEMENT) PORTION OF PROFILE
=1, NOT SYMMETRIC; READ IN COMPLETE PROFILE INCLUDING
NEGATIVE DISPLACEMENT INTENSITIES
IPLDT=0. NO PLOTS GENERATED
=1, BROADENING, STARK/DOPPLER, AND CONVOLVED PROFILES PLOTTED
IREAD=0, INPUT PROFILE DATA ON PJNCHED CARDS
=1, INPUT PROFILE DATA READ IN FROM FILE, CPS07.A0986.CONV
(REQUIRES ADDITIONAL FILE READ JCL AND UTILITY PL/1
PROGRAM TO EDIT FILE DATA IN CARD IMAGE)
WAVEL(I)=DISPLACEMENT ARRAY (ANGSTROMS) OF INSTRUMENT PROFILE
PRFINT(I)=CORRESPONDING INTENSITY ARRAY

DOUBLE PRECISION T<12).PC8), DIMENSION C (5), S(5), A(2), B(2), XF(6), LDENS(5), DINC(200)
DIMENSION TEMP(5), TITLE(15), HLINE(2), WAVE(3), ALPHA(100), STARK(100, 15), DEL(3, 5), WORK(50), ALPHA(3, 5), X(6), XPONET(6), FX(6)
DIMENSION APROFI100), STARKL(100), CONV(100), AREA(5)
DIMENSION XI NTRP(100), YINTRP(100), ALEFT(5), ARIGHT(5), HMA XL(5), HMAX 1R(5), XMID(100), YMID(100), SHAFT(5)
DIMENSION WAVE(100), PRFINT(100), XWAVE(100), XPROFI100)
DATA TEMP/2500, 5000, 10000, 20000, 40000/.
WAVE/4861.33, 4340.46, 4
1101, 73/
READ IN NUMBER OF DATA SETS
READ(5,1) NSETS
1 FORMAT(15)
DO 9999 NUMSET=1,NSETS
READ IN NUMBER OF RUNS FOR THE DATA SET
READ(5,100) NRUNS
100 FORMAT(15)
READ IN INSTRUMENT BROADENING PROFILE FOR THE DATA SET
READ(5,1000) NPOINT, ICONV, ISYM3P, IPLDT
1000 FORMAT(415)
DO 1010 I=1, NPOINT
1010 FORMAT(F10.0, E12.5)
DO 9999 NUMRUN=1, NRUNS
READ IN INFORMATION CARDS FOR A RUN WITHIN THE DATA SET
READ(5, 101) TITLE, HLINE
101 FORMAT(15A4, 2A4)
READ(5, 102) ISKIP, ILINE, NTLow, NTUP, DENS, LDENS
CALCULATE DISPLACEMENT SCALING FACTOR AND HALF-WIDTHS OF DOPPLER BROADENING PROFILE (ICONV=0 USES INTERNAL DOPPLER BROADENING PROFILE AT TEMPERATURE SPECIFIED BY NT UP AND NTLOW)

DENOM=1.25E-9*(DENS**0.6666667)
WRITE(6,50) DENOM
50 FORMAT(1H1, 1D20.25E-09*(NE**(2/3))=,,E12.5)
WRITE(6,55)
55 FORMAT(2A10,*GAUSSIAN PROFILE HALF-WIDTHS*)
WRITE(6,60)
60 FORMAT(1H1, T5,TEMP,T20, LAMDEL(1,T)**T35, LAMDEL(2,T)**T50, LAMDEL(3,T)**T65, ALFDEL(1,T)**T80, ALFDEL(2,T)**T95, ALFDEL(3,T)**T110)
DO 5 I=1,5
DEL(1,I)=0.001733*SQRT(TEMP(I))
DEL(2,I)=0.001548*SQRT(TEMP(I))
DEL(3,I)=0.001462*SQRT(TEMP(I))
ALPHAD(1,I)=DEL(1,I)/DENOM
ALPHAD(2,I)=DEL(2,I)/DENOM
ALPHAD(3,I)=DEL(3,I)/DENOM
DO 70 I=1,5
DO 65 J=1,3
70 WRITE(6,65) TEMP(I),(DEL(J,I)),(ALPHAD(K,I), K=1,3)
65 FORMAT(1A7,1A0.5E12.5)
70 CONTINUE
8 READ(5,103) NALPHA,NCONV,ISYMBP,IPUNCH,IREAD,IPROFL
103 FORMAT(1D15.5)
DO 10 I=1,NALPHA
10 IF(IREAD.EQ.0) GO TO 8
READ(9,104) ALPHAI(I),(STARK(I,J), J=1,5)
GO TO 10
8 READ(5,104) ALPHAI(I),(STARK(I,J), J=1,5)
10 CONTINUE
WRITE(6,105) TITLE
101 FORMAT(/,T20,2A4,5X,F7.2,2X,'ANGSTROMS',5X,'ELECTRON DENSITY = ',',1E11.4)
WRITE(6,200) TITLE
200 FORMAT(/,T10,15A4)
WRITE(6,201) HLINE,WAVE(ILINE),DENS
201 FORMAT(/,T20,2A4,5X,F7.2,2X,'ANGSTROMS',5X,'ELECTRON DENSITY = ',',1E11.4)
WRITE(6,200) TITLE
200 FORMAT(/,T10,15A4)
WRITE(6,201) HLINE,WAVE(ILINE),DENS
201 FORMAT(/,T20,2A4,5X,F7.2,2X,'ANGSTROMS',5X,'ELECTRON DENSITY = ',',1E11.4)
DO 1025 I=2,NPOINT
    J=NPOINT-I+1
    XWAVEL(J)=XWAVEI(I)/DENOM
1025  XPROFL(J)=PRFINT(I)*DENOM
    NPTS=2*NPOINT-1
    GO TO 1040
1030  NPTS=NPOINT
    DO 1035 I=1,NPTS
        XWAVEI(I)=XWAVEL(I)/DENOM
1035  XPROFL(I)=PRFINT(I)*DENOM
    NPTS=2*NPOINT-1
    GO TO 1040
1040  AREAIN=0.00
    BMAX=0.00
    JCHK=(NPTS/2)+1
    DO 1050 I=1,NPTS
        NL=I
        NU=NL+3
        IF(NU.GE.NPTS) NU=NPTS
        N=0
        DO 1045 J=NL,NU
            N=N+1
            X(N)=XAVEH(J)
            XF(N)=XWAVEI(J)
            IF(XAVEI(J).EQ.0.00) JCHK=J
            IF(XPROFL(J).LT.BMAX) GO TO 1045
            BMAX=XPROFL(J)
            JLOW=J-1
            JUP=J+1
        1045  FX(N)=XPROFL(J)
            IER=0
            NUMBER=4
            NTESI=NU-NL+1
            IF(NTEST.LT.4) NUMBER=NTEST
            AINSTR=DCS1U(FX,X,NUMBER,HWORK,IER)
            IF(IER.NE.129) GO TO 1049
            WRITE(6,1046) IER,NL,X(M),M=1,NUMBER
3(M),M=1,NUMBER
        1046  FORMAT(*,10E15.5,5X,15E15.5)
            RSQ=100.0
            MD=2
        1500  M=1,12
            T(M)=0.00
            DO 1501 M=1,2
                A(M)=0.00
            1501  B(M)=0.00
            DO 1502 M=1,8
                P(M)=0.00
            1502  C(M)=0.00
            DO 1503 M=1,5
                S(M)=0.00
            1503  R(M)=100.0
IER=0
ID=0
IF(NUMBER.EQ.2) MD=1
IF(NUMBER.EQ.0) GO TO 1050
CALL RLOPTGH(X,NUMBER,RSQ,MC,ID,P,C,S,A,B,IER)
IF(IER.EQ.129) GO TO 1050
IF(IER.EQ.130) GO TO 1050
CALL RLDOPMC,ID,A,B,T)
FUP=XF(NUMBER)
FLOW=XF(1)
FU2=FUP*FUP
FL2=FLOW*FLOW
FU3=FU2*FUP
FL3=FL2*FLOW
AInstr=9999
IF(ID.EQ.1) C(3)=0.00
AInstr=(C(1)*(FUP-FLOW)) + (C(2)/2.0)*(FU2-FL2) + (C(3)/3.0)*(FU3-FL3))
WRITE(6,1510) AInstr
1510 FORMAT(/,'POLYNOMIAL APPROXIMATION TO AREA USED: AINST= ',E11.4)
1049 AREA1N=AREA1N+AInstr
1050 CONTINUE
BMAX=BMAX/AREA1N
DO 1060 I=1,NPTS
1060 XPROFL(I)=XPROFL(I)/AREA1N
ISHAPE=0
IF(BMAX.GT.XPROFL(JCHK)) ISHAP=1
HALFR=0.00
CALL HMAX(XWAVEL,XPROFL,NPTS,0.0,0.0,JLOW,JUP,BMAX,0.0,HALFR,0.0,ISHAPE)
BHALF=HALFR
BMAX=BMAX
WRITE(6,1061) BMAX,BHALF,AREA1N
1061 FORMAT(/,'AREA AND DISPLACEMENT NORMALIZED INSTRUMENT BROADENING PROFILE: MAX INTENSITY = ',E12.5,2X,'HALF-WIDTH = ',E12.5,2X,'AREA BEFORE NORMALIZATION = ',1X,E12.5)
WRITE(6,1062)
1062 FORMAT(//,'ALPHA',T25,'INTENSITY')
DO 1070 I=1,NPTS
1065 FORMT(T10,E11.4,T25,E11.4)
1070 WRIT£(6,1065) XWAVEL(I),XPROFL(I)
150 FORMAT(//'INPUT DATA')
WRITE(6,151)
151 FORMAT(//'T2',ALPHA',T20,'STARK(2500)',T40,'STARK(5000)',T60,'STAR1K(10000)',T80,'STARK(20000)',T100,'STARK(40000)')
DO 15 I=1,NALPHA
152 FORMAT(T2,E11.4,T20,E11.4,T40,E11.4,T60,E11.4,T80,E11.4,T100,E11.4,1)
15 WRITE(6,152) ALPHA(I),(STARK(I,J),J=1,5)

C COMPLETE PROFILES TO BE CONVOLUTED WITH THE BROADENING PROFILE

C DO 19 I=1,5
19 HMAXL(I)=0.0

C HMAXR(I)=0.00

C IF(ISYMCP.EQ.1) GO TO 1900

C DO 20 I=1,NALPHA
20 APROF(I)=-ALPHA(J)

C DO 25 I=2,NALPHA
25 STARKL(I,K)=STARK(J,K)

C DO 25 I=2,NALPHA
25 APROF(NALPHA)=ALPHA(1)

C DO 25 K=1,5
25 STARKL(J,K)=STARK(I,K)

C GO TO 1950

C 1900 DO 1910 I=1,NALPHA
1910 APROF(I)=ALPHA(I)

C DO 1910 J=1,5
1910 STARKU(I,J)=STARK(I,J)

C GO TO 1950

C 1950 NCONV=NALPHA

C DO 1995 NT=1,5
1995 SHALF(NT)=0.00

C IF(NT.LT.NTL) GO TO 1995

C IF(NT.GT.NTU) GO TO 1995

C JRCHK=(NALPHA/2)+1

C JLC=JRCHK

C DO 1990 I=1,NALPHA
1990 IF(APROF(I).GT.0.0) GO TO 1955

C IF(APROF(I).EQ.0.0) GO TO 1960

C IF(STARKL(I,NT).LT.HMAXL(NT)) GO TO 1990

C HMAXL(NT)=STARKL(I,NT)

C ILSLOW=I-1

C ISUP=I+1

C GO TO 1990

C 1995 IF(STARKL(I,NT).LE.HMAXR(NT)) GO TO 1990

C HMAXR(NT)=STARKL(I,NT)

C ILSLOW=I-1

C IRSUP=I+1

C GO TO 1990

C 1960 JRCHK=I

C JLC=JLCHK

C IF(STARKL(I,NT).GT.HMAXR(NT)) GO TO 1970

C IF(STARKL(I,NT).GT.HMAXL(NT)) GO TO 1970

C HMAXR(NT)=STARKL(I,NT)
ILSLOW=I-1
ILSUP=I+1
GO TO 1990
1970 HMAXR(NT)=STARKL(I,NT)
ISLOW=I-1
ISUP=I+1
1990 CONTINUE
SRMAX=HMAXR(NT)
SLMAX=HMAXL(NT)
DO 1994 J=1,NALPHA
XINTRP(J)=APROF(J)
1994 y INTRP ( J)=STARK1L( J, NT J
HALFR=0.0
HALFL=0.0
ISHAPE=0
IF(SRMAX«GT,YINTRP<JRCHK») ISHAPE=1
IF(SLMAX,GT«YINTRP<JLCHK)) ISHAPE=1
CALL HMAX(XINTRA,YINTRP,NALPHA,1.ILSLOW,ILSUP,SRMAX,SLMAX,HALFR,HALFL,ISHAPE)
SHALF(NT)=(HALFR-HALFL)/2.00
HMAXRfNT>=SRMAX
HMAXL(NT)=SLMAX
1995 CONTINUE
WRITE(6,2000)
2000 FORMAT(//,'COMPLETE PROFILE DATA')
WRITE(6,2001)
2001 FORMAT(//,'ALFA',T20,'STARKL< 2 500 ) • .T40 . • STARKL (5000)',T60,'STARKL< 10000 ) • .T80 . • STARKL (20000)',T100,'STARKL (40000)'
DO 2015 I=1,NALPHA
2002 FORMAT(//,'RIGHT MAX INTENS',T20,'E11.4',T40,'E11.4',T60,'E11.4',T80,'E11.4',T100,'E11.4',E11.4)
2003 FORMAT(//,'AVE HALF-WIDTH',T20,'E11.4',T40,'AVE HALF-WIDTH',T20,'E11.4',T60,'E11.4',T80,'E11.4',T100,'E11.4')
C PERFORM THE CONVOLUTION CALCULATIONS
DO 99 NT=1,5
DO 2990 INUM=1,NALPHA
2990 YINTRP(INUM)=STARKL(INUM,NT)
DO 99 J=1,NCONV
CONV(J,NT)=0.00
IF(NT<NTL3W) GO TO 99
IF(NT<STARKL(NTL3W)) GO TO 99
IF(NT) GO TO 99
IF(ICONV.EQ.1) GO TO 3000
XUP=1.000/DENOM
IF(NT/EQ.3) XUP=1.50/DENOM
IF(NT) XUP=2.00/DENOM
IF(NT.EQ.5) XUP=3.00/DENOM
XLOW=-XUP
RATIO=ALPHAD(ILINE,NT)/SHALF(NT)
KEY=0
IF(RATIO.GE.1.5) KEY=1
GO TO 3010
3000 XUP=XWAVEL(NPTS)
XLOW=XWAVEL(1)
RATIO=BHALF/SHALF(NT)
KEY=0
IF(RATIO.GE.1.5) KEY=1
3010 XAINC=XUP/50.00
XX=XLOW-XAINC
DO 3020 M=1,100
XX=XX+XAINC
3020 DINC(M)=XX
NDET=100
IF(KEY.EQ.1) NDET=NALPHA
DO 98 K=1,NDET,3
NL=K
NU=NL+3
IF(NU.GE.NDET) NU=NDET
N=0
DO 96 I=NL,NU
IF(KEY.EQ.1) X(N)=APROF(J)-APROF(I)
IF(KEY.EQ.1) GO TO 3031
X(N)=DINC(I)
XXX=APROF(J)-X(N)
IF(XXX.LT.APROF(1)) GO TO 3030
IF(XXX.GT.APROF(NALPHA)) GO TO 3030
POLYN=0.00
CALL PLLYNN(APROF,YINTRP,POLYN,XXX,NALPHA,6)
SVALUE=POLYN
GO TO 3031
3030 BXX=ABS(XXX)
SVALUE=2.0*(3.5261*0.03*(BXX**(-2.5))
IF(IPROF.LT.0) SVALUE=0.0
IF(ICONV.EQ.1) GO TO 75
3031 IF(ICNV.EQ.1) SVALUE=0.0
XX2N=ABS(X(N))
XPONETER(N)=-0.99314718*(XX2N**2)/(ALPHAD(ILINE,NT)**2)
XPONETER(N)=EXP(XPONETER(N))*(1.77245*DEL(ILINE,NT))
XPONETER(N)=DENOM*XPONETER(N)*SORT(J,0.99314718)
IF(KEY.EQ.1) SVALUE=STARKL(I,NT)
FX(N)=SVALUE*XPONETER(N)
GO TO 36
72 XPONETER(N)=0.0
FX(N)=0.00
GO TO 86
75 XXX=X(N)
   IF(KEY.EQ.1) SVALUE=STARKL(I,NT)
   IF(XXX.LT.XWAVE(1)) GO TO 80
   IF(XXX.GT.XWAVE(NPTS)) GO TO 80
   POLYN=0.00
   CALL PLLYN(XWAVE,XPROFL,POLYN,XXX,NPTS,6)
   XPONET(N)=POLYN
   GO TO 85
80 XPONET(N)=0.00
85 FX(N)=SVALUE*XPONET(N)
86 CONTINUE
   XF(N)=DINC(I)
   IF(KEY.EQ.1) XF(N)=APROF(I)
   IF(KEY.EQ.1) X(N)=APROF(I)
96 CONTINUE
   IER=0
   NUMBER=4
   NTEST=NU-NL+1
   IF(NTEST.LT.4) NUMBER=NTEST
   CTEST=DCS1QU(FX,X,NUMBER,HWORK,IER)
   IF(JSKIP.EQ.0) GO TO 997
995 FORMAT(T50,CTEST='*E11.4,2X,FOR J='*,I3,2X,'K='*,I3)
   WRITE(6,996) CTEST,J,K
997 IF(IER.NE.129) GO TO 97
105 FORMAT(T10,'****FLAG***IER='*,I5,2X,'RETURNED FOR CONVOLUTION
   1 NUMBER='*,I5,5X,'SUBSET K VALUE = '*'I3)
   WRITE(6,106) APROF(J),NT
106 FORMAT(T50,'ALFA(J)='*,E12.5,2X,'NT = '*'I3)
DO 600 M=1,12
600 T(M)=0.D0
   DO 601 M=1,2
   A(M)=0.00
601 B(M)=0.00
   DO 602 M=1,8
   P(M)=0.00
602 S(M)=0.00
   MD=2
   IER=0
   ID=0
   IF(NUMBER.EQ.1) GO TO 98
   IF(NUMBER.EQ.2) MD=1
   DIF=0.0
   DO 608 M=2,NUMBER
   L=M-1
608 DIF=DIF+(FX(M)-FX(L))**2
XNMBR=NUMBER
DIF=SQRT(DIF)/XNMBR
AVE=0.0
DO 609 M=1,NUMBER
609 AVE=AVE+FX(M)
AVE=AVE/XNMBR
AVTEST=0.001*AVE
IF(DIF*GT*AVTEST) GO TO 604
CTEST=AVE*ABS(NUMBER)-X(1))
GO TO 611
604 CONTINUE
CALL RLFOTH(X,FX,NUMBER,RSQ,MD,I),P,CS,AB,IER)
IF(IER.EQ.129) GO TO 98
IF(IER.EQ.130) GO TO 98
CALL RLDOPM(C,ID,A,B,T)
FUP=XF(NUMBER)
FLOW=XF(1)
FU2=FUP*FUP
FL2=FLOW*FLOW
FU3=FU2*FUP
FL3=FL2*FLOW
CTEST=9999.
IF(ID.EQ.1) C(3)=0.00
CTEST=C(1)*(FUP-FL2)**(C(2)/2.0)*(FU2-FL2)**(C(3)/3.0)*(FU3-FL2)
WRITE(6,610) CTEST,ID
610 FORMAT (T10,'POLYNOMIAL APPROXIMATION TO AREA USED:

1.4,2X,'DEGREE=' ,13)
GO TO 97
611 WRITE(6,615) CTEST
615 FORMAT (T10,'VALUES NEARLY CONSTANT:

1.4,2X,'SQUARE APPROXIMATION TO AREA:

1.4,2X,'CTEST=' ,E12.5)
97 CONV(J,NT)=CONV(J,NT)+CTEST
98 CONTINUE
99 CONTINUE
Determine area of convolved profiles
DO 601 NT=1,5
AREA(NT)=0.00
HMAXL(NT)=0.00
HMAXR(NT)=0.00
ALEFT(NT)=0.00
ALEFT(NT)=0.00
DO 500 I=1,NCONV,3
NL=I
NU=NL+3
IF(NU.GE.NCONV) NU=NCONV
N=0
DO 495 J=NL,NU
N=N+1
XF(N)=APROF(J)
X(N)=APROF(J)

DETERMINE FIRST APPROXIMATIONS TO RIGHT AND LEFT PROFILE
MAXIMUMS USING TABULATED (UNNORMALIZED) CONVOLUTION RESULTS
AREA NORMALIZATION AFTER STATEMENT 501

501 IF(APROF(J) GT 0.00) GO TO 450
502 IF(APROF(J) EQ 0.00) GO TO 460
503 IF(CONV(J,NT) LT HMAXL(NT)) GO TO 495
504 HMAXL(NT)=CONV(J,NT)
505 LJLOW=J-1
506 LJUP=J+1
507 GO TO 495
508 450 IF(CONV(J,NT) LE HMAXR(NT)) GO TO 495
509 HMAXR(NT)=CONV(J,NT)
510 JRLW=J-1
511 JRP=J+1
512 GO TO 495
513 460 IF(CONV(J,NT) GT HMAXR(NT)) GO TO 470
514 IF(CONV(J,NT) LT HMAXL(NT)) GO TO 495
515 HMAXL(NT)=CONV(J,NT)
516 LJLOW=J-1
517 LJUP=J+1
518 GO TO 495
519 470 HMAXR(NT)=CONV(J,NT)
520 JRLW=J-1
521 JRP=J+1
522 495 FX(N)=CONV(J,NT)
523 IER=0
524 NUMBER=4
525 NTEST=NU+NL+1
526 IF(NTEST LE 4) NUMBER=NTEST
527 ATEST=DCSIQU(FX,X,NUMBER,HWORK,IER)
528 IF(IER NE 129) GO TO 497
529 WRITE(6,204) NL,NU,NT
204 FORMAT (T10,13**FLAG*, IER=129 RETURNED FOR ATEST WITH NL= *,I3
1.2X,*NU= *,I3,2X,*NT= *,I3)
530 DO 700 M=1,12
531 T(M)=0.00
532 DO 701 M=1,2
533 A(M)=0.00
534 DO 702 M=1,8
535 B(M)=0.00
536 DO 703 M=1,8
537 C(M)=0.00
538 DO 704 M=1,8
539 RSQ=100.0
540 700 T(M)=0.00
541 DO 701 M=1,2
542 A(M)=0.00
543 DO 702 M=1,8
544 B(M)=0.00
545 DO 703 M=1,8
546 C(M)=0.00
547 DO 704 M=1,8
548 RSQ=100.0
MD=2 551
IER=0 552
IF(NUMBER.EQ.1) GO TO 500 553
IF(NUMBER.EQ.2) MD=1 554
DIF=0.00 555
DO 708 M=2,NUMBER 556
L=M-1 557
708 DIF=DIF+(FX(M)-FX(L))**2 558
XNMBR=NUMBER 559
DIF=SORT(DIF)/XNMBR 560
AVE=0.00 561
DO 709 M=1,NUMBER 562
709 AVE=AVE+FX(M) 563
AVE=AVE/XNMBR 564
AVTEST=0.001*AVE 565
IF(DIF.GT.AVTEST) GO TO 704 566
GO TO 711 567
704 CONTINUE 568
CALL RLFTOH(X,FX(NUMBER),RSQ,MD,I,P,C,S,A,B,IER) 569
IF(IER.EQ.129) GO TO 500 570
IF(IER.EQ.130) GO TO 500 571
CALL RLDOPM(C,ID,A,B,T) 572
FUP=FX(NUMBER) 573
FLOW=FX(1) 574
FUP=FUP+FUP 575
FL2=FLOW*FLOW 576
FUP=FUP+FUP 577
FL3=FL2*FLOW 578
AVTEST=9999. 579
ATEST=(C(1)*(FUP-FLOW))+((C(2)/2.0)*(FUP-FL2))+((C(3)/3.0)*(FUP-FL3)) 580
WRITE(6,710) ATEST 581
710 FORMAT (TIO.'POLYNOMIAL APPROXIMATION TO AREA USED: ATEST= ','E11.4) 582
GO TO 497 583
711 WRITE(6,715) ATEST 584
715 FORMAT (TIO.'VALUES NEARLY CONST: SQUARE APPROX TO AREA: ATEST= ','E12.5) 585
497 AREA(NT)=AREA(NT)+ATEST 586
500 CONTINUE 587
501 CONTINUE 588
C AREA NORMALIZE CONVOLVED PROFILES AND MAX INTENSITY VALUES 589
DO 502 NT=1.5 590
IF(NX.LT.NTLOW) GO TO 502 591
IF(NX.GT.NTUP) GO TO 502 592
C
HMAXL(NT) = HMAXL(NT)/AREA(NT)  
HMAXR(NT) = HMAXR(NT)/AREA(NT)

502 CONTINUE
WRITE(6,203)
203 FORMAT(C1H90,2T20,'AREA NORMALIZED CONVOLUTION RESULTS*')
IF(ICONV.EQ.0) WRITE(6,403)
IF(ICONV.EQ.1) WRITE(6,402)
402 FORMAT(T30,'INSTRUMENT PROFILE CONVOLUTION*')
403 FORMAT(T30,'DOPPLER CONVOLUTION (INTERNALLY GENERATED DOPPLER PROF I*LES)*')
1IF(IPUNCH.EQ.1) WRITE(7,404)
1IF( ICONV.EQ.1) WRITE(6,402)
404 FORMAT(T30,'DOPPLER CONVOLUTION (INTERNALLY GENERATED DOPPLER PROF *)
1LES)*')
1IF(IPUNCH.EQ.1) WRITE(7,210)
210 FORMAT('DELTA ALPHA FOLLOWED BY CONVOLVED PROFILES; 2500, 5000, 1000  
10, 20000, & 40000*')

DO 199 J=1,NCONV  
DO 198 K=1.5  
IF(K.LT.NTLOW) GO TO 198  
IF(K.GT.NTUP) GO TO 198  
CONV(J,K) = CONV(J,K)/AREA(K)
198 CONTINUE
199 WRITE(6,107) APROF(J), (CONV(-,L), L=1.5)

C CALCULATE THE HALF-WIDTH BY USING HALF-MAX INTENSITY VALUES
C FOR BOTH RIGHT AND LEFT SIDES OF THE COMPLETE PROFILE.
C THE MAX INTENSITY VALUE FOR EACH HALF IS DETERMINED BY USING
C THE INTERPOLATING SUBROUTINE, PLYN.
C THE RESPECTIVE HALF-WHTHS FOR EACH SIDE ARE THEN DETERMINED BY
C REVERSING THE INTENSITY AND DISPLACEMENT ARRAYS AND INTERPOLATING
C A VALUE WITH PLLYN

DO 299 I=1,5  
IF(I.LT.NTLOW) GO TO 299  
IF(I.GT.NTUP) GO TO 299  
JRCHK = (NCONV/2)+1  
JLCHK = JRCHK  
DO 249 J=1,NCONV  
XMID(J) = APROF(J)  
IF(APROF(J) .EQ.0.0) JRCHK = J  
JLCHK = JRCHK  
249 YMID(J) = CONV(J,I)  
CRMAX = HMAXR(I)  
CLMAX = HMAXL(I)
HALFR=0.00
HALFL=0.00
ISHAPE=0
IF(CRMAX.GT.YMID(JRCHK)) ISHAPE=1
IF(CLMAX.GT.YMID(JLCHK)) ISHAPE=1
CALL HMAX(XMID,YMID,NCONV,1,LJLOW,LJUP,JRLLOW,JRUP,CRMAX,CLMAX,HALF1R,HALFL,ISHAPE)
ALEFT(I)=HALFL
ARIGHT(I)=HALFR
HMAXR(I)=CRMAX
HMAXL(I)=CLMAX
299 CONTINUE
396 FORMAT(/'RIGHT MAX INTENS',T2,1,5(4X,E11.4))
397 FORMAT(T4,'LEFT MAX INTENS',T2,1,5(4X,E11.4))
399 FORMAT(T4,'LEFT HALF-WIDTH',T2,1,5(4X,E11.4))
WRITE(6,396) (HMAXR(I),I=1,N)
WRITE(6,397) (HMAXL(I),I=1,N)
WRITE(6,399) (ALEFT(I),I=1,N)
WRITE(6,510) (AREACNN),NN=1,5
510 FORMAT(/'AREAd)-AREAr(5)',T2,2,5(3X,E12.5))
IF(IPILOT.NE.1) GO TO 9999
9999 CONTINUE
STOP
END
SUBROUTINE HMAX(X,Y,N.ISYM,ILLOW,ILUP,IRLOW,IRUP,YRMAX,YLMAX,HALFR,HALFL,ISHAPE)
DIMENSION X(N),Y(N),XH(N),YH(N)

SUBROUTINE TO DETERMINE HALF-WIDTHS FOR RIGHT AND (OPTIONALLY) LEFT PROFILES
ISYM=0, SYMMETRIC PROFILE SO ONLY CALCULATE RIGHT HALF-WIDTHS
NE 0, DETERMINE BOTH RIGHT AND LEFT HALF-WIDTHS

NHALF=N/2
IF(ISYM.EQ.0) GO TO 2000
NPLUS=NHALF+1
IF(ISHAPE.EQ.1) NPLUS=ILLOW+1
DO 1010 I=1,NPLUS
XH(I)=Y(I)
1010 YH(I)=X(I)
XINC=(X(ILUP)-X(ILLOW))/100.0
XXX=X(ILLOW)-XINC
DO 1020 J=1,100
XXX=XXX+XINC
201
POLYN=0.00
CALL PLLYN(X,Y,POLYN,XXX,N,6)
IF(POLYN.GT.YLMAX) YLMAX=POLYN

CONTINUE
POLYN=0.00
XXX=YLMAX/2.00
CALL PLLYN(X,Y,POLYN,XXX,NPLUS,4)
HALFL=POLYN

J2=0
J4=0
IF(ISHAPE.EQ.1) NHALF=IRLOW+1
DO 2030 J3=NHALF,N
J4=N-J3+NHALF
J2=J2+1
XH(J2)=Y(J4)

DO 2040 J5=1,100
XXX=XXX+XINC
POLYN=0.00
CALL PLLYN(X,Y,POLYN,XXX,N,6)
IF(POLYN.GT.YRMAX) YRMAX=POLYN

CONTINUE
POLYN=0.00
XXX=YRMAX/2.00
CALL PLLYN(X,Y,POLYN,XXX,12,4)
HALFR=POLYN
RETURN

END

SUBROUTINE PLLYN(X,Y,POLYN,XXX,NMAX,NPOLY)
DIMENSION X(100),Y(100)

N POINT POLYNOMIAL INTERPOLATING SUBROUTINE
TO INTERPOLATE A VALUE FOR XXX THE NPOLY NEAREST KNOWN POINTS ARE
SELECTED AND AN INTERPOLATING POLYNOMIAL OF DEGREE NPOLY-1 IS
FITTED TO THESE POINTS
X AND Y ARE THE ARRAYS OF NMAX KNOWN POINTS ON THE CURVE
THE RESULT IS POLYN

POLYN=0.0
NM=(NPOLY+1)/2
NM1=NM+1
NUP=NMAX+NM1-NPOLY
DO 102 J=NM1,NUP
IF(XXX.LE.X(J)) GO TO 104

CONTINUE
J=NUP

L=J-NM
LLL=L+NPOLY-1
DO 106 K=L,LLL
   TERM=1.0
   DO 105 M=L,LLL
      IF(K.EQ.M) GO TO 105
      TERM=TERM*(X(K)-X(M))
   CONTINUE
   TERM=Y(K)*TERM
105 CONTINUE
106 POLYN=POLYN+TERM
RETURN
END

SUBROUTINE PLOT(APROF,STARKL,CONV,XWAVEL,XPROFL,NTUP,NTLOW,ALPHAD,
ICONV,NPTS,NALPHA,NCONV,ILINE,LDENS)
ILINE(100),XPROFL(100),ALPHAD(3,5),LDENS(5),APROF(100,5),X(100)
3X2(100),Y1(100),Y2(100),LBDT(5)
DATA LBP/*BROAD,NG,P*,RDPI*,ILE*,LSDP/STAR**,K-DO**,P
ICONV,PR*,APROF*,X/LCP/CONV*,XWAVE*,D*,APROF*,ILE*/LT1/T
2EMP,**,2500**,K**,*,LT2/TEMP**,*,5000**,K**
3**,*/LT3/TEMP**,*,1000**,0,K**,**/LT4/TEMP**,*,4000**,0,K**,**
4**,2000**,0,K**,*,/LT5/TEMP**,*,4000**,0,K**,**
IF(ICONV.EQ.1) GO TO 100
DO 10 I=1,NALPHA
   A2=APROF(I)*APROF(J)
   XPNT=-0.96314718*A2/(ALPHAD(I1(INE.1)**2)
   XPTEST=ABS(XPNT)
   IF(XPTEST.GT.45) GO TO 9
   DPROF(J,I)=(SORT(0.69314718)*(EXP(XPNT))/(1.77245*ALPHAD(I1(INE.1))
   1)
   GO TO 10
9 DPROF(J,I)=0.00
10 CONTINUE
NPTS=NALPHA
100 DO 9999 NT=NTLOW,NTUP
   DO 110 I=1,NALPHA
      XI(I)=APROF(I)
      IF(ICONV.EQ.1) GO TO 110
      XWAVEL(I)=APROF(I)
      XPROFL(I)=DPROF(I,NT)
   110 YI(I)=STARKL(I,NT)
   DO 120 I=1,NCONV
      X2(I)=APROF(I)
   120 Y2(I)=CONV(I,NT)
   CALL GRAPH(NPTS,XWAVEL,XPROFL,0,7,8,0,10,0,0,0,0,0,0,ALPHA(NORMALIZED)**,AREA NORM INTENSITY,**,CONVOLUTION PROFILES**,LDENS)
   IF(ILINE.EQ.3) GO TO 300

IF (ILINE.EQ.2) GO TO 200
IF (ILINE.EQ.1) GO TO 125

1000 FORMAT(//,T10,***FLAG***** ERROR: ILINE NOT SPECIFIED CORRECT ILY; NO PLOTS GENERATED*)
WRITE(6,1000)
RETURN

125 CALL GRAPHS(NPTS,XWAVE,LXPROF,0.,107.,LINE1)
IF (NT.EQ.5) GO TO 148
IF (NT.EQ.4) GO TO 146
IF (NT.EQ.3) GO TO 144
IF (NT.EQ.2) GO TO 142
IF (NT.EQ.1) GO TO 140

1010 FORMAT(//,T10,***FLAG***** ERROR IN NTLOW OR NTUP*)
WRITE(6,1010)
RETURN

140 DO 141 N=1,5
141 LBLT(N)=LT1(N)
GO TO 150

142 DO 143 N=1,5
143 LBLT(N)=LT2(N)
GO TO 150

144 DO 145 N=1,5
145 LBLT(N)=LT3(N)
GO TO 150

146 DO 147 N=1,5
147 LBLT(N)=LT4(N)
GO TO 150

148 DO 149 N=1,5
149 LBLT(N)=LT5(N)

150 CALL GRAPHS(NPTS,XWAVE,LXPROF,0.,107.,LBLT)
CALL GRAPHS(NPTS,XWAVE,LXPROF,1.,107.,LBP)
CALL GRAPHS(NALPHA,X1,Y1,2.,107.,LSDP)
CALL GRAPHS(NCDNV,X2,Y2,3.,107.,LCP)
GO TO 9999

200 CALL GRAPHS(NPTS,XWAVE,LXPROF,0.,107.,LINE2)
IF (NT.EQ.5) GO TO 248
IF (NT.EQ.4) GO TO 246
IF (NT.EQ.3) GO TO 244
IF (NT.EQ.2) GO TO 242
IF (NT.EQ.1) GO TO 240

2000 FORMAT(//,T10,***FLAG***** ERROR IN NTLOW OR NTUP*)
WRITE(6,2000)
RETURN

240 DO 241 N=1,5
241 LBLT(N)=LT1(N)
GO TO 250

242 DO 243 N=1,5
243 LBLT(N)=LT2(N)
GO TO 250

244 DO 245 N=1,5
245  LBLT(N)=LT3(N)
GO TO 250
246  DO 247 N=1,5
247  LBLT(N)=LT4(N)
GO TO 250
248  DO 249 N=1,5
249  LBLT(N)=LT5(N)
DO 247 N=1,5
250  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LBLT)
  CALL GRAPHS(NPTS,XWAVEL,XPROFL,1,107,LBP)
  CALL GRAPHS(NLPHA,X1,Y1,2,107,LSDP)
  CALL GRAPHS(NCONV,X2,Y2,3,107,LCP)
GO TO 250
300  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LINE3)
  IF(NT.EQ.5) GO TO 348
  IF(NT.EQ.4) GO TO 346
  IF(NT.EQ.3) GO TO 344
  IF(NT.EQ.2) GO TO 342
  IF(NT.EQ.1) GO TO 340
  CONTINUE
  RETURN
3000 FORMAT(*10,8H****FLAG**** ERR$IN NTLOW OR NTUP*)
  WRITE(6,3000)
  RETURN
340  DO 341 N=1,5
341  LBLT(N)=LT1(N)
GO TO 350
342  DO 343 N=1,5
343  LBLT(N)=LT2(N)
GO TO 350
344  DO 345 N=1,5
345  LBLT(N)=LT3(N)
GO TO 350
346  DO 347 N=1,5
347  LBLT(N)=LT4(N)
GO TO 350
348  DO 349 N=1,5
349  LBLT(N)=LT5(N)
DO 345 N=1,5
350  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LBLT)
  CALL GRAPHS(NPTS,XWAVEL,XPROFL,1,107,LBP)
  CALL GRAPHS(NLPHA,X1,Y1,2,107,LSDP)
  CALL GRAPHS(NCONV,X2,Y2,3,107,LCP)
GO TO 9999
9999 CONTINUE
RETURN
Table D-2. Data card requirements for C337BROD

<table>
<thead>
<tr>
<th>Type</th>
<th># Cards</th>
<th>Columns</th>
<th>Variable Name</th>
<th>Format</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1-5</td>
<td>NSETS</td>
<td>I5</td>
<td>Number of data sets</td>
</tr>
<tr>
<td>2</td>
<td>1/set</td>
<td>1-5</td>
<td>NRUNS</td>
<td>I5</td>
<td>Number of runs within data set</td>
</tr>
<tr>
<td>3</td>
<td>1/run</td>
<td>1-60</td>
<td>TITLE</td>
<td>15A4</td>
<td>Experiment label</td>
</tr>
<tr>
<td></td>
<td></td>
<td>61-68</td>
<td>HLINE</td>
<td>2A4</td>
<td>Name of hydrogen line</td>
</tr>
<tr>
<td>4</td>
<td>1/run</td>
<td>1-5</td>
<td>ILINE</td>
<td>I5</td>
<td>Line identification number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6-10</td>
<td>NRAD</td>
<td>I5</td>
<td>Number of positions for electron density calculations</td>
</tr>
<tr>
<td>5</td>
<td>NRAD</td>
<td>1-10</td>
<td>RAD</td>
<td>F10.0</td>
<td>Radial position array</td>
</tr>
<tr>
<td></td>
<td>/run</td>
<td>11-20</td>
<td>TRAD</td>
<td>F10.0</td>
<td>Corresponding radial temperature array</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21-30</td>
<td>HALF</td>
<td>F10.0</td>
<td>Corresponding radial half-width array</td>
</tr>
</tbody>
</table>
PROGRAM TO CALCULATE ELECTRON NUMBER DENSITY FROM BROADENING DATA FOR THE BALMER SERIES HYDROGEN LINES

NSETS = NUMBER OF SETS OF DATA
NRUNS = NUMBER OF RUNS WITHIN GIVEN DATA SET
TITLE = EXPERIMENT TITLE OF A GIVEN RUN
HLINE = NAME OF BALMER SERIES LINE
(H-BETA, H-GAMMA, H-DELTA)
ILINE = 1, H-BETA CALCULATION
= 2, H-GAMMA CALCULATION
= 3, H-DELTA CALCULATION
NRAD = NUMBER OF RADIAL POSITIONS FOR DENSITY CALCULATION
RAD(N) = RADIAL POSITION ARRAY (N=1 TO NRAD)
TRAD(N) = TEMPERATURE ARRAY CORRESPONDING TO RAD(N)
HALF(N) = FULL (MEASURED) HALF WIDTH AT HALF MAX INTENSITY ARRAY
CORRESPONDING TO RAD(N) AND TRAD(N)

DIMENSION DENS(9), TEMP(5), ALFA(45), TITLE(15), HLINE(2), WAVE(3), HALF(35), RAD(35), TRAD(35), ALFAD(9, 5), X(9), Y(9), XINTRP(5), YINTRP(5), ECE(2NS(35), ALPHAD(35)

READ(5, 110) NRUNS
FORMAT(15)
DO 9999 NSET = 1, NSETS
READ(5, 110) NRUNS
FORMAT(15)
DO 9999 NRUN = 1, NRUNS
READ(5, 120) TITLE, HLINE
FORMAT(15A4, 2A4)
READ(5, 130) ILINE, NRAD
FORMAT(215)
WRITE(6, 1000) TITLE, HLINE, WAVE(Iライン)
FORMAT(1I1, 15X, 15, 'ELECTRON DENSITY BROADENING CALCULATION' //, /
IT10,15A4,*T10,2A4,2X,F7.2)
K=0
DC 140 I=1,45,5
K=K+1
NUP=I+4
L=0
DC 140 J=1,NUP
L=L+1
ALFAD[K,L]=ALFA(J)
WRITE(6,*2000) (TEMP(I),I=1,5)
2000 FORMAT(*,25,*HALF-WIDTH DATA*,*/T15,*ELECTRON DENS*,T30,*F15.0)
1 2001 FORMAT(T15,*E11.4,T33,5(3X,E11.4))
WRITE(6,2001) DENS(I),(ALFAD(I,J),J=1,5)
DO 200 I=1,NRAD
DO 155 J=1,C
DO 155 K=1,5
XINTRP(K)=ALOG10(TEMP(K))
155 YINTRP(K)=ALFD(J,K)
X(J)=ALOG10(DENS(J))
POLYN=0.00
XXX=ALOG10(TRA(I))
CALL PLLYNN(XINTRP,YINTRP,POLYN,XXX,5,3)
Y(J)=POLYN
CONTINUE
ICOUNT=0
XXDEN=14.0
170 POLYN=0.00
ICOUNT=ICOUNT+1
CALL PLLYNN(X,Y,POLYN,XXDEN,9,2)
XXALFA=POLYN
CALDEN=7.9568E+12*((HALF(I)/XXALFA)**1.5)
CALDEN=ALOG10(CALDEN)
TEST=ABS(CALDEN-XXDEN)
IF(TEST.LE.0.00005) GO TO 180
IF(ICOUNT.GT.50) GO TO 190
XXDEN=CALDEN
GC TO 170
180 EDENS(I)=10.0**CALDEN
ALPHA(I)=XXALFA
GC TO 200
190 CALDEN=10.0**CALDEN
WRITE(6,195) RAD(I),TRA(I),HALF(I),CALDEN,XXALFA
195 FORMAT(*,T15,*###*FLAG***** ELECTRON DENSITY ITERATION FAILED TO
ICONVERGE WITHIN 50 ITERATIONS FOR:*/*,715,*RADIUS=*E11.4,2X,*TEMP
2PERATURE=*E11.4,2X,*LAST INTERPOLATED REUCED HALF
3AST CALCULATED DENSITV= *E11.4,2X,LAST INTERPOLATED REDUCED HALF
SUBROUTINE PLLYN(X, Y, POLYN, XXX, NUMX, NPOLY)
DIMENSION X(100), Y(100)
C
C N POINT POLYNOMIAL INTERPOLATING SUBROUTINE
C
C TO INTERPOLATE A VALUE FOR XXX THE NPOLY NEAREST KNOWN POINTS ARE SELECTED AND AN INTERPOLATING POLYNOMIAL OF DEGREE NPOLY-1 IS FITTED TO THESE POINTS
C X AND Y ARE THE ARRAYS OF NUMX KNOWN POINTS ON THE CURVE THE RESULT IS POLYN

POLYN=0.0
N=N+NPOLY+1/2
NM=NM+1
NUP=NUMX+NM1-NPOLY
DO 102 J=NM1, NUP
IF(XXX.LE.X(J)) GO TO 104
102 CONTINUE
J=NUP
104 L=J-NM
LLL=L+NPOLY-1
DO 106 K=L,LLL
TERM=1.0
DO 105 M=L,LLL
IF(K.EQ.M) GO TO 105
TERM=TERM*(XXX-X(M))/(X(K)-X(M))
105 CONTINUE
TERM=TERM*(XXX-X(M))/(X(K)-X(M))
106 CONTINUE
POLYN=POLYN+TERM
RETURN
END