**Numerical Calculation of Impurity
Charge State Distributions**

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E. C. Crume and D. E. Arnurius

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ABSTRACT

The numerical calculation of impurity charge state distributions using the computer program IMPDYN is discussed. The time-dependent corona atomic physics model used in the calculations is reviewed, and general and specific treatments of electron impact ionization and recombination are referenced. The complete program and two examples relating to tokamak plasmas are given on a microfiche so that a user may verify that his version of the program is working properly. In the discussion of the examples, the corona steady-state approximation is shown to have significant defects when the plasma environment, particularly the electron temperature, is changing rapidly.

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1. INTRODUCTION

It is well known that unwanted ions, called impurities, are found in magnetically confined plasmas created for controlled thermonuclear fusion research. The role of impurities in the transport and in the balance of both particles and energy in one of the most promising types of plasma confinement devices, the tokamak,¹ is a topic of intense and widespread current research, both theoretical and experimental. Knowledge of the ionic state (charge state) of a given impurity, or, more generally, of the distribution of charge states of a given impurity element as a function of position in a plasma is critical to such research and its application. For example, the Coulombic friction among various ions and with the electrons which determines classical (i.e., nonturbulent) particle and heat transport depends on the magnitudes of the charge states of the interacting species.² Also, as is well known from atomic physics, the quantity and character of the electromagnetic radiation emitted by ions interacting with electrons depend on the ionic charge, and the amount of such radiation lost from a plasma can be an important part of the plasma energy balance.³ Tokamak plasmas are considered to be "steady state" from the standpoint of equilibrium and stability, but the density and temperatures of the plasma constituents are functions of position in the plasma. Even this "steady-state" plasma must be created from a neutral gas by ionization, and also during the "steady state" there are more or less significant changes in plasma density and temperature as a function of time.

In order to study the temporal evolution of impurity charge states in such plasmas, we have created the computer program IMPDYN⁴ (from IMPurity DYNamics) which can be used either alone with proper input or as a subroutine of another program, such as a tokamak transport code,⁵ which supplies the necessary input. The atomic physics model we use is the time-dependent corona model,⁶ although the code will trivially generate steady-state corona model (corona equilibrium) ionic distributions. The set of coupled first order differential equations describing the model, the rate equations, is integrated in time using an adaptation of a "stiff" equation solver.⁷ The number of possible equations to be

integrated for a given high-Z impurity such as tungsten (atomic number 74 — therefore 75 equations including the neutral species) may itself be large, and there are usually several impurities present, which may yield a large number of equations even if the impurities have low or intermediate atomic numbers.

Thus, the number of equations to be integrated may be cumbersome large and their integration excessively time consuming, especially if the rate equation solver is being used as a subroutine of another program which already may require a large amount of computer core and/or computation time. Consequently, we have implemented in IMPDYN a scheme by which the program decides which equations govern the evolution of the species present in significant quantities at a given time and integrates only these equations. Because rarely as many as half the possible ionic states of an impurity are likely present in significant quantities at a given point in a plasma at a given time, and frequently much fewer, this scheme can more than halve computation time. Because the level of significance is in input quantity, the user can decide how detailed (or crude) an analysis is to be made.

In Sect. 2, the corona atomic physics model is briefly reviewed, and the sources of the rate coefficients we have used are noted. The mathematics of solution of the rate equations, the scheme for integrating only the "significant" equations, and the current version of IMPDYN are discussed in Sect. 3. Two examples illustrative of the use of the program, an approach to corona equilibrium and a neutral injection heating experiment in a tokamak, are given in Sect. 4. In Sect. 5 the conclusions are summarized. A complete program listing with numerous comment cards and the two detailed examples are given on the microfiche enclosed in a pocket on the inside back cover of the report.

2. THE CORONA MODEL RATE EQUATIONS

2.1 THE CORONA MODEL

The corona model in both its steady-state and time-dependent forms is discussed in detail by McWhirter,⁶ so we only summarize here. The time-dependent corona model was evolved from the steady-state corona model, an atomic model proposed to explain certain spectral features of the solar corona.^{8,9} The atomic processes involved are electron collisional ionization, radiative recombination, and excitation and spontaneous decay of excited atomic and ionic states. Jordan¹⁰ has more recently included the additional collisional electronic processes of auto-ionization and dielectronic recombination. For plasmas with electron densities and temperatures in the range of interest,¹ we may decouple the radiation problem (i.e., collisional excitation and spontaneous decay) from the ionic distribution problem and consider only the ground states of the ions (and atoms) involved.⁶ (In fact, we will not consider the radiation problem any further here, except to remark that by applying the appropriate coefficients one can determine the radiation from the ionic distributions and the recombination rates calculated by IMPDYN.) The time-dependent corona model was first used to analyze laboratory plasmas by Breton¹¹ and by Hobbs et al.;¹² the latter workers also coupled the model to a plasma transport model. The steady-state model follows from the time-dependent model by setting all the time derivatives of the ion densities equal to zero, so we treat the steady-state model as a special case.

We may state the assumptions of the time-dependent corona model as follows:

(1) It is assumed that the plasma electron velocity distribution can always be adequately approximated by a Maxwellian distribution of temperature T_e , where T_e may, however, be a function of both time and position within the plasma. This assumption has two aspects. First, thermalization of the distribution following changes in plasma conditions is assumed to occur on a much faster time scale than the time scale of the problem we are considering.⁶ Also, perturbations to the

Maxwellian due to electric currents and to magnetic geometry effects¹ are neglected as being of too high an order. No assumptions as to the form of the ion (or atom) velocity distribution need to be made other than that its "temperature" must be low enough ($T_i \lesssim T_e$) that the relative electron-ion (-atom) velocity may be approximated by the electron velocity.

(2) It is assumed that all atomic processes result from two-body collisions between electrons and atoms or ions in their ground states. This is straightforward for collisional ionization and radiative recombination, but any auto-ionization and dielectronic recombination rate coefficients used must be related to ground state populations. There are also other perturbative corrections, which are summarized in Ref. 10.

(3) It is assumed that any atomic radiation emitted escapes entirely from the plasma (the optically thin approximation).

We may then write the differential equation governing the time evolution of the density $n_j(\vec{r}, t)$ of the ground state of an ion of charge j ,

$$\frac{dn_j}{dt} = n_e [n_{j-1} S_{j-1} + n_{j+1} \alpha_{j+1} - n_j (S_j + \alpha_j)] , \quad (1)$$

where $n_e(\vec{r}, t)$ is the electron density. The ionization rate coefficient $S_j(T_e)$ for the ion of charge j is the moment of the product of the ionization cross section $\sigma_i(|\vec{v}|)$ with the relative velocity $|\vec{v}|$, which we here take to be the electron velocity, over the assumed Maxwellian electron distribution

$$S_j(T_e) = \frac{1}{n_e} \int d^3v \sigma_i(|\vec{v}|) |\vec{v}| f_{e0}(T_e) . \quad (2)$$

The recombination rate coefficient $\alpha_j(T_e)$ is a similar moment of the recombination cross section $\sigma_r(|\vec{v}|)$. We reiterate that auto-ionization, dielectronic recombination, or other effects to be included must have rate coefficients which apply to ground state populations. (Otherwise, obviously, we would have to have an enormously increased number of equations — one for each excited state.) For a given element, there are

$Z + 1$ such coupled equations where j ranges (in integral steps) from $j = 0$ (atoms) to $j = Z$ (fully ionized ion, i.e., the bare nucleus). Although analytic solutions of this set are possible if T_e is constant,⁶ such solutions are of limited value for real plasmas, and we are led to numerical solutions such as those accomplished by IMPDYN. If the left-hand sides of the $Z + 1$ equations for an element are set equal to zero, the well-known steady-state corona model solution,

$$\frac{n_j}{n_{j+1}} = \frac{\alpha_{j+1}}{S_j}, \quad (3)$$

is obtained, expressing the balance between ionization and recombination rates.

Before discussing the sources of the ionization and recombination rate coefficients, we draw attention to the fact that equations of the form of Eq. (1) obviously do not account for sources and sinks which may arise from particle transport or externally, such as from wall sources of neutral atoms. To account for particle transport in a simple manner, one can add a term $-n_j/\tau_j$ to Eq. (1) where $\tau_j(\vec{r}, t)$ is an appropriate decay time. If τ_j is positive the term represents a sink; if negative, a source. We have not included such terms in IMPDYN because of its planned use with tokamak transport codes for problems in which the transport occurs on time scales such that alternating computation of atomic physics processes and transport can be made. We also do not include external source terms. Such terms may have arbitrary forms, and, in any event, we would try to treat them on the same time scale as the transport; i.e., we consider only weak external source terms.

2.2 THE RATE COEFFICIENTS

2.2.1 General

The selection of the coefficients to use in the solution of the coupled equations of the form of Eq. (1) is decidedly problem-dependent. It might occur, especially for low atomic number elements, that the

ionization and recombination rate coefficients are known as accurately as the changing electron temperature and density environment in the problem. On the other hand, it is probably more likely, at least for tokamak research, that there are insufficient experimental data and/or theoretical calculations to determine the desired rate coefficients to within a factor of two or more. If the rate coefficients are entirely obtained from theory, it may be that the overall problem is such that some or all of the theoretical calculations may be done at the same time as the solution of the rate equations. However, if the atomic physics aspect of the problem is only part of the calculation — say, for example, if one is including impurity atomic physics in a tokamak discharge simulation — such theoretical calculations may be too cumbersome and/or time consuming to include. It is not our purpose here to assess the merits of rate coefficients from different sources. Our own criterion for most of the calculations that we perform is that the coefficients include as much physics as possible while retaining a computationally simple form. Because the rate coefficient calculations in IMPDYN are handled in subroutines, the user has the option of providing his own subroutines for that purpose. Besides the references to rate coefficients already listed and those to be given below, we refer the reader to the newsletter *Atomic Data for Fusion*¹³ for the most current references and summaries of new results. We now turn to a brief discussion of the rate coefficients included in the subroutines of IMPDYN.

2.2.2. Ionization Rate Coefficients

Wherever possible, for both ionization and recombination rate coefficients we use tabulations such as those of Jordan¹⁴ and Summers¹⁵ for two reasons. First, more physics went into such calculations (e.g., dielectronic recombination and auto-ionization) than can be put into simple expressions such as the ones we give below for use when such tables are not available. Also, on a computer, interpolation within a table is more rapid than evaluation of a complicated expression. However, when such tabulations are not available, and this is generally true for high atomic number impurities such as molybdenum and tungsten,

we use H. J. Kunze's semiempirical expression for the ionization rate coefficient¹⁶ with the numerical coefficient reduced by a factor of two as he later suggested:¹⁷

$$S_j(T_e) = 3.75 \times 10^{-8} \frac{q_j}{E_j} \left[\left(\ln \frac{40T_e}{E_j} \right)^3 + 40 \right] \times \frac{T_e^{1/2}}{E_j + 3T_e} \exp(-E_j/T_e) \text{ cm}^3 \text{ s}^{-1} . \quad (4)$$

In Eq. (4), q_j is the number of electrons in the outermost shell of the atom or ion, T_e is the electron temperature of the plasma, and E_j is the ionization energy obtained either experimentally¹⁸ or from the theoretical calculations of Carlson et al.¹⁹ when no experimental values are available. We note that we also use Eq. (4) to fill the uncompleted portions of tabulations such as those referred to above.

There are two exceptions to the above discussion, carbon and oxygen. For these two elements we have used unpublished work by Dory²⁰ based on the results of Beigman et al.,²¹ who give

$$S_j(T_e) = A_j (E_j/T_e)^{1/2} / (E_j/T_e + \chi_j) \text{ cm}^3 \text{ s}^{-1} . \quad (5)$$

where the values of A_j and χ_j are given in Table 1.

2.2.3 Recombination Rate Coefficients

The calculation of the dielectronic recombination contribution to the total recombination rate coefficient is generally so complicated that we do not calculate it. Consequently, when tabulations of total recombination rate coefficients are not available, except for the cases of carbon and oxygen, we calculate only the radiative recombination rate with a few minor corrections along the line pursued by Jordan.¹⁰ For radiative recombination from the charge state j we use the expression of Burgess and Seaton,²²

$$\alpha_{jr}(T_e) = 1.12 \times 10^{-13} j^2 E_{j-1}^{1/2} / T_e \text{ cm}^3 \text{ s}^{-1} . \quad (6)$$

Table 1. Parameters for ionization and recombination rate coefficients of carbon and oxygen

Spectroscopic state	A_j ($\times 10^8$)	x_j	B_j ($\times 10^{12}$)	ψ_j
CI	13.0	0.36		
CII	3.6	0.40	0.165	0.1
CIII	2.4	0.73	0.287	0.5
CIV	0.83	0.78	0.576	0.87
CV	0.104	0.62	0.73	0.9
CVI	0.037	0.62	0.38	0.64
CVII			0.56	1.0
OI	11.0	0.285		
OII	3.35	0.285	0.088	0.1
OIII	1.42	0.33	0.255	0.15
OIV	0.9	0.38	0.412	0.53
OV	0.43	0.42	0.583	0.75
OVI	0.17	0.44	0.777	0.82
OVII	0.034	0.62	0.925	0.93
OVIII	0.013	0.62	0.46	0.74
OIX			0.65	1.0

To this we add the correction due to Wilson²³ for radiative decay from bound levels above the thermal principal quantum number limit n_t to those below

$$\alpha_{jb}(T_e) = 9.60 \times 10^{-13} j^4 \exp(x_{tj}/T_e) / n_{tj}^{3/2} \text{ cm}^3 \text{ s}^{-1}, \quad (7)$$

where Wilson^{23,24} gives

$$x_{tj} = 1.29 \times 10^{-4} (E_j/T_e)^{1/7} n_e^{2/7} \quad (8)$$

and Griem²⁵ gives

$$n_{tj} = 1.26 \times 10^2 \left(\frac{j^{12} T_e}{n_e^2 E_H} \right)^{1/17} \exp \left(\frac{4j^2 E_H}{17n_{tj}^3 T_e} \right), \quad (9)$$

where E_H is the ionization energy of the hydrogen atom. Two further corrections by Wilson²³ are included but are generally negligible for tokamak plasmas. The first is for three-body recombination from the continuum,

$$\alpha_{jcb} = 4.45 \times 10^{-29} n_e / (j T_e)^2 \text{ cm}^3 \text{ s}^{-1}, \quad (10)$$

and the second is for collisional de-excitation from levels above the thermal limit n_{tj} ,

$$\alpha_{jcc} = 1.48 \times 10^{-28} n_e \exp(x_{tj}/T_e) / (j n_{tj} T_e)^2 \text{ cm}^3 \text{ s}^{-1}. \quad (11)$$

For carbon and oxygen recombination we use the expression

$$\alpha_j(T_e) = B_j (E_j/T_e)^{3/2} / (E_j/T_e + \psi_j) \text{ cm}^3 \text{ s}^{-1} \quad (12)$$

where Dory's²⁰ values for B_j and ψ_j are given in Table 1.

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3. NUMERICAL SOLUTION OF THE RATE EQUATIONS

3.1 THE NORMALIZED CHARGE STATE DISTRIBUTION VECTOR

It is advantageous to work with the normalized form of Eq. (1), so we define the normalized density or concentration of the $(j-1)$ st charge state of an impurity element as

$$y_j \equiv n_j / \sum_{i=1}^{Z+1} n_i, \quad (13)$$

where $1 \leq j \leq Z + 1$. Thus $j = 1$ corresponds to the neutral atom and $j = Z + 1$ corresponds to the fully ionized ion where Z is the atomic number of the impurity element. The indexing is seen to be different from that in Sect. 2 and has been changed from the more physical notation used there to simplify computer programming. We denote by $y = y(t)$ the complete normalized charge state distribution vector of which $y_j = y_j(t)$ is one component. The normalization of the vector y is expressed in matrix notation as

$$e^T y(t) = 1, \quad (14)$$

where

$$e^T = (1, 1, \dots, 1) \quad (15)$$

and the superscript T is used to indicate the transpose of a matrix.

The vector y is the solution of an initial value problem associated with a system of n linear ordinary differential equations of the form taken by Eq. (1) upon normalization. We designate the ionization rate coefficient for the ion of charge $j - 1$ by I_j , which corresponds to S_{j-1} of Sect. 2. We designate the recombination rate coefficient for the ion of charge j by R_j , corresponding to α_j of Sect. 2. If we define

$$\beta_j = n_e (R_j y_{j+1} - I_j y_j), \quad j = 1, 2, \dots, n - 1, \quad (16a)$$

$$\beta_0 = \beta_n = 0, \quad (16b)$$

then y satisfies the linear, homogeneous system of ordinary differential equations

$$y_j' = -\beta_{j-1} + \beta_j, \quad j = 1, \dots, n, \quad (17)$$

where the prime indicates a time derivative and time dependence usually will not be indicated explicitly. The initial condition is given at $t = t_s$ and satisfies

$$e^T y(t_s) = 1, \quad y(t_s) \geq 0. \quad (18)$$

Equation (17) may be expressed in vector-matrix notation as

$$y' = n_e A y \quad (19)$$

where A is the tridiagonal matrix

$$A = \begin{bmatrix} -I_1 & & R_1 & & & \\ I_1 & -(I_2 + R_1) & R_2 & & & \\ & I_2 & & & & \\ & & & R_{n-2} & & \\ & & I_{n-2} & -(I_{n-1} + R_{n-2}) & R_{n-1} & \\ & & & I_{n-1} & -R_{n-1} & \end{bmatrix}. \quad (20)$$

Because $e^T A = 0$, zero is an eigenvalue of the matrix A . Moreover, it can be shown that the eigenvalues of A are simple, real, and nonpositive. The system of differential equations that y satisfies is called a stiff system because there are some large magnitude negative eigenvalues of the matrix $n_e A$. If a nonstiff numerical integration procedure (e.g., Runge-Kutta or Adams-Moulton) is used to approximate y , a small step size is required to ensure the stability of the integration method, even when the terms associated with the negatively large eigenvalues have become

relatively insignificant. For this reason, an integration procedure designed for stiff systems⁷ is used to approximate the solution y .

It is characteristic of the charge state distribution vector that a significant number, often one-third to one-half, of its components are negligibly small at any given time. However, the components that are negligible vary with time. The computational time required to solve a stiff system as described in Eqs. (19) and (20) is proportional to n , the number of equations in the system. If Eq. (19) can be replaced by a reduced system that adequately describes the significant components of the charge state distribution vector, then a marked saving in computational time can be realized. This approach is discussed in Sect. 3.2.

3.2 A REDUCED CHARGE STATE DISTRIBUTION SYSTEM AND ITS ASSOCIATED ERROR

The elimination of some equations from each end of the homogeneous system of differential equations described in Eq. (19) yields a reduced system with an inhomogeneous term. Let the reduced system comprise equations ℓ through k and define

$$\tilde{y}^T \equiv (y_\ell, y_{\ell+1}, \dots, y_k) . \quad (21)$$

Then the reduced system may be expressed as

$$\tilde{y}' = n_e \tilde{A} \tilde{y} + b \quad (22)$$

where

$$b^T = (-\beta_{\ell-1}, 0, \dots, 0, \beta_k) \quad (23)$$

and

$$\tilde{A} = \begin{bmatrix} -I_\ell & R_\ell & & & \\ I_\ell & -(I_{\ell+1} + R_\ell) & R_{\ell+1} & & \\ & I_{\ell+1} & & & \\ & & & R_{k-2} & \\ & & I_{k-2} & -(I_{k-1} + R_{k-2}) & R_{k-1} \\ & & & I_{k-1} & -R_{k-1} \end{bmatrix} \quad (24)$$

An analytical representation for the solution to the inhomogeneous problem of Eq. (22) is given by

$$\tilde{y}(t) = \phi(t)\phi^{-1}(\tau)\tilde{y}(\tau) + \int_{\tau}^t \phi(t)\phi^{-1}(s)b(s) ds, \quad (25)$$

where

$$\tilde{y}_h(t) \equiv \phi(t)\phi^{-1}(\tau)\tilde{y}(\tau) \quad (26)$$

is the solution to the associated homogeneous problem with the same initial condition at $t = \tau$. Moreover, ϕ is the matrix solution to the matrix initial value problem

$$\phi' = n_e \tilde{A} \phi, \quad \phi(\tau) = I, \quad (27)$$

where I is the identity matrix of order $k - \ell + 1$.

Define the vector e_j to be that vector whose j th component is unity, whose other components are zero, and whose dimension is to be inferred from the context, and let

$$E_f \equiv - \int_{\tau}^t \beta_{\ell-1}(s)\phi(t)\phi^{-1}(s)e_1 ds \quad (28)$$

and

$$E_b \equiv \int_{\tau}^t \beta_k(s) \Phi(t) \Phi^{-1}(s) e_{k-\ell+1} ds . \quad (29)$$

Then

$$\tilde{y}(t) - \tilde{y}_h(t) = E_f(t) + E_b(t) . \quad (30)$$

Define the function $[\]^+$ by

$$[x]^+ \equiv \begin{cases} x & \text{whenever } x \geq 0 \\ 0 & \text{otherwise} \end{cases} . \quad (31)$$

Let

$$E_f^+(t) = \int_{\tau}^t [-\beta_{\ell-1}(s)]^+ \Phi(t) \Phi^{-1}(s) e_1 ds \geq 0 , \quad (32a)$$

$$E_f^-(t) = \int_{\tau}^t [\beta_{\ell-1}(s)]^+ \Phi(t) \Phi^{-1}(s) e_1 ds \geq 0 , \quad (32b)$$

$$E_b^+(t) = \int_{\tau}^t [\beta_k(s)]^+ \Phi(t) \Phi^{-1}(s) e_{k-\ell+1} ds \geq 0 , \quad (32c)$$

$$E_b^-(t) = \int_{\tau}^t [-\beta_k(s)]^+ \Phi(t) \Phi^{-1}(s) e_{k-\ell+1} ds \geq 0 . \quad (32d)$$

With these functions, $\tilde{y}$ may be expressed as

$$\tilde{y}(t) = \tilde{y}_h(t) + [E_f^+(t) + E_b^+(t)] - [E_f^-(t) + E_b^-(t)] . \quad (33)$$

Because

$$[-\beta_{\ell-1}]^+ \leq n_e I_{\ell-1} y_{\ell-1} \quad (34a)$$

and

$$[\beta_{\ell-1}]^+ \leq n_e R_{\ell-1} y_{\ell} , \quad (34b)$$

it follows that

$$E_f^+(t) \leq \int_{\tau}^t n_e I_{\ell-1} y_{\ell-1} \phi(t) \phi^{-1}(s) e_1 \, ds \quad (35a)$$

and

$$E_f^-(t) \leq \int_{\tau}^t n_e R_{\ell-1} y_{\ell} \phi(t) \phi^{-1}(s) e_1 \, ds . \quad (35b)$$

Also, the components of $\phi(t)\phi^{-1}(s)$ are nonnegative and $e^T \phi(t) = e^T$ for $t \geq \tau$; consequently

$$\|E_f^+(t)\|_1 \leq \int_{\tau}^t n_e I_{\ell-1} y_{\ell-1} \, ds \quad (36a)$$

and

$$\|E_f^-(t)\|_1 \leq \int_{\tau}^t n_e R_{\ell-1} y_{\ell} \, ds , \quad (36b)$$

where $\|v\|_1$ denotes the ℓ_1 -norm of the vector $v^T = (v_1, \dots, v_{k-\ell+1})$.

That is,

$$\|v\|_1 = |v_1| + \dots + |v_{k-\ell+1}| . \quad (37)$$

In a similar fashion,

$$\|E_b^+(t)\|_1 \leq \int_{\tau}^t n_e R_k y_{k+1} \, ds \quad (38a)$$

and

$$\|E_b^-(t)\|_1 \leq \int_{\tau}^t n_e I_k y_k ds . \quad (38b)$$

The reduced system to be used is not the inhomogeneous system described in Eq. (22), which is exact, but the associated homogeneous system

$$\tilde{y}_h' = n_e \tilde{A} \tilde{y}_h , \quad \tilde{y}_h(\tau) = \tilde{y}(\tau) . \quad (39)$$

It follows from Eq. (33) that the approximation $\tilde{y}_h$ is low by at most the vector $E_f^+ + E_b^+$ and high by at most the vector $E_f^- + E_b^-$. $E_f^+(t)$ is associated with the gain into the reduced system from the equations eliminated at the front (low index equations) and $E_f^-(t)$ is associated with the loss from the reduced system to those same equations. But the magnitude of the gain at the front over the time interval $[\tau, t]$ is bounded by the magnitude of the loss to the front over the same time interval plus the sum of the concentrations discarded by the truncation at time τ . Thus,

$$\|E_f^+(t)\|_1 \leq \|E_f^-(t)\|_1 + \sum_{j=1}^{\ell-1} y_j(\tau) \quad (40)$$

and

$$\|E_f^+(t) + E_b^+(t)\|_1 \leq \|E_f^-(t) + E_b^-(t)\|_1 + \sum_{j=1}^{\ell-1} y_j(\tau) + \sum_{j=k+1}^n y_j(\tau) . \quad (41)$$

From Eqs. (36b) and (38b) it follows that

$$\|E_f^-(t) + E_b^-(t)\|_1 \leq \int_{\tau}^t n_e (R_{\ell-1} y_{\ell} + I_k y_k) ds . \quad (42)$$

Equations (40) and (41) are used in Sect. 3.4 as the basis for the strategy to alter (add to or delete from) the set of active equations and to monitor the error arising from the use of a truncated set.

3.3 PROPAGATION OF THE CURRENT ERROR

Let us assume that at $t = \tau$ the exact solution of the reduced system is denoted by $y(\tau)$ and that $y(\tau)$ is decomposed into

$$y(\tau) = y_a(\tau) + E^+(\tau) - E^-(\tau), \quad (43)$$

where

$$E^+(\tau) \geq 0, E^-(\tau) \geq 0, [E^+(\tau)]^T E^-(\tau) = 0 \quad (44)$$

and $y_a(\tau)$ is the computed approximation to $y(\tau)$. From the linearity of the problem it follows that

$$\begin{aligned} \Phi(t)\Phi^{-1}(\tau)y(\tau) &= \Phi(t)\Phi^{-1}(\tau)y_a(\tau) + \Phi(t)\Phi^{-1}(\tau)E^+(\tau) \\ &\quad - \Phi(t)\Phi^{-1}(\tau)E^-(\tau), \end{aligned} \quad (45)$$

where Φ is the matrix solution to the problem described in Eq. (27) with $\ell = 1$ and $k = n$. Because $\Phi(t)\Phi^{-1}(\tau) \geq 0$ and because $e^T \Phi(t)\Phi^{-1}(\tau) = e^T$, it follows that

$$\|\Phi(t)\Phi^{-1}(\tau)E^+(\tau)\|_1 = \|E^+(\tau)\|_1 \quad (46a)$$

and

$$\|\Phi(t)\Phi^{-1}(\tau)E^-(\tau)\|_1 = \|E^-(\tau)\|_1. \quad (46b)$$

Thus, the ℓ_1 -norm of each vector term on the right-hand side of Eq. (45) is constant. The accuracy of most integration procedures is expressed in terms of a local truncation error bound, so it would be beneficial if some cancellation in the vector difference in Eq. (45) occurred with time.

Qualitatively there are two basic types of reduced systems. In the first, the reduced system is such that I_j/R_j is large (small) for all j within the reduced system. In this case the tendency is for the distribution to move toward the higher (lower) charge states. This is also true for the associated error vectors. In the second, the reduced system is

such that $I_j/R_j \geq 1$ for some j and $I_j/R_j \leq 1$ for some j . In this situation there is a tendency for the distribution to move toward or reside mainly in the components $j + 1$ for which I_j/R_j is near one. Again, the error vectors have the same tendency. In this second type with the central tendency we would expect good cancellation in the vector difference in Eq. (45). In fact, in the case of constant temperature and density the three vector terms on the right-hand side of Eq. (45) become proportional to the equilibrium charge state distribution vector as time increases. Hence, in this case, maximal cancellation occurs.

If $y^T(t_s) = (1, 0, \dots, 0)$ or $(0, \dots, 0, 1)$, then a significant number of integration steps are often required with the first type of reduced system. Although some cancellation is to be expected with the first type, its degree is indeterminant.

3.4 A STRATEGY FOR MONITORING THE ERROR AND ALTERING THE SET OF ACTIVE EQUATIONS

The results of Sects. 3.2 and 3.3 need to be combined in order to monitor the error more closely on a time interval (τ, t) . We let the set of active equations be equations ℓ through k and in Eq. (43) let the components of $y_a(\tau)$ that correspond to deleted equations be zero. Define $\tilde{E}^+(t)$ to be the vector comprising the ℓ through k components of the vector $\Phi(t)\Phi^{-1}(\tau)E^+(\tau)$ appearing in Eq. (45) and define $\tilde{E}^-(t)$ in the obvious way. Then

$$\|\tilde{E}^+(t)\| \leq \|E^+(\tau)\|_1, \|\tilde{E}^-(t)\| \leq \|E^-(\tau)\|_1. \quad (47)$$

Thus, the representation

$$\tilde{y}(t) = \tilde{y}_h(t) + [\tilde{E}^+(t) + E_f^+(t) + E_b^+(t)] - [\tilde{E}^-(t) + E_f^-(t) + E_b^-(t)] \quad (48)$$

includes the error due to an initial error at time τ , as described in Eq. (43), but with the above alteration as well as the error due to using the reduced system of equations.

With the introduction of zeros into $y_a(\tau)$ it follows that

$$\|E^+(\tau)\|_1 = \|\tilde{E}^+(\tau)\|_1 + \sum_{j=1}^{\ell-1} y_j(\tau) + \sum_{j=k+1}^n y_j(\tau) \quad (49a)$$

and

$$\|E^-(\tau)\|_1 = \|\tilde{E}^-(\tau)\|_1. \quad (49b)$$

Define

$$L(\tau, t) = \int_{\tau}^t n_e(R_{\ell-1} y_{\ell} + I_k y_k) ds. \quad (50)$$

Then on the interval $[\tau, t]$,

$$\|\tilde{E}^+(t) + E_f^+(t) + E_b^+(t)\|_1 \leq \|E^+(\tau)\|_1 + L(\tau, t) \quad (51a)$$

and

$$\|\tilde{E}^-(t) + E_f^-(t) + E_b^-(t)\|_1 \leq \|\tilde{E}^-(\tau)\|_1 + L(\tau, t). \quad (51b)$$

Let us assume that at the initial time $t = t_s$ the initial value is exact. Then on the interval (t_s, t)

$$\|\tilde{E}^+(t) + E_f^+(t) + E_b^+(t)\|_1 \leq L(t_s, t) + p(t) \quad (52a)$$

and

$$\|\tilde{E}^-(t) + E_f^-(t) + E_b^-(t)\|_1 \leq L(t_s, t). \quad (52b)$$

where $p(t)$ is the cumulative sum of the values of the deleted components through time t .

The components of the approximation, $\tilde{y}_h$, may be used in L and p with the result that Eq. (52) remains valid. The functions L and p provide a computationally simple means to monitor the error associated with the current set of active equations and to alter the set of active

equations. In fact, except at points where the set of active equations is altered, the time derivative of the bounds on the right-hand side of Eq. (52) is

$$n_e(R_{\ell-1}y_{\ell} + I_k y_k) . \quad (53)$$

The function L may be effectively restrained by requiring the time derivative in Eq. (53) to be bounded. Indeed, if the value of the expression in Eq. (53) becomes too large, then equations should be added to the back of the current system whenever $I_k y_k \geq R_{\ell-1} y_{\ell}$ or to the front of the system whenever $R_{\ell-1} y_{\ell} > I_k y_k$.

A criterion for deleting equations must take two things into account. First, the proposed new set of active equations must have a sufficiently small value for the time derivative given by Eq. (53). Second, the sum of the components associated with the proposed newly deleted equations must be bounded so that the function p does not become too large.

3.5 COMPUTATIONAL PROGRAMS

A collection of subroutines has been compiled from which it is possible to form two separate computer programs. One program, PROG TI, requires that the temperature and density be constant. Here the suffix (and elsewhere the "argument") TI indicates time independence. The other program, PROG TD, allows the temperature and density functions to be time-dependent. The suffix (and elsewhere "argument") TD indicates time dependence.

Program PROG TI is designed for equilibrium calculations. In this case, the system of linear ordinary differential equations describing the normalized charge state distribution vector

$$y' = n_e A y , \quad y(t_s) = y_0 \quad (54)$$

has a constant coefficient matrix $n_e A$. PROG TI may be requested to: (1) determine the equilibrium vector associated with Eq. (53), (NCH.NE.0); (2) approximate the eigenvalues of the coefficient matrix $n_e A$ in Eq. (54), (NROOTS.GT.0); (3) integrate Eq. (54) over the time interval (t_s, t_f)

with y_0 specified in subroutine YINIT; or (4) integrate Eq. (54) until the current $y(t)$ first becomes within EPSCC of the equilibrium vector associated with Eq. (54), where subroutine CONEQU contains the two criteria for measuring closeness.

Fundamentally, the equilibrium vector associated with Eq. (54) is determined from the relationship

$$y_{j+1} = (I_j/R_j)y_j . \quad (55)$$

However, measures are followed to exclude the occurrence of machine underflows or overflows and to handle zero values for I and R reasonably. The equilibrium vector is approximated within subroutine EQU.

Program PROGTD is designed only to integrate Eq. (54) over the interval (t_s, t_f) where the temperature and density are time-dependent. Subroutines DENTMP(TD), DTDATA, and DTINIT provide for the definition of the temperature and density profiles.

Subroutine MAIN1(TD) is the basic control routine for program PROGTD; subroutine MAIN1(TI) is the basic control routine for program PROGTI. Subroutine DRIVES controls the numerical integration of Eq. (54). Logic schematics of these three subroutines are given in the flow charts in Figs. 1, 2, and 3.

The subroutines, including numerous comment cards, are listed on the accompanying microfiche lexicographically except that the block data routines come first. The block data routine BDPARM comes first, followed by the set of block data routines BDEL, ordered according to the atomic number of the associated impurity element. The parameter EL is replaced by the chemical symbol for the element. The data within BDEL is for use with the rate coefficient routines, SVIONZ and SVRECZ, but NZ, the atomic number of the element, is used in several other routines. The block data routine BDPARM contains descriptions of all the control parameters that may be used in the definition of the problem to be solved with the computer program. All input to the program is through the block data routine BDPARM for the program PROGTI. For program PROGTD, the additional data describing the time-dependent temperature and density profiles are found within subroutine DTDATA in data statements.

FLOW CHART I
SUBR. MAIN1 (TD)

Fig. 1. Logic schematic of IMPDYN program subroutine MAIN1(TD) used when the electron density and temperature are time-dependent.

(*) EITHER LOOPING OVER: (1) TE, DEN INDEPENDENTLY;
OR (2) THE ORDERED PAIRS (TE, DEN).

Fig. 2. Logic schematic of IMPDYN program subroutine MAIN1(TI) used when the electron density and temperature are constant (time-independent).

FLOW CHART III
SUBR. DRIVES

Fig. 3. Logic schematic of IMPDYN program subroutine DRIVES.

Besides describing in the comment cards the kinds of problems the programs PROGTD and PROGTI can solve, the main routine, MAIN, contains two tables that help to reveal the structural organization of the programs and the layout of the labeled commons.

4. EXAMPLES

In this section we discuss the two examples that are included on the microfiche. These examples were chosen to illustrate the use of IMPDYN in its most recent version, to provide benchmarks for checkout of IMPDYN at other installations, and to illustrate some points of physics. Because considerable discussion of input and output for the examples is given on the comment cards associated with the examples on the microfiche, few of the programming details are discussed here and the emphasis is on physics.

4.1 EXAMPLE I: CORONA EQUILIBRIUM

The first example concerns the corona equilibrium charge state distribution of iron in constant plasma conditions where $T_e = 500$ eV, $n_e = 10^{13}$ cm⁻³. For the simple general models of ionization and recombination used, in which auto-ionization and dielectronic recombination are neglected, the equilibrium vector is essentially independent of n_e , although there are small corrections which depend on n_e [see Eqs. (7)-(11)]. However, the time required for the charge state vector to approach to within a specified approximation to the equilibrium vector is directly proportional to n_e . This follows directly from Eq. (1), where the time rate of change of a given charge state is seen to be directly proportional to n_e . On page 3 of the Example I part of the microfiche, the normalized equilibrium vector calculated using Eq. (55) [cf. also Eq. (14)] is listed. Only components with concentrations of $\geq 10^{-6}$ are included in the vector. Components with smaller concentrations are neglected and the vector renormalized. This lower bound is set in the data statement card EQU 18 of subroutine EQU. The eigenvalues of $n_e A$ are also listed on page 3. Note that the known zero eigenvalue is not calculated numerically by this single precision program to vanish identically; however, its computed value is about five orders of magnitude smaller than the next larger eigenvalue.

On page 4 of this example, an approach to equilibrium is illustrated. At time $t = 0$, neutral iron atoms are subjected to the plasma

conditions listed above. Printouts of the distribution have been requested for convergence criteria $EPSE = 0.5, 0.1$, and 0.01 , corresponding to the three values of $EPSCC$ in the block data, card EX.I 50, and at intermediate values controlled by the information on card EX.I 47. The convergence criterion used, $NCRIT = 1$ (cf. cards BDPARM 35-42, page 2 of program listing), is that the ℓ_1 -norm, defined in Eq. (37), of the vector difference between the charge state vector $\tilde{y}_h(t)$ calculated at a given time and the equilibrium vector y_{eq} be less than a prescribed amount. From the listing it is seen that nearly 57 ms are required for $\|\tilde{y}_h - y_{eq}\|_1 < 0.5$. Although this value of $EPSE$ is adequate to get the average charge of the distribution within $\sim 3.5\%$ of its equilibrium value, the concentrations of important states may be incorrect by as much as a factor of two, with possible significant effects on transport and radiation. As would be expected, the lower charge states are overpopulated and the higher states are underpopulated. We also note that 12 equations are current ($K - L + 1$), those for Fe^{13+} through Fe^{24+} , down from the 14 equations needed at the time $t = 0.5$ ms of the first printout. The integration step size H is between 2 and 4 ms (H is listed in seconds), up from the initial step size of 5 ns (input quantity $H0$) needed at the beginning of the integration when the distribution was farthest from equilibrium. It takes nearly 64 ms more to satisfy the next convergence criterion, $EPSE = 0.1$, at which time the average Z is within less than a percent of its equilibrium value. The dominant charge states are within 10% or so of their equilibrium values at this time. In fact, at $t = 110$ ms the dominant charge states were within 15% or so, and even at $t = 80$ ms, within 25% or so. Nevertheless, it is apparent that for this electron density, tens of milliseconds are required for the charge distribution to approach reasonably near to corona equilibrium. These times are on the order of transport times in a tokamak,²⁴ so the effects of transport should be taken into account, as discussed in Sect. 2. We recall, however, that these times are also inversely proportional to the electron density. For the electron temperature chosen for the example, realistically, the electron density should probably be on the order of a factor of two to three higher.²⁴

Consequently, the time estimates should be reduced by the same factor. Such a reduction would still leave the time estimates on the order of transport times, thus leaving open the question of whether corona equilibrium distributions for iron can exist in tokamak plasmas. We address this point further in the next example. We also point out that including auto-ionization and dielectronic recombination in the rate coefficients would change the results for these examples quantitatively (e.g., increase the proportions of the lower charge states) but not qualitatively (i.e., relatively long times are still needed for the approach to corona equilibrium).

4.2 EXAMPLE II: TIME-DEPENDENT T_e AND n_e

In the second example, we study the evolution of the charge state distribution of iron in a plasma environment representative of the central plasma region of the Oak Ridge Tokamak (ORMAK) during electron heating experiments.²⁴ Laser electron temperature and density data were available for seven times within the discharge period studied, starting at 20 ms, and these are listed at the top of page 4 of the Example II part of the microfiche. In the period before data were available, simple models of the density and temperature evolution were used, and these are listed following the data. As is also indicated on the microfiche, linear interpolation is used to obtain necessary density and temperature information between data points. At each printout time, as chosen in the data statements for TPRNT, DTPRNT, and NPRNT, the distribution of charge states is given, along with other information similar to that given for Example I.

We first note that the time step H in this case, in which the electron temperature is evolving with time, exceeds 1 ms only when the temperature is changing very slowly and never exceeds 2.6 ms. This is in contrast to Example I, in which the temperature was constant and H eventually exceeded 10 ms. In order to best illustrate some of the things that can be learned from this example, we have plotted some of the results of the calculations in Fig. 4. In the upper part of Fig. 4, the evolution of the electron density and temperature is illustrated.

Fig. 4. Ratios of time-dependent to corona steady-state densities of iron ions as functions of time in an ORMAK experiment. In the upper part curves showing the evolution of the central plasma electron density and temperature are given. In the lower part curves are given only for ions with concentrations at least 10% of the total iron density at a given time. The following coding is used for the dominant (greatest fraction of total) ion: (1) heavy line – dominant for both time-dependent and steady-state, (2) broken line – dominant for time-dependent only, (3) dotted line – dominant for steady-state only.

In the lower part of the figure, the evolution of charge states comprising more than 10% of the total impurity at the time of plotting is shown in the following way. The curves plotted are the ratios of the densities (concentrations) calculated using PROGTD, i.e., the concentrations given on the microfiche, to densities (concentrations) for coronal steady state calculated using PROGTI (not given on the microfiche).

When a curve is at or near unity, the steady-state approximation is good for that species. Another criterion for the validity of the steady-state approximation is whether it would predict the same dominant (highest concentration) charge state as the time-dependent model. In Fig. 4, the heavy solid line indicates when this is true. When it is not true, the dominant species are indicated as described in the figure caption. As would be expected, the steady-state approximation is worst when the electron temperature is changing relatively rapidly, e.g., in the intervals 30-70 ms and 80-100 ms. Although in the vicinity of 80 ms all the curves are near unity, they have large slopes, so the ratios are changing rapidly. At the end of the calculation, where the temperature has been essentially constant for about 30 ms, the curves are approaching unity. Note that when the temperature is increasing, the time-dependent distribution is weighted toward lower charge states than the equilibrium; when the temperature is decreasing, the opposite is true. Because the excitation rate coefficient for a given species is strongly dependent on the electron temperature,²⁵ this can have the effect of enhancing the intensity of the radiation emitted when the electron temperature is rising but diminishing it when the temperature is falling. Finally, as was also noted in the discussion of Example I, the atomic physics processes are occurring on time scales comparable to plasma transport time scales, so they must generally be treated time-dependently in transport modeling along with the diffusion processes.

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5. SUMMARY AND CONCLUSIONS

In this report, we have discussed a computer program, IMPDYN, that we have found very useful in the study of the evolution of impurities in tokamak plasmas. The program has a number of desirable features, such as minimizing the number of rate equations that need to be solved at any time and allowing any models of ionization and recombination to be used, provided they can be put in a form compatible with the rest of the program. The program has been designed to make this latter step relatively easy by having ionization handled by one subprogram, SVIONZ, and recombination handled by another, SVRECZ, either or both of which may be replaced by equivalent subroutines. The entire program, including two examples which are valuable for checking that the program is working properly, is listed on a microfiche so that the program may be put on any machine. The program is also available from the authors via the National Magnetic Fusion Energy Computer Center.

In the examples we have basically tried to point out that (1) the corona steady-state approximation can be poor when plasma conditions, especially electron temperature, are changing rapidly, and (2) in time-dependent modeling of tokamak discharges there must be interplay between the calculations of the atomic physics processes and the diffusion in order to get them both correct.

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MICROFICHE ENCLOSURE

C *** DIBECIOY FOR THE MICROFICHE	DIR.	1
C ***	DIR.	2
C *** (I). A LISTING OF ALL THE ROUTINES ORDERED LEXICOGRAPHICALLY	DIR.	3
C *** EXCEPT THAT THE BLOCK DATA BDPARM COMES FIRST AND THEN THE COLL.	DIR.	4
C *** OF BLOCK DATA (BDEL) FOR CERTAIN ELEMENTS ORDERED ACCORDING TO	DIR.	5
C *** THEIR ATOMIC NUMBER WHERE EL IS REPLACED WITH THE SYMBOL FOR THE	DIR.	6
C *** ELEMENT. SUBROUTINE MAIN CONTAINS A DESCRIPTION OF THE TYPE OF	DIR.	7
C *** PROBLEMS THAT CAN BE SOLVED AND THE BLOCK DATA BDPARM DEFINES THE	DIR.	8
C *** PARAMETERS THAT NEED TO BE DEFINED BY THE USER. THE CURRENT SPACE	DIR.	9
C *** ALLOCATION IS SUCH THAT ELEMENTS THRU ATOMIC NUMBER 74(H) MAY BE	DIR.	10
C *** HANDLED. THE SPACE ALLOCATION MAY BE CHANGED BY REDEFINING NOM IN	DIR.	11
C *** MAIN TO THE DESIRED VALUE AND ALTER THE SIZE OF THE COMMON ARRAYS	DIR.	12
C *** DEFINED IN MAIN ACCORDING TO THE FORMULAS INDICATED THERE.	DIR.	13
C *** MOREOVER, SUBROUTINE SURECZ, THE MODIFIED CAROLE JORDAN ROUTINE	DIR.	14
C *** FOR APPROXIMATING THE RECOMBINATION RATE COEFF., HAS THREE LOCAL	DIR.	15
C *** ARRAYS THAT MUST HAVE AT LEAST NZ (=ATOMIC NUMBER OF ELEMENT UNDER	DIR.	16
C *** CONSIDERATION) ELEMENTS IN EACH ARRAY. CURRENTLY, THESE ARRAYS	DIR.	17
C *** HAVE NOM=74 ELEMENTS EACH.	DIR.	18
C *** THE ORDER OF THE ROUTINES IS BDPARM, BDC, BDO, BDAL, BDFE, BDNI, BDCU,	DIR.	19
C *** BDW, BDAU, EQU, YNA, MAIN, YOUT, YPAY, MAINI(TD), MAINI(TI), ROOTS, STIFF,	DIR.	20
C *** TESOC, YINIT, YOUTD, CONEQU, DENTMP(TD), DENTMP(TI), DRIVES, DTDATA,	DIR.	21
C *** DTINIT, INTQLI, INTEGC, STRATG, STRTGI, SUIONZ, SURECZ, ZAVERG.	DIR.	22
C ***	DIR.	23
C *** (II). A DESCRIPTION OF EXAMPLE 1 AND THE BLOCK DATA, BDPARM, FOR	DIR.	24
C *** THIS EXAMPLE.	DIR.	25
C ***	DIR.	26
C *** (III). OUTPUT FOR EXAMPLE 1.	DIR.	27
C ***	DIR.	28
C *** (IV). A DESCRIPTION OF EXAMPLE 2 AND THE BLOCK DATA, BDPARM, FOR	DIR.	29
C *** THIS EXAMPLE.	DIR.	30
C ***	DIR.	31
C *** (V). OUTPUT FOR EXAMPLE 2.	DIR.	32

BLOCK DATA

BDPARM 1

C *** ORIGINAL SEQUENCING DONE ON 07-13-77

COMMON/EP5/NCH, NEQU, NEPS, NEPSC, NCRIT, EPSECU, ZAUGEO, EPSCC(10)

BDPARM 2

COMMON/STGY/TF, TELN, TBLN, FL, BL, DC, BDLOSS, BDLOSH, RDEC, ITDEL, NSTRT,

BDPARM 3

NDEL, NEQADD, NEQDEL, NEQDML, BDEL, TSWIT, BDL5MM, JPSTGY

BDPARM 4

COMMON/PRINT/TPRINT, TPRNT(5), DTPRT(5), NPRINT(5), NPRINT1, TPRNTJ, NPR

BDPARM 5

COMMON/SHARE/TE, DEN, HMIN, HMAX, EPS, HF, KFLAG, JDISC, NOM, NOM2, NOMP

BDPARM 6

COMMON/STRAT/IT, NLB, NKB, ISWSTR, IEQU, MH

BDPARM 7

COMMON/MAINBD/NTEMP, NDENS, NLOG, NROOTS, IPAIR, TSTART, TLAST, TEL, DTE,

BDPARM 8

IDENL, DDEN, THRES, HO, TEMP(25), DENS(25)

BDPARM 9

COMMON/STGY2B/FACT, FACT1

BDPARM10

C *** FOR PROGT1 THE USER MAY NEED TO SPECIFY ALL THE PARAMETERS

BDPARM11

C *** DESCRIBED HERE.

BDPARM12

C *** FOR PROGT2 THE USER NEEDS TO DEFINE NLB, NKB, ISWSTR, NPRINT1, IEQU, MH,

BDPARM13

C *** TSTART, TLAST, THRES, EPS, HO AND WHENEVER ISWSTR=2 HE NEEDS TO DEFINE

BDPARM14

C *** BDLOSS, FACT, BDEL, RDEC, TSWIT, FACT1, NEQADD, NEQDEL, NSTRT, NDEL,

BDPARM15

C *** JPSTGY. MOREOVER, HE MUST DEFINE (TPRNT(1), DTPRT(1), NPRINT(1),

BDPARM16

C *** I=1, ..., NPRINT1).

BDPARM17

C *** SUBR, MAIN(JD) DEFINES NCH=0

BDPARM18

C ***

BDPARM19

C *** DEFINITION OF POSSIBLY NEEDED INPUT VALUES.

BDPARM20

C ***

BDPARM21

C *** NTEMP USED ONLY WHEN IPAIR, LE, 0. THEN NTEMP, GT, 0 IMPLIES

BDPARM22

C *** 1ST NTEMP LOC. OF TEMP ARRAY CONTAIN TEMPERATURES.

BDPARM23

C *** NTEMP, LT, 0 CAUSES MAIN1(T1) TO DEFINE

BDPARM24

C *** TEMP(J)=TEL+J*DTE, J=0, ..., -NTEMP-1

BDPARM25

C *** NDENS USED ONLY WHEN IPAIR, LE, 0. THEN NDENS, GT, 0 IMPLIES

BDPARM26

C *** 1ST NDENS LOC. OF DENS ARRAY CONTAIN DENSITIES.

BDPARM27

C *** NDENS, LT, 0 CAUSES MAIN1(T1) TO DEFINE

BDPARM28

C *** DENS(J)=DENL+J*DDEN, J=0, ..., -NDENS-1

BDPARM29

C *** NLOG NLOG, GT, 0 IMPLIES INPUT TEMP. IN FORM LOG10(T), T IN

BDPARM30

C *** DEGREES KELVIN. NLOG, LE, 0 IMPLIES TEMP. IN EV.

BDPARM31

C *** NROOTS NROOTS, GT, 0 REQUESTS EIGENVALUES OF CONSTANT COEFF.

BDPARM32

C *** MATRIX NEXA WHERE Y'=NEXA*Y. NROOTS, LE, 0 YIELDS NONE.

BDPARM33

C *** NEPS NEPS(LE, 10)=NO. EPSILON VALUES IN ARRAY EPSCC.

BDPARM34

C *** NCRIT SELECTS CRITERION TO USE FOR MEASURING CLOSENESS OF

BDPARM35

C *** THE TIME EVOLUTION OF THE DISTRIBUTION TO THE

BDPARM36

C *** EQUILIBRIUM DISTRIBUTION. REPORTS THE DISTRIBUTION

BDPARM37

C *** VECTOR FOR THE 1ST COMPUTED TIME FOR WHICH DIST. VEC.

BDPARM38

C *** IS WITHIN EPSCC(1) OF EQUIL. VEC.

BDPARM39

C *** NCRIT=1 USES L1-NORM OF VECTOR DIFFERENCE, Y-YEQU.

BDPARM40

C *** NCRIT=2 USES ABS((Z(Y)-Z(YEQU))/Z(YEQU)) WHERE

BDPARM41

C *** Z(Y)=SUM I=1 TO NZ OF (1-I)*Y(I).

BDPARM42

C *** C.F. NCRIT, NEPS. NEED EPSCC(1+1) LT EPSCC(1)

BDPARM43

C *** NCH NCH, GT, 0 CAUSES TIME INTEGRATION AND MONITORING OF

BDPARM44

C *** CLOSENESS TO EQUILIBRIUM VEC.. CF. NCRIT ABOVE.

BDPARM45

C *** DENSITY AND TEMPERATURE ARE CONSTANT

BDPARM46

C *** NCH=0 CAUSES TIME INTEGRATION ONLY.

BDPARM47

C *** NCH=-2 CAUSES CALCULATION OF EQUILIBRIUM VECTOR ONLY.

BDPARM48

C *** NCH.NE.-2 AND NCH.LT.0 CAUSES TIME INTEGRATION AND

BDPARM49

C *** CALCULATION OF EQUILIBRIUM VECTOR. (NO MONITORING)

BDPARM50

C *** NLB 1ST DIFFERENTIAL EQ. WILL BE NLB UNLESS

BDPARM51

C *** (1) IEQU=1 IN WHICH CASE NLB DEFINED TO BE 1 IN YINIT

BDPARM52

C *** OR (2) IEQU=2, NCH.NE.0, AND THRES.GT.0 IN WHICH CASE

BDPARM53

C *** NLB IS REDEFINED IN SUBR.YINIT.

BDPARM54

C *** NKB LAST DIFFERENTIAL EQ. WILL BE NKB UNLESS

BDPARM55

C *** (1) IEQU=1, NCH.NE.0, AND THRES.GT.0 IN WHICH CASE

BDPARM56

C *** NKB IS REDEFINED IN SUBR.YINIT. OR

BDPARM57

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C *** (2) IEQU=2 IN WHICH CASE YINIT DEFINES NKB=NZ+1 BDPARM58
C *** ISWSTR SELECTS STRATEGY FOR ALTERING SET OF ACTIVE EQS.. BDPARM59
C *** (1) ISWSTR=1 MEANS DON'T ALTER INITIAL SET OF ACTIVE BDPARM60
C *** EQS. BDPARM61
C *** (2) ISWSTR=2 USES GENERAL STRATEGY DESCRIBED IN REPORT BDPARM62
C *** FOR ALTERING SET OF ACTIVE EQS.: VARIABLE DENSITY, BDPARM63
C *** TEMPERATURE, BDPARM64
C *** NPRINT = NUMBER 'PRINT' CONTROL INTERVALS FOR TIME INTEG. BDPARM65
C *** NPRINT1, LE, 5, CF, ARRAYS TPRT, DTPRT, NPRINT IN COMMON BDPARM66
C *** /PRINT/ BDPARM67
C *** IEQU SELECTS INIT, DIST, VEC, WHENEVER TIME INTEGRATION TO BDPARM68
C *** BE PERFORMED AND HELPS DETERMINE INITIAL SET OF ACT. BDPARM69
C *** EQS. IEQU=1 SETS Y(TSTART)=(1,0,...,0) BDPARM70
C *** IEQU=2 SETS Y(TSTART)=(0,...,0,1) BDPARM71
C *** IEQU=3 INCOMPLETE. DEFINE Y(TSTART) IN YINIT. BDPARM72
C *** IPAIR IPAIR.GT.0 MEANS HAVE IPAIR VALUES IN ARRAY TEMP AND BDPARM73
C *** IN ARRAY DENS. THESE ARE PAIRED ARRAYS. BDPARM74
C *** IPAIR.LE.0 MEANS THE TEMPERATURE AND DENSITY VALUES BDPARM75
C *** VARY INDEPENDENTLY OF ONE ANOTHER (CF, NTEMP, NDENS). BDPARM76
C *** MH USED IN NUMERICAL INTEG. WHEN ORDER OF STIFF METH. BDPARM77
C *** SET TO 1 DEFINE H=(LAST H)/(1+(NQ-1)*MH) WHERE BDPARM78
C *** NQ=ORDER OF STIFF LAST USED. BDPARM79
C *** ISTART INITIAL INTEGRATION TIME IN MILLISEC. BDPARM80
C *** TLAST FINAL INTEGRATION TIME IN MILLISEC. BDPARM81
C *** TEL WHEN NTEMP.LT.0 THE DESIRED TEMPERATURES ARE BDPARM82
C *** TEL+J*DTE, J=0,...,-NTEMP-1. IN EV WHEN NLOG.LE.0 AND BDPARM83
C *** LOG10(DEGREE K) WHEN NLOG.GT.0 BDPARM84
C *** DTE CF. TEL ABOVE. BDPARM85
C *** DENL WHEN NDENS.LT.0 DESIRED DENSITIES ARE BDPARM86
C *** DENL+J*DDEN, J=0,...,-NDENS-1 BDPARM87
C *** DDEN CF. DENL ABOVE. BDPARM88
C *** THRES APPLICABLE ONLY WHEN IEQU=1 OR 2 AND NCH.NE.0 BDPARM89
C *** (CF, SUBR, YINIT) LET COMPONENTS OF IEQU BE YE(I) BDPARM90
C *** (1) IEQU=1 DEFINES NKB SO THAT SUM I=NKB TO NZ+1 OF BDPARM91
C *** YE(I) IS .GE. THRES AND SUM I=NKB+1 TO NZ+1 OF YE(I) BDPARM92
C *** IS .LT. THRES. BDPARM93
C *** (1) IEQU=2 DEFINES NLB SO THAT SUM I=1, NLB OF YE(I) BDPARM94
C *** IS .GE. THRES AND SUM I=1 TO NLB-1 OF YE(I) IS .LT. BDPARM95
C *** THRES. BDPARM96
C *** EPS USED IN INTEGRATION ROUTINE STIFF. ACTUALLY IS BDPARM97
C *** EPS*YMAX WHERE EPS IS THE DESIRED BOUND FOR THE LOCAL BDPARM98
C *** TRUNCATION ERROR AND YMAX IS USED FOR SCALING. BDPARM99
C *** ORIGINALLY YMAX WAS A VECTOR, BUT NOW IS A SCALAR. BDPARM 0
C *** .3.LT.YMAX.LT.6 IS REASONABLE. BDPARM 1
C *** H0 INITIAL STEPSIZE TO TRY AT T=ISTART IS H0(SEC.). BDPARM 2
C *** FOLLOWING PARAMETERS ARE REQUIRED FOR STRATEGY 11 FOR ALTERING BDPARM 3
C *** SET OF ACTIVE EQS. (ISWSTR=2). BDPARM 4
C *** BDLOSS DESIRED MAX. BOUND FOR L1-NORM OF ERROR IN ACTIVE BDPARM 5
C *** COMPONENTS. BDPARM 6
C *** FACT WHEN DELETE FROM FRONT OF SYSTEM REQUIRE FOR NEW L BDPARM 7
C *** THAT NEXT(L-1)*Y(L)*(TF-T).LE.FACT*BDLOSS WHERE BDPARM 8
C *** T(SEC.)= CURRENT TIME, TF(SEC.)=EXPECTED FINAL TIME, BDPARM 9
C *** FROM BACK REQUIRE NEW K SUCH THAT NEXT(K)*Y(K)*(TF-T) BDPARM10
C *** .LE.FACT*BDLOSS. BDPARM11
C *** BDEL REQUIRE SUM OF COMPONENTS AT FRONT(OR BACK) TO BE BDPARM12
C *** .LE.BDEL PRIOR TO DELETION. BDPARM13
C *** RDEC MAY ADD FEWER THAN NEQADD EQS. WHEN ADD TO FRONT OR BDPARM14
C *** BACK. HOWEVER, NEVER ADD BEYOND 1ST RATE COEFF. THAT BDPARM15

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C *** IS LE RDEC*(LAST ONE USED IN CALCULATION) BDPARM16
C *** RDEC SIGNIFIES RELATIVE DECREASE. BDPARM17
C *** TSWIT DISTRIBUTION VECTOR VARIES QUICKLY FOR EARLY TIME. BDPARM18
C *** IN (TSTART/1000, TSWIT(SEC)) DESIRE LI-NORM OF ERROR BDPARM19
C *** IN ACTIVE EOS, TO BE LE FACT*BDLOSS BDPARM20
C *** FACT1 CF. TSWIT ABOVE. BDPARM21
C *** NEQADD ADD AT MOST NEQADD EOS TO FRONT (BACK) AT ONE TIME BDPARM22
C *** CF. RDEC ABOVE. BDPARM23
C *** NEQDEL IF EOS MUST BE ADDED TO ONE END, THEN OTHER END IS BDPARM24
C *** CHECKED SO AS TO DELETE AS MANY EOS. AS POSS. SUBJECT BDPARM25
C *** ONLY TO LIMITATION IMPOSED BY BDEL ABOVE. BDPARM26
C *** NSTRT CHECK CRITERION FOR DELETING EOS. ON INTEGRATION BDPARM27
C *** STEP NUMBERS GIVEN BY NSTRT+(P-1)*NBDEL, P=L2, BDPARM28
C *** DON'T WANT TO TEST CRITERION TOO OFTEN. BDPARM29
C *** NBDEL CF. NSTRT ABOVE. BDPARM30
C *** IPSTGY =1 MEANS DON'T PRINT FROM SUBR.STRATG BDPARM31
C *** =2,3 PRINT WHEN ADD EOS. TO SYSTEM. BDPARM32
C *** =3,4 PRINT WHEN CHECK FOR DELETION OF EOS.. BDPARM33
C *** END OF PARA. FOR STRATEGY 11. BDPARM34
C *** PARAMETERS GOVERNING OUTPUT CONTROL. OUTPUT OF THE DISTRIBUTION BDPARM35
C *** VECTOR IS HANDLED IN SUBR. YNA. (USER MAY WISH TO USE HIS OWN YNA) BDPARM36
C *** YNA IS CALLED BY YOUT WHENEVER CURRENT TIME T IS GE. TPRINT. BDPARM37
C *** TPRINT(J) SUBR. YNA CALLED WHENEVER CURRENT TIME GE. BDPARM38
C *** TPRINT(MS)=TPRNT(1)+J*DTPT(1), J=0,...,NPRNT(1), BDPARM39
C *** LE L...NPRNT(1) (TPRNT(1), DTPT(1) IN MILLISEC) BDPARM40
C *** DTPT(1) CF. TPRNT(1) ABOVE. BDPARM41
C *** NPRNT(1) CF. TPRNT(1) ABOVE. BDPARM42
C *** TEMP AND DENS ARRAYS ARE FOR USE WITH SUBROUTINE MAIN(11). BDPARM43
C *** TEMP(1) CONTAINS IPAIR.GT.0 TEMP. VALUES. BDPARM44
C *** CONTAINS NTEMP.GT.0 TEMP. VALUES (IPAIR.LE.0) BDPARM45
C *** TEMP. UNIT IS EV WHENEVER NLOG.LE.0 AND LOG10(DEG K) BDPARM46
C *** WHENEVER NLOG.GT.0 BDPARM47
C *** DENS(1) CONTAINS IPAIR.GT.0 DENSITY VALUES. BDPARM48
C *** CONTAINS NDENS.GT.0 DENSITY VALUES (IPAIR.LE.0). BDPARM49
C *** BDPARM50
C *** END OF DEFINITION OF POSSIBLY NEEDED INPUT VALUES. BDPARM51
C *** BDPARM52
DATA NTEMP, NDENS, NLOG, NROOTS, NEPS, NCRIT, NCH70, 0, 0, 7, 5, 7, 7 BDPARM53
DATA NLB, NKB, ISWSTR, NPRNT1, IEQU, IPAIR, MH/1, 10, 2, 4, 1, 1, 5/ BDPARM54
DATA TSTART, TLAST, TEL, DTE, DENL, DDEN, THRES, EPS, HO/0., 500., BDPARM55
10., 0., 0., 0., 0., 5.E-6, 1.E-9/ BDPARM56
C *** NEXT GROUP OF PARAMETERS APPLICABLE ONLY IF TSWSTR=2 BDPARM57
DATA BDLOSS, FACT, BDEL, RDEC, TSWIT, FACT1, NEQADD, NEQDEL, NSTRT, NBDEL, BDPARM58
IPSTGY/1.E-5, .5, 1.E-7, .1, 1.E-6, .1, 3, 3, 50, 20, 1/ BDPARM59
C *** NEXT GROUP OF PARAMETERS (AND NPRNT1) GOVERN OUTPUT THRU SUBR. YNA. BDPARM60
DATA TPRNT/0., 2., 25., 225., DTPT/1, 1., 10., 25., NPRNT/19, 19, 19, 13/ BDPARM61
DATA TEMP/388./ BDPARM62
DATA DENS/1.717E13/ BDPARM63
DATA EPSCC/9.75E5, 1.001/ BDPARM64
END BDPARM65

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BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-06-77	BDC	1
C *** E,API,CHI USED IN SUIONZ BY DORY.	BDC	2
C *** E,APR,CHR USED IN SURECZ BY DORY.	BDC	3
C *** USE E'S AND Q'S IN SUIONZ FOR KUNZE IONIZATION AS WELL AS INFO.	BDC	4
C *** IN COMMON/XCION/.	BDC	5
C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION,	BDC	6
C CALC. AV. SIGMA *U FOR RECOMBINATION AND IONIZATION OF	BDC	7
C CARBON R DORY 2/12/73 FUDGED API(2), APR(5,6) TO GIVE	BDC	8
C BETTER FIT TO TABULATION OF LOTZ, ASTROPHYS. J. XIV (1967).	BDC	9
C REF. L. L. REICHMAN, ET AL, ASTRON. JH, 13, 75, (1970)	BDC	10
COMMON/E/NZ, NEQPT, E(6)	BDC	11
COMMON/Q/Q(6)	BDC	12
COMMON/API/API(6)	BDC	13
COMMON/APR/APR(6)	BDC	14
COMMON/CHI/CHI(6)	BDC	15
COMMON/CHR/CHR(6)	BDC	16
COMMON/XCION/NCUT, DELTA, XC(1)	BDC	17
COMMON/ELNAME/ELNAME, NELDES, DES(B)	BDC	18
DATA NCUT/0/	BDC	19
DATA DES/' FIND OUT WHERE E'S CAME FROM. '	BDC	20
DATA NELDES/8/	BDC	21
DATA ELNAME/' C '	BDC	22
C *** NEQPT.LE.0 CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED	BDC	23
C *** IN SUIONZ AND SURECZ.	BDC	24
C *** NEQPT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND	BDC	25
C *** DESCRIPTIVE INFO. IN DES ARRAY.	BDC	26
C *** NEQPT MAY BE ALTERED WITHIN SUIONZ, SURECZ.	BDC	27
INTEGER NZ/6/, NEQPT/1/	BDC	28
REAL E/11.3,24.4,47.9,64.5,392.,7490./	BDC	29
REAL Q/4.,3.,2.,1.,2.,1./	BDC	30
REAL API/13.E-8,3.6E-8,2.4E-8,.83E-8,.7E-8,.037E-8/	BDC	31
REAL APR/1.65E-12,.355E-12,.576E-12,.727E-12,.38E-12,.56E-12/	BDC	32
REAL CHI/.36,.40,.73,.778,.62,.62/	BDC	33
REAL CHR/1.5,87.9,64.1/	BDC	34
END	BDC	35

BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-06-77	BDO	1
C *** E,API,CHI USED IN SUTONZ BY DORY.	BDO	2
C *** E,APR,CHR USED IN SURECZ BY DORY.	BDO	3
C *** USE E'S AND O'S IN SUTONZ FOR KUNZE IONIZATION AS WELL AS INFO.	BDO	4
C *** IN COMMON/XCION/.	BDO	5
C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.	BDO	6
C *** CALC. AV. SIGMA *U FOR RECOMBINATION AND IONIZATION OF	BDO	7
C *** OXYGEN R DORY 2/12/73 FUDGED API(2), APR(5,6) TO GIVE	BDO	8
C *** BETTER FIT TO TABULATION OF LOTZ, ASTROPHYS. J. XIU (1967).	BDO	9
C *** REF. L. L. BEIGHAN, ET AL. ASTRON. J. 75, (1970)	BDO	10
COMMON/E/NZ, NEOPRT, E(8)	BDO	11
COMMON/O/Q(8)	BDO	12
COMMON/API/API(8)	BDO	13
COMMON/APR/APR(8)	BDO	14
COMMON/CHI/CHI(8)	BDO	15
COMMON/CHR/CHR(8)	BDO	16
COMMON/XCION/NCUT, DELTA, XC(1)	BDO	17
COMMON/ELNAME/ELNAME, NELDES, DES(8)	BDO	18
DATA NCUT/0/	BDO	19
DATA DES/' FIND OUT WHERE E'S CAME FROM. '	BDO	20
DATA NELDES/0/	BDO	21
DATA ELNAME/' O '	BDO	22
C *** NEOPRT.LE.O CAUSES NO PRINT OF E AND O VALUES THAT ARE TO BE USED	BDO	23
C *** IN SUTONZ AND SURECZ.	BDO	24
C *** NEOPRT=1 REQUESTS PRINT OF E'S IF NEEDED AND O'S IF NEEDED AND	BDO	25
C *** DESCRIPTIVE INFO. IN DES ARRAY.	BDO	26
C *** NEOPRT MAY BE ALTERED WITHIN SUTONZ, SURECZ.	BDO	27
INTEGER NZ/8/, NEOPRT/1/	BDO	28
REAL E/13.614, 35.15, 54.93, 77.394, 113.87, 138.08, 173.9, 178.71, 172/	BDO	29
REAL O/6.5, 4.3, 2.1, 2.1/	BDO	30
REAL API/11.E-8, 3.35E-8, 1.42E-8, .9E-8, .43E-8, .77E-8, .034E-8,	BDO	31
1.013E-8/	BDO	32
REAL APR/.088E-12, .255E-12, .412E-12, .583E-12, .777E-12, .925E-12,	BDO	33
1.46E-12, .65E-12/	BDO	34
REAL CHI/2*0.285, 0.333, 0.375, 0.417, 0.438, 2*0.627	BDO	35
REAL CHR/0.1, 0.15, 0.53, 0.75, 0.82, 0.93, 0.74, 1.2	BDO	36
END	BDO	37

BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-06-77

BDAL

1

C *** USE E'S AND Q'S IN SUIONZ FOR KUNZE IONIZATION AS WELL AS INFO.

BDAL

2

C *** IN COMMON/XCION/.

BDAL

3

C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.

BDAL

4

COMMON/Q/Q(13)

BDAL

5

COMMON/E/NZ, NEOPRT, E(13)

BDAL

6

COMMON/ELNAME/ELNAME, NELDES, DES(31)

BDAL

7

COMMON/XCION/NCUT, DELTA, XC(13)

BDAL

8

DATA NCUT, DELTA/1,1.E-20/

BDAL

9

C *** NCUT=Q(1) MEANS ARRAY XC UNAVAILABLE(AVAILABLE)

BDAL

10

C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE.GE.XC(1),

BDAL

11

C *** THEN IONIZATION RATE COEFF. LT DELTA

BDAL

12

DATA XC/

BDAL

13

1 29.27, 27.18, 25.89, 25.81, 25.31, 24.84, 24.31, 23.85, 23.35,

BDAL

14

2 22.67, 21.84, 20.25, 19.41/

BDAL

15

DATA NELDES/31/

BDAL

16

DATA DES/ Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 63

BDAL

17

1 1970, E'S FROM DIE NATURWISSENSCHAFTEN, VOL. 2, 1955 BY FINKLEMB

BDAL

18

2RG.

BDAL

19

DATA ELNAME/'AL ' /

BDAL

20

C *** NEOPRT.LE.O CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED

BDAL

21

C *** IN SUIONZ AND SURECZ.

BDAL

22

C *** NEOPRT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND

BDAL

23

C *** DESCRIPTIVE INFO. IN DES ARRAY.

BDAL

24

C *** NEOPRT MAY BE ALTERED WITHIN SUIONZ, SURECZ.

BDAL

25

DATA NZ/13/, NEOPRT/1/

BDAL

26

DATA Q/3.,2.,1.,8.,7.,6.,5.,4.,3.,2.,1.,2.,1./

BDAL

27

DATA E/5.984, 18.82, 28.44, 119.96, 53.8, 90.42, 241.8, 285.13, 330.1,

BDAL

28

1398.6, 441.5, 2071.3, 2298.8/

BDAL

29

END

BDAL

30

H I

BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-05-77

C *** USE E'S AND Q'S IN SUIONZ FOR KUNZE IONIZATION AS WELL AS INFO.

C *** IN COMMON/XCION/.

C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.

COMMON/Q/Q(26)

COMMON/E/NZ, NEOPRT, E(26)

COMMON/ELNAME/ELNAME, NELDES, DES(31)

COMMON/XCION/NCUT, DELTA, XC(26)

DATA NCUT, DELTA/1, 1.E-20/

C *** NCUT=Q(1) MEANS ARRAY XC UNAVAILABLE(AVAILABLE)

C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE*GE*XC(1),

C *** THEN IONIZATION RATE COEFF. LT DELTA

DATA XC/

1 28.46, 26.72, 28.37, 27.37, 26.75, 26.27, 25.87, 25.51, 24.78,

2 24.47, 24.16, 23.83, 23.45, 23.05, 22.42, 21.64, 22.45, 22.18,

3 21.90, 21.61, 21.27, 20.88, 20.36, 19.60, 18.17, 17.42/

DATA NELDES/31/

DATA DES/' Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 63

1 1970, E'S FROM DIE NATURWISSENSCHAFTEN, VOL. 2, 1955 BY FINKLEMBUB

2RG

DATA ELNAME/'FE

C *** NEOPRT, LE, D CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED

C *** IN SUIONZ AND SURECZ:

C *** NEOPRT=L REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND

C *** DESCRIPTIVE INFO. IN DES ARRAY.

C *** NEOPRT MAY BE ALTERED WITHIN SUIONZ, SURECZ.

DATA NZ/26/, NEOPRT/1/

DATA Q/2,

87. , 6. , 5. , 4. , 3. , 2. , 1. , 8. , 7. , 6. , 5. , 4. ,

83. , 2. , 1. , 2. ,

DATA E/7.90 , 16.18 , 30.64 , 57.40 , 83.00 , 108.7 ,

8133.2 , 158.3 , 240.2 , 271.7 , 303.1 , 334.6 , 372.2 ,

8404.0 , 472.4 , 506.0 , 1168. , 1283. , 1399. , 1514. ,

81644. , 1760. , 1923. , 2025. , 8503. , 8969. ,

END

BLOCK DATA

BDN1

1

C *** ORIGINAL SEQUENCING DONE ON 07-06-77

BDN1

2

C *** USE E'S AND Q'S IN SUTONZ FOR KUNZE IONIZATION AS WELL AS INFO.

BDN1

3

C *** IN COMMON/XCION/.

BDN1

4

C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION

BDN1

5

COMMON/Q/Q(28)

BDN1

6

COMMON/E/NZ, NEOPRT, E(28)

BDN1

7

COMMON/ELNAME/ELNAME, NELDES, DES(31)

BDN1

8

COMMON/XCION/NCUT, DELTA, XC(28)

BDN1

9

DATA NCUT, DELTA/1, 1.E-20/

BDN1

10

C *** NCUT=Q(L) MEANS ARRAY XC UNAVAILABLE(AVAILABLE)

BDN1

11

C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE.GE.XC(1),

BDN1

12

C *** THEN IONIZATION RATE COEFF. LT DELTA

BDN1

13

DATA XC/

BDN1

14

1 28.51, 26.55, 28.26, 27.35, 26.75, 26.29, 25.89, 25.55, 25.24,

BDN1

15

2 24.94, 24.31, 24.03, 23.75, 23.45, 23.10, 22.71, 22.10, 21.33,

BDN1

16

3 22.16, 21.21, 21.64, 21.35, 21.02, 20.65, 20.13, 19.39, 17.95,

BDN1

17

4 17.20/

BDN1

18

DATA NELDES/31/

BDN1

19

DATA DES/ Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 63

BDN1

20

1 1970, E'S FROM DIE NATURWISSEN SCHAFTEN, VOL. 2, 1955 BY FINKLEMBU

BDN1

21

2RG.

BDN1

22

DATA ELNAME/'NI' /

BDN1

23

C *** NEOPRT, LE.0 CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED

BDN1

24

C *** IN SUTONZ AND SURECZ.

BDN1

25

C *** NEOPRT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND

BDN1

26

C *** DESCRIPTIVE INFO. IN DES-ARRAY.

BDN1

27

C *** NEOPRT MAY BE ALTERED WITHIN SUTONZ, SURECZ.

BDN1

28

DATA NZ/28/ NEOPRT/1/

BDN1

29

DATA Q/2, 1, 16, 15, 14, 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2,

BDN1

30

1 1.8, 7.6, 5.4, 3.2, 2.1, 2.1,

BDN1

31

DATA E/7.633, 18.15, 36.16, 64.07, 91.90, 119.7, 148.2, 176.4, 204.5,

BDN1

32

1232.7, 330.3, 365.0, 399.7, 434.4, 473.9, 509.0, 587.2, 624.0, 1419.,

BDN1

33

21545., 1671., 1797., 1942., 2069., 2247., 2358., 9915., 10420./

BDN1

34

END

BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-06-77

BDCU 1

C *** USE E'S AND Q'S IN SUTONZ FOR KUNZE IONIZATION AS WELL AS INFO.

BDCU 2

C *** IN COMMON/XCION/.

BDCU 3

C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.

BDCU 4

COMMON/Q/Q(29)

BDCU 5

COMMON/E/NZ, NEQPT, E(29)

BDCU 6

COMMON/ELNAME/ELNAME, NELDES, DES(31)

BDCU 7

COMMON/XCION/NCUT, DELTA, XC(29)

BDCU 8

DATA NCUT, DELTA/1, 1.E-20/

BDCU 9

C *** NCUT=Q(1) MEANS ARRAY XC UNAVAILABLE(AVAILABLE)

BDCU 10

C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE.GE.XC(1),

BDCU 11

C *** THEN IONIZATION RATE COEFF. Δ LT DELTA

BDCU 12

DATA XC/

BDCU 13

1 27.81, 29.23, 28.29, 27.17, 26.66, 26.24, 25.89, 25.57, 25.28,

BDCU 14

2 25.01, 24.74, 24.14, 23.87, 23.59, 23.30, 22.97, 22.58, 21.98,

BDCU 15

3 21.21, 22.04, 21.79, 21.53, 21.24, 20.91, 20.54, 20.03, 19.28,

BDCU 16

4 17.84, 17.09/

BDCU 17

DATA ELNAME/'CU

BDCU 18

DATA NELDES/31/

BDCU 19

DATA DES/' Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 63

BDCU 20

1 1970. E'S FROM DIE NATURWISSENSCHAFTEN, VOL. 2, 1955 BY FINKLE

BDCU 21

2RG.

BDCU 22

C *** NEQPT.LE.0 CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED

BDCU 23

C *** IN SUTONZ AND SURECZ.

BDCU 24

C *** NEQPT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND

BDCU 25

C *** DESCRIPTIVE INFO. IN DES ARRAY.

BDCU 26

C *** NEQPT MAY BE ALTERED WITHIN SUTONZ, SURECZ.

BDCU 27

DATA NZ/29, NEQPT/1/

BDCU 28

DATA Q/1., 18., 17., 16., 15., 14., 13., 12., 11., 10., 9., 8., 7., 6., 5., 4.,

BDCU 29

13., 2., 1., 8., 7., 6., 5., 4., 3., 2., 1., 2., 1.,

BDCU 30

DATA E/7.724, 20.29, 36.83, 75.58, 102.7, 129.9, 157.0, 184.6, 212.0,

BDCU 31

1239.5, 266.9, 371.7, 407.7, 443.7, 479.6, 518.4, 554.9, 638.3, 676.5, 1542.,

BDCU 32

21673., 1805., 1936., 2088., 2221., 2406., 2523., 10650., 11170./

BDCU 33

END

BDCU 34

K I

BLOCK DATA

BDW

1

C *** ORIGINAL SEQUENCING DONE ON 07-05-77

BDW

2

C *** USE E'S AND Q'S IN SUIONZ FOR KUNZE IONIZATION AS WELL AS INFO.

BDW

3

C *** IN COMMON/XCION/.

BDW

4

C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.

BDW

5

COMMON/E/NZ, NEOPRT, E(74)

BDW

6

COMMON/Q/Q(74)

BDW

7

COMMON/ELNAME/ELNAME, NELDES, DES(23)

BDW

8

COMMON/XCION/NCUT, DELTA, XC(74)

BDW

9

DATA NCUT, DELTA/1, 1.E-20/

BDW

10

C *** NCUT=0(1) MEANS ARRAY XC UNAVAILABLE(AVAILABLE)

BDW

11

C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE.GE.XC(1),

BDW

12

C *** THEN IONIZATION RATE COEFF. = LT DELTA

BDW

13

DATA XC/

BDW

14

1 28.45, 26.59, 28.50, 27.77, 27.23, 26.78, 27.18, 25.57, 25.23,

BDW

15

2 24.90, 24.56, 24.10, 23.68, 25.81, 25.57, 22.78, 22.01, 25.17,

BDW

16

3 24.99, 24.82, 24.66, 24.51, 24.36, 24.22, 24.09, 23.95, 23.82,

BDW

17

4 23.70, 23.26, 23.14, 23.02, 22.90, 22.77, 22.64, 22.50, 22.36,

BDW

18

5 22.21, 22.06, 21.76, 21.58, 21.39, 21.17, 20.86, 20.54, 20.04,

BDW

19

6 19.32, 21.53, 21.42, 21.31, 21.19, 21.07, 20.95, 20.80, 20.67,

BDW

20

7 20.53, 20.38, 20.16, 19.99, 19.81, 19.60, 19.25, 18.94, 18.47,

BDW

21

8 17.77, 18.72, 18.55, 18.36, 18.15, 17.78, 17.46, 17.01, 16.30,

BDW

22

9 14.94, 14.23/

BDW

23

DATA NELDES/23/

BDW

24

DATA DES/' E VALUES FOR H FROM CARLSON, ATOMIC DATA, VOL. 2, P. 86

BDW

25

1970. HOWEVER NEUTRAL AND H+ ARE NEW.

BDW

26

C *** NEOPRT=0 CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED

BDW

27

C *** IN SUIONZ AND SURECZ.

BDW

28

C *** NEOPRT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND

BDW

29

C *** DESCRIPTIVE INFO. IN DES ARRAY.

BDW

30

C *** NEOPRT MAY BE ALTERED WITHIN SUIONZ, SURECZ.

BDW

31

DATA ELNAME/' H /, NZ/74/, NEOPRT/1/

BDW

32

DATA Q/2, 1, 12, 11, 10, 9, 32, 8, 7, 6, 5, 4, 3, 31, 30, 2, 1,

BDW

33

129, 28, 27, 26, 25, 24, 23, 22, 21, 20, 19, 18, 17, 16, 15,

BDW

34

214, 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, 1, 18, 17, 16, 15,

BDW

35

314, 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, 1, 8, 7, 6, 5, 4, 3,

BDW

36

42, 1, 2, 1,

BDW

37

DATA E/7.98, 17.7, 25.43, 39.29, 53.75, 67.07, 79.7, 94.8, 102.0, 103.7,

BDW

38

1204.2, 240.5, 263.1, 294.6, 339.9, 369.9, 395.0, 435.5, 480.8, 526.1, 571.4,

BDW

39

2616.7, 664.6, 710.2, 755.8, 801.4, 846.9, 892.5, 1154., 1206., 1259.,

BDW

40

31312, 1365., 1417., 1483., 1537., 1591., 1645., 1870., 1926., 1981., 2037.,

BDW

41

42163., 2223., 2386., 2447., 3734., 3882., 4029., 4177., 4325., 4472., 4684.,

BDW

42

54836., 4987., 5139., 5538., 5671., 5803., 5936., 6468., 6611., 6919., 7055.,

BDW

43

614760., 15140., 15520., 15900., 17630., 18060., 18800., 19150., 77510.,

BDW

44

778990./

BDW

45

END

BLOCK DATA

C *** ORIGINAL SEQUENCING DONE ON 07-06-77	BDAU	1
C *** USE E'S AND Q'S IN SUIONZ FOR KUNZE IONIZATION AS WELL AS INFO:	BDAU	2
C *** IN COMMON/XCION/	BDAU	3
C *** USE E'S IN SURECZ FOR MODIFIED C. JORDAN RECOMBINATION.	BDAU	4
COMMON/Q/Q(79)	BDAU	5
COMMON/E/NZ, NEQPT, E(79)	BDAU	6
COMMON/ELNAME/ELNAME, NELDES, DES(31)	BDAU	7
COMMON/XCION/NCUT, DELTA, XC(79)	BDAU	8
DATA NCUT, DELTA/1, 1.E-20/	BDAU	9
C *** NCUT=0(1) MEANS ARRAY XC UNAVAILABLE(AVAILABLE).	BDAU	10
C *** XC HERE ARE FOR IONIZATION BY KUNZE. IF X=E(1)/TE.GE.XC(1),	BDAU	11
C *** THEN IONIZATION RATE COEFF. LT. DELTA	BDAU	12
DATA XC/	BDAU	13
1 27.55, 29.22, 28.27, 27.66, 27.20, 26.82, 26.49, 26.17, 25.88,	BDAU	14
2 25.61, 25.35, 24.72, 24.45, 24.18, 23.88, 23.48, 23.10, 25.28,	BDAU	15
3 25.07, 22.29, 21.53, 24.73, 24.57, 24.42, 24.27, 24.13, 24.00,	BDAU	16
4 23.86, 23.74, 23.61, 23.49, 23.37, 23.25, 22.86, 22.75, 22.64,	BDAU	17
5 22.52, 22.40, 22.28, 22.14, 22.01, 21.87, 21.72, 21.44, 21.27,	BDAU	18
6 21.08, 20.86, 20.55, 20.23, 19.74, 19.03, 21.25, 21.15, 21.04,	BDAU	19
7 20.93, 20.81, 20.70, 20.55, 20.42, 20.29, 20.14, 19.92, 19.76,	BDAU	20
8 19.58, 19.37, 19.01, 18.70, 18.24, 17.54, 18.50, 18.34, 18.15,	BDAU	21
9 17.94, 17.55, 17.24, 16.79, 16.08, 14.72, 14.02/	BDAU	22
DATA NELDES/31/	BDAU	23
DATA DES/' Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 638	BDAU	24
1970. E'S FROM DIE NATURWISSENSCHAFTEN, VOL. 2, 1955 BY FINKLEHUB	BDAU	25
2RG.	BDAU	26
DATA ELNAME/'AU	BDAU	27
DATA Q/1.18, 17.16, 15.14, 13.12, 11.10, 9.8, 7.6, 5.4,	BDAU	28
13.32, 31.2, 30.29, 28.27, 26.25, 24.23, 22.21, 20.19,	BDAU	29
218.17, 16.15, 14.13, 12.11, 10.9, 8.7, 6.5, 4.3, 2.1,	BDAU	30
318.17, 16.15, 14.13, 12.11, 10.9, 8.7, 6.5, 4.3, 2.1,	BDAU	31
48.7, 6.5, 4.3, 2.1, 2.1/	BDAU	32
C *** NEQPT=LE.O CAUSES NO PRINT OF E AND Q VALUES THAT ARE TO BE USED	BDAU	33
C *** IN SUIONZ AND SURECZ.	BDAU	34
C *** NEQPT=1 REQUESTS PRINT OF E'S IF NEEDED AND Q'S IF NEEDED AND	BDAU	35
C *** DESCRIPTIVE INFO. IN DES ARRAY.	BDAU	36
C *** NEQPT MAY BE ALTERED WITHIN SUIONZ, SURECZ.	BDAU	37
DATA NZ/79/, NEQPT/1/	BDAU	38
DATA E/9.223, 20.5, 37.37, 54.18, 70.99, 87.81,	BDAU	39
8104.6, 123.2, 140.9, 158.6,	BDAU	40
8176.3, 250.3, 274.7, 299.1, 323.5, 365.7, 391.8,	BDAU	41
8432.9, 487.4, 516.8, 545.7,	BDAU	42
8599.7, 654.2, 708.8, 763.3, 817.9, 872.7, 930.9, 986.2,	BDAU	43
81042, 1097, 1152,	BDAU	44
81207, 1516, 1575, 1634, 1692, 1751, 1810, 1888,	BDAU	45
81948, 2009,	BDAU	46
82069, 2325, 2387, 2448, 2510, 2671, 2738, 2924,	BDAU	47
82991, 4516, 4676,	BDAU	48
84837, 4997, 5158, 5318, 5566, 5731, 5896, 6061,	BDAU	49
86500, 6644, 6787,	BDAU	50
86931, 7615, 7772, 8111, 8259, 17090, 17500,	BDAU	51
817910, 18320, 20570,	BDAU	52
821040, 21870, 22260, 89680, 91290,	BDAU	53
END	BDAU	54

```

SUBROUTINE EQU(YEQU,SUIZ,SURZ,NZ,D)
C *** ORIGINAL SEQUENCING DONE ON 07-12-77
DIMENSION YEQU(1),SUIZ(1),SURZ(1),D(1)
C *** NEED DIM. YEQU(NZ+1),SUIZ(NZ),SURZ(NZ),D(NZ)
C *** D IS A SCRATCH ARRAY
C *** SUIZ(1)=IONIZATION RATE FROM SPECTROSCOPIC STATE 1 TO 1+1
C *** SURZ(1)=RECOMBINATION RATE FROM SPECTROSCOPIC STATE 1+1 TO 1
C *** YEQU, THE EQUILIBRIUM DISTRIBUTION VECTOR, IS NORMALIZED SO THAT
C *** SUM OF ITS COMPONENTS = 1.
C *** YEQU IS IN THE NULL SPACE OF THE COEFF. MATRIX, A.
C *** LET RHO(J)=SUIZ(J)/SURZ(J) AND ASSUME SURZ(J) NE 0. MOREOVER, LET
C *** THE 1-TH COMPONENT OF THE NORMALIZED EQUILIBRIUM VECTOR, YEQU, BE
C *** ETA(1), GE 0. THEN ETA(J+1)=RHO(J)*ETA(1)=(PRODUCT OF RHO(J),J=1,
C *** ...,1)*ETA(1).
C *** DETERMINE INDEX OF LARGEST COMPONENT, ETA(1), BY USING LOGS IN
C *** ORDER TO AVOID UNDERFLOWS OR OVERFLOWS. THEN FORM YEQU NORMALIZED
C *** SO ITS LARGEST COMPONENT HAS VALUE 1. THEN NORMALIZE YEQU SO THE
C *** SUM OF ITS COMPONENTS IS ONE.
DATA EPSEQU/1.E-06/
C *** WHENEVER A COMPONENT OF THE NORMALIZED EQUILIBRIUM VECTOR IS
C *** LE EPSEQU TIMES THE LARGEST COMPONENT SET IT TO 0.
C *** COMPUTATIONALLY SOME OF THE COMPUTED RATE COEFF. MAY BE 0.
C *** IF SURZ(J)=0, THEN LOGICALLY REGARD SURZ(J)=0, J=1..J, (4/14/77)
C *** IF SUIZ(J)=0, THEN LOGICALLY REGARD SUIZ(J)=0, J=J..NZ, (4/14/77)
DO 1 I=1,NZ
IF(SURZ(I).LE.0.) GO TO 1
JL=I
GO TO 222
YEQU(I)=0
C *** WON'T FALL THRU
222 JL=JL
DO 11 I=JL,NZ
IF(SURZ(I).GT.0.) GO TO 11
JL=I
11 CONTINUE
IF(JL.EQ.1) GO TO 2
DO 13 J=JL,JL
YEQU(J)=0.
JL=JL+1
2 IH=NZ
22 IF(SUIZ(IH).GT.0.) GO TO 33
YEQU(IH+1)=0.
IH=IH-1
GO TO 22
33 IZ=IH
I=IH-1
35 IF(SUIZ(I).GT.0.) GO TO 34
IZ=I
I=I-1
34 IF(I.GT.0) GO TO 35
IF(IZ.EQ.IH) GO TO 3
DO 36 J=IZ,IH
YEQU(J+1)=0.
IH=IZ-1
3 JH=IH+1
C *** MUST APPROX. COMPONENTS JL THRU JH.
ANUMMX=-1.E8
S=0.

```

EQU	1
EQU	2
EQU	3
EQU	4
EQU	5
EQU	6
EQU	7
EQU	8
EQU	9
EQU	10
EQU	11
EQU	12
EQU	13
EQU	14
EQU	15
EQU	16
EQU	17
EQU	18
EQU	19
EQU	20
EQU	21
EQU	22
EQU	23
EQU	24
EQU	25
EQU	26
EQU	27
EQU	28
EQU	29
EQU	30
EQU	31
EQU	32
EQU	33
EQU	34
EQU	35
EQU	36
EQU	37
EQU	38
EQU	39
EQU	40
EQU	41
EQU	42
EQU	43
EQU	44
EQU	45
EQU	46
EQU	47
EQU	48
EQU	49
EQU	50
EQU	51
EQU	52
EQU	53
EQU	54
EQU	55
EQU	56
EQU	57

```

-----
DO 201 I=JL,JH                                EQU 58
D(I)=SUIZ(I)/SURZ(I)                            EQU 59
C *** MAX(SUIZ,SURZ).LT.1. IF NEITHER 0, THEN SUIZ.LT.SUIZ/SURZ.LT. EQU 60
C *** 1/SURZ, THUS QUOTIENT WONT UNDERFLOW. CHANCE OVERFLOW REMOTE. EQU 61
S=S+ALOG(D(I))                                  EQU 62
IF(S.LE.ANUMMX) GO TO 201                       EQU 63
ANUMMX=S                                         EQU 64
IMAX=I                                           EQU 65
201 CONTINUE                                     EQU 66
YEQU(IMAX+1)=1.                                EQU 67
IF(IMAX.EQ.1H) GO TO 72                        EQU 68
C *** PROCESS BACK, IMAX+2 THRU JH              OR IMAX+1 THRU 1H. EQU 69
J=IMAX+1                                         EQU 70
71 YEQU(I+1)=D(I)*YEQU(I)                       EQU 71
IF(YEQU(I+1).LE.EPSEQU) GO TO 80              EQU 72
I=I+1                                           EQU 73
IF(I.LE.1H) GO TO 71                          EQU 74
C *** PROCESS FRONT, IMAX THRU JL              EQU 75
72 J=IMAX                                         EQU 76
78 YEQU(I)=YEQU(I+1)/D(I)                      EQU 77
IF(YEQU(I).LE.EPSEQU) GO TO 180               EQU 78
I=I-1                                           EQU 79
IF(I.GE.JL) GO TO 78                          EQU 80
C *** SUM COMPONENTS TO GET NORMALIZATION FACTOR EQU 81
76 S=0                                           EQU 82
DO 77 I=JL,JH                                  EQU 83
77 S=S+YEQU(I)                                  EQU 84
C *** NORMALIZE EQUILIBRIUM VECTOR              EQU 85
DO 74 I=JL,JH                                  EQU 86
74 YEQU(I)=YEQU(I)/S                          EQU 87
RETURN                                           EQU 88
C *** PROBABLY MORE CAUTIOUS THAN NEEDED. 80 CORRESPONDS TO BACK, 180 EQU 89
C *** TO FRONT.                                EQU 90
80 S=YEQU(I+1)                                  EQU 91
R=1                                              EQU 92
YEQU(I+1)=0.                                    EQU 93
81 I=I+1                                         EQU 94
IF(I.GT.1H) GO TO 72                          EQU 95
R=R*D(I)                                         EQU 96
IF(R.LE.1.E-4) GO TO 75                      EQU 97
IF(R.LE.1.) GO TO 73                         EQU 98
YEQU(I+1)=R*S                                  EQU 99
GO TO 81                                         EQU 100
73 YEQU(I+1)=0.                                EQU 101
GO TO 81                                         EQU 102
75 YEQU(I+1)=0.                                EQU 103
I=I+1                                           EQU 104
IF(I.LE.1H) GO TO 75                          EQU 105
GO TO 72                                         EQU 106
180 S=YEQU(I)                                  EQU 107
R=1                                              EQU 108
YEQU(I)=0.                                      EQU 109
81 I=I-1                                         EQU 110
IF(I.LT.JL) GO TO 76                          EQU 111
R=R/D(I)                                         EQU 112
IF(R.LE.1.E-4) GO TO 175                     EQU 113
IF(R.LE.1.) GO TO 173                       EQU 114
YEQU(I)=R*S                                     EQU 115

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GO TO 181
173 YEQU(1)=0.

GO TO 181
175 YEQU(1)=0.

J=J-1

IF(I.GE.JL) GO TO 175

GO TO 176

END

EQU 116
EQU 117
EQU 118
EQU 119
EQU 120
EQU 121
EQU 122
EQU 123

P I

SUBROUTINE YNA(Y)

C *** ORIGINAL SEQUENCING DONE ON 07-12-77

DIMENSION Y(1)

COMMON/IO/LOUT,LIN

COMMON/EQ/L,T,H,HUSED,NLRC,NKRC,NL,NLP,NKMI,NK,MXEQM,ISTART,NQ

COMMON/STGY/TF,TFLN,TBLN,FL,BL,DC,BDLOSS,BDLOSM,RDEC,ITDEL,NSTRAT,

INDEL,NEQADD,NEQDEL,NEQDML,BDEL,TSWIT,BDLSHM,JPSTGY

COMMON/PRINT/TPRINT

COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH

C *** SEE SUBR. YOUT. USER SHOULD DISPOSE OF VECTOR Y=Y(TPRINT) HERE.

CALL ZAVERG(ZAUG,Y)

CALL DENTMP(TE,DEN,TPRINT)

JMS=JDDQ,*TPRINT

C *** FL,BL,DC ARE ASSOCIATED WITH STRATEGY II FOR ALTERING SET OF

C *** ACTIVE EQUATIONS. THEY ARE INITIALIZED TO 0 IN DRIVES.

C *** WHEN STRATEGY II IS ACTIVE THEN THE COMPUTED COMPONENTS ARE HIGH

C *** BY AT MOST FL+BL AND LOW BY AT MOST FL+BL+DC. THESE ERRORS DEAL

C *** ONLY WITH ERROR ASSOCIATED WITH USING AN ABBREVIATED SYSTEM OF EQSYNA

WRITE(LOUT,1) JMS,TE,DEN,ZAUG,NL,NK,IT,NQ,HUSED,FL,BL,DC,

1(Y(1),I=NL,NK)

1 FORMAT('0T(MS)='1PE9.3,2X'TE='1E8.2,2X'NE='1E8.2,2X'ZAUG='0PF5.2,

12X'L='12,1X'K='12,2X'IT='14,2X'NQ='11,2X'H='1PE8.2,2X'FL,BL,DC='

2 3E8.1, Y='0P1QF10.6/(3X1QF10.6))

RETURN

END

```

C *** ORIGINAL SEQUENCING DONE ON 07-12-77 MAIN 1
C *** TWO PROGRAMS CAN BE FORMED FROM THE COLLECTION OF SUBROUTINES MAIN 2
C *** GIVEN HERE. ONE IS DESIGNED FOR CONSTANT TEMPERATURE AND CONSTANT MAIN 3
C *** DENSITY AND IS CALLED PROGTI WHERE TI SIGNIFIES THE TIME MAIN 4
C *** INDEPENDENCE OF THE TEMPERATURE AND DENSITY. THE OTHER IS PROGTD MAIN 5
C *** WHERE TD SIGNIFIES THE TIME DEPENDENCE OF THE TEMPERATURE AND/OR MAIN 6
C *** DENSITY. MAIN 7
C *** PROGRAM, PROGTI, DEALS WITH EQUILIBRIUM CALCULATIONS. THAT IS IT MAIN 8
C *** DEALS WITH THE LINEAR SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS MAIN 9
C ***  $Y' = \text{DEN} * X Y$  EQ. (*) MAIN 10
C *** WHERE DEN AND TE ARE REGARDED CONSTANT AND THE MATRIX A IS MAIN 11
C *** TRIJAGONAL. PROGTI MAY BE REQUESTED TO (1) DETERMINE THE MAIN 12
C *** EQUILIBRIUM VECTOR (NCH.NE.0) ASSOCIATED WITH EQUATION (*), (2) TO MAIN 13
C *** APPROXIMATE (NROOTS.GT.0) THE EIGENVALUES OF THE COEFF. MATRIX, MAIN 14
C *** DEN*A, IN (*), (3) TO INTEGRATE (*) OVER THE TIME INTERVAL (TS,TF) MAIN 15
C *** WITH Y(TS) SPECIFIED IN SUBR.YINIT, OR (4) TO INTEGRATE (*) WITH MAIN 16
C *** Y(TS) SPECIFIED UNTIL THE CURRENT Y(T) 1ST BECOMES WITHIN EPSCC OF MAIN 17
C *** THE EQUILIBRIUM VECTOR ASSOCIATED WITH (*) WHERE SUBR.CONEQU MAIN 18
C *** CONTAINS THE 2 CRITERIA FOR MEASURING CLOSENESS. MAIN 19
C *** PROGRAM, PROGTD, DEALS WITH THE TIME EVOLUTION OF THE NORMALIZED MAIN 20
C *** CHARGE STATE, DISTRIBUTION VECTOR. ITS ONLY PURPOSE IS TO. MAIN 21
C *** INTEGRATE  $Y' = \text{DEN} * X Y$ ,  $Y(TS) = Y_0$  OVER (TS,TF) WHERE THE MAIN 22
C *** DENSITY AND TEMPERATURE ARE TIME DEPENDENT FUNCTIONS. THE USER MAIN 23
C *** MOST LIKELY WILL HAVE TO ALTER MAIN(TD) AND DENTMP(TD) TO REFLECT MAIN 24
C *** HIS SITUATION. THE CURRENT DENTMP(TD) USES LINEAR INTERPOLATION TO MAIN 25
C *** ESTIMATE DEN AND TE BETWEEN THE GIVEN EXPERIMENTALLY DETERMINED MAIN 26
C *** VALUES. ANALYTIC EXPRESSIONS ARE USED FOR THE TIME PERIOD BEFORE MAIN 27
C *** THE 1ST EXPERIMENTAL VALUES AND THE LAST EXPERIMENTAL VALUES ARE MAIN 28
C *** USED FOR TIMES GREATER THAN THE LAST EXPERIMENTAL TIME. MAIN 29
C *** LET BDEL DENOTE THE BLOCK DATA NEEDED (USUALLY) BY SUBR.SUIONZ, MAIN 30
C *** SURECZ FOR THE ELEMENT EL. OF COURSE EL IS REPLACED WITH THE MAIN 31
C *** SYMBOL FOR THE ELEMENT. MAIN 32
C *** LET BDPARM DENOTE THE BLOCK DATA IN WHICH THE PROGRAM CONTROL MAIN 33
C *** PARAMETERS ARE DEFINED. MAIN 34
C *** MAIN 35
C *** THEN PROGTI REQUIRES THESE ROUTINES FOR ITS DEFINITION, BDEL, MAIN 36
C *** BDPARM, EQU, YNA, 'EXIT'-TERMINATES JOB, MAIN, YOUT, YPAY, MAIN(TI), MAIN 37
C *** ROOTS, STIFF, TESOC, YINIT, YOUTD, CONEQU, DENTMP(TI), DRIVES, INTOLI, MAIN 38
C *** INTEGC, STRATG, STRGT, SUIONZ, SURECZ, ZAVERG. MAIN 39
C *** MAIN 40
C *** PROGTD REQUIRES THESE ROUTINES FOR ITS DEFINITION, BDEL, BDPARM, MAIN 41
C *** YNA, 'EXIT'-TERMINATES JOB, MAIN, YOUT, YPAY, MAIN(TD), STIFF, MAIN 42
C *** TESOC, YINIT, YOUTD, CONEQU, DENTMP(TD), DRIVES, DTDATA, DTINIT, STRATG, MAIN 43
C *** STRGT, SUIONZ, SURECZ, ZAVERG. MAIN 44
C *** MAIN 45
C *** IN PROGTD SUBR.CONEQU IS NEVER ENTERED. IF ISWSTR=1 IN EITHER MAIN 46
C *** PROGRAM. THEN STRATG AND STRGT MAY BE REPLACED WITH DUMMY MAIN 47
C *** ROUTINES. MAIN 48
C *** MAIN 49
C *** MAIN 50
C *** MAIN 51
C *** THE NUMERICAL INTEGRATION OF THE SYSTEM OF DIFF. EQS. USES MANY OF MAIN 52
C *** THE ROUTINES FROM THE PACKAGE, GEAR, ORDINARY DIFFERENTIAL MAIN 53
C *** EQUATION SOLVER, A.C.HINDMARSH, DECEMBER 1974. UCID-30001 REV.3 MAIN 54
C *** COMPUTER DOCUMENTATION, LLL. THE VERSION OBTAINED CAME FROM THE MAIN 55
C *** ARGONNE CODE CENTER (IN EARLY 1974) AND REPRESENTED A MODIFICATION MAIN 56
C *** OF THE CDC VERSION FOR USE ON IBM 360 LINE COMPUTERS. MANY OF MAIN 57

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C *** THESE ROUTINES HAVE BEEN ALTERED TO TAILOR THE INTEGRATION TO THE MAIN 58
C *** SPECIAL FEATURES OF THE LINEAR SYSTEM OF DIFF. EQS. THAT DESCRIBE MAIN 59
C *** THE TIME RATE OF CHANGE OF THE NORMALIZED CHARGE STATE DISTRIBUTION MAIN 60
C *** N VECTOR. IN THIS CASE, THE SYSTEM IS (1) LINEAR, (2) HAS A MAIN 61
C *** TRIANGULAR JACOBIAN MATRIX, AND (3) IS STIFF. THE ROUTINE NAMES MAIN 62
C *** ASSOCIATED WITH THE GEAR PACKAGE ARE YOUT,YPAY,YNA,STIFF,TESOC, MAIN 63
C *** YOUTD, AND DRIVES. MAIN 64
C *** MAIN 65
C *** MAIN 66
C *** THE SUBROUTINES APPEARING IN THE PROGRAM LISTING ARE ORDERED MAIN 67
C *** LEXICOGRAPHICALLY EXCEPT THAT THE BLOCK DATA ROUTINES COME FIRST. MAIN 68
C *** IN FACT, BDPARM COMES FIRST AND THEN ALL THE BDEL WHERE THE BDEL MAIN 69
C *** HAVE BEEN ORDERED ACCORDING TO THE ATOMIC NUMBER OF THE ASSOCIATED MAIN 70
C *** ELEMENT. IN SOME CASES THE USER NEEDS TO SELECT THE DESIRED MAIN 71
C *** ROUTINE WHEN SEVERAL ARE OFFERED. MAIN 72
C *** SUMMARY OF CALLING SUBROUTINES MAIN 73
C *** SUBROUTINE CALLED BY SUBROUTINES. MAIN 74
C *** EQU MAIN(TI) MAIN 75
C *** YNA YOUT MAIN 76
C *** EXIT MAIN,SURECZ(MODIFIED JORDAN RECOMB.) MAIN 77
C *** MAIN MAIN 78
C *** YOUT DRIVES MAIN 79
C *** YPAY STIFF MAIN 80
C *** MAIN(TD) MAIN MAIN 81
C *** MAIN(TI) MAIN MAIN 82
C *** ROOTS MAIN(TI) MAIN 83
C *** STIFF DRIVES MAIN 84
C *** TESOC STIFF MAIN 85
C *** YINIT MAIN(TI),MAIN(TD) MAIN 86
C *** YOUTD DRIVES MAIN 87
C *** CONEQU DRIVES MAIN 88
C *** DENTMP(TD) DRIVES,YPAY,YNA MAIN 89
C *** DENTMP(TI) DRIVES,YPAY,YNA MAIN 90
C *** DRIVES INTEGC,MAIN(TD) MAIN 91
C *** DTDATA MAIN(TD) MAIN 92
C *** DTINIT MAIN(TD) MAIN 93
C *** INTQ1 ROOTS MAIN 94
C *** INTEGC MAIN(TI) MAIN 95
C *** STRATG DRIVES MAIN 96
C *** STRTGI MAIN(TI),MAIN(TD) MAIN 97
C *** SUIONZ MAIN(TI),DRIVES,YPAY,STRATG MAIN 98
C *** SURECZ MAIN(TI),DRIVES,YPAY,STRATG MAIN 99
C *** ZAVERG MAIN(TI),YNA MAIN 100
C *** END OF SUMMARY OF CALLING SUBROUTINES. MAIN 101
C *** MAIN 102
C *** BDEL=BLOCK DATA FOR ELEMENT, EL. E.G., BDC=BLOCK DATA FOR CARBON. MAIN 103
C *** BDPARM,BLOCK DATA WHERE USER SPECIFIES PROGRAM CONTROL PARAMETERS. MAIN 104
C *** SUMMARY OF COMMON USAGE ORDERED LEXICOGRAPHICALLY. MAIN 105
C *** (TI) CORRESPONDS TO CONSTANT NE, TE AND (TD) TO VARIABLE NE,TE. MAIN 106
C *** ARGUMENTS TO SUBR BELOW INDICATE MORE THAN 1 SUBR WITH SAME NAME MAIN 107
C *** /E/ BDEL,MAIN,MAIN(TD,TI),STRTGI,SUIONZ(DORY,KUNZE), MAIN 108
C *** SURECZ(DORY,MOD.C.JORDAN) MAIN 109
C *** /Q/ BDEL,SUIONZ(KUNZE) MAIN 110
C *** /TO/ YNA,MAIN,MAIN(TD,TI),ROOTS,YINIT,YOUTD,CONEQU,DRIVES, MAIN 111
C *** DTDATA,DTINIT,STRATG,STRTGI,SUIONZ(DORY,KUNZE), MAIN 112
C *** SURECZ(DORY,MOD.C.JORDAN) MAIN 113
C *** /API/ BDC,BDO,SUIONZ(DORY) MAIN 114
C *** /APR/ BDC,BDO,SURECZ(DORY) MAIN 115

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C *** /CHL/ BDC,BDO,SUIONZ(DORY) MAIN 116
C *** /CHR/ BDC,BDO,SURECZ(DORY) MAIN 117
C *** /EPS/ MAINI(TD,TI),YINIT,BDPARM,CONEQU,DRIVES,INTEGC MAIN 118
C *** /EQ1/ YNA,YOUT,YPAY,MAINI(TD,TI),STIFF,YINIT,YOUTD,CONEQU,DRIVESMAIN 119
C *** /INTEGC,STRATG,SUIONZ(DORY,KUNZE),SURECZ(DORY,MOD,C,JORDAN) MAIN 120
C *** /ZAUERG MAIN 121
C *** /STGY/ YNA,BDPARM,DRIVES,STRATG,STRGTJ MAIN 122
C *** /YFCN/ MAIN,MAINI(TD,TI),INTEGC MAIN 123
C *** /EQUIL/ MAIN,MAINI(TI),YINIT,CONEQU MAIN 124
C *** /JACOB/ MAIN,MAINI(TI),STIFF MAIN 125
C *** /PRINT/ YNA,YOUT,MAINI(TD,TI),BDPARM,DRIVES MAIN 126
C *** /RATEC/ MAIN,YPAY,STIFF MAIN 127
C *** /SHARE/ MAIN,YPAY,MAINI(TD,TI),STIFF,YINIT,BDPARM,DENTMP(TI), MAIN 128
C *** /DRIVES,STRATG MAIN 129
C *** /STRAT/ YNA,MAINI(TD,TI),YINIT,BDPARM,STRATG,STRGTJ MAIN 130
C *** /XCION/ BDEL,SUIONZ(KUNZE) MAIN 131
C *** /CONTR/ MAINI(TD,TI),DRIVES,INTEGC,STRATG MAIN 132
C *** /DISCON/ MAINI(TI),DENTMP(TD),DRIVES,DTDATA,DTINIT MAIN 133
C *** /ELNAME/ BDEL,SUIONZ(DORY,KUNZE),SURECZ(DORY,MOD,C,JORDAN) MAIN 134
C *** /MAINBD/ MAINI(TD,TI),BDPARM MAIN 135
C *** /SC1235/ MAIN,YOUT,MAINI(TI),STIFF MAIN 136
C *** /STGY2B/ BDPARM,STRGTJ MAIN 137
C *** /TDPROF/ DENTMP(TD),DTINIT MAIN 138
C *** END OF COMMON SUMMARY. MAIN 139
C *** MAIN 140
COMMON/E/NZ MAIN 141
COMMON/LO/LOUT,LIN MAIN 142
COMMON/YFCN/Y(450) MAIN 143
COMMON/EQUIL/YEQU(75) MAIN 144
COMMON/JACOB/FL(223) MAIN 145
COMMON/RATEC/SUIZ(150) MAIN 146
COMMON/SHARE/TE,DEN,HMIN,AMAX,EPS,HF,KFLAG,JDISC,NOM,NOM2,NOMPI MAIN 147
COMMON/SC1235/FSAVE(150) MAIN 148
C *** NZ IS DEFINED IN A BLOCK DATA STATEMENT MAIN 149
C *** REQUIRE NZ.LE.NOM IN ORDER TO HAVE SUFFICIENT STORAGE SPACE. MAIN 150
C *** DIMENSION FL(3NOM+1),SUIZ(2NOM+2),FSAVE(2NOM+2), MAIN 151
C *** YEQU(NOM+1),Y(6*(NOM+1)), MAIN 152
C *** IN STRATEGY 11 OF 2777 FOR DELETING EQS. USE SURZ(TD)=0=SUIZ(NZ+1) MAIN 153
C *** LIN(LOUT)=LOGICAL UNIT NUMBER OF INPUT(OUTPUT) DEVICE TO BE USED. MAIN 154
LIN=5 MAIN 155
LOUT=6 MAIN 156
C *** NOM=74 ALLOWS US TO DO THRU W, TUNGSTEN. MAIN 157
NOM=74 MAIN 158
NOM2=NOM+NOM MAIN 159
NOMPI=NOM+1 MAIN 160
IF(NZ.LE.NOM) GO TO 1 MAIN 161
WRITE(LOUT,2) NOM,NZ MAIN 162
2 FORMAT(' HAVE SPACE FOR NZ.LE.NOM=13,2X' BUT CURRENT NZ=13' MAIN 163
1' INCREASE ARRAY SIZES IN MAIN PROGRAM AND REDEFINE NOM.') MAIN 164
CALL EXIT MAIN 165
1 CONTINUE MAIN 166
CALL MAINI(SUIZ,SUIZ(NOMPI+2)) MAIN 167
RETURN MAIN 168
END MAIN 169

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SUBROUTINE YOUT(Y,NO,NQ)
C *** ORIGINAL SEQUENCING DONE ON 06-09-77
DIMENSION Y(NO,1)
COMMON/EQ1/T,H,HUSED,NLRC,NKRC,NL,NLPI,NKMI,NK
COMMON/PRINT/TPRINT,TPRNT(5),DTPRT(5),NPRNT(5),NPRNTI,TPRNTL,NPR
COMMON/SCI235/YPRINT(1)
C *** SUBROUTINE YOUT WILL BE CALLED AT THE FIRST DISCRETE TIME.
C *** T(SEC.) GE. (TPRNT(1)+Q*DTPRT(1))/1000., Q=0 TO NPRNT(1), I=1 TO
C *** NPRNTL. THE SYSTEM OF ODE'S IS EXPRESSED IN SECONDS. T AND TPRINT YOUT
C *** ARE IN SEC.. HOWEVER ARRAYS TPRNT AND DTPRT ARE IN MILLISEC..
C *** INTERPOLATION OF AN ORDER CONSISTENT WITH STIFF METHOD IS USED TO
C *** ESTIMATE Y AT TIME TPRINT.
C *** THE ACTIVE SYSTEM OF ODE IS EQS. NL THRU NK.
C *** SUBR.YNA SHOULD DISPOSE OF YPRINT=Y(TPRINT) ACCORDING TO
C *** THE USER'S WISHES.
C *** NPR=0, IPRNTI=1, TPRINT=TPRNT(1)/1000 ARE DEFINED AT BEGINNING OF
C *** DRIVES. TPRNT(1), DTPRT(1), NPRNT(1), NPRNTL NEED TO BE DEFINED
C *** PRIOR TO CALLING DRIVES. (DONE IN BDPAH=BLOCK DATA OF PROG.PARA.)
C *** THEORETICALLY COMPONENTS OF Y ARE NONNEGATIVE.
DO 22 I=NL,NK
IF(Y(I,1).LT.0.) Y(I,1)=0.
22 CONTINUE
5 CONTINUE
S = (TPRINT - T) / H
DO 3 J=NL,NK
YPRINT(I) = Y(I,1)
R = 1.0
L = NQ + 1
DO 3 J=2,L
R = R * S
DO 2 I=NL,NK
2 YPRINT(I) = YPRINT(I) + Y(I,J) * R
3 CONTINUE
C *** YPRINT DEFINED FOR I=NL,NK
CALL YNA(YPRINT)
NPR=NPR+1
IF(NPR.LE.NPRNT(TPRINT)) GO TO 40
IPRNTI=IPRNTI+1
IF(IPRNTI.LE.NPRNTI) GO TO 39
TPRINT=1.E10
GO TO 41
39 NPR=0
40 TPRINT=(TPRNT(IPRNTI)+NPR*DTPRT(IPRNTI))/1000.
IF(TPRINT.LE.T) GO TO 5
41 RETURN
END

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SUBROUTINE YPAY(YDOT,Y)	YPAY	1
C *** ORIGINAL SEQUENCING DONE ON 07-05-77		
DIMENSION Y(1),YDOT(1)	YPAY	2
COMMON/EQ1/T,H,HUSED,NLRC,NKRC,NL,NLP1,NKH1,NK	YPAY	3
COMMON/RATEC/SUIZ(1)	YPAY	4
COMMON/SHARE/TE,DEN,HMIN,HMAX,EPS,MF,KFLAG,JDFSC,NOM,NOM2,NOMP1	YPAY	5
C *** YDOT=Y'=DEN*AY, A IS TRI DIAGONAL	YPAY	6
C *** UPPER DIAG=(R(1),...,R(N-1)), LOWER DIAG=(1(1),...,1(N-1))	YPAY	7
C *** MAINDIAG=(-1(1),-1(2)+R(1)),...,-1(N-1)+R(N-2),-R(N-1))	YPAY	8
C *** DIAG DISPLAY FOR NL=1 AND NK=N.	YPAY	9
CALL DENTMP(TE,DEN,T)	YPAY	10
C *** SUBR.DENTMP RETURNS THE TEMP, TE, AND THE DENSITY, DEN, FOR	YPAY	11
C *** THE GIVEN TIME, T.	YPAY	12
CALL SUIONZ(SUIZ,TE,DEN)	YPAY	13
CALL SURECZ(SUIZ(NOMP1+2),TE,DEN)	YPAY	14
C *** APPROXIMATION TO THE IONIZATION COEFF. IN SUIZ(K), K=NLRC,NKRC AND	YPAY	15
C *** THE RECOMBINATION COEFF. IN SUIZ(NOMP1+2+K), K=NLRC,NKRC FOR THE	YPAY	16
C *** GIVEN TEMPERATURE, TE, AND DENSITY, DEN.	YPAY	17
C *** THE SYSTEM OF ODE'S IS EXPRESSED IN TIME UNIT OF SEC.	YPAY	18
C *** RATE COEFF. ARE IN UNITS OF CM**3/SEC., DENSITY IN CM**3	YPAY	19
C *** SURZ(1)=SUIZ(NOM+3), HAVE SURZ(0)=0.	YPAY	20
YDOT(NL)=DEN*(SUIZ(NOM+NL+2)*Y(NL+1)-SUIZ(NL)*Y(NL))	YPAY	21
DO L (=NLP1,NKH1)	YPAY	22
YDOT(1)=DEN*(SUIZ(1-1)*Y(1-1)-(SUIZ(1)+SUIZ(NOM+1+1))*Y(1))	YPAY	23
L=SUIZ(NOM+1+2)*Y(1+1))	YPAY	24
YDOT(NKH1+1)=DEN*(SUIZ(NKH1)*Y(NKH1)-SUIZ(NOM+NKH1+2)*Y(NKH1+1))	YPAY	25
RETURN	YPAY	26
END	YPAY	27

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SUBROUTINE MAIN(SUIZ,SURZ) MAINI 1
C *** ORIGINAL SEQUENCING DONE ON 07-12-77
C *** SUBROUTINE MAINI(TD) MAINI 2
C *** HAVE TIME DEPENDENT DENSITY AND TEMPERATURE PROFILES (3/29/77). MAINI 3
C *** THIS MAINI IS DESIGNED FOR INTEGRATION OF THE SYSTEM OF DIFF. MAINI 4
C *** EQUATIONS DESCRIBING THE RATE OF CHANGE OF THE NORMALIZED CHARGE MAINI 5
C *** STATE DISTRIBUTION WHERE THE COEFFICIENT MATRIX IS TIME MAINI 6
C *** DEPENDENT. (3/29/77). I.E., TE AND NE ARE TIME DEPENDENT. MAINI 7
      DIMENSION SUIZ(1),SURZ(1) MAINI 8
      DIMENSION DENI(8),TEE(8),TDCON(9) MAINI 9
      COMMON/E/NZNZ MAINI 10
      COMMON/IO/LOUT,LTN MAINI 11
      COMMON/EP5/NCH MAINI 12
      COMMON/EQ1/T,H,HUSED,NLRC,NKRC,NL,NLPT,NKMI,NK,MXEQM,JSTART,NQ MAINI 13
      COMMON/YFCN/Y(1) MAINI 14
      COMMON/PRINT/TPRINT,TPRNT(5),DTPRT(5),NPRNT(5),NPRNT1,IPRNT1,NPR MAINI 15
      COMMON/SHARE/TE,DEN,HMIN,HMAX,EP5,MF,KFLAG,JDISC,NOM,NOM2,NOMP MAINI 16
      COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH MAINI 17
      COMMON/CONTRL/NZ,NZP1 MAINI 18
      COMMON/MAINBD/NTEMP,NDENS,NLOG,NROOTS,IPAIR,TSTART,TLAST,TEL,DTE, MAINI 19
      DENL,BDEN,THRES,H0,TEMP(25),DENS(25) MAINI 20
C *** SUBROUTINE DENTMP(TEMP,DENS,T) RETURNS THE TEMPERATURE, TEMP, MAINI 21
C *** AND THE DENSITY, DENS, FOR THE GIVEN TIME T AND T IS EXPRESSED IN MAINI 22
C *** SECONDS. MAINI 23
C *** SUBR. DTDATA AND DTINIT ARE USED HERE TO GET THINGS SET UP FOR MAINI 24
C *** DENTMP. THE USER WILL MOST LIKELY HAVE TO MODIFY THESE TO SUIT THEM. MAINI 25
C *** FORM OF HIS DATA. MAINI 26
C *** THE POINTS OF DISCONTINUITY IN THE DERIVATIVE OF TEMP(T) OR MAINI 27
C *** DENS(T) MUST BE RECORDED IN ARRAY JDISC FOR USE IN DRIVES. DRIVES MAINI 28
C *** ADJUSTS STEP SO AS TO LAND ON TOP OF DISCONTINUITY. MAINI 29
C *** AT THE DISCONTINUITY THE ORDER OF METHOD IS SET TO 1 AND A SMALL MAINI 30
C *** STEP USED. MAINI 31
C *** BASICALLY THE ORDER OF STIFF METHOD MUST BE CONSISTENT WITH THE MAINI 32
C *** SMOOTHNESS OF TEMP(T) AND DENS(T). MAINI 33
C *** NCH=0 TELLS DRIVES THAT DOING A TIME DEPENDENT INTEGRATION, BUT MAINI 34
C *** THAT NO EQUILIBRIUM VECTOR, YEQU, IS AVAILABLE. MAINI 35
      NCH=0 MAINI 36
C *** NZNZ DEFINED IN A BLOCK DATA USUALLY. MAINI 37
      NZ=NZNZ MAINI 38
      NZP1=NZ+1 MAINI 39
      WRITE(LOUT,40) TSTART,TLAST,H0,EP5,MH MAINI 40
40  FORMAT(' INTEG.PARMS.: TSTART(MS)=',EP5.3,2X'TLAST(MS)=',EP5.3,2X MAINI 41
      1'H0(S)=',EP5.3,2X'EP5(=EP5*YMAX)=',EP5.3/ MAINI 42
      215X'IF ORDER OF STIFF METHOD SET TO 1, THEN NEXT H=(LAST H)/(1+(NOM MAINI 43
      3-1)MH) WHERE NQ=STIFF ORDER LAST USED, MH=',12) MAINI 44
      GO TO (81,82),ISWSTR MAINI 45
82  CALL STRGI(SUIZ,SURZ) MAINI 46
81  CONTINUE MAINI 47
      WRITE(LOUT,29)(1,TPRNT(1),DTPRT(1),NPRNT(1),I=1,NPRNT1) MAINI 48
29  FORMAT('OCALL YNA AT T(MS)=(TPRNT(1)+Q*DTPRT(1)) Q=0 TO NPRNT(1), MAINI 49
      1 I=1 TO NPRNT1. /1X'1'3X'TPRNT'6X'DTPRT'3X'NPRNT' / MAINI 50
      2(12,1P2E10.2,15)) MAINI 51
      T0=TSTART/1000. MAINI 52
      TF=TLAST/1000. MAINI 53
      MF=21 MAINI 54
C *** BASICALLY HAVE LOOP FOR LP1=1,NOLP1 MAINI 55
C *** NOLP1 IS RETURNED FROM SUBR. DTDATA AND = NUMBER OF DIFFERING MAINI 56
C *** PROFILE PAIRS FOR (TE,DEN). MAINI 57

```


C *** GENERALLY NOLPI=NUMBER OF RADIAL POINTS AT WHICH EXPERIMENTAL	MAIN	58
C *** VALUES FOR TE,DEN ARE OBTAINED FROM A LASER SHOT. HENCE LOOP OVER	MAIN	59
C *** RADIAL POINTS WITH LOOP VARIABLE LPI.	MAIN	60
LPI=1	MAIN	61
140 CALL DTDATA(LPI,NOLPI,DEN,TEE,TDCON,NTLAS,NDEN,DN1,DN12,DN13,	MAIN	62
DN21,DN22,TP11,TP12)	MAIN	63
CALL DTINIT(DEN,TEE,TDCON,NDEN,DN1,DN12,DN13,DN21,DN22,TP11,	MAIN	64
TP12,NTLAS)	MAIN	65
CALL YINIT(Y,NZPI,THRES)	MAIN	66
CALL DRIVES(NZPI,TO,TF,Y,H0,EPS,MF,KFLAG,SU12,SUR2)	MAIN	67
C *** KFLAG=0 MEANS EQUATIONS INTEGRATED TO DESIRED END.	MAIN	68
IF(KFLAG.EQ.0) GO TO 113	MAIN	69
WRITE(LOUT,12) KFLAG	MAIN	70
12 FORMAT('ODE-PACKAGE DIDN'T DELIVER OUR REQUEST. KFLAG=13')	MAIN	71
GO TO 222	MAIN	72
113 CONTINUE	MAIN	73
222 CONTINUE	MAIN	74
LPI=LPI+1	MAIN	75
IF(LPI.LE.NOLPI) GO TO 140	MAIN	76
RETURN	MAIN	77
END	MAIN	78

SUBROUTINE MAIN(SUIZ,SURZ)

MAIN 1

C *** ORIGINAL SEQUENCING DONE ON 09-12-77

C *** SUBROUTINE MAIN(TI)

MAIN 2

C *** DENSITY AND TEMP. PROFILES ARE CONST.; I.E., TIME INDEPENDENT(TI)

MAIN 3

C *** EQUILIBRIUM VECTOR CALCULATIONS

MAIN 4

DIMENSION SUIZ(1),SURZ(1)

MAIN 5

C *** NZNZ IS DEFINED IN A BLOCK DATA STATEMENT. FOR FE. NZNZ=26

MAIN 6

COMMON/E/NZNZ

MAIN 7

COMMON/IO/LOUT,LIN

MAIN 8

COMMON/EPN/NCH,NEQU,NEPS,NEPSC,NCRT,EPSEQU,ZAUGEQ,EPSCC(10)

MAIN 9

COMMON/EOI/T,H,HUSED,NLRC,NKRC,NL,NLPL,NKHI,NK,MXEOM,JSTART,NQ

MAIN 10

COMMON/YFCN/Y(1)

MAIN 11

COMMON/EQUIL/YEQU(1)

MAIN 12

COMMON/JACOB/FL(1)

MAIN 13

COMMON/PRINT/TPRINT,TPRNT(5),DTPRT(5),NPRNT(5),NPRNT1,IPRNT1,NPR

MAIN 14

COMMON/SHARE/TE,DEN,HMIN,HMAX,EPS,MF,KFLAG,JDISC,NOM,NOM2,NOMPI

MAIN 15

COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH

MAIN 16

COMMON/CONTRL/NZ,NZPI

MAIN 17

COMMON/DISCON/IDISC

MAIN 18

COMMON/MAINBD/NTMP,NDENS,NLOG,NROOTS,IPAIR,TSTART,TLAST,TEL,DTE,

MAIN 19

IDENL,BDEN,THRES,H0,TEMP(25),DENS(25)

MAIN 20

COMMON/SC1235/PSAVE(1)

MAIN 21

DATA TCONUT/1000, /

MAIN 22

IDISC=0

MAIN 23

C *** SAYS TO DRIVES THERE ARE NO DISCONTINUITIES IN NE AND TE PROFILES

MAIN 24

C *** IN FACT, HERE THESE PROFILES ARE CONSTANT. (IDISC=0)

MAIN 25

IF(NCH,NE,-2) GO TO 19

MAIN 26

IF(IPAIR,GT,0) GO TO 18

MAIN 27

IF(NTMP,LT,0) GO TO 19

MAIN 28

IF(NDENS,GT,0) GO TO 700

MAIN 29

19 CONTINUE

MAIN 30

IF(NCH,EO,-2) GO TO 26

MAIN 31

WRITE(LOUT,40) TSTART,TLAST,H0,EPS,MH

MAIN 32

40 FORMAT(' INTEG.PARMS., TSTART(MS)='E9.3,2X'TLAST(MS)='E9.3,2X

MAIN 33

-1'H0(S)='E9.3,2X'EPS(=EPS*YMAX)='E9.3/

MAIN 34

215X'IF ORDER OF STIFF METHOD SET TO 1, THEN NEXT H=(LAST H)/1+(NOMPI

MAIN 35

3-1)MH) WHERE NO=STIFF ORDER LAST USED, MH='12)

MAIN 36

GO TO (81,82),ISWSTR

MAIN 37

82 CALL STRTGI(SUIZ,SURZ)

MAIN 38

81 CONTINUE

MAIN 39

WRITE(LOUT,29)(1,TPRNT(1),DTPRT(1),NPRNT(1),I=1,NPRNT1)

MAIN 40

29 FORMAT('DCALL YNA AT T(MS)=(TPRNT(1)+0*DTPRT(1)), 0=0 TO NPRNT(1),

MAIN 41

1 I=1 TO NPRNT1, /1X'1'3X'TPRNT'6X'DTPRT'3X'NPRNT'

MAIN 42

2(12,1P2E10.2,15)

MAIN 43

28 IF(IPAIR,LE,0) GO TO 228

MAIN 44

C *** IPAIR OVERRIDES NTEMP AND NDENS WHENEVER IPAIR,GT,0

MAIN 45

18 CONTINUE

MAIN 46

NTEMP=1

MAIN 47

NDENS=IPAIR

MAIN 48

GO TO 703

MAIN 49

228 IF(NTMP,GT,0) GO TO 700

MAIN 50

NT=-NTEMP

MAIN 51

NTEMP=NT

MAIN 52

GO TO 701

MAIN 53

700 NT=0

MAIN 54

701 IF(NDENS,GT,0) GO TO 702

MAIN 55

ND=-NDENS

MAIN 56

NDENS=ND

MAIN 57

GO TO 703	MAIN1	58
702 ND=0	MAIN1	59
703 CONTINUE	MAIN1	60
IF(NCH.LE.0) GO TO 22	MAIN1	61
WRITE(LOUT,850)NCRIT	MAIN1	62
850 FORMAT('/// INTEGRATION CONVRG. MEANS LI-NORM(Y(T)-YEQU).LE.EPSEQU	MAIN1	63
IF NCRIT=L AND ABS(ZAUG(Y(T))-ZAUG(YEQU))/ZAUG(YEQU).LE.EPSEQU IF	MAIN1	64
2NCRIT=2'/' IN THIS CASE NCRIT='1')	MAIN1	65
22 ALM1=0.	MAIN1	66
DO 26 L=1,NDENS	MAIN1	67
IF(IPAIR.LE.0) GO TO 760	MAIN1	68
TE=TEMP(L)	MAIN1	69
GO TO 754	MAIN1	70
760 IF(ND.EQ.0) GO TO 754	MAIN1	71
DEN=DENL+ALM1*DDEN	MAIN1	72
ALM1=ALM1+1.	MAIN1	73
GO TO 756	MAIN1	74
754 DEN=DENS(L)	MAIN1	75
756 CONTINUE	MAIN1	76
AJMI=0.	MAIN1	77
DO 25 J=1,NTEMP	MAIN1	78
IF(IPAIR.GT.0) GO TO 751	MAIN1	79
IF(NT.EQ.0) GO TO 750	MAIN1	80
TE=TE+AJMI*DTE	MAIN1	81
AJMI=AJMI+J	MAIN1	82
GO TO 751	MAIN1	83
750 TE=TEMP(J)	MAIN1	84
751 IF(NLOG.LE.0) GO TO 752	MAIN1	85
TELOG=TE	MAIN1	86
TE=10.**TE/11604.5	MAIN1	87
GO TO 753	MAIN1	88
752 TELOG=ALOG10(11604.5*TE)	MAIN1	89
753 CONTINUE	MAIN1	90
NZ=NZNZ	MAIN1	91
NZPI=NZ+1	MAIN1	92
IF(NCH.EQ.0) GO TO 801	MAIN1	93
C *** THE CURRENT SET OF ACTIVE DIFF. EOS. IS EOS. NL THRU NK.	MAIN1	94
C *** THIS SET REQUIRES RATE COEFFS. NLRC THRU NKRC.	MAIN1	95
C *** REGARD NL,NK,NLRC,NKRC,NLPI,NKMI AS NORMAL INPUT TO SUTONZ,SURECZ.	MAIN1	96
NL=1	MAIN1	97
NLRC=1	MAIN1	98
NLPI=2	MAIN1	99
NKMI=NZNZ	MAIN1	100
NKRC=NKMI	MAIN1	101
NK=NZNZ+1	MAIN1	102
CALL SUTONZ(SUTZ,TE,DEN)	MAIN1	103
CALL SURECZ(SURZ,TE,DEN)	MAIN1	104
CALL EQU(YEQU,SUTZ,SURZ,NZ,FL)	MAIN1	105
CALL ZAVERG(ZAUGEO,YEQU)	MAIN1	106
IF(NZ.GE.20) WRITE(LOUT,202)	MAIN1	107
202 FORMAT('1')	MAIN1	108
WRITE(LOUT,900)DEN,TE,TELOG,ZAUGEO	MAIN1	109
900 FORMAT('0***START***',3X'NE='1PE11.5,3X'TE='E11.5,3X'LOG(11604.5*TE)	MAIN1	110
TE)='E11.5,3X'ZAUG(YEQU)='0PF8.4)	MAIN1	111
DO 345 I=1,NZ	MAIN1	112
IF(SURZ(I).GT.0.) GO TO 347	MAIN1	113
AIDR=-1.	MAIN1	114
GO TO 348	MAIN1	115

347	AIDR=SUZ(1)/SURZ(1)	MAIN	116
348	IMI=1-1	MAIN	117
	IF(1.GT.1) GO TO 223	MAIN	118
	WRITE(LOUT,200)	MAIN	119
200	FORMAT('SPECTRO'15X'RATE COEFFICIENTS'21X'NORMALIZED'/'	MAIN	120
	'-SCOPIC'2X'CHARGE'3X'IONIZATION'3X'RECOMBINATION'6X'1/R'7X	MAIN	121
	2'EQUILIBRIUM'/'	MAIN	122
	3'STATE'4X'STATE'6X'OUT OF'9X'INTO'21X'VECTOR'/'	MAIN	123
223	WRITE(LOUT,346)1,IMI,SUZ(1),SURZ(1),AIDR,YEQU(1)	MAIN	124
346	FORMAT(15,6X,13,1X,1P2E14.4,5X,E10.4,3X,DPF8.6)	MAIN	125
345	CONTINUE	MAIN	126
	WRITE(LOUT,201)NZPI,NZ,YEQU(NZPI)	MAIN	127
201	FORMAT(15,6X,13,47X,PF8.6)	MAIN	128
	IF(NROOTS.GT.0) CALL ROOTS(SUZ,SURZ,NZPI,DEN,FL,PSAVE)	MAIN	129
	IF(NCH.EQ.-2) GO TO 222	MAIN	130
	NEPSC=1	MAIN	131
	EPSEQU=EPSCC(1)	MAIN	132
	IF(NZ.GE.20) WRITE(LOUT,202)	MAIN	133
801	CALL YINIT(Y,NZPI,THRES)	MAIN	134
	CALL INTEGCT(START,TLAST,TEQU,KFLAG,SUZ,SURZ,EP5,H0)	MAIN	135
	IF(KFLAG.EQ.0) GO TO 113	MAIN	136
	WRITE(LOUT,12) KFLAG	MAIN	137
12	FORMAT('MODE-PACKAGE DIDN'T DELIVER OUR REQUEST, KFLAG='13)	MAIN	138
	GO TO 222	MAIN	139
113	IF(NCH.EQ.0) GO TO 222	MAIN	140
	IF(NEQU.EQ.0) GO TO 222	MAIN	141
	TOUT=TCONUT*T	MAIN	142
	WRITE(LOUT,115) TOUT	MAIN	143
115	FORMAT('DIDN'T SATISFY THE EQUILIBRIUM CONDITION.'/'	MAIN	144
	'INTEGRATED TO T(HS)='1PE9.3/)	MAIN	145
222	CONTINUE	MAIN	146
25	CONTINUE	MAIN	147
26	CONTINUE	MAIN	148
	RETURN	MAIN	149
	END	MAIN	150

```

SUBROUTINE ROOTS(SUIZ,SURZ,N,DENS,D,E)
C *** ORIGINAL SEQUENCING DONE ON 08-25-77
C *** THE TRIDIAGONAL COEFF. MATRIX, A, MAY BE TRANSFORMED BY USING A
C *** POSITIVE DIAG. MATRIX, P, INTO A SYMMETRIC TRIDIAG. MATRIX, AS.
C *** RELATE ROOTS OF A DIAGONAL SUBMATRIX OF A TO THOSE OF A. THE
C *** MATRIX Q SELECTS THE SUBMATRIX.
C *** LET Q= IDENTITY MATRIX WITH SOME ADDITIONAL 0 ENTRIES. THEN
C ***  $P(-1)*Q*A*Q*P=Q*P(-1)*A*P*Q=Q*AS*Q$ .
C *** TRIDIAGONAL MATRIX TRANSFORMED TO A SYM. TRIDIAG. MATRIX.
C *** THE SYM. MATRIX HAS MAIN DIAG. = D AND NONTRIVIAL OFF-DIAG. = E.
DIMENSION SUIZ(1),SURZ(1),D(1),E(1)
COMMON/IO/LOUT,LIN
C *** NM1=NZ
NM1=N-1
D(1)=-SUIZ(1)
D(N)=-SURZ(NM1)
DO 1 L=2,NM1
1 D(L)=-(SUIZ(L)+SURZ(L-1))
DO 2 L=L,NM1
C *** GUARD AGAINST UNDERFLOW WITH THE 2 DISTINCT SQUARE ROOTS.
2 E(L+1)=SQRT(SUIZ(L))*SQRT(SURZ(L))
C *** NORMALIZE MATRIX SO LARGEST ELEMENT HAS MAGNITUDE 1.
AM=0
DO 3 I=1,N
3 AM=AMAX1(AM,-D(I))
DO 4 I=2,N
4 AM=AMAX1(AM,E(I))
DO 5 I=1,N
5 D(I)=D(I)/AM
DO 6 I=2,N
6 E(I)=E(I)/AM
CALL INTGL(N,D,E,IERR)
IF(IERR.GT.0) WRITE(LOUT,13) IERR
13 FORMAT('FROM SUBR. ROOTS, IERR='13)
DENT=DENS*AM
DO 12 I=1,N
12 D(I)=DENT*D(I)
WRITE(LOUT,10)(D(I),I=1,N)
10 FORMAT('ROOTS OF NE*A='1P10E11.2/(15X,10E11.2))
AM=-2.303/D(NM1)
WRITE(LOUT,11) AM
11 FORMAT('THE EXPONENTIAL ASSOCIATED WITH THE NEXT TO LAST ROOT =
1) AT TIME T(S)='1PE7.1)
RETURN
END

```

ROOTS 1
ROOTS 2
ROOTS 3
ROOTS 4
ROOTS 5
ROOTS 6
ROOTS 7
ROOTS 8
ROOTS 9
ROOTS 10
ROOTS 11
ROOTS 12
ROOTS 13
ROOTS 14
ROOTS 15
ROOTS 16
ROOTS 17
ROOTS 18
ROOTS 19
ROOTS 20
ROOTS 21
ROOTS 22
ROOTS 23
ROOTS 24
ROOTS 25
ROOTS 26
ROOTS 27
ROOTS 28
ROOTS 29
ROOTS 30
ROOTS 31
ROOTS 32
ROOTS 33
ROOTS 34
ROOTS 35
ROOTS 36
ROOTS 37
ROOTS 38
ROOTS 39
ROOTS 40
ROOTS 41
ROOTS 42
ROOTS 43
ROOTS 44

SUBROUTINE STIFF(Y,NO)

STIFF 1

C *** ORIGINAL SEQUENCING DONE ON 06-09-77

C HAVE TAILORED STIFF FOR OUR LINEAR SYSTEM. (3/77)

STIFF 2

C DIMENSION Y(NO,6),EL(6),TQ(3)

STIFF 3

C *** DIMENSION Y(NO,13),EL(13),TQ(4) FOR NONSTIFF DIMENSIONING

STIFF 4

C *** OF MAX. ORDER.

STIFF 5

C *** ACTIVE EQUATIONS ARE NL THRU NK.

STIFF 6

C *** THE CORRECTOR EQUATION FOR A LINEAR SYSTEM OF DIFFERENTIAL EQS. IS

STIFF 7

C *** ITSELF LINEAR.

STIFF 8

C *** CF., "NUMERICAL INITIAL VALUE PROBLEM IN ORDINARY DIFFERENTIAL

STIFF 9

C *** EQUATION", C. WILLIAM GEAR, PRENTICE-HALL, INC., 1971, P. 215-218.

STIFF 10

C *** LET DIFF. EQS. BE DESCRIBED BY $Y' = F(Y_1, Y_2, \dots, Y_5)$, $i = 1, \dots, 5$.

STIFF 11

C *** IF TRANSPOSE OF $Y = (Y_1, Y_2, \dots, Y_5)$, THEN $Y' = NEX * Y$ WHERE A IS A

STIFF 12

C *** TRIDIAGONAL MATRIX WHOSE NONZERO ENTRIES ARE LINEAR COMBINATIONS

STIFF 13

C *** OF IONIZATION AND RECOMBINATION RATE COEFFICIENTS. THE LETTERS

STIFF 14

C *** PRED FOLLOWING AN EXPRESSION IN PARENTHESES INDICATES AN ESTIMATE

STIFF 15

C *** OBTAINED FROM THE PREDICTOR STEP.

STIFF 16

C *** USING (11.8) ON P. 216 DEFINE

STIFF 17

C *** $G1(W1, W2, \dots, W5) = H * F1((Y1)PRED + L * W1, \dots, (Y5)PRED + L * W5)$

STIFF 18

C *** $- ((H * Y1')PRED + L * W1)$ $i = 1, \dots, 5$.

STIFF 19

C *** $W1, \dots, W5$ ARE DETERMINED FROM $G1 = G2 = \dots = G5 = 0$

STIFF 20

C *** THIS IS EQUIVALENT TO THE VECTOR-MATRIX EQUATION

STIFF 21

C *** $H * NEX * ((Y)PRED + L * W) - ((H * Y')PRED + L * W) = 0$ WHERE $W =$ TRANSPOSE OF

STIFF 22

C *** $(W1, W2, \dots, W5)$. REARRANGING YIELDS THE LINEAR SYSTEM $(L1 = 1)$

STIFF 23

C *** $((L * H * NEX * A) * W = H * (NEX * ((Y)PRED) - (H * Y')PRED)$

STIFF 24

C *** SINCE THE EIGENVALUES OF THE MATRIX A ARE REAL AND NONPOSITIVE,

STIFF 25

C *** THE COEFF. MATRIX IS NONSINGULAR. MOREOVER, IT CAN BE SHOWN THAT

STIFF 26

C *** GAUSSIAN ELIMINATION WITH PARTIAL PIVOTING REQUIRES NO PIVOTING

STIFF 27

C *** AT ALL.

STIFF 28

COMMON/EO/T,H,AUSEO,NLRC,NKRC,NL,NLPI,NKMI,NK,MXEQMI,JSTART,

STIFF 29

COMMON/JACOB/FL(1)

STIFF 30

COMMON/RATEC/SUIZ(1)

STIFF 31

COMMON/SHARE/TE,DEN,HMIN,HMAX,EPS,MF,KFLAG,JDISC,NOM,NOM2,NOMPI

STIFF 32

COMMON/SC235/PSAVE(1)

STIFF 33

C *** $SUIZ(NOM+2+1) = SURZ(1)$, $FL(NOM+1) = FU(1)$, $FL(NOM2+1) = FD(1)$

STIFF 34

C *** NEED $2 * NOM + 2$ ELEMENTS IN $SUIZ$, $3 * NOM + 1$ IN FL , $2 * NOM$ IN $PSAVE$.

STIFF 35

C *** THE TRIDIAGONAL SYSTEM OF LIN. EQS. IS SOLVED BY FACTORING IT INTO

STIFF 36

C *** A UNIT LOWER, L, TIMES AN UPPER, U. FL IS 1ST DIAG OF L AND $FD =$

STIFF 37

C *** $DIAG(U)$, $FU =$ 1ST UPPER DIAG OF U.

STIFF 38

C *** HAVE $SUM Y(I) = 1$, $Y(I) \geq 0$. CHOOSE $YMAX$ TO BE CONSTANT

STIFF 39

C *** FEED IN EPS THE VALUE $YMAX * EPS$.

STIFF 40

C* STIFF PERFORMS ONE STEP OF THE INTEGRATION OF AN INITIAL VALUE

STIFF 41

C* PROBLEM FOR A SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS.

STIFF 42

C* COMMUNICATION WITH STIFF IS DONE WITH THE FOLLOWING VARIABLES.

STIFF 43

C*

STIFF 44

C* Y AN NO BY LMAX ARRAY CONTAINING THE DEPENDENT VARIABLES

STIFF 45

C* AND THEIR SCALED DERIVATIVES. LMAX IS CURRENTLY 13 FOR

STIFF 46

C* THE ADAMS METHODS AND 6 FOR THE GEAR METHODS. LMAX = 1

STIFF 47

C* IS MAXDER, THE MAXIMUM ORDER USED. SEE SUBROUTINE TESOC.

STIFF 48

C* $Y(I, J+1)$ CONTAINS THE J-TH DERIVATIVE OF $Y(I)$, SCALED BY

STIFF 49

C* $H * XJ / FACTORIAL(J)$. ONLY $Y(I)$, $i \leq 1$. LE. 1. LE. N, NEED BE

STIFF 50

C* SET BY THE CALLING PROGRAM ON THE FIRST ENTRY.

STIFF 51

C* IF IT IS DESIRED TO INTERPOLATE TO NON-MESH POINTS,

STIFF 52

C* THE Y ARRAY CAN BE USED. IF THE CURRENT STEP SIZE

STIFF 53

C* IS H AND THE VALUE AT $T + E$ IS NEEDED, FORM

STIFF 54

C* $S = E/H$, AND THEN COMPUTE

STIFF 55

C* NO

STIFF 56

C* $Y(I)(T+E) = SUM Y(I, J+1) * S ** J$

STIFF 57

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C*                                     J=0 STIFF 58
C* THE Y ARRAY SHOULD NOT BE ALTERED BY THE CALLING PROGRAM. STIFF 59
C* WHEN REFERENCING Y AS A 2-DIMENSIONAL ARRAY, USE A STIFF 60
C* COLUMN LENGTH OF NO, AS THIS IS THE VALUE USED IN STIFF. STIFF 61
C* NO A CONSTANT INTEGER GE, N, USED FOR DIMENSIONING PURPOSES. STIFF 62
C* NO MUST NOT BE CHANGED WITHOUT SETTING JSTART = 0. STIFF 63
C* T THE INDEPENDENT VARIABLE, T IS UPDATED ON EACH STEP TAKEN. STIFF 64
C* H THE STEP SIZE TO BE ATTEMPTED ON THE NEXT STEP. STIFF 65
C* H MAY BE ADJUSTED UP OR DOWN BY THE ROUTINE STIFF 66
C* IN ORDER TO ACHIEVE AN ECONOMICAL INTEGRATION. STIFF 67
C* HOWEVER, IF THE H PROVIDED BY THE USER DOES STIFF 68
C* NOT CAUSE A LARGER ERROR THAN REQUESTED, IT STIFF 69
C* WILL BE USED. TO SAVE COMPUTER TIME, THE USER IS STIFF 70
C* ADVISED TO USE A FAIRLY SMALL STEP FOR THE FIRST STIFF 71
C* CALL. IT WILL BE AUTOMATICALLY INCREASED LATER. STIFF 72
C* H CAN BE EITHER POSITIVE OR NEGATIVE, BUT ITS SIGN STIFF 73
C* MUST REMAIN CONSTANT THROUGHOUT THE PROBLEM. STIFF 74
C* HMIN THE MINIMUM ABSOLUTE VALUE OF THE STEP SIZE THAT WILL BE STIFF 75
C* USED FOR THE PROBLEM. ON STARTING THIS MUST BE MUCH STIFF 76
C* SMALLER THAN THE AVERAGE ABS(H) EXPECTED, SINCE STIFF 77
C* A FIRST ORDER METHOD IS USED INITIALLY. STIFF 78
C* HMAX THE MAXIMUM ABSOLUTE VALUE OF THE STEP SIZE THAT WILL STIFF 79
C* BE USED FOR THE PROBLEM. STIFF 80
C* EPS THE RELATIVE ERROR TEST CONSTANT. SINGLE STEP ERROR STIFF 81
C* ESTIMATES DIVIDED BY YMAX(1) MUST BE LESS THAN THIS STIFF 82
C* IN THE EUCLIDEAN NORM. THE STEP AND/OR ORDER IS STIFF 83
C* ADJUSTED TO ACHIEVE THIS. STIFF 84
C *** YMAX AS VECTOR REPLACED BY A SCALAR YMAX. MOREOVER, IT IS STIFF 85
C *** INCORPORATED INTO PARA.EPS. THUS EPS=EPS*YMAX. STIFF 86
C* MF THE METHOD FLAG. MF IS A POSITIVE INTEGER WITH STIFF 87
C* TWO DECIMAL DIGITS--METH AND MITER (MF=10*METH+MITER). STIFF 88
C* METH IS THE BASIC METHOD INDICATOR. STIFF 89
C* METH = 1 MEANS THE ADAMS METHODS. STIFF 90
C* METH = 2 MEANS THE STIFF SYSTEM METHODS OF GEAR. STIFF 91
C* MITER IS THE ITERATION METHOD INDICATOR. STIFF 92
C* MITER = 0 MEANS FUNCTIONAL ITERATION (NO PARTIAL STIFF 93
C* DERIVATIVES NEEDED). STIFF 94
C* MITER = 1 MEANS CHORD METHOD WITH ANALYTIC JACOBIAN. STIFF 95
C* FOR THIS USER SUPPLIES SUBROUTINE STIFF 96
C* PEDERU(N,T,Y,PD,NO). PD IS AN N BY N ARRAY, STIFF 97
C* STORED AS AN NO BY NO ARRAY. PD(I,J) IS STIFF 98
C* TO BE SET TO THE PARTIAL DERIVATIVE OF STIFF 99
C* YDOT(I) WITH RESPECT TO Y(J). STIFF 100
C* MITER = 2 MEANS CHORD METHOD WITH JACOBIAN STIFF 101
C* CALCULATED IN STIFF BY FINITE DIFFERENCES. STIFF 102
C* PEDERU IS NOT CALLED AND A DUMMY CAN BE USED. STIFF 103
C* MITER = 3 MEANS CHORD METHOD WITH JACOBIAN REPLACED STIFF 104
C* BY A DIAGONAL APPROXIMATION BASED ON A STIFF 105
C* DIRECTIONAL DERIVATIVE. STIFF 106
C* YMAX AN ARRAY OF N LOCATIONS WHICH CONTAINS THE MAXIMUM STIFF 107
C* ABSOLUTE VALUE OF EACH Y SEEN SO FAR. STIFF 108
C *** CF. PARAMETER EPS ABOVE. STIFF 109
C* ERROR AN ARRAY OF N ELEMENTS PROPORTIONAL TO THE ESTIMATED STIFF 110
C* ONE STEP ERROR IN EACH COMPONENT. STIFF 111
C* KFLAG A COMPLETION CODE WITH THE FOLLOWING MEANINGS. STIFF 112
C* 0 THE STEP WAS SUCCESSFUL. STIFF 113
C* -1 THE REQUESTED ERROR COULD NOT BE ACHIEVED STIFF 114
C* WITH ABS(H) = HMIN. STIFF 115

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C* -2 THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED FOR THIS PROBLEM. STIFF116
C* -3 CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED FOR ABS(H) .GT. HMIN. STIFF117
C* -5 H WAS SUCH THAT T+H EQ. T ON MACHINE. STIFF118
C* ON A RETURN WITH KFLAG NEGATIVE, THE VALUES OF T AND STIFF119
C* THE Y ARRAY ARE AS OF THE BEGINNING OF THE LAST STEP, AND H IS THE LAST STEP SIZE ATTEMPTED. STIFF120
C* JSTART AN INTEGER USED ON INPUT AND OUTPUT. STIFF121
C* ON INPUT, IT HAS THE FOLLOWING VALUES AND MEANINGS. STIFF122
C* Q PERFORM THE FIRST STEP. THIS VALUE ENABLES THE SUBROUTINE TO INITIALIZE ITSELF. STIFF123
C* .GT.Q TAKE A NEW STEP CONTINUING FROM THE LAST. ASSUMES THE LAST STEP WAS SUCCESSFUL AND USER HAS NOT CHANGED ANY PARAMETERS. STIFF124
C* .LT.Q REPEAT THE LAST STEP WITH A NEW VALUE OF H AND/OR EPS AND/OR MF. THIS MAY BE EITHER IN REDOING A STEP THAT FAILED, OR IN CONTINUING FROM A SUCCESSFUL STEP. STIFF125
C* ON EXIT, JSTART IS SET TO NQ, THE CURRENT ORDER OF THE METHOD. THIS IS ALSO THE ORDER OF THE MAXIMUM DERIVATIVE AVAILABLE IN THE Y ARRAY. AFTER A SUCCESSFUL STEP, JSTART NEED NOT BE RESET FOR THE NEXT CALL. STIFF126
C* THE PARAMETERS WHICH MUST BE INPUT BY THE USER ARE... STIFF127
C* N, NO, J, Y, H, HMIN, HMAX, EPS, MF, JSTART. STIFF128
C* ADDITIONAL SUBROUTINES REQUIRED ARE... STIFF129
C* TESOC(METH,NO,EL,TO,MAXDER) SETS METHOD COEFFICIENTS. STIFF130
C* IT IS PROVIDED IN THE PACKAGE. STIFF131
C* THE CALLING PROGRAM MUST CONTAIN THE COMMON DECLARATIONS GIVEN ABOVE, IN WHICH THE LENGTHS ARE AS GIVEN BY THE DESCRIPTIONS OF THE VARIABLES ABOVE. THE OPTIONAL ROUTINE DRIVES MAY BE USED FOR THIS PURPOSE. STIFF132
C* THE ORIGINAL VERSION OF THIS PROGRAM WAS WRITTEN AT LLL BY A. C. HINDMARSH FOR CDC COMPUTERS. THE CDC VERSION WAS MODIFIED FOR USE ON IBM COMPUTERS AT ARGONNE IN JUNE, 1973. STIFF133
C* LATEST REVISION SEPTEMBER, 1973 STIFF134
C* KFLAG = 0 STIFF135
C* TOLD = T STIFF136
C* IF (JSTART .GT. 0) GO TO 200 STIFF137
C* IF (JSTART .NE. 0) GO TO 120 STIFF138
C* ON THE FIRST CALL, THE ORDER IS SET TO 7 AND THE INITIAL DERIVATIVES ARE CALCULATED. STIFF139
C* RMAX IS THE MAXIMUM RATIO BY WHICH H CAN BE INCREASED IN A SINGLE STEP. IT IS INITIALLY 1.E4 TO COMPENSATE FOR THE SMALL INITIAL H, BUT THEN IS NORMALLY EQUAL TO 10. IF A FAILURE OCCURS (IN CORRECTOR CONVERGENCE OR ERROR TEST), RMAX IS SET AT 2 FOR THE NEXT INCREASE. EPSJ IS USED AS THE RELATIVE INCREMENT TO Y WHEN GETTING PARTIALS BY FINITE DIFFERENCING. STIFF140
C *** STARTING OR RESTARTING AT T. NEED NE(T), TE(T) AND IONIZATION AND RECOMBINATION COEFF. STIFF141
C* CALL YPAY(FSAVE,Y) STIFF142
C* DO 112 I=NL,NK STIFF143
C* 112 Y(I,2)=FSAVE(I)*H STIFF144
C* NQ = 1 STIFF145
C* L = 2 STIFF146

```


BMAX = LQF4

MFOLD = 0

METH = 0°

HOLD = H

STIFF174

STIFF175

STIFF176

STIFF177

C* IF THE CALLER HAS CHANGED METH. OR IF JSTART = 0, TESOC IS CALLED

STIFF178

C* TO SET THE COEFFICIENTS OF THE METHOD. IF THE CALLER HAS CHANGED

STIFF179

C* EPS OR METH, THE CONSTANTS E, EDN, EUP, AND BND MUST BE RESET.

STIFF180

C* E IS A COMPARISON FOR ERRORS OF THE CURRENT ORDER NO. EUP IS

STIFF181

C* TO TEST FOR INCREASING THE ORDER, EDN FOR DECREASING THE ORDER.

STIFF182

C* BND IS USED TO TEST FOR CONVERGENCE OF THE CORRECTOR ITERATES.

STIFF183

C* IF THE CALLER HAS CHANGED H, Y MUST BE RESCALED.

STIFF184

C* IF H OR METH HAS BEEN CHANGED, IDOUB IS RESET TO L + 1 TO PREVENT

STIFF185

C* FURTHER CHANGES IN H FOR THAT MANY STEPS. ALSO, RC IS RESET.

STIFF186

C* RC IS THE RATIO OF NEW TO OLD VALUES OF THE COEFFICIENT L(0)*H.

STIFF187

C* WHEN RC DIFFERS FROM 1 BY MORE THAN 30 PERCENT, OR THE CALLER HAS

STIFF188

C* CHANGED MITER, IWEAL IS SET TO MITER TO FORCE THE PARTIALS TO BE

STIFF189

C* UPDATED, IF PARTIALS ARE USED.

STIFF190

120 IF (MF.EQ.MFOLD) GO TO 150

STIFF191

MEQ = METH

STIFF192

METH = MF / 10

STIFF193

MFOLD = MF

STIFF194

IF (METH.EQ.MEQ) GO TO 150

STIFF195

IDOUB = L + 1

STIFF196

IRET = 1

STIFF197

130 CALL TESOC(METH,NQ,EL,TQ,MAXDER)

STIFF198

140 EDN = (TQ(1) * EPS) ** 2

STIFF199

E = (TQ(2) * EPS) ** 2

STIFF200

EUP = (TQ(3) * EPS) ** 2

STIFF201

GO TO (160, 170, 200), IRET

STIFF202

150 IF (EPS.EQ.EPSOLD) GO TO 160

STIFF203

IRET = 1

STIFF204

GO TO 140

STIFF205

160 LMAX = MAXDER + 1

STIFF206

EPSOLD = EPS

STIFF207

IF (H.EQ.HOLD) GO TO 200

STIFF208

RH = H / HOLD

STIFF209

C *** JDISC IS A DISCONTINUITY SWITCH. IF .NE. 0 TRYING TO LAND

STIFF210

C *** EXACTLY ON TIME OF DISCONTINUITY.

STIFF211

IF(JDISC.EQ.0) GO TO 169

STIFF212

HSAVE=H

STIFF213

GO TO 171

STIFF214

169 H = HOLD

STIFF215

170 RH = AMAXI(RH,HMIN/ABS(H))

STIFF216

RH=AMINI(RH,HMAX/ABS(H))

STIFF217

RH=AMINI(RH,RMAX)

STIFF218

171 RI = 1.0

STIFF219

C *** RESCALE AT TOLD TO REFLECT A NEW H VALUE.

STIFF220

DO 180 J = 2, L

STIFF221

RI = RI * RH

STIFF222

C

STIFF223

DO 180 I = NL,NK

STIFF224

Y(I,J) = Y(I,J) * RI

STIFF225

180 CONTINUE

STIFF226

H = H * RH

STIFF227

IF(JDISC.EQ.0) GO TO 179

STIFF228

H=HSAVE

STIFF229

179 IDOUB = L + 1

STIFF230

```

      IF (T.NE.TOLD) GO TO 690
C* THIS SECTION COMPUTES THE PREDICTED VALUES BY EFFECTIVELY
C* MULTIPLYING THE Y ARRAY BY THE PASCAL TRIANGLE MATRIX.
      200 CONTINUE
      T = T + H
C *** IF MUST SET ORDER OF STIFF TO 1, THEN A SMALL STEPSIZE MAY BE
C *** REQUIRED TO MAINTAIN BOUND FOR LOCAL TRUNCATION ERROR EXPRESSED
C *** IN VARIABLE EPS. THUS T=T+H MAY OCCUR. USUALLY WOULD EXPECT TO
C *** CONTINUE INTEGRATION, SINCE H SHOULD BEGIN TO GROW.
      IF (T.EQ.TOLD) GO TO 685
      HUSED=H
      DO 210 J1 = 1, NQ
      DO 210 J2 = J1, NQ
      J = NQ - J2 + J1
      DO 210 I=NL,NK
      Y(I,J) = Y(I,J) + Y(I,J+1)
      210 CONTINUE
C *** AT NEW T VALUE. NEED NE(T), TE(T) AND ASSOCIATED IONIZATION
C *** AND RECOMBINATION COEFFICIENTS.
      CALL YPAY(FSAVE(NOMP1),Y)
      R=-EL(I)*H*DEN
C *** FORM 1-LO*H*NE*A.
      DO 250 I=NL,NKML
      FL(I)=R*SU1Z(I)
      250 FL(NOM+1)=R*SU1Z(NOM+1+2)
      FL(NOM2+NL)=1.-FL(NL)
      FL(NOM2+NK)=1.-FL(NOM+NKML)
      DO 251 I=NLPI,NKMI
      251 FL(NOM2+1)=1.-(FL(I)+FL(NOM+1-1))
C *** FACTOR TRIANG. MATRIX
C *** THE 'DIAGONALS' OF THE TRIANGULAR MATRIX ARE IN FL,FD,FU.
C *** THE 'L' VECTOR OF THE UNIT LOWER TRIANGULAR MATRIX GOES
C *** INTO FL.
C *** DIAG. OF UPPER TRIANGULAR IS STORED IN FD AND ITS
C *** SUPERDIAG IN FU. N.B., SUPERDIAG IS JUST FU ANYWAY.
      DO 252 I=NL,NKMI
      FL(I)=FL(I)/FL(NOM2+1)
      252 FL(NOM2+1+1)=FL(NOM2+1+1)-FL(I)*FL(NOM+1)
C *** FORM H*(NE*A*(Y)PRED)-(H*Y)PRED IN FSAVE(NOM+1).
      DO 370 I=NL,NK
      370 FSAVE(I+NOM) = FSAVE(I+NOM) * H - Y(I,2)
C *** SOLVE 2-FACTOR TRIANGULAR SYSTEM.
      FSAVE(NL)=FSAVE(NOM+NL)
      DO 90 K=NL,NKMI
      90 FSAVE(K+1)=FSAVE(K+NOMP1)-FL(K)*FSAVE(K)
      FSAVE(NK)=FSAVE(NK)/FL(NOM2+NK)
      K=NKMI
      91 FSAVE(K)=FSAVE(K)-FL(NOM+K)*FSAVE(K+1)/FL(NOM2+K)
      K=K-1
      IF (K.GE.NL) GO TO 91
      D = 0
      DO 460 I=NL,NK
      460 D=D+FSAVE(I)**2
      IF (D.GT.E) GO TO 500
C* AFTER A SUCCESSFUL STEP, UPDATE THE Y ARRAY
C* CONSIDER CHANGING H IF IDOUB = 1. OTHERWISE DECREASE IDOUB BY 1.

```

```

C* IF IDOUB IS THEN 1 AND NO JT, MAXDER, THEN ERROR IS SAVED FOR STIFF290
C* USE IN A POSSIBLE ORDER INCREASE ON THE NEXT STEP. STIFF291
C* IF A CHANGE IN H IS CONSIDERED, AN INCREASE OR DECREASE IN ORDER STIFF292
C* BY ONE IS CONSIDERED ALSO. A CHANGE IN H IS MADE ONLY IF IT IS BY A STIFF293
C* FACTOR OF AT LEAST J. IF NOT, IDOUB IS SET TO JO TO PREVENT STIFF294
C* TESTING FOR THAT MANY STEPS. STIFF295
      KFLAG = 0 STIFF296
      DO 470 J = 1, L STIFF297
        DO 470 I = NL, NK STIFF298
          Y(I,J) = Y(I,J) + EL(J) * FSAVE(I) STIFF299
470 CONTINUE STIFF300
      IF (IDOUB.EQ. 1) GO TO 520 STIFF301
      IDOUB = IDOUB - 1 STIFF302
      IF (IDOUB.GT. 1) GO TO 700 STIFF303
      IF (NO.EQ. MAXDER) GO TO 700 STIFF304
C STIFF305
      DO 490 L = NL, NK STIFF306
490 Y(I,LMAX) = FSAVE(I) STIFF307
C STIFF308
      GO TO 700 STIFF309
C* THE ERROR TEST FAILED. KFLAG KEEPS TRACK OF MULTIPLE FAILURES. STIFF310
C* RESTORE T AND THE Y ARRAY TO THEIR PREVIOUS VALUES, AND PREPARE STIFF311
C* TO TRY THE STEP AGAIN. COMPUTE THE OPTIMUM STEP SIZE FOR THIS OR STIFF312
C* ONE LOWER ORDER. STIFF313
500 KFLAG = KFLAG - 1 STIFF314
      T = TOLD STIFF315
C STIFF316
      DO 510 J1 = 1, NO STIFF317
C STIFF318
        DO 510 J2 = J1, NO STIFF319
          J = NO - J2 + J1 STIFF320
C STIFF321
          DO 510 I = NL, NK STIFF322
            Y(I,J) = Y(I,J) - Y(I,J+1) STIFF323
510 CONTINUE STIFF324
            RMAX = 2. STIFF325
            IF (ABS(H).LE. (HMIN*1.00001)) GO TO 660 STIFF326
            IF (KFLAG.LE. -3) GO TO 640 STIFF327
            PR3 = 1.0E20 STIFF328
            GO TO 540 STIFF329
C* REGARDLESS OF THE SUCCESS OR FAILURE OF THE STEP, FACTORS STIFF330
C* PR1, PR2, AND PR3 ARE COMPUTED, BY WHICH H COULD BE DIVIDED STIFF331
C* AT ORDER NO - 1, ORDER NO, OR ORDER NO + 1, RESPECTIVELY. STIFF332
C* IN THE CASE OF FAILURE, PR3 = 1.0D20 TO AVOID AN ORDER INCREASE. STIFF333
C* THE SMALLEST OF THESE IS DETERMINED AND THE NEW ORDER CHOSEN STIFF334
C* ACCORDINGLY. IF THE ORDER IS TO BE INCREASED, WE COMPUTE ONE STIFF335
C* ADDITIONAL SCALED DERIVATIVE. STIFF336
520 PR3 = 1.0E20 STIFF337
      IF (NO.EQ. MAXDER) GO TO 540 STIFF338
      DI = 0.0 STIFF339
C STIFF340
      DO 530 I = NL, NK STIFF341
530 DI = DI + (FSAVE(I) - Y(I,LMAX))**2 STIFF342
      ENQ3 = 0.5 / FLOAT(L+1) STIFF343
      PR3 = ((DI / EUP) ** ENQ3) * 1.4 + 1.4E-06 STIFF344
540 ENQ2 = 0.5 / FLOAT(L) STIFF345
      PR2 = ((DI / E) ** ENQ2) * 1.2 + 1.2E-06 STIFF346
      PR1 = 1.0E20 STIFF347

```

```
IF (NQ .EQ. 1) GO TO 560
```

```
D = 0.0  
DO 550 I = NL, NK
```

```
550 D = D + Y(I, L) ** 2
```

```
ENQ1 = 0.5 / FLOAT(NQ)
```

```
PR1 = ((D / EDN) ** ENQ1) * 1.3 + 1.3E-06
```

```
560 IF (PR2 .LE. PR3) GO TO 570
```

```
IF (PR3 .LT. PR1) GO TO 590
```

```
570 IF (PR2 .GT. PR1) GO TO 580
```

```
C *** PR2 = MIN(PRI, PR2, PR3)
```

```
NEWQ = NQ
```

```
RH = 1. / PR2
```

```
GO TO 620
```

```
580 NEWQ = NQ - 1
```

```
C *** PRI = MIN(PRI, PR2, PR3)
```

```
RH = 1. / PRI
```

```
GO TO 620
```

```
590 NEWQ = L
```

```
C *** PR3 = MIN(PRI, PR2, PR3)
```

```
RH = 1. / PR3
```

```
IF (RH .LT. 1.1) GO TO 610
```

```
DO 600 I = NL, NK
```

```
600 Y(I, NEWQ+1) = FSAVE(I) * EL(I) / FLOAT(L)
```

```
GO TO 630
```

```
610 IDOUB = 10
```

```
GO TO 700
```

```
620 IF ((KFLAG .EQ. 0).AND.(RH .LT. 1.1DO)) GO TO 610
```

```
C* IF THERE IS A CHANGE OF ORDER, RESET NQ, L, AND THE COEFFICIENTS.
```

```
C* IN ANY CASE H IS RESET ACCORDING TO RH AND THE Y ARRAY IS RESCALED.
```

```
C* THEN EXIT FROM 690 IF THE STEP WAS OK, OR REDO THE STEP OTHERWISE.
```

```
IF (NEWQ .EQ. NQ) GO TO 170
```

```
630 NQ = NEWQ
```

```
L = NQ + 1
```

```
IRET = 2
```

```
GO TO 130
```

```
C* CONTROL REACHES THIS SECTION IF 3 OR MORE FAILURES HAVE OCCURRED.
```

```
C* IT IS ASSUMED THAT THE DERIVATIVES THAT HAVE ACCUMULATED IN THE
```

```
C* Y ARRAY HAVE ERRORS OF THE WRONG ORDER. HENCE THE FIRST
```

```
C* DERIVATIVE IS RECOMPUTED, AND THE ORDER IS SET TO 1. THEN
```

```
C* H IS REDUCED BY A FACTOR OF 10, AND THE STEP IS RETRIED.
```

```
C* AFTER A TOTAL OF 7 FAILURES, AN EXIT IS TAKEN WITH KFLAG = -2.
```

```
640 IF (KFLAG .EQ. -7) GO TO 670
```

```
RH = .1
```

```
RH = AMAX1(HMIN/ABS(H), RH)
```

```
H = H * RH
```

```
C *** GOING BACK TO TOLD. NEED NE(TOLD), TE(TOLD) AND ASSOCIATED
```

```
C *** IONIZATION AND RECOMBINATION COEFF.
```

```
C *** IF AFTER EACH SUCCESSFUL STEP THE ESTIMATED Y' IS REPLACED
```

```
C *** WITH Y' = F(Y), THEN THIS CALL YPAY WOULD BE UNNECESSARY.
```

```
CALL YPAY(FSAVE, Y)
```

```
C
```

```
DO 650 I = NL, NK
```

```
650 Y(I, 2) = H * FSAVE(I)
```

```
C
```

```
IDOUB = 10
```

```
IF (NQ .EQ. 1) GO TO 200
```

```
NQ = 1
```

L = 2
IRET = 3
GO TO 180

C* ALL RETURNS ARE MADE THROUGH THIS SECTION. H IS SAVED IN HOLD
C* TO ALLOW THE CALLER TO CHANGE H ON THE NEXT STEP.

660 KFLAG = -1
GO TO 700
670 KFLAG = -2
GO TO 700

685 KFLAG = -5
GO TO 700

690 RMAX = 10.

700 HOLD = H
JSTART = NO
RETURN
END

STIFF406
STIFF407
STIFF408
STIFF409
STIFF410
STIFF411
STIFF412
STIFF413
STIFF414
STIFF415
STIFF416
STIFF417
STIFF418
STIFF419
STIFF420
STIFF421

C* STIFFLY STABLE GEAR METHODS OF ORDERS L TO 5.

201	EL(1)=1.	TESOC	58
	GO TO 900	TESOC	59
202	EL(1)=2./3.	TESOC	60
	EL(3)=1./3.	TESOC	61
	GO TO 900	TESOC	62
203	EL(1)=6./11.	TESOC	63
	EL(3) = EL(1)	TESOC	64
	EL(4)=1./11.	TESOC	65
	GO TO 900	TESOC	66
204	EL(1)=24./50.	TESOC	67
C ***	EL(1)=.5 ACCORDING TO GEAR'S BOOK. HOWEVER FROM L(T) ABOVE	TESOC	68
C ***	EL(1)=24./50	TESOC	69
	EL(3)=35./50.	TESOC	70
	EL(4)=10./50.	TESOC	71
	EL(5)=1./50.	TESOC	72
	GO TO 900	TESOC	73
205	EL(1)=120./274.	TESOC	74
	EL(3)=225./274.	TESOC	75
	EL(4)=85./274.	TESOC	76
	EL(5)=15./274.	TESOC	77
	EL(6)=1./274.	TESOC	78
900	DO 910 K = L 3	TESOC	79
910	TQ(K) = PERTST(NQ, METH, K)	TESOC	80
C ***	IQ(4) = .5DQ*TQ(2) / DFLOAT(NQ+2)	TESOC	81
	RETURN	TESOC	82
	END	TESOC	83
		TESOC	84

H 3.

```

SUBROUTINE YINIT(Y,NZPI,THRES)
C *** ORIGINAL SEQUENCING DONE ON 06-09-77
DIMENSION Y(1)
COMMON/IO/LOUT,LIN
COMMON/EP5/NCH
COMMON/EQ1/T,H,HUSED,NLRC,NKRC,NL,NLPI,NKMI,NK,MXEQHI,JSTART,NO
COMMON/EQUIL/YEQU(1)
COMMON/SHARE/TE,DEN,HMIN,HMAX,EP5,HF,KFLAG,JDTSC,NOM,NOM2,NOMPI
COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH
C *** DEFINE INITIAL-VALUE VECTOR FOR ODE'S IN 1ST NZ+1 COMPONENTS OF Y.
C *** IEQU=1 IMPLIES Y=(1,0,...,0)
C *** IEQU=2 IMPLIES Y=(0,...,0,1)
C *** IF IEQU=3, USER MUST SUPPLY CODING FOR DESIRED Y AT 30 CONTINUE
C *** NEEDED( OR POSSIBLY NEEDED) INPUT VARIABLE OR ARRAYS (APART FROM
C *** ARGUMENTS) ARE IEQU,NLB,NKB,NCH,ISWSTR,LOUT, AND ARRAY YEQU.
C *** IF YEQU IS USED, IT MUST CONTAIN EQUILIBRIUM, NORMALIZED, CHARGE
C *** STATE DISTRIBUTION VECTOR FOR FIXED TE AND NE=DEN UNDER
C *** CONSIDERATION.
C *** NEEDED OUTPUT VARIABLES APART FROM ARGUMENT ARE NLRC,NKRC,NL,NLPI
C *** NKMI,NK. AT THE BEGINNING THE ACTIVE DIFF.EQ. ARE EQS. NL THRU NK
C *** AND THE NEEDED RATE COEFF.(MAY VARY DUE TO STRATEGY FOR
C *** ALTERING SET OF ACTIVE EQS.) ARE NLRC AND NKRC. OF COURSE NLPI=NL
C *** +1 AND NKMI=NK-1
GO TO (10,20,30), IEQU
10 Y(1)=1
NLB=1
DO 1 I=2,NZPI
1 Y(I)=0.
IF(NCH.EQ.0) GO TO 801
C *** HAVE NORMALIZED EQUILIBRIUM VECTOR YEQU.
IF(THRES.LE.0.) GO TO 801
SUMR=0.
NK1=NZPI
800 IF(SUMR+YEQU(NK1).GE.THRES) GO TO 802
SUMR=SUMR+YEQU(NK1)
NK1=NK1-1
GO TO 800
802 GO TO (101,102), ISWSTR
101 NKB=NK1
C *** INITIAL SET OF ACTIVE EQS. NOT ALTERED DURING INTEGRATION.
WRITE(LOUT,803) THRES,NKB,SUMR
803 FORMAT(' Y(TSTART)=(1,0,...,0), USED THRES=',1PE8.2,'(X) TO DEFINE NKYINIT
1B='13.4X'MAX.ERROR DUE TO DELETED EQS. FROM BACK (LE.'E8.2)
GO TO 801
102 NKB=MINO(NKB,NK1)
7C *** STRATEGY IT ALTERS ACTIVE EQS. DURING TIME INTEGRATION.
GO TO 801
20 Y(NZPI)=1.
NKB=NZPI
NZ=NZPI-1
DO 21 I=1,NZ
21 Y(I)=0.
IF(NCH.EQ.0) GO TO 801
IF(THRES.LE.0.) GO TO 801
SUML=0.
NL1=1
900 IF(SUML+YEQU(NL1).GE.THRES) GO TO 902
SUML=SUML+YEQU(NL1)

```


	NLI=NLI+1	YINIT 58
	GO TO 900	YINIT 59
902	GO TO (111,112), ISHSTR	YINIT 60
111	NLB=NLI	YINIT 61
	WRITE(LOUT,903) THRES,NLB,SUML	YINIT 62
903	FORMAT('Y(TSTART)=(0,...,0,1), USED THRES=TYPE8.2, IX TO DEFINE NLI	YINIT 63
	LB='13.4X' MAX. ERROR DUE TO DELETED EOS. FROM BACK I.E. 'EQ.2)	YINIT 64
	GO TO 801	YINIT 65
112	NLB=MAX0(NLB,NLI)	YINIT 66
	GO TO 801	YINIT 67
30	CONTINUE	YINIT 68
801	NL=NLB	YINIT 69
	NLP1=NLI	YINIT 70
	NK=NKB	YINIT 71
	NKM1=NK-1	YINIT 72
	GO TO (121,122), ISHSTR	YINIT 73
C ***	STRATEGY U. NEED 1 EXTRA IONIZATION AND 1 EXTRA RECOMBINATION	YINIT 74
C ***	COEFF. FOR MONITORING LOSSES OUT ENDS OF CURRENT SET OF ACTIVE EOS	YINIT 75
122	NLRC=MAX0(NL-L, 1)	YINIT 76
	NKRC=MIN0(NK, NZP1-1)	YINIT 77
	GO TO 751	YINIT 78
121	NLRC=NL	YINIT 79
C ***	STRATEGY L MEANS SET OF ACTIVE EOS. REMAIN FIXED THRUOUT	YINIT 80
C ***	INTEGRATION. HENCE NEED ONLY RATE COEFF. ASSOCIATED WITH ACTIVE EOS	YINIT 81
	NKRC=NKM1	YINIT 82
751	RETURN	YINIT 83
	END	YINIT 84

C *** SUBROUTINE YOUTD(Y,NQ)
 ORIGINAL SEQUENCING DONE ON 06-09-77
 DIMENSION Y(1)

YOUTD 1

COMMON/IO/LOUT,LIN

YOUTD 2

COMMON/EO/L,T,H,HUSED,NLRC,NKRC,NL,NLP,L,NKMI,NK

YOUTD 3

C *** DON'T EXPECT TO ENTER HEREIN.

YOUTD 4

WRITE(LOUT,1000) NQ,(L,Y(L),J=NL,NK)

YOUTD 5

1000 FORMAT('FROM SUBR.YOUTD NQ=',12/('1=',13,3X,Y(1)=',1PE13.6))

YOUTD 6

RETURN

YOUTD 7

END

YOUTD 8

YOUTD 9

K 3

```

SUBROUTINE CONEQU(Y,NZPL,NOK)
C *** ORIGINAL SEQUENCING DONE ON 07-12-77
DIMENSION Y(1)
COMMON/IO/LOUT,LIN
COMMON/EP5/NCH,NEQU,NEPS,NEPSC,NCRIT,EPSEQU,ZAUGEQ,EPSCC(1)
COMMON/EQ1/T
COMMON/EQUIL/YEQU(1)
NOK=0
C *** MONITOR CLOSENESS OF DISTRIBUTION VECTOR, Y, TO THE EQUILIBRIUM
C *** VECTOR, YEQU. 2 CLOSENESS CRITERIA. CORRESPOND TO NCRIT=1,2.
C *** NCRIT=1 MEASURES CLOSENESS OF Y TO YEQU IN TERMS OF L1-NORM OF
C *** Y-YEQU.
C *** NCRIT=2 MEASURES CLOSENESS IN TERMS OF REL. CLOSENESS OF ZAUG(Y)
C *** TO ZAUG(YEQU).
C *** CLOSENESS LEVELS ARE GIVEN IN THE VECTOR EPSCC AND THE NUMBER OF
C *** LEVELS IS NEPS.
C *** NEPSC SET TO 1 AND EPSEQU=EPSCC(1) IN MAIN(TI). EPSCC AND NEPS
C *** ARE DEFINED IN BLOCK DATA, BDPARM.
ALOT=0.
AIMI=0.
DZAUG=0.
DO 901 I=1,NZPL
YDIFF=Y(I)-YEQU(I)
DZAUG=DZAUG+AIMI*YDIFF
ALOT=ALOT+ABS(YDIFF)
901 AIMI=AIMI+1.
ZAUG=DZAUG+ZAUGEQ
YDIFF=ABS(DZAUG)/ZAUGEQ
GO TO (1000,1001),NCRIT
1000 IF(ALOT.GT.EPSEQU) GO TO 500
GO TO 1002
1001 IF(YDIFF.GT.EPSEQU) GO TO 500
1002 TMS=1000.*T
WRITE(LOUT,950)TMS,YDIFF,ZAUG,ALOT,EPSEQU
950 FORMAT('OT(MS)='1PE10.4,'ABS(ZAUG(Y(T))-ZAUG(YEQU))/ZAUG(YEQU)='
10PF7.5,'ZAUG(Y(T))='F6.3,'L1(Y(T)-YEQU)='F7.5,'EPSE='F7.5)
WRITE(LOUT,951)(Y(I),I=1,NZPL)
951 FORMAT('Y='10F10.6/13X,10F10.6)
NEPSC=NEPSC+1
IF(NEPSC.LE.NEPS) GO TO 899
C *** NOK=1(0) MEANS THAT CONVERGENCE CRITERIA IN CONEQU HAS(NOT) BEEN
C *** MET WITH EPSCC(NEPS). DRIVES TERMINATES INTEGRATION WHENEVER NOK=
C *** IS RETURNED.
C *** NEQU=0(1) CONVEYS SAME INFORMATION AS NOK=1(0), BUT TO SUBR.
C *** MAIN(TI).
NEQU=0
NOK=1
GO TO 500
899 EPSEQU=EPSCC(NEPSC)
500 RETURN
END

```

CONEQU 1
CONEQU 2
CONEQU 3
CONEQU 4
CONEQU 5
CONEQU 6
CONEQU 7
CONEQU 8
CONEQU 9
CONEQU 10
CONEQU 11
CONEQU 12
CONEQU 13
CONEQU 14
CONEQU 15
CONEQU 16
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CONEQU 36
CONEQU 37
CONEQU 38
CONEQU 39
CONEQU 40
CONEQU 41
CONEQU 42
CONEQU 43
CONEQU 44
CONEQU 45
CONEQU 46
CONEQU 47
CONEQU 48
CONEQU 49
CONEQU 50

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SUBROUTINE DENTMP(TEMP,DENS,T)
C *** ORIGINAL SEQUENCING DONE ON 07-11-77
C *** SUBROUTINE DENTMP(TD)
C *** DENTMP(TD) AND DTDATA AND DTINIT NEED TO BE VIEWED TOGETHER.
COMMON/DISCON/IDISC,NCDIS,TDISC(1)
COMMON/TDPROF/TTP1,TTP12,DDN1,DDN12,DDN13,DDN21,DDN22,NCASE,
LNTIML,DENEXP(8),TMPEXP(8),DDDEN(7),DDTEMP(7)
C *** NCASE=1 MEANS NTIML=1 AND NDEN=1, ONLY DISCONTINUITY IS IN NE
C *** AT T=TDSS=TDISC(1).
C *** NCASE=2 MEANS NTIML=1 AND NDEN=2, NO DISCONTINUITIES.
C *** NCASE=3 MEANS NTIML.GT.L AND NDEN=1, 1ST DISCONTINUITY AT
C *** T=TDSS=TDISC(1).
C *** NCASE=4 MEANS NTIML.GT.L AND NDEN=2, 1ST DISCONTINUITY
C *** AT T=STS=TDISC(2).
C *** NCASE=5 MEANS DENSITY AND TEMPERATURE ARE CONSTANT(NDEN=0).
DATA TEO,DENO/.1,1.E4/
C *** SOME OF IONIZATION, RECOMBINATION ROUTINES BLOW UP WITH 0 TEMP, ORDENTMP16
C *** DEN. HENCE ADD A SMALL NUMBER OF APPROPRIATE ORDER.
C *** SUBR. DENTMP(TD), DTDATA, DTINIT MUST HAVE SAME VALUES FOR TEO,DENO.
GO TO (1,2,3,4,5),NCASE
1 TEMP=TTP1*((T*T)/((T*T)+TTP12))+TEO
IF(T.LE.TDISC(1)) GO TO 100
DENS=DDN12*EXP(DDN13*T)
99 RETURN
100 DENS=DDN1*(T+DENO)
GO TO 99
2 TEMP=TTP1*((T*T)/((T*T)+TTP12))+TEO
DENS=DDN2*((T*T)/((T*T)+DDN22))+DENO
GO TO 99
3 IF(T.LE.TDISC(2)) GO TO 1
C *** LINEAR INTERPOLATION USED ON INTERVALS DETERMINED BY TDISC(2)
C *** TDISC(NTIML+1).
101 DO 102 I=2,NTIML
IF(T.GT.TDISC(I+1)) GO TO 102
DT=T-TDISC(I)
DENS=DENEXP(I-1)+DT*DDDEN(I-1)
TEMP=TMPEXP(I-1)+DT*DDTEMP(I-1)
GO TO 99
102 CONTINUE
DENS=DENEXP(NTIML)
TEMP=TMPEXP(NTIML)
GO TO 99
4 IF(T.LE.TDISC(2)) GO TO 2
GO TO 101
5 TEMP=TMPEXP(1)
DENS=DENEXP(1)
GO TO 99
END

```

SUBROUTINE DENTMP(TEA,DENA,T)	DENTMP 1
C *** ORIGINAL SEQUENCING DONE ON 06-09-77	DENTMP 2
C *** SUBROUTINE DENTMP(TI) TEMPERATURE, DENSITY CONSTANT.	DENTMP 3
C *** T IS TIME IN SECONDS (NCH.NE.0)	DENTMP 4
COMMON SHARE,TE,DEN,HMIN,HMAX,EPS,MF,KFLAG,JDISC,NOM,NOM2,NOMP1	DENTMP 5
TEA=TE	DENTMP 6
DENA=DEN	DENTMP 7
RETURN	DENTMP 8
END	

N 3

```

SUBROUTINE DRIVES(NO, TO, TLAST, Y, HO, EPS, MF, KFLAG, SU1Z, SURZ)
C *** ORIGINAL SEQUENCING DONE ON 09-12-77.
DIMENSION Y(1), SU1Z(1), SURZ(1)
C
C DIMENSION Y(NO,1)
COMMON/IO/LOUT, LIN
COMMON/EP5/NCH
COMMON/EO1/T, H, HUSED, NLRC, NKRC, NL, NLPI, NKMI, NK, MXEQMI, JSTART, NO
COMMON/STGY/TF, TFLN, TBLN, FL, BL, DC, BDLOSS, BDLOSH, RDEC, ITDEL, NSTRT,
INDEL, NEQADD, NEQDEL, NEQDMI, BDEL, TSWIT, BDLMM, IPSTGY
COMMON/PRINT/TPRINT, TPRNT(5), DTPRT(5), NPRNT(5), NPRNT1, IPRNT1, NPR
COMMON/SHARE/TE, DEN, HMIN, HMAX, EPSL, MFL, KFLAG, JDISC, NOM, NOM2, NOMPI
COMMON/STRAT/IT, NLB, NKB, ISWSTR, IEQU, MH
COMMON/CONTRL/NZ, NZPI
COMMON/DISCON/IDISC, NCDIS, TDISC(1)
C* THE INPUT PARAMETERS ARE..
C* NO = THE NUMBER OF DIFFERENTIAL EQUATIONS, INITIALLY.
C* TO = THE INITIAL VALUE OF T, THE INDEPENDENT VARIABLE.
C* TLAST = THE FINAL VALUE OF T.
C* Y = AN NO BY LMAX ARRAY FOR THE COMPUTED SOLUTION, THE SAME
C* AS IN STIFF. THE FIRST COLUMN SHOULD CONTAIN THE
C* INITIAL VALUES OF THE DEPENDENT VARIABLE.
C* CURRENTLY, LMAX IS 13 FOR THE ADAMS METHODS AND
C* 6 FOR THE GEAR METHODS. TO CHANGE THIS, SEE
C* SUBROUTINE TESOC.
C* HO = THE INITIAL VALUE OF H, THE STEP SIZE IN T.
C* EPS = THE RELATIVE ERROR BOUND, THE SAME AS IN STIFF.
C* MF = THE METHOD FLAG, THE SAME AS IN STIFF.
C* ALLOWED VALUES ARE 10, 11, 12, 13, 20, 21, 22, 23.
C *** THIS ADAPTATION REQUIRES MF=2
C* THE OUTPUT PARAMETERS ARE..
C* T = VALUE OF T TO WHICH INTEGRATION HAS BEEN COMPLETED.
C* Y = NO BY LMAX ARRAY OF Y AND ITS SCALED DERIVATIVES.
C* Y(1) FOR I.LE. I.LE. N CONTAINS THE COMPUTED SOLUTION
C* AT TIME T.
C* HUSED = THE VALUE OF THE STEP SIZE H USED LAST TO GET TO CURRENT
C *** H=PROPOSED NEXT STEPSIZE BY SUBR.STIFF, DERIVATIVES IN Y ARRAY
C *** SCALED BY THIS H. USER MAY ALTER H, BUT MUST SET JSTART=-1
C *** HOLD=STEPSIZE THAT DERIVATIVES IN Y ARRAY ARE SCALED BY. DEFINED
C *** LOCALLY IN STIFF. RESCALING OF DERIVATIVES IS DONE IN STIFF.
C* KFLAG = A COMPLETION FLAG WITH THE FOLLOWING VALUES AND MEANINGS.
C* 0 THE PROBLEM WAS COMPLETED SUCCESSFULLY.
C* -1 THE INTEGRATION WAS HALTED AFTER FAILING TO PASS THE
C* ERROR TEST EVEN AFTER REDUCING H BY A FACTOR OF
C* 1.0D10 FROM ITS INITIAL VALUE.
C* -2 AFTER SOME INITIAL SUCCESS, THE INTEGRATION WAS
C* HALTED WHEN A REDUCTION IN H BY A FACTOR OF MORE
C* THAN 1.0D4 WAS INDICATED IN ORDER TO PASS THE ERROR TEST.
C* -3 THE INTEGRATION WAS HALTED AFTER FAILING TO ACHIEVE
C* CORRECTOR CONVERGENCE EVEN AFTER REDUCING H BY A
C* FACTOR OF 1.0D10 FROM ITS INITIAL VALUE.
C* -4 IMMEDIATE HALT BECAUSE OF ILLEGAL VALUES OF INPUT
C* PARAMETERS. SEE PRINTED MESSAGE.
C* -5 H IS SUCH THAT T+H.EQ. T
C* DRIVES CALLS SUBROUTINE YOUT FOR NORMAL OUTPUT
C* AND SUBROUTINE YOUTD FOR OUTPUT IN CASE OF FAILURE BELOW 150 AND 200.
C* THE NAMES AND CALL SEQUENCES OF THESE CAN BE ALTERED AS DESIRED.

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C* IN THE FOLLOWING, SET..
C* LOU = THE LOGICAL UNIT NUMBER FOR THE OUTPUT OF MESSAGES
C* DURING THE INTEGRATION.
C* THE ORIGINAL VERSION OF THIS PROGRAM WAS WRITTEN AT LL BY A. C.
C* HINDMARSH FOR CDC COMPUTERS. THE CDC VERSION WAS MODIFIED FOR
C* USE ON IBM COMPUTERS AT ARGONNE IN JUNE, 1973.
C* LATEST REVISION SEPTEMBER, 1973
C *** DATE OF REVISION FROM ARGONNE IS 9/73.
C *** PROG. FROM ARGONNE TAILORED FOR THE LINEAR SYSTEM DESCRIBING THE
C *** CHARGE STATE DISTRIBUTION VECTOR, DONE FOR E.C. CRUME OF
C *** THERMONUCLEAR. (FUSION ENERGY) (VERSION DATE = 3/25/77).
C **
C *** TO,TF=TLAST,H0,TPRINT,TDISC(1) ARE IN UNITS OF SEC..
C *** THE TIME UNIT OF THE SYSTEM OF ODE'S IS SECONDS.
C *** Y'=DEN*XY, Y=Y(T0) IS SET IN SUBR.YINIT.
C *** J-TH ORDER STIFF METHOD REQUIRES (J-1)-TH DERIVATIVE OF FCN.
C *** DEN AND TE TO BE CONTINUOUS. MAX. ORDER STIFF METHOD IS 5 AND
C *** THIS IS SET IN SUBR.TESOC. MAY NEED TO DEFINE THIS LOWER FOR SOME
C *** APPROXIMATING FCNS. TO DEN AND TE.
C *** IF IDISC=0, THEN FCNS, DEN AND TE ARE SUFFICIENTLY SMOOTH FOR THE
C *** ORDER 5 METHOD.
C *** IF IDISC.NE.0, THEN AT TDISC(1) THE 1ST DISCONTINUITY IS
C *** ENCOUNTERED. ORDER OF STIFF IS SET TO 1 AT TDISC(1) AND PROG.
C *** CONTINUES. ON (T0,TDISC(1)) WILL ALLOW ORDER TO GO TO 5 AS WELL AS
C *** ON (TDISC(1),TDISC(2)). IF HAVE J DISCONTINUITIES, THEN DEFINE
C *** TDISC(J+1)=1.E10.
C *** SETTING ORDER TO 1 MEANS THE DERIVATIVE OF DEN OR TE IS REGARDED
C *** TO BE DISCONTINUOUS AT THAT POINT.
C ***
C *** PRIOR TO CALL DRIVES MUST DEFINE VARIABLES NZ,NZPI=NZ+1,
C *** ,NL,NK,TDISC,NCDIS, AND TDISC(1). NL,NK DEFINED IN SUBR.YINIT.
C *** FOR PROGTD TDISC,NCDIS,TDISC(1) ARE INITIALIZED IN SUBR.DTINIT
C *** FOR PROGT MAIN(T) SETS TDISC=0. (DON'T NEED NCDIS,TDISC IF =0)
C *** IF (EPS.LE.0.) GO TO 400
C *** IF (NO.LE.0.) GO TO 410
C *** IF ((T0-TLAST)*H0.GE.0.) GO TO 420
C ***
C *** IT=0
C *** IDISC=0
C *** T = T0
C *** H = H0
C *** HMIN = ABS(H0)
C *** BEGIN INITIALIZATION FOR STRATEGY II, ISWSTR=2
C *** INCLUDES THAT FOR ISWSTR=1
C *** SURZ(0)=0.
C *** SUIZ(NZ+1)=0.
C *** ITDEL=NSTRT
C *** CALL DENTHP(TE,DEN,T)
C *** CALL SUIONZ(SUIZ,TE,DEN)
C *** CALL SURECZ(SURZ,TE,DEN)
C *** FL=0.
C *** BL=0.
C *** DL=0.
C *** TFLN=DEN*SURZ(NL-1)*Y(NL)
C *** TBLN=DEN*SUIZ(NK)*Y(NK)
C *** END INITIALIZATION FOR STRATEGY II, ISWSTR=2

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C *** IF=LAST
      NQ=0, HUSED=0. IN EVENT CALL YOUT AT T=TD.
      NQ=0
      HUSED=0.
      C *** INITIALIZE IPRINT FOR USE IN SUBR YOUT
      IPRINT=1
      TPRINT=TPRNT(1)/1000.
      HMAX = ABS(TD-TLAST) * .1
      HMIN = AMIN(HMIN, .1*HMAX)
      EPSL = EPS
      MFI = MF
      JSTART = 0
      KFLAG = 0
      C *** MAY WISH TO PRINT INITIAL VALUES THRU YOUT
      IF(T.EQ.TPRINT) CALL YOUT(Y,NO,1)
      10 CONTINUE
      IF(IDISC.EQ.0) GO TO 11
      C *** JDISC=0 IMPLIES NO DISCONTINUITIES IN NE OR IN TE OR THEIR DERIV.
      C *** MOREOVER, MAIN(T) DEFINES IDISC=0
      IF(T+H.LT.TDISC(NCDIS)) GO TO 11
      C *** TDISC INITIALIZED IN SUBR. DTIMIT
      HOLD=H
      H=TDISC(NCDIS)-T
      HSAVE=H
      JDISC=1
      JSTART=-1
      11 CALL STIFF(Y,NO)
      NQ = JSTART
      KGO = 1 - KFLAG
      GO TO ( 20,100,200,300,20,350), KGO
      C KFLAG = 0, -1, -2, -3, -5
      20 IF(T.GE.TPRINT) CALL YOUT(Y,NO,NQ)
      IF(JDISC.EQ.0) GO TO 21
      JDISC=0
      IF(HUSED.LT.HSAVE) GO TO 21
      JSTART=0
      C *** SET INTEGRATION ORDER TO 1, HAVE DISCONTINUITY IN 2ND DERIVATIVE.
      H=HOLD/(1+(NQ-1)*MH)
      NQ=1
      C *** SET NQ=1 IN EVENT THAT CHANGE COMPOSITION OF ACTIVE EQUATIONS.
      C *** SINCE THEN H=H/(1+(NQ-1)*MH)=H.
      NCDIS=NCDIS+1
      C *** HUSED=LAST STEP SIZE USED TO GET TO CURRENT T
      C *** H=SUBR.STIFF'S NEXT PROPOSED STEP SIZE. DERIVATIVES ARE SCALED
      C *** WITH THIS VALUE. USER MAY REDEFINE IT (BUT MUST ALSO REDEFINE
      C *** JSTART)
      21 IF(NCH.LE.0) GO TO 900
      C *** ONLY CALL CONEQU IF HAVE AN EQUILIBRIUM VECTOR. MUST HAVE TE AND
      C *** NE CONST. NOK.NE.0 MEANS CONVRG WITH LAST CONVRG PARA ESTABLISHED
      CALL CONEQU(Y,NZPI,NOK)
      IF(NOK.NE.0) GO TO 500
      900 IT=IT+1
      C *** SUBR. STRATG MAY ALTER THE CURRENT SET OF ACTIVE DIFFERENTIAL
      C *** EQUATIONS. ACTIVE ONES ARE NL THRU NK. COMPUTE RATE COEFFS.
      C *** FROM SPECTROSCOPIC STATE NLRC THRU NKRC.
      GO TO (81,82),15HSTR
      82 CALL STRATG(Y,SU1Z,SURZ)

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81 IF ((T-TLAST)*H .LT. 0.) GO TO 10
GO TO 500
100 CONTINUE
C100 WRITE (LOUT,105) T
C105 FORMAT(//30H KFLAG = -1 FROM STIFF AT T = ,D25.16/
C 30H ERROR TEST FAILED WITH ABS(H) = HMIN/)
110 IF (KHFLAG .EQ. 10) GO TO 150
KHFLAG = KHFLAG + 1
HMIN = HMIN * .1
H = H * .1
C WRITE (LOUT,115) H
C115 FORMAT(24H H HAS BEEN REDUCED TO ,D25.16,
C 26H AND STEP WILL BE RETRIED//)
JSTART = -1
GO TO 10
150 WRITE (LOUT,155)
155 FORMAT(//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)
C* HMIN HAS BEEN CUT BY 10 ORDERS OF MAGNITUDE WITH NO SUCCESS.
C* AT THIS POINT, OUTPUT INFORMATION NEEDED FOR DEBUGGING
CALL YOUTD(Y,NQ)
GO TO 500
200 WRITE (LOUT,205) T,H
205 FORMAT(//30H KFLAG = -2 FROM STIFF AT T = ,D25.16,5H H = ,D25.16/
52H THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)
C* AT THIS POINT, OUTPUT INFORMATION NEEDED FOR DEBUGGING
CALL YOUTD(Y,NQ)
GO TO 500
C *** SINCE SYSTEM IS LINEAR AND STIFF TAKES ADVANTAGE OF THIS,
C *** CORRECTOR CONVERGES IN 1 STEP, HENCE NEVER ARRIVE AT 300.
300 WRITE (LOUT,305) T
305 FORMAT(//30H KFLAG = -3 FROM STIFF AT T = ,D25.16/
45H CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED//)
GO TO 110
350 WRITE (LOUT,355) T,H
355 FORMAT(//30H KFLAG = -5 FROM STIFF AT T = ,D25.16,
5H H = ,D25.16/
2 45H H IS SUCH THAT T+H .EQ. T ON MACHINE.
CALL YOUTD(Y,NQ)
GO TO 500
400 WRITE (LOUT,405)
405 FORMAT(//28H ILLEGAL INPUT.. EPS .(LE. 0.//)
KFLAG = -4
RETURN
410 WRITE (LOUT,415)
415 FORMAT(//25H ILLEGAL INPUT.. N .(LE. 0.//)
KFLAG = -4
RETURN
420 WRITE (LOUT,425)
425 FORMAT(//38H ILLEGAL INPUT.. (T0-TLAST)*H0 .GE. 0.//)
KFLAG = -4
RETURN
500 KFLAG = KFLAG1
RETURN
END

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SUBROUTINE DTDATA(IR,NOIR,DENI,TEA,TDCON,NTLAS,NDEN,DNI,
C *** ORIGINAL SEQUENCING DONE ON 07-11-77
I DN12,DN13,DN21,DN22,TP11,TP12)
C *** ALL ARGUMENTS TO DTDATA ARE OUTPUT ARGUMENTS EXCEPT IR
C *** DIMENSION DENI(1),TEA(1),TDCON(1)
C *** DIMENSION DENE(32),TEE(32),CNE(8),TDISCM(9)
C *** COMMON/IO/LOUT,LIN
C *** COMMON/DISCON/IDISC,NCDIS,TDISC(10)
C *** CALLED BY MAINI(TD), MUST LOOK AT DTDATA,DTINIT, AND DENTMP(TD)
C *** TOGETHER.
C *** MAINI(TD) CALLS DTDATA, DENI,TEA,TDCON ARE DIMENSIONED THERE.
C *** LOGICALLY REQUIRE DIMENSION DENI(NTLAS),TEA(NTLAS),TDCON(NTLAS+1)
C *** SPACE DEFN. FOR ARRAY TDISC MADE HERE. REQUIRE DIM. OF AT LEAST
C *** TDISC(NTLAS+2)
C *** ARRAYS DIMENSIONED SO THAT NTLAS.LE.8 IS ALLOWED.
C *** DIMENSIONALLY NEED DENE(NOIR*NTLAS),TEE(NOIR*NTLAS),CNE(NTLAS),
C *** TDISCM(NTLAS+1)
C *** USE DATA STATEMENT FOR DEFN. OF NEEDED VALUES AND DATA.
C *** NTLAS=NUMBER OF LASER SHOTS
C *** NOIR=NUMBER OF RADIAL POSITIONS ASSOCIATED WITH THE LASER SHOTS.
C *** THE SINGLY DIMENSIONED EXPERIMENTAL DATA ARRAY DENE MAY BE
C *** REGARDED AS THE 2-DIMENSIONAL ARRAY DENE(IR,IT) WHERE IR POINTS
C *** TO THE RADIAL POSITION R(IR) AND IT TELLS THE ASSOCIATED LASER
C *** SHOT. HERE IR=1,2,...,NOIR AND IT=1,...,NTLAS. LOGICALLY THE
C *** DIMENSION OF DENE AS A 2-DIM. ARRAY IS DENE(NOIR,NTLAS). SIMILARLY
C *** FOR THE EXPERIMENTAL DATA ARRAY TEE THAT CONTAINS TEMPERATURE
C *** ESTIMATES IN UNITS OF EV.
C *** DENE(IR,IT) IS THE DENSITY ESTIMATE AT RADIAL POSITION IR FOR THE
C *** LASER SHOT ASSOCIATED WITH IT DIVIDED BY THE FACTOR CNE(IT).
C *** THUS THE RECORDED DENSITY PROFILE FOR A SHOT IS SCALED BY THE
C *** FACTOR CNE(IT). DENSITIES FOR PROGRAM TO BE IN UNIT OF 1/CM**3
C *** THE TIMES OF THE LASER SHOTS ARE GIVEN IN MILLISEC. AND THE
C *** IT-TH SHOT TIME IS RECORDED IN TDISCM(IT+1), INTO TDISCM(1) IS
C *** PLACED THE TIME TDS WHENEVER IT IS NEEDED. HOWEVER,
C *** TDISCM(1) MAY NOT BE USED FOR OTHER INFORMATION BESIDES TDS.
C *** TDS IS USED IN DEFN. OF ANALYTIC EXPRESSION FOR DENSITY TO BE USED
C *** ON (0,TDISCM(2)) WHENEVER NDENA=1, NDENA DEFINED IN DATA STATEMENT
C *** TDISCM STANDS FOR TIME DISCONTINUITY IN MILLISEC. THIS VERSION
C *** USES LIN. INTERPOLATION BETWEEN SHOT TIMES FOR ESTIMATING THE
C *** TEMPERATURE AND DENSITY. THUS, IN GENERAL, AT EACH OF THE SHOT
C *** TIMES THE 1ST DERIVATIVES OF THE APPROXIMATING FUNCTIONS FOR THE
C *** TEMPERATURE AND DENSITY ARE DISCONTINUOUS. THUS AT THESE POINTS
C *** THE NORMALIZED CHARGE STATE DISTRIBUTION VECTOR WILL NOT HAVE A
C *** CONTINUOUS 2ND DERIV. SINCE THE STIFF INTEGRATION ROUTINE ALLOWS
C *** THE ORDER OF THE METHOD TO INCREASE TO 5, THE ORDER OF THE METHOD
C *** NEEDS TO BE SET TO 1 AT EACH OF THE LASER SHOT TIMES. MOREOVER, ONE
C *** OF THE ANALYTIC MODELS FOR DESCRIBING THE DENSITY BEFORE THE TIME
C *** OF THE 1ST SHOT HAS ITS DERIVATIVE DISCONTINUOUS AT TDS WHICH IS
C *** STORED IN TDISCM(1).
C *** N.B., THE ORDER OF THE STIFF INTEGRATION METHOD MUST BE CONSISTENT
C *** WITH THE SMOOTHNESS OF THE EQS. THE SMOOTHNESS OF THE EQS. IS
C *** ASSOCIATED WITH THE COEFF. MATRIX OF THE SYSTEM, HENCE TO THE
C *** DENSITY AND THE RATE COEFFICIENTS.
C *** SUBR.DRIVES USES TDCON=TDISCM/1000. IN ORDER TO LAND RIGHT ON TOP
C *** OF A POINT OF DISCONTINUITY, DRIVES SETS ORDER OF STIFF METHOD
C *** TO 1 AS PASS BEYOND THE POINT OF DISCONTINUITY. CF. SUBR.DRIVES.
C *** ST=TDISCM(2)=TIME OF 1ST LASER IN MILLISECONDS.
C *** TDEL,TR,DDT,TDS,TDISCM(1) IN MILLISEC.

```

```

C *** TDSS, TDCON IN SEC. DTDATA58
C *** SYSTEM OF DIFF. EQS. DESCRIBING THE CHARGE STATE DISTRIBUTION DTDATA59
C *** VECTOR ARE EXPRESSED IN TIME UNIT OF SECONDS. DTDATA60
DATA TDEL/10., TR/10., DDT/5. DTDATA61
DATA DENE/5., 2. DTDATA62
1 4.9, 1.9, .9, DTDATA63
2 4.4, 1.4, .4, DTDATA64
DATA CNE/1.E13, 1.E12, 1.E11 DTDATA65
DATA TEE/500., 200., 10., DTDATA66
1 410., 120., 10., DTDATA67
2 360., 105., 10., DTDATA68
DATA TDISCH/5., 15., 30., 45., NTLAS/1., NOIR/3. DTDATA69
DATA NDENA/2. DTDATA70
DATA TED, DENO/1., 1.E4 DTDATA71
C *** IR IS A LOOPING INDEX AND IT IS EXPECTED TO RANGE OVER VALUES DTDATA72
C *** 1, ..., NOIRA=NOIR. NOTE THAT NOIRA IS DEFINED HERE ON 1ST CALL TO DTDATA73
C *** DTDATA, MOREOVER, NOIR DETERMINES THE LOGICAL PARTITIONING OF THE DTDATA74
C *** ARRAYS TEE AND DENE. DTDATA75
NDEN=NDENA DTDATA76
C *** 3 ANALYTIC MODELS FOR ESTIMATING THE DENSITY ON (0, TDISCH(2)) ARE DTDATA77
C *** AVAILABLE. THE MODEL IS SELECTED BY THE VALUE OF THE PARA, NDEN. DTDATA78
C *** MODEL 1, NDEN=0. HERE DENSITY AND TEMPERATURE ARE TIME INDEPENDENT DTDATA79
C *** FOR ALL TIME WITH VALUES GN. BY DENSITY=CNE(I)*DENE(IR) AND DTDATA80
C *** TEMPERATURE=TEE(IR). DTDATA81
C *** MODEL 1L, NDEN=L. DENSITY(T)=CNE(I)*DENE(IRS)*DID*T/TDSS+D WHERE DTDATA82
C *** D=DENO, DID=EXP(LN(2)*(ST-TDS)/DDT), TDSS=TDS/1000, ST=TDISCH(2), DTDATA83
C *** TDS=TDISCH(1) ON THE INTERVAL (0, TDS). D INCLUDED TO MAKE DENSITY DTDATA84
C *** NONZERO. NEEDED IN SOME RATE COEFF. ROUTINES. ON THE INTERVAL DTDATA85
C *** (TDS, TDISCH(2)) DENSITY(T)=CNE(I)*DENE(IRS)*EXP((LN(2)/DDT)* DTDATA86
C *** (ST-1000*T)). RECALL T IS IN SECONDS. DTDATA87
C *** MODEL 111, NDEN=2. DENSITY(T)=CNE(I)*DENE(IRS)*(1+(TDEL/ST)**2)* DTDATA88
C *** T**2/(T**2+(TDEL/1000)**2)+D WHERE D=DENO. DTDATA89
C *** WHEN NTLAS=1, THEN AN ANALYTIC MODEL IS USED FOR WHOLE TIME DTDATA90
C *** INTEGRATION. THE ANALYTIC FORM THAT IS USED JUST PRIOR TO DTDATA91
C *** TDISCH(2) IS USED FOR LATER TIMES. DTDATA92
C *** SUBR.DENTHP(TD), DTDATA, DTINIT MUST HAVE SAME VALUES FOR TED, DENO. DTDATA93
IF(NTLAS.LE.8) GO TO 200 DTDATA94
WRITE (LOUT, 50) NTLAS DTDATA95
50 FORMAT('D***** SUBR.DTDATA, REQUIRE NTLAS.LE.8 FOR STORAGE. HAVE NDTDATA96
ITLAS='12, 2X'REDEFINED NTLAS=8') DTDATA97
NTLAS=8 DTDATA98
200 NOIRA=NOIR DTDATA99
NTIML=NTLAS DTDATA 0
IRS=IR DTDATA 1
DO 1 I=1, NTLAS DTDATA 2
TEA(I)=TEE(IRS) DTDATA 3
DENE(I)=CNE(I)*DENE(IRS) DTDATA 4
1 IRS=IRS+NOIR DTDATA 5
C *** MAY WISH TO WRITE OUT THE EXPERIMENTAL DATA ASSOCIATED WITH IR. DTDATA 6
M=NTLAS+1 DTDATA 7
DO 2 I=1, M DTDATA 8
C *** TIME UNIT OF DIFF. EQS. IN SECONDS, YET MANY OF DATA TIMES ARE DTDATA 9
C *** GIVEN IN MILLISECONDS. DTDATA10
2 TDCON(I)=TDISCH(I)/1000. DTDATA11
TDS=TDISCH(1) DTDATA12
TDSS=TDCON(I) DTDATA13
ST=TDISCH(2) DTDATA14
DID=EXP(.693147*(ST-TDS)/DDT) DTDATA15

```

```

C *** LN(2)=.693147
TP11=1.+(TR/ST)**2
TRS=TR/1000.
TP12=TRS**2.
70 NDENP1=NDEN+1
GO TO (10,11,12),NDENP1
11 DNI1=DID/TDSS
DNI2=EXP(.693147*(ST/DDT))
DNI3=.693147/DDT
GO TO 20
12 DN21=L+(TDEL/ST)**2
DN22=(TDEL/1000.)*2
GO TO 20
10 CONTINUE
20 WRITE(LOUT,250) IR,NDEN,(TDCON(I+1),I=1,NTLAS)
250 FORMAT(' EXPERIMENTAL DATA',10X' LOOP INDEX IR='12,10X' DENSITY MODE
L, NDEN='11/' T(SEC)='1P12E10,2)
WRITE(LOUT,251) (DENI(I),I=1,NTLAS)
251 FORMAT(' DEN(I)='1P12E10,2)
WRITE(LOUT,252) (TEA(I),I=1,NTLAS)
252 FORMAT(' TE(I)='1P12E10,2)
IF(NDEN.GT.0) GO TO 253
WRITE(LOUT,254)
254 FORMAT(' TE, DEN ARE CONSTANT WITH VALUES OF DATA ABOVE.')
GO TO 401
253 TST=TDCON(2)
IF(NTLAS.EQ.1) TST=1.E10
WRITE(LOUT,255) TST,TEA(1),TE0,TR,ST
255 FORMAT(' ON (0,'1PE8,2,') TE(T)=(TMPEXP(1)-TE0)*(1+(TR/ST)**2)*
1*2/(1**2+(TR/1000)**2)+TE0, TMPEXP(1)='E8,2,2X' TE0='0PF4,2,2X' TR=
2F4,1,2X' ST='F4,1)
GO TO (256,257),NDEN
256 WRITE(LOUT,258) TDSS,DENI(1),DID,DENO
258 FORMAT(' ON (0,TDSS='1PE8,2,') DEN(T)=((DENEXP(1)*DID-DENO)/TDSS)*
1T+DENO, DENEXP(1)='E8,2,2X' DID='E8,2,2X' DENO='E8,2)
WRITE(LOUT,259) TST,ST,DDT
259 FORMAT(' ON (TDSS,'1PE8,2,') DEN(T)=DENEXP(1)*EXP(LN(2)*(ST-1000T
1/DDT), ST='0PF5,2,2X' DDT='F5,2)
GO TO 402
257 WRITE(LOUT,260) TST,DENI(1),DENO,TDEL,ST
260 FORMAT(' ON (0,'1PE8,2,') DEFINE'
1' DEN(T)=(DENEXP(1)-DENO)*(1+(TDEL/ST)**2)*1*2/(1**2+(TDEL/1000)**
22)+DENO, DENEXP(1)='E8,2,2X' DENO='E8,2,2X' TDEL='0PF4,1,2X' ST='F4,
3)
402 IF(NTLAS.EQ.1) GO TO 401
WRITE(LOUT,261)
261 FORMAT(' LIN. INTERPOLATION USED AT TIMES WITHIN TABLE OF EXP. DATA
1VALUES. LAST EXP. VALUE USED FOR TIMES .GT. THOSE OF TABLE.')
401 RETURN
END

```

SUBROUTINE DTINIT(ENE,TEE,TDCON,NDEN,DDN1,DDN2,DDN3,DDN22,DDN22,DTINIT1

C *** ORIGINAL SEQUENCING DONE ON 07-11-77

I TPI1,TPI2,NTLAS)

DIMENSION ENE(1),TEE(1),TDCON(1)

COMMON/LO/LOUT,LIN

COMMON/DISCON/IDISC,NCDIS,TDISC(1)

COMMON/TPROF/TPI1,TPI2,DDN1,DDN2,DDN3,DDN22,NCASE

I NTIML,DENEXP(8),TMPEXP(8),DDEN(7),DDTEMP(7)

C *** CALLED BY MAIN(TD). MUST LOOK AT DTDATA,DTINIT, AND DENTMP(TD)

C *** TOGETHER.

C *** NCDIS POINTS TO NEXT DISCONTINUITY, OCCURS AT T=TDISC(NCDIS)

C *** SET TDISC(NTIML+2)=1.E10 SAYS LAST DISCONTINUITY AT TDISC(NTIML+1)

C *** THIS VERSION GENERATED ON (3/22/77)

C *** RECEIVES AND PROCESSES THE DATA TO BE USED TO GENERATE THE NEXT

C *** TEMPERATURE AND DENSITY PROFILE.

C *** NTLAS=NO. OF LASER TIMES.

C *** TDCON=(POSSIBLE) DISCONTINUITIES IN TIME UNITS OF SEC.

C *** NDEN=SWITCH TO SELECT ANALYTIC MODEL FOR DENSITY FOR EARLY TIME.

C *** NDEN=0 MEANS NE AND TE ARE EACH CONSTANT.

C *** ENE(1) AND TEE(1) ARE THE EXPERIMENTAL VALUES FOR THE DENSITY AND

C *** TEMPERATURE ASSOCIATED WITH THE LASER TIME RECORDED IN TDCON(1+1).

C *** SPACE IS RESERVED FOR TDSS IN TDCON(1) EVEN WHEN NOT USED

DATA TEO,DENO,L,L4/

C *** SUBR.DENTMP(TD),DTDATA,DTINIT MUST HAVE SAME VALUES FOR TEO,DENO.

IDISC=1

C *** IDISC=0 MEANS NO DISCONTINUITY IN DERIVATIVES OF NE AND TE(DRIVES)

TDISC(1)=TDCON(1)

NTIML=NTLAS

IF(NTIML.GT.1) GO TO 100

TMPEXP(1)=TEE(1)

DENEXP(1)=ENE(1)

IF(NDEN.EQ.0) GO TO 500

GO TO (1,2),NDEN

1 NCASE=1

NCDIS=1

C *** HAVE DISCONTINUITY IN NE? AT T=TDSS=TDCON(1), SET NCDIS=1.

TDISC(2)=1.E10

GO TO 300

2 NCASE=2

IDISC=0

GO TO 300

100 DO 200 T=T,NTLAS

DENEXP(1)=ENE(1)

TMPEXP(1)=TEE(1)

200 TDISC(1+1)=TDCON(1+1)

IF(NDEN.EQ.0) GO TO 500

TDISC(NTLAS+2)=1.E10

J=NTLAS-1

DO 20 I=1,J

C *** USING LINEAR INTERPOLATION WITHIN SHOT INTERVALS (3/22/77)

DELT=TDISC(1+2)-TDISC(1+1)

DDEN(1)=(DENEXP(1+1)-DENEXP(1))/DELT

20 DDTEMP(1)=(TMPEXP(1+1)-TMPEXP(1))/DELT

GO TO (1,12),NDEN

11 NCASE=3

NCDIS=1

GO TO 300

12 NCASE=4

```

NCDIS=2
C *** COMBINE CONSTANT FACTORS FOR THE ANALYTIC MODELS.
300 TPI1=TP11*(THPEXP(1)-TE0)
    TPI2=TP12
    GO TO (21,22),NDEN
21 DDN11=DN11*DENEXP(1)-DEN0/TDISC(1)
C *** TDISC(1)=TD55
    DDN12=DN12*DENEXP(1)
    DDN13=-DN13
    GO TO 400
22 DDN21=DN21*(DENEXP(1)-DEN0)
    DDN22=DN22
400 RETURN
500 NCASE=5
C *** TE, DEN ARE CONSTANT FOR ALL TIME.
    TDISC=0
    GO TO 400
END
```

```

DTINIT58
DTINIT59
DTINIT60
DTINIT61
DTINIT62
DTINIT63
DTINIT64
DTINIT65
DTINIT66
DTINIT67
DTINIT68
DTINIT69
DTINIT70
DTINIT71
DTINIT72
DTINIT73
DTINIT74
DTINIT75
```

SUBROUTINE INTQL(N,D,E,IERR)

INTQL L

C *** ORIGINAL SEQUENCING DONE ON 06-08-77

C *** CHANGED FROM DOUBLE PRECISION TO SINGLE PRECISION (5/12/77).

REAL D(N),E(N),MACHEP

C THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE INTQL

C NUM. MATH. 12, 377-383(1968) BY MARTIN AND WILKINSON,

C AS MODIFIED IN NUM. MATH. 15, 450(1970) BY DUBRULLE.

C HANDBOOK FOR AUTO. COMP., VOL.11-LINEAR ALGEBRA, 241-248(1971).

C THIS SUBROUTINE FINDS THE EIGENVALUES OF A SYMMETRIC

C TRIANGULAR MATRIX BY THE IMPLICIT QL METHOD.

C ON INPUT:

C N IS THE ORDER OF THE MATRIX;

C D CONTAINS THE DIAGONAL ELEMENTS OF THE INPUT MATRIX;

C E CONTAINS THE SUBDIAGONAL ELEMENTS OF THE INPUT MATRIX
C IN ITS LAST N-1 POSITIONS. E(1) IS ARBITRARY.

C ON OUTPUT:

C D CONTAINS THE EIGENVALUES IN ASCENDING ORDER. IF AN
C ERROR EXIT IS MADE, THE EIGENVALUES ARE CORRECT AND
C ORDERED FOR INDICES 1,2,...,IERR-1, BUT MAY NOT BE
C THE SMALLEST EIGENVALUES;

C E HAS BEEN DESTROYED;

C IERR IS SET TO

C ZERO

C FOR NORMAL RETURN,

C IF THE J-TH EIGENVALUE HAS NOT BEEN

C DETERMINED AFTER 30 ITERATIONS.

C QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARROW,
C APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORYC JUUUUU MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING
C THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC.

C MACHEP = 16.000**(-13) FOR LONG FORM ARITHMETIC

C ON 5360

C *** MACHEP=16**(-5) FOR SINGLE PREC. ON IBM 360.

C *** MACHEP=16**(-6)/16**(-1) WHERE NUMERATOR INDICATES ERROR OF 1 IN LAST

C *** HEX DIGIT AND DENOMINATOR IS SMALLEST NORMALIZED FRACTION.

C DATA MACHEP/23C100000/

C *** DATA MACHEP/234100000000000000/

C IERR = 0

C IF (N.EQ. 1) GO TO 1001

C DO 100 I = 2, N

C 100 E(I-1) = E(I)

C E(N) = 0.0

INTQL 2

INTQL 3

INTQL 4

INTQL 5

INTQL 6

INTQL 7

INTQL 8

INTQL 9

INTQL 10

INTQL 11

INTQL 12

INTQL 13

INTQL 14

INTQL 15

INTQL 16

INTQL 17

INTQL 18

INTQL 19

INTQL 20

INTQL 21

INTQL 22

INTQL 23

INTQL 24

INTQL 25

INTQL 26

INTQL 27

INTQL 28

INTQL 29

INTQL 30

INTQL 31

INTQL 32

INTQL 33

INTQL 34

INTQL 35

INTQL 36

INTQL 37

INTQL 38

INTQL 39

INTQL 40

INTQL 41

INTQL 42

INTQL 43

INTQL 44

INTQL 45

INTQL 46

INTQL 47

INTQL 48

INTQL 49

INTQL 50

INTQL 51

INTQL 52

INTQL 53

INTQL 54

INTQL 55

INTQL 56

INTQL 57

DO 200 L = L, N

J = 0

C LOOK FOR SMALL SUB-DIAGONAL ELEMENT

105 DO 110 M = L, N

IF (M.EQ.N) GO TO 120

IF (ABS(E(M)) .LE. MACHEP * (ABS(D(M)) + ABS(D(M+1))))

X GO TO 120

110 CONTINUE

C 120 P = D(L)

IF (M.EQ.L) GO TO 215

IF (J.EQ.30) GO TO 1000

J = J + 1

C FORM SHIFT

G = (D(I+1) - P) / (2.0 * E(L))

R = SQRT(G*G+1.0)

G = D(M) - P + E(L) / (G + SIGN(R,G))

S = 1.0

C = L.0

P = 0.0

MML = M - L

C FOR I=M-1 STEP -1 UNTIL L DO --

DO 200 J = L, MML

I = M - 1

F = S * E(I)

B = C * E(I)

IF (ABS(F) .LT. ABS(G)) GO TO 150

C = G / F

R = SQRT(C*C+1.0)

E(I+1) = F * R

S = 1.0 / R

C = C * S

GO TO 160

150 S = F / G

R = SQRT(S*S+1.0)

E(I+1) = G * R

C = 1.0 / R

S = S * C

160 G = D(I+1) - P

R = (D(I) - G) * S + 2.0 * C * B

P = S * R

D(I+1) = G + P

G = C * R - B

200 CONTINUE

C D(L) = D(L) - P

E(L) = G

E(M) = 0.0

GO TO 105

C ORDER EIGENVALUES

215 IF (L.EQ.1) GO TO 250

C FOR I=L STEP -1 UNTIL 2 DO --

DO 230 J = 2, L

I = L + 2 - J

IF (P.GE.D(I-1)) GO TO 270

D(I) = D(I-1)

230 CONTINUE

C

INTOL 158

INTOL 159

INTOL 160

INTOL 161

INTOL 162

INTOL 163

INTOL 164

INTOL 165

INTOL 166

INTOL 167

INTOL 168

INTOL 169

INTOL 170

INTOL 171

INTOL 172

INTOL 173

INTOL 174

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INTOL 200

INTOL 201

INTOL 202

INTOL 203

INTOL 204

INTOL 205

INTOL 206

INTOL 207

INTOL 208

INTOL 209

INTOL 210

INTOL 211

INTOL 212

INTOL 213

INTOL 214

INTOL 215

250 L = L
270 D(I) = P
290 CONTINUE

INTQL116
INTQL117
INTQL118
INTQL119
INTQL120
INTQL121
INTQL122
INTQL123
INTQL124
INTQL125
INTQL126

C GO TO 1001
C : : : : : SET ERROR -- NO CONVERGENCE TO AN
C : : : : : EIGENVALUE AFTER 30 ITERATIONS : : : : :
1000 TERR = L
1001 RETURN
C : : : : : LAST CARD OF INTQL1 : : : : :
END

	SUBROUTINE INTEGC(TSTART,TLAST,TEQU,KFLAG,SUIZ,SURZ,EPS,H0)	INTEGC 1
C ***	ORIGINAL SEQUENCING DONE ON 06-08-77	
	DIMENSION SUIZ(1),SURZ(1)	INTEGC 2
	COMMON/EP5/NCH,NEQU	INTEGC 3
	COMMON/EQ1/T	INTEGC 4
	COMMON/YFCN/Y(1)	INTEGC 5
	COMMON/CONTRL/NZ,NZPI	INTEGC 6
C ***	DIFFERENTIAL EQUATIONS EXPRESSED IN SECONDS.	INTEGC 7
C ***	EXTERNAL TIMES IN MILLISECONDS.	INTEGC 8
	DATA TCONUT/1000./	INTEGC 9
	TQ=TSTART/TCONUT	INTEGC 10
	TF=TLAST/TCONUT	INTEGC 11
	NEQU=1	INTEGC 12
C ***	NEQU SET TO 0 IF EQUILIBRIUM CONDITION MET IN SUBR.CONEQU	INTEGC 13
	NO=NZPI	INTEGC 14
	MF=21	INTEGC 15
C ***	USE STIFF PART OF GEAR-HINDMARSH ODE PACKAGE.	INTEGC 16
	CALL DRIVES(NO,TQ,TF,Y,H0,EP5,MF,KFLAG,SUIZ,SURZ)	INTEGC 17
C ***	KFLAG=0 MEANS ODE PACKAGE COMPLETED REQUESTED INTEGRATION.	INTEGC 18
	IF(NCH.NE.0.AND.NEQU.EQ.0) TEQU=T/TCONUT	INTEGC 19
	RETURN	INTEGC 20
	END	INTEGC 21

```

SUBROUTINE STRATG(Y,SUIZ,SURZ)
C *** ORIGINAL SEQUENCING DONE ON 07-05-77
DIMENSION Y(1),SUIZ(1),SURZ(1)
COMMON/IO/LOUT,LIN
COMMON/EQ1/T,H,HUSED,NLRC,NKRC,NL,NLPI,NKMI,NK,HXEQMI,JSTART,NQ
COMMON/STGY/TF,TFLN,TBLN,FL,BL,DC,BDLOSS,BDLSM,RDEC,ITDEL,NSTRT,
INDEL,NEQADD,NEQDEL,NEQDM,BDEL,TSWIT,BDLSHM,IPSTGY
COMMON/SHARE/TE,DEN
COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH
COMMON/CONTRL/NZ,NZPI
C *** STRATEGY 11 (2/18/77). THIS IS STRATEGY DESCRIBED IN REPORT.
C *** N.B., IN SUBR DRIVES WE DEFINE SURZ(0)=SUIZ(NZPI)=0. ON IBM 360
C *** THE 0-TH ELEMENT OF AN ARRAY IMMEDIATELY PRECEDES THE 1ST ELEMENT.
C *** INTEGRAL APPROX. USING TRAPEZOIDAL RULE.
C *** CONSIDERING ONLY ERRORS DUE TO USING A RESTRICTED SET OF EQS..
C *** BL=EST. OF CUMULATIVE LOSSES OUT BACK OF SYSTEM OF ACTIVE EQS..
C *** BL=INTEGRAL FROM ISTART TO T OF NE*I(K)*Y(K) WHERE I(NZ+1)=0.
C *** FL=EST. OF CUMULATIVE LOSSES OUT FRONT OF SYSTEM OF ACTIVE EQS..
C *** FL=INTEGRAL FROM ISTART TO T OF NE*R(L-1)*Y(L) WHERE R(0)=0.
C *** DC=CUMULATIVE SUM OF ALL COMPONENTS DELETED IN TIME INTEGRATION
C *** FROM ISTART TO T
C *** COMPUTED COMPONENTS ARE HIGH BY AT MOST FL+BL AND LOW BY AT MOST
C *** FL+BL+DC.
C *** DRIVES SETS FL=BL=DC=SURZ(0)=0=SUIZ(NZ+1),ITDEL=NSTRT,TF=TLAST
C *** DEFINE TFLN AND TBLN FOR THE INITIAL CONDITION SPECIFIED AT T=TS.
C *** BDLSHM=FACT1*BDLOSS, BDLSM=FACT*BDLOSS
C *** TE,DEN=TEMPERATURE AND DENSITY FOR TIME T.
C *** NZPI=NZ+1 WHERE NZ=MAX. CHARGE STATE FOR ELEMENT.
NSEQ=0
DT2=.5*HUSED
IF(NL.EQ.1) GO TO 400
TFLO=TFLN
TFLN=DEN*SURZ(NL-1)*Y(NL)
FL=FL+DT2*(TFLO+TFLN)
400 TBLQ=TBLN
TBLN=DEN*SUIZ(NK)*Y(NK)
BL=BL+DT2*(TBLQ+TBLN)
TFMT=TF-T
TRMN=TFLN+TBLN
ERR=FL+BL+DC
IF(T.GT.TSWIT) GO TO 401
IF(TRMN*(TSWIT-T).LE.BDLSHM-ERR) GO TO 100
GO TO 402
401 IF(TRMN*TFMT.LE.BDLOSS-ERR) GO TO 100
C *** NEED TO ADD EQUATIONS TO THE SET OF ACTIVE EQUATIONS.
402 NSEQ=1
NLMI=NL-1
GO TO (501,500,500,500,500),IPSTGY
500 WRITE(LOUT,299)
299 FORMAT(' ADD EQS. (STRATG) ')
WRITE(LOUT,300) IT,NLMI,NK,T,HUSED,FL,BL,DC,TFLN,TBLN
300 FORMAT(' 19X, IT='14,2X,NLMI='14,2X,NK='14,2X,T='1PE15,2X,
13.5,2X,HUSED='E13.5,2X,FL='E13.5,
219X,BL='E13.5,2X,DC='E13.5,2X,TFLN='E13.5,2X,TBLN='E13.5)
WRITE(LOUT,301)(SUIZ(I),I=NLMI,NK)
301 FORMAT(' SUIZ='1P15E8.1)
WRITE(LOUT,311)(SURZ(I),I=NLMI,NK)
311 FORMAT(' SURZ='1P15E8.1)

```

WRITE (LOUT, 302) (Y(I), I=NL, NK)

STRATG58

302 FORMAT(' Y:', IPI0E12.4)

STRATG59

501 IF (TFLN.GT.TBLN) GO TO 102

STRATG60

C *** ADD EQS. TO BACK, BUT 1ST SEE IF CAN DELETE FROM FRONT.

STRATG61

IF (Y(NL).GT.BDDEL) GO TO 103

STRATG62

IF (DEN*SURZ(NL)*Y(NL+1)*TFMT.GT.BDLOSH) GO TO 103

STRATG63

C *** ELIMINATE EQ. L

STRATG64

SUM=0.

STRATG65

104 SUM=SUM+Y(NL)

STRATG66

Y(NL)=0.

STRATG67

NL=NL+1

STRATG68

IF (SUM+Y(NL).GT.BDDEL) GO TO 105

STRATG69

IF (DEN*SURZ(NL)*Y(NL+1)*TFMT.LE.BDLOSH) GO TO 104

STRATG70

105 NLRC=NL-1

STRATG71

NLPI=NL+1

STRATG72

DC=DC+SUM

STRATG73

103 KOLD=NKRC

STRATG74

IF (Y(NK).LT..001) GO TO 110

STRATG75

NK=NK+1

STRATG76

GO TO 111

STRATG77

110 NK=MIND(NK+NEGADD,NZPI)

STRATG78

111 NKRC=MIND(NK,NZ)

STRATG79

CALL SUIONZ(SUIZ,TE,DEN)

STRATG80

CALL SURECZ(SURZ,TE,DEN)

STRATG81

IF (KOLD.EQ.NKRC) GO TO 106

STRATG82

KS=KOLD+1

STRATG83

107 IF (SUIZ(KS).LT.RDEC*SUIZ(KOLD)) GO TO 108

STRATG84

KS=KS+1

STRATG85

IF (KS.LT.NKRC) GO TO 107

STRATG86

106 NKMI=NK-1

STRATG87

GO TO 109

STRATG88

108 NKMI=KS-1

STRATG89

NKRC=KS

STRATG90

NK=KS

STRATG91

GO TO 109

STRATG92

C *** ADD EQS. TO FRONT. CHECK IF CAN DELETE SOME FROM BACK AT SAME TIME

STRATG93

102 IF (Y(NK).GT.BDDEL) GO TO 113

STRATG94

IF (DEN*SUIZ(NKMI)*Y(NKMI)*TFMT.GT.BDLOSH) GO TO 113

STRATG95

C *** ELIMINATE EQ. K.

STRATG96

SUM=0.

STRATG97

114 SUM=SUM+Y(NK)

STRATG98

Y(NK)=0.

STRATG99

NK=NK-1

STRATG 0

IF (SUM+Y(NK).GT.BDDEL) GO TO 115

STRATG 1

IF (DEN*SUIZ(NK-1)*Y(NK-1)*TFMT.LE.BDLOSH) GO TO 114

STRATG 2

115 NKRC=NK

STRATG 3

NKMI=NK-1

STRATG 4

DC=DC+SUM

STRATG 5

113 LOLD=NLRC

STRATG 6

NL=MAX0(NL-NEGADD,1)

STRATG 7

NLRC=MAX0(NL-1,1)

STRATG 8

CALL SUIONZ(SUIZ,TE,DEN)

STRATG 9

CALL SURECZ(SURZ,TE,DEN)

STRATG10

IF (LOLD.EQ.1) GO TO 116

STRATG11

LS=LOLD-1

STRATG12

117 IF (SURZ(LS).LT.RDEC*SURZ(LOLD)) GO TO 118

STRATG13

LS=LS-1

STRATG14

IF (LS.GT.NLRC) GO TO 117

STRATG15

```

116 NLP1=NL+1
GO TO 109
118 NLRC=LS
NL=LS+1
GO TO 116
C *** ARRIVE AT 100 ONLY IF DON'T HAVE TO ADD ANY EQS..
100 IF (IT LT ITDEL) GO TO 1000
ITDEL=ITDEL+NBDEL
NLMI=NL-1
GO TO (502,502,503,503),1PSTGY
503 WRITE(LOUT,298)
298 FORMAT(' CHECK DEL.(STRATG)')
WRITE(LOUT,300) IT,NLMI,NK,T,HUSED,FL,BL,DC,TFLN,TBLN
WRITE(LOUT,301)(SUIZ(I),I=NLMI,NK)
WRITE(LOUT,311)(SURZ(I),I=NLMI,NK)
WRITE(LOUT,302)(Y(I),I=NL,NK)
C *** CHECK TO SEE IF CAN DELETE NEQDEL EQS. FROM FRONT OF ACTIVE SYS.
502 SUM=0.
LS=NL+NEQDMI
DO 200 I=NL,LS
200 SUM=SUM+Y(I)
IF(SUM.GT.BDDEL) GO TO 209
ZRM=DEN*SURZ(LS)*Y(LS+1)
IF(ZRM*TFMT.GT.BDLOSM) GO TO 209
C *** SET DELETED COMPONENTS=0.
DO 201 I=NL,LS
201 Y(I)=0.
DC=DC+SUM
NLRC=LS
NL=LS+1
NLP1=NL+1
NSEQ=1
C *** CHECK IF CAN DELETE NEQDEL EQS. FROM BACK OF CURRENT SET.
209 SUM=0.
LS=NK-NEQDMI
DO 210 I=LS,NK
210 SUM=SUM+Y(I)
IF(SUM.GT.BDDEL) GO TO 109
ZRM=DEN*SUIZ(LS-1)*Y(LS-1)
IF(ZRM*TFMT.GT.BDLOSM) GO TO 109
DO 202 I=LS,NK
202 Y(I)=0.
NSEQ=1
DC=DC+SUM
NK=LS-1
NKRC=NK
NKH1=NK-1
109 CONTINUE
1000 CONTINUE
IF(NSEQ.EQ.0) GO TO 1001
C *** SET OF ACTIVE EQS.. ALTERED.
JSTART=0
H=H/(1+(NQ-1)*MH)
C *** NQ=ORDER OF STIFF METHOD LAST USED TO GET TO CURRENT T, MH IS USER
C *** DEFINED.
TFLN=DEN*SURZ(NL-1)*Y(NL)
TBLN=DEN*SUIZ(NK)*Y(NK)
1001 RETURN

```

STRATG16
 STRATG17
 STRATG18
 STRATG19
 STRATG20
 STRATG21
 STRATG22
 STRATG23
 STRATG24
 STRATG25
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 STRATG65
 STRATG66
 STRATG67
 STRATG68
 STRATG69
 STRATG70
 STRATG71
 STRATG72
 STRATG73

END

STRATIG74 PAGE 60

P 4

SUBROUTINE STRGI(SUIZ,SURZ)

STRGI 1

C *** ORIGINAL SEQUENCING DONE ON 06-08-77

DIMENSION SUIZ(1),SURZ(1)

STRGI 2

COMMON/E/NZ

STRGI 3

COMMON/LO/LOUT,LIN

STRGI 4

COMMON/STGY/TF,TFLN,TBLN,FL,BL,DC,BDLOSS,BDLOSH,RDEC,ITDEL,NSTRT,

STRGI 5

NBDEL,NEQADD,NEQDEL,NEQDML,BDEL,TSWIT,BDLSHM,IPSTGY

STRGI 6

COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH

STRGI 7

COMMON/STGY2B/FACT,FACT1

STRGI 8

BDLOSH=FACT*BDLOSS

STRGI 9

BDLSHM=FACT1*BDLOSS

STRGI 10

WRITE(LOUT,12) BDLOSS,BDEL,TSWIT,FACT1,FACT,NEQADD,RDEC,NEQDEL,

STRGI 11

INSTRT,NBDEL

STRGI 12

12 FORMAT('STRATEGY 11 FOR ALTERING SET OF ACTIVE EQUATIONS (2/18/77)STRGI 13

1)''' DESIRED BOUND FOR ERROR DUE TO ALTERING SET OF DIFF. EQS.=BDLSTRGI 14

20SS='1PE7.1/' SUM OF COMPONENTS DELETED AT ONCE TO BE .LE.BDEL='STRGI 15

3E7.1/' IN THE TIME INTERVAL (TS,TSWIT) WILL ALLOW ERROR BOUND BY FSTRGI 16

4ACT1*BDLOSS WHERE TSWIT(SEC.)='E7.1,1X' AND FACT1='E7.1/'STRGI 17

5' WHEN NEW L THRU DELETION, REQUIRE NE*R(L-1)*Y(L)*(TF-T).LE.FACT*STRGI 18

6BDLOSS WHERE FACT='E7.1/' WHEN GET NEW K THRU DELETION, REQUIRE NESTRGI 19

7*I(NK)*Y(NK)*(TF-T).LE.FACT*BDLOSS,/'STRGI 20

8' WILL ADD EQS. IN GROUPS OF AT MOST NEQADD='12,1X'EQS. '/'STRGI 21

9' HOWEVER, ONLY ADD UNTIL 1ST RATE COEFF. THAT IS .LE.RDEC* OLD PRSTRGI 22

VIOUS RATE COEFF. WHERE RDEC='E7.1/' WILL DELETE EQS. IN GROUPS OSTRGI 23

BF NEQDEL='12,1X'EQS. HOWEVER, WHEN ADD TO 1 END WILL DELETE AS MANSTRGI 24

CY AS CAN FROM OTHER END. '/' WILL CHECK FOR DELETION AT INTEG.STEPSTRGI 25

D NO.=NSTRT+(P-1)*NBDEL WHERE P=1,2, AND NSTRT='13,2X'NBDEL='13)STRGI 26

NEQDML=NEQDEL-1STRGI 27

1 RETURNSTRGI 28

ENDSTRGI 29

SUBROUTINE SUIONZ(SUION,TE,NE)

C *** ORIGINAL SEQUENCING DONE ON 07-05-77

REAL NE

DIMENSION SUION(1)

C *** FOR THE GIVEN TEMPERATURE, TE IN EV, AND DENSITY, NE IN J/CM**3

C *** DETERMINE APPROXIMATIONS FOR THE IONIZATION COEFF.,

C *** (SUION(J), J=NLRC,NKRC), WHERE (J-1) IS THE CHARGE OF THE

C *** IONIZING ION.

C *** NZ, NEQPR1, (E(1), Q(1), I=1, NZ), ELNAME, NELDES, (DES(J), J=1, NELDES) ARE

C *** ALL DEFINED IN BLOCK DATA FOR ELEMENT UNDER CONSIDERATION.

C *** MOREOVER, COMMON/XCION/ IS DEFINED IN BLOCK DATA FOR ELEMENT.

C *** NLRC, NKRC, AND LOUT MUST BE DEFINED PRIOR TO CALLING SUIONZ.

COMMON/E/NZ, NEQPR1, E(1)

COMMON/Q/Q(1)

COMMON/LO/LOUT, LIN

COMMON/EQ1/T, H, HUSED, NLRC, NKRC

COMMON/XCION/NCUT, DELTA, XC(1)

COMMON/ELNAME/ELNAME, NELDES, DES(1)

C ***

C *** KUNZE IONIZATION WITH ORIGINAL CONSTANT FACTOR DIVIDED BY 2

C *** SUION(J) FROM H. J. KUNZE, PHYS REV A, VOL 3, 937(1971)

C *** NUMERICAL FACTOR DIVIDED BY 2 PER KUNZE'S COMMENT IN

C *** SPACE SCIENCE REVIEWS 13, 565(1972)

C ***

C *** IF XC ARRAY AVAILABLE (NCUT=1), THEN $XJ = E(J)/TE.GE.XC(J)$ IMPLIES

C *** SUION(J).LE.DELTA. USED TO DECREASE POTENTIAL FOR UNDERFLOW. IF XC

C *** TO BE USED (NCUT=1), THEN NEED 3 STATEMENTS, IF (XJ.LT.XC(J)) GO

C *** TO 101, SUION(J)=0., GO TO 100, AFTER THE STATEMENT

C *** $XJ = E(J)/TE$, IF NOT USED (NCUT=0), THEN ABOVE 3 STATEMENTS MUST BE

C *** COMMENTED OUT.

C ***

C *** THE COMMON'S TE, T, H, XCION, AND ELNAME MAY BE INITIALIZED IN A

C *** BLOCK DATA ROUTINE. DES IS USUALLY DESCRIPTIVE INFO. CONCERNING

C *** THE E AND Q VALUES.

C *** NCUT=1 MEANS THIS SUIONZ EXPECTS AN XC ARRAY.

C *** NCUT=0 MEANS THIS SUIONZ DOES NOT EXPECT AN XC ARRAY.

DATA NGEN, NCUT, 1, 1

IF (NGEN.EQ.0) GO TO 360

NGEN=0

WRITE(LOUT, 200) ELNAME

200 FORMAT(' FOR ELEMENT='A4, IX'USE IONIZATION BY KUNZE.')

C *** NEQPR1=1 DESIRES PRINT OF E AND Q IF USED IN CALC.

C *** NEQPR1=2(3) MEANS E'S (Q'S) ALREADY PRINTED, NOT Q'S (E'S).

C *** NEQPR1=4 MEANS BOTH PRINTED.

IF (NEQPR1.LE.0) GO TO 300

GO TO (11, 12, 13, 300), NEQPR1

11 WRITE(LOUT, 349) (DES(I), I=1, NELDES)

349 FORMAT(77(32A4))

13 WRITE(LOUT, 350) (E(I), I=1, NZ)

350 FORMAT(7(' E='F9.3, (2F10.3))

NEQPR1=NEQPR1+1

IF (NEQPR1.NE.2) GO TO 300

12 WRITE(LOUT, 351) (Q(I), I=1, NZ)

351 FORMAT(7(' Q='25F5.0))

NEQPR1=NEQPR1+2

300 IF (NCUT.EQ.0) GO TO 360

C *** NCUT=1 MEANS ARRAY XC DEFINED. IN THIS CASE $X = E(1)/TE.GE.XC(1)$

C *** MEANS THAT SUIZ(X).LE.DELTA (ASSUMING XC CORRESPONDS TO IONIZATION)

C *** FUNCTION USED IN SUIONZ J	SUIONZ58
C *** NCUT=0 MEANS XC ARRAY NOT DEFINED(AVAILABLE)	SUIONZ59
IF(NCUT.EQ.0) GO TO 370	SUIONZ60
IF(NEQPRT.GT.0) WRITE(LOUT,352) DELTA,(XC(1),1=1,NZ)	SUIONZ61
352 FORMAT(2,' XJ=E(J)/TE,GE XC(J) IMPLIES SUION(J),LT DELTA=' LP#0.2/	SUIONZ62
1(' XC='0P20F6.2))	SUIONZ63
360 DO 100 J=NLRC,NKRC	SUIONZ64
XJ=E(J)/TE	SUIONZ65
IF(XJ.LT.XC(J)) GO TO 101	SUIONZ66
SUION(J)=0.	SUIONZ67
GO TO 100	SUIONZ68
101 SUION(J)=(3.75E-8*XQ(J)*((ALOG(40./XJ))*3+40.)*EXP(-XJ))/	SUIONZ69
&(E(J)*SQRT(TE)*(XJ+3.))	SUIONZ70
100 CONTINUE	SUIONZ71
380 RETURN	SUIONZ72
370 WRITE(LOUT,353)	SUIONZ73
353 FORMAT(' SUIONZ EXPECTS A XC ARRAY IN COMMON/XCION/, BUT DO NOT HAS	SUIONZ74
IVE ONE.')	SUIONZ75
CALL EXIT	SUIONZ76
GO TO 380	SUIONZ77
END	SUIONZ78

```

SUBROUTINE SURECZ(SUREC,TE,NE)
C *** ORIGINAL SEQUENCING DONE ON 09-01-77
REAL NE
DIMENSION SUREC(1)
DIMENSION AJP(074),AJEJH(074),EID7(074)
C *** FOR THE GIVEN TEMPERATURE, TE IN EV, AND DENSITY, NE IN 1/CM**3
C *** DETERMINE APPROXIMATIONS FOR THE RECOMBINATION COEFFICIENTS.
C *** (SUREC(J),J=NLRC,NKRC), WHERE J IS THE CHARGE OF THE RECOMBINING
C *** ION.
C *** NZ,NEOPRT,(E(I),I=1,NZ),ELNAME,NELDES,(DES(J),J=1,NELDES) ARE ALL
C *** DEFINED IN THE BLOCK DATA FOR ELEMENT UNDER CONSIDERATION.
C *** NLRC,NKRC, AND LOUT MUST BE DEFINED PRIOR TO CALLING SURECZ.
COMMON/E/NZ,NEOPRT,E(1)
COMMON/IO/LOUT,LIN
COMMON/EQ1/T,H,HUSED,NLRC,NKRC
COMMON/ELNAME/ELNAME,NELDES,DES(1)
C ***
C *** C.JORDAN RECOMBINATION LESS DIELECTRONIC RECOMBINATION.
C *** THE ALPHR RADIATIVE RECOMBINATION BY
C *** BURGESS AND SEATON '1964 VIA EQ.(9),C.JORDAN,
C *** M.NOT R.ASTR.SOC.142,501(1969)'
C *** ALPHR = RADIATIVE RECOMBINATION DUE TO BURGESS, SEATON.
C *** ALPHB = RADIATIVE RECOMBINATION VIA BOUND LEVEL (WILSON).
C *** ALPHCB = COLLISIONAL DE-EXCITATION ABOVE THERMAL LIMIT. (WILSON).
C *** ALPHCC = 3-BODY RECOMBINATION FROM THE CONTINUUM. (WILSON).
C ***
C *** REQUIRE THAT THE NZ FOR CURRENT ELEMENT, I.E. NZMAX WHERE NZMAX
C *** DEFINED IN LOCAL DATA STATEMENT AND HAVE DIMENSION AJP(NZMAX),
C *** AJEJH(NZMAX),EID7(NZMAX)
C ***
C *** THE POWER OF X IN EXP IN G(X) WAS CORRECTED FROM 2 TO 3 ON 6/31/77
C *** EXPECT CORRECT SOL. TO BE LESS THAN SOL. TO THE (EARLIER) WRONG
C *** EQUATION.
C ***
C *** NEW ITERATION TO ESTIMATE QUANTUM NUMBER CN INCLUDED (4/29/77).
C *** LET C SATISFY C-G(C)=0. STRAIGHT NEWTON'S WOULD GIVE FOR REL. ERR.
C *** IN APPROX. TO 1ST ORDER
C ***  $(C-CN1)/C=A(12+9A)(C/CN)(G(CN)/CN)((C-CN)/C)**2$ 
C *** WHERE  $A=P2/CN**3$ . NOW  $A.LT.P2/P1**3=(2.5E-6*NE**(6/17))$ 
C ***  $(P1**3(20/17)*J**2/17)$ 
C *** BUT THIS EXPRESSION IS ORDINARILY SMALL. HENCE EXPECT
C ***  $(C-CN1)/C.LT.((C-CN)/C)**2$ 
C *** REMEMBER MODIFIED NEWTON IS FASTER. HENCE 1 ADDITIONAL ITERATE
C *** WOULD TAKE US FROM 2 SIGNIFICANT FIGURES TO 4.
C *** DEFINE ESTGCM=1+2*REB WHERE REB IS THE DESIRED REL. ERR. BND. IN
C *** ESTIMATE FOR CN.
C *** EXPECT CN=C BETWEEN 10 AND 100. (INTEGRAL).
C ***
C *** EH=HYDROGEN LEVEL, NGEN=INTERNAL SWITCH SO AS TO CALL TABLES
C *** AJP, AJEJH, EID7 ONCE. NGEN IS REDEFINED LOCALLY.
DATA NGEN,NZMAX,EH,ESTGCM/1,74,13.598398,1.0002/
G(X)=PI*EXP(P2/(X**X))
IF(NGEN.EQ.0) GO TO 300
IF(NZ.LE.NZMAX) GO TO 201
WRITE(LOUT,202) NZMAX,NZ
202 FORMAT('MAXIMUM NZ ALLOWED = '13,2X'NZ='13,3X'CALL EXIT SUBR.SURECZ
ICZ')

```

```

CALL EXLT
201 AJ=1.
DO 301 J=1,NZ
C *** 12/17 = .7058...
AJPJ(J)=AJ** .705823529
AJEJH(J)=AJ*AJ*SQRT(E(J))
EID7(J)=E(J)** .1428571429
301 AJ=AJ+1.
NGEN=0
WRITE(LOUT,200) ELNAME
200 FORMAT(' FOR ELEMENT='A4,IX'USE MODIFIED C. JORDAN RECOMBINATION.
1 PART DUE TO BURGESS, SEATON AND 3 TO WILSON.')
IF(NEQPT.LE.0) GO TO 300
GO TO (1,300,12,300), NEQPT
C *** Q'S NOT NEEDED IN THIS RECOMBINATION EXPRESSION.
11 WRITE(LOUT,349) (DES(I),I=1,NELDES)
349 FORMAT(4(32A4))
12 NEQPT=NEQPT+1
WRITE(LOUT,350) (E(J),J=1,NZ)
350 FORMAT(/(' E='F9.3,12F10.3))
C *** 1/7 = .1428...
300 TEID7=TE** .1428571429
CON=J J2E-13/TE
C *** 2/7 = .2857142857
D1=L.29E-4*NE** .2857142857
C *** 1/17 = .05882...
D2=L.26E2*(TE/(EH*NE*NE))** .05882352941
D3=6.39925/TE
C *** D3=2*D3=2*(4*EH)/(17*TE)
CFB=9.60E-13/(TE*SQRT(TE))
CFCB=L.48E-28*(NE/(TE*TE))
CFCC=4.45E-29*(NE/(TE*TE))
C *** CN = QUANTUM NO. (EQ. DUE TO GRIEM)
C *** CN = COLLISIONAL LIMIT ENERGY
CNL=0
AJ=NLRC
DO 100 J=NLRC,NKRC
AJ5=AJ*AJ
TP2=TD3*AJ5
P2=.5*TP2
C *** FOR FIXED TE, NE A LARGER J VALUE MEANS ROOT OF P1*EXP(P2/X**2)=X
C *** INCREASES.
C *** FIND POSITIVE ZERO OF X-G(X)=0. USE NEWTON'S APPROXIMATION.
C *** IF INITIAL APPROX. IS LOW, THEN ALL WILL BE LOW.
C *** X0=P1.GT.0 IS A LOW ESTIMATE. TRY TO USE LAST APPROX. OF
C *** PREVIOUSLY DETERMINED COEFF..
P1=D2*AJPJ(J)
CN=AMAX1(CNL,P1)
10 CNL=CN
C *** AUGMENT OUR PREVIOUS NEWTON'S ESTIMATE, CNL, BY THE FACTOR ESIGCN.
C *** THIS IS CNT. APPLY NEWTON'S METHOD AT CNT. IF RESULTING CN.LT.CNT,
C *** THEN CNT IS A HIGH EST. OF ROOT OF X-G(X)=0. HENCE ROOT IN
C *** (CNL,CNT) AND MIDPT. OF INTERVAL IS AN EST. WITH A RELATIVE
C *** ACCURACY BOUNDED BY REB. OF COURSE, CN.GT.CNT GIVES A BETTER EST.
C *** THAN IF HAD USED CNL.
CNT=ESIGCN*CNL
C=TP2/(CNT*CNT)
GCNT=G(CNT)

```

SURECZ58
 SURECZ59
 SURECZ60
 SURECZ61
 SURECZ62
 SURECZ63
 SURECZ64
 SURECZ65
 SURECZ66
 SURECZ67
 SURECZ68
 SURECZ69
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 SURECZ90
 SURECZ91
 SURECZ92
 SURECZ93
 SURECZ94
 SURECZ95
 SURECZ96
 SURECZ97
 SURECZ98
 SURECZ99
 SURECZ 0
 SURECZ 1
 SURECZ 2
 SURECZ 3
 SURECZ 4
 SURECZ 5
 SURECZ 6
 SURECZ 7
 SURECZ 8
 SURECZ 9
 SURECZ10
 SURECZ11
 SURECZ12
 SURECZ13
 SURECZ14
 SURECZ15

$CN = ((L + C) * GCNT) / (1 + (C * GCNT) / CNT)$
IF(CN.GT.CNT) GO TO 10
C *** HAVE ACCEPTABLE ESTIMATE OF ROOT
 $CN = .5 * (CNL + CNT)$
 $EC = D1 * EIDZ(J) / TEID7$
 $ALPHR = CON * AJEJH(J)$
 $D4 = EXP(EC / TE)$
 $ALPHB = (CFB * AJS * AJS * D4) / CN$
 $ALPHCB = (CFCB * D4) / (AJS * CN * CN)$
 $ALPHCC = CFCC / AJS$
 $SUREC(J) = ALPHR + ALPHB + ALPHCB + ALPHCC$
100 AJ = AJ + 1
RETURN
END

SURECZ16
SURECZ17
SURECZ18
SURECZ19
SURECZ20
SURECZ21
SURECZ22
SURECZ23
SURECZ24
SURECZ25
SURECZ26
SURECZ27
SURECZ28
SURECZ29

SUBROUTINE ZAVERG(ZAUG, Y)

ZAVERG 1

C *** ORIGINAL SEQUENCING DONE ON 06-08-77

C *** FORM THE AVERAGE Z USING ONLY THE ACTIVE COMPONENTS NL THRU NK.

ZAVERG 2

DIMENSION Y(1)

ZAVERG 3

COMMON/EO L, L, H, HUSED, NLRC, NKRC, NL, NLP, NKMI, NK

ZAVERG 4

ZAUG=0.

ZAVERG 5

AKMI=NL-1

ZAVERG 6

DO 700 K=NL, NK

ZAVERG 7

ZAUG=ZAUG+AKMI*Y(K)

ZAVERG 8

700 AKMI=AKMI+1.

ZAVERG 9

RETURN

ZAVERG 10

END

ZAVERG 11

H 5

```

C ***** EXAMPLE 1 *****
C *** IN EX. 1 THE TEMP. AND DEN. ARE TIME INDEPENDENT WITH VALUES
C *** TE=500EV AND NE=DEN=1.E13/CM**3. IN EX.1 PROG1 IS USED TO FIND
C *** (I) THE NORMALIZED, CHARGE-STATE, DISTRIBUTION VECTOR, (II) APPROXEX.
C *** FOR THE EIGENVALUES (ROOTS) OF THE COEFF. MATRIX, DEN*A, OF THE
C *** LIN.SYSTEM OF DIFF.EQS., (III) THE TIME EVOLUTION OF THE DISTR.VEC EX.
C *** Y(T) UNTIL THE (NCRT=1) L-NORM OF (Y(T)-YEQU) IS 1ST LESS THAN EX.
C *** EPSCC(NEPS)=.01. SPECIAL REPORT INFORMATION IS GIVEN AT THE TIME EX.
C *** LI(Y(T)-YEQU), LT, EPSCC(I) FOR I=1,...,NEPS WITH THE TIME EVOL. EX.
C *** TERMINATED WHEN INEQ. WITH I=NEPS IS 1ST SATISFIED. MOREOVER, EX.
C *** OTHER GENERAL REPORT TIMES ARE GIVEN THRU THE ARRAYS TPRNT, DTPRT, EX.
C *** AND NPRINT AND THE VARIABLE NPRINTI. THE GEN. REPORT INFORMATION AT EX.
C *** A GIVEN TIME TELLS US THE TEMPERATURE, TE, IN EV, THE DENSITY, NE, EX.
C *** IN CM**3, THE AVERAGE Z VALUE, THAT THE ACTIVE SET OF DIFF. EQS. EX.
C *** ARE THE L-TH THRU THE K-TH, THAT IT INTEGRATION STEPS HAVE BEEN EX.
C *** PERFORMED TO ARRIVE AT THIS TIME, THAT THE CURRENT ORDER OF THE EX.
C *** STIFF INTEGRATION METHOD IS NO, THAT THE LAST STEPSIZE WAS H(SEC) EX.
C *** FL,BL,DC GIVE INFORMATION ASSOCIATED WITH STRATEGY 1, (ISWSTR=2), EX.
C *** FOR ALTERING THE SET OF ACTIVE DIFF. EQS., IN THIS CASE FL BOUNDS EX.
C *** THE LOSSES OUT THE FRONT END OF THE ABBREV. SYSTEMS, BL BOUNDS THE EX.
C *** LOSSES OUT BACK END, AND DC BOUNDS SUM OF ALL COMPONENTS DELETED EX.
C *** FROM THE FRONT OR THE BACK. EX.
C *** THE Y VALUES OF THE NORMALIZED, CHARGE-STATE, DISTR.VEC EX.
C *** CORRESPOND TO Y(I) WHERE I=L,...,K. EX.
C *** BELOW WE HAVE THE BLOCK DATA, BDPARM, FOR THIS EXAMPLE, BUT EX.
C *** WITHOUT ANY OF THE COMMENT CARDS. CONSULT THE EARLIER BDPARM IN EX.
C *** THE GENERAL PROGRAM LISTINGS FOR THE DEFINITION OF THE VARIABLES EX.
C *** IN THE DATA STATEMENTS. EX.
C *** EX.
C *** THE CPU TIME REQUIRED TO RUN EXAMPLE 1 ON THE IBM 360/91 AT ORNL EX.
C *** WAS 1.05 SECONDS. EX.
C *** EX.
C *** BLOCK DATA EX.
COMMON/EPSC/NECH,NEQU,NEPS,NEPSC,NCRTI,EPSEQU,ZAUGEQ,EPSCC(10) EX.
COMMON/STGY/TF,IFLN,TBLN,FL,BL,DC,BDLOSS,BDLOSH,RDEC,ITDEL,NSTRT, EX.
INBDEL,NEQADD,NEQDEL,NEQDM,BDDEL,TSHIT,BDLSHM,IPSTGY EX.
COMMON/PRINT/TPRINT,IPRINT(5),DTPRT(5),NPRINT(5),NPRINTI,IPRNTI,NPR EX.
COMMON/SHARE/TE,DEN,HMIN,HMAX,EPS,MF,KFLAG,JDISC,NOM,NOM2,NOMPI EX.
COMMON/STRAT/IT,NLB,NKB,ISWSTR,IEQU,MH EX.
COMMON/HAINBD/NTEMP,NDENS,NLOG,NROOTS,IPATR,TSTART,TLAST,TEL,DTE, EX.
IDENL,DDEN,THRES,H0,TEMP(25),DENS(25) EX.
COMMON/STGY2B/FACT,FACTI EX.
DATA NTEMP,NDENS,NLOG,NROOTS,NEPS,NCRTI,NCH/0,0,0,1,3,1,1/ EX.
DATA NLB,NKB,ISWSTR,NPRINTI,IEQU,IPATR,MH/1,5,2,4,1,1,5/ EX.
DATA TSTART,TLAST,TEL,DTE,DENL,DDEN,THRES,EPS,H0/0.,250., EX.
150.,5.E-5,5.E-9/ EX.
DATA BDLOSS,FACT,BDDEL,RDEC,TSHIT,FACTI,NEQADD,NEQDEL,NSTRT,NBDEL EX.
IPSTGY/1.E-5,7,1.E-7,1,1.E-5,1,3,3,100,20,1/ EX.
DATA TPRNT/5,10,20,250,/,DTPRT/5,5,30,50,/,NPRINT/0,0,6,5/ EX.
DATA TEMP/500./ EX.
DATA DENS/1.E13/ EX.
DATA EPSCC/5,1,.01/ EX.
END EX.

```

INTEG. PARMS. TSTART(MS)=0.0 TLAST(MS)=2.500E 02 HQ(S)=5.000E-09 EPS(=EPS*YMAX)=5.000E-05
IF ORDER OF STIFF METHOD SET TO 1, THEN NEXT H=(LAST H)/(1+(NQ-1)MH) WHERE NQ=STIFF ORDER LAST USED, MH= 5

STRATEGY 11 FOR ALTERING SET OF ACTIVE EQUATIONS (2/18/77)
DESIRED BOUND FOR ERROR DUE TO ALTERING SET OF DIFF. EQS.=BDLOSS=1.0E-05
SUM OF COMPONENTS DELETED AT ONCE TO BE .LE.BDDEL=1.0E-07
IN THE TIME INTERVAL (TS,TSHIT) WILL ALLOW ERROR BOUND BY FACT*BDLOSS WHERE TSHIT(SEC.)=1.0E-05 AND FACT=1.0E-01
WHEN NEW L THRU DELETION, REQUIRE NE*(L-1)*Y(L)*(TF-T).LE.FACT*BDLOSS WHERE FACT=7.0E-01
WHEN GET NEW K THRU DELETION, REQUIRE NE*(NK)*Y(NK)*(TF-T).LE.FACT*BDLOSS.
WILL ADD EQS. IN GROUPS OF AT MOST NEQADD= 3 EQS.
HOWEVER, ONLY ADD UNTIL 1ST RATE COEFF. THAT IS .LE.RDEC* OLD PREVIOUS RATE COEFF. WHERE RDEC=1.0E-01
WILL DELETE EQS. IN GROUPS OF NEQDEL= 3 EQS. HOWEVER, WHEN ADD TO 1 END WILL DELETE AS MANY AS CAN FROM OTHER END.
WILL CHECK FOR DELETION AT INTEG.STEP. NO.=NSTRT+(P-1)*NDEL WHERE P=1,2 AND NSTRT=100 NDEL=20

CALL YNA AT T(MS)=(TPRNT(I)+Q*DTPRT(I)), Q=0 TO NPRNT(I), I=1 TO NPRNTI.

I	TPRNT	DTPRT	NPRNT
1	5.00E-01	5.00E 00	0
2	1.00E 01	5.00E 00	0
3	2.00E 01	3.00E 01	6
4	2.50E 02	5.00E 01	5

INTEGRATION CONVRG. MEANS $1 - \text{NORM}(Y(T) - Y_{\text{EQU}})$.LE.EPSEQU IF NCRIT=1 AND $\text{ABS}(Z_{\text{AUG}}(Y(T)) - Z_{\text{AUG}}(Y_{\text{EQU}})) / Z_{\text{AUG}}(Y_{\text{EQU}})$.LE.EPSEQU IF NCRIT=2
IN THIS CASE NCRIT=1
FOR ELEMENT=FE USE IONIZATION BY KUNZE.

Q'S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL.2, P.63 1970. E'S FROM DIE NATURWISSEN SCHAFTEN, VOL.2, 1955 BY FINKLEBURG.

E=	7.900	16.180	30.640	57.400	83.000	108.100	133.200	158.300	240.200	271.700	303.100	334.600	372.200
E=	404.000	472.400	506.000	168.000	283.000	399.000	514.000	644.000	760.000	923.000	2025.000	8503.000	8969.000
Q=	2.	1.	14.	13.	12.	11.	10.	9.	8.	7.	6.	5.	4.
Q=	1.												

XJ=E(J)/TE.GE.XC(J) IMPLIES SU(ON(J).LT.DELTA=1.00E-20
XC= 28.46 25.72 28.37 27.37 26.75 26.27 25.87 25.51 24.78 24.47 24.16 23.83 23.45 23.05 22.42 21.64 22.45 22.18 21.90 21.61
XC= 21.27 20.88 20.36 19.60 18.17 17.42
FOR ELEMENT=FE USE MODIFIED C.JORDAN RECOMBINATION, 1 PART DUE TO BURGESS, SEATON AND 3 TO WILSON.

START NE=1.00000E 13 TE=5.00000E 02 LOG(11604.5*TE)=6.76360E 00 ZAUG(YEQU)=18.8930

SPECTRO -SCOPIC STATE	CHARGE STATE	RATE COEFFICIENTS IONIZATION OUT OF	RECOMBINATION INTO	L/R	NORMALIZED EQUILIBRIUM VECTOR
1	0	7.2235E-08	6.4826E-16	1.1143E-08	0.0
2	1	1.3267E-08	3.7871E-15	3.5032E-06	0.0
3	2	7.3513E-08	1.1855E-14	6.2010E-06	0.0
4	3	2.6152E-08	2.8949E-14	9.0340E-05	0.0
5	4	1.3297E-08	5.4762E-14	2.4282E-05	0.0
6	5	7.7910E-09	9.0668E-14	8.5930E-04	0.0
7	6	4.8984E-09	1.3802E-13	3.5491E-04	0.0
8	7	3.2113E-09	1.9798E-13	1.6221E-04	0.0
9	8	1.2554E-09	3.0715E-13	4.0872E-03	0.0
10	9	8.4584E-10	4.0594E-13	2.0836E-03	0.0
11	10	5.7004E-10	5.2213E-13	1.0917E-03	0.0
12	11	3.7932E-10	6.5696E-13	5.7738E-02	0.0
13	12	2.3605E-10	8.1746E-13	2.8875E-02	0.0
14	13	1.4492E-10	9.9367E-13	1.4584E-02	0.0
15	14	6.4760E-11	1.2350E-12	5.2436E-01	0.000018
16	15	2.6939E-11	1.4626E-12	1.8419E-01	0.000941
17	16	1.3099E-11	2.4232E-12	5.4055E-00	0.017331
18	17	7.6700E-12	2.8541E-12	2.6874E-00	0.093683
19	18	4.4461E-12	3.3287E-12	1.3357E-00	0.251760
20	19	2.5440E-12	3.8464E-12	6.6139E-01	0.336272
21	20	1.3468E-12	4.4282E-12	3.0414E-01	0.222408
22	21	7.0541E-13	5.0411E-12	1.3993E-01	0.067643
23	22	2.8764E-13	5.7668E-12	4.9879E-02	0.009465
24	23	1.0645E-13	6.4625E-12	1.6472E-02	0.000472
25	24	3.2964E-20	1.3661E-11	2.4130E-09	0.000008
26	25	0.0	1.5195E-11	0.0	0.0
27	26				0.0

ROOTS OF NE*A= -7.35E 05 -7.22E 05 -2.62E 05 -1.33E 05 -1.33E 05 -7.79E 04 -4.90E 04 -3.21E 04 -1.26E 04 -8.46E 03
-5.71E 03 -3.80E 03 -2.37E 03 -1.45E 03 -6.61E 02 -2.90E 02 -1.72E 02 -1.52E 02 -1.37E 02 -1.15E 02
-8.69E 01 -7.43E 01 -6.51E 01 -5.36E 01 -3.94E 01 -2.17E 01 -2.25E 04

THE EXPONENTIAL ASSOCIATED WITH THE NEXT TO LAST ROOT = .1 AT TIME T(S)=1.1E-01

K 5

T(MS)=5.000E-01 TE=5.00E-02 NE=1.00E-13 ZAVG=10.92 L=7 K=20 IT=164 NQ=3 H=1.77E-05 FL,BL,DC= 5.8E-11 1.1E-07 5.6E-08
 Y= 0.000000 0.000002 0.006620 0.079214 0.267632 0.357114 0.218705 0.061713 0.008528 0.000429
 0.000008 0.000000 0.000000 0.000000

T(MS)=1.000E-01 TE=5.00E-02 NE=1.00E-13 ZAVG=16.15 L=11 K=23 IT=242 NQ=4 H=4.89E-04 FL,BL,DC= 5.0E-09 1.2E-07 5.5E-08
 Y= 0.000000 0.000000 0.000001 0.000124 0.011893 0.205326 0.467282 0.255492 0.054576 0.005040
 0.000212 0.000004 0.000000

T(MS)=2.000E-01 TE=5.00E-02 NE=1.00E-13 ZAVG=17.04 L=11 K=23 IT=256 NQ=4 H=9.84E-04 FL,BL,DC= 5.0E-09 1.5E-07 5.5E-08
 Y= 0.000000 0.000000 0.000000 0.000006 0.000828 0.031995 0.258012 0.410541 0.236907 0.055694
 0.005712 0.000248 0.000005

T(MS)=5.000E-01 TE=5.00E-02 NE=1.00E-13 ZAVG=18.12 L=14 K=25 IT=282 NQ=4 H=2.12E-03 FL,BL,DC= 2.8E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000070 0.003438 0.054485 0.218963 0.369274 0.262390 0.080558 0.010204 0.000549
 0.000010 0.000000

T(MS)=5.6809E-01 ABS(ZAVG(Y(T))-ZAVG(YEQU))/ZAVG(YEQU)=0.03452, ZAVG(Y(T))=18.247, LI(Y(T)-YEQU)=0.46942, EPSE=0.50000
 Y= 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.000000 0.000055 0.002747 0.044974 0.192703 0.357935 0.286242
 0.099939 0.014440 0.000887 0.000018 0.000000 0.0 0.0

T(MS)=8.000E-01 TE=5.00E-02 NE=1.00E-13 ZAVG=18.52 L=14 K=25 IT=290 NQ=4 H=4.91E-03 FL,BL,DC= 3.6E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000033 0.001686 0.029321 0.141648 0.317547 0.325566 0.151670 0.029871 0.002525
 0.000072 0.000001

T(MS)=1.100E-02 TE=5.00E-02 NE=1.00E-13 ZAVG=18.71 L=14 K=25 IT=296 NQ=4 H=7.32E-03 FL,BL,DC= 4.1E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000024 0.001245 0.022354 0.114947 0.284865 0.337048 0.188434 0.045936 0.004904
 0.000179 0.000002

T(MS)=1.2067E-02 ABS(ZAVG(Y(T))-ZAVG(YEQU))/ZAVG(YEQU)=0.00772, ZAVG(Y(T))=18.747, LI(Y(T)-YEQU)=0.09575, EPSE=0.10000
 Y= 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.000000 0.000022 0.001170 0.021127 0.109935 0.277691 0.337903
 0.196132 0.050095 0.005643 0.000218 0.000003 0.0 0.0

T(MS)=1.400E-02 TE=5.00E-02 NE=1.00E-13 ZAVG=18.80 L=14 K=25 IT=300 NQ=4 H=7.32E-03 FL,BL,DC= 4.5E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000021 0.001081 0.019673 0.103845 0.268477 0.338177 0.205781 0.055839 0.006757
 0.000283 0.000004

T(MS)=1.700E-02 TE=5.00E-02 NE=1.00E-13 ZAVG=18.84 L=14 K=25 IT=303 NQ=4 H=1.12E-02 FL,BL,DC= 4.8E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000019 0.001009 0.018479 0.098728 0.260290 0.337646 0.214088 0.061368 0.007945
 0.000360 0.000005

T(MS)=2.000E-02 TE=5.00E-02 NE=1.00E-13 ZAVG=18.87 L=14 K=25 IT=306 NQ=4 H=1.12E-02 FL,BL,DC= 5.1E-07 2.4E-07 6.9E-08
 Y= 0.000000 0.000019 0.000975 0.017909 0.096239 0.256142 0.337084 0.218175 0.064339 0.008639
 0.000409 0.000006

T(MS)=2.3421E-02 ABS(ZAVG(Y(T))-ZAVG(YEQU))/ZAVG(YEQU)=0.00069, ZAVG(Y(T))=18.880, LI(Y(T)-YEQU)=0.00794, EPSE=0.01000
 Y= 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.000000 0.000018 0.000957 0.017600 0.094875 0.253817 0.336877
 0.220422 0.066062 0.009061 0.000440 0.000007 0.0 0.0

```

C ***** EXAMPLE 11 *****
C *** IN EX.11 THE FUNCTIONS TE AND DENE VARY WITH TIME. PROGTD IS
C *** USED TO DESCRIBE THE TIME EVOLUTION OF THE NORMALIZED, CHARGE-
C *** STATE, DISTRIBUTION VECTOR. SEE EX.1 DESCRIPTION FOR THE MEANING
C *** OF THE REPORTED INFORMATION. BELOW THE BLOCK DATA, BDPARM, IS
C *** GIVEN. MOST UNNEEDED PARAMETERS ARE NOT DEFINED. SEE THE EARLIER
C *** BDPARM IN THE GENERAL PROGRAM LISTINGS FOR THE DEFINITION OF THE
C *** VARIABLES IN THE DATA STATEMENTS. BELOW THE BDPARM ARE DATA
C *** STATEMENTS THAT GO IN SUBR.DTDATA TO REPLACE CARDS DTDATA61 THRU
C *** DTDATA70.
C *** THE CPU TIME REQUIRED TO RUN EXAMPLE 11 ON THE IBM 360/91 AT ORNL
C *** WAS 1.44 SECONDS.
C ***
C *** BDPARM
C *** BLOCK DATA
COMMON/EP5/NCH, NEQU, NEPS, NEPSC, NCRIT, EPSEQU, ZAUGEQ, EPSCC(10)
COMMON/STGY/TE, TFLN, TBLN, FL, BL, DC, BDLOSS, BDLOSM, RDEC, ITDEL, NSTRT,
INBDEL, NEQADD, NEQDEL, NEQDM1, BDEL, TSWIT, BDLSMH, IPSTGY
COMMON/PRINT/TPRINT, TPRT(5), DTPRT(5), NPRNT(5), NPRNT1, IPRNT1, NPR
COMMON/SHARE/TE, DEN, HMIN, HMAX, EPS, HF, KFLAG, JDISC, NOM, NOM2, NOMP1
COMMON/STRAT/IT, NLB, NKB, ISWSTR, IEQU, MH
COMMON/MAINBD/NTEMP, NDENS, NLOG, NROOTS, IPAIR, TSTART, TLAST, TEL, DTE,
IDENL, DDEN, THRES, HO, TEMP(25), DENS(25)
COMMON/STGY2B/FACT, FACT1
DATA NLB, NKB, ISWSTR, NPRNT1, IEQU, MH/1, 5, 2, 2, 1, 5/
DATA TSTART, TLAST, THRES, EPS, HO/0., 130., 0., 5.E-5, 5.E-9/
DATA BDLOSS, FACT, BDEL, RDEC, TSWIT, FACT1, NEQADD, NEQDEL, NSTRT, NBDEL,
IPSTGY/1.E-5, .7, 1.E-7, .1, 1.E-5, .1, 3, 3, 100, 20, 1/
DATA TPRT/10, 16, 2, DTPRT/10, 14, 2, NPRNT/10, 1/
END
C ***
C *** DATA STATEMENTS THAT GO INTO SUBR.DTDATA.
DATA TR, DDT/2., 5./
DATA DENE/2.7, 2.5, 4.5, 4.4, 4.4, 4.05, 3.3, 2.6, 2.1/
DATA CNE/8*1.E13/
DATA TEE/280., 290., 550., 700., 760., 630., 630., 630./
DATA TDISCH/8, 20, 35, 48, 60, 75, 95, 116, 130/
DATA NDENA, NYLAS, NOIR/1, 8, 1/

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INTEG.PARMS., TSTART(MS)=0.0 TLAST(MS)=1.300E 02 H0(5)=5.000E-09 EPS(-EPS*YMAX)=5.000E-05
IF ORDER OF STIFF METHOD SET TO 1, THEN NEXT H=(LAST H)/(1+(N0-1)MH) WHERE N0=STIFF ORDER LAST USED, MH= 5

STRATEGY 11 FOR ALTERING SET OF ACTIVE EQUATIONS (2/18/77)
DESIRED BOUND FOR ERROR DUE TO ALTERING SET OF DIFF. EQS.=BDLOSS=1.0E-05
SUM OF COMPONENTS DELETED AT ONCE TO BE .LE.BDDEL=1.0E-07
IN THE TIME INTERVAL (TS,TSHIT) WILL ALLOW ERROR BOUND BY FACT1*BDLOSS WHERE TSHIT(SEC.)=1.0E-05 AND FACT1=1.0E-01
WHEN NEW I THRU DELETION, REQUIRE $NE * R(I-1) * Y(I) * (TF-T)$.LE.FACT*BDLOSS WHERE FACT=7.0E-01
WHEN GET NEW K THRU DELETION, REQUIRE $NE * I(NK) * Y(NK) * (TF-T)$.LE.FACT*BDLOSS.
WILL ADD EQS. IN GROUPS OF AT MOST NEADD= 3 EQS.
HOWEVER, ONLY ADD UNTIL 1ST RATE COEFF. THAT IS .LE.RDEC* OLD PREVIOUS RATE COEFF. WHERE RDEC=1.0E-01
WILL DELETE EQS. IN GROUPS OF NEDEL= 3 EQS. HOWEVER, WHEN ADD TO 1 END WILL DELETE AS MANY AS CAN FROM OTHER END.
WILL CHECK FOR DELETION AT INTEG.STEP NO.=NSTRT+(P-1)*NBDEL WHERE P=1,2, AND NSTRT=100 NBDEL= 20

CALL YNA AT T(MS)=(TPRNT(I)+Q*DTPRNT(I)), Q=0 TO NPRNT(I), I=1 TO NPRNT1.

I	TPRNT	DTPRNT	NPRNT
1	1.00E 01	1.00E 01	10
2	1.46E 02	1.40E 01	1

N 5

EXPERIMENTAL DATA LOOP INDEX IR= 1 DENSITY MODEL, NDEN=1
 SEC)= 2.00E-02 3.50E-02 4.80E-02 6.00E-02 7.50E-02 9.50E-02 1.16E-01 1.30E-01
 N(T)= 2.70E 13 2.50E 13 4.50E 13 4.40E 13 4.05E 13 3.30E 13 2.60E 13 2.10E 13
 (T) = 2.80E 02 2.90E 02 5.50E 02 7.00E 02 7.60E 02 6.30E 02 6.30E 02 6.30E 02
 (0,2.00E-02) TE(T)=(TMEXP(I)-TE0)*(1+(TR/ST)**2)*T**2/(T**2+(TR/1000)**2)+TE0, TMEXP(I)=2.80E 02 TE0=0.10 TR= 2.0 ST=20.0
 (0,TDSS=8.00E-03) DEN(T)=((DENEXP(I)*DID-DENO)/TDSS)*T+DENO, DENEXP(I)=2.70E 13 DID=5.28E 00 DENO=1.00E 04
 (TDSS,2.00E-02) DEN(T)=DENEXP(I)*EXP(LN(2)*(ST-1000T)/DDT), ST=20.00 DDT= 5.00
 IN INTERPOLATION USED AT TIMES WITHIN TABLE OF EXP. DATA VALUES. LAST EXP. VALUE USED FOR TIMES .GT. THOSE OF TABLE.
 OR ELEMENT=FE USE IONIZATION BY KUNZE.

S AND SOME E'S FROM CARLSON, ATOMIC DATA, VOL. 2, P. 63, 1970. E'S FROM DIE NATURWISSENSCHAFTEN, VOL. 2, 1955 BY FINKLEMBURG.

7.900	16.180	30.640	57.400	83.000	108.100	133.200	158.300	240.200	271.700	303.100	334.600	372.200
404.000	472.400	506.000	1168.000	1283.000	1399.000	1514.000	1644.000	1760.000	1923.000	2025.000	8503.000	8969.000

2.	1.	14.	13.	12.	11.	10.	9.	8.	7.	6.	5.	4.	3.	2.	1.	8.	7.	6.	5.	4.	3.	2.	1.	2.
----	----	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

J=E(J)/TE, GE, XC(J) IMPLIES SVION(J), LT, DELTA=1.00E-20

C= 28.46	26.72	28.37	27.37	26.75	26.27	25.87	25.51	24.78	24.47	24.16	23.83	23.45	23.05	22.42	21.64	22.45	22.18	21.90	21.61
----------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

C= 21.27 20.88 20.36 19.60 18.17 17.42

OR ELEMENT=FE USE MODIFIED C. JORDAN RECOMBINATION, 1 PART DUE TO BURGESS, SEATON AND 3 TO WILSON.

0 5

T(MS)=1.000E 01 TE=2.72E 02 NE=1.08E 14 ZAVG=15.95 L=11 K=23 IT= 338 NQ=3 H=2.39E-04 FL,BL,DC= 8.1E-09 6.1E-08-2.2E-09
 Y= 0.000000 0.000000 0.000009 0.000626 0.019818 0.194684 0.612674 0.157124 0.014511 0.000495
 0.000006 0.000000 0.000000

T(MS)=2.000E 01 TE=2.80E 02 NE=2.70E 13 ZAVG=16.07 L=11 K=23 IT= 356 NQ=3 H=3.28E-04 FL,BL,DC= 8.2E-09 6.1E-08-2.2E-09
 Y= 0.000000 0.000000 0.000005 0.000400 0.014265 0.160592 0.590672 0.204641 0.027842 0.001495
 0.000032 0.000000 0.000000

T(MS)=3.000E 01 TE=2.87E 02 NE=2.57E 13 ZAVG=16.12 L=11 K=23 IT= 365 NQ=3 H=2.52E-03 FL,BL,DC= 8.2E-09 6.1E-08-2.2E-09
 Y= 0.000000 0.000000 0.000004 0.000323 0.012257 0.147581 0.580350 0.223350 0.033963 0.002063
 0.000050 0.000000 0.000000

T(MS)=4.000E 01 TE=3.90E 02 NE=3.27E 13 ZAVG=16.46 L=11 K=23 IT= 383 NQ=4 H=5.96E-04 FL,BL,DC= 8.2E-09 6.1E-08-2.2E-09
 Y= 0.000000 0.000000 0.000000 0.000050 0.003560 0.077733 0.480219 0.343142 0.086325 0.008553
 0.000351 0.000006 0.000000

T(MS)=5.000E 01 TE=5.75E 02 NE=4.48E 13 ZAVG=18.26 L=13 K=25 IT= 414 NQ=3 H=3.92E-04 FL,BL,DC= 8.8E-09 1.6E-07-2.2E-09
 Y= 0.000000 0.000000 0.000038 0.002249 0.038759 0.188923 0.366207 0.290418 0.098602 0.013881
 0.000838 0.000018 0.000000

T(MS)=6.000E 01 TE=7.00E 02 NE=4.40E 13 ZAVG=19.71 L=13 K=25 IT= 430 NQ=4 H=7.17E-04 FL,BL,DC= 8.8E-09 1.6E-07-2.2E-09
 Y= 0.000000 0.000000 0.000001 0.000053 0.001546 0.018790 0.108034 0.287802 0.352714 0.185071
 0.042395 0.003434 0.000090

T(MS)=7.000E 01 TE=7.40E 02 NE=4.17E 13 ZAVG=20.48 L=13 K=25 IT= 449 NQ=4 H=1.10E-03 FL,BL,DC= 8.8E-09 1.6E-07-2.2E-09
 Y= 0.000000 0.000000 0.000000 0.000006 0.000215 0.003685 0.032418 0.144357 0.319895 0.323855
 0.149251 0.024892 0.001351

T(MS)=8.000E 01 TE=7.28E 02 NE=3.86E 13 ZAVG=20.82 L=16 K=25 IT= 467 NQ=3 H=1.06E-03 FL,BL,DC= 2.0E-07 1.7E-07 2.0E-08
 Y= 0.000002 0.000097 0.001815 0.018081 0.095326 0.262128 0.347611 0.219040 0.051745 0.004075
 0.000002 0.000097 0.001815

T(MS)=9.000E 01 TE=6.63E 02 NE=3.49E 13 ZAVG=20.73 L=16 K=25 IT= 476 NQ=3 H=1.34E-03 FL,BL,DC= 1.3E-06 1.8E-07 2.0E-08
 Y= 0.000005 0.000190 0.002921 0.024431 0.110915 0.271252 0.334200 0.203561 0.048454 0.003990
 0.000005 0.000190 0.002921

T(MS)=1.000E 02 TE=6.30E 02 NE=3.13E 13 ZAVG=20.49 L=13 K=25 IT= 490 NQ=3 H=2.44E-03 FL,BL,DC= 2.0E-06 1.8E-07 2.0E-08
 Y= 0.000000 0.000000 0.000000 0.000015 0.000461 0.005864 0.040174 0.149256 0.300438 0.308630
 0.159617 0.033025 0.002436

T(MS)=1.100E 02 TE=6.30E 02 NE=2.80E 13 ZAVG=20.35 L=13 K=25 IT= 494 NQ=3 H=2.44E-03 FL,BL,DC= 2.0E-06 1.8E-07 2.0E-08
 Y= 0.000000 0.000000 0.000000 0.000021 0.000628 0.007664 0.049628 0.171365 0.315733 0.292557
 0.135606 0.025052 0.001660

T(MS)=1.160E 02 TE=6.30E 02 NE=2.60E 13 ZAVG=20.30 L=13 K=25 IT= 496 NQ=3 H=1.79E-03 FL,BL,DC= 2.0E-06 1.8E-07 2.0E-08
 Y= 0.000000 0.000000 0.000000 0.000023 0.000684 0.008274 0.052829 0.178802 0.320734 0.287014
 0.127655 0.022484 0.001416

T(MS)=1.300E 02 TE=6.30E 02 NE=2.10E 13 ZAVG=20.25 L=13 K=25 IT= 505 NQ=3 H=2.29E-03 FL,BL,DC= 2.0E-06 1.8E-07 2.0E-08
 Y= 0.000000 0.000000 0.000000 0.000025 0.000752 0.009013 0.056726 0.187872 0.326791 0.280181
 0.118009 0.019414 0.001130