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

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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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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

Page

Page

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)

$$I_{qp}(X) = \frac{d}{4\pi} A_{qp} \; h \; \nu_{qp} \; n_q(X) \qquad (1)$$

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 $q \longrightarrow p$,

h = Planck's constant,

ν_{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

$$I_{qp}(X) = \frac{d}{4\pi} A_{qp} \; h \; \nu_{qp} \; \frac{g_q}{g_o} \; n_o(X) \; \exp \left\{ - \frac{E_q}{k \; T(X)} \right\} \qquad (2)$$

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) = 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)

$$\ell n \left(\frac{g_q A_{qp} \nu_{qp}}{J_{qp}(R)} \right) = \frac{E_q}{kT(R)} + \ell n \left(\frac{4\pi g_o}{h\, n_o(R)} \right) \qquad (3)$$

where R denotes the radial position in the plasma. For emission lines originating from the same ionization stage a plot of $\ell n \frac{gA\nu}{J}$ 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 and t→s) to yield the radial "two-line" temperature defined by the following expression:

$$T(R) = 0.6247(E_q - E_t) \Big/ \left[\log_{10} \left(\frac{g_q A_{qp} \nu_{qp}}{g_t A_{ts} \nu_{ts}} \frac{J_{ts}(R)}{J_{qp}(R)} \right) \right] \qquad (4)$$

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 μm). 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 (30,40). 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.[1] 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.

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[1]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)

λ(nm)[a]	E_q(cm^{-1})[b]	g_q[c]	Relative Transition Probabilities[d]		
			R	BH	HP
381.584	38175	7	0.948	1.540	1.530
382.043	33096	9	0.638	0.656	0.882
382.444	26140	7	0.0283	0.0292	---
382.588	33507	7	0.567	0.610	---

[a] λ = wavelength of the transition q ——> p, and for subsequent tables.

[b] E_q = excitation energy of the emitting level, and for subsequent tables.

[c] g_q = statistical weight of the emitting level, and for subsequent tables.

[d] Relative transition probabilities normalized to the Fe I 371.994 nm line by $A_{371.994} = 0.163$: R = 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

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[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.

Table II. Fe I emission line data (ten-line set)

λ(nm)	E_q(cm^{-1})	g_q	Relative Transition Probabilities		
			R	BH	HP
367.992	27167	9	0.0138	0.0151	0.0169
370.557	27395	7	0.0328	0.0341	0.0372
371.994	26875	11	0.163	0.163	0.163
372.256	27560	5	0.0505	0.0531	0.0580
373.487	33695	11	0.886	0.776	0.867
373.713	27167	9	0.143	0.140	0.143
374.826	27560	5	0.0904	0.0870	0.0994
374.949	34040	9	0.744	0.681	0.798
375.824	34329	7	0.611	0.611	0.674
376.379	34547	5	0.523	0.610	0.622

Table III. Ar I emission line data

λ(nm)	E_q (cm^{-1})	g_q	A_{qp} x 10^{-7} (sec^{-1})[a]					
			AP	MC	CS	BTW	G	BW
425.118	116,660	3	0.0085	0.0089	0.0132	0.0075	0.0079	0.0076
425.936	118,871	1	0.360	0.3665	0.450	0.3643	0.360	0.320
426.629	117,184	5	0.028	0.0265	0.036	0.0294	0.028	0.023
427.217	117,151	3	0.071	0.0688	0.090	0.0769	0.071	0.063
430.010	116,999	5	0.034	0.0318	0.042	0.0366	0.034	0.031
433.356	118,469	5	0.049	0.0506	0.074	0.0551	0.049	0.048
433.535	118,459	3	0.0333	0.0308	0.044	0.0385	0.040	0.029
434.545	118,408	3	0.028	0.0273	0.041	0.0278	0.028	0.022

[a]Absolute transition probabilities: AP = Adcock and Plumtree (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 (∿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 ∿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 $Y_2 = X + \Delta X$ (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 dectector 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 gAλ 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)

$$n_e(R) = 4.83 \times 10^{15} \frac{J^{\circ}(R)}{J^{+}(R)} \frac{g^{+}A^{+}\lambda^{\circ}}{g^{\circ}A^{\circ}\lambda^{+}} T(R)^{3/2} \times \exp\left\{\frac{E^{+}-E^{\circ}-E_i^{\circ}+\Delta E_i^{\circ}}{k\,T(R)}\right\} \quad (5)$$

where, $(^{\circ}),(^{+})$ denote the neutral atom and singly ionized species, respectively,

λ = wavelength of the emission transition,

E_i° = ionization energy of the neutral atom species,

ΔE_i° = lowering of the ionization energy.

A ΔE_i° 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 ΔE_i° have been reported (31,36,59). When the Unsöld formula (31) was applied, a value of $\Delta E_i^{\circ} = 403\ cm^{-1}$ (0.05 eV) was found

Table IV. Emission line data for Saha-Eggert's electron number density calculations

Species	λ(nm)	$E_q(cm^{-1})$	g_q	$\frac{g^o A^o \lambda^+}{g^+ A^+ \lambda^o}$ Ratios[a]	Average Ratio
Ca I	422.673	23652	3		
Ca II	396.847	25192	2	2.1738(SL), 2.0488(SG), 2.1029(NBS)[b]	2.0911 ± 0.0379
Mg I	285.213	35087	3		
Mg II	279.553	35732	4	1.4317(SL), 1.504(ADJS), 1.333(SG), 1.3578(NBS)	1.4066 ± 0.0773
Mg II	280.270	35652	2	2.8708(SL), 3.0161(ADJS), 2.6649(SG), 2.743(NBS)	2.8273 ± 0.154
Fe I	252.285	39626	9		
Fe II	258.588	38660	8	3.4050(AS 1), 2.8658(BH/H)	3.1354 ± 0.270
Cd I	228.802	43692	3		
Cd II	226.502	44136	2	2.6575(AS 2), 3.3949(BS)	3.0262 ± 0.369
Zn I	213.86	46745	3		
Zn II	206.19	48481	2	3.0290(AS 2), 2.5203(BS)	2.7747 ± 0.254

[a]Numerals I,II and superscripts (^{o}),($^+$) denote neutral atom and first ion species, respectively.

[b]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)

$$\frac{n_X{}^+(R)}{n_X{}^o(R)} = \frac{J^+(R)}{J^o(R)} \cdot \frac{g^o A^o \lambda^+}{g^+ A^+ \lambda^o} \cdot \frac{Z^+[T(R)]}{Z^o[T(R)]} \cdot \exp\left\{\frac{E^+ - E^o}{kT(R)}\right\} \qquad (6)$$

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_β line The H_β 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 (∿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_β 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_β line is related to n_e by (94-96,98)

$$n_e(R) = \left\{ \frac{\Delta\lambda^S_{\frac{1}{2}}(R)}{2\alpha_{\frac{1}{2}}(2.61\ e)} \right\}^{3/2} \qquad (7)$$

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

$\alpha_{\frac{1}{2}}$ = 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, $\alpha'_{\frac{1}{2}}$, which could be compared directly with experimentally observed H_β half-widths, $\Delta\lambda^o_{\frac{1}{2}}(R)$. When these quantities were substituted for $\Delta\lambda^S_{\frac{1}{2}}(R)$ and $\alpha_{\frac{1}{2}}$ in Equation 7 and the constants were evaluated, the radial n_e was given by

$$n_e(R) = 7.9658 \times 10^{12} \left\{ \frac{\Delta\lambda^o_{\frac{1}{2}}(R)}{\alpha'_{\frac{1}{2}}} \right\}^{3/2} \qquad (8)$$

A discussion of the details and accuracy of the convolution procedure and of the H_β 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)

$$\Delta\lambda^{S}_{\frac{1}{2}} \simeq 2w[1 + 1.75\ A\ (1-0.75\ R')] \qquad (9)$$

where w = electron impact width, proportional to n_e,

A = ion broadening parameter, proportional to $(n_e)^{\frac{1}{4}}$,

R' = ratio of the mean distance between ions, r_1, to the Debye radius ρ_D.

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

$$R' = r_1/\rho_D = 1.82\ \pi^{1/6}\ \frac{e}{(kT)^{\frac{1}{2}}}\ (n_e)^{1/6} \qquad (10)$$

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 $\Delta\lambda^{S}_{\frac{1}{2}}$ values were obtained for each line at the temperatures listed and for

n_e 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 V. Experimental facilities and operating conditions

Plasma Generation	
Radiofrequency generator	Fixed frequency (27.12 MHz), 1.5 kW crystal controlled oscillator and air-cooled amplifier (International Plasma Corporation, Hayward, CA). A feedback circuit was added to this facility to maintain constant forward power in the transmission line (type RG-8U coaxial cable) to the impedence matching network by controlling the screen voltage of the oscillator. Forward power in the transmission line was measured with a Thruline Wattmeter (Model 43, 2500-H Element, Bird Electronics Corp., Cleveland, OH).
Impedence matching network	Variable (30-turn) vacuum capacitor coupling circuit (International Plasma Corporation, Hayward, CA) as described in reference 100. Copper, two-turn, water-cooled load coil, 5 mm o.d.
Plasma torch	Concentric quartz tube arrangement similar to that described previously (101). Inner and outer tubes were clear precision quartz tubing (Wilmad Glass Co., Buena, NJ). Spacing between inner and outer tubes and, position of aerosol injector tube accurately set with a machined brass alignment plug during torch construction.
coolant tube	Outer tube, 20 ± 0.025 mm o.d., 18.05 ± 0.025 mm i.d.
plasma tube	Inner tube, 15 ± 0.025 mm o.d., 13 ± 0.025 mm i.d.

Table V. (Continued)

aerosol tube	Clear fused quartz, 6 mm o.d., 4 mm i.d., tapered orifice, 1.5 mm i.d.
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.
	Aerosol Generation
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	
Spectrometer	0.5 meter, Ebert mount, scanning monochromator (Jarrell-Ash Division, Fisher Scientific Co., Waltham, MA, Model No. 82000).
Grating	1180 rulings/mm, blazed at 2500 Å, first order.
Slits	Fixed, 15 μm entrance and exit, entrance slit height masked to 3 mm.
Reciprocal linear dispersion	16 Å/mm, first order.
Detector	EMI 6256B photomultiplier, S-13 response (Gencom Division, Emitronics, Inc., Plainview, NY)
Optical transfer system	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.
Amplifier	Linear picoammeter with zero suppression (Keithly Instruments, Cleveland, OH, Model 417)
Integrator	Digital readout system, hard copy only (Infotronics, Houston, TX, Model CRS-80).
Recorder	X-Y recorder (Moseley Division, Hewlett-Packard, Pasadena, CA, Model 7001-A).

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,

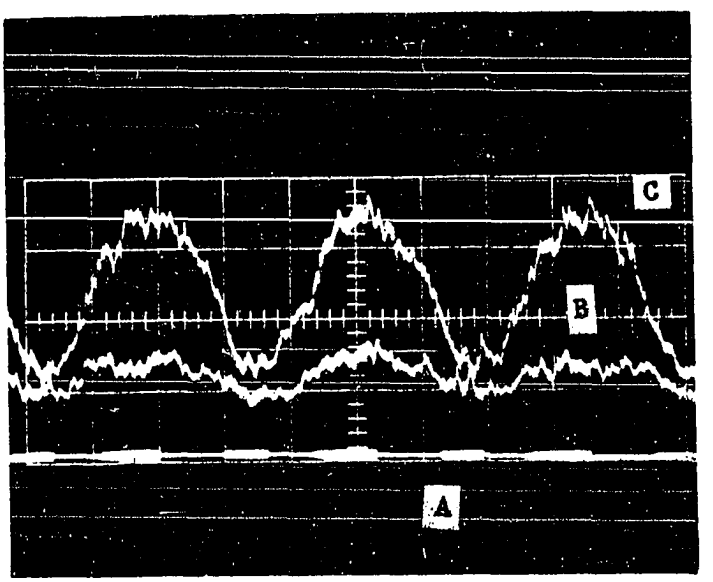


Figure 1. Oscilloscope tracings showing emission intensity modulation with a 60 Hz ripple on the forward power to the plasma: (A) dark current, (B) Fe I 382.444 nm, (C) Fe I 381.584 nm

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 ∿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 ∿9% peak-to-peak magnitude, remained. The 120 Hz ripple was reduced to ∿3% near maximum power and to <1% at 900 W by increasing the generator high voltage filtering network capacitance from 4μF to 12μF. For the latter the reflected power was reduced from ∿10 W to ∿1 W when the 60 Hz ripple was eliminated.

Computer Facilities

Off-line computer calculations were handled by PL1 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

Region	Relative Intensity		Ratio[a]	Temperature (K)	
	Fe I 381.584	Fe I 382.444		R[b]	BH
peak	3.3	1.4	0.42	6500	5600
valley	1.3	0.85	0.65	5600	4900

[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 $(g^{o}A^{o}\lambda^{+}/g^{+}A^{+}\lambda^{o})$ ratios given in Table IV. Radial number density ratios $(n_{X+}(R)/n_{Xo}(R))$ 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

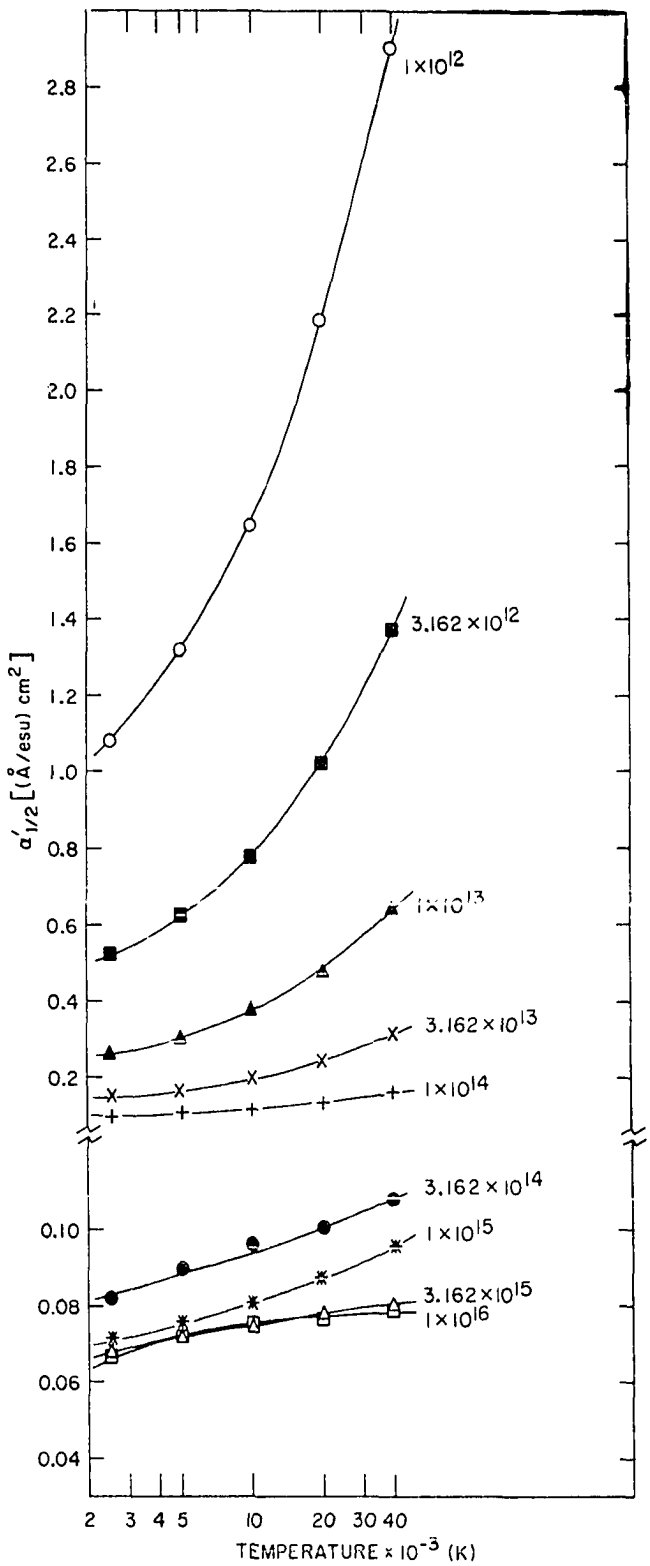
H_β line

Wavelength scans over the H_β line profile were obtained at successive lateral displacements across the plasma discharge. First, each scan was divided into ∿25 constituent wavelengths spanning the entire interval of the H_β line profile. Second, lateral profiles were constructed for each constituent wavelength and the spectral background was interpolated from the continuum emission beyond the H_β 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 H_β profile at each radial position was reconstructed from the radial intensity data; the radial half-widths, $\Delta\lambda^{o}_{\frac{1}{2}}(R)$, were measured from these H_β 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 $\alpha'_{\frac{1}{2}}$ *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 $\Delta\lambda^{o}_{\frac{1}{2}}(R)$ obtained as described above was inserted into Equation 8 to evaluate the $[\Delta\lambda^{o}_{\frac{1}{2}}(R)]^{3/2}$ term. Third, $[\alpha'_{\frac{1}{2}}, n_e(R)]$ pairs were calculated by appropriate interpolation methods (98) for the Fe I excitation temperature, T(R), at radius R. Fourth, an approximate $[\alpha'_{\frac{1}{2}}]_0$ 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 $[\alpha'_{\frac{1}{2}}]_1$ value was interpolated from the $\alpha'_{\frac{1}{2}}$ *vs.* $n_e(R)$ relationship and from the value of $[n_e(R)]_0$. This value for $[\alpha'_{\frac{1}{2}}]_1$ was used in Equation 8 to give a

Figure 2. Reduced Stark profile half-widths, $\alpha'_{\frac{1}{2}}$, corrected for Doppler and instrument broadening plotted *vs.* $\log_{10} T$ for electron densities from 10^{12} to 10^{16} cm^{-3} for the H_β 486.13 nm line

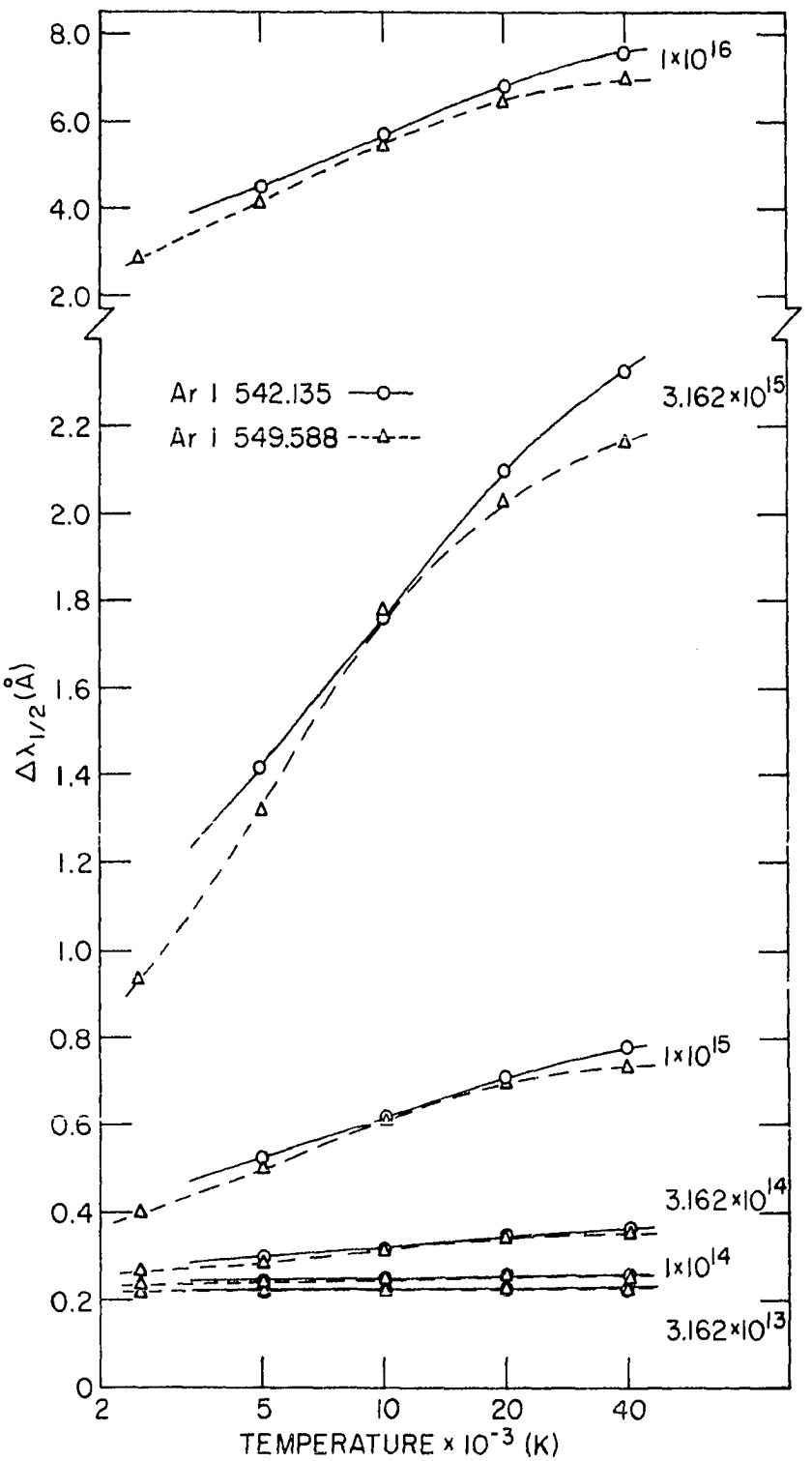

1×10^12
3.162×10^12
1×10^13
3.162×10^13
1×10^14
3.162×10^14
1×10^15
3.162×10^15
1×10^16
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.10
0.08
0.06
0.04
2 3 4 5 10 20 30 40
TEMPERATURE × 10^-3 (K)
a'1/2 [(Å/esu) cm^2]

first-order electron density, $[n_e(R)]_1$. Finally, this procedure was repeated iteratively until a self-consistent pair of $[\alpha'_{\frac{1}{2}}, n_e(R)]$ 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., $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda^G_{\frac{1}{2}}$ and $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda_{\frac{1}{2}}$, could be used to calculate the expected experimental half-width, $\Delta\lambda_{\frac{1}{2}}$, at the appropriate n_e and temperature combinations. The $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda_{\frac{1}{2}}$ ratios were plotted as a function of the $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda^G_{\frac{1}{2}}$ ratios for the values given in reference 93. Equation 9 was used to calculate the $\Delta\lambda^S_{\frac{1}{2}}$ values and the $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda^G_{\frac{1}{2}}$ ratio was obtained from the Stark half-width and the known value for $\Delta\lambda^G_{\frac{1}{2}}$. The corresponding $\Delta\lambda^S_{\frac{1}{2}}/\Delta\lambda_{\frac{1}{2}}$ ratio was interpolated from the plot and the $\Delta\lambda_{\frac{1}{2}}$ value was calculated from this ratio. This procedure was used to obtain $\Delta\lambda_{\frac{1}{2}}$ values for each Ar I line at each n_e and temperature combination considered. The semi-log plots of $\Delta\lambda_{\frac{1}{2}}$ 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, $\Delta\lambda_{\frac{1}{2}}$ *vs.* $\log_{10} T$ for electron density from $10^{13.5}$ to 10^{16} cm^{-3}


8.0
6.0
4.0
2.0
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
$\Delta\lambda_{1/2}$ (Å)
Ar I 542.135
Ar I 549.588
1×10^16
3.162×10^15
1×10^15
3.162×10^14
1×10^14
3.162×10^13
2
5
10
20
40
TEMPERATURE × 10^-3 (K)

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

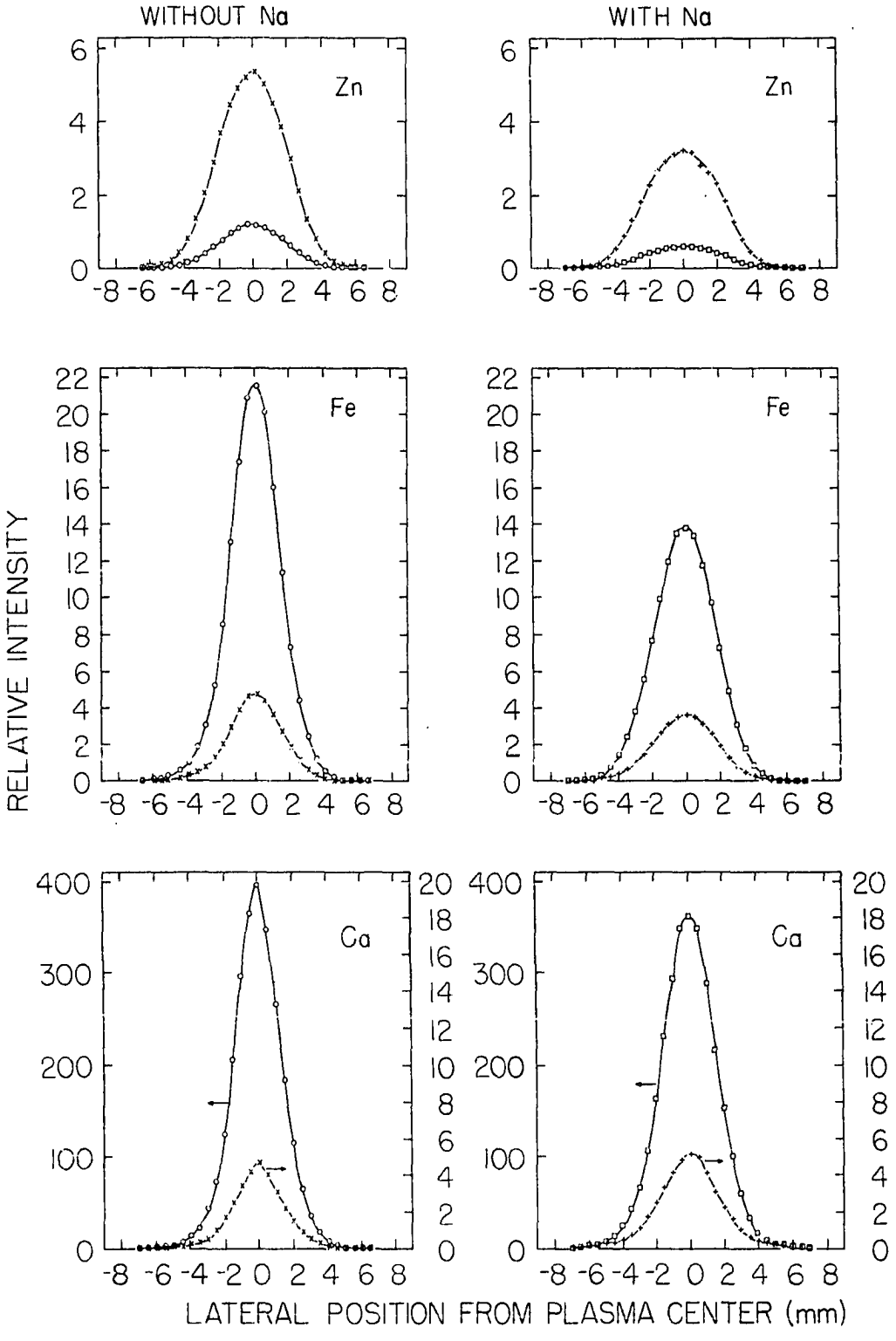
The bell-type lateral intensity distributions which were obtained for Fe I thermometric emission lines complied well with the circular symmetry requirement discussed in Chapter II. The bell-type profiles of the emission lines given in Table IV for Saha-Eggert's n_e calculations were also in compliance 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_β 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

		without Na	with 6900 µg Na/mℓ
10 µg Zn/mℓ:	Zn II 206.19 nm	(—○—)	(—□—)
	Zn I 213.88 nm	(— X —)	(— + —)
150 µg Fe/mℓ:	Fe II 258.588 nm	(—○—)	(—□—)
	Fe I 252.285 nm	(— X —)	(— + —)
10 µg Ca/mℓ:	Ca II 396.847 nm	(—○—)	(—□—)
	Ca I 422.673 nm	(— X —)	(— + —)


WITHOUT Na
WITH Na
Zn
Fe
Ca
RELATIVE INTENSITY
LATERAL POSITION FROM PLASMA CENTER (mm)

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 (1c).

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

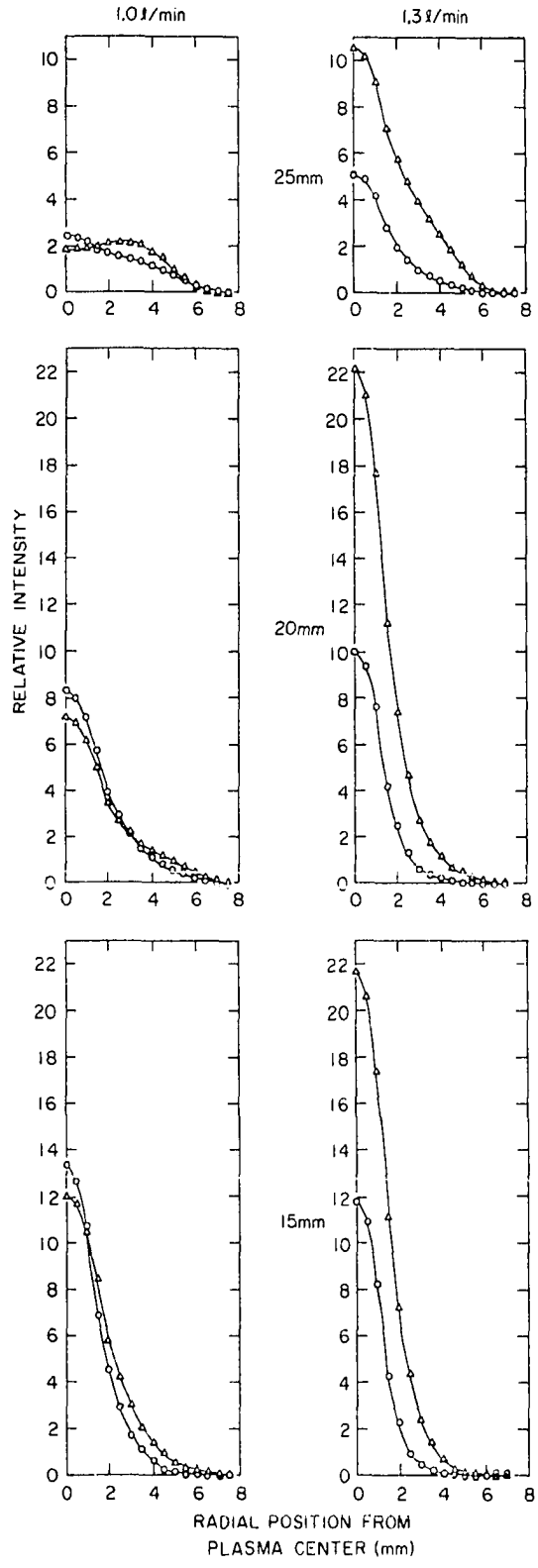
Species	I^+/I^o Ratios[a]		$\frac{(I^+/I^o)Na}{(I^+/I^o)}$
	Without Na	With 6900 µg Na/mℓ	
Zn	0.22	0.18	0.82
Cd	0.88	0.67	0.76
Fe	4.6	3.8	0.83
Mg[b]	10.4	9.9	0.95
Mg[c]	5.3	5.1	0.96
Ca	85	70	0.82

[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 (—○—) and 150 µg Fe/mℓ + 6900 µg Na/mℓ (—△—)


1.0ℓ/min
1.3ℓ/min
25mm
20mm
15mm
RELATIVE INTENSITY
RADIAL POSITION FROM
PLASMA CENTER (mm)

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

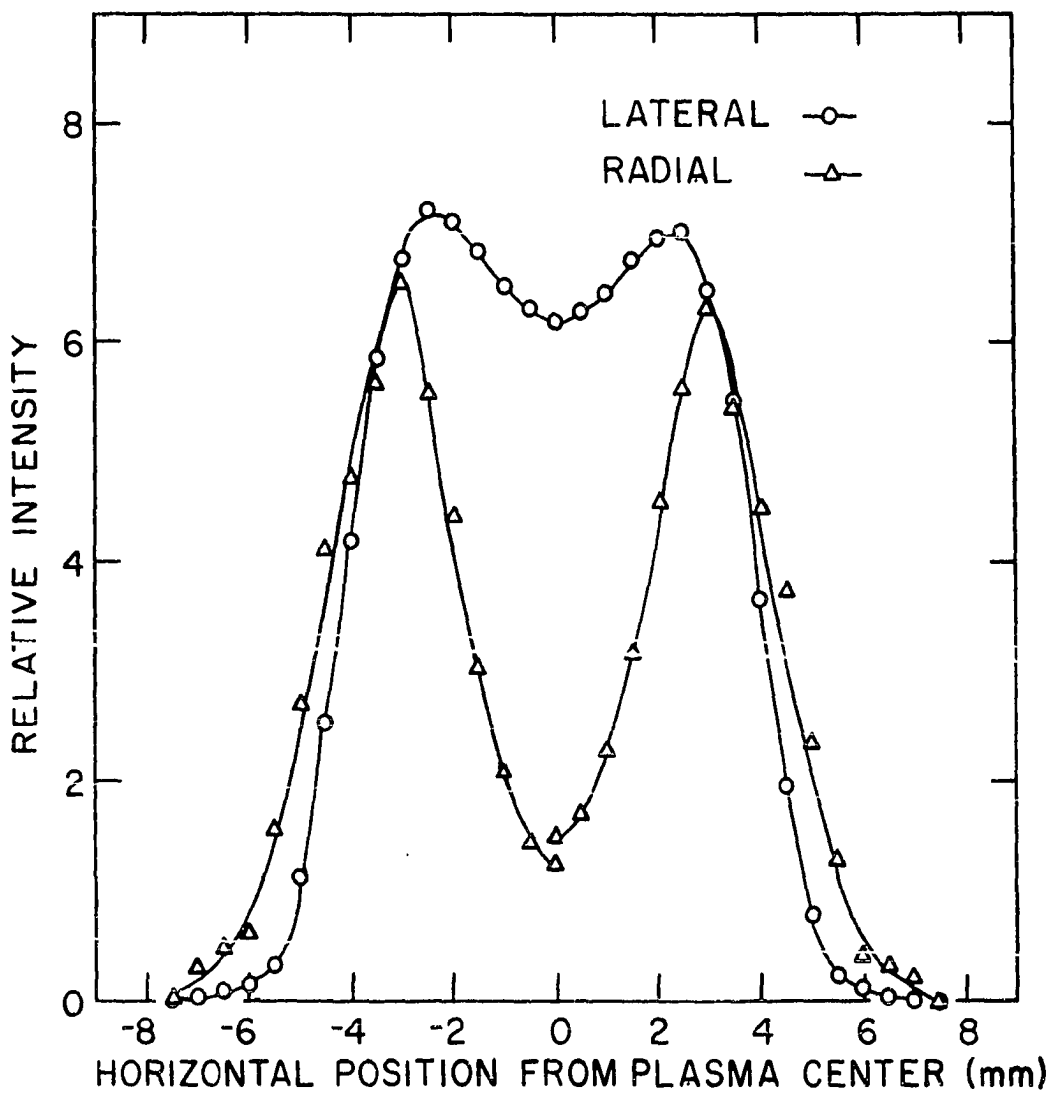


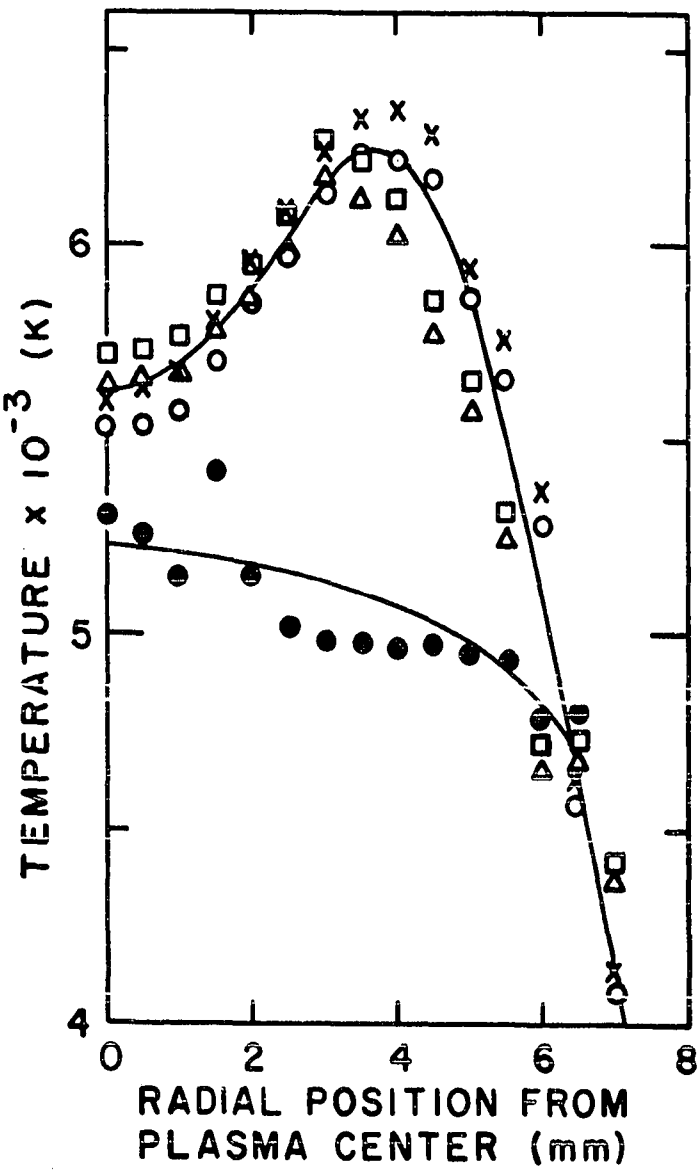
Figure 6. Toroidal lateral and radial relative intensity distributions for the Ar I 425.936 nm line at 15 mm, 1000W and 1.0 ℓ/min aerosol carrier gas flow

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_β 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%

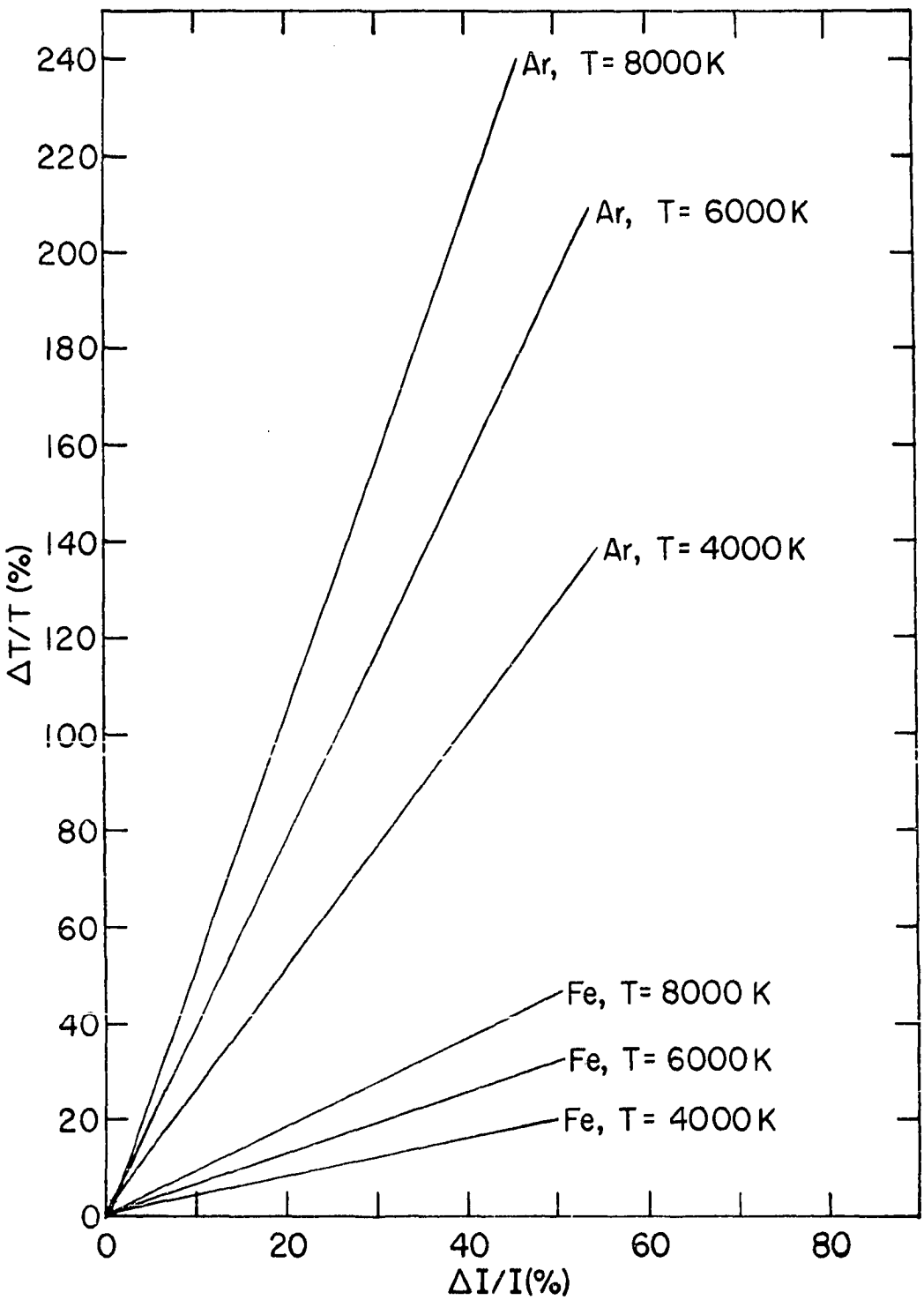
Figure 7. Radial excitation temperatures at 15 mm, 1000W and 1.0 ℓ/min aerosol carrier gas flow. Ar I eight-line with Corliss and Shumaker (77) transition probability data (—●—); Fe I ten-line with Huber and Parkinson (67) data (—X—) and with Reif (30) and Banfield and Huber (66) data (—○—); Fe I three-line with Reif data (—△—) and with Banfield and Huber data (—□—)


TEMPERATURE x 10^{-3} (K)
6
5
4
0
2
4
6
8
RADIAL POSITION FROM
PLASMA CENTER (mm)

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 $\Delta I/I$ 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


240
220
200
180
160
140
120
100
80
60
40
20
0
ΔT/T (%)
0
20
40
60
80
ΔI/I(%)
Ar, T= 8000K
Ar, T= 6000K
Ar, T= 4000K
Fe, T= 8000 K
Fe, T= 6000K
Fe, T= 4000K

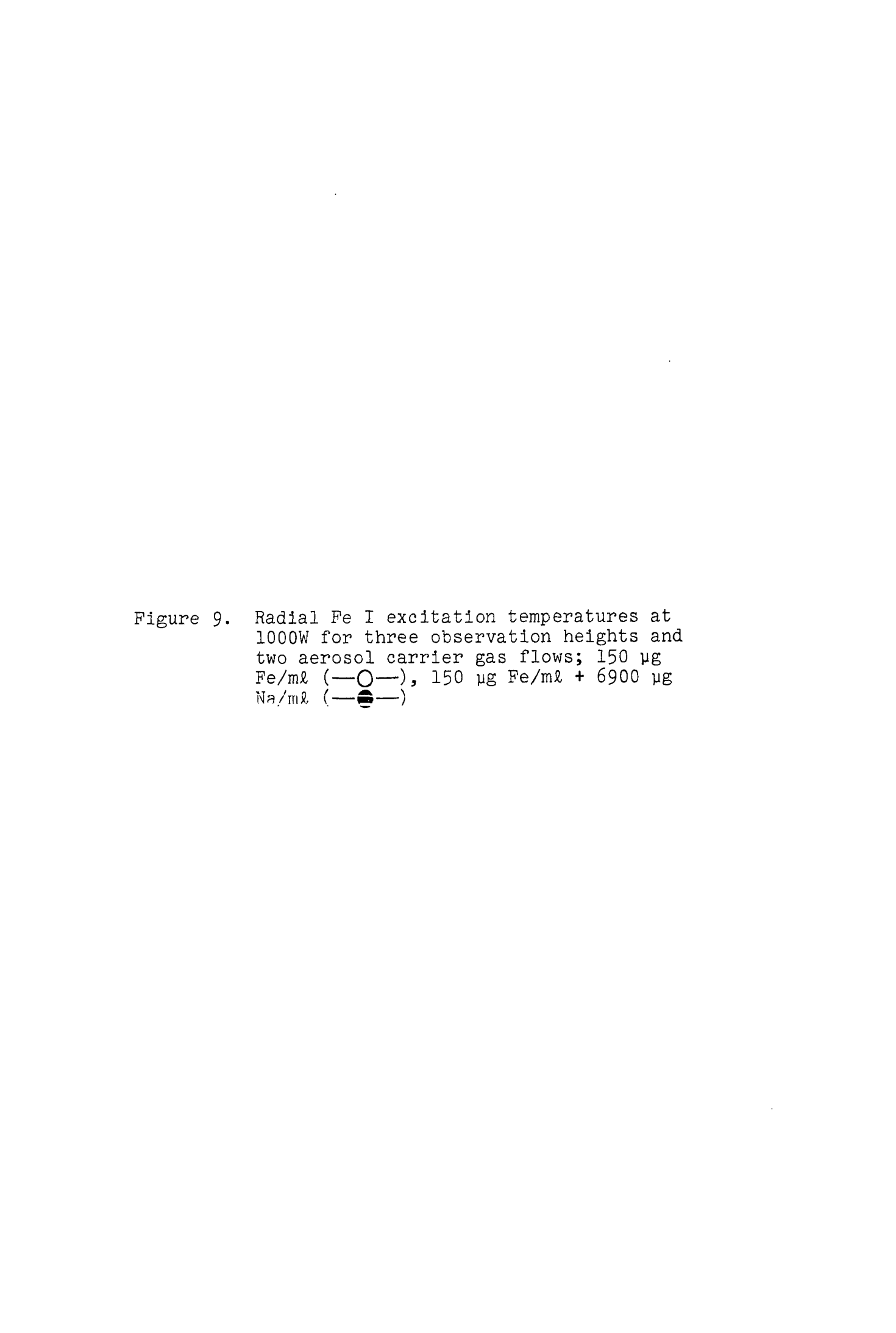
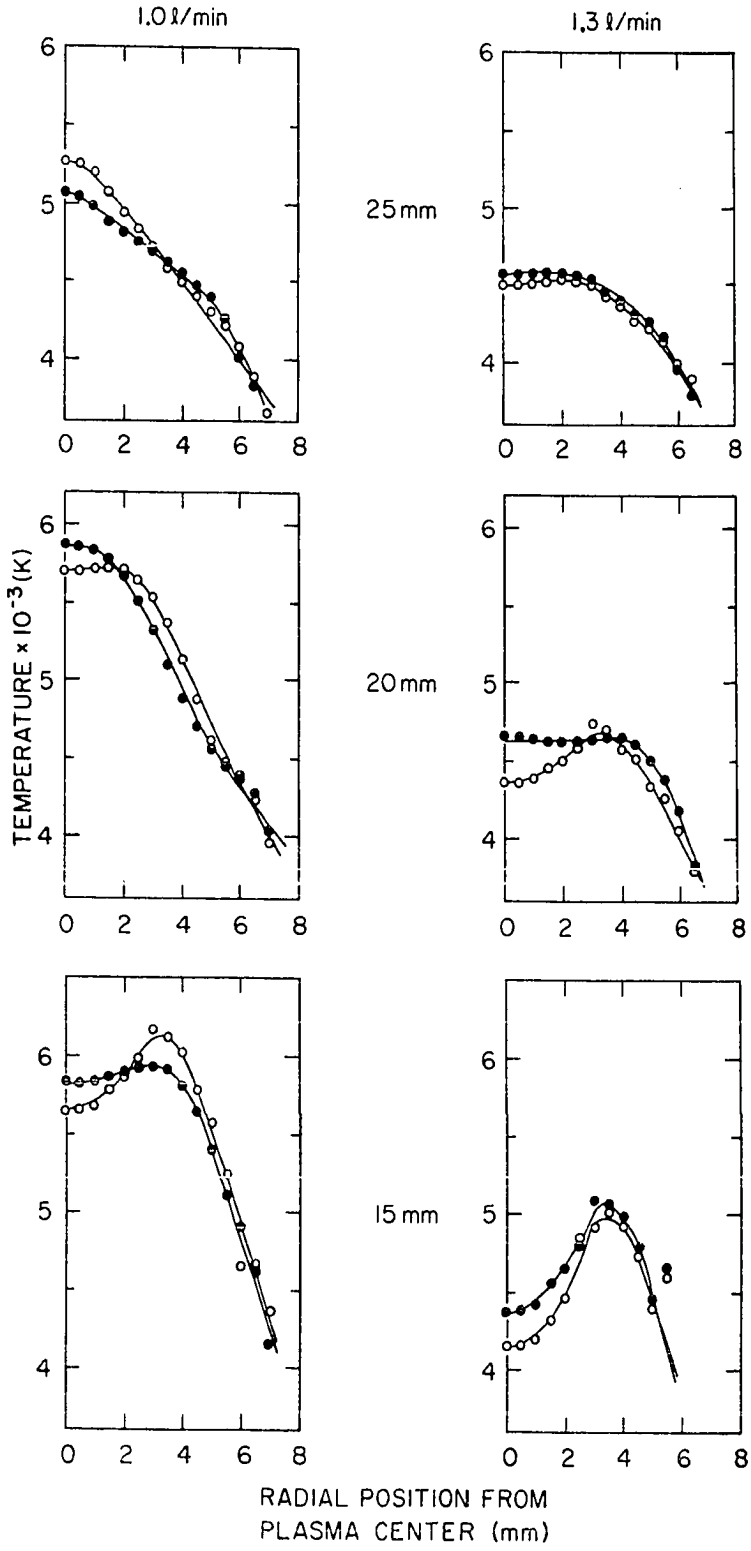


Figure 9. Radial Fe I excitation temperatures at 1000W for three observation heights and two aerosol carrier gas flows; 150 µg Fe/mℓ (—○—), 150 µg Fe/mℓ + 6900 µg Na/mℓ (—◒—)


1.0 ℓ/min
1.3 ℓ/min
25 mm
20 mm
15 mm
TEMPERATURE × 10⁻³ (K)
RADIAL POSITION FROM
PLASMA CENTER (mm)

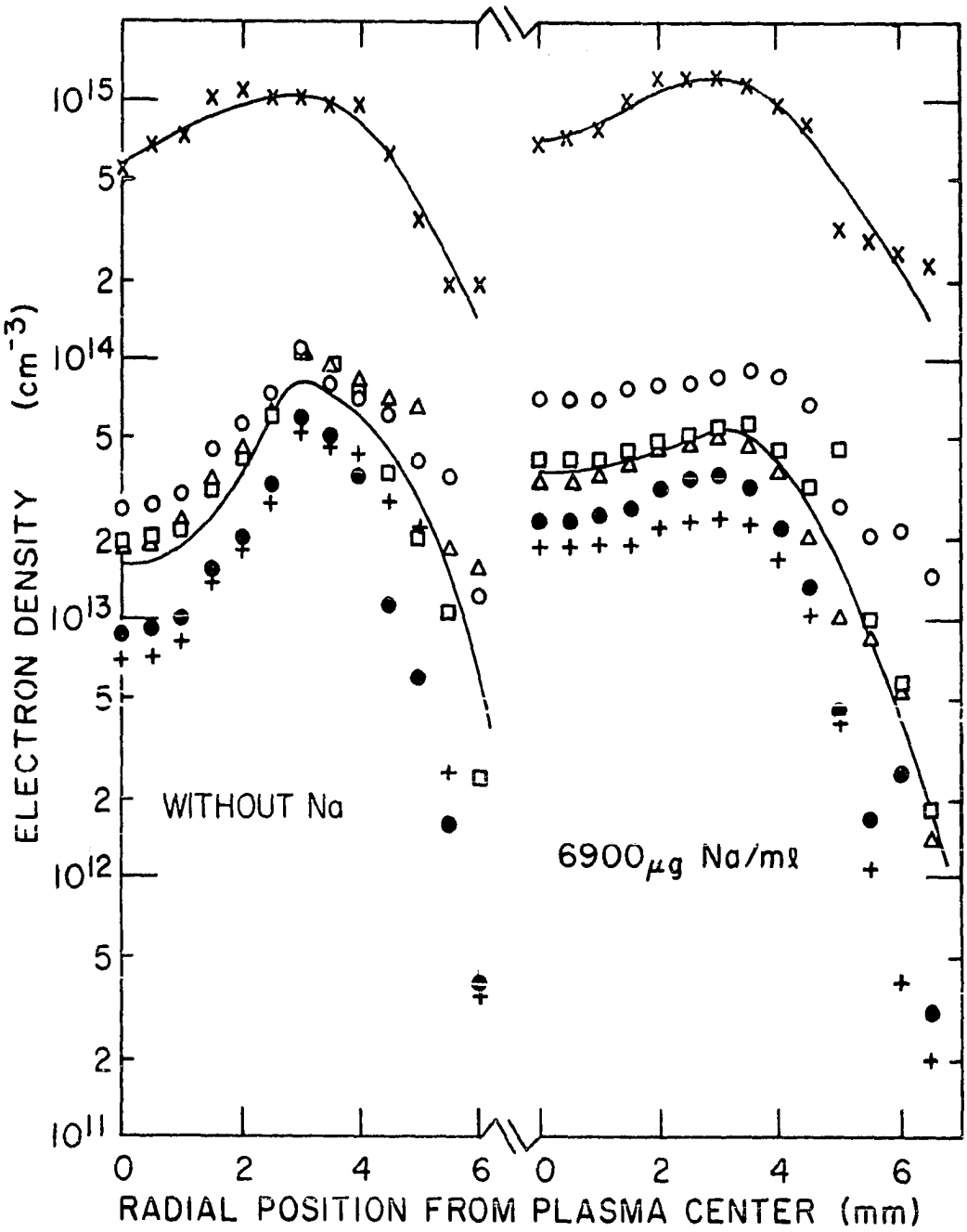
Examination of this figure reveals several important features. First, the excitation temperature distributions obtained at the respective aerosol carrier gas flows and observation heights are not significantly changed upon addition of Na as an EIE. Second, the temperatures for the higher flow are significantly 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 ℓ/min aerosol carrier gas flow and ∿15-20 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_β 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_β 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})
10^{15}
5
2
10^{14}
5
2
10^{13}
5
2
10^{12}
5
2
10^{11}
WITHOUT Na
6900μg Na/mℓ
0
2
4
6
0
2
4
6
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

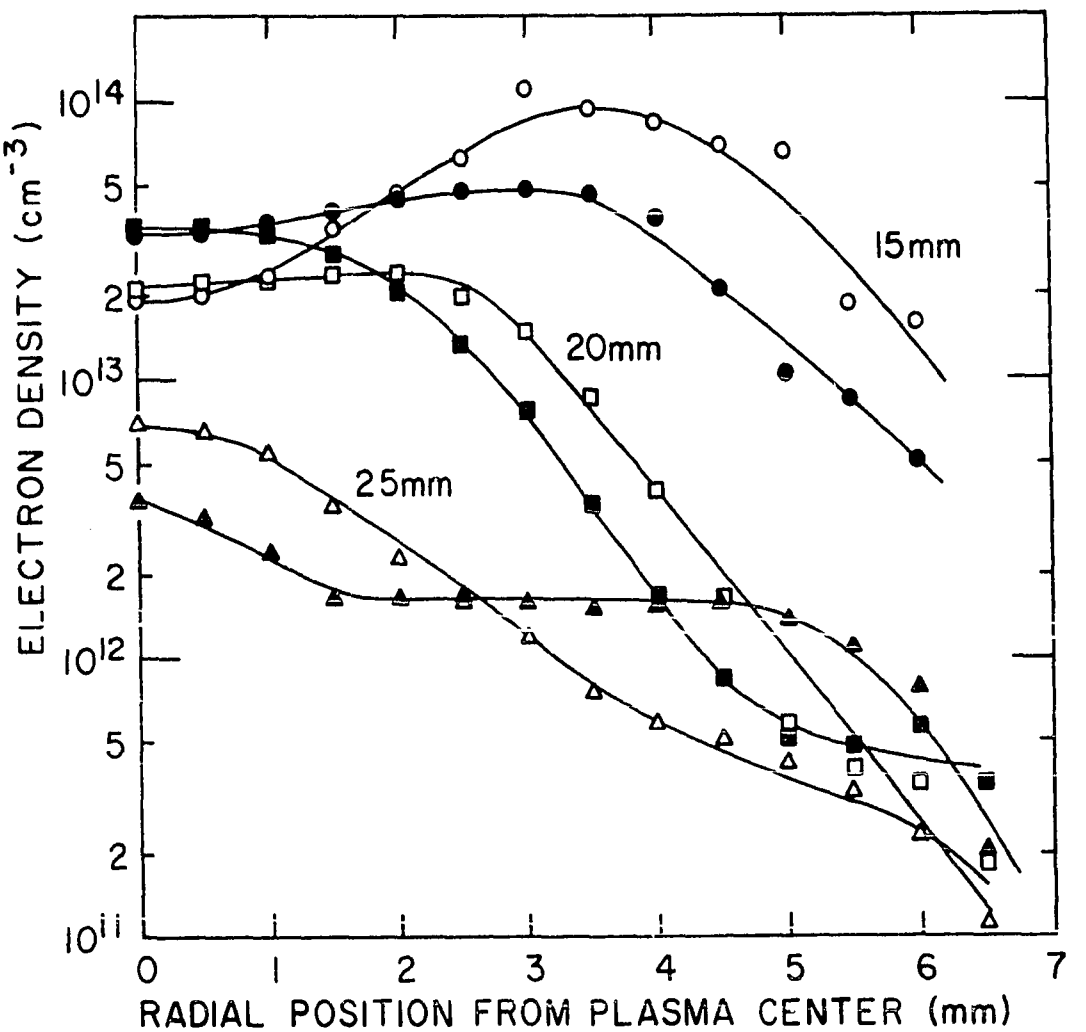
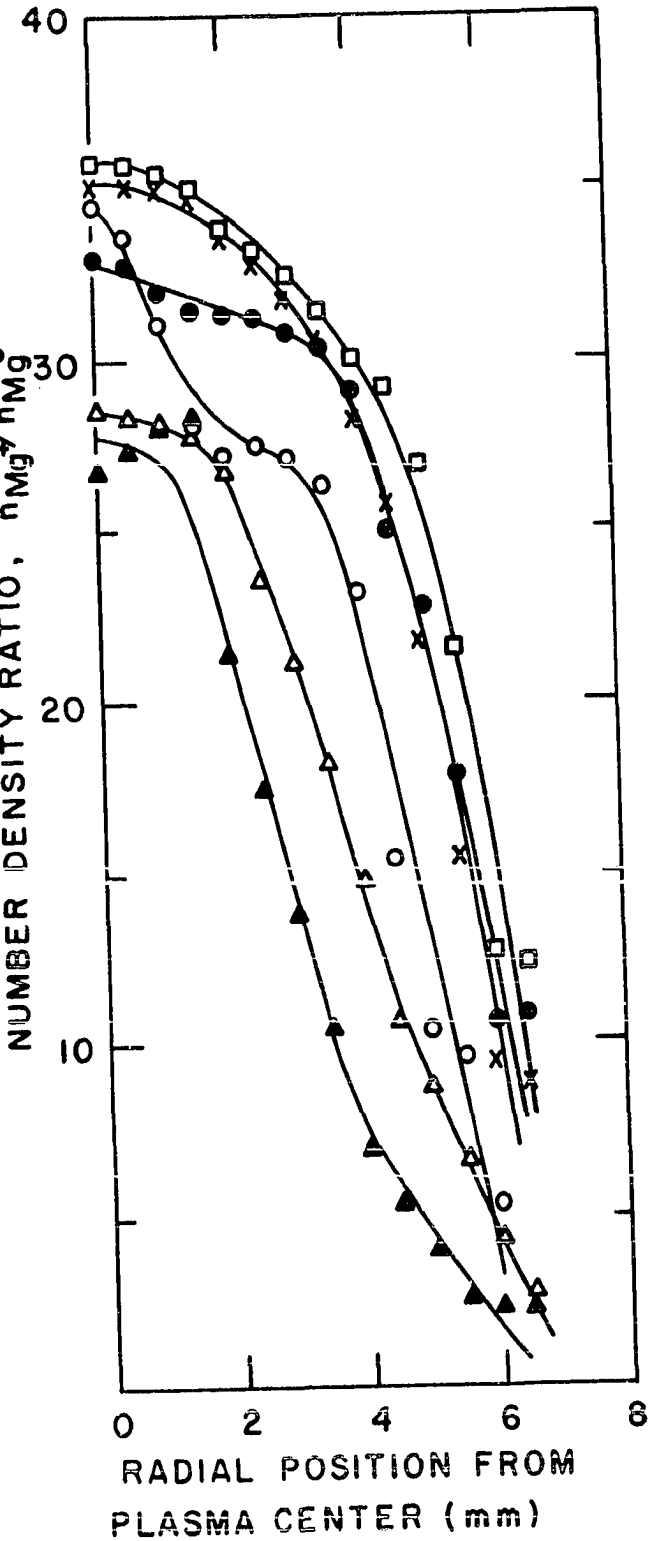


Figure 11. Radial Saha-Eggert's electron density distributions at 15, 20, and 25 mm for Mg atom/ion line combinations; 10 µg Mg/mℓ (—○—, —□—, —△—), 10 µg Mg/mℓ + 6900 µg Na/mℓ (—●—, —■—, —▲—)

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^+}/n_{Mg^o} 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_{Mg^0}, 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 (—Δ—); 10 µg Mg/mℓ + 6900 µg Na/mℓ at 15 mm (—●—), 20 mm (—X—), and 25 mm (—▲—)


40
30
20
10
0
2
4
6
8
NUMBER DENSITY RATIO, n_{Mg^+}/n_{Mg^0}
RADIAL POSITION FROM PLASMA CENTER (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 Souilliart 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, $n_{X^+}(R)/n_{XO}(R)$, for Zn, Cd, Fe and Ca with and without added Na at 1000W, 1.0 ℓ/min, and 15 mm height

	Without Na				With 6900 μg Na/mℓ			
Radius (mm)	Zn	Cd	Fe	Ca	Zn	Cd	Fe	Ca
0.0	2.1	6.2	18	610	1.5	4.4	15	300
0.5	2.1	6.2	18	590	1.5	4.4	15	300
1.0	2.1	5.9	17	540	1.5	4.5	15	310
1.5	2.0	5.2	16	440	1.5	4.6	15	280
2.0	1.9	5.0	16	430	1.5	4.6	16	320
2.5	1.9	4.8	16	410	1.5	4.6	15	340
3.0	1.8	4.6	15	310	1.5	4.6	15	320
3.5	1.8	4.2	15	380	1.4	4.6	13	310
4.0	1.8	3.5	14	390	1.5	4.6	12	260
4.5	1.9	3.0	14	190	1.4	4.9	11	230
5.0	1.9	2.7	13	190	1.4	4.9	8.6	240
5.5	1.9	3.8	10	170	1.0	4.3	7.1	170
6.0	2.0	2.9	8.8	160	0.3	4.2	4.9	100
6.5	---	---	---	---	0.8	4.3	4.5	100

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

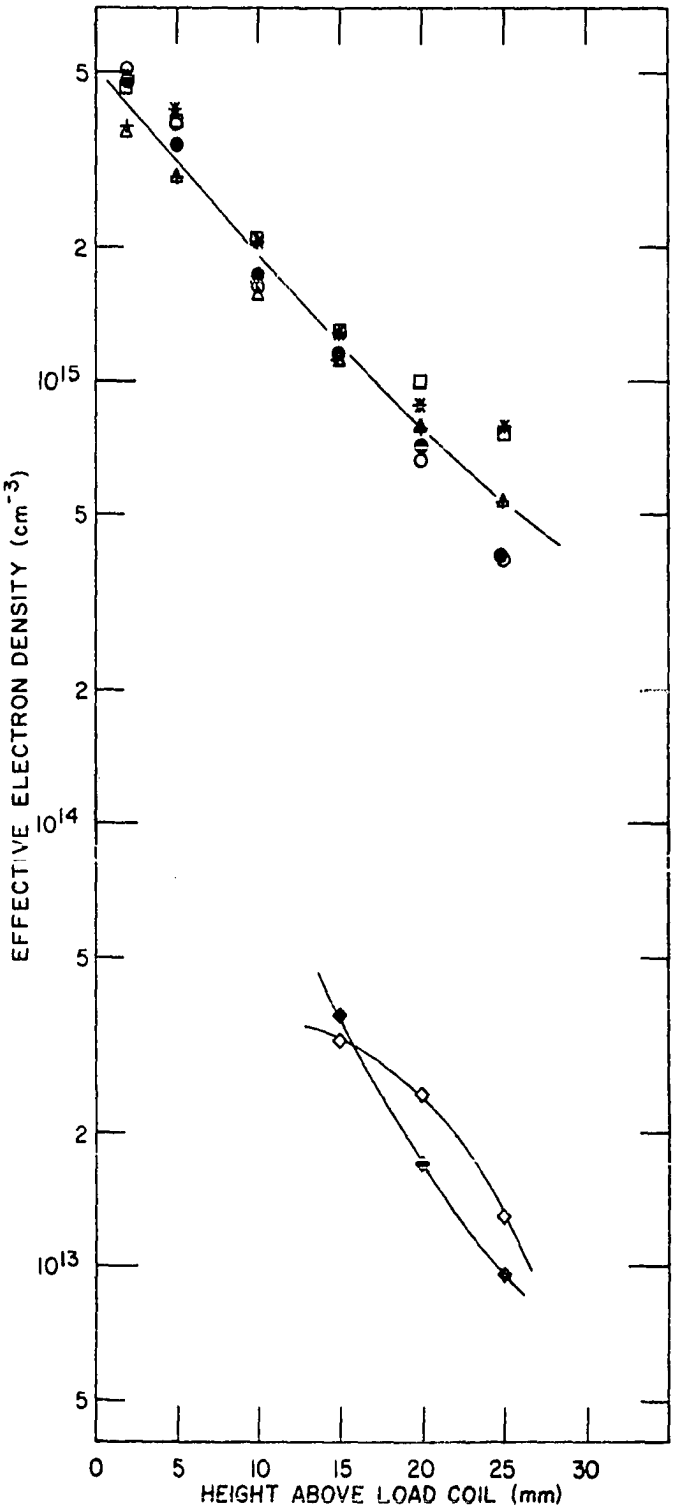
Table IX. Effective half-widths[a] of H_β and Ar I lines measured at the plasma axis for 1000W forward power and 1.0 ℓ/min aerosol carrier gas flow

Observation Height (mm)	Ar I 542.135 nm		Ar I 549.588 nm		H_β 486.13 nm	
	Without Na	With Na[b]	Without Na	With Na	Without Na	With Na
2	2.36	2.49	1.79	1.88	5.47	5.25
5	1.88	2.01	1.40	1.40	4.49	4.16
10	1.05	1.04	0.808	0.851	2.63	2.74
15	0.674	0.656	0.565	0.568	2.08	2.08
20	0.522	0.487	0.434	0.435	1.53	1.59
25	0.432	0.443	0.346	0.348	1.15	1.15

[a]Half-widths expressed in units of Angstroms (Å), 10 Å = 1 nm.

[b]6900 µg 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_β 486.13 nm (—○—), Ar I 542.14 nm (—□—), Ar I 549.59 nm (—△—). Stark broadening with 6900 µg Na/mℓ nebulized; H_β 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 + 6900 µg Na/mℓ (—◆—)


EFFECTIVE ELECTRON DENSITY (cm^{-3})
5
2
10^{15}
5
2
10^{14}
5
2
10^{13}
5
0
5
10
15
20
25
30
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_β line in a static electric field (96,116, 117) reveals that ∿20,000 volts/cm would account for the increased broadening. Magnetic fields of ∿10,000 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 (1c,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.

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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, $n \geq 2$. 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

Type #	# Cards	Columns	Variable Name	Format	Remarks
1	1	1- 5	NSETS	I5	Number of profile data sets
2	1/set	1-60	TITLE	15A4	Experiment description label
		61-80	DLAB	5A4	Plot description label
3	1/set	1- 5	LKODE	I5	Indicates Fe/Ar or other lines used
		6-10	IARTP	I5	Selects Ar transition probability data set
		11-30	ELNAME	5A4	Name of element other than Fe or Ar (punch LKODE = 99, this is redefined to be LKODE = 3 in subroutine PNTORG)
4	1/set	1- 5	NLZ	I5	Number of lines (4 max)
		6-10	IWT	I5	End point weighting selection (used with subroutine SPLINE)
5	1/set	1-28	WAVE	4F7.2	Line wavelength array (Angstrom units)
		31-70	DELA	4F10.0	Transition probability uncertainty array
6	1/set	1- 5	L1	I5	Intensity plot option switch
		6-10	L2	I5	Spline fit option switch
		11-15	L3	I5	Two-line temperature calculation option (Fe lines only)
		21-25	L5	I5	Slope temperature calculation option
		26-30	NL	I5	Pointer to starting F-test value
		31-35	NH	I5	Pointed to ending F-test value
		36-40	KPLOT1	I5	Option to plot Fe two-line T's
		41-45	KPLOT2	I5	Option to plot average Fe two-line T's
		46-50	KPLOT3	I5	Option to plot slope T's

Table A-1. (Continued)

Type #	# Cards	Columns	Variable Name	Format	Remarks
		51-55	KLINE1	I5	Option to select Fe two-line T's to plot
		56-60	KLINE2	I5	
		61-65	KPNED1	I5	Option to punch lateral T's on cards
		66-70	KPNED2	I5	Option to punch radial T's on cards
7	1/set	1- 2	N	I2	Number of lateral intensities (15 max)
8a	N/set	1-10	RBP(i,1)	F10.0	Lateral displacement array for line #1
		11-20	ARI(i,1)	F10.0	Corresponding lateral intensity array
8b	N/set		RBP(i,2)		Same as 8a except for line #2
			ARI(i,2)		Same as 8a except for line #2
8c	N/set		RBP(i,3)		Same as 8a except for line #3
			ARI(i,3)		Same as 8a except for line #3
8d	N/set		RBP(i,4)		Same as 8a except for line #4
			ARI(i,4)		Same as 8a except for line #4
9a-1	1/line	1- 5	NPTS	I5	Number of points for segmented spline fit
		6-10	NS1	I5	Defines number of zones for Abel inversion poly fit
		16-35	ELEMNT	5A4	Element identifier in subroutine SPLINE
		36-45	ZPNT	F10.0	Distance between successive radial intensity calculations
		46-50	LSHIFT	I5	Option to zero correct lateral displacements
		51-60	XZERO	F10.0	Zero position for lateral displacement array (used when LSHIFT = 1 specified)

Table A-1. (Continued)

Type #	# Cards	Columns	Variable Name	Format	Remarks
		61-65	NFACTR	I5	Weight factor selection for endpoints of spline fits
		66-70	KWT	I5	Option to select reading uncertainty array for lateral intensities from cards
9a-2	NPTS/ line	1-10	XDIST	F10.0	Smoothed lateral displacement array
		11-20	YINT	F10.0	Corresponding lateral intensity array
		21-30	SIGMAY	F10.0	Corresponding uncertainty array
9b-1	1/line	1- 5	IMA	I5	Number of points in lateral intensity array
		6-10	NS1	I5	Defines number of zones for Abel inversion poly fit (same as 9a-1 NS1)
		11-20	XPNT	F10.0	Distance between successive radial intensity calculations (same as 9a-1 ZNPT)
		21-30	XBIG	F10.4	Lateral position of profile maximum
9b-2	IMA/ line		XDIST		Same as 9a-2 XDIST
			YINT		Same as 9a-2 YINT
			SIGMAY		Same as 9a-2 SIGMAY

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 A-1. (Continued)

Type #	# Cards	Columns	Variable Name	Format	Remarks
10a	1/set	1-40	GA	4F10.0	OPTIONAL: $g_q A_{qp}$ array for Ar I lines listed in comment card section, used when LKODE = 2 and IARTP > 6
10b-1	1/set	1-40	EQ	4F10.0	OPTIONAL: Excitation energy of ELNAME lines employed, used when LKODE = 3
10b-2	1/set	1-40	GA	4F10.0	OPTIONAL: $g_q A_{qp}$ array for ELNAME lines, used when LKODE = 3

```
C                                                                       1
C                                                                       2
C        **********    C337TEM2    **********                           3
C     *** DEFINITION OF IMPORTANT VARIABLES AND INDEXES USED ***        4
C                                                                       5
C              TITLE = DESCRIPTION OF EXPERIMENT                        6
C              DLAB  = MONITORED REGION OF EMISSION SOURCE (FOR PLOT ID) 7
C                                                                       8
C         ** CONTROL SWITCHES **                                        9
C                                                                       10
C              L1 =0, NO LATERAL OR RADIAL INTENSITY PLOTS              11
C              L1 =1, SUPERIMPOSED PLOTS OF LATERAL AND RADIAL INTENSITY 12
C              L2=0, MEASURED INTENSITY FIT BY SEGMENTED SPLINE AND ZERO 13
C                    CORRECTED IF NECESSARY (LSHIFT=1)                  14
C                 =1,SPLINE FIT NOT NECESSARY; SMOOTHED LATERAL PROFILE 15
C                    (ZERO CORRECTED) SUPPLIED AND SUBROUTINE XYCALC     16
C                    USED                                               17
C              L3 =0, AVERAGE LINE PAIR TEMPERATURE AND PLOT            18
C              L3 =1, TEMPERATURES OF INDIVIDUAL LINE PAIRS AND PLOT    19
C              L5 =0, TEMPERATURES CALCULATED FROM I(X) & I(R) DATA     20
C              L5 =1, ONLY RADIAL INTENSITIES CALCULATED---TEMP BY-PASSE 21
C     F - TEST FOR 0.5 TO 50.0 PERCENT PROBABILITY OF EXCEEDING THE     22
C          F-VALUE;  NL DEFINES THE LOWER LIMIT, NH DEFINES UPPER LIMIT 23
C          MAX NH=7, MIN NL=1                                           24
C                                                                       25
C          PERCENT      NL     ALLOWED NH VALUES                       26
C            0.5         1          1,2,3,4,5,6,7                      27
C            1.0         2          2,3,4,5,6,7                        28
C            2.5         3          3,4,5,6,7                          29
C            5.0         4          4,5,6,7                            30
C           10.0         5          5,6,7                              31
C           25.0         6          6,7                                32
C           50.0         7          7                                  33
C              LKODE = 1, FE LINES USED                                 34
C              LKODE = 2, AR LINES USED                                 35
C              KPLOT1 = 1, 2-LINE T'S NOT PLOTTED                       36
C              KPLOT2 = 1, AVE. 2-LINE T'S NOT PLOTTED                  37
C              KPLOT3 = 1, SLOPE T NOT PLOTTED                          38
C              KLINE1 < 2, ALL 2-LINE T'S PLOTTED                       39
C                     = 2, 1ST 2-LINE T NOT PLOTTED                     40
C                     = 3, 1ST, 2ND 2-LINE T'S NOT PLOTTED              41
C                     = 4, 1ST,...,3RD 2-LINE T'S NOT PLOTTED           42
C                     = 5, 1ST,...,4TH " " " " "                        43
C                     = 6, 1ST,...,5TH " " " " "                        44
C                     = 7, ALL NOT PLOTTED                              45
C                     > 7, ALL NOT PLOTTED                              46
C              KLINE2 = 0, ALL 2-LINE T'S PLOTTED                       47
C                     = 1, 1ST LP T NOT PLOTTED                         48
C                     = 2, 2ND " " "     "                              49
C                     = 3, 3RD " " "     "                              50
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C                = 4. 4TH "  "  "      "                                    51
C                = 5. 5TH "  "  "      "                                    52
C                = 6. 6TH "  "  "      "                                    53
C                > 6. ALL 2-LINE T'S PLOTTED                                54
C        KPNED1  = 1. LATERAL SLOPE T'S PUNCHED ON CARDS FOR USE IN         55
C                     THE ELECTRON DENSITY PROGRAM (C337EDEN)               56
C        KPNED2  = 1. RADIAL SLOPE T'S PUNCHED ON CARDS FOR USE IN          57
C                     THE ELECTRON DENSITY PROGRAM (C337EDEN)               58
C        IARTP   = 1. MALONE AND CORCORAN GA VALUES: ARGON LINES            59
C                = 2. WUJEC GA                                              60
C                = 3. ADDOCK AND PLUMTREE GA                                61
C                = 4. CORLISS AND SHUMAKER GA                               62
C                = 5. WENDE GA                                              63
C                = 6. GERICKE GA                                            64
C                 > 6. READ IN GA DATA CARD AT END OF DATA DECK.            65
C                      4F10.0 FORMAT                                        66
C                ARGON LINES USED: 4251.2,4259.4,4266.3,4272.2 ANGS         67
C                                                                           68
C        LKODE=1. IARTP=9. BANFIELD AND HUBER (1973) GA VALUES              69
C                          USED FOR FE I LINES                              70
C        LKODE=99. INPUT SPECIES IDENTIFIER AS ELNAME AND READ IN           71
C                  GA,EQ VALUES FOR SLOPE TEMP CALCULATION                  72
C                  (TEMP CALCN OPTIONAL. SEE L5 SPECIFICATION)              73
C                                                                           74
C                                                                           75
C                                                                           76
C     ** ARRAYS **                                                          77
C                                                                           78
C        RBP = EXPERIMENTALLY MEASURED LATERAL DISTANCE ARRAY               79
C        ARI =          "                "      PEAK INTENSITY ARRAY       80
C              CORRESPONDING TO 'RBP' ARRAY                                 81
C        N = NUMBER OF ELEMENTS IN 'RBP' OR 'ARI' ARRAY (NOT MORE           82
C        XDIST = MEASURED AND SMOOTHED LATERAL DISTANCE ARRAY.              83
C                ORIGIN ZERO SHIFT CORRECTED WITH RESPECT TO                84
C                EXPT MEASURED RBP ARRAY SO THAT XDIST=0                    85
C                CORRESPONDS TO GEOMETRIC CENTER                            86
C        YINT = CORRESPONDING MEASURED AND SMOOTHED LATERAL INTENS          87
C        SIGMAY=CORRESPONDING ARRAY OF SIGMA VALUES FOR YINT                88
C               ARRAY                                                       89
C        RAD = INTERMEDIATE RADIAL INTENSITY ARRAY                          90
C        RDI =       "          "    DISTANCE    "   CORRESPONDING T        91
C              'RAD' ARRAY                                                  92
C        RADINT = FINAL RADIAL DISTANCE ARRAY CONTAINING ELEMENTS           93
C                 CORRESPONDING TO 'RADINT' ARRAY                           94
C                                                                           95
C                                                                           96
C     ** INDEXES **                                                         97
C                                                                           98
C                                                                           99
C        KT = NUMBER OF ELEMENTS IN 'RAD' OR 'ARI' ARRAY                   100
```

```
C              NSETS = NUMBER OF SETS OF PROFILE DATA TO BE PROCESSED,      101
C                      INDEX FOR PRIMARY DO LOOP                            102
C              NLZ = NUMBER OF LINES USED (NOT MORE THAN 4)                 103
C              LAM = DATA ARRAY INDEX FOR PRIMARY DO LOOP                   104
C              LZ = SPECTRAL LINE INDEX FOR PRIMARY DO LOOP,                105
C                   NOTE:                                                   106
C                        LZ = 1, CORRESPONDS TO FE-I- 3815.84 ANGSTROMS     107
C                        LZ = 2       "       "    " "  3820.43     "      108
C                        LZ = 3       "       "    " "  3824.44     "      109
C                        LZ = 4       "       "    " "  3825.88     "      110
C                   THIS LABELLING MUST BE RIGOROUSLY FOLLOWED IN ORDER     111
C              THAT THIS PROGRAM FUNCTION PROPERLY                          112
C                                                                           113
C                                                                           114
C         ** INPUT CONSTAINTS AND VARIABLES **                              115
C                                                                           116
C                                                                           117
C              IMA = NUMBER OF SMOOTHED DATA POINTS IN ARRAY 'XDIST' OR     118
C                    (NOT MORE THAN 51)                                     119
C              NS1=3, 3 ZONE POLY FIT                                       120
C              NS1=4, 4 ZONE POLY FIT                                       121
C              NS1=5, 5 ZONE POLY FIT                                       122
C              IWT=0, NO WEIGHTING ON POLY FIT                              123
C                 =1, YINT VALUES WEIGHTED WITH SIGMAY ARRAY                124
C              XPNT = RADIAL DISTANCE (MM) BETWEEN TWO SUCCESSIVELY CALC    125
C                     RADIAL INTENSITIES = R(N+1) - R(N)                    126
C              WAVE = WAVELENGTHS OF SPECTRAL LINES (ANGSTROMS)             127
C              XBIG=POSITION OF INT MAX IN LATERAL DIST ARRAY (SUPPLIED     128
C                   AS INPUT WHEN SPLINE NOT USED IE, XYCALC USED)          129
C         FOLLOWING INPUT CODES NECESSARY ONLY WHEN SUBROUTINE SPLINE US    130
C              KWT=1, INPUT ARRAY OF INTEN SIGMAS FOR POLY FIT              131
C                  0, SIGMAS SET =0  SO THAT WEIGHT=1.0 IN POLY FIT         132
C              NFACTR=1, SPLINE FIT ENDPOINTS X 0.825                       133
C              NFACTR=2,     "      "       "   X 0.850                     134
C              NFACTR=3,     "      "       "   X 0.875                     135
C              NFACTR=4,     "      "       "   X 0.900                     136
C              NFACTR=5,     "      "       "   X 0.925                     137
C              NFACTR=6,     "      "       "   X 0.950                     138
C              LSHIFT=1, LATERAL INTENSITIES ZERO CORRECTED BY XZERO        139
C              XZERO=POSITION OF GEOMETRIC CENTER ON ORIGINAL LATERAL       140
C                   DISPLACEMENT SCALE                                      141
C              NPTS=NUMBER OF POINTS FOR SEGMENTED SPLINE FIT               142
C                 *****NPTS MUST BE GREATOR THAN OR EQUAL TO 10             143
C                                                                           144
C                                                                           145
C                                                                           146
      DIMENSION DLAB(5),TITLE(15),WAVE(4),XDTR(51),RBP(15,4),ARI(15,4),     147
     1SIGMAY(51)     ,XDIST(51),YINT(51),RAD( 51),RDI( 51),RADINT( 51,4,7   148
     2),RADIST( 51,4,7),ILZ(4,7),XBIG(4),DELA(4),DELIR(51),DELINT(51,4,7    149
     3),FNUM(7),ELNAME(5)                                                   150
```

```
      DATA FNUM/0.5,1.0,2.5,5.0,10.0,25.0,50.0/                          151
      READ (5,1003) NSETS                                                152
 1003 FORMAT (I5)                                                        153
      DO 10 NUM=1,NSETS                                                  154
      READ (5,100) TITLE,DLAB                                            155
  100 FORMAT (15A4,5A4)                                                  156
      WRITE (6,101) TITLE,DLAB                                           157
  101 FORMAT (1H1,10X,15A4,5A4,///)                                      158
      READ(5,1001) LKODE,IARTP,ELNAME                                    159
      READ(5,1000) NLZ,IWT                                               160
 1000 FORMAT(2I5)                                                        161
 1001 FORMAT(2I5,5A4)                                                    162
      READ (5,102) (WAVE(I),I=1,NLZ),(DELA(J),J=1,NLZ)                   163
  102 FORMAT (4F7.2,2X,4F10.0)                                           164
      CALL LINDEX (L1,L2,L3,L4,L5,NL,NH,KPLOT1,KPLOT2,KPLOT3,KLINE1,     165
     1KLINE2,KPNED1,KPNED2)                                              166
      READ (5,106) N                                                     167
  106 FORMAT (I2)                                                        168
      DO 1 J=1,NLZ                                                       169
      DO 1 I=1,N                                                         170
  107 FORMAT (2F10.0)                                                    171
    1 READ (5,107) RBP(I,J),ARI(I,J)                                     172
      DO 8 LZ=1,NLZ                                                      173
      LAM=1                                                              174
      CALL PNTORG(LZ,KM,WAVE,RBP,ARI,N,LKODE,ELNAME)                     175
      GO TO (2,3),L2                                                     176
    2 CALL SPLINE (IMA,NS1,XDIV,XDIST,YINT,LAM,XPNT,LZ,XDTR,XD,XBIG,SIGM 177
     1AY,WAVE,IWT)                                                       178
      GO TO 4                                                            179
    3 CALL XYCALC (IMA,NS1,XDIV,XDIST,YINT,LAM,XPNT,LZ,XDTR,XD,XBIG,SIGM 180
     1AY)                                                                181
    4 DO 8 NZ=NL,NH                                                      182
      CALL DKABEL (XDTR,YINT,IMA,NS1,NZ,XPNT,RAD,RDI,KT,XD,XBIG,LZ,DELIR 183
     1,SIGMAY,L1,IWT)                                                    184
      IF(KPNED2.NE.1) GO TO 5                                            185
      DO 199 IPUNCH=1,KT                                                 186
 2001 FORMAT(3F10.4,2X,'LINE',I3,2X,'FTEST PROB',F5.2,1X,5A4)            187
  199 WRITE(7,2001) RAD(IPUNCH),RDI(IPUNCH),DELIR(IPUNCH),LZ,FNUM(NZ),DL 188
     1AB                                                                 189
    5 GO TO (7,6),L1                                                     190
    6 CALL RADPL (IMA,XDIST,YINT,N,RBP,ARI,          LZ,RAD,RDI,LAM,   DLA 191
     1B,KT,NZ)                                                           192
    7 CALL PNTMAP (LZ,KT,RAD,RDI,KM,ILZ,RADINT,RADIST,DELIR,DELINT)      193
    8 CONTINUE                                                           194
   11 GO TO (9,10),L5                                                    195
    9 CALL TEMP  (N,KT,RBP,ARI,RADIST,RADINT,NLZ,DLAB,L3,KM,NL,NH,LKODE, 196
     1KPLOT1,KPLOT2,KLINE1,KLINE2,DELA,DELINT,IARTP)                     197
   13 CALL SLOPET (N,KT,RBP,ARI,RADIST,RADINT,NLZ,DLAB,WAVE,KM,NL,NH,LKO 198
     1DE,KPLOT3,KPNED1,KPNED2,DELA,DELINT,IARTP)                         199
   10 CONTINUE                                                           200
```

```
      STOP                                                                  201
      END                                                                   202
      SUBROUTINE LINDEX (L1,L2,L3,L4,L5,NL,NH,KPLOT1,KPLOT2,KPLOT3,         203
     1KLINE1,KLINE2,KPNED1,KPNED2)                                          204
      READ (5,101) L1,L2,L3,L4,L5,NL,NH,KPLOT1,KPLOT2,KPLOT3,KLINE1,       205
     1KLINE2,KPNED1,KPNED2                                                  206
  101 FORMAT(14I5)                                                          207
      L4=1                                                                  208
      IF (NL) 4,3,1                                                         209
    1 IF (NH-NL) 4,2,2                                                      210
    3 IF (NH) 4,5,4                                                         211
    5 NL=1                                                                  212
      NH=1                                                                  213
    2 IF (L4) 6,6,7                                                         214
    7 IF (L1) 8,10,10                                                       215
   10 IF (L3) 8,11,11                                                       216
   11 L1=L1+1                                                               217
      L2=L2+1                                                               218
      L3=L3+1                                                               219
      L5=L5+1                                                               220
      RETURN                                                                221
    4 WRITE (6,102)                                                         222
      GO TO 12                                                              223
    6 WRITE (6,103)                                                         224
      GO TO 12                                                              225
    8 WRITE (6,104)                                                         226
   12 STOP                                                                  227
  102 FORMAT (//10X'INPUT ERROR IN SWITCH NL OR NH')                        228
  103 FORMAT (//10X'INPUT ERROR IN SWITCH L4')                              229
  104 FORMAT (//10X'INPUT ERROR IN SWITCH L1      OR L3')                   230
      END                                                                   231
      SUBROUTINE PNTORG(LZ,KM,WAVE,RBP,ARI,N,LKODE,ELNAME)                  232
      DIMENSION ELNAME(5)                                                   233
      DIMENSION WAVE(1),RBP(15,4),ARI(15,4)                                 234
      KM=0                                                                  235
      IF(LKODE.EQ.99) LKODE=3                                               236
      GO TO (2,1,1,1),LZ                                                    237
    1 WRITE (6,100)                                                         238
    2 GO TO (4,5,7),LKODE                                                   239
    4 WRITE (6,101) LZ,WAVE(LZ)                                             240
      GO TO 6                                                               241
    5 WRITE (6,103) LZ,WAVE(LZ)                                             242
      GO TO 6                                                               243
    7 WRITE(6,104) LZ,ELNAME,WAVE(LZ)                                       244
  104 FORMAT(5X,'LINE',I3,5X,5A4,F7.2//,14X,'EXPERIMENTALLY MEASURED LAT    245
     1ERAL INTENSITY DATA'/21X,'CORRECTED FOR SPECTRAL RESPONSE'//26X,'X     246
     2',11X,'I(X)'//)                                                       247
  100 FORMAT (1H1)                                                          248
  101 FORMAT (5X,'LINE',I3,5X,'-  FE I -  ',F7.2,//14X,'EXPERIMENTALLY      249
     1MEASURED LATERAL INTENSITY DATA'/21X,'CORRECTED FOR SPECTRAL RESPO    250
```

```
   2NSE'//26X,'X',11X,'I(X)'//)                                          251
103 FORMAT (5X,'LINE',I3,5X,'- AR I - ',F7.2,//14X,'EXPERIMENTALLY       252
   1MEASURED LATERAL INTENSITY DATA'/21X,'CORRECTED FOR SPECTRAL RESPO   253
   2NSE'//26X,'X',11X,'I(X)'//)                                          254
  6 DO 3 I=1,N                                                           255
  3 WRITE (6,102) RBP(I,LZ),ARI(I,LZ)                                    256
102 FORMAT (22X,F8.4,6X,F8.4)                                            257
    RETURN                                                               258
    END                                                                  259
    SUBROUTINE XYCALC (IMA,NS1,          XDIV,XDIST,YINT,LAM,XPNT,LZ,    260
   1XDTR,XD,XBIG,SIGMAY)                                                 261
    DIMENSION SIGMAY(1)                                                  262
    DIMENSION XDIST(1),YINT(1),XBIG(4),XDTR(1)                           263
    READ (5,100) IMA,NS1,XPNT,XBIG(LZ)                                   264
100 FORMAT (2I5,2(F10.4))                                                265
    IF(XBIG(LZ).LT.0.0) GO TO 8                                          266
    IF (LAM-1) 2,2,1                                                     267
  1 WRITE (6,101)                                                        268
101 FORMAT (1H1)                                                         269
  2 WRITE (6,102) IMA                                                    270
102 FORMAT(//14X,'LATERAL INTENSITY DISTRIBUTION HAS BEEN EXPERIMENTAL   271
   1LY MEASURED WITHOUT SPLINE INTERPOLATION'/14X,'INPUT LATERAL DATA    272
   2HAS BEEN ZERO CORRECTED FOR',I3,2X,'POINTS',//T25,'X',T38,'U(X)',T   273
   360,'SIGMA(U(X))',//)                                                 274
    DO 3 I=1,IMA                                                         275
103 FORMAT (3F10.0)                                                      276
104 FORMAT (T20,F10.4,T33,F10.4,T60,E11.4)                               277
    READ (5,103) XDIST(I),YINT(I),SIGMAY(I)                              278
  3 WRITE(6,104) XDIST(I),YINT(I),SIGMAY(I)                              279
    XD=ABS(XDIST(IMA))                                                   280
    DO 7 I=1,IMA                                                         281
  7 XDTR(I)=XDIST(I)/XD                                                  282
    XDIV=ABS(XDTR(2)-XDTR(1))                                            283
    XPNT=XPNT/XD                                                         284
    RETURN                                                               285
  8 WRITE (6,105)                                                        286
105 FORMAT (10X'ERROR IN XBIG INPUT')                                    287
    STOP                                                                 288
    END                                                                  289
    SUBROUTINE PNTMAP (LZ,KT,RAD,RDI,KM,ILZ,RADINT,RADIST,DELIR,DELINT   290
   1)                                                                    291
    DIMENSION RAD(1),RDI(1),RADINT(51,4,7),RADIST(51,4,7),ILZ(4,7)       292
   1,XHOLD(51),YHOLD(51),DELIR(51),DELINT(51,4,7)                        293
    KTHOLD=KT                                                            294
    KM=KM+1                                                              295
    WRITE (6,100) LZ,KT                                                  296
    DO 4 I=1,5                                                           297
    IF (KT - 30*I) 1,1,4                                                 298
  1 J=KT/I                                                               299
    IF (KT - I*J) 3,3,2                                                  300
```

```
    2 J=J+1                                                                 301
    3 GO TO (5,6,7,8,9), I                                                  302
    4 CONTINUE                                                              303
      WRITE (6,101)                                                         304
      STOP                                                                  305
    5 WRITE (6,102)                                                         306
      GO TO 10                                                              307
    6 WRITE (6,103)                                                         308
      GO TO 10                                                              309
    7 WRITE (6,104)                                                         310
      GO TO 10                                                              311
    8 WRITE (6,105)                                                         312
      GO TO 10                                                              313
    9 WRITE (6,106)                                                         314
   10 DO 16 L=1,J                                                           315
      L1=L+J                                                                316
      L2=L+2*J                                                              317
      L3=L+3*J                                                              318
      L4=L+4*J                                                              319
      GO TO (11,12,13,14,15),I                                              320
   11 WRITE (6,107) RDI(L),RAD(L)                                           321
      GO TO 16                                                              322
   12 WRITE (6,108) RDI(L),RAD(L),RDI(L1),RAD(L1)                           323
      GO TO 16                                                              324
   13 WRITE (6,109) RDI(L),RAD(L),RDI(L1),RAD(L1),RDI(L2),RAD(L2)           325
      GO TO 16                                                              326
   14 WRITE (6,110) RDI(L),RAD(L),RDI(L1),RAD(L1),RDI(L2),RAD(L2),          327
     1RDI(L3),RAD(L3)                                                       328
      GO TO 16                                                              329
   15 WRITE (6,111) RDI(L),RAD(L),RDI(L1),RAD(L1),RDI(L2),RAD(L2),          330
     1RDI(L3),RAD(L3),RDI(L4),RAD(L4)                                       331
   16 CONTINUE                                                              332
      WRITE (6,1000)                                                        333
 1000 FORMAT  (1H1)                                                         334
      WRITE (6,1001)                                                        335
 1001 FORMAT (20X,'J',8X,'LZ',8X,'KM',8X,'RADIST(J,LZ,KM)',6X,'RADINT(J,    336
     1LZ,KM)',6X,'DELINT(J,LZ,KM)')                                         337
      IF (RDI(1).GE.0.) GO TO 22                                            338
      INZERO=0                                                              339
      DO 20 IN=1,KT                                                         340
      IF (RDI(IN).LT.0.) GO TO 20                                           341
      INZERO=INZERO+1                                                       342
      XHOLD(INZERO)=RDI(IN)                                                 343
      YHOLD(INZERO)=RAD(IN)                                                 344
   20 CONTINUE                                                              345
      DO 21 IOUT=1,INZERO                                                   346
      RAD(IOUT)=YHOLD(IOUT)                                                 347
   21 RDI(IOUT)=XHOLD(IOUT)                                                 348
      KT=INZERO                                                             349
   22 ILZ(LZ,KM)=KT                                                         350
```

```
      DO 17 I=1,KT                                                          351
      J=KT-I+1                                                              352
      RADIST(J,LZ,KM)=RDI(I)                                                353
      RADINT(J,LZ,KM)=RAD(I)                                                354
      DELINT(J,LZ,KM)=DELIR(I)                                              355
      WRITE (6,1002) J,LZ,KM,RADIST(J,LZ,KM),RADINT(J,LZ,KM),DELINT(J,LZ    356
     1,KM)                                                                  357
 1002 FORMAT (20X,3(I3,8X),3(E11.4,10X))                                    358
      RAD(I)=0.0                                                            359
   17 RDI(I)=0.0                                                            360
      KT=KTHOLD                                                             361
      RETURN                                                                362
  100 FORMAT (//19X,'LINE ',I1,' - RADIAL INTENSITIES FOR ',I3,             363
     1' RADIAL POSITIONS IN SOURCE'//)                                      364
  101 FORMAT (19X,'PRINT ERROR')                                            365
  102 FORMAT (42X,'R',12X,'I(R)'//)                                         366
  103 FORMAT (31X,'R',8X,'I(R)',20X,'R',8X,'I(R)'//)                        367
  104 FORMAT (31X,'R',8X,'I(R)',10X,'R',8X,'I(R)',10X,'R',8X,'I(R)'//)      368
  105 FORMAT (31X,'R',8X,'I(R)',3(10X,'R',8X,'I(R)')//)                     369
  106 FORMAT ( 8X,'R',8X,'I(R)',4(10X,'R',8X,'I(R)')//)                     370
  107 FORMAT (39X,F7.4,6X,F9.5)                                             371
  108 FORMAT (28X,F7.4,2X,F9.5,15X,F7.4,2X,F9.5)                            372
  109 FORMAT (28X,F7.4,2X,F9.5,2(5X,F7.4,2X,F9.5))                          373
  110 FORMAT (28X,F7.4,2X,F9.5,3(5X,F7.4,2X,F9.5))                          374
  111 FORMAT  (5X,F7.4,2X,F9.5,4(5X,F7.4,2X,F9.5))                          375
      END                                                                   376
      SUBROUTINE SPLINE (IMA,NS1,ZDIV,ZDIST,ZINT,LAM,ZPNT,LZ,ZDTR,ZD,ZBI    377
     1G,ZSIG,ZWAVE,IWT)                                                     378
      IMPLICIT REAL*8(B-H,O-Y)                                              379
      DIMENSION ZDIST(1),ZINT(1),ELEMNT(5),ZSIG(1),ZWAVE(1),FACTOR(6),YO    380
     1UT(101,3),YINT(51),XDIST(51),SIGMAY(51),YMID(50,3),SIGMAS(50),ZDTR    381
     2(1),WAVE(4),ZBIG(4)                                                   382
      DATA FACTOR/0.825D0,0.85D0,0.875D0,0.90D0,0.925D0,0.95D0/             383
C                                                                           384
C     EXECUTE SPLINE FIT AND VARIANCE ESTIMATE FO MIDPTS FOR EACH LINE:     385
C     TOT SIGMA = SQRT(FIT SIGMA**2+DATA SIGMA**2) DATA SIGMA IS TAKEN      386
C     AS AVERAGE OF SIGMA OF FOUR NEIGHBORING INPUT DATA POINTS EXCEPT      387
C     FOR THE ENDPOINTS WHERE IT IS TAKEN AS THE AVERAGE OF THE ENDPOINT    388
C     SIGMA AND THE TWO  ADJACENT INTERIOR POINT SIGMA VALUES               389
C                                                                           390
      WAVE(LZ)=ZWAVE(LZ)                                                    391
      I=LZ                                                                  392
      CALL READS(NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMAY,LSHIFT,SCHK,    393
     1NFACTR,NS1,ZPNT,KWT)                                                  394
      IWT=KWT                                                               395
      CALL INTERP (NPTS,YINT,XDIST,I,SCHK,YMID,NFACTR,FACTOR)               396
      SIGMAS(1)=YMID(1,3)                                                   397
      SIG=(SIGMAY(1)+SIGMAY(2)+SIGMAY(3))/3.D0                              398
      YMID(1,3)=DSQRT(SIG**2+SIGMAS(1)**2)                                  399
      NPTSS=NPTS-1                                                          400
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```
      DO 10 N=3,NPTSS                                                    401
      J=N-1                                                              402
      JJ=N-2                                                             403
      NN=N+1                                                             404
      SIGMAS(J)=YMID(J,3)                                                405
      SIG=(SIGMAY(JJ)+SIGMAY(J)+SIGMAY(N)+SIGMAY(NN))/4.D0               406
   10 YMID(J,3)=DSQRT(SIGMAS(J)**2+SIG**2)                               407
      N=NPTSS-1                                                          408
      SIGMAS(NPTSS)=YMID(NPTSS,3)                                        409
      SIG=(SIGMAY(N)+SIGMAY(NPTSS)+SIGMAY(NPTS))/3.D0                    410
      YMID(NPTSS,3)=DSQRT(SIG**2+SIGMAS(NPTSS)**2)                       411
      NUP=NPTS+NPTS-1                                                    412
      DO 30 N=1,NUP                                                      413
      NN=(N/2)*2                                                         414
      IF(NN.NE.N) GO TO 25                                               415
      LL=N/2                                                             416
      DO 24 L=1,3                                                        417
   24 YOUT(N,L)=YMID(LL,L)                                               418
      GO TO 30                                                           419
   25 LLL=(N+1)/2                                                        420
      YOUT(N,1)=XDIST(LLL)                                               421
      YOUT(N,2)=YINT(LLL)                                                422
      YOUT(N,3)=SIGMAY(LLL)                                              423
   30 CONTINUE                                                           424
C                                                                        425
CC    CORRECT YOUT FOR ZERO SHIFT                                        426
C                                                                        427
      ITAG=0                                                             428
      IF(LSHIFT.NE.1) GO TO 41                                           429
      JSTART=1                                                           430
      DO 40 J=1,NUP                                                      431
      YOUT(J,1)=YOUT(J,1)-XZERO                                          432
      IF(YOUT(J,1).GE.0.0) GO TO 40                                      433
      JSTART=J+1                                                         434
   40 CONTINUE                                                           435
   41 IF(LSHIFT.NE.1) JSTART=1                                           436
      DO 45 J=JSTART,NUP                                                 437
      ITAG=ITAG+1                                                        438
      ZDIST(ITAG)=YOUT(J,1)                                              439
      ZINT(ITAG)=YOUT(J,2)                                               440
   45 ZSIG(ITAG)=YOUT(J,3)                                               441
      IMA=ITAG                                                           442
C                                                                        443
CC    DETERMINE POSITION OF MAX IN LATERAL INTENSITY ARRAY               444
C                                                                        445
      ZBIG(LZ)=ZDIST(3)                                                  446
      DO 60 J=4,IMA                                                      447
      JJJ=J-1                                                            448
      IF(ZINT(J).GE.ZINT(JJJ)) ZBIG(LZ)=ZDIST(J)                         449
   60 CONTINUE                                                           450
```

```
      IF(LAM-1) 65,65,64                                                    451
   64 WRITE(6,1000)                                                         452
 1000 FORMAT(1H1)                                                           453
   65 WRITE(6,1001) IMA                                                     454
 1001 FORMAT(///14X,'LATERAL INTENSITY DISTRN HAS BEEN FIT BY SEGMENTED    455
     1SPLINE, MIDPOINTS INTERPOLATED, AND SIGMAS DETERMINED',/,14X,'RESU    456
     2LTING LATERAL DATA HAS BEEN ZERO CORRECTED FOR',I3,2X,'POINTS',//T    457
     325,'X',T38,'U(X)',T60,'SIGMA(U(X))',//)                               458
      DO 66 J=1,IMA                                                         459
 1002 FORMAT (T20,F10.4,T33,F10.4,T60,E11.4)                                460
   66 WRITE(6,1002) ZDIST(J),ZINT(J),ZSIG(J)                                461
      ZD=ABS(ZDIST(IMA))                                                    462
      DO 67 J=1,IMA                                                         463
   67 ZDTR(J)=ZDIST(J)/ZD                                                   464
      ZDIV=ABS(ZDTR(2)-ZDTR(1))                                             465
      ZPNT=ZPNT/ZD                                                          466
      RETURN                                                                467
      END                                                                   468
      SUBROUTINE READS (NPTS,YINT,XDIST,ELEMNT,WAVE,XZERO,I,SIGMAY,LSHIF    469
     1T,SCHK,NFACTR,NS1,ZPNT,KWT)                                           470
      IMPLICIT REAL*8(A-H,O-Y)                                              471
      DIMENSION YINT(1),XDIST(1),ELEMNT(5),WAVE(1),SIGMAY(1)                472
C                                                                           473
CC    READ INPUT X,Y PAIRS FOR LINE I                                       474
C                                                                           475
      READ(5,100) NPTS,NS1,ELEMNT,ZPNT,LSHIFT,XZERO,NFACTR,KWT              476
  100 FORMAT(2I5,5X,5A4,F10.0,I5,F10.0,2I5)                                 477
      DO 10 J=1,NPTS                                                        478
  101 FORMAT (3F10.0)                                                       479
   10 READ (5,101) XDIST(J),YINT(J),SIGMAY(J)                               480
      SCHK=XDIST(NPTS)                                                      481
      RETURN                                                                482
      END                                                                   483
      SUBROUTINE INTERP (NPTS,YINT,XDIST,I,SCHK,YMID,NFACTR,FACTOR)         484
      IMPLICIT REAL*8(A-H,O-Z)                                              485
      DIMENSION YHOLD(50,5),XNORM(6),YNORM(6),XMID(5),YSTOR(50,5),YAVE(5    486
     10),COEF(6,4),FACTOR(1),YINT(1),XDIST(1),YMID(50,3),SIGMA(50)          487
C                                                                           488
CC    CALCULATE SPLINE FIT FOR 6 PT INTERVALS BEGINNING AT XDIST(1) AND     489
CC    CONTINUE TO STOP:  TABULATE MIDPOINT DIST, AVE VALUE,AND SIGMA        490
C                                                                           491
      DO 5 J=1,35                                                           492
      YAVE(J)=0.D0                                                          493
    5 SIGMA(J)=0.D0                                                         494
      KOUNT=0                                                               495
      DO 999 J=1,NPTS                                                       496
      JJ=J+5                                                                497
      IF(JJ.GT.NPTS) GO TO 9999                                             498
      IF(XDIST(JJ).LE.SCHK) GO TO 6                                         499
      WRITE (6,888)                                                         500
```

```
  888 FORMAT (//,T25,'********** TRANSFER ERROR IN XDIST(NPTS) TO INTERP    501
     1, END RUN **********')                                               502
      STOP                                                                503
    6 KOUNT=KOUNT+1                                                       504
      HSIZE=1.D0/3.D0                                                     505
      K=J+1                                                               506
      YMID(KOUNT,1)=(XDIST(J)+XDIST(K))/2.D0                              507
      XNORM(1)=-HSIZE                                                     508
      DO 10 L=2,6                                                         509
      XL=L-2                                                              510
   10 XNORM(L)=XL*HSIZE                                                   511
      YNORM(1)=FACTOR(NFACTR)*YINT(KOUNT)                                 512
   11 L=KOUNT                                                             513
      DO 20 LL=2,6                                                        514
      L=L+1                                                               515
   20 YNORM(LL)=YINT(L)                                                   516
      YNORM(6)=FACTOR(NFACTR)*YNORM(6)                                    517
C                                                                         518
CC                                                                        519
C     CALL MATRIX INVERSION ROUTINE TO SOLVE FOR SPLINE COEFFICIENTS AND  520
C     CALCULATE MIDPOINT X VALUES AND SPLINE FIT INTENSITY VALUES         521
C                                                                         522
C                                                                         523
   29 CALL XMATRX(6,YNORM,COEF,I,HSIZE,KOUNT)                             524
      DO 30 LL=2,6                                                        525
      L=LL-1                                                              526
   30 XMID(L)=(XNORM(LL)+XNORM(L))/2.D0                                   527
      CALL CALCY (I,6,COEF,XMID,HSIZE,YHOLD,KOUNT)                        528
      XINC=XDIST(2)-XDIST(1)                                              529
      DO 40 JJ=1,4                                                        530
      JJJ=KOUNT+JJ                                                        531
      XJJ=JJ                                                              532
   40 YMID(JJJ,1)=YMID(KOUNT,1)+(XJJ*XINC)                                533
      DO 50 L=1,5                                                         534
      LL=KOUNT+L-1                                                        535
   50 YAVE(LL)=YAVE(LL)+YHOLD(KOUNT,L)                                    536
C                                                                         537
C     DEFINE STORAGE ARRAY 'YSTOR' FOR SIGMA CALCULATION                  538
C                                                                         539
   85 IF(KOUNT.LT.5) GO TO 100                                            540
      DO 90 N1=1,5                                                        541
      N2=N1-1                                                             542
      N3=KOUNT-N2                                                         543
      YSTOR(KOUNT,N1)=YHOLD(N3,N1)                                        544
   90 CONTINUE                                                            545
      KN=NPTS-5                                                           546
      IF(KOUNT.LT.KN) GO TO 999                                           547
      DO 91 N1=1,4                                                        548
      N2=KOUNT+N1                                                         549
      NN=N1+1                                                             550
```

```
      DO 91 NNN=NN,5                                                    551
      N3=NNN-N1                                                         552
      N4=KOUNT+1-N3                                                     553
   91 YSTOR(N2,N3)=YHOLD(N4,NNN)                                        554
      GO TO 999                                                         555
  100 IF(KOUNT.GT.1) GO TO 101                                          556
      YSTOR(1,1)=YHOLD(1,1)                                             557
      GO TO 999                                                         558
  101 DO 102 N1=1,KOUNT                                                 559
      N2=N1-1                                                           560
      N3=KOUNT-N2                                                       561
  102 YSTOR(KOUNT,N1)=YHOLD(N3,N1)                                      562
  999 CONTINUE                                                          563
C                                                                       564
C     CALCULATE SIGMA AND STORE 'YAVE' AND 'SIGMA' IN 'YMID' AS         565
C     YMID(J,2) AND YMID(J,3), RESPECTIVELY                             566
C                                                                       567
 9999 J=NPTS-1                                                          568
      DO 70 JJ=1,J                                                      569
      IF(JJ.LT.5) GO TO 57                                              570
      KK=NPTS-5                                                         571
      IF(JJ.GT.KK) GO TO 65                                             572
      YMID(JJ,2)=YAVE(JJ)/5.D0                                          573
      DO 56 II=1,5                                                      574
   56 SIGMA(JJ)=(YSTOR(JJ,II)-YMID(JJ,2))**2                            575
      SIGMA(JJ)=DSQRT(SIGMA(JJ)/4.D0)                                   576
      YMID(JJ,3)=SIGMA(JJ)                                              577
      GO TO 70                                                          578
   57 XJJ=JJ                                                            579
      YMID(JJ,2)=YAVE(JJ)/XJJ                                           580
      IF(JJ.GT.1) GO TO 58                                              581
      YMID(JJ,3)=0.D0                                                   582
      GO TO 70                                                          583
   58 DO 59 II=1,JJ                                                     584
   59 SIGMA(JJ)=(YSTOR(JJ,II)-YMID(JJ,2))**2                            585
      XII=XJJ-1.D0                                                      586
      SIGMA(JJ)=DSQRT(SIGMA(JJ)/XII)                                    587
      YMID(JJ,3)=SIGMA(JJ)                                              588
      GO TO 70                                                          589
   65 XKK=NPTS-JJ                                                       590
      YMID(JJ,2)=YAVE(JJ)/XKK                                           591
      IF(JJ.LT.J) GO TO 66                                              592
      YMID(JJ,3)=0.D0                                                   593
      GO TO 70                                                          594
   66 III=NPTS-JJ                                                       595
      DO 67 II=1,III                                                    596
   67 SIGMA(JJ)=(YSTOR(JJ,II)-YMID(JJ,2))**2                            597
      XII=III-1                                                         598
      SIGMA(JJ)=DSQRT(SIGMA(JJ)/XII)                                    599
      YMID(JJ,3)=SIGMA(JJ)                                              600
```

```
   70 CONTINUE                                                          601
      RETURN                                                            602
      END                                                               603
      SUBROUTINE XMATRX(NPTS,YINT,COEF,I,HSIZE,KOUNT)                   604
      IMPLICIT REAL*8(A-H,O-Z)                                          605
      DIMENSION YINT(6),S(6,6),COEF(6,4),SCALC(6,6),SOUT(36),YCAL(6)    606
C                                                                       607
C     DETERMINE COEFS OF SPLINE FIT WITH FORTRAN SSP ROUTINE 'DGELG' AND 608
C     RETURN TO INTERP AS 'COEF'                                        609
C                                                                       610
      DO 10 M=1,NPTS                                                    611
      DO 10 L=1,NPTS                                                    612
      K=M-L                                                             613
      J=L-M                                                             614
      IF(K.EQ.1) GO TO 8                                                615
      IF(J.EQ.1) GO TO 8                                                616
      IF(L.EQ.M) GO TO 9                                                617
      S(M,L)=0.D0                                                       618
      GO TO 10                                                          619
    8 S(M,L)=0.25D0                                                     620
      GO TO 10                                                          621
    9 S(M,L)=1.D0                                                       622
   10 CONTINUE                                                          623
      DO 15 J=1,NPTS                                                    624
      DO 15 K=1,NPTS                                                    625
   15 SCALC(J,K)=S(J,K)                                                 626
      DO 16 J=1,NPTS                                                    627
   16 YCAL(J)=YINT(J)                                                   628
      IF(NPTS.EQ.6) GO TO 25                                            629
      IX=0                                                              630
      DO 17 L=1,NPTS                                                    631
      DO 17 K=1,NPTS                                                    632
      IX=IX+1                                                           633
   17 SOUT(IX)=SCALC(K,L)                                               634
      GO TO 26                                                          635
   25 CALL DGELG (YCAL,SCALC,6,1,1.0E-16,IER)                           636
      GO TO 27                                                          637
   26 CALL DGELG (YCAL,SOUT,NPTS,1,1.0E-16,IER)                         638
   27 CONTINUE                                                          639
      DO 30 K=1,NPTS                                                    640
   30 COEF(K,I)=YCAL(K)                                                 641
      IF(IER.NE.0) GO TO 99999                                          642
      RETURN                                                            643
99999 WRITE(6,2000) IER,KOUNT                                           644
 2000 FORMAT(/////,T15,'***** IER =',I3,2X,'KOUNT =',I4)                645
      RETURN                                                            646
      END                                                               647
      SUBROUTINE CALCY (I,NPTS,COEF,XMID,HSIZE,YHOLD,KOUNT)             648
      IMPLICIT REAL*8(A-H,O-Z)                                          649
      DIMENSION X(5),F(5),COEF(6,4),XMID(5),YHOLD(50,5)                 650
```

```
C                                                                       651
C     CALCULATE MIDPOINT INTERPOLATED VALUES AND RETURN TO 'INTERP' AS  652
C     ARRAY 'YHOLD'                                                     653
C                                                                       654
      DO 10 J=1,5                                                       655
   10 X(J)=XMID(J)                                                      656
      DO 20 J=1,5                                                       657
      F(J)=0.D0                                                         658
      DO 15 K=1,NPTS                                                    659
      XK=K                                                              660
      X1=X(J)-((XK-2.D0)*HSIZE)                                         661
      HL=-2.D0*HSIZE                                                    662
      HU=2.D0*HSIZE                                                     663
      IF(X1.GE.HL) GO TO 11                                             664
      F(J)=F(J)+0.D0                                                    665
      GO TO 15                                                          666
   11 H=-HSIZE                                                          667
      IF(X1.GT.H) GO TO 12                                              668
      F(J)=F(J)+(((X1+(2.D0*HSIZE))**3.D0)/(4.D0*(HSIZE**3.D0))*COEF(K,I 669
     1))                                                                670
      GO TO 15                                                          671
   12 IF(X1.GT.0.D0) GO TO 13                                           672
      TERM=(HSIZE**3.D0)+((3.D0*(HSIZE**2.D0))*(X1+HSIZE))+((3.D0*HSIZE) 673
     1*((X1+HSIZE)**2.D0))-(3.D0*((X1+HSIZE)**3.D0))                    674
      TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)                        675
      F(J)=F(J)+TERM                                                    676
      GO TO 15                                                          677
   13 IF(X1.GT.HSIZE) GO TO 14                                          678
      TERM=(HSIZE**3.D0)+((3.D0*(HSIZE**2.D0))*(HSIZE-X1))+((3.D0*HSIZE) 679
     1*((HSIZE-X1)**2.D0))-(3.D0*((HSIZE-X1)**3.D0))                    680
      TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)                        681
      F(J)=F(J)+TERM                                                    682
      GO TO 15                                                          683
   14 IF(X1.GT.HU) GO TO 16                                             684
      TERM=((2.D0*HSIZE)-X1)**3.D0                                      685
      TERM=(TERM/(4.D0*(HSIZE**3.D0)))*COEF(K,I)                        686
      F(J)=F(J)+TERM                                                    687
      GO TO 15                                                          688
   16 F(J)=F(J)+0.D0                                                    689
   15 CONTINUE                                                          690
   20 CONTINUE                                                          691
      DO 40 N=1,5                                                       692
   40 YHOLD(KOUNT,N)=F(N)                                               693
      RETURN                                                            694
      END                                                               695
      SUBROUTINE DKABEL (XDTR,YINT,IMA,NS1,NZ,XPNT,RAD,RDI,KT,XD,XBIG,LZ 696
     1,DELIR,SIGMAY,L1,IWT)                                             697
      DIMENSION XDTR(1),YINT(1),RAD(1),RDI(1),XBIG(1),DELIR(1),SEGEND(5) 698
     1,SIGMAY(1),COEF(5,5),DELCOF(5,5),RA(2),XA(51),YA(51),YCHECK(51,5), 699
     2DIFY(51),PERCNT(51),AVEPCT(12),STDDEV(5),DEVAVE(5),YC(51,5),NTAG(5 700
```

```
     3),RDST(5)                                                          701
      DATA NTAG/0.0,0.0,0.0/                                             702
      DATA RDST/1.0,1.0,1.0,1.0,1.0/                                     703
      WRITE (6,1000)                                                     704
 1000 FORMAT (/////,T2,'INPUT DATA TRANSFERRED TO DKABEL')               705
      WRITE (6,1001)                                                     706
 1001 FORMAT (/,T4,"IDEX",T25,'XDTR',T50,'YINT')                         707
      DO 100 IDEX=1,IMA                                                  708
 1002 FORMAT (/,T6,I2,T20,E11.4,T45,E11.4)                               709
  100 WRITE (6,1002) IDEX,XDTR(IDEX),YINT(IDEX)                          710
      DO 5 J=1,5                                                         711
      SEGEND(J)=0.0                                                      712
      DO 5 I=1,5                                                         713
      COEF(I,J)=0.0                                                      714
    5 DELCOF(I,J)=0.0                                                    715
C                                                                        716
C     SET  UP ZONE SEGMENTS FOR POLY FIT (3 TO 5 ZONES)                  717
C                                                                        718
      NSEGS=NS1                                                          719
      XBIG(LZ)=XBIG(LZ)/XD                                               720
      IF(NSEGS-4) 10,25,29                                               721
   10 CHECK=XBIG(LZ)-0.3333333                                           722
      CHECK=ABS(CHECK)                                                   723
      IF(CHECK.GT.0.100) GO TO 12                                        724
      IF(XBIG(LZ)-0.3333333) 11,11,12                                    725
   11 SEGEND(1)=0.450                                                    726
      SEGEND(2)=0.750                                                    727
      SEGEND(3)=1.000                                                    728
      NSEGS=3                                                            729
      GO TO 30                                                           730
   12 CHECK=XBIG(LZ)-0.6666667                                           731
      CHECK=ABS(CHECK)                                                   732
      IF(CHECK.GT.0.100) GO TO 14                                        733
      IF(XBIG(LZ)-0.6666667) 13,13,14                                    734
   13 SEGEND(1)=0.350                                                    735
      SEGEND(2)=0.750                                                    736
      SEGEND(3)=1.000                                                    737
      NSEGS=3                                                            738
      GO TO 30                                                           739
   14 IF(XBIG(LZ)-0.2333333) 15,15,16                                    740
   15 SEGEND(1)=0.3333333                                                741
      SEGEND(2)=0.6666667                                                742
      SEGEND(3)=1.0000000                                                743
      NSEGS=3                                                            744
      GO TO 30                                                           745
   16 IF(XBIG(LZ)-0.6666667) 17,19,19                                    746
   17 IF(XBIG(LZ)-0.4333333) 18,18,19                                    747
   18 SEGEND(1)=0.250                                                    748
      SEGEND(2)=0.650                                                    749
      SEGEND(3)=1.000                                                    750
```

```
      NSEGS=3                                                                751
      GO TO 30                                                               752
   19 IF(XBIG(LZ)-0.7666667) 20,20,21                                        753
   20 SEGEND(1)=0.300                                                        754
      SEGEND(2)=0.550                                                        755
      SEGEND(3)=1.000                                                        756
      NSEGS=3                                                                757
      GO TO 30                                                               758
   21 SEGEND(1)=0.3333333                                                    759
      SEGEND(2)=0.6666667                                                    760
      SEGEND(3)=1.0000000                                                    761
      NSEGS=3                                                                762
      GO TO 30                                                               763
   25 SEGEND(1)=0.250                                                        764
      SEGEND(2)=0.500                                                        765
      SEGEND(3)=0.750                                                        766
      SEGEND(4)=1.000                                                        767
      NSEGS=4                                                                768
      GO TO 30                                                               769
   29 NSEGS=5                                                                770
      SEGEND(1)=0.2                                                          771
      SEGEND(2)=0.4                                                          772
      SEGEND(3)=0.6                                                          773
      SEGEND(4)=0.8                                                          774
      SEGEND(5)=1.0                                                          775
   30 CONTINUE                                                               776
C                                                                            777
C     CALL ROUTINE SEGMNT FOR ZONE COEFS AND SIGMA VALUES                    778
C                                                                            779
      CALL SEGMNT (XDTR,YINT,IMA,NS1,NSEGS,NZ,COEF,DELCOF,SEGEND,SIGMAY,     780
     1NTAG,IWT)                                                              781
      DO 35 I=1,IMA                                                          782
      XA(I)=XDTR(I)                                                          783
   35 YA(I)=YINT(I)                                                          784
C                                                                            785
C     COMPARE CALCULATED TO INPUT Y VALUES FOR EACH ZONE                     786
C                                                                            787
      WRITE (6,2000)                                                         788
 2000 FORMAT (/////,T10,'REGION',T22,'DIST',T33,'CALCY',T45,'REALY',T56,     789
     1'DIFF',T73,'PERCENT',T88,'AVE PERCENT',T102,'WEIGHTED STD DEV')        790
      IMS1=NTAG(1)                                                           791
      NSEG=NSEGS                                                             792
      IZONE=1                                                                793
      SUMPCT=0.0                                                             794
      SUMERR=0.0                                                             795
      AVEDEV=0.0                                                             796
      YSUM=0.0                                                               797
      DO 75 I=1,IMS1                                                         798
      XCHEC2=XA(I)*XA(I)                                                     799
      XCHEC4=XCHEC2*XCHEC2                                                   800
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      XCHEC6=XCHEC4*XCHEC2                                                      801
      XCHEC8=XCHEC6*XCHEC2                                                      802
      YCHECK(I,1)=COEF(1,1)+(COEF(2,1)*XCHEC2)+(COEF(3,1)*XCHEC4)+(COEF(        803
     14,1)*XCHEC6)+(COEF(5,1)*XCHEC8)                                           804
      DIFY(I)=YA(I)-YCHECK(I,1)                                                 805
      PERCNT(I)=(DIFY(I)*100.)/YA(I)                                            806
      PERCNT(I)=ABS(PERCNT(I))                                                  807
      SUMPCT=SUMPCT+PERCNT(I)                                                   808
      SUMERR=SUMERR+(DIFY(I)*DIFY(I)/YA(I))                                     809
      AVEDEV=AVEDEV+(DIFY(I)*DIFY(I))                                           810
      YSUM=YSUM+YA(I)                                                           811
      IF(I.NE.IMS1) GO TO 74                                                    812
      XI=I                                                                      813
      AVEPCT(1)=SUMPCT/XI                                                       814
      STDDEV(1)=SQRT(SUMERR/(XI-1.0))                                           815
      DEVAVE(1)=SQRT(AVEDEV/(XI-1.0))/(YSUM/XI)                                 816
      WRITE (6,3000) IZONE,XA(I),YCHECK(I,1),YA(I),DIFY(I),PERCNT(I),AVE        817
     1PCT(1),STDDEV(1),DEVAVE(1)                                                818
3000 FORMAT (T12,I2,T20,F8.4,T32,F8.4,T44,F8.4,T54,E11.4,T72,E11.4,T87,        819
     1E11.4,T105,E11.4,T117,E11.4)                                              820
      GO TO 75                                                                  821
   74 WRITE(6,2001) IZONE ,XA(I),YCHECK(I,1),YA(I),DIFY(I),PERCNT(I)            822
2001 FORMAT (T12,I2,T20,F8.4,T32,F8.4,T44,F8.4,T54,E11.4,T72,E11.4)             823
   75 CONTINUE                                                                  824
      DO 80 J=2,NSEG                                                            825
      NHOLD=0                                                                   826
      JJ=J-1                                                                    827
      N1=NTAG(JJ)+1                                                             828
      N2=NTAG(J)                                                                829
      SUMPCT=0.0                                                                830
      SUMERR=0.0                                                                831
      AVEDEV=0.0                                                                832
      YSUM=0.0                                                                  833
      IF (J.NE.NSEG) GO TO 78                                                   834
      N2=IMA                                                                    835
   78 DO 79 K=N1,N2                                                             836
   76 XCHEC1=XA(K)                                                              837
      XCHEC2=XA(K)*XA(K)                                                        838
      XCHEC3=XCHEC2*XA(K)                                                       839
      XCHEC4=XCHEC3*XA(K)                                                       840
   77 YCHECK(K,J)=COEF(1,J)+(COEF(2,J)*XCHEC1)+(COEF(3,J)*XCHEC2)+(COEF(        841
     14,J)*XCHEC3)+(COEF(5,J)*XCHEC4)                                           842
      DIFY(K)=YA(K)-YCHECK(K,J)                                                 843
      DIFYI=DIFY(K)*DIFY(K)                                                     844
      IF (YA(K).EQ.0.0) GO TO 200                                               845
      PERCNT(K)=ABS((DIFY(K)*100.)/YA(K))                                       846
      DIF2=DIFY(K)*DIFY(K)/YA(K)                                                847
      GO TO 201                                                                 848
  200 PERCNT(K)=0.0                                                             849
      DIF2=DIFY(K)*DIFY(K)                                                      850
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      NHOLD=NHOLD+1                                                     851
  201 SUMPCT=SUMPCT+PERCNT(K)                                           852
      AVEDEV=AVEDEV+DIFYI                                               853
      YSUM=YSUM+YA(K)                                                   854
      SUMERR=SUMERR+DIF2                                                855
      IF(K.NE.N2) GO TO 202                                             856
      XK=N2-N1+1-NHOLD                                                  857
      AVEPCT(J)=SUMPCT/XK                                               858
      XFREE=N2-N1                                                       859
      IF(XFREE.LE.0.0) XFREE=1.0                                        860
      STDDEV(J)=SQRT(SUMERR/XFREE)                                      861
      DEVAVE(J)=SQRT(AVEDEV/XFREE)/(YSUM/(XFREE+1.0))                   862
      WRITE (6,3001) J,XA(K),YCHECK(K,J),YA(K),DIFY(K),PERCNT(K),AVEPCT(863
     1J),STDDEV(J),DEVAVE(J)                                            864
 3001 FORMAT (T12,I2,T20,F8.4,T32,F8.4,T44,F8.4,T54,E11.4,T72,E11.4,T87,865
     1E11.4,T105,E11.4,T117,E11.4)                                      866
      GO TO 79                                                          867
  202 WRITE (6,2002) J,XA(K),YCHECK(K,J),YA(K),DIFY(K),PERCNT(K)        868
 2002 FORMAT (T12,I2,T20,F8.4,T32,F8.4,T44,F8.4,T54,E11.4,T72,E11.4)    869
   79 CONTINUE                                                          870
   80 CONTINUE                                                          871
      WRITE (6,3999)                                                    872
 3999 FORMAT (/////,T10,'WEIGHTED STD DEV DEFINED AS:',/,T15,'SQUARE ROO873
     1T OF:  (SUM(DIFF**2/REALY))/(NUM PTS IN ZONE - 1)',///,T10,'LAST C874
     2OLUMN:  (SQRT(SUM(DIFF**2/(NPTS-1)))/(MEAN VALUE REALY FOR ZONE)')875
      WRITE (6,4000)                                                    876
 4000 FORMAT (/////,T10,'REGION',T22,'DIST',T33,'CALCY')                877
      IZ=1                                                              878
      DO 49 I=2,IMS1                                                    879
      J=I-1                                                             880
      XAVE=(XA(I)+XA(J))/2.                                             881
      XC2=XAVE*XAVE                                                     882
      XC4=XC2*XC2                                                       883
      XC6=XC4*XC2                                                       884
      XC8=XC6*XC2                                                       885
      YC(J,1)=COEF(1,1)+(COEF(2,1)*XC2)+(COEF(3,1)*XC4)+(COEF(4,1)*XC6)+886
     1(COEF(5,1)*XC8)                                                   887
      WRITE (6,4001) IZ,XAVE,YC(J,1)                                    888
 4001 FORMAT (T12,I2,T20,F8.4,T32,F8.4)                                 889
   49 CONTINUE                                                          890
      DO 48 J=2,NSEG                                                    891
      JJ=J-1                                                            892
      N1=NTAG(JJ)+2                                                     893
      N2=NTAG(J)                                                        894
      IF(J.NE.NSEG) GO TO 46                                            895
      N2=IMA                                                            896
   46 DO 47 K=N1,N2                                                     897
      K2=K-1                                                            898
      XAVE=(XA(K)+XA(K2))/2.                                            899
      XC1=XAVE                                                          900
```

```
      XC2=XAVE*XAVE                                                          901
      XC3=XC2*XAVE                                                           902
      XC4=XC3*XAVE                                                           903
      YC(K2,J)=COEF(1,J)+(COEF(2,J)*XC1)+(COEF(3,J)*XC2)+(COEF(4,J)*XC3)     904
     1+(COEF(5,J)*XC4)                                                       905
      WRITE (6,4002) J,XAVE,YC(K2,J)                                         906
 4002 FORMAT (T12,I2,T20,F8.4,T32,F8.4)                                      907
   47 CONTINUE                                                               908
   48 CONTINUE                                                               909
C                                                                            910
CC    CALCULATE RADIAL INTENSITY VALUES BASED ON POLY FIT                    911
C                                                                            912
  500 RM=0.0                                                                 913
      X=SEGEND(1)                                                            914
      X3=X**3                                                                915
      X5=X**5                                                                916
      X7=X**7                                                                917
      RA1=COEF(2,1)*X+2.*COEF(3,1)*X3/3.+3.*COEF(4,1)*X5/5.+4.*COEF(5,1)     918
     1*X7/7.                                                                 919
      RA2=-2.*RA1/3.141593                                                   920
      DO 521 J=2,NSEGS                                                       921
      I=1                                                                    922
      XLC=SEGEND(J)                                                          923
  518 RA(I)=COEF(2,J)*ALOG(XLC)+2.*COEF(3,J)*XLC+3.*COEF(4,J)*XLC*XLC/2.     924
     1+4.*COEF(5,J)*XLC*XLC*XLC/3.                                           925
      GO TO (519,520),I                                                      926
  519 I=2                                                                    927
      XLC=SEGEND(J-1)                                                        928
      GO TO 518                                                              929
  520 RM1=-(RA(1)-RA(2))/3.141593                                            930
      RM=RM1+RM                                                              931
  521 CONTINUE                                                               932
      RAD(1)=RA2+RM                                                          933
      RDI(1)=0.0                                                             934
      KT=1                                                                   935
      R=0.0                                                                  936
      LC=1                                                                   937
  550 R=R+XPNT                                                               938
      IF(R.GT.SEGEND(NSEGS)) GO TO 600                                       939
      IF(R.GT.SEGEND(LC)) LC=LC+1                                            940
      KT=KT+1                                                                941
      RDI(KT)=R                                                              942
      RM=0.0                                                                 943
      R2=R*R                                                                 944
      GO TO (575,555,555,555,555),LC                                         945
  555 X=SEGEND(LC)                                                           946
      X2=X*X                                                                 947
      B=SQRT(X2-R2)                                                          948
      B3=B*B*B                                                               949
  556 RA1=COEF(2,LC)*ALOG((X+B)/R)+2.*COEF(3,LC)*B+3./2.*COEF(4,LC)*(X*B     950
```

```
     1+R2*ALOG((X+B)/R))+4.*COEF(5,LC)*(B3/3.+R2*B)                          951
      RA2=-RA1/3.141593                                                     952
      IF(LC.LT.NSEGS) GO TO 557                                             953
      RAD(KT)=RA2+RM                                                        954
      GO TO 550                                                             955
  557 LCUP=LC+1                                                             956
      RM=0.0                                                                957
      DO 565 J=LCUP,NSEGS                                                   958
      I=1                                                                   959
      XLC=SEGEND(J)                                                         960
  558 X2LC=XLC*XLC                                                          961
      A=SQRT(X2LC-R2)                                                       962
      A3=A*A*A                                                              963
      RA(I)=COEF(2,J)*ALOG(XLC+A)+2.*COEF(3,J)*A+3./2.*COEF(4,J)*(XLC*A+    964
     1R2*ALOG(XLC+A))+4.*COEF(5,J)*(A3/3.+R2*A)                             965
      GO TO (559,560),I                                                     966
  559 I=2                                                                   967
      XLC=SEGEND(J-1)                                                       968
      GO TO 558                                                             969
  560 RM1=-(RA(1)-RA(2))/3.141593                                           970
      RM=RM1+RM                                                             971
  565 CONTINUE                                                              972
      RAD(KT)=RA2+RM                                                        973
      GO TO 550                                                             974
  575 X=SEGEND(1)                                                           975
      X2=X*X                                                                976
      B=SQRT(X2-R2)                                                         977
      R4=R2*R2                                                              978
      R6=R2*R4                                                              979
      B2=B*B                                                                980
      B3=B2*B                                                               981
      B5=B2*B3                                                              982
      B7=B2*B5                                                              983
      RA1=2.*COEF(2,1)*B+4.*COEF(3,1)*(B3/3.+R2*B)+6.*COEF(4,1)*(R4*B+2.    984
     1*R2*B3/3.+B5/5.)+8.*COEF(5,1)*(R6*B+R4*B3+3.*R2*B5/5.+B7/7.)          985
      RA2=-RA1/3.141593                                                     986
      GO TO 557                                                             987
  600 DO 610 I=1,KT                                                         988
  610 RDI(I)=RDI(I)*XD                                                      989
      WRITE (6,5002) NSEGS,NSEGS,(SEGEND(I),I=1,NSEGS)                      990
 5002 FORMAT (///,T5,'ZONE DIVISIONS FOR',I3,2X,'SEGMENTS',//,T5,'REGION    991
     1(1)-----REGION(',I1,')= ',5(E11.4,5X))                                992
C                                                                           993
C     CALCULATE SIGMA VALUES FOR RADIAL INTENSITIES                         994
C                                                                           995
      DO 66 I=1,NSEGS                                                       996
   66 RDST(I)=SEGEND(I)                                                     997
      DO 67 I1=1,KT                                                         998
   67 RDI(I1)=RDI(I1)/XD                                                    999
      DO 90 I=1,KT                                                          1000
```

```
      IF(RDI(I).GT.RDST(1)) GO TO 82                                    1001
      G=SQRT(RDST(1)**2.-RDI(I)**2.)                                    1002
      DEL1=(2.*ABS(G)*DELCOF(2,1))+(4.*ABS(((G**3.)/3.)+((RDI(I)**2.)*G)1003
     1)*DELCOF(3,1))+(6.*ABS(((RDI(I)**4.)*G)+((2./3.)*(RDI(I)**2.)*(G**1004
     23.))+((1./5.)*(G**5.)))*DELCOF(4,1))+(8.*ABS(((RDI(I)**6.)*G)+((RD1005
     3I(I)**4.)*(G**3.))+((3./5.)*(RDI(I)**2.)*(G**5.))+((1./7.)*(G**7.)1006
     4))*DELCOF(5,1))                                                   1007
      DEL2=0.0                                                          1008
      DO 89 J=2,NSEGS                                                   1009
      K=J-1                                                             1010
      GJ=SQRT(RDST(J)**2.-RDI(I)**2.)                                   1011
      GK=SQRT(RDST(K)**2.-RDI(I)**2.)                                   1012
      ADD=(ABS(ALOG((RDST(J)+GJ)/(RDST(K)+GK)))*DELCOF(2,J))+(2.*ABS(GJ-1013
     1GK)*DELCOF(3,J))+(1.5*ABS((RDST(J)*GJ)-(RDST(K)*GK)+((RDI(I)**2.)*1014
     2ALOG((RDST(J)+GJ)/(RDST(K)+GK))))*DELCOF(4,J))+(4.*ABS(((GJ**3.)/31015
     3.)-((GK**3.)/3.)+((RDI(I)**2.)*(GJ-GK)))*DELCOF(5,J))             1016
   89 DEL2=DEL2+ADD                                                     1017
      DELIR(I)=((DEL1+DEL2)/3.141593)*100.0                             1018
      DELIR(I)=DELIR(I)/RAD(I)                                          1019
      GO TO 90                                                          1020
   82 IF(RDI(I).LE.RDST(2)) L=2                                         1021
      IF(RDI(I).LE.RDST(3)) L=3                                         1022
      IF(RDI(I).LE.RDST(4)) L=4                                         1023
      IF(RDI(I).LE.RDST(5)) L=5                                         1024
      IF(RDI(I).GT.RDST(5)) GO TO 92                                    1025
      G=SQRT(RDST(L)**2.-RDI(I)**2.)                                    1026
      RDI2=RDI(I)*RDI(I)                                                1027
      XTMLOG=ALOG((RDST(L)+G)/RDI(I))                                   1028
      DEL1=(ABS(XTMLOG)*DELCOF(2,L))+(2.*ABS(G)*DE_COF(3,L))+(1.5*ABS((R1029
     1DST(L)*G)+(RDI2*XTMLOG))*DELCOF(4,L))+(4.*ABS(((G**3.)/3.)+(RDI2*G1030
     2))*DELCOF(5,L))                                                   1031
      IF(L.LT.NSEGS) GO TO 87                                           1032
      DELIR(I)=(DEL1/3.141593)*100.0                                    1033
      DIFRNC=RAD(I)-0.0                                                 1034
      ABDIF=ABS(DIFRNC)                                                 1035
      IF(ABDIF.LT.0.0000001) GO TO 90                                   1036
      DELIR(I)=DELIR(I)/RAD(I)                                          1037
      GO TO 90                                                          1038
   87 N1=L+1                                                            1039
      DEL2=0.0                                                          1040
      DO 88 M=N1,NSEGS                                                  1041
      N=M-1                                                             1042
      GM=SQRT(RDST(M)**2.-RDI(I)**2.)                                   1043
      GN=SQRT(RDST(N)**2.-RDI(I)**2.)                                   1044
      ADD=(ABS(ALOG((RDST(M)+GM)/(RDST(N)+GN)))*DELCOF(2,M))+(2.*ABS(GM-1045
     1GN)*DELCOF(3,M))+(1.5*ABS((RDST(M)*GM)-(RDST(N)*GN)+((RDI(I)**2.)*1046
     2ALOG((RDST(M)+GM)/(RDST(N)+GN))))*DELCOF(4,M))+(4.*ABS(((GM**3.)/31047
     3.)-((GN**3.)/3.)+((RDI(I)**2.)*(GN-GN)))*DELCOF(5,M))             1048
   88 DELI=DEL2+ADD                                                     1049
      DELIR(I)=((DEL1+DEL2)/3.141593)*100.0                             1050
```

```
      DELIR(I)=DELIR(I)/RAD(I)                                          1051
   90 CONTINUE                                                          1052
      IF(I.EQ.KT) GO TO 93                                              1053
   92 KT=I-1                                                            1054
   93 DO 91 I2=1,KT                                                     1055
   91 RDI(I2)=RDI(I2)*XD                                                1056
      SUMR=0.                                                           1057
      WRITE (6,6000)                                                    1058
 6000 FORMAT (/////,T29,'I',T45,'RDI(I)',T67,'RAD(I)',T83,'DELTA RAD IN  1059
     1PERCENT')                                                         1060
      DO 23 K=1,KT                                                      1061
  101 FORMAT (27X,I3,2(12X,E11.4),T90,E11.4)                            1062
      SUMR=SUMR+RAD(K)                                                  1063
   23 WRITE (6,101) K,RDI(K),RAD(K),DELIR(K)                            1064
      WRITE (6,102) SUMR                                                1065
  102 FORMAT (///,T80,'SUM RAD = ',2X,E11.4)                            1066
      WRITE (6,5000)                                                    1067
 5000 FORMAT (/////,T10,'J',T15,'I',T30,'DELCOF(I,J)')                  1068
      DO 28 J=1,NSEG                                                    1069
      DO 28 I=2,5                                                       1070
 5001 FORMAT (T9,I2,T14,I2,T30,E11.4)                                   1071
   28 WRITE (6,5001) J,I,DELCOF(I,J)                                    1072
      IF (L1.EQ.2) GO TO 300                                            1073
      DO 299 NABS=1,KT                                                  1074
  299 RAD(NABS)=ABS(RAD(NABS))                                          1075
  300 RETURN                                                            1076
      END                                                               1077
      SUBROUTINE SEGMNT (XA,YA,IMA,NS1,NSEGS,NZ,COEF,DELCOF,SEG,SIGA,NTA 1078
     1G,IWT)                                                            1079
      DIMENSION RELCOF(5,5),SRELC(5,5),FTEST5(5),FTEST6(5),FTEST7(5)    1080
      DIMENSION XA(1),YA(1),COEF(5,5),DELCOF(5,5),SEG(1),SIGA(1),PERCT(7 1081
     1),FTEST1(5),FTEST2(5),FTEST3(5),FTEST4(5),NTAG(5),XSTOR(11,5),YSTO 1082
     2R(11,5),SSTOR(11,5),XFIT(35),YFIT(35),SFIT(35),FTEST(5),YCALC(35), 1083
     3REALC(5),SIGMAC(5),RELC(5),SIGMAR(5),CHISQR(5)                    1084
      DATA FTEST1/16200.0,198.0,55.6,31.3,22.8/,FTEST2/4050.0,98.5,34.1, 1085
     121.2,16.3/,FTEST3/648.0,38.5,17.4,12.2,10.0/,FTEST4/161.0,18.5,10. 1086
     21,7.71,6.61/,PERCT/0.5,1.0,2.5,5.0,10.0,25.0,50.0/                1087
      DATA FTEST5/39.9,8.53,5.54,4.54,4.06/,FTEST6/5.83,2.57,2.02,1.81,1 1088
     1.69/,FTEST7/1.00,0.667,0.585,0.549,0.528/                         1089
      GO TO (1,3,5,7,11,21,31),NZ                                       1090
    1 DO 2 I=1,5                                                        1091
    2 FTEST(I)=FTEST1(I)                                                1092
      GO TO 9                                                           1093
    3 DO 4 I=1,5                                                        1094
    4 FTEST(I)=FTEST2(I)                                                1095
      GO TO 9                                                           1096
    5 DO 6 I=1,5                                                        1097
    6 FTEST(I)=FTEST3(I)                                                1098
      GO TO 9                                                           1099
    7 DO 8 I=1,5                                                        1100
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    8 FTEST(I)=FTEST4(I)                                                    1101
      GO TO 9                                                               1102
   11 DO 12 I=1,5                                                           1103
   12 FTEST(I)=FTEST5(I)                                                    1104
      GO TO 9                                                               1105
   21 DO 22 I=1,5                                                           1106
   22 FTEST(I)=FTEST6(I)                                                    1107
      GO TO 9                                                               1108
   31 DO 32 I=1,5                                                           1109
   32 FTEST(I)=FTEST7(I)                                                    1110
    9 WRITE (6,1000) PERCT(NZ),NSEGS                                        1111
 1000 FORMAT (1H1,T15,'RADIAL INTENSITY DISTRIBUTION CALCULATION',//,T15    1112
     1,'ABEL INVERSION UTILIZING WEIGHTED LEAST-SQUARES POLYNOMIAL FITTI     1113
     2NG OF THE LATERAL INTENSITY DISTRIBUTION',/,T20,'F-TEST FOR SIGNIF     1114
     3ICANCE OF ADDED COEFFICIENT FOR',F6.2,2X,'PERCENT PROBABILITY OF E     1115
     4XCEEDING THE F-VALUE',//,T25,"THE LATERAL I(X) PROFILE HAS BEEN DI     1116
     5VIDED INTO',I3,2X,'ZONES')                                            1117
      WRITE (6,1001)                                                        1118
 1001 FORMAT (/////,T15,'ZONE DIVISIONS ON REDUCED RADIUS SCALE',/,T15,'    1119
     1ZONE NUMBER',T35,'DISTANCE')                                          1120
      DO 10 I=1,NSEGS                                                       1121
 1002 FORMAT (T20,I2,T32,E14.7)                                             1122
   10 WRITE (6,1002) I,SEG(I)                                               1123
      WRITE (6,2000) (FTEST(I),I=1,5)                                       1124
 2000 FORMAT (//,T15,'FTEST(1)---FTEST(5)=',5(2X,E13.6))                    1125
      WRITE (6,1003)                                                        1126
 1003 FORMAT (///,T20,'THE FOLLOWING COEFFICIENTS WERE OBTAINED',//,T27,    1127
     1'POLY',5X,'Y',5X,'=',6X,'A',6X,'+',5X,'B*X',5X,'+',6X,'C*X**2',4X,    1128
     2'+',4X,'D*X**3',4X,'+',4X,'E*X**4',//,T20,'REGION',2X,'DEG',19X,'A    1129
     3',14X,'B',14X,'C',14X,'D',14X,'E',///)                                1130
      DO 15 J=1,NSEGS                                                       1131
      DO 15 I=1,IMA                                                         1132
      IF(XA(I).GT.SEG(J)) GO TO 15                                          1133
      NTAG(J)=I                                                             1134
   15 CONTINUE                                                              1135
      N1=NTAG(1)                                                            1136
      DO 20 I=1,N1                                                          1137
      XSTOR(I,1)=XA(I)                                                      1138
      YSTOR(I,1)=YA(I)                                                      1139
   20 SSTOR(I,1)=SIGA(I)                                                    1140
      DO 25 LC=2,NSEGS                                                      1141
      N1=LC-1                                                               1142
      N2=NTAG(N1)+1                                                         1143
      N3=NTAG(LC)                                                           1144
      I=0                                                                   1145
      DO 25 J=N2,N3                                                         1146
      I=I+1                                                                 1147
      XSTOR(I,LC)=XA(J)                                                     1148
      YSTOR(I,LC)=YA(J)                                                     1149
   25 SSTOR(I,LC)=SIGA(J)                                                   1150
```

```
      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)
  115 SFIT(I)=SSTOR(I,1)
      I=N
      DO 116 J=1,3
      I=I+1
      XFIT(I)=XSTOR(J,2)**2
      YFIT(I)=YSTOR(J,2)
  116 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)
  125 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)
  126 SFIT(I)=SSTOR(J,2)
      DO 127 J=1,3
      I=I+1
      XFIT(I)=XSTOR(J,3)
      YFIT(I)=YSTOR(J,3)
  127 SFIT(I)=SSTOR(J,3)
      NFIT=I
      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)
  135 SFIT(I)=SSTOR(J,2)
      DO 136 J=1,N3
      I=I+1
      XFIT(I)=XSTOR(J,3)
```

```
      YFIT(I)=YSTOR(J,3)                                                1201
  136 SFIT(I)=SSTOR(J,3)                                                1202
      NFIT=I                                                            1203
      GO TO 500                                                         1204
  200 GO TO (210,220,230,240),LC                                        1205
  210 N1=NTAG(1)                                                        1206
      N2=NTAG(2)-NTAG(1)                                                1207
      I=0                                                               1208
      DO 215 J=1,N1                                                     1209
      I=I+1                                                             1210
      XFIT(I)=XSTOR(J,1)**2                                             1211
      YFIT(I)=YSTOR(J,1)                                                1212
  215 SFIT(I)=SSTOR(J,1)                                                1213
      DO 216 J=1,N2                                                     1214
      I=I+1                                                             1215
      XFIT(I)=XSTOR(J,2)**2                                             1216
      YFIT(I)=YSTOR(J,2)                                                1217
  216 SFIT(I)=SSTOR(J,2)                                                1218
      NFIT=I                                                            1219
      GO TO 500                                                         1220
  220 N1=NTAG(1)*3/4                                                    1221
      N2=NTAG(1)-N1+1                                                   1222
      N3=NTAG(1)                                                        1223
      N4=NTAG(2)-NTAG(1)                                                1224
      N5=(NTAG(3)-NTAG(2))*3/4                                          1225
      I=0                                                               1226
      DO 225 J=N2,N3                                                    1227
      I=I+1                                                             1228
      XFIT(I)=XSTOR(J,1)                                                1229
      YFIT(I)=YSTOR(J,1)                                                1230
  225 SFIT(I)=SSTOR(J,1)                                                1231
      DO 226 J=1,N4                                                     1232
      I=I+1                                                             1233
      XFIT(I)=XSTOR(J,2)                                                1234
      YFIT(I)=YSTOR(J,2)                                                1235
  226 SFIT(I)=SSTOR(J,2)                                                1236
      DO 227 J=1,N5                                                     1237
      I=I+1                                                             1238
      XFIT(I)=XSTOR(J,3)                                                1239
      YFIT(I)=YSTOR(J,3)                                                1240
  227 SFIT(I)=SSTOR(J,3)                                                1241
      NFIT=I                                                            1242
      GO TO 500                                                         1243
  230 N1=(NTAG(2)-NTAG(1))*3/4                                          1244
      N2=(NTAG(2)-NTAG(1))-N1+1                                         1245
      N3=NTAG(2)-NTAG(1)                                                1246
      N4=NTAG(3)-NTAG(2)                                                1247
      N5=(NTAG(4)-NTAG(3))*3/4                                          1248
      I=0                                                               1249
      DO 235 J=N2,N3                                                    1250
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```
      I=I+1                                                             1251
      XFIT(I)=XSTOR(J,2)                                                1252
      YFIT(I)=YSTOR(J,2)                                                1253
  235 SFIT(I)=SSTOR(J,2)                                                1254
      DO 236 J=1,N4                                                     1255
      I=I+1                                                             1256
      XFIT(I)=XSTOR(J,3)                                                1257
      YFIT(I)=YSTOR(J,3)                                                1258
  236 SFIT(I)=SSTOR(J,3)                                                1259
      DO 237 J=1,N5                                                     1260
      I=I+1                                                             1261
      XFIT(I)=XSTOR(J,4)                                                1262
      YFIT(I)=YSTOR(J,4)                                                1263
  237 SFIT(I)=SSTOR(J,4)                                                1264
      NFIT=I                                                            1265
      GO TO 500                                                         1266
  240 N1=NTAG(3)-NTAG(2)                                                1267
      N2=NTAG(4)-NTAG(3)                                                1268
      I=0                                                               1269
      DO 245 J=1,N1                                                     1270
      I=I+1                                                             1271
      XFIT(I)=XSTOR(J,3)                                                1272
      YFIT(I)=YSTOR(J,3)                                                1273
  245 SFIT(I)=SSTOR(J,3)                                                1274
      DO 246 J=1,N2                                                     1275
      I=I+1                                                             1276
      XFIT(I)=XSTOR(J,4)                                                1277
      YFIT(I)=YSTOR(J,4)                                                1278
  246 SFIT(I)=SSTOR(J,4)                                                1279
      NFIT=I                                                            1280
      GO TO 500                                                         1281
  300 GO TO (310,320,320,320,330),LC                                    1282
  310 N1=NTAG(1)                                                        1283
      N2=NTAG(2)-NTAG(1)                                                1284
      I=0                                                               1285
      DO 315 J=1,N1                                                     1286
      I=I+1                                                             1287
      XFIT(I)=XSTOR(J,1)**2                                             1288
      YFIT(I)=YSTOR(J,1)                                                1289
  315 SFIT(I)=SSTOR(J,1)                                                1290
      DO 316 J=1,N2                                                     1291
      I=I+1                                                             1292
      XFIT(I)=XSTOR(J,2)**2                                             1293
      YFIT(I)=YSTOR(J,2)                                                1294
  316 SFIT(I)=SSTOR(J,2)                                                1295
      NFIT=I                                                            1296
      GO TO 500                                                         1297
  320 IF(LC.NE.2) GO TO 32?                                             1298
      N1=NTAG(1)                                                        1299
      N2=NTAG(2)-NTAG(1)                                                1300
```

```
      N3=NTAG(3)-NTAG(2)                                                1301
      GO TO 324                                                         1302
  321 LCL1=LC-1                                                         1303
      LCL2=LC-2                                                         1304
      LCU=LC+1                                                          1305
      N1=NTAG(LCL1)-NTAG(LCL2)                                          1306
      N2=NTAG(LC)-NTAG(LCL1)                                            1307
      N3=NTAG(LCU)-NTAG(LC)                                             1308
  324 I=0                                                               1309
      DO 325 J=1,N1                                                     1310
      I=I+1                                                             1311
      XFIT(I)=XSTOR(J,LC-1)                                             1312
      YFIT(I)=YSTOR(J,LC-1)                                             1313
  325 SFIT(I)=SSTOR(J,LC-1)                                             1314
      DO 326 J=1,N2                                                     1315
      I=I+1                                                             1316
      XFIT(I)=XSTOR(J,LC)                                               1317
      YFIT(I)=YSTOR(J,LC)                                               1318
  326 SFIT(I)=YSTOR(J,LC)                                               1319
      DO 327 J=1,N3                                                     1320
      I=I+1                                                             1321
      XFIT(I)=XSTOR(J,LC+1)                                             1322
      YFIT(I)=YSTOR(J,LC+1)                                             1323
  327 SFIT(I)=SSTOR(J,LC+1)                                             1324
      NFIT=I                                                            1325
      GO TO 500                                                         1326
  330 N1=NTAG(4)-NTAG(3)                                                1327
      N2=NTAG(5)-NTAG(4)                                                1328
      I=0                                                               1329
      DO 335 J=1,N1                                                     1330
      I=I+1                                                             1331
      XFIT(I)=XSTOR(J,4)                                                1332
      YFIT(I)=YSTOR(J,4)                                                1333
  335 SFIT(I)=SSTOR(J,4)                                                1334
      DO 336 J=1,N2                                                     1335
      I=I+1                                                             1336
      XFIT(I)=XSTOR(J,5)                                                1337
      YFIT(I)=YSTOR(J,5)                                                1338
  336 SFIT(I)=SSTOR(J,5)                                                1339
      NFIT=I                                                            1340
  500 SUMS=0.0                                                          1341
      DO 510 I=1,IMA                                                    1342
  510 SUMS=SUMS+SIGA(I)                                                 1343
      IF(SUMS.GT.0.0) GO TO 520                                         1344
      IWT=0                                                             1345
  520 NEVEN=0                                                           1346
      NORDER=4                                                          1347
      MODE=IWT                                                          1348
      NUMCOF=0                                                          1349
      MFIT=NFIT-1                                                       1350
```

```
      IF((MFIT-NORDER).GT.0) GO TO 524                                  1351
      NORDER=3                                                          1352
      IF((MFIT-NORDER).GT.0) GO TO 524                                  1353
      NORDER=2                                                          1354
      IF((MFIT-NORDER).GT.0) GO TO 524                                  1355
      NORDER=1                                                          1356
  524 CALL FITPOL(XFIT,YFIT,SFIT,NFIT,NORDER,NEVEN,MODE,FTEST,YCALC,REAL 1357
     1C,SIGMAC,RELC,SIGMAR,CHI,NUMCOF)                                  1358
      CHISQR(LC)=CHI                                                    1359
      DO 525 I=1,NUMCOF                                                 1360
      COEF(I,LC)=REALC(I)                                               1361
      DELCOF(I,LC)=SIGMAC(I)                                            1362
      RELCOF(I,LC)=RELC(I)                                              1363
  525 SRELC(I,LC)=SIGMAR(I)                                             1364
      NPLUS=NUMCOF+1                                                    1365
      IF(NPLUS.GT.5) GO TO 527                                          1366
      DO 526 I=NPLUS,5                                                  1367
      REALC(I)=0.0                                                      1368
      RELCOF(I,LC)=0.0                                                  1369
  526 SRELC(I,LC)=0.0                                                   1370
  527 DO 530 I=1,5                                                      1371
      TEST=ABS(COEF(I,LC))                                              1372
      IF(TEST.GT.0.0) GO TO 530                                         1373
      NPOLY=I-2                                                         1374
      GO TO 532                                                         1375
  530 IF(I.EQ.5) NPOLY=4                                                1376
  532 WRITE(6,1004) LC,NPOLY,(REALC(I),I=1,5)                           1377
 1004 FORMAT(T22,I1,6X,I1,14X,E13.6,4(2X,E13.6))                        1378
      WRITE(6,1008) (RELCOF(I,LC),I=1,5)                                1379
 1008 FORMAT (T22,'RELATIVE COEFS = ',3X,5(2X,E13.6))                   1380
      WRITE(6,1005) LC,CHISQR(LC),INT,NUMCOF                            1381
 1005 FORMAT(T40,'REDUCED CHI-SQUARE FOR REGION',I2,' = ',E13.6,2X,'WEIG 1382
     1HT CODE=',I2,2X,'NO. COEFS=',I2,//)                               1383
  999 CONTINUE                                                          1384
      RETURN                                                            1385
      END                                                               1386
      SUBROUTINE FITPOL(X,Y,SIGMAY,NPTS,NORDER,NEVEN,MODE,FTEST,YFIT,A,S 1387
     1IGMAA,B,SIGMAB,CHISQR,NTERMS)                                     1388
      DOUBLE PRECISION P,BETA,ALPHA,CHISQ,DSQRT                         1389
      DIMENSION X(1),Y(1),SIGMAY(1),FTEST(1),YFIT(1),A(1),SIGMAA(1),B(1) 1390
     1,SIGMAB(1)                                                        1391
      DIMENSION WEIGHT(51),P(51,5),BETA(5),ALPHA(5,5)                   1392
C                                                                       1393
C     ACCUMULATE WEIGHTS AND POWER SERIES TERMS                         1394
C                                                                       1395
   11 NTERMS=1                                                          1396
      NCOEFF=1                                                          1397
      JMAX=NORDER+1                                                     1398
   20 DO 40 I=1,NPTS                                                    1399
   21 IF(MODE) 22,27,29                                                 1400
```

```
   22 IF(Y(I)) 25,27,23                                                  1401
   23 WEIGHT(I)=1.0/Y(I)                                                 1402
      GO TO 31                                                           1403
   25 WEIGHT(I)=1.0/(-Y(I))                                              1404
      GO TO 31                                                           1405
   27 WEIGHT(I)=1.0                                                      1406
      GO TO 31                                                           1407
   29 WEIGHT(I)=1.0/(SIGMAY(I)**2)                                       1408
   31 P(I,1)=1.D0                                                        1409
      DO 36 L=1,NORDER                                                   1410
   36 P(I,L+1)=X(I)**L                                                   1411
   40 CONTINUE                                                           1412
C                                                                        1413
CC    ACCUMULATE MATRICES ALPHA AND BETA                                 1414
C                                                                        1415
   51 DO 54 J=1,NTERMS                                                   1416
      BETA(J)=0.D0                                                       1417
      DO 54 K=1,NTERMS                                                   1418
   54 ALPHA(J,K)=0.D0                                                    1419
   61 DO 66 I=1,NPTS                                                     1420
      DO 66 J=1,NTERMS                                                   1421
      BETA(J)=BETA(J)+P(I,J)*Y(I)*WEIGHT(I)                              1422
      DO 66 K=J,NTERMS                                                   1423
      ALPHA(J,K)=ALPHA(J,K)+P(I,J)*P(I,K)*WEIGHT(I)                      1424
   66 ALPHA(K,J)=ALPHA(J,K)                                              1425
C                                                                        1426
CC    DELETE FIXED COEFFICIENTS                                          1427
C                                                                        1428
   70 IF(NEVEN) 71,91,81                                                 1429
   71 DO 76 J=3,NTERMS,2                                                 1430
      BETA(J)=0.D0                                                       1431
      DO 75 K=1,NTERMS                                                   1432
      ALPHA(J,K)=0.D0                                                    1433
   75 ALPHA(K,J)=0.D0                                                    1434
   76 ALPHA(J,J)=1.D0                                                    1435
      GO TO 91                                                           1436
   81 DO 86 J=2,NTERMS,2                                                 1437
      BETA(J)=0.D0                                                       1438
      DO 85 K=1,NTERMS                                                   1439
      ALPHA(J,K)=0.D0                                                    1440
   85 ALPHA(K,J)=0.D0                                                    1441
   86 ALPHA(J,J)=1.D0                                                    1442
C                                                                        1443
CC    INVERT CURVATURE MATRIX ALPHA                                      1444
C                                                                        1445
   91 DO 95 J=1,JMAX                                                     1446
      A(J)=0.0                                                           1447
      SIGMAA(J)=0.0                                                      1448
      B(J)=0.0                                                           1449
   95 SIGMAB(J)=0.0                                                      1450
```

```
      DO 97 I=1,NPTS                                                    1451
   97 YFIT(I)=0.0                                                       1452
  101 CALL MATINV(ALPHA,NTERMS,DET)                                     1453
      IF(DET) 111,103,111                                               1454
  103 CHISQR=0.0                                                        1455
      GO TO 170                                                         1456
C                                                                       1457
C     CALCULATE COEFFICIENTS, FIT, AND CHI SQUARE                       1458
C                                                                       1459
  111 DO 115 J=1,NTERMS                                                 1460
      DO 113 K=1,NTERMS                                                 1461
  113 A(J)=A(J)+BETA(K)*ALPHA(J,K)                                      1462
      DO 115 I=1,NPTS                                                   1463
  115 YFIT(I)=YFIT(I)+A(J)*P(I,J)                                       1464
  121 CHISQ=0.D0                                                        1465
      DO 123 I=1,NPTS                                                   1466
  123 CHISQ=CHISQ+(Y(I)-YFIT(I))**2*WEIGHT(I)                           1467
      FREE=NPTS-NCOEFF                                                  1468
      CHISQR=CHISQ/FREE                                                 1469
C                                                                       1470
C     TEST FOR END OF FIT                                               1471
C                                                                       1472
  131 IF(NTERMS-JMAX) 132,151,151                                       1473
  132 IF(NCOEFF-2) 133,134,141                                          1474
  133 IF(NEVEN) 137,137,135                                             1475
  134 IF(NEVEN) 135,137,135                                             1476
  135 NTERMS=NTERMS+2                                                   1477
      GO TO 138                                                         1478
  137 NTERMS=NTERMS+1                                                   1479
  138 NCOEFF=NCOEFF+1                                                   1480
      CHISQ1=CHISQ                                                      1481
      GO TO 51                                                          1482
  141 FVALUE=(CHISQ1-CHISQ)/CHISQR                                      1483
      IF(FTEST(NTERMS)-FVALUE) 134,143,143                              1484
  143 IF(NEVEN) 144,146,144                                             1485
  144 NTERMS=NTERMS-2                                                   1486
      GO TO 147                                                         1487
  146 NTERMS=NTERMS-1                                                   1488
  147 NCOEFF=NCOEFF-1                                                   1489
      JMAX=NTERMS                                                       1490
  149 GO TO 51                                                          1491
C                                                                       1492
C     CALCULATE REMAINDER OF OUTPUT                                     1493
C                                                                       1494
  151 IF(MODE) 152,154,152                                              1495
  152 VARNCE=1.0                                                        1496
      GO TO 155                                                         1497
  154 VARNCE=CHISQR                                                     1498
  155 DO 156 J=1,NTERMS                                                 1499
  156 SIGMAA(J)=DSQRT(VARNCE*ALPHA(J,J))                                1500
```

```
  161 IF(A(1)) 162,170,162                                                      1501
  162 DO 166 J=2,NTERMS                                                         1502
      IF(A(J)) 164,166,164                                                      1503
  164 B(J)=A(J)/A(1)                                                            1504
  165 SIGMAB(J)=B(J)*DSQRT((SIGMAA(J)/A(J))**2+(SIGMAA(1)/A(1))**2-2.0*V        1505
     IARNCE*ALPHA(J,1)/(A(J)*A(1)))                                             1506
  166 CONTINUE                                                                  1507
      B(1)=1.0                                                                  1508
  170 RETURN                                                                    1509
      END                                                                       1510
      SUBROUTINE MATINV(ARRAY,NORDER,DET)                                       1511
      DOUBLE PRECISION ARRAY,AMAX,SAVE,DABS                                     1512
      DIMENSION ARRAY(5,5),IK(5),JK(5)                                          1513
   10 DET=1.0                                                                   1514
   11 DO 100 K=1,NORDER                                                         1515
C                                                                               1516
CC    FIND LARGEST ELEMENT ARRAY(I,J) IN REST OF MATRIX                         1517
C                                                                               1518
      AMAX=0.D0                                                                 1519
   21 DO 30 I=K,NORDER                                                          1520
      DO 30 J=K,NORDER                                                          1521
   23 IF(DABS(AMAX)-DABS(ARRAY(I,J))) 24,24,30                                  1522
   24 AMAX=ARRAY(I,J)                                                           1523
      IK(K)=I                                                                   1524
      JK(K)=J                                                                   1525
   30 CONTINUE                                                                  1526
C                                                                               1527
CC    INTERCHANGE ROWS AND COLUMNS TO PUT AMAX IN ARRAY(K,K)                    1528
C                                                                               1529
   31 IF(AMAX) 41,32,41                                                         1530
   32 DET=0.0                                                                   1531
      GO TO 140                                                                 1532
   41 I=IK(K)                                                                   1533
      IF(I-K) 21,51,43                                                          1534
   43 DO 50 J=1,NORDER                                                          1535
      SAVE=ARRAY(K,J)                                                           1536
      ARRAY(K,J)=ARRAY(I,J)                                                     1537
   50 ARRAY(I,J)=-SAVE                                                          1538
   51 J=JK(K)                                                                   1539
      IF(J-K) 21,61,53                                                          1540
   53 DO 60 I=1,NORDER                                                          1541
      SAVE=ARRAY(I,K)                                                           1542
      ARRAY(I,K)=ARRAY(I,J)                                                     1543
   60 ARRAY(I,J)=-SAVE                                                          1544
C                                                                               1545
CC    ACCUMULATE ELEMENTS OF INVERSE MATRIX                                     1546
C                                                                               1547
   61 DO 70 I=1,NORDER                                                          1548
      IF(I-K) 63,70,63                                                          1549
   63 ARRAY(I,K)=-ARRAY(I,K)/AMAX                                               1550
```

```
   70 CONTINUE                                                                  1551
   71 DO 80  I=1,NORDER                                                         1552
      DO 80  J=1,NORDER                                                         1553
      IF(I-K) 74,80,74                                                          1554
   74 IF(J-K) 75,80,75                                                          1555
   75 ARRAY(I,J)=ARRAY(I,J)+ARRAY(I,K)*ARRAY(K,J)                               1556
   80 CONTINUE                                                                  1557
   81 DO 90 J=1,NORDER                                                          1558
      IF(J-K) 83,90,83                                                          1559
   83 ARRAY(K,J)=ARRAY(K,J)/AMAX                                                1560
   90 CONTINUE                                                                  1561
      ARRAY(K,K)=1.0/AMAX                                                       1562
  100 DET=DET*AMAX                                                              1563
C                                                                               1564
CC    RESTORE ORDERING OF MATRIX                                                1565
C                                                                               1566
  101 DO 130 L=1,NORDER                                                         1567
      K=NORDER-L+1                                                              1568
      J=IK(K)                                                                   1569
      IF(J-K) 111,111,105                                                       1570
  105 DO 110 I=1,NORDER                                                         1571
      SAVE=ARRAY(I,K)                                                           1572
      ARRAY(I,K)=-ARRAY(I,J)                                                    1573
  110 ARRAY(I,J)=SAVE                                                           1574
  111 I=JK(K)                                                                   1575
      IF(I-K) 130,130,113                                                       1576
  113 DO 120 J=1,NORDER                                                         1577
      SAVE=ARRAY(K,J)                                                           1578
      ARRAY(K,J)=-ARRAY(I,J)                                                    1579
  120 ARRAY(I,J)=SAVE                                                           1580
  130 CONTINUE                                                                  1581
  140 RETURN                                                                    1582
      END                                                                       1583
      SUBROUTINE RADPL (IMA,XDIST,YINT,N,RBP,ARI,          LZ,RAD,RDI,LAM,      1584
     1   DLAB,KT,NZ)                                                            1585
      DIMENSION XDIST(1),YINT(1),RBP(15,4),ARI(15,4),                RAD(1      1586
     1),RDI(1),X(51),Y(51),XL1(5),YL1(5),IGL(5),DLAB(1),DL1(5),DL2(5),DL       1587
     23(5),DL4(5),DL5(5),XX(51),YY(51),XA(15),YA(15)                            1588
      DIMENSION DL6(5),DL7(5),DL8(5)                                            1589
     1,DL9(5),DL10(5),DL11(5)                                                   1590
      DATA XL1/'X AN','D R ','(MM)','    ','    ','    '/,                     1591
     1YL1/'I(X)','  AND','  I(R','  ,','    ','    '/,                        1592
     2IGL/'I PR','OFIL','E, L','INE ','    ','  0'/                           1593
      DATA DL1/'SMOO','THED','  I(X','  ,','    ','    '/                     1594
      DATA DL2/'INIT','IAL ','I(X)','    ','    ','    '/                     1595
      DATA DL3/'DKAB','EL W','ITH ','F-TE','ST  ','    '/                     1596
      DATA DL4/'0.5 ','PERC','ENT ','PROB','  FOR'/,DL5/'1.0 ','PERC','EN     1597
     1T ','PROB','  FOR'/,DL6/'2.5 ','PERC','ENT ','PROB','  FOR'/,DL7/'5.     1598
     20 ','PERC','ENT ','PROB','  FOR'/,DL8/'EXCE','EDIN','G F-','VALU','      1599
     1E   '/                                                                    1600
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      DATA  DL9/'10.0','PERC','ENT ','PROB',' FOR'/                    1601
      DATA DL10/'25.0','PERC','ENT ','PROB',' FOR'/                    1602
      DATA DL11/'50.0','PERC','ENT ','PROB',' FOR'/                    1603
      IZERO=0                                                          1604
      DO 1 I=1,IMA                                                     1605
      IF (XDIST(I).LT.0.) GO TO 1                                      1606
      IZERO=IZERO+1                                                    1607
      X(IZERO)=XDIST(I)                                                1608
      Y(IZERO)=YINT(I)                                                 1609
    1 CONTINUE                                                         1610
      IZE=IMA                                                          1611
      IMA=IZERO                                                        1612
      NZERO=0                                                          1613
      DO 4 IJ=1,N                                                      1614
      IF (RBP(IJ,LZ).LT.0.) GO TO 4                                    1615
      NZERO=NZERO+1                                                    1616
      XA(NZERO)=RBP(IJ,LZ)                                             1617
      YA(NZERO)=ARI(IJ,LZ)                                             1618
    4 CONTINUE                                                         1619
      NHOLD=N                                                          1620
      N=NZERO                                                          1621
      IGL(5)=IGL(5)+LZ                                                 1622
      CALL GRAPH (IMA,X,Y,0,2,7.00,9.00,0.0,0.0,0.0,XL1,YL1,IGL,DLAB)  1623
      CALL GRAPHS (IMA,X,Y,4,107,DL1)                                  1624
      CALL GRAPHS (N,XA,YA,1,107,DL2)                                  1625
      IGL(5)=IGL(5)-LZ                                                 1626
      LZERO=0                                                          1627
      DO 6 LDEX=1,KT                                                   1628
      IF (RDI(LDEX).LT.0.) GO TO 6                                     1629
      LZERO=LZERO+1                                                    1630
      XX(LZERO)=RDI(LDEX)                                              1631
      YY(LZERO)=RAD(LDEX)                                              1632
    6 CONTINUE                                                         1633
      KTHOLD=KT                                                        1634
      KT=LZERO                                                         1635
    8 GO TO (9,10,11,15,16,16,16),NZ                                   1636
    9 CALL GRAPHS(KT,XX,YY,2,111,DL3)                                  1637
      CALL GRAPHS(KT,XX,YY,0,107,DL4)                                  1638
      CALL GRAPHS(KT,XX,YY,0,107,DL8)                                  1639
      GO TO 12                                                         1640
   10 CALL GRAPHS(KT,XX,YY,2,111,DL3)                                  1641
      CALL GRAPHS(KT,XX,YY,0,107,DL5)                                  1642
      CALL GRAPHS(KT,XX,YY,0,107,DL8)                                  1643
      GO TO 12                                                         1644
   11 CALL GRAPHS(KT,XX,YY,2,111,DL3)                                  1645
      CALL GRAPHS(KT,XX,YY,0,107,DL6)                                  1646
      CALL GRAPHS(KT,XX,YY,0,107,DL8)                                  1647
      GO TO 12                                                         1648
   15 CALL GRAPHS(KT,XX,YY,2,111,DL3)                                  1649
      CALL GRAPHS(KT,XX,YY,0,107,DL7)                                  1650
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      CALL GRAPHS(KT,XX,YY,0,107,DL8)                                    1651
      GO TO 12                                                           1652
   16 CALL GRAPHS (KT,XX,YY,2,111,DL3)                                   1653
      NN=NZ-4                                                            1654
      GO TO (17,18,19),NN                                                1655
   17 CALL GRAPHS (KT,XX,YY,0,107,DL9)                                   1656
      GO TO 20                                                           1657
   18 CALL GRAPHS (KT,XX,YY,0,107,DL10)                                  1658
      GO TO 20                                                           1659
   19 CALL GRAPHS (KT,XX,YY,0,107,DL11)                                  1660
   20 CALL GRAPHS (KT,XX,YY,0,107,DL8)                                   1661
   12 KT=KTHOLD                                                          1662
      IMA=IZE                                                            1663
      N=NHOLD                                                            1664
      DO 13 IPOS=1,KT                                                    1665
   13 RAD(IPOS)=ABS(RAD(IPOS))                                           1666
      RETURN                                                             1667
      END                                                                1668
      SUBROUTINE TEMP (NT,IMAT,RBP,ARI,RADIST,RADINT,NLZT,DLAB,L3,KM,NL, 1669
     1NH,LKODE,KPLOT1,KPLOT2,KLINE1,KLINE2,DELA,DELINT,IARTP)            1670
      DIMENSION FNUM(7)                                                  1671
      DIMENSION RBP(15,4),ARI(15,4),RADIST(51,4,7),RADINT(51,4,7),TLAT1( 1672
     A51),X(15),RDIST(51),RA(6,51),LA(6,51),Y1(15),Y2(51),               1673
     1TLAT2(51),TLAT3(51),TLAT4(51),TLAT5(51),TRAD1(51),TRAD2(51),TRAD3( 1674
     251),TRAD4(51),TRAD5(51),DLAB(5),IXL(5),IXR(5)                      1675
     3,SUMLAT(51),AVELAT(51),SUMRAD(51),AVERAD(51),DELINT(51,4,7)        1676
     4,XTHOLD(15,4),YTHOLD(15,4),TLAT6(51),TRAD6(51),DELA(4),DELTR(6,51) 1677
      DATA FNUM/0.5,1.0,2.5,5.0,10.0,25.0,50.0/                          1678
      DATA IXL/' TL0',4*' '/,                                            1679
     1IXR/' TR0',4*' '/                                                  1680
      DO 6 NLINE=1,NLZT                                                  1681
      KODEN=0                                                            1682
      IF (RBP(1,NLINE).GE.0.0) GO TO 3                                   1683
      KODEN=KODEN+1                                                      1684
      ITZERO=0                                                           1685
      DO 2 NTSHIF=1,NT                                                   1686
      IF (RBP(NTSHIF,NLINE).LT.0.0) GO TO 2                              1687
      ITZERO=ITZERO+1                                                    1688
      XTHOLD(ITZERO,NLINE)=RBP(NTSHIF,NLINE)                             1689
      YTHOLD(ITZERO,NLINE)=ARI(NTSHIF,NLINE)                             1690
    2 CONTINUE                                                           1691
      DO 4 NSUB1=1,ITZERO                                                1692
      RBP(NSUB1,NLINE)=XTHOLD(NSUB1,NLINE)                               1693
    4 ARI(NSUB1,NLINE)=YTHOLD(NSUB1,NLINE)                               1694
    3 IF (NLINE.LT.NLZT) GO TO 6                                         1695
      IF (KODEN.EQ.0) GO TO 6                                            1696
      NT=ITZERO                                                          1697
    6 CONTINUE                                                           1698
      IMAT=IMAT-1                                                        1699
      NT=NT-1                                                            1700
```

```
      NL=NL-1                                                                   1701
      IF (LKODE.EQ.1) GO TO 97                                                  1702
      RETURN                                                                    1703
   97 IF (NLZT.GE.2) GO TO 1                                                    1704
      WRITE (6,1000)                                                            1705
 1000 FORMAT (//,10X,'TEMPS. CANNOT BE CALCULATED; ONLY ONE LINE')              1706
      RETURN                                                                    1707
    1 DO 96 NPOLY=1,KM                                                          1708
      NL=NL+1                                                                   1709
      WRITE (6,1001)                                                            1710
 1001 FORMAT (1H1)                                                              1711
      WRITE (6,3000) NT,KODEN                                                   1712
 3000 FORMAT (T10,'TEMP CONTROL PARAMETERS'///,T15,'NT = ',I2,5X,               1713
     2'KODEN = ',I2)                                                            1714
      IF (KM.EQ.1) GO TO 5                                                      1715
      WRITE (6,100) FNUM(NL)                                                    1716
  100 FORMAT (10X,'OKABEL MULTIPLE F-TEST POLYNOMIAL TEMPERATURE CALCULA        1717
     1TIONS FOR'/T15,F5.2,'  PERCENT PROBABILITY OF EXCEEDING THE F-VALU        1718
     2E')                                                                       1719
    5 WRITE (6,1002)                                                            1720
 1002 FORMAT (10X,'CALCULATION OF LATERAL AND RADIAL TEMPERATURESF 2-LIN        1721
     1E METHOD',//)                                                             1722
      WRITE (6,1003)                                                            1723
 1003 FORMAT (10X,'SYMBOL KEY')                                                 1724
      WRITE (6,1004)                                                            1725
 1004 FORMAT (5X,'SYMBOL      LINE1      LINE2      EQ1       EQ2       INTEN.  1726
     1USED')                                                                    1727
      WRITE (6,1005)                                                            1728
 1005 FORMAT (//,5X,'TLAT1      3815.84    3820.43    38175     33096      LAT   1729
     1ERAL')                                                                    1730
      WRITE (6,1006)                                                            1731
 1006 FORMAT (/,5X,"TLAT2         "        3824.44      "       26140        "  1732
     1')                                                                        1733
      WRITE (6,1007)                                                            1734
 1007 FORMAT (/,5X,"TLAT3      3820.43       "        33096       "           "  1735
     1')                                                                        1736
      WRITE (6,1008)                                                            1737
 1008 FORMAT (/,5X,"TLAT4      3815.84    3825.88    38175     33507          "  1738
     1')                                                                        1739
      WRITE (6,1009)                                                            1740
 1009 FORMAT (/,5X,"TLAT5      3824.44       "        26140       "           "  1741
     1')                                                                        1742
      WRITE (6,4000)                                                            1743
 4000 FORMAT (/,5X,'TLAT6      3820.43       "        33096       "           "  1744
     1')                                                                        1745
      WRITE (6,1010)                                                            1746
 1010 FORMAT (/,5X,'TRAD1 THRU TRAD6 SIMILAR EXCEPT RADIAL INTEN. USED',        1747
     1/////)                                                                    1748
      WRITE (6,5000) (DELA(I),I=1,NLZT)                                         1749
 5000 FORMAT (T10,'DELA(1)= ',F5.2,10X,'DELA(2)= ',F5.2,10X,'DELA(3)= ',        1750
```

```
     1F5.2,10X,'DELA(4)= ',F5.2)                                                1751
      IF(IARTP.EQ.9) WRITE(6,5001)                                              1752
5001  FORMAT(///,T10,'*****BANFIELD AND HUBER (1973) GA VALUES',///)            1753
      WRITE (6,1011) NT                                                         1754
1011  FORMAT (40X,'LATERAL TEMPERATURES FOR',I4,2X,'EXPERIMENTAL LATERAL        1755
     1 POSITIONS IN EMISS.  SOURCE',//,T20,'X      TLAT1(X)      TLAT2(X)      1756
     2    TLAT3(X)      TLAT4(X)      TLAT5(X)      TLAT6(X)',//)              1757
      DO 10 I=1,NT                                                              1758
      TLAT1(I)=3173./ALOG10(1.1605*(ARI(I,2)/ARI(I,1)))                         1759
      IF(IARTP.EQ.9) TLAT1(I)=TLAT1(I)/(1.0+6.218E-5*TLAT1(I))                  1760
      IF (NLZT.EQ.2) GO TO 10                                                   1761
      TLAT2(I)=7518./ALOG10(33.937*(ARI(I,3)/ARI(I,1)))                        1762
      IF(IARTP.EQ.9) TLAT2(I)=TLAT2(I)/(1.0+2.559E-5*TLAT2(I))                  1763
      TLAT3(I)=4345./ALOG10(29.244*(ARI(I,3)/ARI(I,2)))                         1764
      IF(IARTP.EQ.9) TLAT3(I)=TLAT3(I)/(1.0-1.031E-6*TLAT3(I))                  1765
      IF (NLZT.EQ.3) GO TO 10                                                   1766
      TLAT4(I)=2916./ALOG10(1.676*(ARI(I,4)/ARI(I,1)))                         1767
      IF(IARTP.EQ.9) TLAT4(I)=TLAT4(I)/(1.0+6.144E-5*TLAT4(I))                  1768
      TLAT5(I)=-4608./ALOG10(0.0494*(ARI(I,4)/ARI(I,3)))                        1769
      IF(IARTP.EQ.9) TLAT5(I)=TLAT5(I)/(1.0+2.906E-6*TLAT5(I))                  1770
      TLAT6(I)=-256.9/ALOG10(1.444*(ARI(I,4)/ARI(I,2)))                         1771
      IF(IARTP.EQ.9) TLAT6(I)=TLAT6(I)/(1.0+6.894E-5*TLAT6(I))                  1772
1012  FORMAT (15X,F8.3,6(4X,F8.1))                                              1773
  10  WRITE (6,1012) RBP(I,1),TLAT1(I),TLAT2(I),TLAT3(I),TLAT4(I),TLAT5(       1774
     1I),TLAT6(I)                                                               1775
      WRITE (6,1013) IMAT                                                       1776
1013  FORMAT (//////////,40X,'RADIAL TEMPERATURES FOR',I4,2X,'RADIAL POS        1777
     1ITIONS IN THE EMISSION SOURCE',//,T20,'R      TRAD1(R)      TRAD2(R)     1778
     2      TRAD3(R)      TRAD4(R)      TRAD5(R)      TRAD6(R)',//)            1779
      DO 20 J=1,IMAT                                                            1780
      K=(IMAT-J)+2                                                              1781
      TRAD1(J)=3173./ALOG10(1.1605*(RADINT(K,2,NPOLY)/RADINT(K,1,NPOLY))       1782
     1)                                                                         1783
      IF(IARTP.EQ.9) TRAD1(J)=TRAD1(J)/(1.0+6.218E-5*TRAD1(J))                  1784
      DELTR(1,J)=(TRAD1(J)/(1.439*5079.))*(DELA(1)+DELA(2)+DELINT(K,1,NP        1785
     1OLY)+DELINT(K,2,NPOLY))                                                   1786
      IF (NLZT.EQ.2) GO TO 20                                                   1787
      TRAD2(J)=7518./ALOG10(33.937*(RADINT(K,3,NPOLY)/RADINT(K,1,NPOLY))       1788
     1)                                                                         1789
      IF(IARTP.EQ.9) TRAD2(J)=TRAD2(J)/(1.0+2.559E-5*TRAD2(J))                  1790
      DELTR(2,J)=(TRAD2(J)/(1.439*12035.))*(DELA(1)+DELA(3)+DELINT(K,1,N        1791
     1POLY)+DELINT(K,3,NPOLY))                                                  1792
      TRAD3(J)=4345./ALOG10(29.244*(RADINT(K,3,NPOLY)/RADINT(K,2,NPOLY))       1793
     1)                                                                         1794
      IF(IARTP.EQ.9) TRAD3(J)=TRAD3(J)/(1.0-1.031E-6*TRAD3(J))                  1795
      DELTR(3,J)=(TRAD3(J)/(1.439*6956.))*(DELA(2)+DELA(3)+DELINT(K,2,NP        1796
     1OLY)+DELINT(K,3,NPOLY))                                                   1797
      IF (NLZT.EQ.3) GO TO 20                                                   1798
      TRAD4(J)=2916./ALOG10(1.676*(RADINT(K,4,NPOLY)/RADINT(K,1,NPOLY)))       1799
      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,NP
     1OLY)+DELINT(K,4,NPOLY))
      TRAD5(J)=-4608./ALOG10(0.0494*(RADINT(K,4,NPOLY)/RADINT(K,3,NPOLY)
     1))
      IF(IARTP.EQ.9) TRAD5(J)=TRAD5(J)/(1.0+2.906E-6*TRAD5(J))
      DELTR(5,J)=(TRAD5(J)/(1.439*7367.))*(DELA(3)+DELA(4)+DELINT(K,3,NP
     1OLY)+DELINT(K,4,NPOLY))
      TRAD6(J)=-256.9/ALOG10(1.444*(RADINT(K,4,NPOLY)/RADINT(K,2,NPOLY))
     1)
      IF(IARTP.EQ.9) TRAD6(J)=TRAD6(J)/(1.0+6.894E-6*TRAD6(J))
      DELTR(6,J)=(TRAD6(J)/(1.439*411.))*(DELA(2)+DELA(4)+DELINT(K,2,NPO
     1LY)+DELINT(K,4,NPOLY))
1014  FORMAT (15X,F8.3,6(4X,F8.1))
   20 WRITE (6,1014) RADIST(K,1,NPOLY),TRAD1(J),TRAD2(J),TRAD3(J),TRAD4(
     1J),TRAD5(J),TRAD6(J)
      WRITE (6,2999)
2999  FORMAT (/////,T10,'RADIAL POS',T26,'DELTA TRAD1',T43,'DELTA TRAD2'
     1,T60,'DELTA TRAD3',T76,'DELTA TRAD4',T94,'DELTA TRAD5',T111,'DELTA
     1 TRAD6')
      DO 29 I=1,IMAT
      J=(IMAT-I)+2
3001  FORMAT (T8,E11.4,T26,5(E11.4,6X),E11.4)
   29 WRITE (6,3001) RADIST(J,1,NPOLY),(DELTR(K,I),K=1,6)
      DO 30 L=1,IMAT
      KK=(IMAT-L)+2
   30 RDIST(L)=RADIST(KK,1,NPOLY)
      DO 40 M=1,NT
   40 X(M)=RBP(M,1)
      NN=IMAT
      IF (KPLOT1.EQ.1) GO TO 65
      IF (NLZT.EQ.2) GO TO 15
      IF (NLZT.EQ.3) GO TO 21
      IF (NLZT.EQ.4) GO TO 21
      RETURN
   15 CALL GRAPH (NT,X,TLAT1,0.,2.,7.0,9.,0,0,0.2500,,'X AND R (MM);','T(X
     1) AND T(R);','TEMPERATURE PROFILE;',DLAB)
      CALL GRAPHS (NT,X,TLAT1,4,107.,'LATERAL TEMPS.;')
      CALL GRAPHS (NN,RDIST,TRAD1,1,111,'RADIAL TEMPS.;')
      GO TO 12
   21 DO 22 N=1,NT
      LA(1,N)=TLAT1(N)
      IF (NLZT.EQ.2) GO TO 22
      LA(2,N)=TLAT2(N)
      LA(3,N)=TLAT3(N)
      IF (NLZT.EQ.3) GO TO 22
      LA(4,N)=TLAT4(N)
      LA(5,N)=TLAT5(N)
      LA(6,N)=TLAT6(N)
   22 CONTINUE
      DO 23 II=1,IMAT
```

```
      RA(1,II)=TRAD1(II)                                                        1851
      IF (NLZT.EQ.2) GO TO 23                                                   1852
      RA(2,II)=TRAD2(II)                                                        1853
      RA(3,II)=TRAD3(II)                                                        1854
      IF (NLZT.EQ.3) GO TO 23                                                   1855
      RA(4,II)=TRAD4(II)                                                        1856
      RA(5,II)=TRAD5(II)                                                        1857
      RA(6,II)=TRAD6(II)                                                        1858
   23 CONTINUE                                                                  1859
      IF (NLZT.EQ.4) GO TO 50                                                   1860
      DO 35 JJ=1,3                                                              1861
      IF (JJ.LT.KLINE1) GO TO 34                                                1862
      IF (JJ.EQ.KLINE2) GO TO 34                                                1863
      DO 24 KK=1,NT                                                             1864
   24 Y1(KK)=LA(JJ,KK)                                                          1865
      DO 25 LL=1,IMAT                                                           1866
   25 Y2(LL)=RA(JJ,LL)                                                          1867
      IXL(1)=IXL(1)+1                                                           1868
      IXR(1)=IXR(1)+1                                                           1869
      CALL GRAPH (NT,X,Y1,0,2,7.0,9.,0,0,0,2500.,'X AND R (MM);',T(X) A         1870
     1ND T(R);',' TEMPERATURE PROFILE;',DLAB)                                   1871
      CALL GRAPHS (NT,X,Y1,4,107,IXL)                                           1872
      CALL GRAPHS (NN,RDIST,Y2,1,111,IXR)                                       1873
      GO TO 35                                                                  1874
   34 IXL(1)=IXL(1)+1                                                           1875
      IXR(1)=IXR(1)+1                                                           1876
   35 CONTINUE                                                                  1877
      IXL(1)=IXL(1)-3                                                           1878
      IXR(1)=IXR(1)-3                                                           1879
      GO TO 12                                                                  1880
   50 DO 60 JK=1,6                                                              1881
      IF (JK.LT.KLINE1) GO TO 59                                                1882
      IF (JK.EQ.KLINE2) GO TO 59                                                1883
      DO 51 KL=1,NT                                                             1884
   51 Y1(KL)=LA(JK,KL)                                                          1885
      DO 52 LM=1,IMAT                                                           1886
   52 Y2(LM)=RA(JK,LM)                                                          1887
      IXL(1)=IXL(1)+1                                                           1888
      IXR(1)=IXR(1)+1                                                           1889
      CALL GRAPH (NT,X,Y1,0,2,7.0,9.,0,0,0,2500.,'X AND R (MM);',T(X) A         1890
     1ND T(R);',' TEMPERATURE PROFILE;',DLAB)                                   1891
      CALL GRAPHS (NT,X,Y1,4,107,IXL)                                           1892
      CALL GRAPHS (NN,RDIST,Y2,1,111,IXR)                                       1893
      GO TO 60                                                                  1894
   59 IXL(1)=IXL(1)+1                                                           1895
      IXR(1)=IXR(1)+1                                                           1896
   60 CONTINUE                                                                  1897
      IXL(1)=IXL(1)-6                                                           1898
      IXR(1)=IXR(1)-6                                                           1899
   12 IF (L3.EQ.1) GO TO 65                                                     1900
```

```
      IF (NPOLY.LT.KM) GO TO 96                                                 1901
      RETURN                                                                    1902
   65 DO 75 IJK=1,NT                                                            1903
      SUMLAT(IJK)=0.0                                                           1904
      SUMLAT(IJK)=SUMLAT(IJK)+TLAT1(IJK)                                        1905
      IF (NLZT.EQ.2) GO TO 66                                                   1906
      SUMLAT(IJK)=SUMLAT(IJK)+TLAT2(IJK)+TLAT3(IJK)                             1907
      IF (NLZT.EQ.3) GO TO 67                                                   1908
      SUMLAT(IJK)=SUMLAT(IJK)+TLAT4(IJK)+TLAT5(IJK)+TLAT6(IJK)                  1909
      AVELAT(IJK)=SUMLAT(IJK)/6.                                                1910
      GO TO 75                                                                  1911
   66 AVELAT(IJK)=SUMLAT(IJK)                                                   1912
      GO TO 75                                                                  1913
   67 AVELAT(IJK)=SUMLAT(IJK)/3.                                                1914
   75 CONTINUE                                                                  1915
      DO 85 LMN=1,IMAT                                                          1916
      SUMRAD(LMN)=0.0                                                           1917
      SUMRAD(LMN)=SUMRAD(LMN)+TRAD1(LMN)                                        1918
      IF (NLZT.EQ.2) GO TO 76                                                   1919
      SUMRAD(LMN)=SUMRAD(LMN)+TRAD2(LMN)+TRAD3(LMN)                             1920
      IF (NLZT.EQ.3) GO TO 77                                                   1921
      SUMRAD(LMN)=SUMRAD(LMN)+TRAD4(LMN)+TRAD5(LMN)+TRAD6(LMN)                  1922
      AVERAD(LMN)=SUMRAD(LMN)/6.                                                1923
      GO TO 85                                                                  1924
   76 AVERAD(LMN)=SUMRAD(LMN)                                                   1925
      GO TO 85                                                                  1926
   77 AVERAD(LMN)=SUMRAD(LMN)/3.                                                1927
   85 CONTINUE                                                                  1928
      WRITE (6,2000)                                                            1929
 2000 FORMAT(10X,'DISTANCE          AVE. RADIAL T')                            1930
      DO 90 NNN=1,IMAT                                                          1931
 2001 FORMAT (T10,E11.4,8X,E11.4)                                               1932
   90 WRITE (6,2001) RDIST(NNN),AVERAD(NNN)                                     1933
      WRITE (6,2002)                                                            1934
 2002 FORMAT (////////////,10X,'DISTANCE          AVE. LATERAL T')             1935
      DO 95 MMM=1,NT                                                            1936
 2003 FORMAT (T10,E11.4,8X,E11.4)                                               1937
   95 WRITE (6,2003) X(MMM),AVELAT(MMM)                                         1938
      IF (KPLOT2.EQ.1) GO TO 96                                                 1939
      CALL GRAPH (NT,X,AVELAT,0.2,7.0,9.,0,0.0,2500.,'X AND R (MM);','AV        1940
     1E. LINE PAIR TEMP.','AVE. LP TEMP PROFILE',DLAB)                          1941
      CALL GRAPHS (NT,X,AVELAT,4.107,'AVE. LATERAL TEMPS.;')                    1942
      CALL GRAPHS (IMAT,RDIST,AVERAD,1.111,'AVE. RADIAL TEMPS.;')               1943
   96 CONTINUE                                                                  1944
      RETURN                                                                    1945
      END                                                                       1946
      SUBROUTINE SLOPET (NT,IMAT,RBP,ARI,RADIST,RADINT,NLZT,DLAB,WAVE,KM        1947
     1,NL,NH,LKODE,KPLOT3,KPNED1,KPNED2,DELA,DELINT,IARTP)                      1948
C  LEAST SQUARES SLOPE METHOD OF TEMPERATURE CALCULATION                        1949
      DIMENSION FNUM(7)                                                         1950
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```
      DIMENSION YCALCN(51,4),YINLA(51),TS(5),TLA(51),DLAB(5),RBP(15,4),
     1ARI(15,4),RADINT(51,4,7),RADIST(51,4,7),SLOPEL(51),ERRORL(51),
     2RAYIN(51),WAVE(4),EQ(4),GA(4),RAT(51),RSLOPE(51),RERROR(51)
     3,X1(15),X2(51),D(51,4)
     4,CALYLA(51,4),YLA(51,4),YLADIF(51,4),CALYRA(51,4),YRA(51,4)
     5,YRADIF(51,4),DELA(4),DELINT(51,4,7),DELTRS(51),COEFT(4)
      DATA FNUM/0.5,1.0,2.5,5.0,10.0,25.0,50.0/
      DATA TS/0.0,12.706,4.303,3.182,2.776/
      IF (LKODE.EQ.2) GO TO 30
      IF(LKODE.EQ.3) GO TO 1999
      NL=NL-KM
      DATA EQ/38175.,33096.,26140.,33507./,GA/7.49,6.462,0.2212,4.480/
      IF(IARTP.NE.9) GO TO 35
      WRITE (6,9999)
9999  FORMAT (///,T10,'***** BAINFIELD AND HUBER GA VALUES USED*****')
      GA(1)=10.25
      GA(2)=5.619
      GA(3)=0.1994
      GA(4)=4.059
      GO TO 35
   30 CONTINUE
      EQ(1)=116634.
      EQ(2)=118893.
      EQ(3)=117199.
      EQ(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)=20.64
      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                                                          2001
      GA(1)=3.96                                                        2002
      GA(2)=45.0                                                        2003
      GA(3)=18.0                                                        2004
      GA(4)=27.0                                                        2005
      GO TO 35                                                          2006
  104 CONTINUE                                                          2007
      GA(1)=2.28                                                        2008
      GA(2)=32.0                                                        2009
      GA(3)=11.5                                                        2010
      GA(4)=18.9                                                        2011
      GO TO 35                                                          2012
  105 CONTINUE                                                          2013
      GA(1)=2.37                                                        2014
      GA(2)=36.0                                                        2015
      GA(3)=14.0                                                        2016
      GA(4)=21.3                                                        2017
   35 IF (NLZT.GE.3) GO TO 1                                            2018
      WRITE (6,99)                                                      2019
   99 FORMAT (15X,'INSUFFICIENT NUMBER OF DATA POINTS TO CALCULATE SLOPE 2020
     1 TEMP.')                                                          2021
      RETURN                                                            2022
    1 DO 25 NPOLY=1,KM                                                  2023
      NL=NL+1                                                           2024
      WRITE (6,1005)                                                    2025
 1005 FORMAT (/////)                                                    2026
      IF (KM.EQ.1) GO TO 15                                             2027
      WRITE (6,1006) FNUM(NL)                                           2028
 1006 FORMAT (10X,'0KABEL MULTIPLE F-TEST POLYNOMIAL TEMPERATURE CALCULA 2029
     1TIONS FOR'/T15,F5.2,'  PERCENT PROBABILITY OF EXCEEDING THE F-VALU 2030
     2E')                                                               2031
   15 WRITE (6,1000)                                                    2032
 1000 FORMAT (5X,'CALCULATION OF TEMPERATURE BY THE LEAST-SQUARES SLOPE  2033
     1METHOD')                                                          2034
      DO 2 II=1,NLZT                                                    2035
      DO 2 IJ=1,NT                                                      2036
    2 YCALCN(IJ,II)=ARI(IJ,II)                                          2037
      CALL LSQ (NT,YCALCN,NLZT,TS,GA,EQ,YINLA,TLA,SLOPEL,ERRORL,WAVE,   2038
     1CALYLA,YLA,YLADIF)                                                2039
      WRITE (6,1001)                                                    2040
 1001 FORMAT ('            X          T(X)          SLOPE(X)        95 CL 2041
     1   Y-INTERCEPT')                                                  2042
      DO 3 I=1,NT                                                       2043
 1002 FORMAT (T2,E11.4,1X,E11.4,2X,E11.4,2(4X,E11.4))                   2044
    3 WRITE (6,1002) RBP(I,1),TLA(I),SLOPEL(I),ERRORL(I),YINLA(I)       2045
      IF (KPNED1.NE.1) GO TO 28                                         2046
      WRITE (7,7000) DLAB                                               2047
 7000 FORMAT (10X,'LATERAL SLOPE TEMP. DATA FOR',5X,5A4,5X,'RUN')       2048
      DO 29 I2=1,NT                                                     2049
 7001 FORMAT (2F10.3)                                                   2050
```

```
   29 WRITE (7,7001) TLA(I2),RBP(I2,1)                                    2051
      WRITE (6,7002) DLAB                                                 2052
 7002 FORMAT (///,T10,'LATERAL SLOPE TEMP DATA HAS BEEN PUNCHED FOR USE   2053
     1IN THE ELECTRON',/,T10,'DENSITY PROGRAM FOR THE DATA RUN',5X,5A4)    2054
   28 DO 4 KK=1,NLZT                                                      2055
      DO 4 KL=1,IMAT                                                      2056
      K=(IMAT-KL)+2                                                       2057
    4 YCALCN(KL,KK)=RADINT(K,KK,NPOLY)                                    2058
      CALL LSQ (IMAT,YCALCN,NLZT,TS,GA,EQ,RAYIN,RAT,RSLOPE,RERROR,WAVE,   2059
     1CALYRA,YRA,YRADIF)                                                  2060
      DO 40 I=1,NLZT                                                      2061
      DO 40 J=1,IMAT                                                      2062
      K=(IMAT-J)+2                                                        2063
   40 D(J,I)=DELINT(K,I,NPOLY)                                            2064
      SUMEQ=0.0                                                           2065
      SUMEQ2=0.0                                                          2066
      DO 39 L=1,NLZT                                                      2067
      SUMEQ=SUMEQ+EQ(L)                                                   2068
   39 SUMEQ2=SUMEQ2+(EQ(L)*EQ(L))                                         2069
      DENOMT=ABS((NLZT*SUMEQ2)-(SUMEQ*SUMEQ))                             2070
      DO 38 M=1,NLZT                                                      2071
   38 COEFT(M)=ABS((NLZT*EQ(M))-SUMEQ)                                    2072
      DO 37 N=1,IMAT                                                      2073
      XMULT=RAT(N)/(1.439*DENOMT)                                         2074
      TERM=0.0                                                            2075
      DO 36 M=1,NLZT                                                      2076
   36 TERM=TERM+(COEFT(M)*(DELA(M)+D(N,M)))                               2077
   37 DELTRS(N)=XMULT*TERM                                                2078
      WRITE (6,1003)                                                      2079
 1003 FORMAT ('          R          T(R)          SLOPE(R)        95 CL   2080
     1  Y-INTERCEPT',6X,'DELTA T(R) IN PERCENT')                         2081
      DO 5 J=1,IMAT                                                       2082
      K1=(IMAT-J)+2                                                       2083
 1004 FORMAT (T2,E11.4,1X,E11.4,2X,E11.4,2(4X,E11.4),12X,E11.4)           2084
    5 WRITE (6,1004) RADIST(K1,1,NPOLY),RAT(J),RSLOPE(J),RERROR(J),RAYIN  2085
     1(J),DELTRS(J)                                                       2086
      IF (KPNED2.NE.1) GO TO 33                                           2087
      WRITE (7,8000) DLAB                                                 2088
 8000 FORMAT (10X,'RADIAL SLOPE TEMP. DATA FOR',5X,5A4,5X,'RUN')          2089
      DO 34 J2=1,IMAT                                                     2090
      K2=(IMAT-J2)+2                                                      2091
 8001 FORMAT (2F10.3,15X,'DEGREE',I5,5A4)                                 2092
   34 WRITE (7,8001) RAT(J2),RADIST(K2,1,NPOLY),NL,DLAB                   2093
      WRITE (6,8002) DLAB                                                 2094
 8002 FORMAT (///,T10,'RADIAL SLOPE TEMP. DATA HAS BEEN PUNCHED FOR USE   2095
     1IN THE ELECTRON',/,T10,'DENSITY PROGRAM FOR THE DATA RUN',5X,5A4)    2096
   33 WRITE (6,3000)                                                      2097
 3000 FORMAT (/////)                                                      2098
      WRITE (6,3001)                                                      2099
 3001 FORMAT (T25,'LATERAL INTENSITY DATA,  Y=LOG(GA/WAVE*I(X))',///)      2100
```

```
      DO 6 N1=1,NT                                                          2101
      WRITE (6,3002) RBP(N1,1),TLA(N1)                                      2102
3002  FORMAT(/T15,'LATERAL DISTANCE = ',E11.4,2X,'T(X) = ',E11.4)           2103
      WRITE (6,3003)                                                        2104
3003  FORMAT (/T3,'WAVELENGTH      CALC Y         EXPT Y         DEL Y      2105
     1EXC. POT.',/)                                                         2106
      DO 6 N2=1,NLZT                                                        2107
3004  FORMAT (T2,5(E11.4,2X))                                               2108
    6 WRITE (6,3004) WAVE(N2),CALYLA(N1,N2),YLA(N1,N2),YLADIF(N1,N2),EQ(    2109
     1N2)                                                                   2110
      WRITE (6,3005)                                                        2111
3005  FORMAT (//////////,T25,'RADIAL INTENSITY DATA, Y=LOG(GA/WAVE*I(R))    2112
     1',///)                                                                2113
      DO 7 N3=1,IMAT                                                        2114
      KKK=(IMAT-N3)+2                                                       2115
      WRITE (6,3006) RADIST(KKK,1,NPOLY),RAT(N3)                            2116
3006  FORMAT (/T15,'RADIAL DISTANCE = ',E11.4,2X,'T(R) = ',E11.4)           2117
      WRITE (6,3007)                                                        2118
3007  FORMAT (/T3,'WAVELENGTH      CALC Y         EXPT Y         DEL Y      2119
     1EXC. POT.',/)                                                         2120
      DO 7 N4=1,NLZT                                                        2121
3008  FORMAT (T2,5(E11.4,2X))                                               2122
    7 WRITE (6,3008) WAVE(N4),CALYRA(N3,N4),YRA(N3,N4),YRADIF(N3,N4),EQ(    2123
     1N4)                                                                   2124
      IF (KPLOT3.EQ.1) GO TO 25                                             2125
      DO 10 M=1,NT                                                          2126
   10 X1(M)=RBP(M,1)                                                        2127
      DO 20 N=1,IMAT                                                        2128
      K2=(IMAT-N)+2                                                         2129
   20 X2(N)=RADIST(K2,1,NPOLY)                                              2130
      CALL GRAPH (NT,X1,TLA,0.2,7.0,9.,0.0,0.0,2500.,'X AND R (MM)',',',SLOP 2131
     1E T(X) AND T(R)',',SLOPE TEMP. PROFILE',DLAB)                         2132
      CALL GRAPHS (NT,X1,TLA,4,107,'LATERAL SLOPE TEMP.',')                 2133
      CALL GRAPHS (IMAT,X2,RAT,1,111,'RADIAL SLOPE TEMP.',')                2134
   25 CONTINUE                                                              2135
      RETURN                                                                2136
      END                                                                   2137
      SUBROUTINE LSQ (INDEX,YCALCN,NLZT,TS,GA,EQ,YIN,TEMP,SLOPE,ERRORM,     2138
     1WAVE,CALCY,Y,YDIF)                                                    2139
      DIMENSION YCALCN(51,4),TS(5),GA(4),EQ(4),YIN(51),TEMP(51),SLOPE(51    2140
     1),ERRORM(51),SUMX(51),SUMY(51),SUMXX(51),SUMXY(51),WAVE(4),DENOM(5    2141
     21),SSE(51),SSEX(51),XBAR(51),DIFY(4),DIFX(4)                          2142
     3,CALCY(51,4),Y(51,4),YDIF(51,4)                                       2143
    8 DO 50 I=1,INDEX                                                       2144
      SUMX(I)=0.0                                                           2145
      SUMY(I)=0.0                                                           2146
      SUMXX(I)=0.0                                                          2147
      SUMXY(I)=0.0                                                          2148
      DO 2 J=1,NLZT                                                         2149
      SUMX(I)=SUMX(I)+EQ(J)                                                 2150
```

```
      SUMY(I)=SUMY(I)+ALOG10(GA(J)/(WAVE(J)*YCALCN(I,J)))                    2151
      SUMXX(I)=SUMXX(I)+(EQ(J)*EQ(J))                                        2152
    2 SUMXY(I)=SUMXY(I)+(EQ(J)*ALOG10(GA(J)/(WAVE(J)*YCALCN(I,J))))          2153
      D=NLZT                                                                 2154
      DENOM(I)=(D*SUMXX(I))-(SUMX(I)*SUMX(I))                                2155
      SLOPE(I)=((D*SUMXY(I))-(SUMX(I)*SUMY(I)))/DENOM(I)                     2156
      YIN(I)= ((SUMXX(I)*SUMY(I))-(SUMXY(I)*SUMX(I)))/DENOM(I)               2157
      SSE(I)=0.0                                                             2158
      SSEX(I)=0.0                                                            2159
      XBAR(I)=SUMX(I)/D                                                      2160
      DO 3 L=1,NLZT                                                          2161
      CALCY(I,L)=SLOPE(I)*EQ(L)+YIN(I)                                       2162
      Y(I,L)=ALOG10(GA(L)/(WAVE(L)*YCALCN(I,L)))                             2163
      YDIF(I,L)=Y(I,L)-CALCY(I,L)                                            2164
      DIFY(L)=YDIF(I,L)*YDIF(I,L)                                            2165
      SSE(I)=SSE(I)+DIFY(L)                                                  2166
      XDIF=EQ(L)-XBAR(I)                                                     2167
      DIFX(L)=XDIF*XDIF                                                      2168
    3 SSEX(I)=SSEX(I)+DIFX(L)                                                2169
      SSEX(I)=SQRT(SSEX(I))                                                  2170
      S=SQRT(SSE(I)/(D-2.))                                                  2171
      ERRORM(I)=(TS(NLZT)*S)/SSEX(I)                                         2172
      TEMP(I)=1./(1.60013*SLOPE(I))                                          2173
   50 CONTINUE                                                               2174
      RETURN                                                                 2175
      END                                                                    2176
```

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]

$$I(X) = 2\int_0^{Y(X)} J(R)\, dY \qquad (B1)$$

The factor of 2 in Equation B1 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

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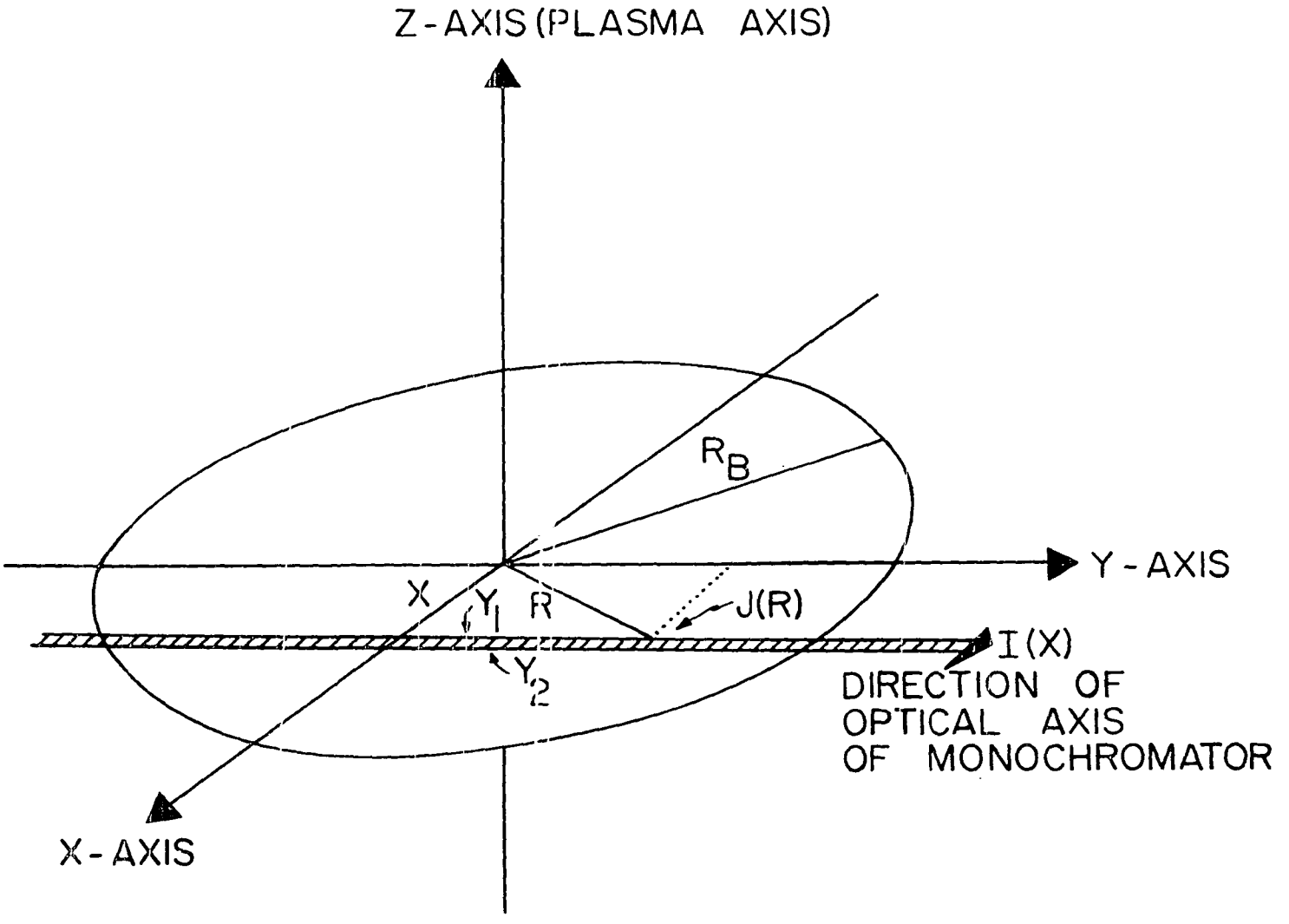
[1] It is important to realize that Equation B1 expresses the geometrical relationship between the spatially resolved emission, which is projected from unit volume of a horizontal section of the source parallel to the Y-axis, i.e., J(R) and, the space integrated intensity radiated over the depth of that 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


Z-AXIS (PLASMA AXIS)
R_B
Y - AXIS
X
Y_1
R
J(R)
I(X)
Y_2
DIRECTION OF
OPTICAL AXIS
OF MONOCHROMATOR
X - AXIS

$$R^2 = X^2 + Y^2$$
$$Y = (R^2 - X^2)^{1/2} \qquad \text{(B2)}$$
$$dY = R(R^2 - X^2)^{-1/2}\, dR$$

is performed, Equation B1 becomes

$$I(X) = 2\int_X^{R_B} R\, J(R)\, (R^2 - X^2)^{-1/2}\, dR \qquad \text{(B3)}$$

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, $$\text{(B4)}$$
$$R = R_B \quad \text{at} \quad Y = Y(X)$$

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 (36,40,129).

$$J(R) = -\frac{1}{\pi}\int_R^{R_B} \frac{I'(X)}{(X^2 - R^2)^{1/2}}\, dX \qquad \text{(B5)}$$

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.,

$$I'(X) = d(I(X))/dX$$

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. Hormann (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

$$v = R^2 \text{ and } u = X^2 \tag{B6}$$

Equation B5 became

$$J(R(v)) = -(1/\pi)\int_{v}^{R_B^2} I'(u)\,(u - v)^{-1/2}\,du \tag{B7}$$

where, the following relationships were employed

$$\begin{aligned} dX &= (1/2)\,u^{-1/2}\,du \\ (X^2 - R^2)^{1/2} &= (u - v)^{1/2} \\ d(I(u))/du &= (d(I(X))/dX)(d(g(u))/du) \end{aligned} \tag{B8}$$

and,

$$\begin{aligned} g(u) &= X = u^{1/2} \\ I'(X) &= 2\,u^{1/2}\,I'(u) \end{aligned} \tag{B9}$$

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

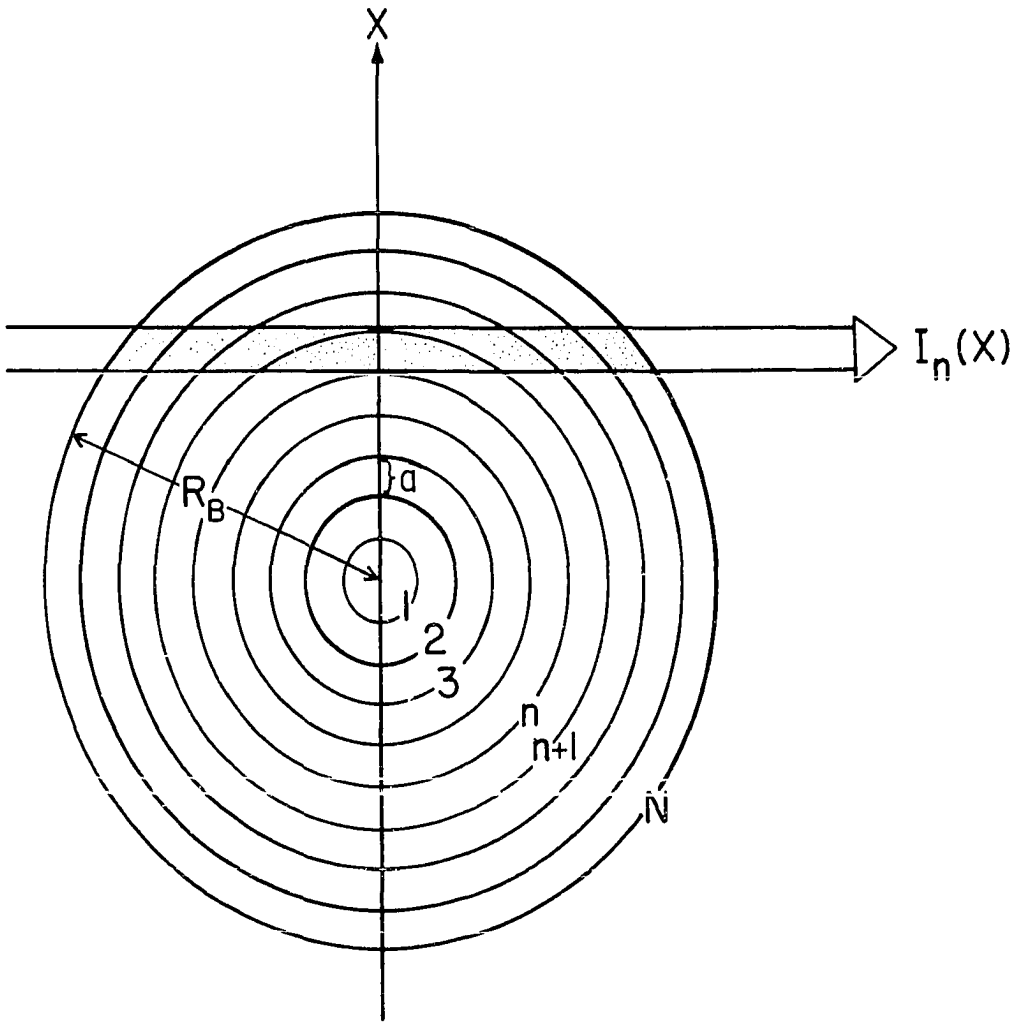


Figure B-2. Two-dimensional representation of a circularly symmetric source divided into N zones of equal width, a

for any zone, k

$$J_k = J(ak) = (-1/\pi) \sum_{n=k}^{N-1} I_n'(u) \int_{(an)^2}^{(a(n+1))^2} (u - (ak)^2)^{-1/2} \, du \qquad \text{(B10)}$$

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

$$I_n'(u) = \frac{(I_{n+1}(u) - I_n(u))}{a^2((n+1)^2 - n^2)} \qquad \text{(B11)}$$

Substitution of Equation B11 into B10 and subsequent integration yielded

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N-1} (I_{n+1}(u) - I_n(u)) \times \frac{((n+1)^2 - k^2)^{1/2} - (n^2 - k^2)^{1/2}}{(2n + 1)} \qquad \text{(B12)}$$

A transformation to the original coordinate system yielded

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N-1} A_{kn} (I_{n+1}(X) - I_n(X)) \qquad \text{(B13)}$$

where,

$$A_{kn} = \frac{((n+1)^2 - k^2)^{1/2} - (n^2 - k^2)^{1/2}}{(2n + 1)} \qquad \text{(B14)}$$

Equation B14 was further simplified to yield

$$J_k = -\frac{2}{a\pi} \sum_{n=k}^{N} B_{kn} I_n \qquad \text{(B15)}$$

where,

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

and (B16)

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

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

$$I(X) = C_o + C_1X + C_2X^2 + \cdots + C_nX^n \qquad (B17)$$

with the corresponding derivative function

$$I'(X) = C_1 + 2C_2X + 3C_3X^2 + \cdots + nC_nX^{n-1} \qquad (B18)$$

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

$$J(R) = -\frac{1}{\pi}\int_R^{R_B} \frac{(C_1 + 2C_2X + \cdots + nC_nX^{n-1})}{(X^2 - R^2)^{1/2}}\,dX \qquad (B19)$$

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

$$I_k(X) = {}_kC_o + \sum_{i=1}^{n} {}_kC_i \, X^i, \quad \text{for } k = 1, 2, \ldots, m \qquad \text{(B20)}$$

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

$$S_k = - I_k'(X)/((X^2 - R^2)^{1/2}) \qquad \text{(B21)}$$

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

$$R_{k-1} \leq R \leq R_k \qquad \text{(B22)}$$

the radial intensity is given by

$$J(R) = {}_kF_o(R) + F_1(R) \tag{B23}$$

where, ${}_kF_o(R)$ and $F_1(R)$ are defined by

$${}_kF_o(R) = \int_R^{R_k} S_k \, dX \tag{B24}$$

and

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

$$= 0 \qquad\qquad\qquad\qquad \text{for} \quad k = m \tag{B25}$$

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 $R_o=0$ 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 R = 0. When Equation B20 was differentiated the following form was obtained

$$I_k'(X) = {}_kC_1 + \sum_{i=2}^{n} ({}_kC_i) \, i \, X^{i-1} \tag{B26}$$

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

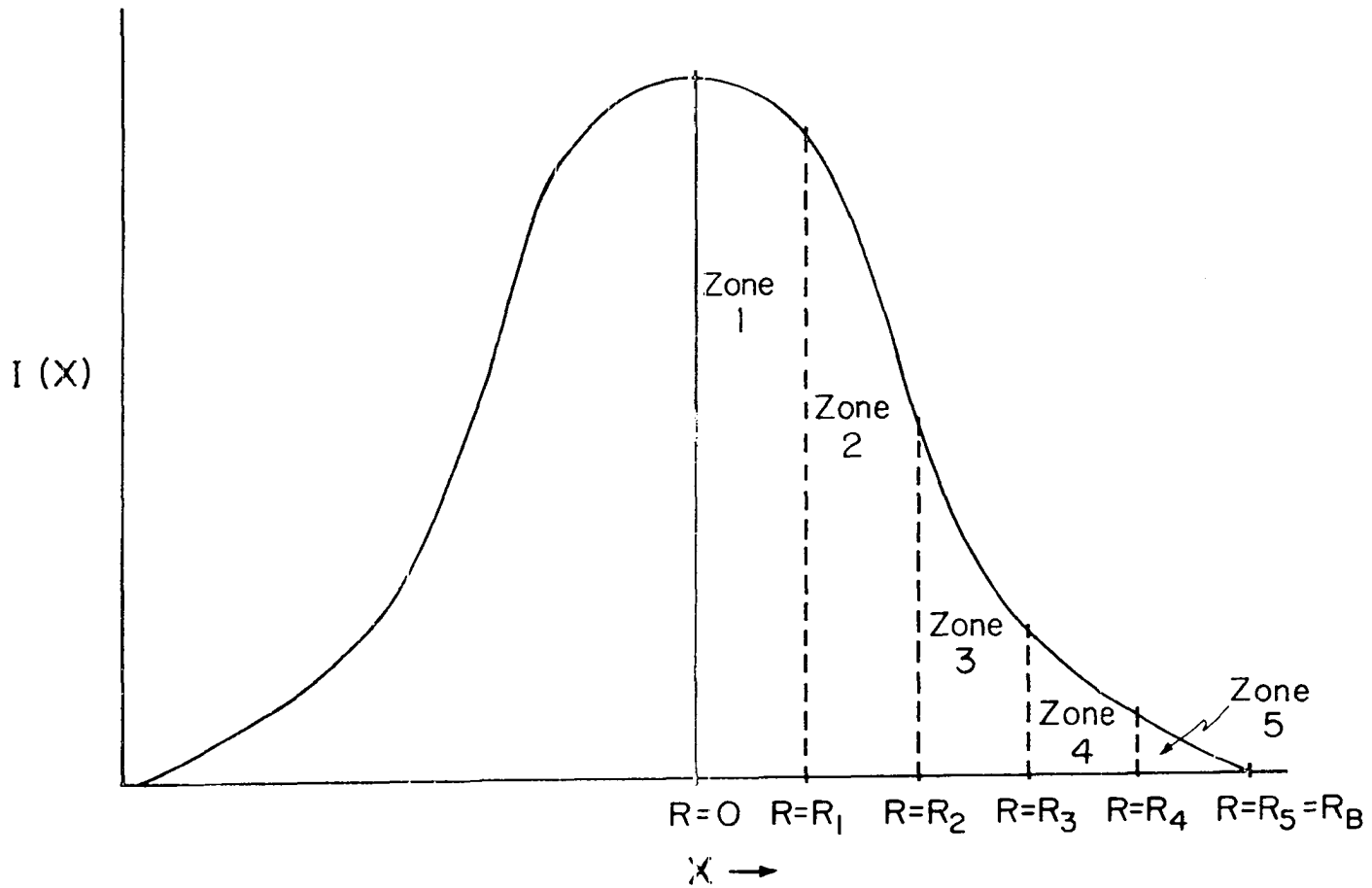


Figure B-3. Schematic representation of five zone subdivision of the I(X) profile (bell-type curve case)

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.,

$$I_1(X) = {}_1C_o + \sum_{i=1}^{n} {}_1C_i \, X^{2i} \tag{B27}$$

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 ${}_kF_o(R)$ and $F_1(R)$. Substitution of the 4-th degres polynomial of the form given by Equation B20 into Equation B24 yielded

$${}_kF_o(R) = -\frac{1}{\pi}\left(\int_R^{R_k} \frac{{}_kC_1}{G(X,R)}\,dX + 2\int_R^{R_k} \frac{{}_kC_2\,X}{G(X,R)}\,dX + 3\int_R^{R_k} \frac{{}_kC_3\,X^2}{G(X,R)}\,dX + 4\int_R^{R_k} \frac{{}_kC_4\,X^3}{G(X,R)}\,dX\right) \tag{B28}$$

where, n = 4 and

$$G(X,R) = (X^2 - R^2)^{1/2} \tag{B29}$$

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

$$\begin{aligned} {}_kF_o(R) = -\frac{1}{\pi}\Big[& {}_kC_1 \ln(X + G(X,R)) + 2\ {}_kC_2\ G(X,R) \\ & + \frac{3}{2}\ {}_kC_3\ (X\ G(X,R) + R^2 \ln(X + G(X,R))) \\ & + 4\ {}_kC_4\ (G^3(X,R)/3 + R^2\ G(X,R))\Big]_R^{R_k} \end{aligned} \tag{B30}$$

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

$$\begin{aligned} {}_kF_o(R) = -\frac{1}{\pi}\Big(& {}_kC_1 \ln\Big(\frac{R_k + G(R_k,R)}{R}\Big) + 2\ {}_kC_2\ G(R_k,R) \\ & + \frac{3}{2}\ {}_kC_3\ (R_k\ G(R_k,R) + R^2 \ln\Big(\frac{R_k + G(R_k,R)}{R}\Big)) \\ & + 4\ {}_kC_4\ (G^3(R_k,R)/3 + R^2\ G(R_k,R))\Big) \end{aligned} \tag{B31}$$

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

$$\ell n(X + G(X,R)) = \ell n(R) \quad \text{for} \quad X = R$$

For a given R such that $R_4 \leq R \leq R_5$, ${}_5F_0(R)$ 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.,

$$\begin{aligned} F_1(R) = \sum_{i=k+1}^{5} (-\tfrac{1}{\pi}) \, (({}_iC_1 \, \ell n(R_i + G(R_i,R)) \\ + 2 \, {}_iC_2 \, G(R_i,R)) + \tfrac{3}{2} \, {}_iC_3 \, (R_i \, G(R_i,R) \\ + R^2 \, \ell n(R_i + G(R_i,R))) + 4 \, {}_iC_4 \, (G^3(R_i,R)/3 \\ + R^2 \, G(R_i,R))) - ({}_iC_1 \, \ell n(R_{i-1} + G(R_{i-1},R)) \\ + 2 \, {}_iC_2 \, G(R_{i-1},R) + \tfrac{3}{2} \, {}_iC_3 \, (R_{i-1} \, G(R_{i-1},R) \\ + R^2 \, \ell n(R_{i-1} + G(R_{i-1},R))) \\ + 4 \, {}_iC_4 \, (G^3(R_{i-1},R)/3 + R^2 \, G(R_{i-1},R)))) \end{aligned} \tag{B32}$$

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

$$ {}_1F_o(R) = \left(-\frac{2}{\pi}\right)\left(\int_R^{R_1} \frac{{}_1C_1\, X}{G(X,R)}\, dX + 2\int_R^{R_1} \frac{{}_1C_2\, X^3}{G(X,R)}\, dX + 3\int_R^{R_1} \frac{{}_1C_3\, X^5}{G(X,R)}\, dX + 4\int_R^{R_1} \frac{{}_1C_4\, X^7}{G(X,R)}\, dX\right) \qquad \text{(B33)} $$

where, n = 4 and the notation of Equation B29 was used. When the integration was performed and the limits were evaluated, ${}_1F_o(R)$ was given by

$$ \begin{aligned} {}_1F_o(R) = \left(-\frac{2}{\pi}\right)\Big({}_1C_1\, G(R_1,R) &+ 2\,{}_1C_2\,\left(G^3(R_1,R)/3 + R^2\, G(R_1,R)\right) \\ &+ 3\,{}_1C_3\,\left(R^4\, G(R_1,R) + \frac{2}{3} R^2\, G^3(R_1,R) + \frac{1}{5} G^5(R_1,R)\right) \\ &+ 4\,{}_1C_4\,\left(R^6\, G(R_1,R) + R^4\, G^3(R_1,R) + \frac{3}{5} R^2\, G^5(R_1,R) + \frac{1}{7} G^7(R_1,R)\right)\Big) \end{aligned} \qquad \text{(B34)} $$

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

$$I(X=0) = 2\int_0^{R_B} J(R)\, dR \qquad (B35)$$

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 ∿1 to 5% for bell-type profiles and ∿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, ${}_1C_j$, and the radial position R. When the uncertainty in R was assumed to be negligible, a maximum differential error treatment yielded

$$\Delta J(R)_k \approx \sum_{j=1}^{4} \left\{ \left| \frac{\partial_k F_o(R)}{\partial_k C_j} \right| \Delta_k C_j + \sum_{i=k+1}^{5} \left| \frac{\partial F_1(R)}{\partial_i C_j} \right| \Delta_i C_j \right\} \tag{B36}$$

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 ${}_1F_o(R)$ and $F_1(R)$, 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 $J(R)_k$ 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 ($\Delta_i C_j$) were obtained from the error analysis techniques incorporated within the polynomial fitting method employed (reference 81, Chapter 8).

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)

$$Z^{z-1}(T) = \sum_{n} g_n \exp(-\frac{E_n}{kT}) \qquad (C1)$$

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_1^{z-1}) of the species is approached, the sum in Equation C1 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, ΔE_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)

$$E_i^{z-1} - E_{n\ell}^{z-1} = \frac{z^2 E_H}{n^2} \qquad (C2)$$

where, E_H is the ionization energy of atomic hydrogen (109,679 cm^{-1}) and $n \geq 4$. The statistical weight of the level

$E_{n\ell}^{z-1}$, 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

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

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

$$n^* = n - \alpha - \frac{z^2}{n^2}\beta \tag{C4}$$

where, z = 1 for neutral atoms, z = 2 for singly charged ions, z = 3 for doubly charged ions, etc., and α,β 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 α and β, 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

$$n^* = n_{max} \leq \left(\frac{z^2 E_H}{E_i^{z-1}}\right)^{1/2} \tag{C5}$$

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

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

$$\times \sum_{n=n'+1}^{n_{max}} 2n^2 \exp\left(-\frac{E_i^{z-1} - (z^2 E_H/n^2)}{kT}\right) \tag{C6}$$

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_{max}); (2) a weighted maximum principal quantum number, n_w, was calculated according to the total degeneracy of each series term ($n_w = (2S+1)(2L+1)(n_{max})$); (3) a weighted average maximum principal quantum number was defined by

$$n_{wa} = \frac{1}{N_d} \sum_{i=1}^{N} (n_w)_i \qquad (C7)$$

where, N_d = sum of the degeneracies of the observed spectral terms,

$$N_d = \sum_{j=1}^{N} (n_{max})_j \qquad (C8)$$

and, N = number of observed spectral terms; (4) n' was taken as the largest integer satisfying the inequality $n' \leq n_{wa}$; and (5) the correction was begun at $n'' = (n'+1)$ where, n'' was the smallest integer which satisfied the condition, $n_{wa} \leq n''$. 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_{max} values) and, the correction for missing levels was begun above a weighted average of these n_{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.

Table C-1. Data card requirements for C337EDNS

Type #	# Cards	Columns	Variable Name	Format	Remarks
1	1	1- 5	NSETS	I5	Number of data sets; one data set per Saha element
2	500	1- 8	TSYM	2A4	Element identifier of partition function arrays
	(max)	11-20	TTEST	F10.0	Temperature array for partition functions
		21-30	QTEST(1,i)	F10.0	Partition function array for neutral atom species
		31-40	QTEST(2,i)	F10.0	Partition function array for first ion species
		41-50	QTEST(3,i)	F10.0	Partition function array for second ion species
3	1/set	1- 5	NRUNS	I5	Number of runs in a given data set
4	1/run	1-70	XIDENT	35A2	Data set identification label
		71-75	NUMAQP	I5	Number of transition probability sources (5 max)
5	1/run	1-10	WAVEA	F10.0	Wavelength of atomic line (Angstrom units)
		11-20	WAVEI	F10.0	Wavelength of ionic line (Angstrom units)
		21-30	GATOM	F10.0	Degeneracy of atomic line emitting level
		31-40	GION	F10.0	Degeneracy of ionic line emitting level
		41-50	EQATOM	F10.0	Excitation energy of atomic line (cm^{-1} units)

Table C-1. (Continued)

Type #	# Cards	Columns	Variable Name	Format	Remarks
		51-60	EQION	F10.0	Excitation energy of ionic line (cm^{-1} units)
6a	1/run	1-50	A(1,j)	5F10.0	Transition probability array for atomic line (5 max)
6b	1/run		A(2,j)		Same as 6a except for ionic line
7	1/run	1-10	XIP	F10.0	Ionization energy of atomic species (cm^{-1} units)
		11-20	DELXIP	F10.0	Ionization energy lowering
8	1/run	1- 5	NR	I5	Number of radial positions
9	NR/run	1-10	TR	F10.0	Radial temperature array
		11-20	R	F10.0	Corresponding radial position array
10a	NR/run	1-10	XI(i,1)	F10.0	Radial intensity array for atomic line
		21-30	DELIR(i,1)	F10.4	Corresponding relative uncertainty array (%)
10b	NR/run		XI(i,2)		Same as 10a except for ionic line
			DELIR(i,2)		Same as 10a except for ionic line

```
C                                                                       1
C                                                                       2
C                                                                       3
C                                                                       4
C        **********    C337EDNS    *********                          5
C                                                                       6
C                                                                       7
C     PROGRAM TO CALCULATE ELECTRON DENSITIES FROM RADIAL TEMPERATURE   8
C     AND ATOM,ION LINE INTENSITIES                                     9
C                                                                       10
C                                                                       11
C     NUMAQP=NUMBER OF TRANSITION PROBABILITY PAIRS (5 MAX)             12
C     NSETS=NUMBER OF DATA SETS                                         13
C     TSYM=ELEMENT IDENTIFIER FOR QTEST ARRAY  ALSO STOPS TTEST READ    14
C     TTEST=TEMP ARRAYFOR INPUT PARTITION FUNCTIONS                     15
C     QTEST(1,I)=PARTITION FUNCTION ARRAY FOR ATOM                      16
C     QTEST(2,I)=      "          "      "    1ST ION                  17
C     QTEST(3,I)=      "          "      "    2ND ION                  18
C     NRUNS=NUMBER OF RUNS PER DATA SET                                 19
C     XIDENT=IDENTIFICATION OF DATA SET                                 20
C     WAVEA=ATOM LINE WAVELENGTH (ANGSTROM UNITS)                       21
C     WAVEI=ION    "       "       "      "                             22
C     GATOM=UPPER LEVEL DEGENERACY FOR ATOM LINE                        23
C     GION=  "      "       "      "   ION   "                          24
C     EQATOM=EXCITATION POTENTIAL OF ATOM LINE (RECIPROCAL CM UNITS)    25
C     EQION=     "        "      "  ION   "       "        "    "      26
C     A(1,J)=TRANS PROB ARRAY FOR ATOM LINE(5 MAX)                      27
C     A(2,J)=  "     "    "    "   ION   "       "                     28
C     XIP=IONIZATION POTENTIAL OF ATOM SPECIES (RECIPROCAL CM UNITS)    29
C     DELIXP=LOWERING OF IONIZATION POTENTIAL       "        "    "     30
C     NR=NUMBER OF RADIAL POSITIONS                                     31
C     TR(I)=RADIAL TEMP ARRAY                                           32
C     R(I)=    "    DIST   "                                            33
C     XI(I,1)=RADIAL INTENSITY ARRAY FOR ATOM LINE                      34
C     XI(I,2)=  "       "       "    "   ION   "                       35
C     DELIR(I,1) = RADIAL ERROR ARRAY (PERCENT) FOR ATOM LINE           36
C     DELIR(I,2) = RADIAL ERROR ARRAY (PERCENT) FOR ION  LINE           37
C                                                                       38
C                                                                       39
      DIMENSION SUMDEN(51),SUMRAT(51),SUMS(51),DELIR(51,2)              40
      DIMENSION TTEST(500),S(51)                                        41
      DIMENSION TSYM(2),QTEST(3,500),QZERO(51),QPLUS(51),RATION(51)     42
      DIMENSION XIDENT(35),TR(51),R(51),XI(51,2),EDENS(51),A(2,5)       43
      DATA CHECKT/'ENDT'/                                               44
      READ(5,100) NSETS                                                 45
  100 FORMAT(I5)                                                        46
      DO 999 INDEX=1,NSETS                                              47
      DO 5 I=1,500                                                      48
    4 FORMAT(2A4,2X,F10.0,3F10.4)                                       49
      READ(5,4) TSYM,TTEST(I),QTEST(1,I),QTEST(2,I),QTEST(3,I)          50
```

```
      IF(TSYM(1).EQ.CHECKT) GO TO 6                                          51
    5 CONTINUE                                                               52
    6 ITEST=I-1                                                              53
      READ(5,99) NRUNS                                                       54
   99 FORMAT(I5)                                                             55
      DO 999 ILOOP=1,NRUNS                                                   56
      READ(5,101) XIDENT,NUMAQP                                              57
  101 FORMAT(35A2,I5)                                                        58
      READ(5,102) WAVEA,WAVEI,GATOM,GION,EQATOM,EQION                        59
  102 FORMAT(6F10.0)                                                         60
      DO 200 I=1,2                                                           61
  201 FORMAT(5F10.0)                                                         62
  200 READ (5,201) (A(I,J),J=1,NUMAQP)                                       63
      READ(5,103) XIP,DELXIP                                                 64
  103 FORMAT(2F10.0)                                                         65
      READ(5,104) NR                                                         66
  104 FORMAT(I5)                                                             67
      DO 10 I=1,NR                                                           68
  105 FORMAT(2F10.0)                                                         69
      READ(5,105) TR(I),R(I)                                                 70
      DO 9 J=1,ITEST                                                         71
      IF(ABS(TR(I)-TTEST(J)).GT.5.0) GO TO 9                                 72
      QZERO(I)=QTEST(1,J)                                                    73
      QPLUS(I)=QTEST(2,J)                                                    74
      GO TO 10                                                               75
    9 CONTINUE                                                               76
   10 CONTINUE                                                               77
      DO 20 J=1,2                                                            78
      DO 20 I=1,NR                                                           79
  106 FORMAT(F10.0,10X,F10.4)                                                80
   20 READ(5,106) XI(I,J),DELIR(I,J)                                         81
      DO 25 I=1,NR                                                           82
      SUMDEN(I)=0.0                                                          83
      SUMRAT(I)=0.0                                                          84
   25 SUMS(I)=0.0                                                            85
      DO 998 IDEX=1,NUMAQP                                                   86
      AATOM=A(1,IDEX)                                                        87
      AION=A(2,IDEX)                                                         88
      DO 30 I=1,NR                                                           89
      EFAC=EQATOM-EQION-XIP+DELXIP                                           90
      EFAC=EFAC/0.69505                                                      91
      ERRFAC=(1.50-(EFAC/TR(I)))*100.0                                       92
      ERRFAC=(ERRFAC**2)/100.0                                               93
      EXP=2.71828**(EFAC/TR(I))                                              94
      TTERM=TR(I)**1.5                                                       95
      RATIO=(XI(I,1)*WAVEA*GION*AION)/(XI(I,2)*WAVEI*GATOM*AATOM)            96
      EXPFAC=(EQION-EQATOM)/0.69505                                          97
      EXPN=2.71828**(EXPFAC/TR(I))                                           98
      ZRATIO=QPLUS(I)/QZERO(I)                                               99
      EIP=-(XIP-DELXIP)                                                      100
```

```
      EIP=EIP/0.69505                                                    101
      EXPIP=2.71828**(EIP/TR(I))                                         102
      SSTAR=4.8296E15*TTERM*ZRATIO*EXPIP                                 103
      RATION(I)=EXPN*ZRATIO/RATIO                                        104
      EDENS(I)=4.8296E15*RATIO*TTERM*EXP                                 105
      ERR1=200.+(DELIR(I,1)**2)+(DELIR(I,2)**2)+ERRFAC                   106
      S(I)=SQRT(ERR1*EDENS(I)*EDENS(I))                                  107
      S(I)=S(I)/EDENS(I)                                                 108
      SUMDEN(I)=SUMDEN(I)+EDENS(I)                                       109
      SUMRAT(I)=SUMRAT(I)+RATION(I)                                      110
   30 SUMS(I)=SUMS(I)+S(I)                                               111
      WRITE(6,1000) XIDENT                                               112
 1000 FORMAT(1H1,T10,'ELECTRON DENSITY CALCULATION; IDENT= ',35A2)        113
      WRITE(6,1001) WAVEA,GATOM,EQATOM,AATOM                             114
 1001 FORMAT(/////,T15,'ATOM LINE DATA:  WAVELENGTH = ',F10.4,2X,'GQ = '  115
     1,F10.4,2X,'EQ = ',F10.4,2X,'AQP = ',F10.4)                         116
      WRITE(6,1002) WAVEI,GION,EQION,AION                                117
 1002 FORMAT(//,T15,'ION LINE DATA:  WAVELENGTH = ',F10.4,2X,'GQ = ',F10  118
     1.4,2X,'EQ = ',F10.4,2X,'AQP = ',F10.4)                             119
      WRITE(6,1003) XIP,DELXIP                                           120
 1003 FORMAT(/////,T15,'IONIZATION POTENTIAL = ',F10.3,2X,'LOWERING OF I  121
     1ONIZATION POTENTIAL = ',F10.4)                                     122
      WRITE(6,1004)                                                      123
 1004 FORMAT(/////,T10,'RADIUS',T20,'TEMPERATURE',T35,'ION LINE INT',T55  124
     1,'ATOM LINE INT',T75,'ELECTRON DENSITY',T95,'ION/ATOM RATIO',T110,  125
     2'DELTA NE, PERCENT')                                               126
      DO 40 N=1,NR                                                       127
 1005 FORMAT(T5,F10.4,T20,F10.4,T35,E12.5,T55,E12.5,T75,E12.5,T95,E12.5,  128
     1T110,E12.5)                                                        129
   40 WRITE(6,1005) R(N),TR(N),XI(N,2),XI(N,1),EDENS(N),RATION(N),S(N)   130
  998 CONTINUE                                                           131
      WRITE(6,1006)                                                      132
 1006 FORMAT(1H1,//,T10,'AVERAGE VALUES')                                133
      WRITE(6,1004)                                                      134
      DO 50 N=1,NR                                                       135
 1007 FORMAT(T5,F10.4,T20,F10.4,T35,E12.5,T55,E12.5,T75,E12.5,T95,E12.5,  136
     1T110,E12.5)                                                        137
      SUMDEN(N)=SUMDEN(N)/NUMAQP                                         138
      SUMRAT(N)=SUMRAT(N)/NUMAQP                                         139
      SUMS(N)=SUMS(N)/NUMAQP                                             140
   50 WRITE(6,1007) R(N),TR(N),XI(N,2),XI(N,1),SUMDEN(N),SUMRAT(N),SUMS(  141
     1N)                                                                 142
  999 CONTINUE                                                           143
      STOP                                                               144
      END                                                                145
```

APPENDIX D:

CONVOLUTION AND H_β ELECTRON DENSITY CALCULATIONS

We consider the convolution integral for the "folding" of lorentzian and gaussian line profiles (61,93)

$$I^F(\Delta\lambda^*) = \int_{-\infty}^{+\infty} I^G(\Delta\lambda)\ I^L(\Delta\lambda^* - \Delta\lambda)\ d(\Delta\lambda) \qquad (D1)$$

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.e., $I^L(\Delta\lambda^* - \Delta\lambda)$. 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

$$\int_{-\infty}^{+\infty} I^{G}(\Delta\lambda)\, d(\Delta\lambda) = \int_{-\infty}^{+\infty} I^{L}(\Delta\lambda)\, d(\Delta\lambda) = 1 \qquad \text{(D2)}$$

and, consequently

$$\int_{-\infty}^{+\infty} I^{F}(\Delta\lambda)\, d(\Delta\lambda) = 1 \qquad \text{(D3)}$$

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

$$\Delta\lambda' = \Delta\lambda^{*} - \Delta\lambda \qquad \text{(D4)}$$

then,

$$\Delta\lambda = \Delta\lambda^{*} - \Delta\lambda'$$

and (D5)

$$d(\Delta\lambda') = d(\Delta\lambda^{*}) - d(\Delta\lambda)$$

but,

$$d(\Delta\lambda^{*}) = 0 \qquad \text{(D6)}$$

thus,

$$d(\Delta\lambda') = -\, d(\Delta\lambda) \qquad \text{(D7)}$$

The change in the integration limits is given by

$$\Delta\lambda = -\infty \Longrightarrow \Delta\lambda' = +\infty$$

and (D8)

$$\Delta\lambda = +\infty \Longrightarrow \Delta\lambda' = -\infty$$

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

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

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

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

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_β 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)

$$\text{DENOM} = 1.25 \times 10^{-9} \, n_e^{2/3} \tag{D11}$$

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., $\Delta\lambda^G_{\frac{1}{2}}/\Delta\lambda^S_{\frac{1}{2}}$ 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 (98) 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 DCS1QU 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 H_β 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.

H_β Electron Density Program

The FORTRAN IV computer program which was written to perform the electron density calculations from Stark broadening measurements on the H_β 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 ($\alpha'_{\frac{1}{2}}$), which were calculated for the H_β 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 D-1. Data card requirements for C337CONV

Type #	# Cards	Columns	Variable Name	Format	Remarks
1	1	1- 5	NSETS	I5	Number of data sets
2	1/set	1- 5	NRUNS	I5	Number of runs for a given data set
3	1/set	1- 5	NPOINT	I5	Number of points in the instrument profile array
		6-10	ICONV	I5	Doppler/instrument profile convolution selection
		11-15	ISYMBP	I5	Symmetric/asymmetric instrument profile switch
		16-20	IPLOT	I5	Plot option switch
4	NPOINT /set	1-10	WAVE	F10.0	Wavelength displacement array of instrument profile (Angstrom units)
		11-22	PRFINT	E12.5	Corresponding instrument profile intensity array
5	1/run	1-60	TITLE	15A4	Experiment label for run calculations
		61-68	HLINE	2A4	Name of hydrogen line corresponding to ILINE value
6	1/run	1- 5	ISKIP	I5	Option to print calculation iterations (normally 0, i.e., not printed)
		6-10	ILINE	I5	Number corresponding to H_β, H_γ, or H_δ convolution
		11-15	NTLOW	I5	Beginning NT value for convolutions (see comment cards and reference 98)
		16-20	NTUP	I5	Ending NT value
		21-32	DENS	E12.5	Electron density for the run
		36-55	LDENS	5A4	Graph label for plot identification

Table D-1. (Continued)

Type #	# Cards	Columns	Variable Name	Format	Remarks
7	1/run	1- 5	NALPHA	I5	Number of Stark profile data points
		6-10	NCONV	I5	Number of convolutions
		11-15	ISYMCP	I5	Symmetric/asymmetric Stark profiles to be convoluted with instrument broadening profile
		15-20	IPUNCH	I5	Option to punch convoluted (folded) profiles
		21-25	IREAD	I5	Option to input profile data from disk file (see comment cards)
		26-30	IPROFL	I5	Option to apply asymptotic wing formula in convolution calculation (see comment cards)
8	NAPHA /run	1-10	ALPHA	F10.0	Reduced displacement array for Stark profiles
		11-70	STARK	5E12.5	Stark profile intensity arrays for temperatures from NTLOW to NTUP (see comment cards and reference 98)

```
C                                                                       1
C                                                                       2
C                                                                       3
C     **********    C337CONV    *********                             4
C                                                                       5
C                                                                       6
C   PROGRAM TO CALCULATE CONVOLUTION INTEGRAL OF UNEQUALLY SPACED       7
C   NUMERICAL DATA                                                      8
C                                                                       9
C      NSETS=NUMBER OF DISTINCT DATA SETS;  ONE SET PER GIVEN INSTRUMENT 10
C            BROADENING PROFILE                                         11
C      NRUNS=NUMBER OF RUNS TO BE MADE WITHIN A GIVEN BROADENING PROFILE 12
C            SET                                                        13
C      TITLE=LABEL FOR CALCULATION FOR A GIVEN RUN                      14
C      ILINE=1, H-BETA CONVOLUTION CALCULATION                          15
C           =2, H-GAMMA     "              "                           16
C           =3, H-DELTA     "              "                           17
C      NT=1, TEMPERATURE =  2500 K                                      18
C        =2,       "     =  5000 K                                     19
C        =3,       "     = 10000 K                                     20
C        =4,       "     = 20000 K                                     21
C        =5,       "     = 40000 K                                     22
C      HLINE=LABEL FOR LINE CORRESPONDING TO ILINE                      23
C      DENS=ELECTRON DENSITY FOR A GIVEN RUN                            24
C      LDENS=GRAPH LABEL TO IDENTIFY PLOTS (IF IPLOT=1 SPECIFIED)       25
C      NALPHA=NUMBER OF REDUCED DISPLACEMENTS FOR WHICH THERE ARE STARK 26
C             PROFILE POINTS TABULATED                                  27
C      NCONV=NUMBER OF CONVOLUTIONS TO BE DONE WITHIN GIVEN RUN         28
C            (SET EQUAL TO NALPHA)                                      29
C      ISYMCP=0, SYMMETRIC PROFILE TO BE CONVOLVED WITH THE BROADENING  30
C                PROFILE:  READ IN RIGHT HALF (POS DISPLACEMENT)        31
C             =1, NOT SYMMETRIC; READ IN COMPLETE PROFILES              32
C      ISKIP=0, SKIP PRINTING ITERATIVE VALUES                          33
C           NE 0, PRINT INTERMEDIATE VALUES                             34
C      IPUNCH=0, CONVOLVED PROFILES NOT PUNCHED                         35
C             =1, CONVOLVED PROFILES PUNCHED ON CARDS                   36
C      IPROFL=0, PURE STARK OR STARK/DOPPLER PROFILES TO BE CONVOLVED   37
C                WITH THE BROADENING PROFILE --- ASYMPTOTIC WING        38
C                FORMULA; 2*3.5261E-03*(ALPHA**(-2.5)) , APPLIED        39
C                FOR DISPLACEMENTS BEYOND TABULATED PROFILE DATA        40
C             NE 0, ASYMPTOTIC STARK/DOPPLER WING FORMULAS NOT APPLIED  41
C      NTLOW=STARTING NT VALUE FOR CONVOLUTION CALCN.                   42
C      NTUP=ENDING     "  "    "       "     "                         43
C      STARK(I,NT)=TABULATED BROADENING INPUT DATA ARRAY AT TEMPERATURE 44
C                  CORRESPONDING TO NT;  5E12.5, CLOUMNS 11 - 70        45
C      ALPHA(I)=PROFILE REDUCED DISPLACEMENT ARRAY CORRESPONDING TO     46
C               STARK(I,NT) DATA;   COLUMNS  1 - 10                     47
C      NPOINT=NO. POINTS IN THE INSTRUMENT PROFILE ARRAY                48
C      ICONV=0, DOPPLER CONVOLUTION                                     49
C           =1, INSTRUMENT CONVOLUTION                                  50
```

```
C      ISYMBP=0, SYMMETRIC BROADENING PROFILE; READ IN FROM ZERO                51
C                DISPLACEMENT TO PRFINT(NPOINT):  PROGRAM GENERATES             52
C                LEFT (NEGATIVE DISPLACEMENT) PORTION OF PROFILE                53
C             =1, NOT SYMMETRIC; READ IN COMPLETE PROFILE INCLUDING             54
C                NEGATIVE DISPLACEMENT INTENSITIES                              55
C      IPLOT=0, NO PLOTS GENERATED                                              56
C           =1, BROADENING, STARK/DOPPLER, AND CONVOLVED PROFILES PLOTTED       57
C      IREAD=0, INPUT PROFILE DATA ON PUNCHED CARDS                             58
C           =1, INPUT PROFILE DATA READ IN FROM FILE, CPS07.A0986.CONV          59
C               (REQUIRES ADDITIONAL FILE READ JCL AND UTILITY PL/1             60
C               PROGRAM TO EDIT FILE DATA IN CARD IMAGE)                        61
C      WAVEL(I)=DISPLACEMENT ARRAY (ANGSTROMS) OF INSTRUMENT PROFILE            62
C      PRFINT(I)=CORRESPONDING INTENSITY ARRAY                                  63
C                                                                               64
       DOUBLE PRECISION T(12),P(8)                                              65
       DIMENSION C(5),S(5),A(2),B(2),XF(6),LDENS(5),DINC(200)                   66
       DIMENSION TEMP(5),TITLE(15),HLINE(2),WAVE(3),ALPHA(100),STARK(100,       67
      15),DEL(3,5),HWORK( 50),ALPHAD(3,5),X( 6),XPONET( 6),FX( 6)               68
       DIMENSION APROF(100),STARKL(100,5),CONV(100,5),AREA(5)                   69
       DIMENSION XINTRP(100),YINTRP(100),ALEFT(5),ARIGHT(5),HMAXL(5),HMAX       70
      1R(5),XMID(100),YMID(100),SHALF(5)                                        71
       DIMENSION WAVEL(100),PRFINT(100),XWAVEL(100),XPROFL(100)                 72
       DATA TEMP/2500.,5000.,10000.,20000.,40000./,WAVE/4861.33,4340.46,4       73
      1101.73/                                                                  74
C                                                                               75
C      READ IN NUMBER OF DATA SETS                                              76
C                                                                               77
       READ(5,1) NSETS                                                          78
     1 FORMAT(I5)                                                               79
       DO 9999 NUMSET=1,NSETS                                                   80
C                                                                               81
C      READ IN NUMBER OF RUNS FOR THE DATA SET                                  82
C                                                                               83
       READ(5,100) NRUNS                                                        84
   100 FORMAT(I5)                                                               85
C                                                                               86
C      READ IN INSTRUMENT BROADENING PROFILE FOR THE DATA SET                   87
C                                                                               88
       READ(5,1000) NPOINT,ICONV,ISYMBP,IPLOT                                   89
  1000 FORMAT(4I5)                                                              90
       DO 1010 I=1,NPOINT                                                       91
  1001 FORMAT(F10.0,E12.5)                                                      92
  1010 READ(5,1001) WAVEL(I),PRFINT(I)                                          93
       DO 9999 NUMRUN=1,NRUNS                                                   94
C                                                                               95
C      READ IN INFORMATION CARDS FOR A RUN WITHIN THE DATA SET                  96
C                                                                               97
       READ(5,101) TITLE,HLINE                                                  98
   101 FORMAT(15A4,2A4)                                                         99
       READ(5,102) ISKIP,ILINE,NTLOW,NTUP,DENS,LDENS                           100
```

```
  102 FORMAT(4I5,E12.5,3X,5A4)                                          101
      WRITE(6,200) TITLE                                                102
  200 FORMAT(1H1,//T10,15A4)                                            103
      WRITE(6,201) HLINE,WAVE(ILINE),DENS                               104
  201 FORMAT(//,T20,2A4,5X,F7.2,2X,'ANGSTROMS',5X,'ELECTRON DENSITY = ',  105
     1E11.4)                                                            106
C                                                                       107
C     CALCULATE DISPLACEMENT SCALING FACTOR AND HALF-WIDTHS OF DOPPLER  108
C     BROADENING PROFILE (ICONV=0 USES INTERNAL DOPPLER BROADENING      109
C     PROFILE AT TEMPERATURE SPECIFIED BY NT UP AND NTLOW)              110
C                                                                       111
      DENOM=1.25E-9*(DENS**0.6666667)                                   112
      WRITE(6,50) DENOM                                                 113
   50 FORMAT(/,T20,'1.25E-09*(NE**(2/3))= ',E12.5)                      114
      WRITE(6,55)                                                       115
   55 FORMAT(///,T10,'GAUSSIAN PROFILE HALF-WIDTHS')                    116
      WRITE(6,60)                                                       117
   60 FORMAT(/,T5,'TEMP',T20,'LAMDEL(1,T)',T35,'LAMDEL(2,T)',T50,'LAMDEL  118
     1(3,T)',T65,'ALFDEL(1,T)',T80,'ALFDEL(2,T)',T95,'ALFDEL(3,T)')     119
      DO 5 I=1,5                                                        120
      DEL(1,I)=0.001733* SQRT(TEMP(I))                                  121
      DEL(2,I)=0.001548* SQRT(TEMP(I))                                  122
      DEL(3,I)=0.001462* SQRT(TEMP(I))                                  123
      ALPHAD(1,I)=DEL(1,I)/DENOM                                        124
      ALPHAD(2,I)=DEL(2,I)/DENOM                                        125
    5 ALPHAD(3,I)=DEL(3,I)/DENOM                                        126
      DO 70 I=1,5                                                       127
   65 FORMAT(T1,7(4X,E11.4))                                            128
   70 WRITE(6,65) TEMP(I),(DEL(J,I),J=1,3),(ALPHAD(K,I),K=1,3)          129
C                                                                       130
C     READ IN PROFILE DATA TO BE CONVOLUTED WITH THE BROADENING PROFILE 131
C                                                                       132
      READ(5,103) NALPHA,NCONV,ISYMCP,IPUNCH,IREAD,IPROFL               133
  103 FORMAT(6I5)                                                       134
      DO 10 I=1,NALPHA                                                  135
  104 FORMAT(F10.0,5E12.5)                                              136
      IF(IREAD.EQ.0) GO TO 8                                            137
      READ(9,104) ALPHA(I),(STARK(I,J),J=1,5)                           138
      GO TO 10                                                          139
    8 READ(5,104) ALPHA(I),(STARK(I,J),J=1,5)                           140
   10 CONTINUE                                                          141
C                                                                       142
C     COMPLETE AND AREA NORMALIZE THE BROADENING PROFILE                143
C                                                                       144
      IF(ISYMBP.EQ.1) GO TO 1030                                        145
      DO 1020 I=1,NPOINT                                                146
      J=NPOINT+1-I                                                      147
      XWAVEL(I)=-WAVEL(J)/DENOM                                         148
 1020 XPROFL(I)=PRFINT(J)*DENOM                                         149
      XWAVEL(NPOINT)=WAVEL(1)                                           150
```

```
      DO 1025 I=2,NPOINT                                                    151
      J=NPOINT-1+I                                                          152
      XWAVEL(J)=WAVEL(I)/DENOM                                              153
1025  XPROFL(J)=PRFINT(I)*DENOM                                             154
      NPTS=2*NPOINT-1                                                       155
      GO TO 1040                                                            156
1030  NPTS=NPOINT                                                           157
      DO 1035 I=1,NPTS                                                      158
      XWAVEL(I)=WAVEL(I)/DENOM                                              159
1035  XPROFL(I)=PRFINT(I)*DENOM                                             160
1040  AREAIN=0.00                                                           161
      BMAX=0.00                                                             162
      JCHK=(NPTS/2)+1                                                       163
      DO 1050 I=1,NPTS,3                                                    164
      NL=I                                                                  165
      NU=NL+3                                                               166
      IF(NU.GE.NPTS) NU=NPTS                                                167
      N=0                                                                   168
      DO 1045 J=NL,NU                                                       169
      N=N+1                                                                 170
      X(N)=XWAVEL(J)                                                        171
      XF(N)=XWAVEL(J)                                                       172
      IF(XWAVEL(J).EQ.0.00) JCHK=J                                          173
      IF(XPROFL(J).LT.BMAX) GO TO 1045                                      174
      BMAX=XPROFL(J)                                                        175
      JLOW=J-1                                                              176
      JUP=J+1                                                               177
1045  FX(N)=XPROFL(J)                                                       178
      IER=0                                                                 179
      NUMBER=4                                                              180
      NTEST=NU-NL+1                                                         181
      IF(NTEST.LT.4) NUMBER=NTEST                                           182
      AINSTR=DCS1QU(FX,X,NUMBER,HWORK,IER)                                  183
      IF(IER.NE.129) GO TO 1049                                             184
      WRITE(6,1046) IER,NL,(X(M),M=1,NUMBER),(FX(MM),MM=1,NUMBER)           185
1046  FORMAT(/,T10,'*****FLAG, IER= ',I3,2X,'FOR INITIAL SEGMENT VALUE',    186
     1I4,/,T15,'X(1)---X(N) = ',4(2X,E11.4),/,T15,'FX(1)---FX(N) =',4(2X    187
     2,E11.4))                                                              188
      DO 1500 M=1,12                                                        189
1500  T(M)=0.D0                                                             190
      DO 1501 M=1,2                                                         191
      A(M)=0.00                                                             192
1501  B(M)=0.00                                                             193
      DO 1502 M=1,8                                                         194
1502  P(M)=0.D0                                                             195
      DO 1503 M=1,5                                                         196
      C(M)=0.00                                                             197
1503  S(M)=0.00                                                             198
      RSQ=100.0                                                             199
      MD=2                                                                  200
```

```
      IER=0                                                                    201
      ID=0                                                                     202
      IF(NUMBER.EQ.2) MD=1                                                     203
      IF(NUMBER.EQ.1) GO TO 1050                                               204
      CALL RLFOTH(X,FX,NUMBER,RSQ,MD,ID,P,C,S,A,B,IER)                         205
      IF(IER.EQ.129) GO TO 1050                                                206
      IF(IER.EQ.130) GO TO 1050                                                207
      CALL RLDOPM(C,ID,A,B,T)                                                  208
      FUP=XF(NUMBER)                                                           209
      FLOW=XF(1)                                                               210
      FU2=FUP*FUP                                                              211
      FL2=FLOW*FLOW                                                            212
      FU3=FU2*FUP                                                              213
      FL3=FL2*FLOW                                                             214
      AINSTR=9999.                                                             215
      IF(ID.EQ.1) C(3)=0.00                                                    216
      AINSTR=(C(1)*(FUP-FLOW))+((C(2)/2.0)*(FU2-FL2))+((C(3)/3.0)*(FU3-F       217
     1L3))                                                                     218
      WRITE(6,1510) AINSTR                                                     219
 1510 FORMAT(/,T10,'POLYNOMIAL APPROXIMATION TO AREA USED:  AINSTR= ',E1       220
     11.4)                                                                     221
 1049 AREAIN=AREAIN+AINSTR                                                     222
 1050 CONTINUE                                                                 223
      BMAX=BMAX/AREAIN                                                         224
      DO 1060 I=1,NPTS                                                         225
 1060 XPROFL(I)=XPROFL(I)/AREAIN                                               226
      ISHAPE=0                                                                 227
      IF(BMAX.GT.XPROFL(JCHK)) ISHAPE=1                                        228
      HALFR=0.00                                                               229
      CALL HMAX(XWAVEL,XPROFL,NPTS,0.0,0.0,JLOW,JUP,BMAX,0.0,HALFR,0.0,ISH     230
     1APE)                                                                     231
      BHALF=HALFR                                                              232
      BMAX=BMAX                                                                233
      WRITE(6,1061) BMAX,BHALF,AREAIN                                          234
 1061 FORMAT(/////,T25,'AREA AND DISPLACEMENT NORMALIZED INSTRUMENT BROAD       235
     1ENING PROFILE',/,T35,'MAX INTENSITY = ',E12.5,2X,'HALF-WIDTH = ',E       236
     212.5,2X,'AREA BEFORE NORMALIZATION =',1X,E12.5)                          237
      WRITE(6,1062)                                                            238
 1062 FORMAT(///,T10,'ALPHA',T25,'INTENSITY')                                  239
      DO 1070 I=1,NPTS                                                         240
 1065 FORMAT(T10,E11.4,T25,E11.4)                                              241
 1070 WRITE(6,1065) XWAVEL(I),XPROFL(I)                                        242
      WRITE(6,150)                                                             243
  150 FORMAT(//,T10,'INPUT DATA')                                              244
      WRITE(6,151)                                                             245
  151 FORMAT(//,T2,'ALPHA',T20,'STARK(2500)',T40,'STARK(5000)',T60,'STAR       246
     1K(10000)',T80,'STARK(20000)',T100,'STARK(40000)')                        247
      DO 15 I=1,NALPHA                                                         248
  152 FORMAT(T2,E11.4,T20,E11.4,T40,E11.4,T60,E11.4,T80,E11.4,T100,E11.4       249
     1)                                                                        250
```

```
   15 WRITE(6,152) ALPHA(I),(STARK(I,J),J=1,5)                          251
C                                                                       252
C      COMPLETE PROFILES TO BE CONVOLUTED WITH THE BROADENING PROFILE   253
C                                                                       254
       DO 19 I=1,5                                                      255
       HMAXL(I)=0.0                                                     256
   19  HMAXR(I)=0.00                                                    257
       IF(ISYMCP.EQ.1) GO TO 1900                                       258
       DO 20 I=1,NALPHA                                                 259
       J=NALPHA+1-I                                                     260
       APROF(I)=-ALPHA(J)                                               261
       DO 20 K=1,5                                                      262
   20  STARKL(I,K)=STARK(J,K)                                           263
       APROF(NALPHA)=ALPHA(1)                                           264
       DO 25 I=2,NALPHA                                                 265
       J=NALPHA-1+I                                                     266
       APROF(J)=ALPHA(I)                                                267
       DO 25 K=1,5                                                      268
   25  STARKL(J,K)=STARK(I,K)                                           269
       NALPHA=2*NALPHA-1                                                270
       GO TO 1950                                                       271
 1900  DO 1910 I=1,NALPHA                                               272
       APROF(I)=ALPHA(I)                                                273
       DO 1910 J=1,5                                                    274
 1910  STARKL(I,J)=STARK(I,J)                                           275
 1950  NCONV=NALPHA                                                     276
       DO 1995 NT=1,5                                                   277
       SHALF(NT)=0.00                                                   278
       IF(NT.LT.NTLOW) GO TO 1995                                       279
       IF(NT.GT.NTUP) GO TO 1995                                        280
       JRCHK=(NALPHA/2)+1                                               281
       JLCHK=JRCHK                                                      282
       DO 1990 I=1,NALPHA                                               283
       IF(APROF(I).GT.0.0) GO TO 1955                                   284
       IF(APROF(I).EQ.0.0) GO TO 1960                                   285
       IF(STARKL(I,NT).LT.HMAXL(NT)) GO TO 1990                         286
       HMAXL(NT)=STARKL(I,NT)                                           287
       ILSLOW=I-1                                                       288
       ILSUP=I+1                                                        289
       GO TO 1990                                                       290
 1955  IF(STARKL(I,NT).LE.HMAXR(NT)) GO TO 1990                         291
       HMAXR(NT)=STARKL(I,NT)                                           292
       IRSLOW=I-1                                                       293
       IRSUP=I+1                                                        294
       GO TO 1990                                                       295
 1960  JRCHK=I                                                          296
       JLCHK=I                                                          297
       IF(STARKL(I,NT).GT.HMAXR(NT)) GO TO 1970                         298
       IF(STARKL(I,NT).LT.HMAXL(NT)) GO TO 1990                         299
       HMAXL(NT)=STARKL(I,NT)                                           300
```

```
      ILSLOW=I-1                                                        301
      ILSUP=I+1                                                         302
      GO TO 1990                                                        303
 1970 HMAXR(NT)=STARKL(I,NT)                                            304
      IRSLOW=I-1                                                        305
      IRSUP=I+1                                                         306
 1990 CONTINUE                                                          307
      SRMAX=HMAXR(NT)                                                   308
      SLMAX=HMAXL(NT)                                                   309
      DO 1994 J=1,NALPHA                                                310
      XINTRP(J)=APROF(J)                                                311
 1994 YINTRP(J)=STARKL(J,NT)                                            312
      HALFR=0.0                                                         313
      HALFL=0.00                                                        314
      ISHAPE=0                                                          315
      IF(SRMAX.GT.YINTRP(JRCHK)) ISHAPE=1                               316
      IF(SLMAX.GT.YINTRP(JLCHK)) ISHAPE=1                               317
      CALL HMAX(XINTRP,YINTRP,NALPHA,1,ILSLOW,ILSUP,IRSLOW,IRSUP,SRMAX,S 318
     1LMAX,HALFR,HALFL,ISHAPE)                                          319
      SHALF(NT)=(HALFR-HALFL)/2.00                                      320
      HMAXR(NT)=SRMAX                                                   321
      HMAXL(NT)=SLMAX                                                   322
 1995 CONTINUE                                                          323
      WRITE(6,2000)                                                     324
 2000 FORMAT(//,T10,'COMPLETE PROFILE DATA')                            325
      WRITE(6,2001)                                                     326
 2001 FORMAT(//,T2,'ALFA',T20,'STARKL(2500)',T40,'STARKL(5000)',T60,'STA 327
     1RKL(10000)',T80,'STARKL(20000)',T100,'STARKL(40000)')             328
      DO 2015 I=1,NALPHA                                                329
 2002 FORMAT(T2,E11.4,T20,E11.4,T40,E11.4,T60,E11.4,T80,E11.4,T100,E11.4 330
     1)                                                                 331
 2015 WRITE(6,2002) APROF(I),(STARKL(I,J),J=1,5)                        332
      WRITE(6,2003) (HMAXR(I),I=1,5),(HMAXL(J),J=1,5),(SHALF(K),K=1,5)  333
 2003 FORMAT(//,T2,'RIGHT MAX INTENS',T20,E11.4,4(9X,E11.4),/,T3,'LEFT M 334
     1AX INTENS',T20,E11.4,4(9X,E11.4),//,T4,'AVE HALF-WIDTH',T20,E11.4, 335
     24(9X,E11.4))                                                      336
C                                                                       337
C     PERFORM THE CONVOLUTION CALCULATIONS                              338
C                                                                       339
      DO 99 NT=1,5                                                      340
      DO 2990 INUM=1,NALPHA                                             341
 2990 YINTRP(INUM)=STARKL(INUM,NT)                                      342
      DO 99 J=1,NCONV                                                   343
      CONV(J,NT)=0.00                                                   344
      IF(NT.LT.NTLOW) GO TO 99                                          345
      IF(NT.GT.NTUP) GO TO 99                                           346
      IF(ICONV.EQ.1) GO TO 3000                                         347
      XUP=1.000/DENOM                                                   348
      IF(NT.EQ.3) XUP=1.50/DENOM                                        349
      IF(NT.EQ.4) XUP=2.00/DENOM                                        350
```

```
      IF(NT.EQ.5) XUP=3.00/DENOM                                        351
      XLOW=-XUP                                                         352
      RATIO=ALPHAD(ILINE,NT)/SHALF(NT)                                  353
      KEY=0                                                             354
      IF(RATIO.GE.1.5) KEY=1                                            355
      GO TO 3010                                                        356
 3000 XUP=XWAVEL(NPTS)                                                  357
      XLOW=XWAVEL(1)                                                    358
      RATIO=BHALF/SHALF(NT)                                             359
      KEY=0                                                             360
      IF(RATIO.GE.1.5) KEY=1                                            361
 3010 XAINC=XUP/50.00                                                   362
      XX=XLOW-XAINC                                                     363
      DO 3020 M=1,100                                                   364
      XX=XX+XAINC                                                       365
 3020 DINC(M)=XX                                                        366
      NDET=100                                                          367
      IF(KEY.EQ.1) NDET=NALPHA                                          368
      DO 98 K=1,NDET,3                                                  369
      NL=K                                                              370
      NU=NL+3                                                           371
      IF(NU.GE.NDET) NU=NDET                                            372
      N=0                                                               373
      DO 96 I=NL,NU                                                     374
      N=N+1                                                             375
      IF(KEY.EQ.1) X(N)=APROF(J)-APROF(I)                               376
      IF(KEY.EQ.1) GO TO 3031                                           377
      X(N)=DINC(I)                                                      378
      XXX=APROF(J)-X(N)                                                 379
      IF(XXX.LT.APROF(1)) GO TO 3030                                    380
      IF(XXX.GT.APROF(NALPHA)) GO TO 3030                               381
      POLYN=0.00                                                        382
      CALL PLLYNN(APROF,YINTRP,POLYN,XXX,NALPHA,6)                      383
      SVALUE=POLYN                                                      384
      GO TO 3031                                                        385
 3030 BXX=ABS(XXX)                                                      386
      SVALUE=2.0*3.5261E-03*(BXX**(-2.5))                               387
      IF(IPROFL.NE.0) SVALUE=0.                                         388
 3031 IF(ICONV.EQ.1) GO TO 75                                           389
      XX2N=ABS(X(N))                                                    390
      XPONET(N)=-0.69314718*(XX2N**2.)/(ALPHAD(ILINE,NT)**2.)           391
      XPTEST=ABS(XPONET(N))                                             392
      IF(XPTEST.GT.60) GO TO 72                                         393
      XPONET(N)=EXP(XPONET(N))/(1.77245*DEL(ILINE,NT))                  394
      XPONET(N)=DENOM*XPONET(N)* SQRT(0.69314718)                       395
      IF(KEY.EQ.1) SVALUE=STARKL(I,NT)                                  396
      FX(N)=SVALUE*XPONET(N)                                            397
      GO TO 86                                                          398
   72 XPONET(N)=0.0                                                     399
      FX(N)=0.00                                                        400
```

```
      GO TO 86                                                          401
   75 XXX=X(N)                                                          402
      IF(KEY.EQ.1) SVALUE=STARKL(I,NT)                                  403
      IF(XXX.LT.XWAVEL(1)) GO TO 80                                     404
      IF(XXX.GT.XWAVEL(NPTS)) GO TO 80                                  405
      POLYN=0.00                                                        406
      CALL PLLYNN(XWAVEL,XPROFL,POLYN,XXX,NPTS,6)                       407
      XPONET(N)=POLYN                                                   408
      GO TO 85                                                          409
   80 XPONET(N)=0.00                                                    410
   85 FX(N)=SVALUE*XPONET(N)                                            411
   86 CONTINUE                                                          412
      XF(N)=DINC(I)                                                     413
      IF(KEY.EQ.1) XF(N)=APROF(I)                                       414
      IF(KEY.EQ.1) X(N)=APROF(I)                                        415
   96 CONTINUE                                                          416
      IER=0                                                             417
      NUMBER=4                                                          418
      NTEST=NU-NL+1                                                     419
      IF(NTEST.LT.4) NUMBER=NTEST                                       420
      CTEST=DCS1QU(FX,X,NUMBER,HWORK,IER)                               421
      IF(ISKIP.EQ.0) GO TO 997                                          422
  995 FORMAT(T50,'CTEST= ',E11.4,2X,'FOR J= ',I3,2X,'K= ',I3)           423
      WRITE(6,996) CTEST,J,K                                            424
  997 IF(IER.NE.129) GO TO 97                                           425
      WRITE(6,105) IER,J,K                                              426
  105 FORMAT    (T10,'****FLAG****,IER= ',I5,2X,'RETURNED FOR CONVOLUTION 427
     1 NUMBER ',I5,5X,'SUBSET K VALUE = ',I3)                           428
      WRITE(6,106) APROF(J),NT                                          429
  106 FORMAT(T15,'ALFA(J)= ',E12.5,2X,'NT = ',I3)                       430
      DO 600 M=1,12                                                     431
  600 T(M)=0.D0                                                         432
      DO 601 M=1,2                                                      433
      A(M)=0.00                                                         434
  601 B(M)=0.00                                                         435
      DO 602 M=1,8                                                      436
  602 P(M)=0.D0                                                         437
      DO 603 M=1,5                                                      438
      C(M)=0.00                                                         439
  603 S(M)=0.00                                                         440
      RSQ=100.0                                                         441
      MD=2                                                              442
      IER=0                                                             443
      ID=0                                                              444
      IF(NUMBER.EQ.1) GO TO 98                                          445
      IF(NUMBER.EQ.2) MD=1                                              446
      DIF=0.0                                                           447
      DO 608 M=2,NUMBER                                                 448
      L=M-1                                                             449
  608 DIF=DIF+(FX(M)-FX(L))**2                                          450
```

```
      XNMBR=NUMBER                                                              451
      DIF=SQRT(DIF)/XNMBR                                                       452
      AVE=0.0                                                                   453
      DO 609 M=1,NUMBER                                                         454
  609 AVE=AVE+FX(M)                                                             455
      AVE=AVE/XNMBR                                                             456
      AVTEST=0.001*AVE                                                          457
      IF(DIF.GT.AVTEST) GO TO 604                                               458
      CTEST=AVE*(X(NUMBER)-X(1))                                                459
      GO TO 611                                                                 460
  604 CONTINUE                                                                  461
      CALL RLFOTH(X,FX,NUMBER,RSQ,MD,ID,P,C,S,A,B,IER)                          462
      IF(IER.EQ.129) GO TO 98                                                   463
      IF(IER.EQ.130) GO TO 98                                                   464
      CALL RLDOPM(C,ID,A,B,T)                                                   465
      FUP=XF(NUMBER)                                                            466
      FLOW=XF(1)                                                                467
      FU2=FUP*FUP                                                               468
      FL2=FLOW*FLOW                                                             469
      FU3=FU2*FUP                                                               470
      FL3=FL2*FLOW                                                              471
      CTEST=9999.                                                               472
      IF(ID.EQ.1) C(3)=0.00                                                     473
      CTEST=(C(1)*(FUP-FLOW))+((C(2)/2.0)*(FU2-FL2))+((C(3)/3.0)*(FU3-FL        474
     13))                                                                       475
      WRITE(6,610) CTEST,ID                                                     476
  610 FORMAT  (T10,'POLYNOMIAL APPROXIMATION TO AREA USED:  CTEST= ',E11        477
     1.4,2X,'DEGREE= ',I3)                                                      478
      GO TO 97                                                                  479
  611 WRITE(6,615) CTEST                                                        480
  615 FORMAT  (T10,'FX(N) VALUES NEARLY CONSTANT:  SQUARE APPROXIMATION         481
     1TO AREA;  CTEST= ',E12.5)                                                 482
   97 CONV(J,NT)=CONV(J,NT)+CTEST                                               483
   98 CONTINUE                                                                  484
   99 CONTINUE                                                                  485
C                                                                               486
C     DETERMINE AREA OF CONVOLVED PROFILES                                      487
C                                                                               488
      DO 501 NT=1,5                                                             489
      AREA(NT)=0.00                                                             490
      HMAXL(NT)=0.00                                                            491
      HMAXR(NT)=0.00                                                            492
      ALEFT(NT)=0.00                                                            493
      ARIGHT(NT)=0.00                                                           494
      DO 500 I=1,NCONV,3                                                        495
      NL=I                                                                      496
      NU=NL+3                                                                   497
      IF(NU.GE.NCONV) NU=NCONV                                                  498
      N=0                                                                       499
      DO 495 J=NL,NU                                                            500
```

```
      N=N+1                                                                  501
      XF(N)=APROF(J)                                                         502
      X(N)=APROF(J)                                                          503
C                                                                            504
C     DETERMINE FIRST APPROXIMATIONS TO RIGHT AND LEFT PROFILE               505
C     MAXIMUMS USING TABULATED (UNNORMALIZED) CONVOLUTION RESULTS            506
C     AREA NORMALIZATION AFTER STATEMENT 501                                 507
C                                                                            508
      IF(APROF(J).GT.0.00) GO TO 450                                         509
      IF(APROF(J).EQ.0.00) GO TO 460                                         510
      IF(CONV(J,NT).LT.HMAXL(NT)) GO TO 495                                  511
      HMAXL(NT)=CONV(J,NT)                                                   512
      LJLOW=J-1                                                              513
      LJUP=J+1                                                               514
      GO TO 495                                                              515
  450 IF(CONV(J,NT).LE.HMAXR(NT)) GO TO 495                                  516
      HMAXR(NT)=CONV(J,NT)                                                   517
      JRLOW=J-1                                                              518
      JRUP=J+1                                                               519
      GO TO 495                                                              520
  460 IF(CONV(J,NT).GT.HMAXR(NT)) GO TO 470                                  521
      IF(CONV(J,NT).LT.HMAXL(NT)) GO TO 495                                  522
      HMAXL(NT)=CONV(J,NT)                                                   523
      LJLOW=J-1                                                              524
      LJUP=J+1                                                               525
      GO TO 495                                                              526
  470 HMAXR(NT)=CONV(J,NT)                                                   527
      JRLOW=J-1                                                              528
      JRUP=J+1                                                               529
  495 FX(N)=CONV(J,NT)                                                       530
      IER=0                                                                  531
      NUMBER=4                                                               532
      NTEST=NU-NL+1                                                          533
      IF(NTEST.LT.4) NUMBER=NTEST                                            534
      ATEST=DCS1QU(FX,X,NUMBER,HWORK,IER)                                    535
      IF(IER.NE.129) GO TO 497                                               536
      WRITE(6,204) NL,NU,NT                                                  537
  204 FORMAT    (T10,'*****FLAG, IER=129 RETURNED FOR ATEST WITH NL= ',I3    538
     1,2X,'NU= ',I3,2X,'NT= ',I3)                                            539
      DO 700 M=1,12                                                          540
  700 T(M)=0.D0                                                              541
      DO 701 M=1,2                                                           542
      A(M)=0.00                                                              543
  701 B(M)=0.00                                                              544
      DO 702 M=1,8                                                           545
  702 P(M)=0.D0                                                              546
      DO 703 M=1,5                                                           547
      C(M)=0.00                                                              548
  703 S(M)=0.00                                                              549
      RSQ=100.0                                                              550
```

```
      MD=2                                                              551
      IER=0                                                             552
      ID=0                                                              553
      IF(NUMBER.EQ.1) GO TO 500                                         554
      IF(NUMBER.EQ.2) MD=1                                              555
      DIF=0.00                                                          556
      DO 708 M=2,NUMBER                                                 557
      L=M-1                                                             558
  708 DIF=DIF+(FX(M)-FX(L))**2                                          559
      XNMBR=NUMBER                                                      560
      DIF=SQRT(DIF)/XNMBR                                               561
      AVE=0.00                                                          562
      DO 709 M=1,NUMBER                                                 563
  709 AVE=AVE+FX(M)                                                     564
      AVE=AVE/XNMBR                                                     565
      AVTEST=0.001*AVE                                                  566
      IF(DIF.GT.AVTEST) GO TO 704                                       567
      ATEST=AVE*(X(NUMBER)-X(1))                                        568
      GO TO 711                                                         569
  704 CONTINUE                                                          570
      CALL RLFOTH(X,FX,NUMBER,RSQ,MD,ID,P,C,S,A,B,IER)                  571
      IF(IER.EQ.129) GO TO 500                                          572
      IF(IER.EQ.130) GO TO 500                                          573
      CALL RLDOPM(C,ID,A,B,T)                                           574
      FUP=XF(NUMBER)                                                    575
      FLOW=XF(1)                                                        576
      FU2=FUP*FUP                                                       577
      FL2=FLOW*FLOW                                                     578
      FU3=FU2*FUP                                                       579
      FL3=FL2*FLOW                                                      580
      ATEST=9999.                                                       581
      IF(ID.EQ.1) C(3)=0.0                                              582
      ATEST=(C(1)*(FUP-FLOW))+((C(2)/2.0)*(FU2-FL2))+((C(3)/3.0)*(FU3-FL 583
     13))                                                               584
      WRITE(6,710) ATEST                                                585
  710 FORMAT  (T10,'POLYNOMIAL APPROXIMATION TO AREA USED:  ATEST= ',E11 586
     1.4)                                                               587
      GO TO 497                                                         588
  711 WRITE(6,715) ATEST                                                589
  715 FORMAT  (T10,'FX(N) VALUES NEARLY CONST:  SQUARE APPROX TO AREA:   590
     1 ATEST= ',E12.5)                                                  591
  497 AREA(NT)=AREA(NT)+ATEST                                           592
  500 CONTINUE                                                          593
  501 CONTINUE                                                          594
C                                                                       595
CC    AREA NORMALIZE CONVOLVED PROFILES AND MAX INTENSITY VALUES        596
C                                                                       597
      DO 502 NT=1,5                                                     598
      IF(NT.LT.NTLOW) GO TO 502                                         599
      IF(NT.GT.NTUP) GO TO 502                                          600
```

```
      HMAXL(NT)=HMAXL(NT)/AREA(NT)                                      601
      HMAXR(NT)=HMAXR(NT)/AREA(NT)                                      602
  502 CONTINUE                                                          603
      WRITE(6,203)                                                      604
  203 FORMAT(1H1,//,T20,'AREA NORMALIZED CONVOLUTION RESULTS')          605
      IF(ICONV.EQ.0) WRITE(6,403)                                       606
      IF(ICONV.EQ.1) WRITE(6,402)                                       607
  402 FORMAT(T30,'INSTRUMENT PROFILE CONVOLUTION')                      608
  403 FORMAT(T30,'DOPPLER CONVOLUTION (INTERNALLY GENERATED DOPPLER PROF 609
     1'LES)')                                                           610
      IF(IPUNCH.EQ.1) WRITE(7,110) HLINE,WAVE(ILINE),DENS               611
  110 FORMAT(2A4,2X,F7.2,2X,'ANGSTROMS',2X,'ELEC DENS = ',E13.6)        612
      WRITE(6,202) (TEMP(I),I=1,5)                                      613
  202 FORMAT(//,T13,'ALPHA',T25,F6.0,' K',T40,F6.0,' K',T55,F6.0,' K',T7 614
     10,F6.0,' K',T85,F6.0,' K')                                        615
      IF(IPUNCH.EQ.1) WRITE(7,210)                                      616
  210 FORMAT('DELTA ALPHA FOLLOWED BY CONVOLVED PROFILES; 2500,5000,1000 617
     10,20000, & 40000')                                                618
      DO 199 J=1,NCONV                                                  619
      DO 198 K=1,5                                                      620
      IF(K.LT.NTLOW) GO TO 198                                          621
      IF(K.GT.NTUP) GO TO 198                                           622
      CONV(J,K)=CONV(J,K)/AREA(K)                                       623
  198 CONTINUE                                                          624
      IF(IPUNCH.NE.1) GO TO 199                                         625
  109 FORMAT(F10.6,5E12.5)                                              626
      WRITE(7,109) APROF(J),(CONV(J,M),M=1,5)                           627
  107 FORMAT(T8,E11.4,T21,5(4X,E11.4))                                  628
  199 WRITE(6,107) APROF(J),(CONV(J,L),L=1,5)                           629
C                                                                       630
C     CALCULATE THE HALF-WIDTH BY USING HALF-MAX INTENSITY VALUES       631
C     FOR BOTH RIGHT AND LEFT SIDES OF THE COMPLETE PROFILE.            632
C     THE MAX INTENSITY VALUE FOR EACH HALF IS DETERMINED BY USING      633
C     THE INTERPOLATING SUBROUTINE, PL_YNN.                             634
C     THE RESPECTIVE HALF-WITHS FOR EACH SIDE ARE THEN DETERMINED BY    635
C     REVERSING THE INTENSITY AND DISPLACEMENT ARRAYS AND INTERPOLATING 636
C     A VALUE WITH PLLYNN                                               637
C                                                                       638
      DO 299 I=1,5                                                      639
      IF(I.LT.NTLOW) GO TO 299                                          640
      IF(I.GT.NTUP) GO TO 299                                           641
      JRCHK=(NCONV/2)+1                                                 642
      JLCHK=JRCHK                                                       643
      DO 249 J=1,NCONV                                                  644
      XMID(J)=APROF(J)                                                  645
      IF(APROF(J).EQ.0.00) JRCHK=J                                      646
      JLCHK=JRCHK                                                       647
  249 YMID(J)=CONV(J,I)                                                 648
      CRMAX=HMAXR(I)                                                    649
      CLMAX=HMAXL(I)                                                    650
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```
      HALFR=0.00                                                        651
      HALFL=0.00                                                        652
      ISHAPE=0                                                          653
      IF(CRMAX.GT.YMID(JRCHK)) ISHAPE=1                                 654
      IF(CLMAX.GT.YMID(JLCHK)) ISHAPE=1                                 655
      CALL HMAX(XMID,YMID,NCONV,1,LJLOW,LJUP,JRLOW,JRUP,CRMAX,CLMAX,HALF 656
     1R,HALFL,ISHAPE)                                                   657
      ALEFT(I)=HALFL                                                    658
      ARIGHT(I)=HALFR                                                   659
      HMAXR(I)=CRMAX                                                    660
      HMAXL(I)=CLMAX                                                    661
  299 CONTINUE                                                          662
  396 FORMAT(/,T3,'RIGHT MAX INTENS',T21,5(4X,E11.4))                   663
  397 FORMAT(T4,'LEFT MAX INTENS',T21,5(4X,E11.4))                      664
  398 FORMAT(/,T3,'RIGHT HALF-WIDTH',T21,5(4X,E11.4))                   665
  399 FORMAT(T4,'LEFT HALF-WIDTH',T21,5(4X,E11.4))                      666
      WRITE(6,396) (HMAXR(N1),N1=1,5)                                   667
      WRITE(6,397) (HMAXL(N2),N2=1,5)                                   668
      WRITE(6,398) (ARIGHT(I1),I1=1,5)                                  669
      WRITE(6,399) (ALEFT(I2),I2=1,5)                                   670
      WRITE(6,510) (AREA(NN),NN=1,5)                                    671
  510 FORMAT(//,T3,'AREA(1)-AREA(5)',T22,5(3X,E12.5))                   672
      IF(IPLOT.NE.1) GO TO 9999                                         673
      CALL PLOT(APROF,STARKL,CONV,XWAVEL,XPROFL,NTUP,NTLOW,ALPHAD,ICONV, 674
     1NPTS,NALPHA,NCONV,ILINE,LDENS)                                    675
 9999 CONTINUE                                                          676
      STOP                                                              677
      END                                                               678
      SUBROUTINE HMAX(X,Y,N,ISYM,ILLOW,ILUP,IRLOW,IRUP,YRMAX,YLMAX,HALFR 679
     1,HALFL,ISHAPE)                                                    680
      DIMENSION X(100),Y(100),XH(51),YH(51)                             681
C                                                                       682
CC    SUBROUTINE TO DETERMINE HALF-WIDTHS FOR RIGHT AND (OPTIONALLY)    683
C     LEFT PROFILES                                                     684
C                                                                       685
C     ISYM=0, SYMMETRIC PROFILE SO ONLY CALCULATE RIGHT HALF-WIDTH      686
C         NE 0, DETERMINE BOTH RIGHT AND LEFT HALF-WIDTHS               687
CC                                                                      688
C                                                                       689
      NHALF=N/2                                                         690
      IF(ISYM.EQ.0) GO TO 2000                                          691
      NPLUS=NHALF+1                                                     692
      IF(ISHAPE.EQ.1) NPLUS=ILLOW+1                                     693
      DO 1010 I=1,NPLUS                                                 694
      XH(I)=Y(I)                                                        695
 1010 YH(I)=X(I)                                                        696
      XINC=(X(ILUP)-X(ILLOW))/100.0                                     697
      XXX=X(ILLOW)-XINC                                                 698
      DO 1020 J=1,100                                                   699
      XXX=XXX+XINC                                                      700
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```
      POLYN=0.00                                                        701
      CALL PLLYNN(X,Y,POLYN,XXX,N,6)                                    702
      IF(POLYN.GT.YLMAX) YLMAX=POLYN                                    703
 1020 CONTINUE                                                          704
      POLYN=0.00                                                        705
      XXX=YLMAX/2.00                                                    706
      CALL PLLYNN(XH,YH,POLYN,XXX,NPLUS,4)                              707
      HALFL=POLYN                                                       708
 2000 J2=0                                                              709
      J4=0                                                              710
      IF(ISHAPE.EQ.1) NHALF=IRLOW+1                                     711
      DO 2030 J3=NHALF,N                                                712
      J4=N-J3+NHALF                                                     713
      J2=J2+1                                                           714
      XH(J2)=Y(J4)                                                      715
 2030 YH(J2)=X(J4)                                                      716
      XINC=(X(IRUP)-X(IRLOW))/100.0                                     717
      XXX=X(IRLOW)-XINC                                                 718
      DO 2040 J5=1,100                                                  719
      XXX=XXX+XINC                                                      720
      POLYN=0.00                                                        721
      CALL PLLYNN(X,Y,POLYN,XXX,N,6)                                    722
      IF(POLYN.GT.YRMAX) YRMAX=POLYN                                    723
 2040 CONTINUE                                                          724
      POLYN=0.00                                                        725
      XXX=YRMAX/2.00                                                    726
      CALL PLLYNN(XH,YH,POLYN,XXX,J2,4)                                 727
      HALFR=POLYN                                                       728
      RETURN                                                            729
      END                                                               730
      SUBROUTINE PLLYNN(X,Y,POLYN,XXX,NUMX,NPOLY)                       731
      DIMENSION X(100),Y(100)                                           732
C                                                                       733
CC    N POINT POLYNOMIAL INTERPOLATING SUBROUTINE                       734
CC                                                                      735
CC    TO INTERPOLATE A VALUE FOR XXX THE NPOLY NEAREST KNOWN POINTS ARE 736
C     SELECTED AND AN INTERPOLATING POLYNOMIAL OF DEGREE NPOLY-1 IS     737
C     FITTED TO THESE POINTS                                            738
C     X AND Y ARE THE ARRAYS OF NUMX KNOWN POINTS ON THE CURVE          739
C     THE RESULT IS POLYN                                               740
C                                                                       741
  101 POLYN=0.0                                                         742
      NM=(NPOLY+1)/2                                                    743
      NM1=NM+1                                                          744
      NUP=NUMX+NM1-NPOLY                                                745
      DO 102 J=NM1,NUP                                                  746
      IF(XXX.LE.X(J)) GO TO 104                                         747
  102 CONTINUE                                                          748
      J=NUP                                                             749
  104 L=J-NM                                                            750
```

```
      LLL=L+NPOLY-1                                                     751
      DO 106 K=L,LLL                                                    752
      TERM=1.0                                                          753
      DO 105 M=L,LLL                                                    754
      IF(K.EQ.M) GO TO 105                                              755
      TERM=TERM*(XXX-X(M))/(X(K)-X(M))                                  756
  105 CONTINUE                                                          757
      TERM=Y(K)*TERM                                                    758
  106 POLYN=POLYN+TERM                                                  759
      RETURN                                                            760
      END                                                               761
      SUBROUTINE PLOT(APROF,STARKL,CONV,XWAVEL,XPROFL,NTUP,NTLOW,ALPHAD,762
     1ICONV,NPTS,NALPHA,NCONV,ILINE,LDENS)                              763
      DIMENSION LBP(5),LSDP(5),LCP(5),LT1(5),LT2(5),LT3(5),LT4(5),LT5(5)764
     1,LINE1(5),LINE2(5),LINE3(5),APROF(100),STARKL(100,5),CONV(100,5),X765
     2WAVEL(100),XPROFL(100),ALPHAD(3,5),LDENS(5),DPROF(100,5),X1(100),766
     3X2(100),Y1(100),Y2(100),LBLT(5)                                   767
      DATA LBP/'BROA','DENI','NG P','ROFI','LE  '/,LSDP/'STAR','K-DO','P768
     1PLE','R PR','OF  '/,LCP/'CONV','OLVE','D   ','PROF','ILE '/,LT1/'T769
     2EMP','    ','2500','  K ','   '/,LT2/'TEMP','    ','5000','  K ',770
     3'   '/,LT3/'TEMP','    ','1000','0 K ','   '/,LT4/'TEMP','    ',771
     4'2000','0 K ','   '/,LT5/'TEMP','    ','4000','0 K ','   '/      772
      DATA LINE1/'H-BE','TA  ','4861','.33 ','A   '/,LINE2/'H-GA','MMA '773
     1,'4340','.46 ','A   '/,LINE3/'H-DE','LTA ','4101','.73 ','A   '/ 774
      IF(ICONV.EQ.1) GO TO 100                                          775
      DO 10 I=1,5                                                       776
      DO 10 J=1,NALPHA                                                  777
      A2=APROF(J)*APROF(J)                                              778
      XPNT=-0.963147l8*A2/(ALPHAD(ILINE,I)**2)                          779
      XPTEST=ABS(XPNT)                                                  780
      IF(XPTEST.GT.45) GO TO 9                                          781
      DPROF(J,I)=(SQRT(0.693147l8))*(EXP(XPNT))/(1.77245*ALPHAD(ILINE,I)782
     1)                                                                 783
      GO TO 10                                                          784
    9 DPROF(J,I)=0.00                                                   785
   10 CONTINUE                                                          786
      NPTS=NALPHA                                                       787
  100 DO 9999 NT=NTLOW,NTUP                                             788
      DO 110 I=1,NALPHA                                                 789
      X1(I)=APROF(I)                                                    790
      IF(ICONV.EQ.1) GO TO 110                                          791
      XWAVEL(I)=APROF(I)                                                792
      XPROFL(I)=DPROF(I,NT)                                             793
  110 Y1(I)=STARKL(I,NT)                                                794
      DO 120 I=1,NCONV                                                  795
      X2(I)=APROF(I)                                                    796
  120 Y2(I)=CONV(I,NT)                                                  797
      CALL GRAPH (NPTS,XWAVEL,XPROFL,0.7,8.0,10.0,0.0,0.0,0.,'ALPHA (NORMAL798
     1IZED)','AREA NORM INTENSITY','CONVOLUTION PROFILES',LDENS)        799
      IF(ILINE.EQ.3) GO TO 300                                          800
```

```
      IF(ILINE.EQ.2) GO TO 200                                          801
      IF(ILINE.EQ.1) GO TO 125                                          802
1000  FORMAT(//,T10,'*****FLAG*****  ERROR:  ILINE NOT SPECIFIED CORRECT  803
     1LY; NO PLOTS GENERATED')                                          804
      WRITE(6,1000)                                                     805
      RETURN                                                            806
 125  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LINE1)                       807
      IF(NT.EQ.5) GO TO 148                                             808
      IF(NT.EQ.4) GO TO 146                                             809
      IF(NT.EQ.3) GO TO 144                                             810
      IF(NT.EQ.2) GO TO 142                                             811
      IF(NT.EQ.1) GO TO 140                                             812
1010  FORMAT(/,T10,'*****FLAG*****  ERROR IN NTLOW OR NTUP')            813
      WRITE(6,1010)                                                     814
      RETURN                                                            815
 140  DO 141 N=1,5                                                      816
 141  LBLT(N)=LT1(N)                                                    817
      GO TO 150                                                         818
 142  DO 143 N=1,5                                                      819
 143  LBLT(N)=LT2(N)                                                    820
      GO TO 150                                                         821
 144  DO 145 N=1,5                                                      822
 145  LBLT(N)=LT3(N)                                                    823
      GO TO 150                                                         824
 146  DO 147 N=1,5                                                      825
 147  LBLT(N)=LT4(N)                                                    826
      GO TO 150                                                         827
 148  DO 149 N=1,5                                                      828
 149  LBLT(N)=LT5(N)                                                    829
 150  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LBLT)                        830
      CALL GRAPHS(NPTS,XWAVEL,XPROFL,1,107,LBP)                         831
      CALL GRAPHS(NALPHA,X1,Y1,2,107,LSDP)                              832
      CALL GRAPHS(NCONV,X2,Y2,3,107,LCP)                                833
      GO TO 9999                                                        834
 200  CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LINE2)                       835
      IF(NT.EQ.5) GO TO 248                                             836
      IF(NT.EQ.4) GO TO 246                                             837
      IF(NT.EQ.3) GO TO 244                                             838
      IF(NT.EQ.2) GO TO 242                                             839
      IF(NT.EQ.1) GO TO 240                                             840
2000  FORMAT(/,T10,'*****FLAG*****  ERROR IN NTLOW OR NTUP')            841
      WRITE(6,2000)                                                     842
      RETURN                                                            843
 240  DO 241 N=1,5                                                      844
 241  LBLT(N)=LT1(N)                                                    845
      GO TO 250                                                         846
 242  DO 243 N=1,5                                                      847
 243  LBLT(N)=LT2(N)                                                    848
      GO TO 250                                                         849
 244  DO 245 N=1,5                                                      850
```

```
  245 LBLT(N)=LT3(N)                                                    851
      GO TO 250                                                         852
  246 DO 247 N=1,5                                                      853
  247 LBLT(N)=LT4(N)                                                    854
      GO TO 250                                                         855
  248 DO 249 N=1,5                                                      856
  249 LBLT(N)=LT5(N)                                                    857
  250 CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LBLT)                        858
      CALL GRAPHS(NPTS,XWAVEL,XPROFL,1,107,LBP)                         859
      CALL GRAPHS(NALPHA,X1,Y1,2,107,LSDP)                              860
      CALL GRAPHS(NCONV,X2,Y2,3,107,LCP)                                861
      GO TO 9999                                                        862
  300 CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LINE3)                       863
      IF(NT.EQ.5) GO TO 348                                             864
      IF(NT.EQ.4) GO TO 346                                             865
      IF(NT.EQ.3) GO TO 344                                             866
      IF(NT.EQ.2) GO TO 342                                             867
      IF(NT.EQ.1) GO TO 340                                             868
 3000 FORMAT(/,T10,'*****FLAG*****  ERROR IN NTLOW OR NTUP')            869
      WRITE(6,3000)                                                     870
      RETURN                                                            871
  340 DO 341 N=1,5                                                      872
  341 LBLT(N)=LT1(N)                                                    873
      GO TO 350                                                         874
  342 DO 343 N=1,5                                                      875
  343 LBLT(N)=LT2(N)                                                    876
      GO TO 350                                                         877
  344 DO 345 N=1,5                                                      878
  345 LBLT(N)=LT3(N)                                                    879
      GO TO 350                                                         880
  346 DO 347 N=1,5                                                      881
  347 LBLT(N)=LT4(N)                                                    882
      GO TO 350                                                         883
  348 DO 349 N=1,5                                                      884
  349 LBLT(N)=LT5(N)                                                    885
  350 CALL GRAPHS(NPTS,XWAVEL,XPROFL,0,107,LBLT)                        886
      CALL GRAPHS(NPTS,XWAVEL,XPROFL,1,107,LBP)                         887
      CALL GRAPHS(NALPHA,X1,Y1,2,107,LSDP)                              888
      CALL GRAPHS(NCONV,X2,Y2,3,107,LCP)                                889
 9999 CONTINUE                                                          890
      RETURN                                                            891
      END                                                               892
```

Table D-2. Data card requirements for C337BROD

Type #	# Cards	Columns	Variable Name	Format	Remarks
1	1	1- 5	NSETS	I5	Number of data sets
2	1/set	1- 5	NRUNS	I5	Number of runs within data set
3	1/run	1-60	TITLE	15A4	Experiment label
		61-68	HLINE	2A4	Name of hydrogen line
4	1/run	1- 5	ILINE	I5	Line identification number
		6-10	NRAD	I5	Number of positions for electron density calculations
5	NRAD /run	1-10	RAD	F10.0	Radial position array
		11-20	TRAD	F10.0	Corresponding radial temperature array
		21-30	HALF	F10.0	Corresponding radial half-width array

```
C                                                                               1
C                                                                               2
C                                                                               3
C     **********  C3378ROD  **********                                          4
C                                                                               5
C                                                                               6
C     PROGRAM TO CALCULATE ELECTRON NUMBER DENSITY FROM BROADENING DATA         7
C     FOR THE BALMER SERIES HYDROGEN LINES                                      8
C                                                                               9
C                                                                              10
C     NSETS=NUMBER OF SETS OF DATA                                             11
C     NRUNS=NUMBER OF RUNS WITHIN GIVEN DATA SET                               12
C     TITLE=EXPERIMENT TITLE OF A GIVEN RUN                                    13
C     HLINE=NAME OF BALMER SERIES LINE                                         14
C           (H-BETA, H-GAMMA, H-DELTA)                                         15
C     ILINE=1, H-BETA  CALCULATION                                             16
C          =2, H-GAMMA CALCULATION                                             17
C          =3, H-DELTA CALCULATION                                             18
C     NRAD=NUMBER OF RADIAL POSITIONS FOR DENSITY CALCULATION                  19
C     RAD(N)=RADIAL POSITION ARRAY (N=1, TO NRAD)                              20
C     TRAD(N)=TEMPERATURE ARRAY CORRESPONDING TO RAD(N)                        21
C     HALF(N)=FULL (MEASURED) HALF-WIDTH AT HALF MAX INTENSITY ARRAY           22
C             CORRESPONDING TO RAD(N) AND TRAD(N)                              23
C                                                                              24
C                                                                              25
C                                                                              26
      DIMENSION DENS(9),TEMP(5),ALFA(45),TITLE(15),HLINE(2),WAVE(3),HALF       27
     1(35),RAD(35),TRAD(35),ALFAD(9,5),X(9),Y(9),XINTRP(5),YINTRP(5),EDE       28
     2NS(35),ALPHA(35)                                                         29
      DATA TEMP/2500.,5000.,10000.,20000.,40000./,DENS/1.000E+12,3.162E+       30
     112,1.000E+13,3.162E+13,1.000E+14,3.162E+14,1.000E+15,3.162E+15,1.0       31
     200E+16/,WAVE/4861.33,4340.46,4101.73/                                    32
      DATA ALFA/1.082,1.315,1.647,2.184,2.907,0.5200,0.6260,0.7759,1.017       33
     1,1.372,0.2572,0.3017,0.3780,0.4809,0.6428,0.1435,0.1618,0.1921,0.2       34
     2428,0.3117,0.0990,0.1050,0.1168,0.1370,0.1651,0.0835,0.0890,0.0945       35
     3,0.1010,0.1085,0.07086,0.07539,0.0806,0.08742,0.09587,0.06774,0.07       36
     418,0.07474,0.07738,0.08069,0.06584,0.07161,0.07508,0.07684,0.07791       37
     5/                                                                        38
      READ(5,100) NSETS                                                        39
  100 FORMAT(I5)                                                               40
      DO 9999 NSET=1,NSETS                                                     41
      READ(5,110) NRUNS                                                        42
  110 FORMAT(I5)                                                               43
      DO 9999 NRUN=1,NRUNS                                                     44
      READ(5,120) TITLE,HLINE                                                  45
  120 FORMAT(15A4,2A4)                                                         46
      READ(5,130) ILINE,NRAD                                                   47
  130 FORMAT(2I5)                                                              48
      WRITE(6,1000) TITLE,HLINE,WAVE(ILINE)                                    49
 1000 FORMAT(1H1,/////,T15,'ELECTRON DENSITY BROADENING CALCULATION',//,       50
```

```
     1T10,15A4,/,T10,2A4,2X,F7.2)                                                    51
      K=0                                                                            52
      DO 140 I=1,45,5                                                                53
      K=K+1                                                                          54
      NUP=I+4                                                                        55
      L=0                                                                            56
      DO 140 J=I,NUP                                                                 57
      L=L+1                                                                          58
  140 ALFAD(K,L)=ALFA(J)                                                             59
      WRITE(6,2000) (TEMP(I),I=1,5)                                                  60
 2000 FORMAT(//,T25,'HALF-WIDTH DATA',/,T15,'ELECTRON DENS',T30,5(F15.0)             61
     1)                                                                             62
      DO 145 I=1,9                                                                   63
 2001 FORMAT(T15,E11.4,T33,5(3X,E11.4))                                              64
  145 WRITE(6,2001) DENS(I),(ALFAD(I,J),J=1,5)                                       65
      DO 200 I=1,NRAD                                                                66
  150 FORMAT(3F10.0)                                                                 67
      READ(5,150) RAD(I),TRAD(I),HALF(I)                                             68
      DO 160 J=1,9                                                                   69
      DO 155 K=1,5                                                                   70
      XINTRP(K)=ALOG10(TEMP(K))                                                      71
  155 YINTRP(K)=ALFAD(J,K)                                                           72
      X(J)=ALOG10(DENS(J))                                                           73
      POLYN=0.00                                                                     74
      XXX=ALOG10(TRAD(I))                                                            75
      CALL PLLYNN(XINTRP,YINTRP,POLYN,XXX,5,3)                                       76
      Y(J)=POLYN                                                                     77
  160 CONTINUE                                                                       78
      ICOUNT=0                                                                       79
      XXDENS=14.0                                                                    80
  170 POLYN=0.00                                                                     81
      ICOUNT=ICOUNT+1                                                                82
      CALL PLLYNN(X,Y,POLYN,XXDENS,9,2)                                              83
      XXALFA=POLYN                                                                   84
      CALDEN=7.9568E+12*((HALF(I)/XXALFA)**1.5)                                      85
      CALDEN=ALOG10(CALDEN)                                                          86
      TEST=ABS(CALDEN-XXDENS)                                                        87
      IF(TEST.LE.0.00005) GO TO 180                                                  88
      IF(ICOUNT.GT.50) GO TO 190                                                     89
      XXDENS=CALDEN                                                                  90
      GO TO 170                                                                      91
  180 EDENS(I)=10.0**CALDEN                                                          92
      ALPHA(I)=XXALFA                                                                93
      GO TO 200                                                                      94
  190 CALDEN=10.0**CALDEN                                                            95
      WRITE(6,195) RAD(I),TRAD(I),HALF(I),CALDEN,XXALFA                              96
  195 FORMAT(/,T15,'****FLAG**** ELECTRON DENSITY ITERATION FAILED TO                97
     1CONVERGE WITHIN 50 ITERATIONS FOR:',/,T15,'RADIUS= ',E11.4,2X,'TEM            98
     2PERATURE= ',E11.4,2X,'FULL WIDTH HALF MAX INTENS= ',E11.4,/,T15,'L            99
     3AST CALCULATED DENSITY= ',E11.4,2X,'LAST INTERPOLATED REDUCED HALF            100
```

```
     4 WIDTH= ',E11.4)                                                          101
       EDENS(I)=0.00                                                            102
       ALPHA(I)=0.00                                                            103
   200 CONTINUE                                                                 104
       WRITE(6,1001)                                                            105
  1001 FORMAT(/////,T2,'RADIUS',T15,'TEMP (K)',T30,'FWHMI',T45,'ELEC DENS      106
      1',T60,'REDUCED HALF-WIDTH')                                              107
       DO 300 N=1,NRAD                                                          108
  1002 FORMAT(T2,E12.5,T15,E12.5,T28,4(3X,E12.5))                               109
   300 WRITE(6,1002) RAD(N),TRAD(N),HALF(N),EDENS(N),ALPHA(N)                   110
  9999 CONTINUE                                                                 111
       STOP                                                                     112
       END                                                                      113
       SUBROUTINE PLLYNN(X,Y,POLYN,XXX,NUMX,NPOLY)                              114
       DIMENSION X(100),Y(100)                                                  115
C                                                                               116
CC     N POINT POLYNOMIAL INTERPOLATING SUBROUTINE                              117
C                                                                               118
CC     TO INTERPOLATE A VALUE FOR XXX THE NPOLY NEAREST KNOWN POINTS ARE        119
CC     SELECTED AND AN INTERPOLATING POLYNOMIAL OF DEGREE NPOLY-1 IS            120
CC     FITTED TO THESE POINTS                                                   121
CC     X AND Y ARE THE ARRAYS OF NUMX KNOWN POINTS ON THE CURVE                 122
CC     THE RESULT IS POLYN                                                      123
C                                                                               124
   101 POLYN=0.0                                                                125
       NM=(NPOLY+1)/2                                                           126
       NM1=NM+1                                                                 127
       NUP=NUMX+NM1-NPOLY                                                       128
       DO 102 J=NM1,NUP                                                         129
       IF(XXX.LE.X(J)) GO TO 104                                                130
   102 CONTINUE                                                                 131
       J=NUP                                                                    132
   104 L=J-NM                                                                   133
       LLL=L+NPOLY-1                                                            134
       DO 106 K=L,LLL                                                           135
       TERM=1.0                                                                 136
       DO 105 M=L,LLL                                                           137
       IF(K.EQ.M) GO TO 105                                                     138
       TERM=TERM*(XXX-X(M))/(X(K)-X(M))                                         139
   105 CONTINUE                                                                 140
       TERM=Y(K)*TERM                                                           141
   106 POLYN=POLYN+TERM                                                         142
       RETURN                                                                   143
       END                                                                      144
```