Anode Sheath Contributions in Plasma Thrusters

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Submitted in partial fulfillment
of the requirements for the degrees of

AERONAUTICAL & ASTRONAUTICAL ENGINEER
and
MASTER OF SCIENCE IN ASTRONAUTICAL ENGINEERING

from the

NAVAL POSTGRADUATE SCHOOL
March 1994

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE March 1994	3. REPORT TYPE AND DATES COVERED Engineer's and Master's Thesis

4. TITLE AND SUBTITLE ANODE SHEATH CONTRIBUTIONS IN PLASMA THRUSTERS

5. FUNDING NUMBERS

6. AUTHOR(S) Riggs, John Forrest

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Naval Postgraduate School
Monterey CA 93943-5000

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES The views expressed in this thesis are those of the author and do not reflect the official policy or position of the Department of Defense or the U.S. Government.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE
A

13. ABSTRACT *(maximum 200 words)*

Contributions of the anode to Magnetoplasmadynamic (MPD) thruster performance are considered. High energy losses at this electrode, surface erosion, and sheath/ionization effects must be controlled in designs of practical interest. Current constriction or spotting at the anode, evolving into localized surface damage and considerable throat erosion, is shown to be related to the electron temperature's (T_e) rise above the gas temperature (T_o). An elementary one-dimensional description of a collisional sheath which highlights the role of T_e is presented. Computations to model the one-dimensional sheath are attempted using a set of five coupled first-order, nonlinear differential equations describing the electric field, as well as the species current and number densities. For a large temperature nonequilibrium (i.e., $T_e >> T_o$), the one-dimensional approach fails to give reasonable answers and a multidimensional description is deemed necessary. Thus, anode spotting may be precipitated by the elevation of T_e among other factors. A review of transpiration cooling as a means of recouping some anode power is included. Active anode cooling via transpiration cooling would result in (1) quenching T_e, (2) adding "hot" propellant to exhaust, and (3) reducing the local electron Hall parameter. However, significant technical problems remain.

15. NUMBER OF PAGES 106

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. 239-18

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ACKNOWLEDGMENT

I dedicate this work to my dear wife Lin, for her support and understanding during my absence as a geographical bachelor of almost three years.

My sincere thanks to my parents for encouraging me to pursue my ambitions from childhood on, and to Oscar Biblarz, Ph.D., for patiently helping me to understand plasma physics.

I. INTRODUCTION

Several types of space flight propulsion systems have been developed over the years. These include chemical, nuclear, electric and solar propulsion. The majority of space thrusters to date have been chemical rockets. Although the Chinese used rockets over 800 years ago, true development of rocket propulsion took place during this century [Ref. 1]. Chemical thrusters give high thrust-to-weight ratios, larger than unity, and have been fully developed in the form of space launch vehicles and attitude control thrusters. In contrast, other propulsion systems have been developed only to the proof-of-concept stage, and essentially remain at this stage of development. Nuclear propulsion was studied with the NERVA (Nuclear Engine for Rocket Vehicle Application) thruster in the 1960's, and abandoned [Ref. 2:pp. 517-519]. Electric propulsion flights during the 1960's included the U.S. SERT-1 (Space Electric Rocket Test) in 1964 and the U.S.S.R. Yantari-1 rocket in 1966. Solar-electric propulsion was demonstrated via the SERT-2 rocket in 1970, powering the electric thruster from power generated by solar cells. Further electric propulsion research flights in the 1980's included the U.S. Navy's NOVA-1 satellite in 1981, and Japan's MS-T4 satellite,launched from the Space Shuttle. Beyond this, nonchemical thrusters have only been used in auxiliary roles, such as station-keeping and attitude control on geosynchronous satellites. NASA's Project PATHFINDER in the mid-1980's proposed the use of a megawatt-level electric plasma thruster for a manned Mars mission. However, development of this project was never funded.

In comparing the different propulsion schemes, a primary performance indicator is specific impulse, defined as the ratio of thrust to the rate of propellant usage, or alternately, propellant effective exhaust velocity (u_e), divided by the sea-level gravitational constant, (g_o).

$$I_{sp} = \frac{\dot{m} u_e}{\dot{m} g_o} = \frac{u_e}{g_o} \quad \text{sec} \tag{1}$$

Chemical rockets are inherently limited in performance by the total energy available in the fuel/oxidizer combustion process, so that the total enthalpy available for conversion into exhaust kinetic energy is limited. Exhaust velocity is also limited by material heating limitations of the combustion chamber and nozzle throat, and "frozen flow Losses" (unrecoverable energy deposition in internal modes of the gas) [Ref. 3:pp. 4-5]. Peak specific impulse for liquid chemical propellants is presently on the order of 450 seconds. This capability is completely sufficient for the tasks of launch to low earth orbit (LEO), attitude control, station keeping, and such missions. However, for missions such as manned interplanetary exploration, chemical propulsion can be shown to be clearly inadequate. A comparative analysis of a Mars mission using chemical and electric propulsion systems shows the large difference in mass payload ratio (final mass/initial launch mass) for the two systems. A chemical system using a high impulse Hohman ellipse trajectory delivers a maximum of approximately 10% to 18% of the launch mass to the Martian surface [Ref. 4:p. 115]. In comparison, an electric system using a low impulse spiral trajectory could deliver from 20% to 60% of the launch mass, depending on the desired transit time. Each mission assumes transit from low Earth orbit to Mars orbit. An electric propulsion system would still need a high thrust propulsion system to reach the Martian surface Ref. 5:pp. 344-346]. The large difference in payload ratio is due to the much larger exhaust velocity and more efficient use of fuel by electric propulsion. Thus, some form of electric or hybrid electric thruster would seem to be in order for such interplanetary missions. However, due to the low thrust-to-weight ratio of electric thrusters, they must be launched into orbit by other means. Their usefulness is restricted to space thrusters, not to launch systems.

With specific impulses of as high as 10,000 seconds, electric propulsion offers the performance envelope needed for manned interplanetary missions. Electric propulsion is divided into three types of thrusters: electrostatic, electrothermal, and electromagnetic. The type relevant to this work is the magnetoplasmadynamic (MPD) thruster, an electromagnetic propulsion system that utilizes the Lorentz force created by an electric current together with its induced magnetic field to propel a gas that has been heated to the plasma state. According to electromagnetic theory, a conductor carrying a current produces an induced magnetic force perpendicular to the current. The applied electric field and its induced magnetic field interact to produce the Lorentz force ($\vec{F} = \vec{j} \times \vec{B}$) perpendicular to both fields on the conductors. This briefly summarizes the concept behind the "self-field" MPD accelerator [Ref. 2:pp. 485-486]. MPD performance is enhanced by adding magnetic coils to the thruster, thus strengthening the magnetic field and, as a consequence, the Lorentz force and thrust. This thruster is appropriately called an "applied-field" MPD thruster. MPD thrusters have shown specific impulses of up to 7,000 seconds and efficiencies as high as 70% [Ref. 6:pp. 2-3]. Performance of MPD thrusters is limited by several factors, including electrode erosion, current spotting, frozen flow losses, and electrode power deposition. Specifically, anode power deposition is the single largest power loss mechanism in MPD thrusters operating at submegawatt power levels [Ref. 7]. In the following work, we review and analytically model the MPD anode, including the sheath and anode potential drop.

II. LITERATURE REVIEW

Anode losses significantly limit magnetoplasmadynamic (MPD) thruster performance. Much effort has been placed on characterizing these losses and on the nature of power deposition in the anode [Refs. 8-14]. As much as 80% of thruster total power may end up being deposited in the anode at sub-megawatt power levels [Refs. 8,15]. This power deposition together with current constriction at the anode surface present serious problems to thruster cooling and performance, as well as to anode lifetime. Before any practical design can be achieved, a more thorough understanding of the phenomena at the anode, particularly the anode sheath, must be gained. Studies have shown that the anode power fraction depends on thruster power, current, mass flow rate, and the parameter $J^2/\dot{m}$ [Refs. 8,12,13,16]. It has also been shown that the anode fall voltage is inversely proportional to anode current density [Refs. 13,16]. It is believed that a better understanding of the role of an elevated electron temperature, of current flow dimensionality, and of current unsteadiness are prerequisites for the evolution of any practical MPD thruster design.

Computer codes that accurately describe observed data from steady-state MPD thrusters have been developed [Refs. 17-19]. However, these codes do not adequately describe observed data from quasi-steady thruster experiments. It has been suggested that the lack of proper electrode modelling (i.e., sheaths and fall potentials) in these codes may explain this discrepancy [Ref. 6]. Limited analytical work has been done in modelling the sheath and ambipolar regions at the anode, influenced perhaps by the difficult set of coupled, nonlinear partial differential equations involved. Hugel [Ref. 12] and Subramaniam [Ref. 20] address the influence of the sheath region, but do not model the electric field, temperature, or sheath fall voltage.

Given the minuscule extent of the sheath versus thruster anode curvature, the problem at first appears one-dimensional in nature. A one-dimensional, collisional, equilibrium solution can satisfactorily reproduce the observed electric field and charge density distributions for the entire sheath and ambipolar regions for a sheath where the electron temperature equals that of the heavy species [Ref. 21]. However, this model cannot describe any decrease in current density away from the surface, or current constriction, at the anode surface which might be necessary in nonequilibrium. A two-dimensional model, developed by Biblarz and Dolson [Ref. 14], represents these phenomena and predicts the voltage drop in the region. It is shown that the sheath must account for a majority of the anode voltage drop, and that the sheath extent must be greater than the Debye length [Refs. 14,21]. Thus, a combination of one- and two-dimensional approaches appears to better describe sheath behavior. Incorporation of modelling of this sort may improve the ability of the computer codes cited above to properly describe quasi-steady thrusters.

Next, a description of the anode region is presented in order to delineate some of the possible effects of temperature.

III. ANODE DESCRIPTION

A. THRUSTER GEOMETRY DESCRIPTION

The majority of plasma thrusters to date have consisted of a central cathode rod surrounded by an annular shell anode, as shown in Figure 1 [Ref. 23]. The thruster illustrated is sufficient to produce needed thrust at current levels above one kiloamp. Below this level, an external magnetic field produced by an annular magnet is needed to ensure sufficient Lorentz force on the plasma propellant to meet thrust requirements. [Ref. 8]. As illustrated in Figure 1, the $\vec{j}\times\vec{B}$ body force simplifies into an axial $(j_r B_\theta)$ body force, which provides direct electromagnetic thrust ("blowing"), and a radial $(-j_z B_\theta)$ body force, which provides electromagnetic compression of the plasma and a subsequent pressure force along the cathode surface ("pumping"). [Ref. 6]

A notable exception to this geometry is the Stationary Plasma Thruster (SPT), a design from the former Soviet Union. The SPT is an example of a plasma propulsion system known as a Hall Current Plasma accelerator. An electric field is applied axially to a stream of flowing plasma, in addition to a magnetic field with a strong radial component, which is applied by an external electromagnet. When the axial electric field is applied and a current flows through the plasma, an azimuthal component of current is induced, i.e., the "Hall" current.

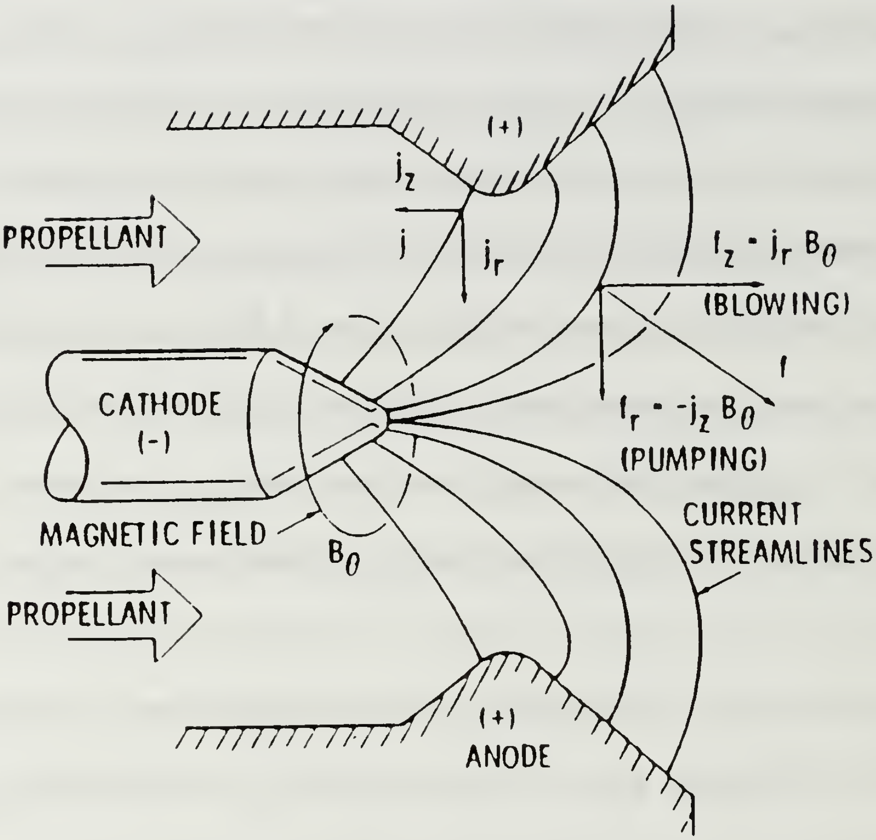

Figure 1 - Magnetoplasmadynamic (MPD) Thruster, with Axial and Radial Forces on Plasma Indicated. [Ref. 23]

Thrust is produced by electrostatically accelerating the ions in the plasma, as well as through the induced Lorentz force mentioned above. A strong radial magnetic field is applied to the plasma, whose properties are controlled to make the electron Larmor radius[1] small compared to the mean free path[2], while the ion Larmor radius is comparatively large. As a consequence, electron mobility in the axial direction is greatly reduced. Thus, the electric field energy is given mainly to the ions, producing axial ion acceleration. Collisions with neutral particles serve to accelerate the entire neutral plasma. [Ref. 24]

A pair of the final prototype design developed, the SPT-100, have been acquired by NASA recently from Fakel Enterprise in Kaliningrad, Russia, and are undergoing performance evaluation at the Jet Propulsion Laboratory. Designed at the Kurchatov Institute of Atomic Energy (IAE) in Moscow, USSR in the 1960's, smaller versions of the SPT-100 (SPT-50 and SPT-70) were flown beginning in 1972[3]. A specific impulse of 1,600 seconds and 50% efficiency, as well as space flights of fifty similar thrusters is claimed. The specific operational characteristics of the thruster are not well understood presently. Bohm diffusion of electrons and a phenomenon called "near-wall conductivity" have been proposed to explain the thruster's operation. This thruster is shown in Figure 2. [Ref. 25]

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[1] Larmor radius is the radius of the helix traversed by a charged particle moving in a magnetic field.

[2] Mean free path is the distance traveled by a particle before making a collision.

[3] The suffix (i.e.,"-70") indicates the characteristic diameter of the thruster in millimeters.

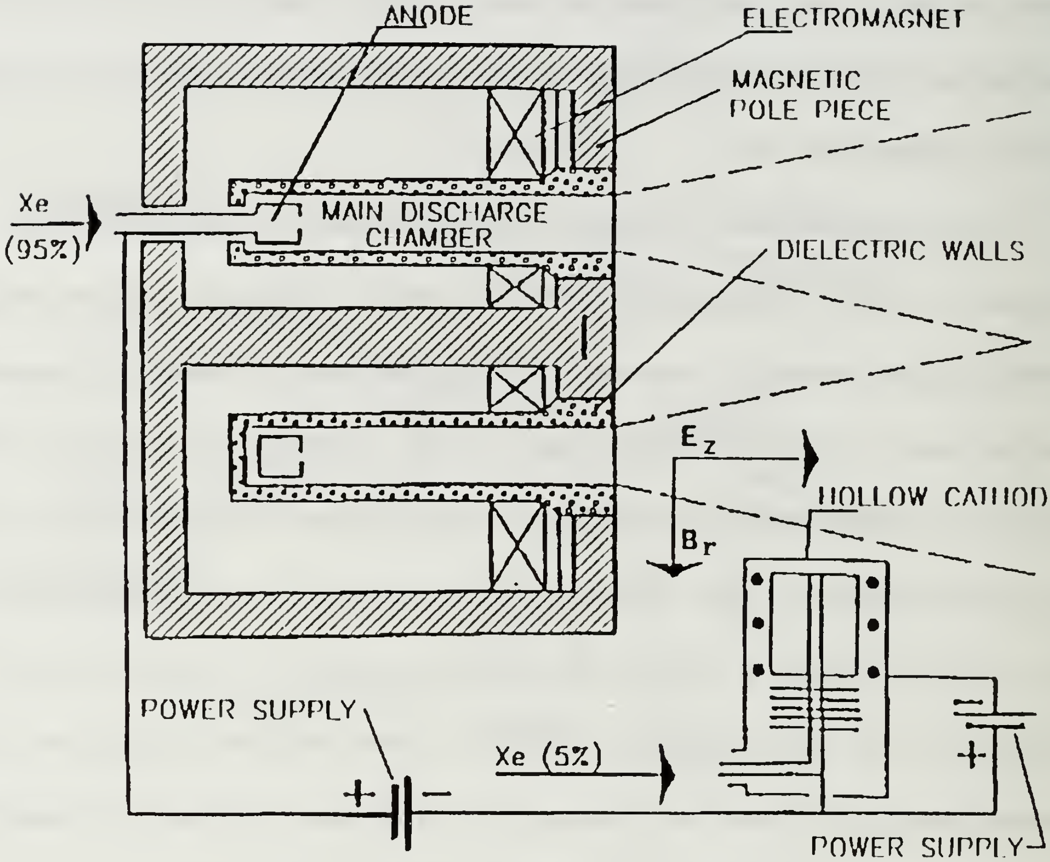

Figure 2 - Stationary Plasma Thruster [Ref. 25]

B. ELEMENTARY SHEATH FORMULAE DESCRIPTION

1. Discussion

Voltage losses and anode power deposition account for most of the inefficiency of plasma thrusters. In order to understand these losses, the anode region must be understood and related phenomena explained and modelled. As shown in Figure 3, a substantial drop in voltage occurs in a short distance from the anode surface.

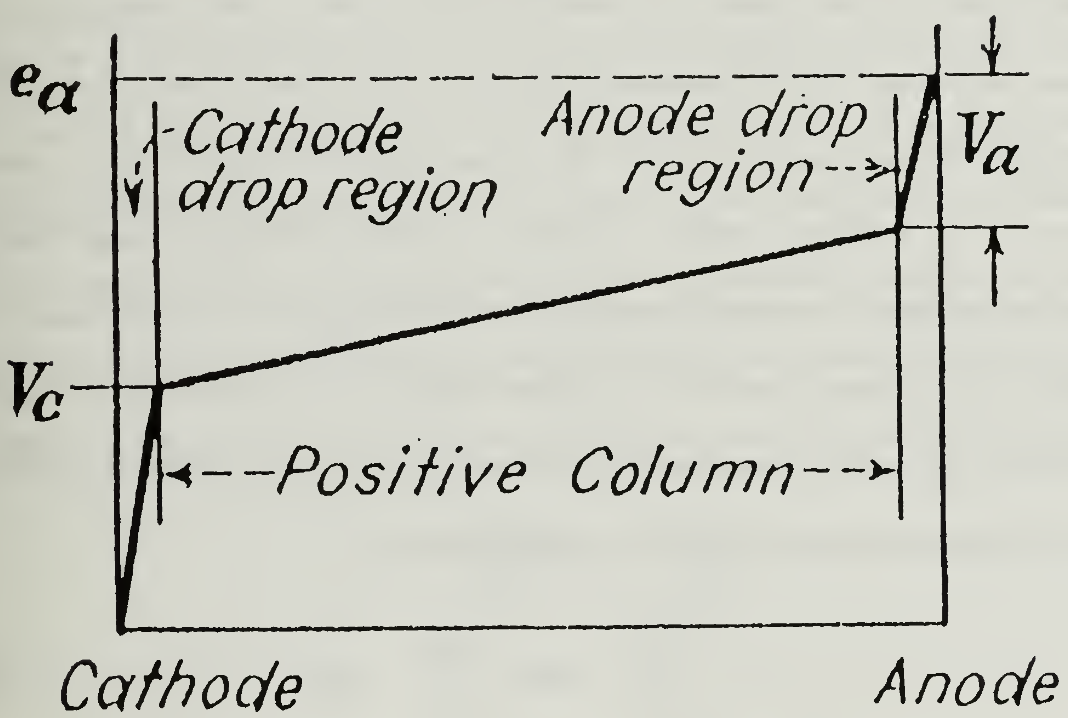

Figure 3 - Electric Field Between Two Electrodes, Including "Positive Column". [Ref. 27]

The anode fall region may be divided into two parts, the sheath and ambipolar regions. The plasma attempts to adjust itself near electrodes so as to shield the main body of the plasma from the electric field [Ref. 26]. The sheath is the region closest to the anode surface within which the ion and electron number densities are unequal, with the electrons dominating the region. A high electron space charge exists at the anode surface. This is caused by the anode collecting incoming electrons in completing the arc current with the cathode. Positive ions are produced within the sheath by electron impact of neutral gas molecules, and the ions are repelled toward the cathode. At the cathode end of the anode drop region, the density of positive ions is high enough to almost neutralize the electron space charge, thus forming the positive column or core plasma. The essential positive ion current is created in this way near the anode. A more complete description of this process may be found in Cobine [Ref. 27] and von Engel [Ref. 28]. A fundamental characteristic of plasma behavior is its tendency toward electrical neutrality. Whenever local charge concentrations arise or external potentials are introduced into a system, these are shielded out in a distance known as the "Debye length"[4]. This distance must be much smaller than the system dimension for the ionized gas to be considered a plasma [Ref. 29]. Equation (2) gives the Debye length [Ref. 26].

$$\lambda_d = \sqrt{\frac{\epsilon_0 kT}{n_\infty e^2}} = 69.0\sqrt{\frac{T}{n_\infty}} \quad \text{(m)} \tag{2}$$

---

[4] The Debye length effectively describes the radius of a shell around a charged particle outside of which the potential of the particle is not seen.

Another distance of interest is the electron mean free path, or distance traveled by a particle before making a collision. Equation (3) is from a derivation of Lin, Resler, and Kantrowitz [Refs. 30,31] giving the mean free path, with λ_s being the approximate sheath length.

$$\lambda = 0.12\left(\frac{1}{n_e(e^2/3kT)^2\ln(\lambda_s e^2/3kT)}\right) \qquad (3)$$

Since the sheath extends at most a few mean-free lengths from the anode surface, curvature of the anode does not affect the governing equations in high pressure discharges. Thus, the region may be described in one dimension, the distance "y" from the anode surface. While the Debye length is sometimes assumed as the sheath extent, Reference 22 showed that the sheath thickness is a function of the anode fall voltage and the electron temperature. Equation (4) gives the appropriate form.

$$\lambda_s \approx \sqrt{\frac{\epsilon_o \Phi_a}{e n_\infty}} = \lambda_D \sqrt{\frac{e\Phi_a}{kT_e}} \qquad (4)$$

An example case with a fall voltage of 100 volts gives a sheath extent of $\lambda_s = 2.352\times10^{-5}\ m$. This compares to a computed Debye length of $\lambda_D = 1.690\times10^{-6}\ m$. Therefore, the sheath can be an order of magnitude larger than the Debye length.

Nasser [Ref. 32] discusses an elementary theoretical approach to the glow discharge problem. He suggests a set of four one-dimensional ordinary differential equations, including the electron and ion current and number density equations, in addition to Poisson's equation. Most solution attempts have failed, with the boundary conditions being identified as the culprit. A similar attempt for the plasma thruster is discussed below.

2. Simplified Formulation

The steady probe equations are first written [Ref. 21] in their simplest form. The anode is assumed to operate as a heavily biased probe, which is true for low enough currents when the anode is not a source of ions. Whenever the temperature can be considered fixed, the energy equations are implicitly satisfied and, since ion inertia is neglected, the resulting set consists only of two species continuity equations and Poisson's equation. These equations are written in terms of y, which is the coordinate outward from the planar positive surface. Constants and variables are listed in Table 1.

TABLE 1 - NOMENCLATURE

a...characteristic length of plasma

$D_{i,e}$...species diffusion coefficient

e...elementary charge constant

E...electric field

E_o...electric field at anode surface

E_∞...electric field at core plasma

$j_{i,e}$...species current density

J...total current

k...Boltzmann's constant

K...current parameter

$n_{i,e}$...species number density

$\dot{n}_e$...time rate-of-change of n_e

n_∞...species number density at core plasma

N...total number density

T...temperature

T_o...neutral species temperature

α...two-body recombination coefficient

ϵ_o...permittivity constant

ν...ionization coefficient

$\mu_{i,e}$...species mobility coefficient

Φ_a...anode fall potential

λ...mean-free distance

λ_d...Debye length

λ_s...Sheath thickness

Note: Species subscripts denote ions (i) and electrons (e).

$$j_i = e\mu_i n_i E - (eD_i)\frac{dn_i}{dy} \tag{5}$$

$$j_e = e\mu_e n_e E + (eD_e)\frac{dn_e}{dy} \tag{6}$$

$$\frac{dE}{dy} = \frac{e}{\epsilon_o}(n_i - n_e) \tag{7}$$

$$J = j_i + j_e \tag{8}$$

$$\mu_{i,e} = \frac{eD_{i,e}}{kT_{i,e}} \tag{9}$$

Here, the j's are species contributions to the total current density. The existence of negative charges as free electrons is pivotal in the formulation. Next, the Einstein relation, equation (9), is introduced to write the mobilities in terms of the diffusion coefficients. We assume that the diffusion coefficients remain constant in the problem.

Equations (5) and (6) are next solved for $dn_{i,e}/dy$. The species current density equations are found from the net reaction rate of the plasma. Equations (10) and (11) combine to produce space derivatives for species current density.

$$\dot{n}_e = \nu_i n_e - \alpha n_i n_e \qquad (10)$$

$$\frac{dj_i}{dy} = \frac{-dj_e}{dy} = e\dot{n}_e \qquad (11)$$

Combining equations (5)-(11) produces a set of five coupled, non-linear differential equations describing the sheath. These are nondimensionalized to adjust all variables to the first order, and are rewritten below as equations (12)-(16), with nondimensionalized variables denoted by "$\tilde{x}$". Nondimensionalization can be accomplished as follows: The species number densities n_e,n_i, are divided by their values at infinity to produce output from the anode surface to unity at the ambipolar boundary. The current densities j_e,j_i are divided by the total current, allowing the output to show the "mirror behavior" of the two currents. The electric field is divided by the initial anode value to give output starting from unity at the surface and decreasing to the final core field value. The variable "y" is divided by the characteristic length[5] of the plasma, "a", producing $\tilde{y}$. These corrections allow all output to vary in the range from zero to one, as a function of distance from the anode.

---

[5] The characteristic length is defined so as to cancel the multiplying factor in the electric field equation, (14), ($a = 1.107 \times 10^{-6}$). This allows a physical interpretation of the ion/electron number densities, as well as the decay rate of the electric field.

$$\frac{d\tilde{n}_i}{d\bar{y}} = \left(\frac{aeE_o}{kT_o}\right) \tilde{n}_i \bar{E} - \left(\frac{aeE_\infty}{kT_o}\right) \bar{j}_i \tag{12}$$

$$\frac{d\tilde{n}_e}{d\bar{y}} = -\left(\frac{aeE_o}{kT_o}\right) \tilde{n}_e \bar{E} + \left(\frac{aeE_\infty}{kT_o}\right) \bar{j}_e \tag{13}$$

$$\frac{d\bar{E}}{d\bar{y}} = \left(\frac{aen_\infty}{E_o \epsilon_o}\right) (\tilde{n}_i - \tilde{n}_e) \tag{14}$$

$$\frac{d\bar{j}_e}{d\bar{y}} = -\left(\frac{akT_o \nu_i}{eE_\infty D_e}\right) \tilde{n}_e \, (\bar{v}_i - \alpha \tilde{n}_i) \tag{15}$$

$$\frac{d\bar{j}_i}{d\bar{y}} = \left(\frac{akT_o \nu_i}{eE_\infty D_e}\right) \tilde{n}_e \, (\bar{v}_i - \alpha \tilde{n}_i) \tag{16}$$

Attempts to solve this equation set using the computer code discussed below shows the set to be extremely sensitive to initial conditions. The computer code solver uses a "marching" scheme from the anode to the undisturbed plasma. The initial conditions are chosen to produce the electric field potential drop observed in actual thrusters. First and second space derivatives of the electric field are used as diagnostic checks to ensure reasonable output values and indicate instability of the integration process. Figure 4 shows the required resulting curves for the electric field and its first and second derivatives.

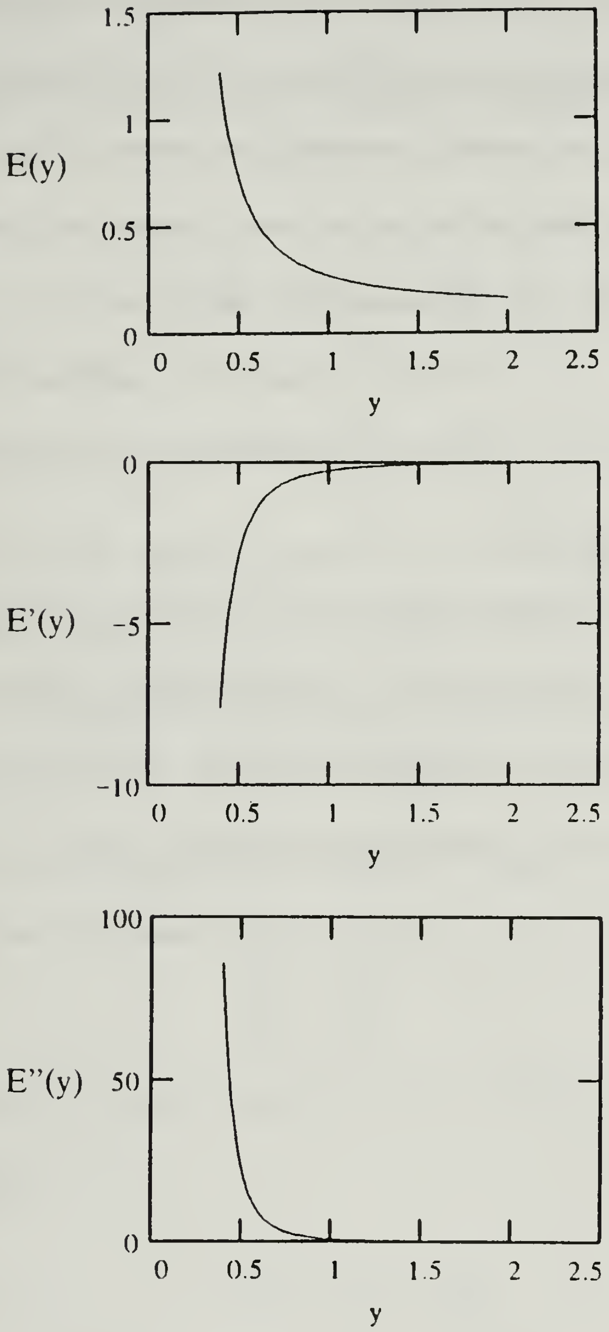

Figure 4 - Electric Field and First Two Space Derivatives Used as Diagnostic Checks for Integrator Output. (Plotted for a Generic Exponential Function).

Ecker characterizes the plasma at the anode as a double sheath, with the inner section called the "inertia sheath", and an outer section called the "energy loss section". The inner section shows a potential rise of the order of one volt, with the outer section showing the exponential potential drop shown in Figure 4. While this double sheath may in fact describe the actual sheath region, the formulation above only models the potential drop portion of the sheath, and does not attempt to produce the potential rise of the inner sheath. In addition, Ecker's current constrictions are of a "macroscopic" nature, whereas those of Reference 14 and this work are "microscopic" [Ref. 33].

Data for a 6,000°K Nitrogen plasma were used to test the equation set [Ref. 21]. Producing a proper solution required adjusting the initial conditions to force the curve shapes discussed above. Using Equations (2), (3), and (4), the mean free path, Debye length, and approximate sheath extent are calculated as $\lambda = 9.352\times10^{-3}$ m, $\lambda_D = 1.690\times10^{-6}$ m, and $\lambda_S = 2.352\times10^{-5}$ m (this assumes a drop voltage of 100 volts).

3. Approximate Formulation

Reference 21 explores the above equation set by taking advantage of the symmetry among the equations, and introducing two parameters, K^+ and K^-, shown below.

$$K^+ \equiv \frac{j_i}{eD_i} + \frac{j_e}{eD_e} \tag{17}$$

$$-K^- \equiv \frac{j_i}{eD_i} - \frac{j_e}{eD_e} \tag{18}$$

It can be shown that the resulting equations can be manipulated to yield a single, ordinary differential equation for the K's in terms of the electric field. The resulting equation can be scrutinized for two distinct temperature regimes. Note that while the total current density, J, is constant in a steady, one-dimensional case, the K's can vary and will in turn also depend on the degree of reactivity of the plasma ($\dot{n}_e$), i.e.,

$$\frac{dj_i}{dy} = \frac{-dj_e}{dy} = e\dot{n}_e \tag{19}$$

Because ion diffusion is much slower than electron diffusion, it can be shown that the K's are related by

$$K^+ \approx -K^- + \frac{2J}{eD_e} \tag{20}$$

As will be evident, at the electrode surface the K's are equal to each other and at the undisturbed plasma, $K^- = 0$. The total current density may be evaluated from

$$J = e n_{\infty} v_{e\infty} \tag{21}$$

where $v_{e\infty}$ is the electron drift velocity beyond the ambipolar region which is strictly a function of E_{∞}/N, (i.e., of the ratio of undisturbed electric field to the total number density).

a. *Effects of Temperature on Anode Constriction*

It is useful to investigate the overall effects of temperature. Since temperature will be considered constant, it comes in as a parameter in this formulation whereas charge density and electric field remain as variables. Intuitive arguments will be introduced which suggest that the electron and ion/neutral temperatures play a rather singular role in determining the intrinsic dimensionality of the problem, (i.e., there are cases when the geometry of the current lines is not necessarily impressed by the electrode geometry). Since the problem is described by moderate pressure, largely collisional sheaths, the ion and neutral temperatures are anticipated to remain reasonably equal. Depending on the gas, the electron temperature, on the other hand, can be elevated from the gas temperature at the anode where actual magnitudes depend on the local value of E/N. In order to get a perspective on the effects of temperature, we shall consider two extremes, namely, the case where the electron and ion temperature are the same (the equilibrium case) and the case where the electron temperature is substantially elevated from that of the ions/neutrals (the two-temperature case).

(1) Case I: $T_e = T_i = T_o$ *(Equilibrium)*

The charge densities can be eliminated by combining equations (5)-(9), (17) and (18). The resulting equation can be shown to be

$$\frac{kT_o}{e}\left(\frac{K^{*}}{E}\right)' + K^{*} = \frac{2J}{eD_e} - \left(\frac{kT_o \epsilon_o}{e^2}\right)\frac{1}{E^2}\left[EE'' - (E')^2 - \frac{1}{4}\left(\frac{e}{kT_o}\right)^2 E^4\right]' \tag{22}$$

If the electric field decreases monotonically from the wall to the undisturbed plasma (i.e., from $E_o \rightarrow E_\infty$), then as $y \rightarrow \infty$, $E \rightarrow E_\infty$, $E' \rightarrow 0$, $E'' \rightarrow 0$.

So that in equation (22) above the "outer solution" becomes:

$$K^{*} = \frac{2J}{eD_e} \tag{23}$$

Now this represents an acceptable solution from a physical point of view. Moreover, as $y \rightarrow \infty$,

$$\dot{n}_{e\infty} \approx D_i (K^{*})' \approx 0 \tag{24}$$

which is also acceptable for an equilibrium situation at the undisturbed plasma. Results [Ref. 21] are shown in Figure 5 for the case of nitrogen at 6000°K using an approximate electric field distribution.

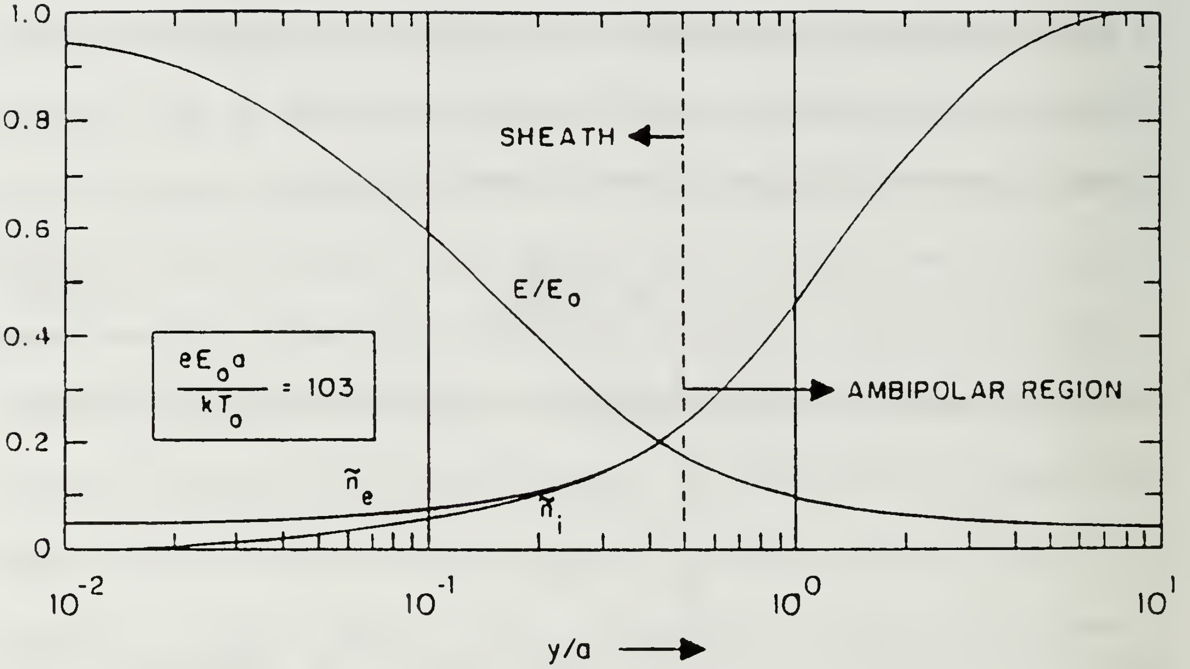

Figure 5 - Electric Field and Species as a Function of $\tilde{y}$, Distance From Anode. An Approximation Using a Shaped Electric Field and Isothermal Plasma [Ref. 21].

(2) *Case II:* $T_e >> T_i = T_o$ *(Two-Temperature)*

In this case the same procedure as before yields the following equation where terms divided by T_e have been dropped when compared to their counterparts divided by T_o.

$$(K^+)' - \frac{K^+}{E} E' = \frac{2EJ}{kT_oD_e} + \frac{2\epsilon_o}{kT_o} EE'' + \frac{\epsilon_o}{eE} E''E' - \frac{\epsilon_o}{e} E''' \qquad (25)$$

Assuming the same monotonic decrease as before for the electric field from the wall to the plasma proper, as $y \rightarrow \infty$, $E \rightarrow E_\infty$, $E' \rightarrow 0$, $E'' \rightarrow 0$.

Then the outer solution becomes

$$\frac{dK^+}{dy} \approx \frac{2eEJ}{kT_oeD_e} \quad \text{with } \dot{n}_{e\infty} > 0 \qquad (26)$$

Or, $K^+ \rightarrow (\text{constant})\, y + \text{constant}$, and $\dot{n}_{e\infty}$ keeps increasing with y.

This is <u>not</u> the proper outer solution for the one-dimensional, equilibrium plasma that we seek because the net ionization rate continues to increase well inside the plasma proper where conditions should saturate, yielding a constant electric field. Therefore, as formulated, Case II is not amenable to a one-dimensional solution. References 14 and 21 show how this case can be analyzed under a multidimensional approach. These references also discuss a method for describing the electron temperature as a function of E/N, then how to couple a simplified energy relation which satisfactorily describes a two-temperature plasma. The necessary ingredient to make equation (26) approach zero beyond the decrease of E to E_∞ is to allow J to fan out as indicated in Figure 6. Thus, in equation (26), the product "EJ" can bring down the charge production rate to arbitrarily low values. Alternatively, it is possible to explore techniques of bringing the electron temperature down to be in closer equilibrium with the ions and neutrals. Transpiration cooling is one such means.

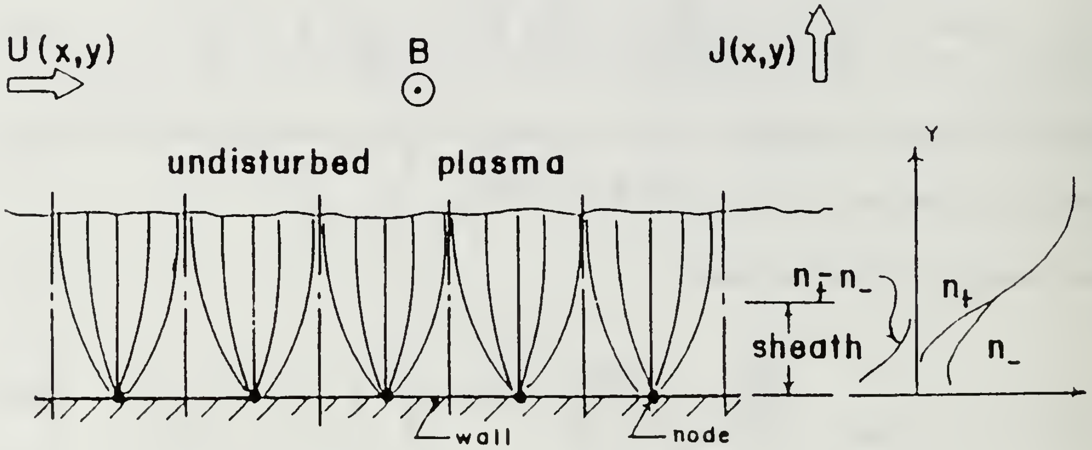

Figure 6 - Two-Dimensional Model of Current Paths Showing Periodic Structure. Thermal Instabilities and Inhomogeneities Would Favor One Site Over Others and a Single Macroscopic Constriction May Then Be Produced. [Refs. 14, 34]

b. Similarity to Vacuum Arc Phenomena

Instability phenomena observed in vacuum arcs [Ref. 35] are very similar to those observed in self-field thrusters [Ref. 12]. After the establishment of the current, the anode region operates in a vapor that issues from the electrodes. In vacuum arcs, Miller characterizes the anode region as operating in one of five distinct modes, ranging from a passive, low current mode to a high current, fully developed spot mode [Ref. 36]. Given the similarities mentioned above, vacuum arc anode research should be helpful in the understanding of MPD thruster transition to the anode spot mode. Existence diagrams after Miller [Ref. 36] are shown in Figure 7, which divide operating modes into regions as a function of anode current versus electrode geometry. Figure 7 shows the transition from glow to spot mode.

Anode spot formation at high currents is clearly a factor in limiting anode lifetime. Various phenomena have been related to anode spotting. Hugel [Ref. 12] relates the transition to spotting mode to an increase in $J^2/\dot{m}$ above a critical level. A separate factor connected with the spot mode is surface temperature of the anode. Rich, et.al., [Ref. 37] show that anode spotting is preceded by a luminous "footpoint" and followed by local melting prior to spot formation. Separately, Schuocker [Ref. 38] finds a connection between spotting initiation and the factors of anode evaporation and magnetic constriction in vacuum arcs with high currents. Experimental investigations must be performed to see if the above-mentioned vacuum arc criteria apply to self-field thrusters.

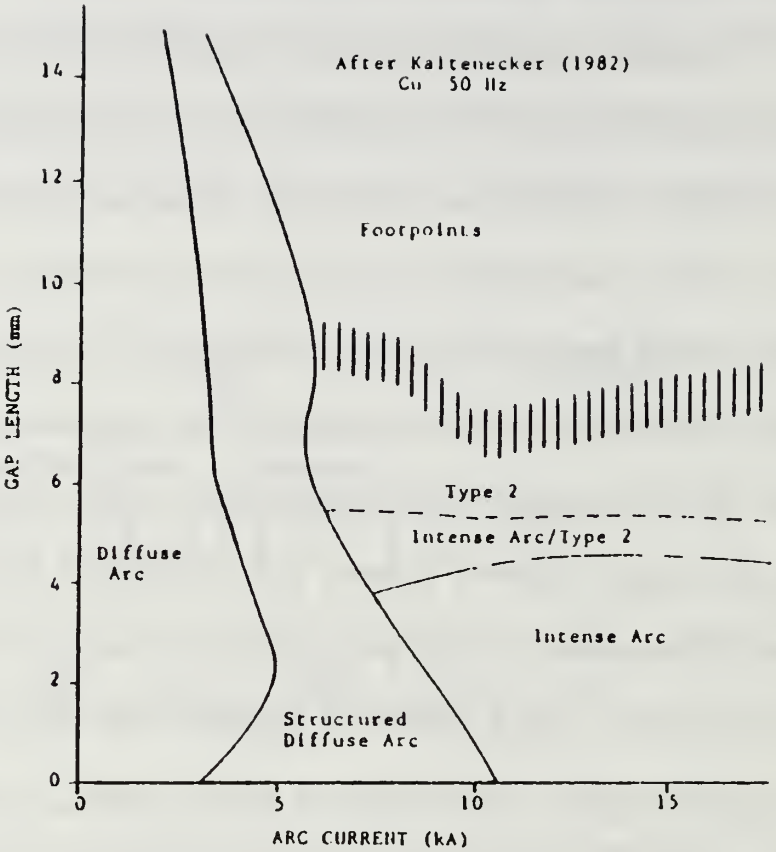

Figure 7 - Anode Discharge Modes as a Function of Current and Gap Length. [Ref. 36]

C. COMPUTER CODE

Rather than using linear approximations to equations (12)-(16), the nonlinear set was used, with initial conditions adjusted in an attempt to produce observed electric fields from probe data. First and second space derivatives of the electric field were used as diagnostic checks to ensure computed output was reasonable. Initial conditions computed from the approximate formulae in Reference 21 were used. The equation set above presents a difficult problem for two reasons, nonlinearity and multiple time constants. The species number density equations, (12) and (13), both contain a nonlinear term, each with a time constant of its own. In addition, the electric field equation, (14), adds a possible third time constant. This constitutes a "stiff" set of equations. Attempts were made to solve the set with the data discussed above, using Gear's method of backward differentiation, in hopes that the variables would change slowly enough with each iteration to render a convergent iterative process. As described in Reference 39, if some reactions are slow and others fast among a set of coupled equations, the fast ones will control the stability of the method. This is addressed in the DGEAR program available from the International Mathematical & Statistical Library (IMSL). The latter software contains an Adams predictor-corrector method, as well as Gear's method, which is well known for its success at solving stiff equation sets. The DGEAR software allows for a choice of functional or chord iteration methods, as well as a choice of Jacobian matrices. A more detailed discussion of this software can be found in Reference 39 and in the IMSL library. [Ref. 39]

D. COMPUTATIONAL RESULTS

Numerous computer runs were completed using the initial conditions taken from Reference 21. In addition, data for the ionization coefficient ν, Figure 8, was taken from References 40 and 41.

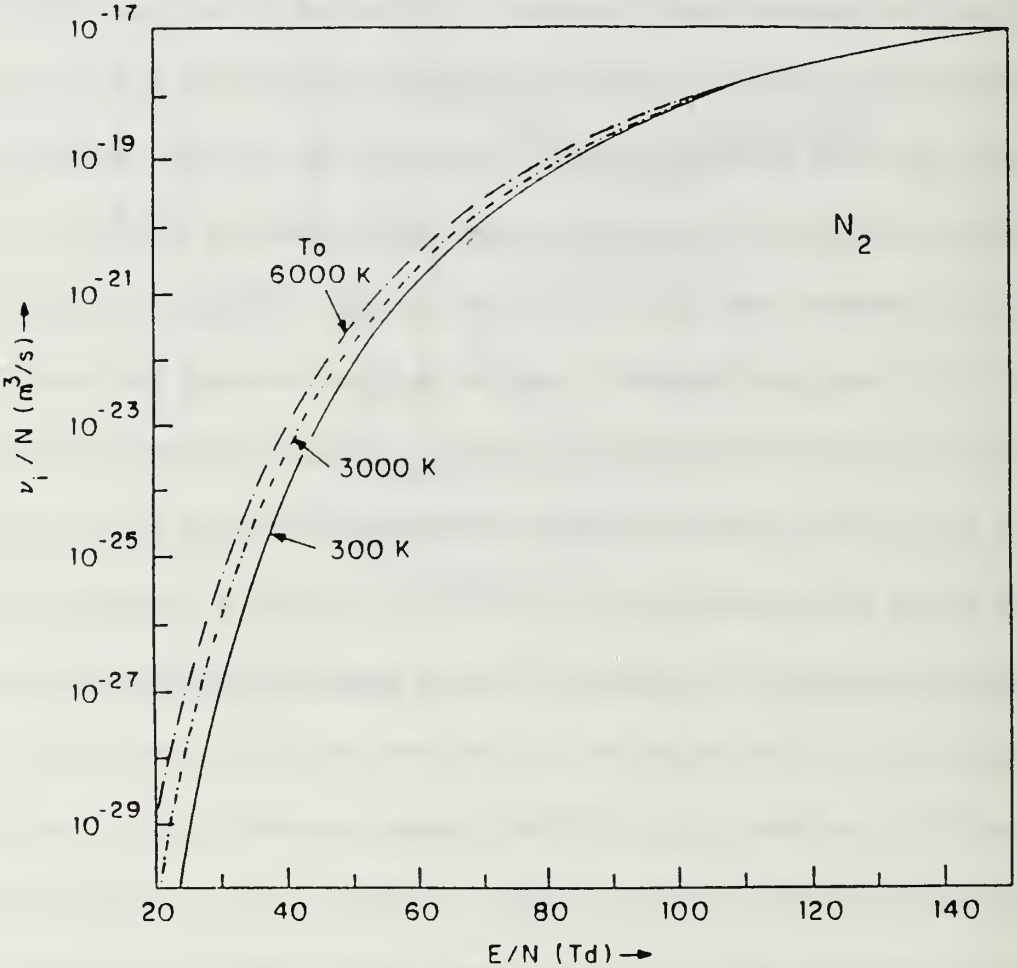

Figure 8. Ionization Coefficient ν as a Function of E/N for Nitrogen for Various Vibrational Temperatures (Refs. 40,41).

Various combinations of initial conditions and ionization coefficient were used. As mentioned above, the electric field and its space derivatives were used as diagnostic/reasonability checks on the output. Individual, as well as multiple computer runs were attempted to model the sheath region. Nonlinearities in the equation set are clearly seen in Figure 9. The ion number density does not reach that of the electrons, and the latter population growth rate continues to grow without bound. The shape of the electron population curve is very sensitive to its initial value. As shown in Figure 9, the latter population has too high a growth rate when compared to the ion population, and the latter does not "catch up". Increasing the initial value of $\tilde{n}_e$ flattens out this curve to a reasonable shape. Above an initial value of approximately 0.06, however, the plot of $\tilde{n}_e$ "dips" after a certain distance and then continues to increase as expected. This gives an approximate upper value for this initial value. To avoid instabilities like this, small "slices" were taken of the output after a small number of integration steps and multiple runs were used to form a "cut and paste" plot of the region. When a reasonable plot shape was produced, the value of ionization coefficient was varied in the "slices" to attempt to produce the required end values for electric field and species population. Both multiple and equilibrium values for the ionization coefficient were used. When the data showed signs of instability and failure to follow the required forms of Figure 4, a "slice" was made in the data stream, and the data points from this point used to start a new computer run. This approach was taken in the hope of avoiding singularities in the integration from anode surface to ambipolar region. In addition to the diagnostic checks shown in Figure 4, an additional data check is provided by the transition from the sheath to the ambipolar region.

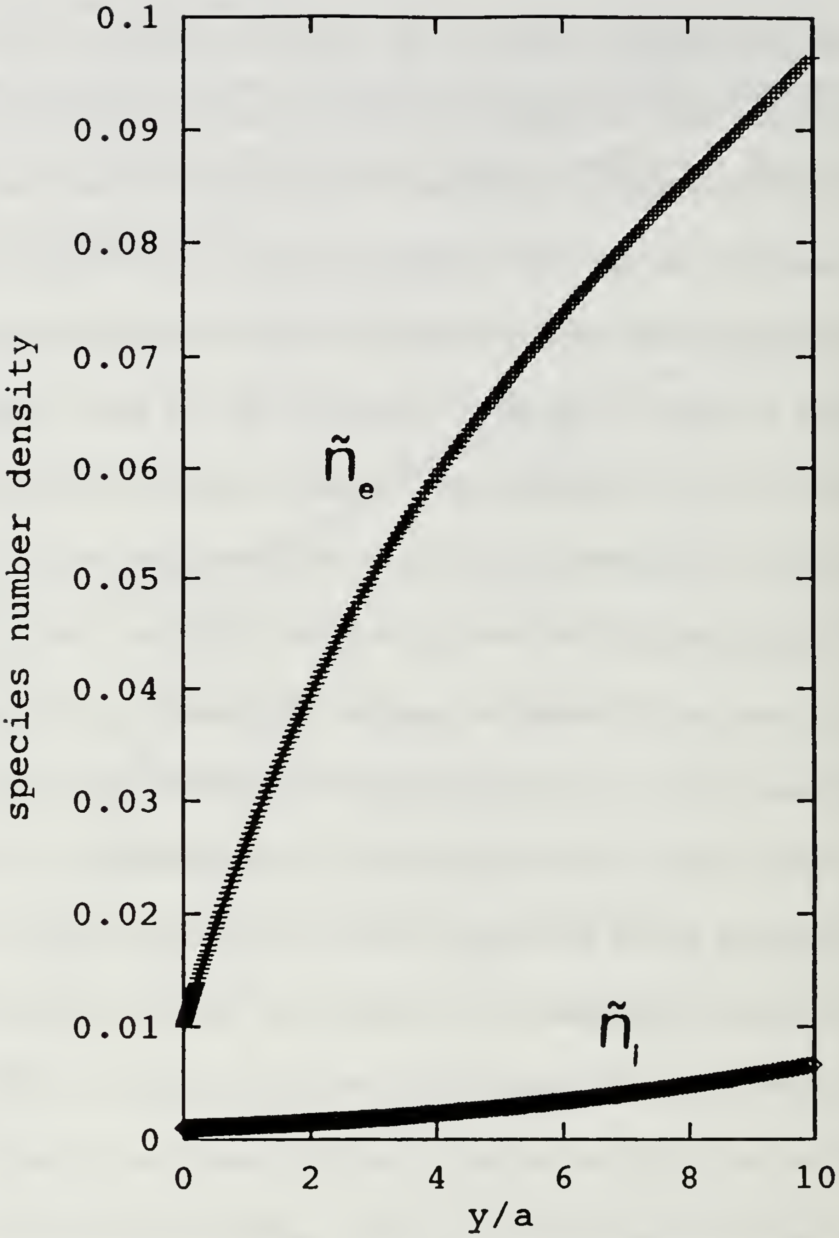

Figure 9. Species Number Density plots for Individual Computer Run, Showing Divergent Tracks for Ion and Electron Populations, and Effect of Nonlinearity.

As shown in Figure 5, the species number densities are equivalent in this region, as are their change rate. Thus, setting Equations (12) and (15) equal to each other and solving for $\tilde{n}$ yields a value of 0.5 in the ambipolar region. As indicated in Figures

10-11, the output produces the desired plot slopes for electric field and species number density. However, the number density plots cross long before approaching the required value of 0.5. In addition, neither electric field nor species number density approaches an equilibrium value or shows sign of levelling off. Apparently, the multiple time constants and nonlinear portions of the number density equations combine to create a seemingly intractable system. Solutions for this system may be possible for specific, individual initial condition sets, but the problem does not appear amenable to this approach in general. A one-dimensional system such as this may be better described through the approach of boundary layer theory or nonlinear dynamics and chaos. Given the effort and difficulty involved in the latter, a one-dimensional approach such as that modelled above does not appear useful. A combination of one- and two-dimensional modelling would appear to be more useful, as discussed in Reference 14. A one-dimensional model may be useful, but only in an approximation approach, with a shaped electric field, such as that used in Reference 21.

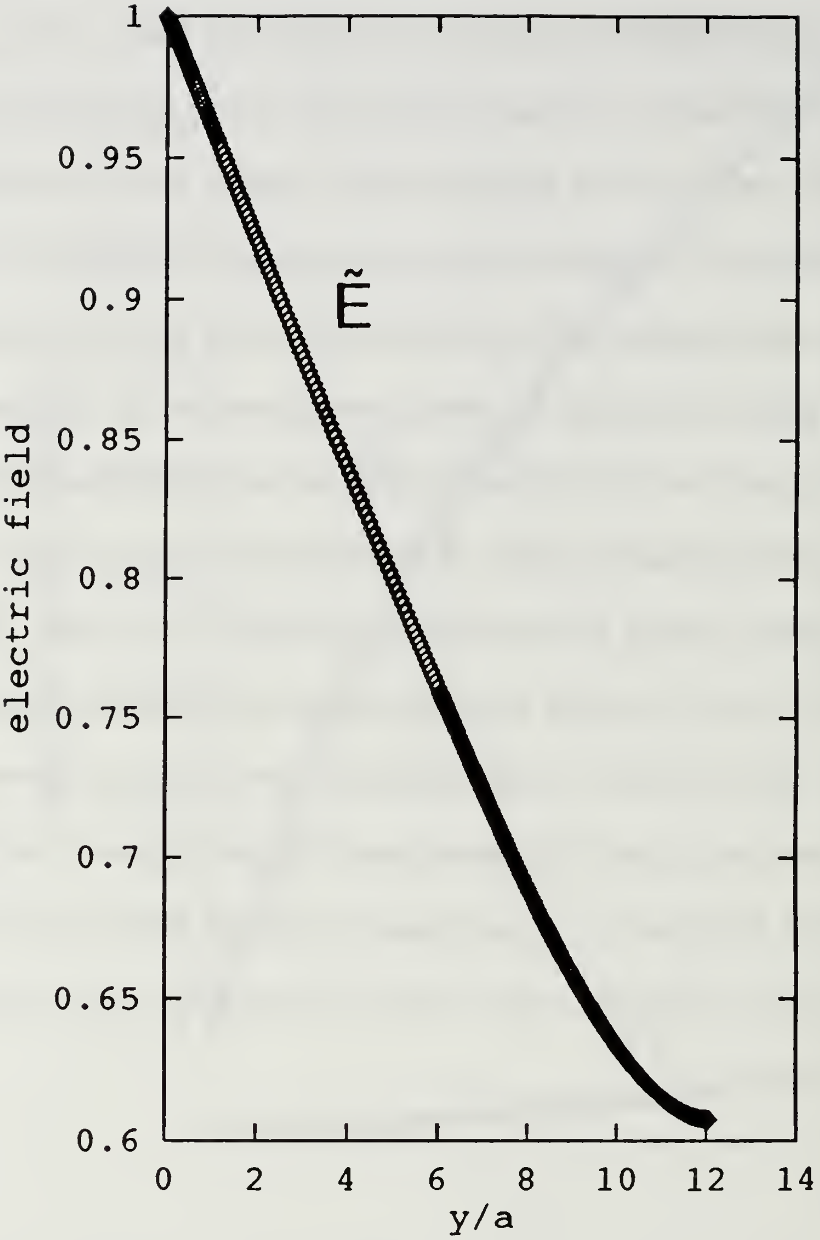

Figure 10. Electric Field as a Function of $\tilde{y}$, Distance From Anode, Using Equations (12)-(16).

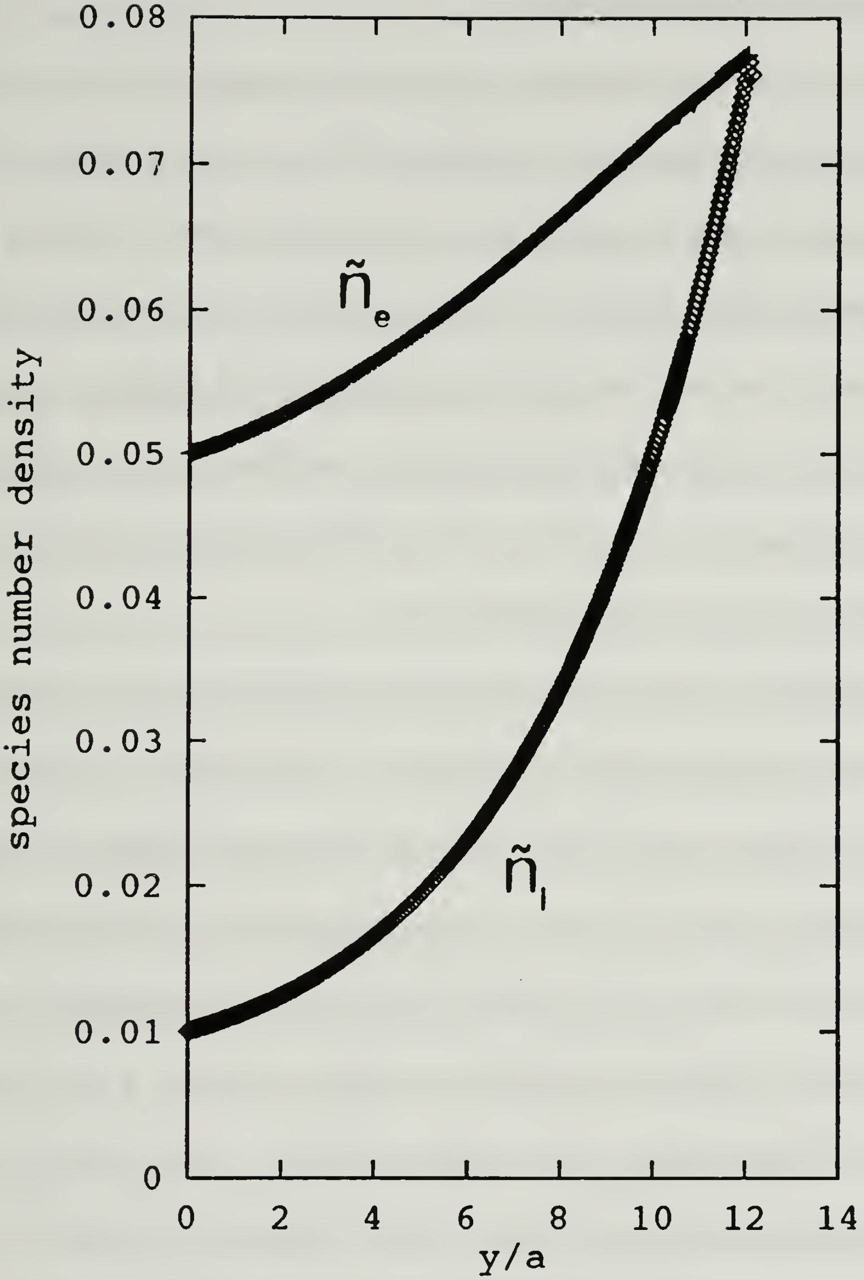

Figure 11. Species Number Density as a Function of $\tilde{y}$, Distance From Anode, Using Equations (12)-(16).

E. ANODE FALL VOLTAGE

The arc discharge operates with an anode voltage drop (V_{af}) which should be on the order of the ionization potential of the gas as it is in glow discharges. This voltage drop is largely non-ohmic because the anode region is typically very thin and space-charge controlled. Since a significant portion of the anode heating comes via the oncoming electrons accelerating through the fall voltage, it is of interest to minimize this voltage, which can range from less than ten to over 40 volts in argon. The question arises as to what governs this anode drop and why is it such a noticeable function of current? [Ref. 42]

In collisional sheaths, the anode voltage drop is largely governed by a positive ion generation region which forms in front of the anode. The production of ions reduces the space charge density and thereby permits operation at lower voltages than otherwise possible. Ions are most often created by electrons within their last few mean-free-paths before entering the anode; these ions slowly drift away from the anode, thereby effectively neutralizing the space charge, at a speed proportional to the ratio of their mobility to that of the electrons. At the anode, the electric field is a maximum and the electron mean energy displays a corresponding high.

At moderate pressures, the sheath is very thin and breakdown can be visualized as occurring between the undisturbed plasma (which acts as a rich source of electrons) and the anode surface. This arrangement has the attributes that represent "thermionic arc breakdown" [Ref. 43], a source of electrons which is independent of the breakdown itself and relatively small spacings. For gases that allow cumulative ionization (with some help from the tail of the Maxwellian distribution of electron energies), what results is a breakdown voltage appreciably below the ionization potential. This then could be an explanation for the low voltage breakdown observations [Ref. 42]. Clearly, gases with low ionization potentials and lots of atomic electron energy levels are preferred (such as cesium and barium) but low-voltage breakdown has been observed with most gases.

The increase of the anode fall voltage above the ionization potential has been related to the electron Hall parameter, since a reduction of this parameter decreases that voltage and corresponding losses. Control of the local magnetic field through the use of and array of permanent magnets as well as implementation of transpiration cooling (which increases the electron collision frequency) have both yielded some encouraging results. Because the anode fall also scales up with $J^2/\dot{m}$, it is conceivable that current inhomogeneities and plasma instabilities which are reflected in this parameter are in the picture as well. [Ref. 44]

In summary, any possible reduction of the anode fall voltage will hinge on a thorough understanding of the anode region, with its associated sheath and ambipolar regions, where electron temperature effects, ionization effects, and magnetic field effects play a pivotal role. If transpiration cooling is present, then additional phenomena of fluid-dynamic nature may come into play. Experimental observations with atmospheric discharges indicate the possible presence of convective effects at the anode. [Ref. 45]

IV. TRANSPIRATION COOLING

Transpiration cooling of the anode has often been promoted as an attractive means of recovering a large portion of the power deposited there. Additionally, the onset of melting may be minimized or even avoided by active anode cooling. Rich, et.al., related high anode temperatures to anode spotting [Ref. 37]. Similarly, Park and Choi showed that low thermal diffusion leads to erosion and, consequently, anode damage [Ref. 46]. Active anode cooling via transpiration is one means of ensuring high thermal diffusion and extending anode lifetime. Early work by Schoeck, et. al., [Ref. 47] showed that up to 80% of the energy deposited in the anode is recoverable via transpiration cooling. While this study used non-convective, high-intensity argon arcs, it is reasonable to assume that this effect would apply in MPD arcs using other propellants. Although this cooling method has not been studied for incorporation in plasma thrusters for some time, it has been recently considered as a means of cooling the fuselage of the National Aerospace Plane (NASP). Plasma thruster designs could undoubtedly gain from this database, and due consideration should be given to this cooling approach for the anode.

For a given mass transfer flow rate, the heat flux reduction to a surface is inversely proportional to the molecular weight of the injected gas. Use of the propellant as coolant as well as fuel would eliminate the need for additional tankage and pumps, simplifying the design considerably. Lithium has been considered to be the propellant of choice, primarily because of its low molecular weight, its favorable ionization potential, and its low-volume tankage properties. It has a relatively low first ionization potential of 5.4 eV and a high second ionization potential of 75.6 eV. This single ionization potential range of over 70 eV compares to approximately 20 eV for Cesium and 27 eV for Potassium [Ref. 48]. This provides a broad temperature range within which only single ionization will occur. Large temperatures must be reached within the gas before double ionization occurs. As the gas temperature is increased several thousand degrees Kelvin, it undergoes ionization and disassociation. Thermal energy deposited can be recovered through nozzle expansion at the exit. However, residence time of the gas is not long enough to ensure recombination. Thus, the energy invested in ionization and disassociation will be lost. [Ref. 49] Lithium has been shown to produce specific impulse figures in excess of 7,000 seconds at 70% efficiency in steady-state thrusters, [Ref. 50] whereas all other propellants have been limited to less than 3,000 seconds specific impulse at less than 40% efficiency [Ref. 6]. Subramaniam has concluded that:

> ...regenerative cooling of anodes (at the specific impulse values in the MPD regime) is possible only with hydrogen or with alkali-metal propellants, notably lithium. In the latter case, the ideal anode operating mode would be evaporation and ionization of the propellant on the porous or wetted anode surface, resulting in increased ion current fraction, reduced anode voltage fall and utilization of part of the anode loss energy [Ref. 51].

Liquid coolants, as well as reducing storage requirements, offer the advantage of providing latent heat of vaporization for energy disposal. However, design problems can occur if the liquid is allowed to vaporize within the porous structure. Problems arise due to the abrupt increase in pressure gradient as the coolant vaporizes. Since coolant flow generally have three-dimensional characteristics, the flow will be diverted around the vapor bubbles and hot spots often develop. The technical practicality of using molten lithium to cool a porous tungsten anode would seem to be beyond current technology. On the other hand, the products of decomposition of hydrazine (gaseous hydrogen and ammonia) have proven to be efficient and practical coolants [Ref. 52].

Given the performance figures above, using an auxiliary coolant gas even with high molecular weight (e.g., NH_3, N_2, CH_4, etc.) which could serve as a propellant once released from a porous hot tungsten anode surface would seem to more practical, vice dealing with molten lithium. Experimental studies would be needed to compare the approaches. Kuriki and Suzuki performed experiments with a quasi-steady MPD thruster to study the effect of anode gas injection (Argon). At high currents of up to 10 kA, increases in thrust, specific impulse, and flow discharge stability were observed [Ref. 53].

There is some question as to the likelihood of current constriction resulting from anode gas injection. In such a case, swirling or circulating the propellant gas would help to move any footpoints that developed around the anode surface and prevent them from becoming fully-developed spots. Additionally, an applied magnetic field could serve to circulate the footpoints as well. The unique advantage of transpiration cooling hinges on providing effective anode cooling while supplying hot propellant, but the real benefit will depend on how small the amount of coolant required really will be.

Transpiration cooling has proven to be as desirable as it is challenging. It is complicated to implement, with associated reliability problems and difficulty of analytical predictions. While the production of thicker boundary layers is largely ineffective against the electron flux heating, the cooling itself is most efficient and a substantial fraction of the energy transferred to the anode is recoverable. The arguments of Chapter Three indicate that a reduction of the electron temperature in the anode would have the desirable effect of reducing the initial current spotting which can be conjectured to be the path that leads to anode arc spots. This electron temperature reduction can be done most effectively by polyatomic gases (which have a high δ-loss factor) emanating from the anode surface [Ref. 54].

The arguments relating to transpiration cooling might be summarized as follows:

Favorable Outcomes

- No separate cooling mechanism for anode required,
- Adds "hot" propellant to exhaust "recovering" most of the electrical power loss to the anode,
- Quenches T_e thus likely to postpone anode spotting and reduce the heating associated with the electron thermal energy ($5kT_e/2e$),
- Reduces bulk convective heating,
- Reduces the local electron Hall parameter by increasing the collision frequency,

Favorable Outcomes (cont'd.)

- Allows for some radiation cooling from the hot tungsten surface (about 120 watts/cm^2 at 2800°K [Ref. 51]),
- Hydrogen/ammonia gases flowing through hot porous (sintered) tungsten represent a compatible, proven technology.

Unfavorable Outcomes

- May decrease the electrical conductivity in the anode region,
- May destabilize the ionization processes in the sheath and bring about significant fluctuations in the current,
- Disrupts "cathode jet" in front of the anode with unpredictable consequences,
- Introduces propellant which may not be hot enough, not ionized enough, or not in the proper place for $\vec{j} \times \vec{B}$ acceleration,
- Transpiration cooling through a porous (tungsten) anode is a difficult design problem.

V. CONCLUSIONS AND RECOMMENDATIONS

Plasma thrusters offer distinct advantages in terms of payload delivered for interplanetary missions, as well as for orbital transfer. A recent comparison completed by Choueiri, Kelly, and Jahn shows a mass savings of 65 tons for an orbital transfer from low Earth orbit to geosynchronous Earth orbit using a quasisteady MPD thruster as opposed to an advanced chemical thruster.[6] This superior performance comes at the expense of low thrust-to-weight ratio and long transit time. However, given the large cargo/logistic requirements of a manned interplanetary mission, delivery of payload must be maximized. Thus, further work to characterize more fully thruster behavior and anode contributions in particular are certainly warranted. [Ref. 55]

The "cut-and-paste" method used to generate Figures 10 and 11 is not of practical use as a modelling method, due to the large effort involved. It did produce the expected electric field and species number and current density plots near the anode, but failed to produce the entire sheath out to the ambipolar region. The nonlinearity of the equation set led to a quickly deteriorating solution. A more practical approach using nonlinear dynamics and/or chaos must be developed to model the sheath numerically.

---

[6] This assumes a specific impulse of 2,000 seconds, 600 kW of input power, and a 270-day transit time.

Depending on the propellant mass fraction used for cooling, the transpiration scheme discussed above presents some rather unique advantages. A hot anode which uses only a small amount of propellant for cooling need not be penalized for any lost thrust. If in addition, we increase anode lifetime by delaying the formation of anode arc spots, then the scheme is all the more desirable. A decrease of the electron temperature in the vicinity of the anode may bring about a more homogeneous flow of current and a reduction in the heating effect associated with the high electron kinetic energy. Recovery of the heat deposited at the anode would be most important if the propellant fraction is high. In such case, nozzle expansion of the hot-propellant/coolant-gas might be implemented.

Means of limiting anode losses through decreasing anode fall voltages were discussed, including the control of the local Hall parameter and the implementation of thermionic arc breakdown. The electrical conductivity (of a nonreacting plasma) could possibly decrease as a result of transpiration cooling and this might increase the anode fall voltage.

Additional work needs to be done in the following areas:

- Investigate effectiveness of nonlinear dynamics and chaos in solving sheath equation set,
- Incorporate adequate one- or two-dimensional sheath modelling in quasisteady MPD numerical codes,

- Investigate the role that fluid dynamic effects play in MPD thruster anode discharges,
- Investigate the effect of transpiration cooling on current and plasma stability, as well as on thruster performance and lifetime,
- Determine effectiveness of transpiration cooling's increase of the collision frequency parameter,
- Compare performance of gaseous propellant/coolants versus hybrid designs with lithium propellant/gaseous coolant,
- Determine if required percentage of propellant gas as coolant is practical (e.g., less than 10%),
- Investigate effect of surface imperfections as focal points for current constrictions and as precursors to anode spotting.

APPENDIX A

The following software includes the calling program, SHEATH, its two subroutines, FCNJ and YDOT, and the DGEAR integrator. The latter is quite extensive in length and includes ten subroutines, including the following: DGRST, DGRCS, DGRPS, DGRIN, LUDATF, LUELMF, LEQT1B, UERTST, UGETIO, and USPKD. A detailed discussion may be found in IMSL literature or Reference 39.

```
******************************************************************************
      Program Sheath                                                    000010
C                                                                       000020
C-----Calling program for DGEAR integrator. Initial conditions are      000030
C     input via READ statements and keyboard entry. Output is to data   000040
C     files via the DGRST subroutine. Diagnostic check of output via    000050
C     Figure 4 printed to data file from DGRST subroutine. Consult      000060
C     DGEAR comments for variable descriptions not listed below.        000061
C----------------------                                                 000062
      REAL E,K,EPS,TI,EF,EFINF,DI,DE,NUINF,C1,K1,A                      000070
      INTEGER N,METH,MITER,INDEX,IWK(1),IER,STEP                        000080
      REAL*8 X,H,Y(5),XEND,TOL,WK                                       000090
      EXTERNAL YDOT, FCNJ, DGEAR                                        000100
      COMMON/CONST/E,K,EPS,TI,EF,EFINF,NINF,DI,DE,VINF,C1,K1,A          000110
C                                                                       000120
C-------------Constants                                                 000121
C     C1 and K1 are constants describing the ionization coefficient.    000122
C     They are taken from the data plotted in Figure 8. The             000123
C     coefficient is equal to the nondimensionalized electric potential 000124
C     raised to the K1 power and then multiplied by C1.                 000125
C     In this way, the ionization coefficient is allowed to vary in     000126
C     proportion to the strength of the electric potential.             000127
C--------------                                                         000128
      WRITE(*,*)'Input value for C1 (format 6E3):'                      000129
      READ(*,*)C1                                                       000130
      WRITE(*,*)C1                                                      000131
      WRITE(*,*)'Input value for K1 (format 6E3):'                      000132
      READ(*,*)K1                                                       000133
      WRITE(*,*)K1                                                      000134
C     Initial conditions for species number density, electric potential 000135
C     and species current density are now input (ni,ne,E,je,ji).        000136
C---------------                                                        000137
      WRITE(*,*)'Input values for y(1) through y(5) (format 5(6E3)):'   000138
      READ(*,*)y(1),y(2),y(3),y(4),y(5)                                 000139
      WRITE(*,*)y(1),y(2),y(3),y(4),y(5)                                000140
C     Following constants are for plasma described in Reference 21      000141
C     (6,000 K, Init E=20,000 V/m, Final E=1,200 V/m)                   000142
      E=1.6E-19                                                         000143
      K=1.38E-23                                                        000150
      EPS=8.854E-12                                                     000160
      TI=6E3                                                            000170
      EF=2E5                                                            000180
      EFINF=1.2E4                                                       000190
      DI=1.724E-4                                                       000200
      DE=1.724E-1                                                       000210
      VIO = 2.E6                                                        000215
      VINF = 4.93E-7                                                    000220
C                                                                       000230
```

```
C     A is plasma characteristic length which shows potential drop.
C     A = ((EPS*EF)/(E*NINF)) = 1.107E-6
      A = 1.107E-5
      X = 0.01
      XEND = 10.
      H = 1e-6
      TOL = 1E-6
      METH = 2
      MITER = 1
      INDEX = 1
      N=5
      IWK(1) = 5
      WK = 18000.
      IER = 0
      OPEN(UNIT=8,FILE='SHEATH.DAT',STATUS='UNKNOWN')
      CALL DGEAR2(N,YDOT,FCNJ,X,H,Y,XEND,TOL,METH,MITER,INDEX,IWK,WK,
     +IER,STEP)
      DO 3 I=0,N
   DO 2 J=0,100
      WRITE(*,*)J,Y(I)
      WRITE(8,1)J,Y(I)
  1   FORMAT(T2,F5.1,5(5X,D9.2))
  2     CONTINUE
  3   CONTINUE
      WRITE(*,*)'Total Steps = ',STEP,'Final Step Size = ',H,
     +'Error Code = ',IER
      CLOSE(UNIT=8)
      STOP
      END
C************************************
C DUMMY SUBROUTINE FCNJ
C************************************
      SUBROUTINE FCNJ(N,X,Y,PD)
      INTEGER N
      REAL Y(N),PD(N,N),X
      RETURN
      END
C************************************
C SUBROUTINE YDOT
C************************************
      SUBROUTINE YDOT(N,X,Y,YPRIME,eprime,eprime2)
      REAL*8 X, Y(5),YPRIME(5),NUI,eprime,eprime2
       REAL E,K,EPS,TI,EF,EFINF,NINF,DI,DE,VINF,C1,K1,A,B1,B2,B3,B4
        COMMON/CONST/E,K,EPS,TI,EF,EFINF,NINF,DI,DE,VIO,VINF,C1,K1,A
      VI = C1 * (Y(3)**K1)
      VIT = VI / VIO
C     Following constants are the bracketed values in Equations 12-16.
C     A is left as a variable.
C-----------------
C     B1 = ((E*EPS)/(K*TI)) * A
      B1= 3.86E5 * A
C     B2 = ((E*EFINF)/(K*TI)) * A
      B2 = 2.32E4 * A
C     B3 = ((E*NINF)/(EF*EPS)) * A
      B3 = 9.04E5 * A
C     B4 = ((VINF*K*TI)/(E*DE*EFINF)) * A
      B4 = 2.62E-21 * A
C     Alpha = 2-body recombination coefficient (fm. Laser Kinetics
C     Handbook (AFWL-TR-74-216, 1974)) (cm3/sec)
      Alpha = 9.e-8
```

```
C---------------------------
 C FIVE FIRST ORDER EQUATIONS - Equations 12-16
C---------------------------
C     Ni
      YPRIME(1) =  (B * Y(1) * Y(3)) - Y(5)
C     Ne
      YPRIME(2) = -(B * Y(2) * Y(3)) + Y(4)
C     E
      YPRIME(3) =  B3 * (Y(1) - Y(2))
C     je
      YPRIME(4) = -B4 * Y(2) * (VIT - (ALPHA * Y(1)))
C     ji
      YPRIME(5) =  B4 * Y(2) * (VIT - (ALPHA * Y(1)))
C
C---Diagnostic Check of first,second derivatives-----
C
      eprime = y(1) - y(2)
      eprime2 = yprime(1) - yprime(2)
C
      RETURN
      END
```

```
C   IMSL ROUTINE NAME   - DGEAR
C
C--modified to return # of steps via variable "step" in subroutine call +
C
C   COMPUTER            - IBM/DOUBLE
C
C   LATEST REVISION     - NOVEMBER 1, 1984
C
C   PURPOSE             - DIFFERENTIAL EQUATION SOLVER - VARIABLE ORDER
C                           ADAMS PREDICTOR CORRECTOR METHOD OR
C                           GEARS METHOD
C
C   USAGE               - CALL DGEAR (N,FCN,FCNJ,X,H,Y,XEND,TOL,METH,
C                           MITER,INDEX,IWK,WK,IER)
C
C   ARGUMENTS    N      - INPUT NUMBER OF FIRST-ORDER DIFFERENTIAL
C                           EQUATIONS.
C                FCN    - NAME OF SUBROUTINE FOR EVALUATING FUNCTIONS.
C                           (INPUT)
C                         THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED
C                           BY THE USER AND IT SHOULD BE OF THE
C                           FOLLOWING FORM
C                             SUBROUTINE FCN (N,X,Y,YPRIME)
C                             REAL X,Y(N),YPRIME(N)
C                                  .
C                                  .
C                                  .
C                         FCN SHOULD EVALUATE YPRIME(1),...,YPRIME(N)
C                           GIVEN N,X, AND Y(1),...,Y(N). YPRIME(I)
C                           IS THE FIRST DERIVATIVE OF Y(I) WITH
C                           RESPECT TO X.
C                         FCN MUST APPEAR IN AN EXTERNAL STATEMENT IN
C                           THE CALLING PROGRAM AND N,X,Y(1),...,Y(N)
C                           MUST NOT BE ALTERED BY FCN.
C                FCNJ   - NAME OF THE SUBROUTINE FOR COMPUTING THE
C                           JACOBIAN MATRIX OF PARTIAL DERIVATIVES.
C                           (INPUT)
C                         THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED
C                           BY THE USER.
C                         IF MITER=1 IT SHOULD BE OF THE FOLLOWING
C                           FORM
C                             SUBROUTINE FCNJ (N,X,Y,PD)
C                             REAL X,Y(N),PD(N,N)
C                                  .
C                                  .
C                         FCNJ MUST EVALUATE PD(I,J), THE PARTIAL
C                           DERIVATIVE OF YPRIME(I) WITH RESPECT TO
C                           Y(J), FOR I=1,N AND J=1,N.
C                         IF MITER= -1 IT SHOULD BE OF THE FOLLOWING
C                           FORM
C                             SUBROUTINE FCNJ (N,X,Y,PD)
C                             REAL X,Y(N),PD(1)
C                                  .
C                                  .
C                         FCNJ MUST EVALUATE PD IN BAND STORAGE MODE.
C                           THAT IS, PD(N*(J-I+NLC)+I) IS THE PARTIAL
C                           DERIVATIVE OF YPRIME(I) WITH RESPECT TO
C                           Y(J).  NLC IS THE NUMBER OF LOWER
C                           CODIAGONALS FOR THE BAND MATRIX.
C                         FCNJ MUST APPEAR IN AN EXTERNAL STATEMENT IN
C                           THE CALLING PROGRAM AND N,X,Y(1),...,Y(N)
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C                           MUST NOT BE ALTERED BY FCNJ.               DGEA0620
C                         FCNJ IS USED ONLY IF MITER IS EQUAL TO       DGEA0630
C                           1 OR -1. OTHERWISE A DUMMY ROUTINE CAN     DGEA0640
C                           BE SUBSTITUTED. SEE REMARK 1.              DGEA0650
C               X      - INDEPENDENT VARIABLE. (INPUT AND OUTPUT)      DGEA0660
C                         ON INPUT, X SUPPLIES THE INITIAL VALUE       DGEA0670
C                           AND IS USED ONLY ON THE FIRST CALL.        DGEA0680
C                         ON OUTPUT, X IS REPLACED WITH THE CURRENT    DGEA0690
C                            VALUE OF THE INDEPENDENT VARIABLE AT WHICHDGEA0700
C                           INTEGRATION HAS BEEN COMPLETED.            DGEA0710
C                H      - INPUT/OUTPUT.                                DGEA0720
C                         ON INPUT, H CONTAINS THE NEXT STEP SIZE IN   DGEA0730
C                           X. H IS USED ONLY ON THE FIRST CALL.       DGEA0740
C                         ON OUTPUT, H CONTAINS THE STEP SIZE USED     DGEA0750
C                           LAST, WHETHER SUCCESSFULLY OR NOT.         DGEA0760
C               Y      - DEPENDENT VARIABLES, VECTOR OF LENGTH N.      DGEA0770
C                          (INPUT AND OUTPUT)                          DGEA0780
C                         ON INPUT, Y(1),...,Y(N) SUPPLY INITIAL       DGEA0790
C                            VALUES.                                   DGEA0800
C                         ON OUTPUT, Y(1),...,Y(N) ARE REPLACED WITH   DGEA0810
C                            A COMPUTED VALUE AT XEND.                 DGEA0820
C               XEND    - INPUT VALUE OF X AT WHICH SOLUTION IS DESIRED DGEA0830
C                          NEXT. INTEGRATION WILL NORMALLY GO          DGEA0840
C                          BEYOND XEND AND THE ROUTINE WILL INTERPOLATEDGEA0850
C                          TO X = XEND.                                DGEA0860
C                        NOTE THAT (X-XEND)*H MUST BE LESS THAN        DGEA0870
C                          ZERO (X AND H AS SPECIFIED ON INPUT).       DGEA0880
C               TOL     - INPUT RELATIVE ERROR BOUND. TOL MUST BE      DGEA0890
C                          GREATER THAN ZERO. TOL IS USED ONLY ON THE  DGEA0900
C                          FIRST CALL UNLESS INDEX IS EQUAL TO -1.     DGEA0910
C                          TOL SHOULD BE AT LEAST AN ORDER OF          DGEA0920
C                          MAGNITUDE LARGER THAN THE UNIT ROUNDOFF     DGEA0930
C                          BUT GENERALLY NOT LARGER THAN .001.         DGEA0940
C                          SINGLE STEP ERROR ESTIMATES DIVIDED BY      DGEA0950
C                          YMAX(I) WILL BE KEPT LESS THAN TOL IN       DGEA0960
C                          ROOT-MEAN-SQUARE NORM (EUCLIDEAN NORM       DGEA0970
C                          DIVIDED BY SQRT(N)). THE VECTOR YMAX OF     DGEA0980
C                          WEIGHTS IS COMPUTED INTERNALLY AND STORED   DGEA0990
C                          IN WORK VECTOR WK. INITIALLY YMAX(I) IS     DGEA1000
C                          THE ABSOLUTE VALUE OF Y(I), WITH A DEFAULT  DGEA1010
C                          VALUE OF ONE IF Y(I) IS EQUAL TO ZERO.      DGEA1020
C                          THEREAFTER, YMAX(I) IS THE LARGEST VALUE    DGEA1030
C                          OF THE ABSOLUTE VALUE OF Y(I) SEEN SO FAR,  DGEA1040
C                          OR THE INITIAL VALUE OF YMAX(I) IF THAT IS  DGEA1050
C                           LARGER.                                    DGEA1060
C                METH   - INPUT BASIC METHOD INDICATOR.                DGEA1070
C                          USED ONLY ON THE FIRST CALL UNLESS INDEX IS DGEA1080
C                           EQUAL TO -1.                               DGEA1090
C                        METH = 1, IMPLIES THAT THE ADAMS METHOD IS    DGEA1100
C                           TO BE USED.                                DGEA1110
C                        METH = 2, IMPLIES THAT THE STIFF METHODS OF   DGEA1120
C                          GEAR, OR THE BACKWARD DIFFERENTIATION       DGEA1130
C                          FORMULAE ARE TO BE USED.                    DGEA1140
C                MITER  - INPUT ITERATION METHOD INDICATOR.            DGEA1150
C                          MITER = 0, IMPLIES THAT FUNCTIONAL          DGEA1160
C                            ITERATION IS USED. NO PARTIAL             DGEA1170
C                            DERIVATIVES ARE NEEDED. A DUMMY FCNJ      DGEA1180
C                            CAN BE USED.                              DGEA1190
C                          MITER = 1, IMPLIES THAT THE CHORD METHOD    DGEA1200
C                            IS USED WITH AN ANALYTIC JACOBIAN. FOR    DGEA1210
C                            THIS METHOD, THE USER SUPPLIES            DGEA1220
C                            SUBROUTINE FCNJ.                          DGEA1230
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C                           MITER = 2, IMPLIES THAT THE CHORD METHOD    DGEA1240
C                             IS USED WITH THE JACOBIAN CALCULATED      DGEA1250
C                             INTERNALLY BY FINITE DIFFERENCES.         DGEA1260
C                             A DUMMY FCNJ CAN BE USED.                 DGEA1270
C                           MITER = 3, IMPLIES THAT THE CHORD METHOD    DGEA1280
C                             IS USED WITH THE JACOBIAN REPLACED BY     DGEA1290
C                             A DIAGONAL APPROXIMATION BASED ON A       DGEA1300
C                             DIRECTIONAL DERIVATIVE.                   DGEA1310
C                             A DUMMY FCNJ CAN BE USED.                 DGEA1320
C                           MITER = -1 OR -2, IMPLIES USE THE SAME      DGEA1330
C                             METHOD AS FOR MITER= 1 OR 2, RESPECTIVELY,DGEA1340
C                             BUT USING A BANDED JACOBIAN MATRIX.  IN   DGEA1350
C                             THESE TWO CASES BANDWIDTH INFORMATION     DGEA1360
C                             MUST BE PASSED TO DGEAR THROUGH THE       DGEA1370
C                              COMMON BLOCK                             DGEA1380
C                                 COMMON /DBAND/ NLC,NUC                DGEA1390
C                             WHERE NLC=NUMBER OF LOWER CODIAGONALS     DGEA1400
C                                   NUC=NUMBER OF UPPER CODIAGONALS     DGEA1410
C                INDEX  - INPUT AND OUTPUT PARAMETER USED TO INDICATE   DGEA1420
C                           THE TYPE OF CALL TO THE SUBROUTINE.  ON     DGEA1430
C                           OUTPUT INDEX IS RESET TO 0 IF INTEGRATION   DGEA1440
C                           WAS SUCCESSFUL.  OTHERWISE, THE VALUE OF    DGEA1450
C                            INDEX IS UNCHANGED.                        DGEA1460
C                         ON INPUT, INDEX = 1, IMPLIES THAT THIS IS THE DGEA1470
C                            FIRST CALL FOR THIS PROBLEM.               DGEA1480
C                         ON INPUT, INDEX = 0, IMPLIES THAT THIS IS NOT DGEA1490
C                           THE FIRST CALL FOR THIS PROBLEM.            DGEA1500
C                         ON INPUT, INDEX = -1, IMPLIES THAT THIS IS NOTDGEA1510
C                           THE FIRST CALL FOR THIS PROBLEM, AND THE    DGEA1520
C                            USER HAS RESET TOL.                        DGEA1530
C                         ON INPUT, INDEX = 2, IMPLIES THAT THIS IS NOT DGEA1540
C                           THE FIRST CALL FOR THIS PROBLEM. INTEGRATIONDGEA1550
C                           IS TO CONTINUE AND XEND IS TO BE HIT EXACTLYDGEA1560
C                           (NO INTERPOLATION IS DONE). THIS VALUE OF   DGEA1570
C                           INDEX ASSUMES THAT XEND IS BEYOND THE       DGEA1580
C                            CURRENT VALUE OF X.                        DGEA1590
C                         ON INPUT, INDEX = 3, IMPLIES THAT THIS IS NOT DGEA1600
C                           THE FIRST CALL FOR THIS PROBLEM. INTEGRATIONDGEA1610
C                           IS TO CONTINUE AND CONTROL IS TO BE RETURNEDDGEA1620
C                           TO THE CALLING PROGRAM AFTER ONE STEP. XEND DGEA1630
C                            IS IGNORED.                                DGEA1640
C                IWK    - INTEGER WORK VECTOR OF LENGTH N. USED ONLY IF DGEA1650
C                            MITER = 1 OR 2                             DGEA1660
C                WK     - REAL WORK VECTOR OF LENGTH 4*N+NMETH+NMITER.  DGEA1670
C                           THE VALUE OF NMETH DEPENDS ON THE VALUE OF  DGEA1680
C                              METH.                                    DGEA1690
C                              IF METH IS EQUAL TO 1,                   DGEA1700
C                                NMETH IS EQUAL TO N*13.                DGEA1710
C                              IF METH IS EQUAL TO 2,                   DGEA1720
C                                NMETH IS EQUAL TO N*6.                 DGEA1730
C                           THE VALUE OF NMITER DEPENDS ON THE VALUE OF DGEA1740
C                              MITER.                                   DGEA1750
C                              IF MITER IS EQUAL TO 1 OR 2,             DGEA1760
C                                NMITER IS EQUAL TO N*(N+1)             DGEA1770
C                              IF MITER IS EQUAL TO -1 OR -2,           DGEA1780
C                                NMITER IS EQUAL TO (2*NLC+NUC+3)*N     DGEA1790
C                                 WHERE NLC=NUMBER OF LOWER CODIAGONALS DGEA1800
C                                       NUC=NUMBER OF UPPER CODIAGONALS DGEA1810
C                              IF MITER IS EQUAL TO 3,                  DGEA1820
C                                NMITER IS EQUAL TO N.                  DGEA1830
C                              IF MITER IS EQUAL TO 0,                  DGEA1840
C                                NMITER IS EQUAL TO 1.                  DGEA1850
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C                          WK MUST REMAIN UNCHANGED BETWEEN SUCCESSIVE DGEA1860
C                           CALLS DURING INTEGRATION.                  DGEA1870
C                IER    - ERROR PARAMETER. (OUTPUT)                    DGEA1880
C                         WARNING ERROR                                DGEA1890
C                           IER = 33, IMPLIES THAT X+H WILL EQUAL X ON DGEA1900
C                             THE NEXT STEP. THIS CONDITION DOES NOT   DGEA1910
C                             FORCE THE ROUTINE TO HALT. HOWEVER, IT   DGEA1920
C                             DOES INDICATE ONE OF TWO CONDITIONS.     DGEA1930
C                             THE USER MIGHT BE REQUIRING TOO MUCH     DGEA1940
C                             ACCURACY VIA THE INPUT PARAMETER TOL.    DGEA1950
C                             IN THIS CASE THE USER SHOULD CONSIDER    DGEA1960
C                             INCREASING THE VALUE OF TOL. THE OTHER   DGEA1970
C                             CONDITION WHICH MIGHT GIVE RISE TO THIS  DGEA1980
C                             ERROR MESSAGE IS THAT THE SYSTEM OF      DGEA1990
C                             DIFFERENTIAL EQUATIONS BEING SOLVED      DGEA2000
C                             IS STIFF (EITHER IN GENERAL OR OVER      DGEA2010
C                             THE SUBINTERVAL OF THE PROBLEM BEING     DGEA2020
C                             SOLVED AT THE TIME OF THE ERROR). IN     DGEA2030
C                             THIS CASE THE USER SHOULD CONSIDER       DGEA2040
C                             USING A NONZERO VALUE FOR THE INPUT      DGEA2050
C                             PARAMETER MITER.                         DGEA2060
C                         WARNING WITH FIX ERROR                       DGEA2070
C                           IER = 66, IMPLIES THAT THE ERROR TEST      DGEA2080
C                             FAILED. H WAS REDUCED BY .1 ONE OR MORE  DGEA2090
C                             TIMES AND THE STEP WAS TRIED AGAIN       DGEA2100
C                             SUCCESSFULLY.                            DGEA2110
C                           IER = 67, IMPLIES THAT CORRECTOR           DGEA2120
C                             CONVERGENCE COULD NOT BE ACHIEVED.       DGEA2130
C                             H WAS REDUCED BY .1 ONE OR MORE TIMES AND DGEA2140
C                             THE STEP WAS TRIED AGAIN SUCCESSFULLY.   DGEA2150
C                         TERMINAL ERROR                               DGEA2160
C                           IER = 132, IMPLIES THE INTEGRATION WAS     DGEA2170
C                             HALTED AFTER FAILING TO PASS THE ERROR   DGEA2180
C                             TEST EVEN AFTER REDUCING H BY A FACTOR   DGEA2190
C                             OF 1.0E10 FROM ITS INITIAL VALUE.        DGEA2200
C                             SEE REMARKS.                             DGEA2210
C                           IER = 133, IMPLIES THE INTEGRATION WAS     DGEA2220
C                             HALTED AFTER FAILING TO ACHIEVE          DGEA2230
C                             CORRECTOR CONVERGENCE EVEN AFTER         DGEA2240
C                             REDUCING H BY A FACTOR OF 1.0E10 FROM    DGEA2250
C                             ITS INITIAL VALUE. SEE REMARKS.          DGEA2260
C                           IER = 134, IMPLIES THAT AFTER SOME INITIAL DGEA2270
C                             SUCCESS, THE INTEGRATION WAS HALTED EITHERDGEA2280
C                             BY REPEATED ERROR TEST FAILURES OR BY    DGEA2290
C                             A TEST ON TOL. SEE REMARKS.              DGEA2300
C                           IER = 135, IMPLIES THAT ONE OF THE INPUT   DGEA2310
C                             PARAMETERS N,X,H,XEND,TOL,METH,MITER, OR DGEA2320
C                             INDEX WAS SPECIFIED INCORRECTLY.         DGEA2330
C                           IER = 136, IMPLIES THAT INDEX HAD A VALUE  DGEA2340
C                             OF -1 ON INPUT, BUT THE DESIRED CHANGES  DGEA2350
C                             OF PARAMETERS WERE NOT IMPLEMENTED       DGEA2360
C                             BECAUSE XEND WAS NOT BEYOND X.           DGEA2370
C                             INTERPOLATION TO X = XEND WAS PERFORMED. DGEA2380
C                             TO TRY AGAIN, SIMPLY CALL AGAIN WITH     DGEA2390
C                             INDEX EQUAL TO -1 AND A NEW VALUE FOR    DGEA2400
C                             XEND.                                    DGEA2410
C                    Step -    # of integration steps taken              +
C                                                                      DGEA2420
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32                        DGEA2430
C                       - SINGLE/H36,H48,H60                           DGEA2440
C                                                                      DGEA2450
C   REQD. IMSL ROUTINES - DGRCS,DGRIN,DGRPS,DGRST,LUDATF,LUELMF,LEQT1B, DGEA2460
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C                          UERTST,UGETIO                                DGEA2470
C                                                                       DGEA2480
C  NOTATION             - INFORMATION ON SPECIAL NOTATION AND           DGEA2490
C                         CONVENTIONS IS AVAILABLE IN THE MANUAL        DGEA2500
C                         INTRODUCTION OR THROUGH IMSL ROUTINE UHELP    DGEA2510
C                                                                       DGEA2520
C  REMARKS  1.  THE EXTERNAL SUBROUTINE FCNJ IS USED ONLY WHEN          DGEA2530
C               INPUT PARAMETER MITER IS EQUAL TO 1 OR -1. OTHERWISE,   DGEA2540
C               A DUMMY FUNCTION CAN BE USED. THE DUMMY SUBROUTINE      DGEA2550
C               SHOULD BE OF THE FOLLOWING FORM                         DGEA2560
C                 SUBROUTINE FCNJ (N,X,Y,PD)                            DGEA2570
C                 INTEGER N                                             DGEA2580
C                 REAL Y(N),PD(N,N),X                                   DGEA2590
C                 RETURN                                                DGEA2600
C                 END                                                   DGEA2610
C           2.  AFTER THE INITIAL CALL, IF A NORMAL RETURN OCCURRED     DGEA2620
C               (IER=0) AND A NORMAL CONTINUATION IS DESIRED, SIMPLY    DGEA2630
C               RESET XEND AND CALL DGEAR AGAIN. ALL OTHER              DGEA2640
C               PARAMETERS WILL BE READY FOR THE NEXT CALL. A CHANGE    DGEA2650
C               OF PARAMETERS WITH INDEX EQUAL TO -1 CAN BE MADE        DGEA2660
C               AFTER EITHER A SUCCESSFUL OR AN UNSUCCESSFUL RETURN.    DGEA2670
C           3.  THE COMMON BLOCKS /DBAND/ AND /GEAR/ NEED TO BE         DGEA2680
C               PRESERVED BETWEEN CALLS TO DGEAR. IF IT IS NECESSARY    DGEA2690
C               FOR THE COMMON BLOCKS TO EXIST IN THE CALLING PROGRAM   DGEA2700
C               THE FOLLOWING STATEMENTS SHOULD BE INCLUDED             DGEA2710
C                 COMMON  /DBAND/ NLC,NUC                               DGEA2720
C                 COMMON  /GEAR/ DUMMY(48),SDUMMY(4),IDUMMY(38)         DGEA2730
C               WHERE DUMMY, SDUMMY, AND IDUMMY ARE VARIABLE NAMES NOT DGEA2740
C               USED ELSEWHERE IN THE CALLING PROGRAM.  (FOR DOUBLE     DGEA2750
C               PRECISION DUMMY IS TYPE DOUBLE AND SDUMMY IS TYPE REAL)DGEA2760
C           4.  THE CHOICE OF VALUES FOR METH AND MITER MAY REQUIRE     DGEA2770
C               SOME EXPERIMENTATION, AND ALSO SOME CONSIDERATION OF    DGEA2780
C               THE NATURE OF THE PROBLEM AND OF STORAGE REQUIREMENTS. DGEA2790
C               THE PRIME CONSIDERATION IS STIFFNESS. IF                DGEA2800
C               THE PROBLEM IS NOT STIFF, THE BEST CHOICE IS PROBABLY   DGEA2810
C               METH = 1 WITH MITER = 0. IF THE PROBLEM IS STIFF TO A   DGEA2820
C               SIGNIFICANT DEGREE, THEN METH SHOULD BE 2 AND MITER     DGEA2830
C               SHOULD BE 1,2,-1,-2 OR 3. IF THE USER HAS NO KNOWLEDGE DGEA2840
C               OF THE INHERENT TIME CONSTANTS OF THE PROBLEM, WITH     DGEA2850
C               WHICH TO PREDICT ITS STIFFNESS, ONE WAY TO DETERMINE    DGEA2860
C               THIS IS TO TRY METH = 1 AND MITER = 0 FIRST, AND LOOK   DGEA2870
C               AT THE BEHAVIOR OF THE SOLUTION COMPUTED AND THE STEP   DGEA2880
C               SIZES USED. IF THE TYPICAL VALUES OF H ARE MUCH         DGEA2890
C               SMALLER THAN THE SOLUTION BEHAVIOR WOULD SEEM TO        DGEA2900
C               REQUIRE (THAT IS, MORE THAN 100 STEPS ARE TAKEN OVER    DGEA2910
C               AN INTERVAL IN WHICH THE SOLUTIONS CHANGE BY LESS       DGEA2920
C               THAN ONE PERCENT), THEN THE PROBLEM IS PROBABLY STIFF   DGEA2930
C               AND THE DEGREE OF STIFFNESS CAN BE ESTIMATED FROM THE   DGEA2940
C               VALUES OF H USED AND THE SMOOTHNESS OF THE SOLUTION.    DGEA2950
C               IF THE DEGREE OF STIFFNESS IS ONLY SLIGHT, IT MAY BE    DGEA2960
C               THAT METH=1 IS MORE EFFICIENT THAN METH=2.              DGEA2970
C               EXPERIMENTATION WOULD BE REQUIRED TO DETERMINE THIS.    DGEA2980
C               REGARDLESS OF METH, THE LEAST EFFECTIVE VALUE OF        DGEA2990
C               MITER IS 0, AND THE MOST EFFECTIVE IS 1,-1,2,OR -2.     DGEA3000
C               MITER = 3 IS GENERALLY SOMEWHERE IN BETWEEN. SINCE      DGEA3010
C               THE STORAGE REQUIREMENTS GO UP IN THE SAME ORDER AS     DGEA3020
C               EFFECTIVENESS, TRADE-OFF CONSIDERATIONS ARE             DGEA3030
C               NECESSARY. FOR REASONS OF ACCURACY AND SPEED, THE       DGEA3040
C               CHOICE OF ABS(MITER)=1 IS GENERALLY PREFERRED TO        DGEA3050
C               ABS(MITER)=2, UNLESS THE SYSTEM IS FAIRLY COMPLICATED   DGEA3060
C                (AND FCNJ IS THUS NOT FEASIBLE TO CODE). THE           DGEA3070
C               ACCURACY OF THE FCNJ CALCULATION CAN BE CHECKED BY      DGEA3080
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C              COMPARISON OF THE JACOBIAN WITH THAT GENERATED WITH    DGEA3090
C              ABS(MITER)=2. IF THE JACOBIAN MATRIX IS SIGNIFICANTLY  DGEA3100
C              DIAGONALLY DOMINANT, THEN THE OPTION MITER = 3 IS      DGEA3110
C              LIKELY TO BE NEARLY AS EFFECTIVE AS ABS(MITER)=1 OR 2, DGEA3120
C              AND WILL SAVE CONSIDERABLE STORAGE AND RUN TIME.       DGEA3130
C              IT IS POSSIBLE, AND POTENTIALLY QUITE DESIRABLE, TO    DGEA3140
C              USE DIFFERENT VALUES OF METH AND MITER IN DIFFERENT    DGEA3150
C              SUBINTERVALS OF THE PROBLEM. FOR EXAMPLE, IF THE       DGEA3160
C              PROBLEM IS NON-STIFF INITIALLY AND STIFF LATER,        DGEA3170
C              METH = 1 AND MITER = 0 MIGHT BE SET INITIALLY, AND     DGEA3180
C              METH = 2 AND MITER = 1 LATER.                          DGEA3190
C          5.  THE INITIAL VALUE OF THE STEP SIZE, H, SHOULD BE       DGEA3200
C              CHOSEN CONSIDERABLY SMALLER THAN THE AVERAGE VALUE     DGEA3210
C              EXPECTED FOR THE PROBLEM, AS THE FIRST-ORDER METHOD    DGEA3220
C              WITH WHICH DGEAR BEGINS IS NOT GENERALLY THE MOST      DGEA3230
C              EFFICIENT ONE. HOWEVER, FOR THE FIRST STEP, AS FOR     DGEA3240
C              EVERY STEP, DGEAR TESTS FOR THE POSSIBILITY THAT       DGEA3250
C              THE STEP SIZE WAS TOO LARGE TO PASS THE ERROR TEST     DGEA3260
C              (BASED ON TOL), AND IF SO ADJUSTS THE STEP SIZE        DGEA3270
C              DOWN AUTOMATICALLY. THIS DOWNWARD ADJUSTMENT, IF       DGEA3280
C              ANY, IS NOTED BY IER HAVING THE VALUES 66 OR 67,       DGEA3290
C              AND SUBSEQUENT RUNS ON THE SAME OR SIMILAR PROBLEM     DGEA3300
C              SHOULD BE STARTED WITH AN APPROPRIATELY SMALLER        DGEA3310
C              VALUE OF H.                                            DGEA3320
C          6.  SOME OF THE VALUES OF INTEREST LOCATED IN THE          DGEA3330
C              COMMON BLOCK /GEAR/ ARE                                DGEA3340
C              A. HUSED, THE STEP SIZE H LAST USED SUCCESSFULLY       DGEA3350
C                 (DUMMY(8))                                          DGEA3360
C              B. NQUSED, THE ORDER LAST USED SUCCESSFULLY            DGEA3370
C                 (IDUMMY(6))                                         DGEA3380
C              C. NSTEP, THE CUMULATIVE NUMBER OF STEPS TAKEN         DGEA3390
C                 (IDUMMY(7))                                         DGEA3400
C              D. NFE, THE CUMULATIVE NUMBER OF FCN EVALUATIONS       DGEA3410
C                 (IDUMMY(8))                                         DGEA3420
C              E. NJE, THE CUMULATIVE NUMBER OF JACOBIAN              DGEA3430
C                 EVALUATIONS, AND HENCE ALSO OF MATRIX LU            DGEA3440
C                 DECOMPOSITIONS (IDUMMY(9))                          DGEA3450
C          7.  THE NORMAL USAGE OF DGEAR MAY BE SUMMARIZED AS FOLLOWS DGEA3460
C              A. SET THE INITIAL VALUES IN Y.                        DGEA3470
C              B. SET N, X, H, TOL, METH, AND MITER.                  DGEA3480
C              C. SET XEND TO THE FIRST OUTPUT POINT, AND INDEX TO 1. DGEA3490
C              D. CALL DGEAR                                          DGEA3500
C              E. EXIT IF IER IS GREATER THAN 128.                    DGEA3510
C              F. OTHERWISE, DO DESIRED OUTPUT OF Y.                  DGEA3520
C              G. EXIT IF THE PROBLEM IS FINISHED.                    DGEA3530
C              H. OTHERWISE, RESET XEND TO THE NEXT OUTPUT POINT, AND DGEA3540
C                 RETURN TO STEP D.                                   DGEA3550
C          8.  THE ERROR WHICH IS CONTROLLED BY WAY OF THE PARAMETER  DGEA3560
C              TOL IS AN ESTIMATE OF THE LOCAL TRUNCATION ERROR, THAT DGEA3570
C              IS, THE ERROR COMMITTED ON TAKING A SINGLE STEP WITH   DGEA3580
C              THE METHOD, STARTING WITH DATA REGARDED AS EXACT. THIS DGEA3590
C              IS TO BE DISTINGUISHED FROM THE GLOBAL TRUNCATION      DGEA3600
C              ERROR, WHICH IS THE ERROR IN ANY GIVEN COMPUTED VALUE  DGEA3610
C              OF Y(X) AS A RESULT OF THE LOCAL TRUNCATION ERRORS     DGEA3620
C              FROM ALL STEPS TAKEN TO OBTAIN Y(X). THE LATTER ERROR  DGEA3630
C              ACCUMULATES IN A NON-TRIVIAL WAY FROM THE LOCAL        DGEA3640
C              ERRORS, AND IS NEITHER ESTIMATED NOR CONTROLLED BY     DGEA3650
C              THE ROUTINE. SINCE IT IS USUALLY THE GLOBAL ERROR THAT DGEA3660
C              A USER WANTS TO HAVE UNDER CONTROL, SOME               DGEA3670
C              EXPERIMENTATION MAY BE NECESSARY TO GET THE RIGHT      DGEA3680
C              VALUE OF TOL TO ACHIEVE THE USERS NEEDS. IF THE        DGEA3690
C              PROBLEM IS MATHEMATICALLY STABLE, AND THE METHOD USED  DGEA3700
```

```
C                IS APPROPRIATELY STABLE, THEN THE GLOBAL ERROR AT A     DGEA3710
C                GIVEN X SHOULD VARY SMOOTHLY WITH TOL IN A MONOTONE     DGEA3720
C                 INCREASING MANNER.                                     DGEA3730
C            9.  IF THE ROUTINE RETURNS WITH IER VALUES OF 132, 133,     DGEA3740
C                OR 134, THE USER SHOULD CHECK TO SEE IF TOO MUCH        DGEA3750
C                ACCURACY IS BEING REQUIRED. THE USER MAY WISH TO        DGEA3760
C                SET TOL TO A LARGER VALUE AND CONTINUE. ANOTHER         DGEA3770
C                POSSIBLE CAUSE OF THESE ERROR CONDITIONS IS AN          DGEA3780
C                ERROR IN THE CODING OF THE EXTERNAL FUNCTIONS FCN       DGEA3790
C                OR FCNJ. IF NO ERRORS ARE FOUND, IT MAY BE NECESSARY    DGEA3800
C                TO MONITOR INTERMEDIATE QUANTITIES GENERATED BY THE     DGEA3810
C                ROUTINE. THESE QUANTITIES ARE STORED IN THE WORK VECTORDGEA3820
C                WK AND INDEXED BY SPECIFIC ELEMENTS IN THE COMMON BLOCKDGEA3830
C                /GEAR/. IF IER IS 132 OR 134, THE COMPONENTS CAUSING    DGEA3840
C                THE ERROR TEST FAILURE CAN BE IDENTIFIED FROM LARGE     DGEA3850
C                 VALUES OF THE QUANTITY                                 DGEA3860
C                   WK(IDUMMY(11)+I)/WK(I), FOR I=1,...,N.               DGEA3870
C                ONE CAUSE OF THIS MAY BE A VERY SMALL BUT NONZERO       DGEA3880
C                 INITIAL VALUE OF ABS(Y(I)).                            DGEA3890
C                IF IER IS 133, SEVERAL POSSIBILITIES EXIST.             DGEA3900
C                IT MAY BE INSTRUCTIVE TO TRY DIFFERENT VALUES OF MITER.DGEA3910
C                ALTERNATIVELY, THE USER MIGHT MONITOR SUCCESSIVE        DGEA3920
C                CORRECTOR ITERATES CONTAINED IN WK(IDUMMY(12)+I), FOR   DGEA3930
C                I=1,...,N. ANOTHER POSSIBILITY MIGHT BE TO MONITOR      DGEA3940
C                THE JACOBIAN MATRIX, IF ONE IS USED, STORED, BY         DGEA3950
C                COLUMN, IN WK(IDUMMY(10)+I), FOR I=1,...,N*N IF         DGEA3960
C                ABS(MITER) IS EQUAL TO 1 OR 2, OR FOR I=1,...,N IF      DGEA3970
C                 MITER IS EQUAL TO 3.                                   DGEA3980
C                                                                        DGEA3990
C   COPYRIGHT           - 1984 BY IMSL, INC.  ALL RIGHTS RESERVED.       DGEA4000
C                                                                        DGEA4010
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN  DGEA4020
C                           APPLIED TO THIS CODE.  NO OTHER WARRANTY,    DGEA4030
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.         DGEA4040
C                                                                        DGEA4050
C-----------------------------------------------------------------------DGEA4060
C                                                                        DGEA4070
      SUBROUTINE DGEAR  (N,FCN,FCNJ,X,H,Y,XEND,TOL,METH,MITER,INDEX,     DGEA4080
     1                   IWK,WK,IER,step)                                   +
C                                  SPECIFICATIONS FOR ARGUMENTS          DGEA4100
      INTEGER            N,METH,MITER,INDEX,IWK(1),IER,step                 +
      DOUBLE PRECISION   X,H,Y(N),XEND,TOL,WK(1)                         DGEA4120
C                                  SPECIFICATIONS FOR LOCAL VARIABLES    DGEA4130
      INTEGER            NERROR,NSAVE1,NSAVE2,NPW,NY,NC,MFC,KFLAG,       DGEA4140
     1                   JSTART,NSQ,NQUSED,NSTEP,NFE,NJE,I,N0,NHCUT,KGO,DGEA4150
     2                   JER,KER,NN,NEQUIL,IDUMMY(21),NLC,NUC            DGEA4160
      REAL               SDUMMY(4)                                       DGEA4170
      DOUBLE PRECISION   T,HH,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,TOUTP,    DGEA4180
     1                   AYI,D,DN,SEPS,DUMMY(39)                         DGEA4190
      EXTERNAL           FCN,FCNJ                                        DGEA4200
      COMMON /DBAND/     NLC,NUC                                         DGEA4210
      COMMON /GEAR/      T,HH,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,    DGEA4220
     1                   TOUTP,SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,    DGEA4230
     2                   NSTEP,NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,  DGEA4240
     3                   NY,IDUMMY,N0,NHCUT                              DGEA4250
      DATA               SEPS/Z3410000000000000/                         DGEA4260
C                                  FIRST EXECUTABLE STATEMENT            DGEA4270
      IF (MITER.GE.0) NLC = -1                                           DGEA4280
      KER = 0                                                            DGEA4290
      JER = 0                                                            DGEA4300
      UROUND = SEPS                                                      DGEA4310
C                                  COMPUTE WORK VECTOR INDICIES          DGEA4320
```

```
      NERROR = N                                                        DGEA4330
      NSAVE1 = NERROR+N                                                 DGEA4340
      NSAVE2 = NSAVE1+N                                                 DGEA4350
      NY = NSAVE2+N                                                     DGEA4360
      IF (METH.EQ.1) NEQUIL = NY+13*N                                   DGEA4370
      IF (METH.EQ.2) NEQUIL = NY+6*N                                    DGEA4380
      NPW = NEQUIL + N                                                  DGEA4390
      IF (MITER.EQ.0.OR.MITER.EQ.3) NPW = NEQUIL                        DGEA4400
      MFC = 10*METH+IABS(MITER)                                         DGEA4410
C                                  CHECK FOR INCORRECT INPUT PARAMETERS DGEA4420
C                                                                       DGEA4430
      IF (MITER.LT.-2.OR.MITER.GT.3) GO TO 85                           DGEA4440
      IF (METH.NE.1.AND.METH.NE.2) GO TO 85                             DGEA4450
      IF (TOL.LE.0.D0) GO TO 85                                         DGEA4460
      IF (N.LE.0) GO TO 85                                              DGEA4470
      IF ((X-XEND)*H.GE.0.D0) GO TO 85                                  DGEA4480
      IF (INDEX.EQ.0) GO TO 10                                          DGEA4490
      IF (INDEX.EQ.2) GO TO 15                                          DGEA4500
      IF (INDEX.EQ.-1) GO TO 20                                         DGEA4510
      IF (INDEX.EQ.3) GO TO 25                                          DGEA4520
      IF (INDEX.NE.1) GO TO 85                                          DGEA4530
C                                  IF INITIAL VALUES OF YMAX OTHER THAN DGEA4540
C                                    THOSE SET BELOW ARE DESIRED, THEY  DGEA4550
C                                    SHOULD BE SET HERE. ALL YMAX(I)    DGEA4560
C                                    MUST BE POSITIVE. IF VALUES FOR    DGEA4570
C                                    HMIN OR HMAX, THE BOUNDS ON        DGEA4580
C                                    DABS(HH), OTHER THAN THOSE BELOW   DGEA4590
C                                    ARE DESIRED, THEY SHOULD BE SET    DGEA4600
C                                     BELOW.                            DGEA4610
      DO 5 I=1,N                                                        DGEA4620
         WK(I) = DABS(Y(I))                                             DGEA4630
         IF (WK(I).EQ.0.D0) WK(I) = 1.D0                                DGEA4640
         WK(NY+I) = Y(I)                                                DGEA4650
    5 CONTINUE                                                          DGEA4660
      NC = N                                                            DGEA4670
      T = X                                                             DGEA4680
      HH = H                                                            DGEA4690
      IF ((T+HH).EQ.T) KER = 33                                         DGEA4700
      HMIN = DABS(H)                                                    DGEA4710
      HMAX = DABS(X-XEND)*10.D0                                         DGEA4720
      EPSC = TOL                                                        DGEA4730
      JSTART = 0                                                        DGEA4740
      N0 = N                                                            DGEA4750
      NSQ = N0*N0                                                       DGEA4760
      EPSJ = DSQRT(UROUND)                                              DGEA4770
      NHCUT = 0                                                         DGEA4780
      DUMMY(2) = 1.0D0                                                  DGEA4790
      DUMMY(14) = 1.0D0                                                 DGEA4800
      GO TO 30                                                          DGEA4810
C                                  TOUTP IS THE PREVIOUS VALUE OF XEND  DGEA4820
C                                     FOR USE IN HMAX.                  DGEA4830
   10 HMAX = DABS(XEND-TOUTP)*10.D0                                     DGEA4840
      GO TO 45                                                          DGEA4850
C                                                                       DGEA4860
   15 HMAX = DABS(XEND-TOUTP)*10.D0                                     DGEA4870
      IF ((T-XEND)*HH.GE.0.D0) GO TO 95                                 DGEA4880
      GO TO 50                                                          DGEA4890
C                                                                       DGEA4900
   20 IF ((T-XEND)*HH.GE.0.D0) GO TO 90                                 DGEA4910
      JSTART = -1                                                       DGEA4920
      NC = N                                                            DGEA4930
      EPSC = TOL                                                        DGEA4940
```

```
C                                                                       DGEA4950
   25 IF ((T+HH).EQ.T) KER = 33                                         DGEA4960
      write(*,*),'error code = ',ker                                       +
C                                                                       DGEA4970
   30 NN = N0                                                           DGEA4980
      step = step + 1                                                      +
      write(*,*)'step = ',step                                             +
      CALL DGRST (FCN,FCNJ,WK(NY+1),WK,WK(NERROR+1),WK(NSAVE1+1),       DGEA4990
     1 WK(NSAVE2+1),WK(NPW+1),WK(NEQUIL+1),IWK,NN,step)                    +
C                                                                       DGEA5010
      KGO = 1-KFLAG                                                     DGEA5020
      GO TO (35,55,70,80), KGO                                          DGEA5030
C                                   KFLAG = 0, -1, -2, -3               DGEA5040
   35 CONTINUE                                                          DGEA5050
C                                  NORMAL RETURN FROM INTEGRATOR. THE   DGEA5060
C                                    WEIGHTS YMAX(I) ARE UPDATED. IF    DGEA5070
C                                    DIFFERENT VALUES ARE DESIRED, THEY DGEA5080
C                                    SHOULD BE SET HERE. A TEST IS MADE DGEA5090
C                                    FOR TOL BEING TOO SMALL FOR THE    DGEA5100
C                                    MACHINE PRECISION. ANY OTHER TESTS DGEA5110
C                                    OR CALCULATIONS THAT ARE REQUIRED  DGEA5120
C                                    AFTER EVERY STEP SHOULD BE         DGEA5130
C                                    INSERTED HERE. IF INDEX = 3, Y IS  DGEA5140
C                                    SET TO THE CURRENT SOLUTION ON     DGEA5150
C                                    RETURN. IF INDEX = 2, HH IS        DGEA5160
C                                    CONTROLLED TO HIT XEND (WITHIN     DGEA5170
C                                    ROUNDOFF ERROR), AND THEN THE      DGEA5180
C                                    CURRENT SOLUTION IS PUT IN Y ON    DGEA5190
C                                    RETURN. FOR ANY OTHER VALUE OF     DGEA5200
C                                    INDEX, CONTROL RETURNS TO THE      DGEA5210
C                                    INTEGRATOR UNLESS XEND HAS BEEN    DGEA5220
C                                    REACHED. THEN INTERPOLATED VALUES  DGEA5230
C                                    OF THE SOLUTION ARE COMPUTED AND   DGEA5240
C                                     STORED IN Y ON RETURN.            DGEA5250
C                                     IF INTERPOLATION IS NOT           DGEA5260
C                                    DESIRED, THE CALL TO DGRIN SHOULD  DGEA5270
C                                    BE REMOVED AND CONTROL TRANSFERRED DGEA5280
C                                    TO STATEMENT 95 INSTEAD OF 105.    DGEA5290
      D = 0.D0                                                          DGEA5300
      DO 40 I=1,N                                                       DGEA5310
         AYI = DABS(WK(NY+I))                                           DGEA5320
         WK(I) = DMAX1(WK(I),AYI)                                       DGEA5330
   40 D = D+(AYI/WK(I))**2                                              DGEA5340
      D = D*(UROUND/TOL)**2                                             DGEA5350
      DN = N                                                            DGEA5360
      IF (D.GT.DN) GO TO 75                                             DGEA5370
      IF (INDEX.EQ.3) GO TO 95                                          DGEA5380
      IF (INDEX.EQ.2) GO TO 50                                          DGEA5390
   45 IF ((T-XEND)*HH.LT.0.D0) GO TO 25                                 DGEA5400
      NN = N0                                                           DGEA5410
      CALL DGRIN (XEND,WK(NY+1),NN,Y)                                   DGEA5420
      X = XEND                                                          DGEA5430
      GO TO 105                                                         DGEA5440
   50 IF (((T+HH)-XEND)*HH.LE.0.D0) GO TO 25                            DGEA5450
      IF (DABS(T-XEND).LE.UROUND*DMAX1(10.D0*DABS(T),HMAX)) GO TO 95    DGEA5460
      IF ((T-XEND)*HH.GE.0.D0) GO TO 95                                 DGEA5470
      HH = (XEND-T)*(1.D0-4.D0*UROUND)                                  DGEA5480
      JSTART = -1                                                       DGEA5490
      GO TO 25                                                          DGEA5500
C                                   ON AN ERROR RETURN FROM INTEGRATOR, DGEA5510
C                                     AN IMMEDIATE RETURN OCCURS IF     DGEA5520
C                                     KFLAG = -2, AND RECOVERY ATTEMPTS DGEA5530
```

```
C                                  ARE MADE OTHERWISE. TO RECOVER, HH
C                                  AND HMIN ARE REDUCED BY A FACTOR
C                                  OF .1 UP TO 10 TIMES BEFORE GIVING
C                                  UP.
   55 JER = 66
   60 IF (NHCUT.EQ.10) GO TO 65
      NHCUT = NHCUT+1
      HMIN = HMIN*.1D0
      HH = HH*.1D0
      JSTART = -1
      GO TO 25
C
   65 IF (JER.EQ.66) JER = 132
      IF (JER.EQ.67) JER = 133
      GO TO 95
C
   70 JER = 134
      GO TO 95
C
   75 JER = 134
      KFLAG = -2
      GO TO 95
C
   80 JER = 67
      GO TO 60
C
   85 JER = 135
      GO TO 110
C
   90 JER = 136
      NN = N0
      CALL DGRIN (XEND,WK(NY+1),NN,Y)
      X = XEND
      GO TO 110
C
   95 X = T
      DO 100 I=1,N
  100 Y(I) = WK(NY+I)
  105 IF (JER.LT.128) INDEX = KFLAG
      TOUTP = X
      IF (KFLAG.EQ.0) H = HUSED
      IF (KFLAG.NE.0) H = HH
  110 IER = MAX0(KER,JER)
 9000 CONTINUE
      IF (KER.NE.0.AND.JER.LT.128) CALL UERTST (KER,6HDGEAR )
      IF (JER.NE.0) CALL UERTST (JER,6HDGEAR )
 9005 RETURN
      END
```

```
C   IMSL ROUTINE NAME   - DGRST                                         DGRS0010
C                                                                       DGRS0020
C-modified to print sheath and diagnostic output to files "sheatha.dat" +
C and "diag.dat"                                                         +
C   COMPUTER            - IBM/DOUBLE                                    DGRS0050
C                                                                       DGRS0060
C   LATEST REVISION     - JUNE 1, 1982                                  DGRS0070
C                                                                       DGRS0080
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR  DGRS0090
C                                                                       DGRS0100
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32                         DGRS0110
C                       - SINGLE/H36,H48,H60                            DGRS0120
C                                                                       DGRS0130
C   REQD. IMSL ROUTINES - DGRCS,DGRPS,LUDATF,LUELMF,LEQT1B,UERTST,      DGRS0140
C                           UGETIO                                      DGRS0150
C                                                                       DGRS0160
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND           DGRS0170
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL      DGRS0180
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  DGRS0190
C                                                                       DGRS0200
C   COPYRIGHT           - 1982 BY IMSL, INC. ALL RIGHTS RESERVED.       DGRS0210
C                                                                       DGRS0220
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN DGRS0230
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,    DGRS0240
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.        DGRS0250
C                                                                       DGRS0260
C-----------------------------------------------------------------------DGRS0270
C                                                                       DGRS0280
      SUBROUTINE DGRST  (FCN,FCNJ,Y,YMAX,ERROR,SAVE1,SAVE2,PW,EQUIL,    DGRS0290
     1                   IPIV,N0,step)                                   +
C                                  SPECIFICATIONS FOR ARGUMENTS         DGRS0310
      INTEGER            IPIV(1),N0                                     DGRS0320
      DOUBLE PRECISION   Y(N0,1),YMAX(1),ERROR(1),SAVE1(1),SAVE2(1),    DGRS0330
     1                   PW(1),EQUIL(1),eprime,eprime(2)                 +
C                                  SPECIFICATIONS FOR LOCAL VARIABLES   DGRS0350
      INTEGER            N,MF,KFLAG,JSTART,NQUSED,NSTEP,NFE,NJE,NSQ,    DGRS0360
     1                   I,METH,MITER,NQ,L,IDOUB,MFOLD,NOLD,IRET,MEO,   DGRS0370
     2                   MIO,IWEVAL,MAXDER,LMAX,IREDO,J,NSTEPJ,J1,J2,   DGRS0380
     3                   M,IER,NEWQ,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY, DGRS0390
     4                   MITER1,IDUMMY(2),NLC,NUC,NWK,JER               DGRS0400
      REAL               TQ(4)                                          DGRS0410
      DOUBLE PRECISION   T,H,HMIN,HMAX,EPS,UROUND,HUSED,EL(13),OLDL0,   DGRS0420
     1                   TOLD,RMAX,RC,CRATE,EPSOLD,HOLD,FN,EDN,E,EUP,   DGRS0430
     2                   BND,RH,R1,CON,R,HL0,R0,D,PHL0,PR3,D1,ENQ3,ENQ2,DGRS0440
     3                   PR2,PR1,ENQ1,EPSJ,DUMMY,tcum                    +
      EXTERNAL           FCN,FCNJ                                       DGRS0460
      COMMON /DBAND/     NLC,NUC                                        DGRS0470
      COMMON /GEAR/      T,H,HMIN,HMAX,EPS,UROUND,EPSJ,HUSED,           DGRS0480
     1                   EL,OLDL0,TOLD,RMAX,RC,CRATE,EPSOLD,HOLD,FN,    DGRS0490
     2                   EDN,E,EUP,BND,RH,R1,R,HL0,R0,D,PHL0,PR3,D1,    DGRS0500
     3                   ENQ3,ENQ2,PR2,PR1,ENQ1,DUMMY,TQ,               DGRS0510
     4                   N,MF,KFLAG,JSTART,NSQ,NQUSED,NSTEP,NFE,NJE,    DGRS0520
     5                   NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,            DGRS0530
     6                   I,METH,MITER,NQ,L,IDOUB,MFOLD,NOLD,IRET,MEO,   DGRS0540
     7                   MIO,IWEVAL,MAXDER,LMAX,IREDO,J,NSTEPJ,J1,J2,   DGRS0550
     8                   M,NEWQ,IDUMMY                                  DGRS0560
C                                  FIRST EXECUTABLE STATEMENT           DGRS0570
      open(unit=8,file='sheatha.dat',status='unknown')                   +
      open(unit=9,file='diag.dat',status='unknown')                      +
      KFLAG = 0                                                         DGRS0580
      TOLD = T                                                          DGRS0590
C                                  THIS ROUTINE PERFORMS ONE STEP OF    DGRS0600
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C                                    THE INTEGRATION OF AN INITIAL      DGRS0610
C                                    VALUE PROBLEM FOR A SYSTEM OF      DGRS0620
C                                    ORDINARY DIFFERENTIAL EQUATIONS.   DGRS0630
      IF (JSTART.GT.0) GO TO 50                                         DGRS0640
      IF (JSTART.NE.0) GO TO 10                                         DGRS0650
C                                  ON THE FIRST CALL, THE ORDER IS SET  DGRS0660
C                                    TO 1 AND THE INITIAL YDOT IS       DGRS0670
C                                    CALCULATED. RMAX IS THE MAXIMUM    DGRS0680
C                                    RATIO BY WHICH H CAN BE INCREASED  DGRS0690
C                                    IN A SINGLE STEP. IT IS INITIALLY  DGRS0700
C                                    1.E4 TO COMPENSATE FOR THE SMALL   DGRS0710
C                                    INITIAL H, BUT THEN IS NORMALLY    DGRS0720
C                                    EQUAL TO 10. IF A FAILURE OCCURS   DGRS0730
C                                    (IN CORRECTOR CONVERGENCE OR ERROR DGRS0740
C                                    TEST), RMAX IS SET AT 2 FOR THE    DGRS0750
C                                    NEXT INCREASE.                     DGRS0760
      CALL FCN (N,T,Y,SAVE1,eprime,eprime2)                               +
      DO 5 I=1,N                                                        DGRS0780
    5 Y(I,2) = H*SAVE1(I)                                               DGRS0790
      METH = MF/10                                                      DGRS0800
      MITER = MF-10*METH                                                DGRS0810
      NQ = 1                                                            DGRS0820
      L = 2                                                             DGRS0830
      IDOUB = 3                                                         DGRS0840
      RMAX = 1.D4                                                       DGRS0850
      RC = 0.D0                                                         DGRS0860
      CRATE = 1.D0                                                      DGRS0870
      HOLD = H                                                          DGRS0880
      MFOLD = MF                                                        DGRS0890
      NSTEP = 0                                                         DGRS0900
      NSTEPJ = 0                                                        DGRS0910
      NFE = 1                                                           DGRS0920
      NJE = 0                                                           DGRS0930
      IRET = 3                                                          DGRS0940
      GO TO 15                                                          DGRS0950
C                                  IF THE CALLER HAS CHANGED METH,      DGRS0960
C                                    DGRCS IS CALLED TO SET THE         DGRS0970
C                                    COEFFICIENTS OF THE METHOD. IF THE DGRS0980
C                                    CALLER HAS CHANGED N, EPS, OR      DGRS0990
C                                    METH, THE CONSTANTS E, EDN, EUP,   DGRS1000
C                                    AND BND MUST BE RESET. E IS A      DGRS1010
C                                    COMPARISON FOR ERRORS OF THE       DGRS1020
C                                    CURRENT ORDER NQ. EUP IS TO TEST   DGRS1030
C                                    FOR INCREASING THE ORDER, EDN FOR  DGRS1040
C                                    DECREASING THE ORDER. BND IS USED  DGRS1050
C                                    TO TEST FOR CONVERGENCE OF THE     DGRS1060
C                                    CORRECTOR ITERATES. IF THE CALLER  DGRS1070
C                                    HAS CHANGED H, Y MUST BE RESCALED. DGRS1080
C                                    IF H OR METH HAS BEEN CHANGED,     DGRS1090
C                                    IDOUB IS RESET TO L + 1 TO PREVENT DGRS1100
C                                    FURTHER CHANGES IN H FOR THAT MANY DGRS1110
C                                     STEPS.                            DGRS1120
   10 IF (MF.EQ.MFOLD) GO TO 25                                         DGRS1130
      MEO = METH                                                        DGRS1140
      MIO = MITER                                                       DGRS1150
      METH = MF/10                                                      DGRS1160
      MITER = MF-10*METH                                                DGRS1170
      MFOLD = MF                                                        DGRS1180
      IF (MITER.NE.MIO) IWEVAL = MITER                                  DGRS1190
      IF (METH.EQ.MEO) GO TO 25                                         DGRS1200
      IDOUB = L+1                                                       DGRS1210
      IRET = 1                                                          DGRS1220
```

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   15 CALL DGRCS (METH,NQ,EL,TQ,MAXDER)                                 DGRS1230
      LMAX = MAXDER+1                                                   DGRS1240
      RC = RC*EL(1)/OLDL0                                               DGRS1250
      OLDL0 = EL(1)                                                     DGRS1260
   20 FN = N                                                            DGRS1270
      EDN = FN*(TQ(1)*EPS)**2                                           DGRS1280
      E = FN*(TQ(2)*EPS)**2                                             DGRS1290
      EUP = FN*(TQ(3)*EPS)**2                                           DGRS1300
      BND = FN*(TQ(4)*EPS)**2                                           DGRS1310
      EPSOLD = EPS                                                      DGRS1320
      NOLD = N                                                          DGRS1330
      GO TO (30,35,50), IRET                                            DGRS1340
   25 IF ((EPS.EQ.EPSOLD).AND.(N.EQ.NOLD)) GO TO 30                     DGRS1350
      IF (N.EQ.NOLD) IWEVAL = MITER                                     DGRS1360
      IRET = 1                                                          DGRS1370
      GO TO 20                                                          DGRS1380
   30 IF (H.EQ.HOLD) GO TO 50                                           DGRS1390
      RH = H/HOLD                                                       DGRS1400
      H = HOLD                                                          DGRS1410
      IREDO = 3                                                         DGRS1420
      GO TO 40                                                          DGRS1430
   35 RH = DMAX1(RH,HMIN/DABS(H))                                       DGRS1440
   40 RH = DMIN1(RH,HMAX/DABS(H),RMAX)                                  DGRS1450
      R1 = 1.D0                                                         DGRS1460
      DO 45 J=2,L                                                       DGRS1470
         R1 = R1*RH                                                     DGRS1480
      DO 45 I=1,N                                                       DGRS1490
   45 Y(I,J) = Y(I,J)*R1                                                DGRS1500
      H = H*RH                                                          DGRS1510
      RC = RC*RH                                                        DGRS1520
      IDOUB = L+1                                                       DGRS1530
      IF (IREDO.EQ.0) GO TO 285                                         DGRS1540
C                                   THIS SECTION COMPUTES THE PREDICTED DGRS1550
C                                     VALUES BY EFFECTIVELY MULTIPLYING DGRS1560
C                                     THE Y ARRAY BY THE PASCAL TRIANGLE DGRS1570
C                                     MATRIX. RC IS THE RATIO OF NEW TO DGRS1580
C                                     OLD VALUES OF THE COEFFICIENT     DGRS1590
C                                     H*EL(1). WHEN RC DIFFERS FROM 1 BY DGRS1600
C                                     MORE THAN 30 PERCENT, OR THE      DGRS1610
C                                     CALLER HAS CHANGED MITER, IWEVAL  DGRS1620
C                                     IS SET TO MITER TO FORCE THE      DGRS1630
C                                     PARTIALS TO BE UPDATED, IF        DGRS1640
C                                     PARTIALS ARE USED. IN ANY CASE,   DGRS1650
C                                     THE PARTIALS ARE UPDATED AT LEAST DGRS1660
C                                     EVERY 20-TH STEP.                 DGRS1670
   50 IF (DABS(RC-1.D0).GT.0.3D0) IWEVAL = MITER                        DGRS1680
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL = MITER                            DGRS1690
      T = T+H                                                           DGRS1700
      DO 55 J1=1,NQ                                                     DGRS1710
      DO 55 J2=J1,NQ                                                    DGRS1720
         J = (NQ+J1)-J2                                                 DGRS1730
      DO 55 I=1,N                                                       DGRS1740
   55 Y(I,J) = Y(I,J)+Y(I,J+1)                                          DGRS1750
C                                   UP TO 3 CORRECTOR ITERATIONS ARE    DGRS1760
C                                     TAKEN. A CONVERGENCE TEST IS MADE DGRS1770
C                                     ON THE R.M.S. NORM OF EACH        DGRS1780
C                                     CORRECTION, USING BND, WHICH IS   DGRS1790
C                                     DEPENDENT ON EPS. THE SUM OF THE  DGRS1800
C                                     CORRECTIONS IS ACCUMULATED IN THE DGRS1810
C                                     VECTOR ERROR(I). THE Y ARRAY IS   DGRS1820
C                                     NOT ALTERED IN THE CORRECTOR LOOP. DGRS1830
C                                     THE UPDATED Y VECTOR IS STORED    DGRS1840
```

```
C                                     TEMPORARILY IN SAVE1.             DGRS1850
   60 DO 65 I=1,N                                                       DGRS1860
   65 ERROR(I) = 0.D0                                                   DGRS1870
      M = 0                                                             DGRS1880
      CALL FCN (N,T,Y,SAVE2,eprime,eprime2)                                 +
      NFE = NFE+1                                                       DGRS1900
      IF (IWEVAL.LE.0) GO TO 95                                         DGRS1910
C                                   IF INDICATED, THE MATRIX P = I -    DGRS1920
C                                     H*EL(1)*J IS REEVALUATED BEFORE   DGRS1930
C                                     STARTING THE CORRECTOR ITERATION. DGRS1940
C                                     IWEVAL IS SET TO 0 AS AN INDICATOR DGRS1950
C                                     THAT THIS HAS BEEN DONE. IF MITER DGRS1960
C                                     = 1 OR 2, P IS COMPUTED AND       DGRS1970
C                                     PROCESSED IN PSET. IF MITER = 3,  DGRS1980
C                                     THE MATRIX USED IS P = I -        DGRS1990
C                                     H*EL(1)*D, WHERE D IS A DIAGONAL  DGRS2000
C                                     MATRIX.                           DGRS2010
      IWEVAL = 0                                                        DGRS2020
      RC = 1.D0                                                         DGRS2030
      NJE = NJE+1                                                       DGRS2040
      NSTEPJ = NSTEP                                                    DGRS2050
      GO TO (75,70,80), MITER                                           DGRS2060
   70 NFE = NFE+N                                                       DGRS2070
   75 CON = -H*EL(1)                                                    DGRS2080
      MITER1 = MITER                                                    DGRS2090
      CALL DGRPS (FCN,FCNJ,Y,N0,CON,MITER1,YMAX,SAVE1,SAVE2,PW,EQUIL,   DGRS2100
     1 IPIV,IER)                                                        DGRS2110
      IF (IER.NE.0) GO TO 155                                           DGRS2120
      GO TO 125                                                         DGRS2130
   80 R = EL(1)*.1D0                                                    DGRS2140
      DO 85 I=1,N                                                       DGRS2150
   85 PW(I) = Y(I,1)+R*(H*SAVE2(I)-Y(I,2))                              DGRS2160
      CALL FCN (N,T,PW,SAVE1,eprime,eprime2)                                +
      NFE = NFE+1                                                       DGRS2180
      HL0 = H*EL(1)                                                     DGRS2190
      DO 90 I=1,N                                                       DGRS2200
         R0 = H*SAVE2(I)-Y(I,2)                                         DGRS2210
         PW(I) = 1.D0                                                   DGRS2220
         D = .1D0*R0-H*(SAVE1(I)-SAVE2(I))                              DGRS2230
         SAVE1(I) = 0.D0                                                DGRS2240
         IF (DABS(R0).LT.UROUND*YMAX(I)) GO TO 90                       DGRS2250
         IF (DABS(D).EQ.0.D0) GO TO 155                                 DGRS2260
         PW(I) = .1D0*R0/D                                              DGRS2270
         SAVE1(I) = PW(I)*R0                                            DGRS2280
   90 CONTINUE                                                          DGRS2290
      GO TO 135                                                         DGRS2300
   95 IF (MITER.NE.0) GO TO (125,125,105), MITER                        DGRS2310
C                                                                       DGRS2320
C                                   IN THE CASE OF FUNCTIONAL ITERATION, DGRS2330
C                                     UPDATE Y DIRECTLY FROM THE RESULT DGRS2340
C                                     OF THE LAST FCN CALL.             DGRS2350
      D = 0.D0                                                          DGRS2360
      DO 100 I=1,N                                                      DGRS2370
         R = H*SAVE2(I)-Y(I,2)                                          DGRS2380
         D = D+((R-ERROR(I))/YMAX(I))**2                                DGRS2390
         SAVE1(I) = Y(I,1)+EL(1)*R                                      DGRS2400
  100 ERROR(I) = R                                                      DGRS2410
      GO TO 145                                                         DGRS2420
C                                   IN THE CASE OF THE CHORD METHOD,    DGRS2430
C                                     COMPUTE THE CORRECTOR ERROR, F SUB DGRS2440
C                                     (M), AND SOLVE THE LINEAR SYSTEM  DGRS2450
C                                     WITH THAT AS RIGHT-HAND SIDE AND P DGRS2460
```

```
C                                    AS COEFFICIENT MATRIX, USING THE   DGRS2470
C                                    LU DECOMPOSITION IF MITER = 1 OR   DGRS2480
C                                    2. IF MITER = 3, THE COEFFICIENT   DGRS2490
C                                    H*EL(1) IN P IS UPDATED.           DGRS2500
  105 PHL0 = HL0                                                        DGRS2510
      HL0 = H*EL(1)                                                     DGRS2520
      IF (HL0.EQ.PHL0) GO TO 115                                        DGRS2530
      R = HL0/PHL0                                                      DGRS2540
      DO 110 I=1,N                                                      DGRS2550
         D = 1.D0-R*(1.D0-1.D0/PW(I))                                   DGRS2560
         IF (DABS(D).EQ.0.D0) GO TO 165                                 DGRS2570
  110 PW(I) = 1.D0/D                                                    DGRS2580
  115 DO 120 I=1,N                                                      DGRS2590
  120 SAVE1(I) = PW(I)*(H*SAVE2(I)-(Y(I,2)+ERROR(I)))                   DGRS2600
      GO TO 135                                                         DGRS2610
  125 DO 130 I=1,N                                                      DGRS2620
  130 SAVE1(I) = H*SAVE2(I)-(Y(I,2)+ERROR(I))                           DGRS2630
      IF (NLC .EQ. -1) GO TO 131                                        DGRS2640
      NWK = (NLC+NUC+1)*N0+1                                            DGRS2650
      CALL LEQT1B(PW,N,NLC,NUC,N0,SAVE1,1,N0,2,PW(NWK),JER)             DGRS2660
      GO TO 135                                                         DGRS2670
  131 CALL LUELMF (PW,SAVE1,IPIV,N,N0,SAVE1)                            DGRS2680
  135 D = 0.D0                                                          DGRS2690
      DO 140 I=1,N                                                      DGRS2700
         ERROR(I) = ERROR(I)+SAVE1(I)                                   DGRS2710
         D = D+(SAVE1(I)/YMAX(I))**2                                    DGRS2720
  140 SAVE1(I) = Y(I,1)+EL(1)*ERROR(I)                                  DGRS2730
C                                  TEST FOR CONVERGENCE. IF M.GT.0, THE DGRS2740
C                                    SQUARE OF THE CONVERGENCE RATE     DGRS2750
C                                    CONSTANT IS ESTIMATED AS CRATE,    DGRS2760
C                                    AND THIS IS USED IN THE TEST.      DGRS2770
  145 IF (M.NE.0) CRATE = DMAX1(.9D0*CRATE,D/D1)                        DGRS2780
      IF ((D*DMIN1(1.D0,2.D0*CRATE)).LE.BND) GO TO 170                  DGRS2790
      D1 = D                                                            DGRS2800
      M = M+1                                                           DGRS2810
      IF (M.EQ.3) GO TO 150                                             DGRS2820
      CALL FCN (N,T,SAVE1,SAVE2,eprime,eprime2)                           +
      GO TO 95                                                          DGRS2840
C                                  THE CORRECTOR ITERATION FAILED TO    DGRS2850
C                                    CONVERGE IN 3 TRIES. IF PARTIALS   DGRS2860
C                                    ARE INVOLVED BUT ARE NOT UP TO     DGRS2870
C                                    DATE, THEY ARE REEVALUATED FOR THE DGRS2880
C                                    NEXT TRY. OTHERWISE THE Y ARRAY IS DGRS2890
C                                    RETRACTED TO ITS VALUES BEFORE     DGRS2900
C                                    PREDICTION, AND H IS REDUCED, IF   DGRS2910
C                                    POSSIBLE. IF NOT, A NO-CONVERGENCE DGRS2920
C                                     EXIT IS TAKEN.                    DGRS2930
  150 NFE = NFE+2                                                       DGRS2940
      IF (IWEVAL.EQ.-1) GO TO 165                                       DGRS2950
  155 T = TOLD                                                          DGRS2960
      RMAX = 2.D0                                                       DGRS2970
      DO 160 J1=1,NQ                                                    DGRS2980
      DO 160 J2=J1,NQ                                                   DGRS2990
         J = (NQ+J1)-J2                                                 DGRS3000
      DO 160 I=1,N                                                      DGRS3010
  160 Y(I,J) = Y(I,J)-Y(I,J+1)                                          DGRS3020
      IF (DABS(H).LE.HMIN*1.00001D0) GO TO 280                          DGRS3030
      RH = .25D0                                                        DGRS3040
      IREDO = 1                                                         DGRS3050
      GO TO 35                                                          DGRS3060
  165 IWEVAL = MITER                                                    DGRS3070
      GO TO 60                                                          DGRS3080
```

```
C                                    THE CORRECTOR HAS CONVERGED. IWEVAL  DGRS3090
C                                      IS SET TO -1 IF PARTIAL            DGRS3100
C                                      DERIVATIVES WERE USED, TO SIGNAL   DGRS3110
C                                      THAT THEY MAY NEED UPDATING ON     DGRS3120
C                                      SUBSEQUENT STEPS. THE ERROR TEST   DGRS3130
C                                      IS MADE AND CONTROL PASSES TO      DGRS3140
C                                      STATEMENT 190 IF IT FAILS.         DGRS3150
  170 IF (MITER.NE.0) IWEVAL = -1                                         DGRS3160
      NFE = NFE+M                                                         DGRS3170
      D = 0.D0                                                            DGRS3180
      DO 175 I=1,N                                                        DGRS3190
  175 D = D+(ERROR(I)/YMAX(I))**2                                         DGRS3200
      IF (D.GT.E) GO TO 190                                               DGRS3210
C                                    AFTER A SUCCESSFUL STEP, UPDATE THE  DGRS3220
C                                      Y ARRAY. CONSIDER CHANGING H IF    DGRS3230
C                                      IDOUB = 1. OTHERWISE DECREASE      DGRS3240
C                                      IDOUB BY 1. IF IDOUB IS THEN 1 AND DGRS3250
C                                      NQ .LT. MAXDER, THEN ERROR IS      DGRS3260
C                                      SAVED FOR USE IN A POSSIBLE ORDER  DGRS3270
C                                      INCREASE ON THE NEXT STEP. IF A    DGRS3280
C                                      CHANGE IN H IS CONSIDERED, AN      DGRS3290
C                                      INCREASE OR DECREASE IN ORDER BY   DGRS3300
C                                      ONE IS CONSIDERED ALSO. A CHANGE   DGRS3310
C                                      IN H IS MADE ONLY IF IT IS BY A    DGRS3320
C                                      FACTOR OF AT LEAST 1.1. IF NOT,    DGRS3330
C                                      IDOUB IS SET TO 10 TO PREVENT      DGRS3340
C                                      TESTING FOR THAT MANY STEPS.       DGRS3350
      KFLAG = 0                                                           DGRS3360
      IREDO = 0                                                           DGRS3370
      NSTEP = NSTEP+1                                                     DGRS3380
      HUSED = H                                                           DGRS3390
      NQUSED = NQ                                                         DGRS3400
      DO 180 J=1,L                                                        DGRS3410
      DO 180 I=1,N                                                        DGRS3420
  180 Y(I,J) = Y(I,J)+EL(J)*ERROR(I)                                      DGRS3430
      IF (IDOUB.EQ.1) GO TO 200                                           DGRS3440
      IDOUB = IDOUB-1                                                     DGRS3450
      IF (IDOUB.GT.1) GO TO 290                                           DGRS3460
      IF (L.EQ.LMAX) GO TO 290                                            DGRS3470
      DO 185 I=1,N                                                        DGRS3480
  185 Y(I,LMAX) = ERROR(I)                                                DGRS3490
      GO TO 290                                                           DGRS3500
C                                    THE ERROR TEST FAILED. KFLAG KEEPS   DGRS3510
C                                      TRACK OF MULTIPLE FAILURES.        DGRS3520
C                                      RESTORE T AND THE Y ARRAY TO THEIR DGRS3530
C                                      PREVIOUS VALUES, AND PREPARE TO    DGRS3540
C                                      TRY THE STEP AGAIN. COMPUTE THE    DGRS3550
C                                      OPTIMUM STEP SIZE FOR THIS OR ONE  DGRS3560
C                                       LOWER ORDER.                      DGRS3570
  190 KFLAG = KFLAG-1                                                     DGRS3580
      T = TOLD                                                            DGRS3590
      DO 195 J1=1,NQ                                                      DGRS3600
      DO 195 J2=J1,NQ                                                     DGRS3610
         J = (NQ+J1)-J2                                                   DGRS3620
      DO 195 I=1,N                                                        DGRS3630
  195 Y(I,J) = Y(I,J)-Y(I,J+1)                                            DGRS3640
      RMAX = 2.D0                                                         DGRS3650
      IF (DABS(H).LE.HMIN*1.00001D0) GO TO 270                            DGRS3660
      IF (KFLAG.LE.-3) GO TO 260                                          DGRS3670
      IREDO = 2                                                           DGRS3680
      PR3 = 1.D+20                                                        DGRS3690
      GO TO 210                                                           DGRS3700
```

```
C                                   REGARDLESS OF THE SUCCESS OR FAILURE DGRS3710
C                                     OF THE STEP, FACTORS PR1, PR2, AND DGRS3720
C                                     PR3 ARE COMPUTED, BY WHICH H COULD DGRS3730
C                                     BE DIVIDED AT ORDER NQ - 1, ORDER  DGRS3740
C                                     NQ, OR ORDER NQ + 1, RESPECTIVELY. DGRS3750
C                                     IN THE CASE OF FAILURE, PR3 =      DGRS3760
C                                     1.E20 TO AVOID AN ORDER INCREASE.  DGRS3770
C                                     THE SMALLEST OF THESE IS           DGRS3780
C                                     DETERMINED AND THE NEW ORDER       DGRS3790
C                                     CHOSEN ACCORDINGLY. IF THE ORDER   DGRS3800
C                                     IS TO BE INCREASED, WE COMPUTE ONE DGRS3810
C                                     ADDITIONAL SCALED DERIVATIVE.      DGRS3820
  200 PR3 = 1.D+20                                                       DGRS3830
      IF (L.EQ.LMAX) GO TO 210                                           DGRS3840
      D1 = 0.D0                                                          DGRS3850
      DO 205 I=1,N                                                       DGRS3860
  205 D1 = D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2                          DGRS3870
      ENQ3 = .5D0/(L+1)                                                  DGRS3880
      PR3 = ((D1/EUP)**ENQ3)*1.4D0+1.4D-6                                DGRS3890
  210 ENQ2 = .5D0/L                                                      DGRS3900
      PR2 = ((D/E)**ENQ2)*1.2D0+1.2D-6                                   DGRS3910
      PR1 = 1.D+20                                                       DGRS3920
      IF (NQ.EQ.1) GO TO 220                                             DGRS3930
      D = 0.D0                                                           DGRS3940
      DO 215 I=1,N                                                       DGRS3950
  215 D = D+(Y(I,L)/YMAX(I))**2                                          DGRS3960
      ENQ1 = .5D0/NQ                                                     DGRS3970
      PR1 = ((D/EDN)**ENQ1)*1.3D0+1.3D-6                                 DGRS3980
  220 IF (PR2.LE.PR3) GO TO 225                                          DGRS3990
      IF (PR3.LT.PR1) GO TO 235                                          DGRS4000
      GO TO 230                                                          DGRS4010
  225 IF (PR2.GT.PR1) GO TO 230                                          DGRS4020
      NEWQ = NQ                                                          DGRS4030
      RH = 1.D0/PR2                                                      DGRS4040
      GO TO 250                                                          DGRS4050
  230 NEWQ = NQ-1                                                        DGRS4060
      RH = 1.D0/PR1                                                      DGRS4070
      IF (KFLAG.NE.0.AND.RH.GT.1.D0) RH = 1.D0                           DGRS4080
      GO TO 250                                                          DGRS4090
  235 NEWQ = L                                                           DGRS4100
      RH = 1.D0/PR3                                                      DGRS4110
      IF (RH.LT.1.1D0) GO TO 245                                         DGRS4120
      DO 240 I=1,N                                                       DGRS4130
  240 Y(I,NEWQ+1) = ERROR(I)*EL(L)/L                                     DGRS4140
      GO TO 255                                                          DGRS4150
  245 IDOUB = 10                                                         DGRS4160
      GO TO 290                                                          DGRS4170
  250 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1D0)) GO TO 245                      DGRS4180
C                                                                        DGRS4190
C                                   IF THERE IS A CHANGE OF ORDER, RESET DGRS4200
C                                     NQ, L, AND THE COEFFICIENTS. IN    DGRS4210
C                                     ANY CASE H IS RESET ACCORDING TO   DGRS4220
C                                     RH AND THE Y ARRAY IS RESCALED.    DGRS4230
C                                     THEN EXIT FROM 285 IF THE STEP WAS DGRS4240
C                                     OK, OR REDO THE STEP OTHERWISE.    DGRS4250
      IF (NEWQ.EQ.NQ) GO TO 35                                           DGRS4260
  255 NQ = NEWQ                                                          DGRS4270
      L = NQ+1                                                           DGRS4280
      IRET = 2                                                           DGRS4290
      GO TO 15                                                           DGRS4300
C                                   CONTROL REACHES THIS SECTION IF 3 OR DGRS4310
C                                     MORE FAILURES HAVE OCCURED. IT IS  DGRS4320
```

```
C                                          ASSUMED THAT THE DERIVATIVES THAT  DGRS4330
C                                          HAVE ACCUMULATED IN THE Y ARRAY    DGRS4340
C                                          HAVE ERRORS OF THE WRONG ORDER.    DGRS4350
C                                          HENCE THE FIRST DERIVATIVE IS      DGRS4360
C                                          RECOMPUTED, AND THE ORDER IS SET   DGRS4370
C                                          TO 1. THEN H IS REDUCED BY A       DGRS4380
C                                          FACTOR OF 10, AND THE STEP IS      DGRS4390
C                                          RETRIED. AFTER A TOTAL OF 7        DGRS4400
C                                          FAILURES, AN EXIT IS TAKEN WITH    DGRS4410
C                                          KFLAG = -2.                        DGRS4420
  260 IF (KFLAG.EQ.-7) GO TO 275                                              DGRS4430
      RH = .1D0                                                               DGRS4440
      RH = DMAX1(HMIN/DABS(H),RH)                                             DGRS4450
      H = H*RH                                                                DGRS4460
      CALL FCN (N,T,Y,SAVE1,eprime,eprime2)                                     +
      NFE = NFE+1                                                             DGRS4480
      DO 265 I=1,N                                                            DGRS4490
  265 Y(I,2) = H*SAVE1(I)                                                     DGRS4500
      IWEVAL = MITER                                                          DGRS4510
      IDOUB = 10                                                              DGRS4520
      IF (NQ.EQ.1) GO TO 50                                                   DGRS4530
      NQ = 1                                                                  DGRS4540
      L = 2                                                                   DGRS4550
      IRET = 3                                                                DGRS4560
      GO TO 15                                                                DGRS4570
C                                        ALL RETURNS ARE MADE THROUGH THIS    DGRS4580
C                                          SECTION. H IS SAVED IN HOLD TO     DGRS4590
C                                          ALLOW THE CALLER TO CHANGE H ON    DGRS4600
C                                          THE NEXT STEP.                     DGRS4610
  270 KFLAG = -1                                                              DGRS4620
      GO TO 290                                                               DGRS4630
  275 KFLAG = -2                                                              DGRS4640
      GO TO 290                                                               DGRS4650
  280 KFLAG = -3                                                              DGRS4660
      GO TO 290                                                               DGRS4670
  285 RMAX = 10.D0                                                            DGRS4680
  290 HOLD = H                                                                DGRS4690
      JSTART = NQ                                                             DGRS4700
C--Diagnostic Check of first and second derivatives of E                         +
      if(tcum.eq.told)go to 310                                                  +
      write(8,300)tcum,step,y(1,1),y(2,1),y(3,1),y(4,1),y(5,1)                   +
  300 format(1x,e11.4,1x,I5,5(1x,e11.4))                                         +
      write(9,305)step,eprime,eprime2                                            +
  305 format(1x,I5,2(1x,e20.13))                                                 +
      RETURN                                                                  DGRS4710
      END                                                                     DGRS4720
```

```
C   IMSL ROUTINE NAME   - DGRCS
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - IBM/DOUBLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - NONE REQUIRED
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   COPYRIGHT           - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.
C
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
C
      SUBROUTINE DGRCS  (METH,NQ,EL,TQ,MAXDER)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER            METH,NQ,MAXDER
      REAL               TQ(1)
      DOUBLE PRECISION   EL(1)
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER            K
      REAL               PERTST(12,2,3)
      DATA               PERTST/1.,1.,2.,1.,.3158,.7407E-1,
     1                  .1391E-1,.2182E-2,.2945E-3,.3492E-4,
     2                  .3692E-5,.3524E-6,1.,1.,.5,.1667,
     3                  .4167E-1,7*1.,2.,12.,24.,37.89,
     4                  53.33,70.08,87.97,106.9,126.7,
     5                  147.4,168.8,191.0,2.0,4.5,7.333,
     6                  10.42,13.7,7*1.,12.0,24.0,37.89,
     7                  53.33,70.08,87.97,106.9,126.7,
     8                  147.4,168.8,191.0,1.,3.0,6.0,
     9                  9.167,12.5,8*1./
C                                  FIRST EXECUTABLE STATEMENT
      GO TO (5,10), METH
    5 MAXDER = 12
      GO TO (15,20,25,30,35,40,45,50,55,60,65,70), NQ
   10 MAXDER = 5
      GO TO (75,80,85,90,95), NQ
C                                  THE FOLLOWING COEFFICIENTS SHOULD BE
C                                    DEFINED TO MACHINE ACCURACY. FOR A
C                                    GIVEN ORDER NQ, THEY CAN BE
C                                    CALCULATED BY USE OF THE
C                                    GENERATING POLYNOMIAL L(T), WHOSE
C                                    COEFFICIENTS ARE EL(I).. L(T) =
C                                    EL(1) + EL(2)*T + ... +
C                                    EL(NQ+1)*T**NQ. FOR THE IMPLICIT
C                                    ADAMS METHODS, L(T) IS GIVEN BY
C                                    DL/DT = (T+1)*(T+2)* ...
C                                    *(T+NQ-1)/K, L(-1) = 0, WHERE K =
```

```
C                                     FACTORIAL(NQ-1). FOR THE GEAR      DGRC0630
C                                     METHODS, L(T) = (T+1)*(T+2)* ...   DGRC0640
C                                     *(T+NQ)/K, WHERE K =               DGRC0650
C                                     FACTORIAL(NQ)*(1 + 1/2 + ... +     DGRC0660
C                                     1/NQ). THE ORDER IN WHICH THE      DGRC0670
C                                     GROUPS APPEAR BELOW IS.. IMPLICIT  DGRC0680
C                                     ADAMS METHODS OF ORDERS 1 TO 12,   DGRC0690
C                                     BACKWARD DIFFERENTIATION METHODS   DGRC0700
C                                     OF ORDERS 1 TO 5.                  DGRC0710
   15 EL(1) = 1.0D0                                                      DGRC0720
      GO TO 100                                                          DGRC0730
   20 EL(1) = 0.5D0                                                      DGRC0740
      EL(3) = 0.5D0                                                      DGRC0750
      GO TO 100                                                          DGRC0760
   25 EL(1) = 4.166666666666667D-01                                      DGRC0770
      EL(3) = 0.75D0                                                     DGRC0780
      EL(4) = 1.666666666666667D-01                                      DGRC0790
      GO TO 100                                                          DGRC0800
   30 EL(1) = 0.375D0                                                    DGRC0810
      EL(3) = 9.166666666666667D-01                                      DGRC0820
      EL(4) = 3.333333333333333D-01                                      DGRC0830
      EL(5) = 4.166666666666667D-02                                      DGRC0840
      GO TO 100                                                          DGRC0850
   35 EL(1) = 3.486111111111111D-01                                      DGRC0860
      EL(3) = 1.041666666666667D0                                        DGRC0870
      EL(4) = 4.861111111111111D-01                                      DGRC0880
      EL(5) = 1.041666666666667D-01                                      DGRC0890
      EL(6) = 8.333333333333333D-03                                      DGRC0900
      GO TO 100                                                          DGRC0910
   40 EL(1) = 3.298611111111111D-01                                      DGRC0920
      EL(3) = 1.141666666666667D+00                                      DGRC0930
      EL(4) = 0.625D+00                                                  DGRC0940
      EL(5) = 1.770833333333333D-01                                      DGRC0950
      EL(6) = 0.025D+00                                                  DGRC0960
      EL(7) = 1.388888888888889D-03                                      DGRC0970
      GO TO 100                                                          DGRC0980
   45 EL(1) = 3.155919312169312D-01                                      DGRC0990
      EL(3) = 1.225D+00                                                  DGRC1000
      EL(4) = 7.518518518518519D-01                                      DGRC1010
      EL(5) = 2.552083333333333D-01                                      DGRC1020
      EL(6) = 4.861111111111111D-02                                      DGRC1030
      EL(7) = 4.861111111111111D-03                                      DGRC1040
      EL(8) = 1.984126984126984D-04                                      DGRC1050
      GO TO 100                                                          DGRC1060
   50 EL(1) = 3.042245370370370D-01                                      DGRC1070
      EL(3) = 1.296428571428571D+00                                      DGRC1080
      EL(4) = 8.685185185185185D-01                                      DGRC1090
      EL(5) = 3.357638888888889D-01                                      DGRC1100
      EL(6) = 7.777777777777778D-02                                      DGRC1110
      EL(7) = 1.064814814814815D-02                                      DGRC1120
      EL(8) = 7.936507936507937D-04                                      DGRC1130
      EL(9) = 2.480158730158730D-05                                      DGRC1140
      GO TO 100                                                          DGRC1150
   55 EL(1) = 2.948680004409171D-01                                      DGRC1160
      EL(3) = 1.358928571428571D+00                                      DGRC1170
      EL(4) = 9.765542328042328D-01                                      DGRC1180
      EL(5) = 4.171875D-01                                               DGRC1190
      EL(6) = 1.113541666666667D-01                                      DGRC1200
      EL(7) = 0.01875D+00                                                DGRC1210
      EL(8) = 1.934523809523810D-03                                      DGRC1220
      EL(9) = 1.116071428571429D-04                                      DGRC1230
      EL(10)= 2.755731922398589D-06                                      DGRC1240
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      GO TO 100                                                         DGRC1250
   60 EL(1) = 2.869754464285714D-01                                     DGRC1260
      EL(3) = 1.414484126984127D+00                                     DGRC1270
      EL(4) = 1.077215608465609D+00                                     DGRC1280
      EL(5) = 4.985670194003527D-01                                     DGRC1290
      EL(6) = 1.484375D-01                                              DGRC1300
      EL(7) = 2.906057098765432D-02                                     DGRC1310
      EL(8) = 3.720238095238095D-03                                     DGRC1320
      EL(9) = 2.996858465608466D-04                                     DGRC1330
      EL(10)= 1.377865961199295D-05                                     DGRC1340
      EL(11)= 2.755731922398589D-07                                     DGRC1350
      GO TO 100                                                         DGRC1360
   65 EL(1) = 2.801895964439367D-01                                     DGRC1370
      EL(3) = 1.464484126984127D+00                                     DGRC1380
      EL(4) = 1.171514550264550D+00                                     DGRC1390
      EL(5) = 5.793581900352734D-01                                     DGRC1400
      EL(6) = 1.883228615520282D-01                                     DGRC1410
      EL(7) = 4.143036265432099D-02                                     DGRC1420
      EL(8) = 6.211144179894180D-03                                     DGRC1430
      EL(9) = 6.252066798941799D-04                                     DGRC1440
      EL(10)= 4.041740152851264D-05                                     DGRC1450
      EL(11)= 1.515652557319224D-06                                     DGRC1460
      EL(12)= 2.505210838544172D-08                                     DGRC1470
      GO TO 100                                                         DGRC1480
   70 EL(1) = 2.742655400315991D-01                                     DGRC1490
      EL(3) = 1.509938672438672D+00                                     DGRC1500
      EL(4) = 1.260271164021164D+00                                     DGRC1510
      EL(5) = 6.592341820987654D-01                                     DGRC1520
      EL(6) = 2.304580026455027D-01                                     DGRC1530
      EL(7) = 5.569724610523222D-02                                     DGRC1540
      EL(8) = 9.439484126984127D-03                                     DGRC1550
      EL(9) = 1.119274966931217D-03                                     DGRC1560
      EL(10) = 9.093915343915344D-05                                    DGRC1570
      EL(11) = 4.822530864197531D-06                                    DGRC1580
      EL(12)= 1.503126503126503D-07                                     DGRC1590
      EL(13)= 2.087675698786810D-09                                     DGRC1600
      GO TO 100                                                         DGRC1610
C                                                                       DGRC1620
   75 EL(1) = 1.0D+00                                                   DGRC1630
      GO TO 100                                                         DGRC1640
   80 EL(1) = 6.666666666666667D-01                                     DGRC1650
      EL(3) = 3.333333333333333D-01                                     DGRC1660
      GO TO 100                                                         DGRC1670
   85 EL(1) = 5.454545454545455D-01                                     DGRC1680
      EL(3) = EL(1)                                                     DGRC1690
      EL(4) = 9.090909090909091D-02                                     DGRC1700
      GO TO 100                                                         DGRC1710
   90 EL(1) = 0.48D+00                                                  DGRC1720
      EL(3) = 0.7D+00                                                   DGRC1730
      EL(4) = 0.2D+00                                                   DGRC1740
      EL(5) = 0.02D+00                                                  DGRC1750
      GO TO 100                                                         DGRC1760
   95 EL(1) = 4.379562043795620D-01                                     DGRC1770
      EL(3) = 8.211678832116788D-01                                     DGRC1780
      EL(4) = 3.102189781021898D-01                                     DGRC1790
      EL(5) = 5.474452554744526D-02                                     DGRC1800
      EL(6) = 3.649635036496350D-03                                     DGRC1810
C                                                                       DGRC1820
  100 DO 105 K=1,3                                                      DGRC1830
          TQ(K) = PERTST(NQ,METH,K)                                     DGRC1840
  105 CONTINUE                                                          DGRC1850
      TQ(4) = .5D0*TQ(2)/(NQ+2)                                         DGRC1860
```

```
      RETURN                                                            DGRC1870
      END                                                               DGRC1880
```

```
C   IMSL ROUTINE NAME   - DGRPS
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - IBM/DOUBLE
C
C   LATEST REVISION     - NOVEMBER 1, 1984
C
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - LUDATF,LEQT1B,UERTST,UGETIO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   COPYRIGHT           - 1984 BY IMSL, INC.  ALL RIGHTS RESERVED.
C
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                           APPLIED TO THIS CODE.  NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
C
      SUBROUTINE DGRPS (FCN,FCNJ,Y,N0,CON,MITER,YMAX,SAVE1,SAVE2,PW,
     *                   EQUIL,IPIV,IER)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER            N0,MITER,IPIV(1),IER
      DOUBLE PRECISION   Y(N0,1),CON,YMAX(1),SAVE1(1),SAVE2(1),PW(1),
     *                   EQUIL(1)
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
C
      INTEGER            NC,MFC,KFLAG,JSTART,NQUSED,NSTEP,NFE,NJE,NPW,
     *                   NSQ,I,J1,J,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     *                   IDUMMY(23),NLIM,II,IJ,LIM1,LIM2,NB,NLC,NUC,NWK
      REAL               SDUMMY(4)
      DOUBLE PRECISION   T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,D,R0,YJ,R,
     *                   D1,D2,WA,DUMMY(40)
      COMMON /DBAND/     NLC,NUC
      COMMON /GEAR/      T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,
     *                   SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,NSTEP,
     *                   NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     *                   IDUMMY
C                                  THIS ROUTINE IS CALLED BY DGRST TO
C                                    COMPUTE AND PROCESS THE MATRIX P =
C                                    I - H*EL(1)*J , WHERE J IS AN
C                                    APPROXIMATION TO THE JACOBIAN. J
C                                    IS COMPUTED, EITHER BY THE USER-
C                                    SUPPLIED ROUTINE FCNJ IF MITER =
C                                    1, OR BY FINITE DIFFERENCING IF
C                                    MITER = 2. J IS STORED IN PW AND
C                                    REPLACED BY P, USING CON =
C                                    -H*EL(1). THEN P IS SUBJECTED TO
C                                    LU DECOMPOSITION IN PREPARATION
C                                    FOR LATER SOLUTION OF LINEAR
C                                    SYSTEMS WITH P AS COEFFICIENT
C                                    MATRIX. IN ADDITION TO VARIABLES
C                                    DESCRIBED PREVIOUSLY,
C                                    COMMUNICATION WITH DGRPS USES THE
```

```
C                                  FOLLOWING EPSJ = DSQRT(UROUND),     DGRP0630
C                                  USED IN THE NUMERICAL JACOBIAN      DGRP0640
C                                   INCREMENTS.                        DGRP0650
C                                                                      DGRP0660
C                                FIRST EXECUTABLE STATEMENT            DGRP0670
      IF (NLC.EQ.-1) GO TO 45                                          DGRP0680
C                                BANDED JACOBIAN CASE                  DGRP0690
      NB = NLC+NUC+1                                                   DGRP0700
      NWK = NB*N0+1                                                    DGRP0710
      IF (MITER.EQ.2) GO TO 15                                         DGRP0720
C                                MITER = 1                             DGRP0730
      NLIM = NB*N0                                                     DGRP0740
      DO 5 I=1,NLIM                                                    DGRP0750
         PW(I) = 0.0D0                                                 DGRP0760
    5 CONTINUE                                                         DGRP0770
      CALL FCNJ(NC,T,Y,PW)                                             DGRP0780
      DO 10 I=1,NLIM                                                   DGRP0790
         PW(I) = PW(I)*CON                                             DGRP0800
   10 CONTINUE                                                         DGRP0810
      GO TO 35                                                         DGRP0820
C                                MITER = 2                             DGRP0830
   15 D = 0.0D0                                                        DGRP0840
      DO 20 I=1,NC                                                     DGRP0850
   20 D = D+SAVE2(I)**2                                                DGRP0860
      R0 = DABS(H)*DSQRT(D)*1.0D+03*UROUND                             DGRP0870
      DO 30 J=1,NC                                                     DGRP0880
         YJ = Y(J,1)                                                   DGRP0890
         R = EPSJ*YMAX(J)                                              DGRP0900
         R = DMAX1(R,R0)                                               DGRP0910
         Y(J,1) = Y(J,1)+R                                             DGRP0920
         D = CON/R                                                     DGRP0930
         CALL FCN(NC,T,Y,SAVE1)                                        DGRP0940
         LIM1 = MAX0(1,J-NUC)                                          DGRP0950
         LIM2 = MIN0(N0,J+NLC)                                         DGRP0960
         DO 25 I=LIM1,LIM2                                             DGRP0970
            IJ = (J-I+NLC)*N0+I                                        DGRP0980
            PW(IJ) = (SAVE1(I)-SAVE2(I))*D                             DGRP0990
   25    CONTINUE                                                      DGRP1000
         Y(J,1) = YJ                                                   DGRP1010
   30 CONTINUE                                                         DGRP1020
C                                ADD IDENTITY MATRIX.                  DGRP1030
   35 DO 40 I=1,NC                                                     DGRP1040
         II = NLC*N0+I                                                 DGRP1050
         PW(II) = PW(II)+1.0D0                                         DGRP1060
   40 CONTINUE                                                         DGRP1070
C                                DO LU DECOMPOSITION ON P              DGRP1080
C                                                                      DGRP1090
      CALL LEQT1B(PW,NC,NLC,NUC,N0,EQUIL,1,N0,1,PW(NWK),IER)           DGRP1100
      RETURN                                                           DGRP1110
C                                FULL JACOBIAN CASE                    DGRP1120
   45 IF (MITER.EQ.2) GO TO 55                                         DGRP1130
C                                MITER = 1                             DGRP1140
      CALL FCNJ(NC,T,Y,PW)                                             DGRP1150
      DO 50 I=1,NSQ                                                    DGRP1160
   50 PW(I) = PW(I)*CON                                                DGRP1170
      GO TO 75                                                         DGRP1180
C                                MITER = 2                             DGRP1190
   55 D = 0.0D0                                                        DGRP1200
      DO 60 I=1,NC                                                     DGRP1210
   60 D = D+SAVE2(I)**2                                                DGRP1220
      R0 = DABS(H)*DSQRT(D)*1.0D+03*UROUND                             DGRP1230
      J1 = 0                                                           DGRP1240
```

```
      DO 70 J=1,NC                                                      DGRP1250
         YJ = Y(J,1)                                                    DGRP1260
         R = EPSJ*YMAX(J)                                               DGRP1270
         R = DMAX1(R,R0)                                                DGRP1280
         Y(J,1) = Y(J,1)+R                                              DGRP1290
         D = CON/R                                                      DGRP1300
         CALL FCN(NC,T,Y,SAVE1)                                         DGRP1310
         DO 65 I=1,NC                                                   DGRP1320
   65    PW(I+J1) = (SAVE1(I)-SAVE2(I))*D                               DGRP1330
         Y(J,1) = YJ                                                    DGRP1340
         J1 = J1+N0                                                     DGRP1350
   70 CONTINUE                                                          DGRP1360
C                                  ADD IDENTITY MATRIX.                 DGRP1370
   75 J = 1                                                             DGRP1380
      DO 80 I=1,NC                                                      DGRP1390
         PW(J) = PW(J)+1.0D0                                            DGRP1400
         J = J+(N0+1)                                                   DGRP1410
   80 CONTINUE                                                          DGRP1420
C                                  DO LU DECOMPOSITION ON P.            DGRP1430
C                                                                       DGRP1440
      CALL LUDATF(PW,PW,NC,N0,0,D1,D2,IPIV,EQUIL,WA,IER)                DGRP1450
      RETURN                                                            DGRP1460
      END                                                               DGRP1470
```

```
C   IMSL ROUTINE NAME   - DGRIN                                         DGRI0010
C                                                                       DGRI0020
C-----------------------------------------------------------------------DGRI0030
C                                                                       DGRI0040
C   COMPUTER            - IBM/DOUBLE                                    DGRI0050
C                                                                       DGRI0060
C   LATEST REVISION     - JANUARY 1, 1978                               DGRI0070
C                                                                       DGRI0080
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR  DGRI0090
C                                                                       DGRI0100
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32                         DGRI0110
C                       - SINGLE/H36,H48,H60                            DGRI0120
C                                                                       DGRI0130
C   REQD. IMSL ROUTINES - NONE REQUIRED                                 DGRI0140
C                                                                       DGRI0150
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND           DGRI0160
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL      DGRI0170
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  DGRI0180
C                                                                       DGRI0190
C   COPYRIGHT           - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.       DGRI0200
C                                                                       DGRI0210
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN DGRI0220
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,    DGRI0230
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.        DGRI0240
C                                                                       DGRI0250
C-----------------------------------------------------------------------DGRI0260
C                                                                       DGRI0270
      SUBROUTINE DGRIN  (TOUT,Y,N0,Y0)                                  DGRI0280
C                                  SPECIFICATIONS FOR ARGUMENTS         DGRI0290
      INTEGER            N0                                             DGRI0300
      DOUBLE PRECISION   TOUT,Y0(N0),Y(N0,1)                            DGRI0310
C                                  SPECIFICATIONS FOR LOCAL VARIABLES   DGRI0320
      INTEGER            NC,MFC,KFLAG,I,L,J,JSTART,NSQ,NQUSED,NSTEP,    DGRI0330
     1                   NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,    DGRI0340
     2                   IDUMMY(23)                                     DGRI0350
      REAL               SDUMMY(4)                                      DGRI0360
      DOUBLE PRECISION   T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,S,S1,     DGRI0370
     1                   DUMMY(40)                                      DGRI0380
      COMMON /GEAR/      T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,    DGRI0390
     1                   SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,NSTEP,   DGRI0400
     2                   NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,    DGRI0410
     3                   IDUMMY                                         DGRI0420
C                                  FIRST EXECUTABLE STATEMENT           DGRI0430
      DO 5 I = 1,NC                                                     DGRI0440
         Y0(I) = Y(I,1)                                                 DGRI0450
    5 CONTINUE                                                          DGRI0460
C                                  THIS SUBROUTINE COMPUTES INTERPOLATEDDGRI0470
C                                    VALUES OF THE DEPENDENT VARIABLE   DGRI0480
C                                    Y AND STORES THEM IN Y0. THE       DGRI0490
C                                    INTERPOLATION IS TO THE            DGRI0500
C                                    POINT T = TOUT, AND USES THE       DGRI0510
C                                    NORDSIECK HISTORY ARRAY Y, AS      DGRI0520
C                                    FOLLOWS..                          DGRI0530
C                                                NQ                     DGRI0540
C                                    Y0(I)  =  SUM  Y(I,J+1)*S**J ,     DGRI0550
C                                               J=0                     DGRI0560
C                                    WHERE S = -(T-TOUT)/H.             DGRI0570
      L = JSTART + 1                                                    DGRI0580
      S = (TOUT - T)/H                                                  DGRI0590
      S1 = 1.0D0                                                        DGRI0600
      DO 15 J = 2,L                                                     DGRI0610
         S1 = S1*S                                                      DGRI0620
```

```
          DO 10 I = 1,NC                                                DGRI0630
             Y0(I) = Y0(I) + S1*Y(I,J)                                  DGRI0640
  10      CONTINUE                                                      DGRI0650
  15   CONTINUE                                                         DGRI0660
       RETURN                                                           DGRI0670
       END                                                              DGRI0680
```

```
C   IMSL ROUTINE NAME   - LUDATF                                        LUDA0010
C                                                                       LUDA0020
C-----------------------------------------------------------------------LUDA0030
C                                                                       LUDA0040
C   COMPUTER            - IBM/DOUBLE                                    LUDA0050
C                                                                       LUDA0060
C   LATEST REVISION     - JANUARY 1, 1978                               LUDA0070
C                                                                       LUDA0080
C   PURPOSE             - L-U DECOMPOSITION BY THE CROUT ALGORITHM      LUDA0090
C                           WITH OPTIONAL ACCURACY TEST.                LUDA0100
C                                                                       LUDA0110
C   USAGE               - CALL LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,       LUDA0120
C                           EQUIL,WA,IER)                               LUDA0130
C                                                                       LUDA0140
C   ARGUMENTS   A       - INPUT MATRIX OF DIMENSION N BY N CONTAINING   LUDA0150
C                           THE MATRIX TO BE DECOMPOSED.                LUDA0160
C               LU      - REAL OUTPUT MATRIX OF DIMENSION N BY N        LUDA0170
C                           CONTAINING THE L-U DECOMPOSITION OF A       LUDA0180
C                           ROWWISE PERMUTATION OF THE INPUT MATRIX.    LUDA0190
C                           FOR A DESCRIPTION OF THE FORMAT OF LU, SEE  LUDA0200
C                           EXAMPLE.                                    LUDA0210
C               N       - INPUT SCALAR CONTAINING THE ORDER OF THE      LUDA0220
C                           MATRIX A.                                   LUDA0230
C               IA      - INPUT SCALAR CONTAINING THE ROW DIMENSION OF  LUDA0240
C                           MATRICES A AND LU EXACTLY AS SPECIFIED IN   LUDA0250
C                           THE CALLING PROGRAM.                        LUDA0260
C               IDGT    - INPUT OPTION.                                 LUDA0270
C                           IF IDGT IS GREATER THAN ZERO, THE NON-ZERO  LUDA0280
C                           ELEMENTS OF A ARE ASSUMED TO BE CORRECT TO  LUDA0290
C                           IDGT DECIMAL PLACES.  LUDATF PERFORMS AN    LUDA0300
C                           ACCURACY TEST TO DETERMINE IF THE COMPUTED  LUDA0310
C                           DECOMPOSITION IS THE EXACT DECOMPOSITION    LUDA0320
C                           OF A MATRIX WHICH DIFFERS FROM THE GIVEN    LUDA0330
C                           ONE BY LESS THAN ITS UNCERTAINTY.           LUDA0340
C                         IF IDGT IS EQUAL TO ZERO, THE ACCURACY TEST   LUDA0350
C                           IS BYPASSED.                                LUDA0360
C               D1      - OUTPUT SCALAR CONTAINING ONE OF THE TWO       LUDA0370
C                           COMPONENTS OF THE DETERMINANT. SEE          LUDA0380
C                           DESCRIPTION OF PARAMETER D2, BELOW.         LUDA0390
C               D2      - OUTPUT SCALAR CONTAINING ONE OF THE           LUDA0400
C                           TWO COMPONENTS OF THE DETERMINANT. THE      LUDA0410
C                           DETERMINANT MAY BE EVALUATED AS (D1)(2**D2).LUDA0420
C               IPVT    - OUTPUT VECTOR OF LENGTH N CONTAINING THE      LUDA0430
C                           PERMUTATION INDICES. SEE DOCUMENT           LUDA0440
C                           (ALGORITHM).                                LUDA0450
C               EQUIL   - OUTPUT VECTOR OF LENGTH N CONTAINING          LUDA0460
C                           RECIPROCALS OF THE ABSOLUTE VALUES OF       LUDA0470
C                           THE LARGEST (IN ABSOLUTE VALUE) ELEMENT     LUDA0480
C                           IN EACH ROW.                                LUDA0490
C               WA      - ACCURACY TEST PARAMETER, OUTPUT ONLY IF       LUDA0500
C                           IDGT IS GREATER THAN ZERO.                  LUDA0510
C                           SEE ELEMENT DOCUMENTATION FOR DETAILS.      LUDA0520
C               IER     - ERROR PARAMETER. (OUTPUT)                     LUDA0530
C                         TERMINAL ERROR                                LUDA0540
C                           IER = 129 INDICATES THAT MATRIX A IS        LUDA0550
C                             ALGORITHMICALLY SINGULAR. (SEE THE        LUDA0560
C                             CHAPTER L PRELUDE).                       LUDA0570
C                         WARNING ERROR                                 LUDA0580
C                           IER = 34 INDICATES THAT THE ACCURACY TEST   LUDA0590
C                             FAILED.  THE COMPUTED SOLUTION MAY BE IN  LUDA0600
C                             ERROR BY MORE THAN CAN BE ACCOUNTED FOR   LUDA0610
C                             BY THE UNCERTAINTY OF THE DATA.  THIS     LUDA0620
```

```
C                            WARNING CAN BE PRODUCED ONLY IF IDGT IS
C                            GREATER THAN 0 ON INPUT.  SEE CHAPTER L
C                            PRELUDE FOR FURTHER DISCUSSION.
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - UERTST,UGETIO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      A TEST FOR SINGULARITY IS MADE AT TWO LEVELS:
C                1.  A ROW OF THE ORIGINAL MATRIX A IS NULL.
C               2.  A COLUMN BECOMES NULL IN THE FACTORIZATION PROCESS.
C
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C
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
C
      SUBROUTINE LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,EQUIL,WA,IER)
C
      DIMENSION          A(IA,1),LU(IA,1),IPVT(1),EQUIL(1)
      DOUBLE PRECISION  A,LU,D1,D2,EQUIL,WA,ZERO,ONE,FOUR,SIXTN,SIXTH,
     *                  RN,WREL,BIGA,BIG,P,SUM,AI,WI,T,TEST,Q
      DATA              ZERO,ONE,FOUR,SIXTN,SIXTH/0.D0,1.D0,4.D0,
     *                   16.D0,.0625D0/
C                                  FIRST EXECUTABLE STATEMENT
C                                  INITIALIZATION
      IER = 0
      RN = N
      WREL = ZERO
      D1 = ONE
      D2 = ZERO
      BIGA = ZERO
      DO 10 I=1,N
         BIG = ZERO
         DO 5 J=1,N
            P = A(I,J)
            LU(I,J) = P
            P = DABS(P)
            IF (P .GT. BIG) BIG = P
    5    CONTINUE
         IF (BIG .GT. BIGA) BIGA = BIG
         IF (BIG .EQ. ZERO) GO TO 110
         EQUIL(I) = ONE/BIG
   10 CONTINUE
      DO 105 J=1,N
         JM1 = J-1
         IF (JM1 .LT. 1) GO TO 40
C                                  COMPUTE U(I,J), I=1,...,J-1
         DO 35 I=1,JM1
            SUM = LU(I,J)
            IM1 = I-1
            IF (IDGT .EQ. 0) GO TO 25
C                                  WITH ACCURACY TEST
            AI = DABS(SUM)
```

```
            WI = ZERO                                                   LUDA1250
            IF (IM1 .LT. 1) GO TO 20                                    LUDA1260
            DO 15 K=1,IM1                                               LUDA1270
               T = LU(I,K)*LU(K,J)                                      LUDA1280
               SUM = SUM-T                                              LUDA1290
               WI = WI+DABS(T)                                          LUDA1300
   15       CONTINUE                                                    LUDA1310
            LU(I,J) = SUM                                               LUDA1320
   20       WI = WI+DABS(SUM)                                           LUDA1330
            IF (AI .EQ. ZERO) AI = BIGA                                 LUDA1340
            TEST = WI/AI                                                LUDA1350
            IF (TEST .GT. WREL) WREL = TEST                             LUDA1360
            GO TO 35                                                    LUDA1370
C                                  WITHOUT ACCURACY                     LUDA1380
   25       IF (IM1 .LT. 1) GO TO 35                                    LUDA1390
            DO 30 K=1,IM1                                               LUDA1400
               SUM = SUM-LU(I,K)*LU(K,J)                                LUDA1410
   30       CONTINUE                                                    LUDA1420
            LU(I,J) = SUM                                               LUDA1430
   35    CONTINUE                                                       LUDA1440
   40    P = ZERO                                                       LUDA1450
C                                  COMPUTE U(J,J) AND L(I,J), I=J+1,...,LUDA1460
         DO 70 I=J,N                                                    LUDA1470
            SUM = LU(I,J)                                               LUDA1480
            IF (IDGT .EQ. 0) GO TO 55                                   LUDA1490
C                                  WITH ACCURACY TEST                   LUDA1500
            AI = DABS(SUM)                                              LUDA1510
            WI = ZERO                                                   LUDA1520
            IF (JM1 .LT. 1) GO TO 50                                    LUDA1530
            DO 45 K=1,JM1                                               LUDA1540
               T = LU(I,K)*LU(K,J)                                      LUDA1550
               SUM = SUM-T                                              LUDA1560
               WI = WI+DABS(T)                                          LUDA1570
   45       CONTINUE                                                    LUDA1580
            LU(I,J) = SUM                                               LUDA1590
   50       WI = WI+DABS(SUM)                                           LUDA1600
            IF (AI .EQ. ZERO) AI = BIGA                                 LUDA1610
            TEST = WI/AI                                                LUDA1620
            IF (TEST .GT. WREL) WREL = TEST                             LUDA1630
            GO TO 65                                                    LUDA1640
C                                  WITHOUT ACCURACY TEST                LUDA1650
   55       IF (JM1 .LT. 1) GO TO 65                                    LUDA1660
            DO 60 K=1,JM1                                               LUDA1670
               SUM = SUM-LU(I,K)*LU(K,J)                                LUDA1680
   60       CONTINUE                                                    LUDA1690
            LU(I,J) = SUM                                               LUDA1700
   65       Q = EQUIL(I)*DABS(SUM)                                      LUDA1710
            IF (P .GE. Q) GO TO 70                                      LUDA1720
            P = Q                                                       LUDA1730
            IMAX = I                                                    LUDA1740
   70    CONTINUE                                                       LUDA1750
C                                  TEST FOR ALGORITHMIC SINGULARITY     LUDA1760
         IF (RN+P .EQ. RN) GO TO 110                                    LUDA1770
         IF (J .EQ. IMAX) GO TO 80                                      LUDA1780
C                                  INTERCHANGE ROWS J AND IMAX          LUDA1790
         D1 = -D1                                                       LUDA1800
         DO 75 K=1,N                                                    LUDA1810
            P = LU(IMAX,K)                                              LUDA1820
            LU(IMAX,K) = LU(J,K)                                        LUDA1830
            LU(J,K) = P                                                 LUDA1840
   75    CONTINUE                                                       LUDA1850
         EQUIL(IMAX) = EQUIL(J)                                         LUDA1860
```

```
   80    IPVT(J) = IMAX                                                 LUDA1870
         D1 = D1*LU(J,J)                                                LUDA1880
   85    IF (DABS(D1) .LE. ONE) GO TO 90                                LUDA1890
         D1 = D1*SIXTH                                                  LUDA1900
         D2 = D2+FOUR                                                   LUDA1910
         GO TO 85                                                       LUDA1920
   90    IF (DABS(D1) .GE. SIXTH) GO TO 95                              LUDA1930
         D1 = D1*SIXTN                                                  LUDA1940
         D2 = D2-FOUR                                                   LUDA1950
         GO TO 90                                                       LUDA1960
   95    CONTINUE                                                       LUDA1970
         JP1 = J+1                                                      LUDA1980
         IF (JP1 .GT. N) GO TO 105                                      LUDA1990
C                                 DIVIDE BY PIVOT ELEMENT U(J,J)        LUDA2000
         P = LU(J,J)                                                    LUDA2010
         DO 100 I=JP1,N                                                 LUDA2020
            LU(I,J) = LU(I,J)/P                                         LUDA2030
  100    CONTINUE                                                       LUDA2040
  105 CONTINUE                                                          LUDA2050
C                                 PERFORM ACCURACY TEST                 LUDA2060
      IF (IDGT .EQ. 0) GO TO 9005                                       LUDA2070
      P = 3*N+3                                                         LUDA2080
      WA = P*WREL                                                       LUDA2090
      IF (WA+10.D0**(-IDGT) .NE. WA) GO TO 9005                         LUDA2100
      IER = 34                                                          LUDA2110
      GO TO 9000                                                        LUDA2120
C                                 ALGORITHMIC SINGULARITY               LUDA2130
  110 IER = 129                                                         LUDA2140
      D1 = ZERO                                                         LUDA2150
      D2 = ZERO                                                         LUDA2160
 9000 CONTINUE                                                          LUDA2170
C                                 PRINT ERROR                           LUDA2180
      CALL UERTST(IER,6HLUDATF)                                         LUDA2190
 9005 RETURN                                                            LUDA2200
      END                                                               LUDA2210
```

```
C   IMSL ROUTINE NAME   - LUELMF                                        LUEF0010
C                                                                       LUEF0020
C-----------------------------------------------------------------------LUEF0030
C                                                                       LUEF0040
C   COMPUTER            - IBM/DOUBLE                                    LUEF0050
C                                                                       LUEF0060
C   LATEST REVISION     - JANUARY 1, 1978                               LUEF0070
C                                                                       LUEF0080
C   PURPOSE             - ELIMINATION PART OF SOLUTION OF AX=B          LUEF0090
C                           (FULL STORAGE MODE)                         LUEF0100
C                                                                       LUEF0110
C   USAGE               - CALL LUELMF (A,B,IPVT,N,IA,X)                 LUEF0120
C                                                                       LUEF0130
C   ARGUMENTS    A      - A = LU (THE RESULT COMPUTED IN THE IMSL       LUEF0140
C                           ROUTINE LUDATF) WHERE L IS A LOWER          LUEF0150
C                           TRIANGULAR MATRIX WITH ONES ON THE MAIN     LUEF0160
C                           DIAGONAL. U IS UPPER TRIANGULAR. L AND U    LUEF0170
C                           ARE STORED AS A SINGLE MATRIX A AND THE     LUEF0180
C                           UNIT DIAGONAL OF L IS NOT STORED. (INPUT)   LUEF0190
C                B      - B IS A VECTOR OF LENGTH N ON THE RIGHT HAND   LUEF0200
C                           SIDE OF THE EQUATION AX=B. (INPUT)          LUEF0210
C                IPVT   - THE PERMUTATION MATRIX RETURNED FROM THE      LUEF0220
C                           IMSL ROUTINE LUDATF, STORED AS AN N LENGTH  LUEF0230
C                           VECTOR. (INPUT)                             LUEF0240
C                N      - ORDER OF A AND NUMBER OF ROWS IN B. (INPUT)   LUEF0250
C                IA     - ROW DIMENSION OF A EXACTLY AS SPECIFIED IN    LUEF0260
C                           THE DIMENSION STATEMENT IN THE CALLING      LUEF0270
C                           PROGRAM. (INPUT)                            LUEF0280
C                X      - THE RESULT X. (OUTPUT)                        LUEF0290
C                                                                       LUEF0300
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32                         LUEF0310
C                       - SINGLE/H36,H48,H60                            LUEF0320
C                                                                       LUEF0330
C   REQD. IMSL ROUTINES - NONE REQUIRED                                 LUEF0340
C                                                                       LUEF0350
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND           LUEF0360
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL      LUEF0370
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  LUEF0380
C                                                                       LUEF0390
C   COPYRIGHT           - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.       LUEF0400
C                                                                       LUEF0410
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN LUEF0420
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,    LUEF0430
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.        LUEF0440
C                                                                       LUEF0450
C-----------------------------------------------------------------------LUEF0460
C                                                                       LUEF0470
      SUBROUTINE LUELMF (A,B,IPVT,N,IA,X)                               LUEF0480
C                                                                       LUEF0490
      DIMENSION          A(IA,1),B(1),IPVT(1),X(1)                      LUEF0500
      DOUBLE PRECISION   A,B,X,SUM                                      LUEF0510
C                                  FIRST EXECUTABLE STATEMENT           LUEF0520
C                                  SOLVE LY = B FOR Y                   LUEF0530
      DO 5 I=1,N                                                        LUEF0540
    5 X(I) = B(I)                                                       LUEF0550
      IW = 0                                                            LUEF0560
      DO 20 I=1,N                                                       LUEF0570
         IP = IPVT(I)                                                   LUEF0580
         SUM = X(IP)                                                    LUEF0590
         X(IP) = X(I)                                                   LUEF0600
         IF (IW .EQ. 0) GO TO 15                                        LUEF0610
         IM1 = I-1                                                      LUEF0620
```

```
         DO 10 J=IW,IM1                                                 LUEF0630
            SUM = SUM-A(I,J)*X(J)                                       LUEF0640
   10    CONTINUE                                                       LUEF0650
         GO TO 20                                                       LUEF0660
   15    IF (SUM .NE. 0.D0) IW = I                                      LUEF0670
   20 X(I) = SUM                                                        LUEF0680
C                                 SOLVE UX = Y FOR X                    LUEF0690
      DO 30 IB=1,N                                                      LUEF0700
         I = N+1-IB                                                     LUEF0710
         IP1 = I+1                                                      LUEF0720
         SUM = X(I)                                                     LUEF0730
         IF (IP1 .GT. N) GO TO 30                                       LUEF0740
         DO 25 J=IP1,N                                                  LUEF0750
            SUM = SUM-A(I,J)*X(J)                                       LUEF0760
   25   CONTINUE                                                        LUEF0770
   30 X(I) = SUM/A(I,I)                                                 LUEF0780
      RETURN                                                            LUEF0790
      END                                                               LUEF0800
```

```
C   IMSL ROUTINE NAME   - LEQT1B                                        LE1B0010
C                                                                       LE1B0020
C-----------------------------------------------------------------------LE1B0030
C                                                                       LE1B0040
C   COMPUTER            - IBM/DOUBLE                                    LE1B0050
C                                                                       LE1B0060
C   LATEST REVISION     - JANUARY 1, 1978                               LE1B0070
C                                                                       LE1B0080
C   PURPOSE             - LINEAR EQUATION SOLUTION - BAND STORAGE       LE1B0090
C                           MODE - SPACE ECONOMIZER SOLUTION            LE1B0100
C                                                                       LE1B0110
C   USAGE               - CALL LEQT1B (A,N,NLC,NUC,IA,B,M,IB,IJOB,XL,   LE1B0120
C                           IER)                                        LE1B0130
C                                                                       LE1B0140
C   ARGUMENTS    A      - INPUT/OUTPUT MATRIX OF DIMENSION N BY         LE1B0150
C                           (NUC+NLC+1). SEE PARAMETER IJOB.            LE1B0160
C                N      - ORDER OF MATRIX A AND THE NUMBER OF ROWS IN   LE1B0170
C                           B. (INPUT)                                  LE1B0180
C                NLC    - NUMBER OF LOWER CODIAGONALS IN MATRIX A.      LE1B0190
C                           (INPUT)                                     LE1B0200
C                NUC    - NUMBER OF UPPER CODIAGONALS IN MATRIX A.      LE1B0210
C                           (INPUT)                                     LE1B0220
C                IA     - ROW DIMENSION OF MATRIX A EXACTLY AS          LE1B0230
C                           SPECIFIED IN THE DIMENSION STATEMENT IN THE LE1B0240
C                           CALLING PROGRAM. (INPUT)                    LE1B0250
C                B      - INPUT/OUTPUT MATRIX OF DIMENSION N BY M.      LE1B0260
C                           ON INPUT, B CONTAINS THE M RIGHT-HAND SIDES LE1B0270
C                           OF THE EQUATION AX = B. ON OUTPUT, THE      LE1B0280
C                           SOLUTION MATRIX X REPLACES B. IF IJOB = 1,  LE1B0290
C                           B IS NOT USED.                              LE1B0300
C                M      - NUMBER OF RIGHT HAND SIDES (COLUMNS IN B).    LE1B0310
C                           (INPUT)                                     LE1B0320
C                IB     - ROW DIMENSION OF MATRIX B EXACTLY AS          LE1B0330
C                           SPECIFIED IN THE DIMENSION STATEMENT IN THE LE1B0340
C                           CALLING PROGRAM. (INPUT)                    LE1B0350
C                IJOB   - INPUT OPTION PARAMETER. IJOB = I IMPLIES WHEN LE1B0360
C                           I = 0, FACTOR THE MATRIX A AND SOLVE THE    LE1B0370
C                             EQUATION AX = B. ON INPUT, A CONTAINS THE LE1B0380
C                             COEFFICIENT MATRIX OF THE EQUATION AX = B,LE1B0390
C                             WHERE A IS ASSUMED TO BE AN N BY N BAND   LE1B0400
C                             MATRIX. A IS STORED IN BAND STORAGE MODE  LE1B0410
C                             AND THEREFORE HAS DIMENSION N BY          LE1B0420
C                             (NLC+NUC+1). ON OUTPUT, A IS REPLACED     LE1B0430
C                             BY THE U MATRIX OF THE L-U DECOMPOSITION  LE1B0440
C                             OF A ROWWISE PERMUTATION OF MATRIX A. U   LE1B0450
C                             IS STORED IN BAND STORAGE MODE.           LE1B0460
C                           I = 1, FACTOR THE MATRIX A. A CONTAINS THE  LE1B0470
C                             SAME INPUT/OUTPUT INFORMATION AS IF       LE1B0480
C                             IJOB = 0.                                 LE1B0490
C                           I = 2, SOLVE THE EQUATION AX = B. THIS      LE1B0500
C                             OPTION IMPLIES THAT LEQT1B HAS ALREADY    LE1B0510
C                             BEEN CALLED USING IJOB = 0 OR 1 SO THAT   LE1B0520
C                             THE MATRIX A HAS ALREADY BEEN FACTORED.   LE1B0530
C                             IN THIS CASE, OUTPUT MATRICES A AND XL    LE1B0540
C                             MUST HAVE BEEN SAVED FOR REUSE IN THE     LE1B0550
C                             CALL TO LEQT1B.                           LE1B0560
C                XL     - WORK AREA OF DIMENSION N*(NLC+1). THE FIRST   LE1B0570
C                           NLC*N LOCATIONS OF XL CONTAIN COMPONENTS OF LE1B0580
C                           THE L MATRIX OF THE L-U DECOMPOSITION OF A  LE1B0590
C                           ROWWISE PERMUTATION OF A. THE LAST N        LE1B0600
C                           LOCATIONS CONTAIN THE PIVOT INDICES.        LE1B0610
C                IER    - ERROR PARAMETER. (OUTPUT)                     LE1B0620
```

```
C                         TERMINAL ERROR                                LE1B0630
C                           IER = 129 INDICATES THAT MATRIX A IS        LE1B0640
C                             ALGORITHMICALLY SINGULAR. (SEE THE        LE1B0650
C                             CHAPTER L PRELUDE).                       LE1B0660
C                                                                       LE1B0670
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32                         LE1B0680
C                       - SINGLE/H36,H48,H60                            LE1B0690
C                                                                       LE1B0700
C   REQD. IMSL ROUTINES - UERTST,UGETIO                                 LE1B0710
C                                                                       LE1B0720
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND           LE1B0730
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL      LE1B0740
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  LE1B0750
C                                                                       LE1B0760
C   COPYRIGHT           - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.       LE1B0770
C                                                                       LE1B0780
C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN LE1B0790
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,    LE1B0800
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.        LE1B0810
C                                                                       LE1B0820
C-----------------------------------------------------------------------LE1B0830
C                                                                       LE1B0840
      SUBROUTINE LEQT1B (A,N,NLC,NUC,IA,B,M,IB,IJOB,XL,IER)             LE1B0850
C                                                                       LE1B0860
      DIMENSION          A(IA,1),XL(N,1),B(IB,1)                        LE1B0870
      DOUBLE PRECISION   A,XL,B,P,Q,ZERO,ONE,RN                         LE1B0880
      DATA               ZERO/0.D0/,ONE/1.0D0/                          LE1B0890
C                                  FIRST EXECUTABLE STATEMENT           LE1B0900
      IER = 0                                                           LE1B0910
      JBEG = NLC+1                                                      LE1B0920
      NLC1 = JBEG                                                       LE1B0930
      IF (IJOB .EQ. 2) GO TO 80                                         LE1B0940
      RN = N                                                            LE1B0950
C                                  RESTRUCTURE THE MATRIX               LE1B0960
C                                  FIND RECIPROCAL OF THE LARGEST       LE1B0970
C                                  ABSOLUTE VALUE IN ROW I              LE1B0980
      I = 1                                                             LE1B0990
      NC = JBEG+NUC                                                     LE1B1000
      NN = NC                                                           LE1B1010
      JEND = NC                                                         LE1B1020
      IF (N .EQ. 1 .OR. NLC .EQ. 0) GO TO 25                            LE1B1030
    5 K = 1                                                             LE1B1040
      P = ZERO                                                          LE1B1050
      DO 10 J = JBEG,JEND                                               LE1B1060
         A(I,K) = A(I,J)                                                LE1B1070
         Q =  DABS(A(I,K))                                              LE1B1080
         IF (Q .GT. P) P = Q                                            LE1B1090
         K = K+1                                                        LE1B1100
   10 CONTINUE                                                          LE1B1110
      IF (P .EQ. ZERO) GO TO 135                                        LE1B1120
      XL(I,NLC1) = ONE/P                                                LE1B1130
      IF (K .GT. NC) GO TO 20                                           LE1B1140
      DO 15 J = K,NC                                                    LE1B1150
         A(I,J) = ZERO                                                  LE1B1160
   15 CONTINUE                                                          LE1B1170
   20 I = I+1                                                           LE1B1180
      JBEG = JBEG-1                                                     LE1B1190
      IF (JEND-JBEG .EQ. N) JEND = JEND-1                               LE1B1200
      IF (I .LE. NLC) GO TO 5                                           LE1B1210
      JBEG = I                                                          LE1B1220
      NN = JEND                                                         LE1B1230
   25 JEND = N-NUC                                                      LE1B1240
```

```
      DO 40 I = JBEG,N                                                  LE1B1250
         P = ZERO                                                       LE1B1260
         DO 30 J = 1,NN                                                 LE1B1270
            Q =  DABS(A(I,J))                                           LE1B1280
            IF (Q .GT. P) P = Q                                         LE1B1290
   30    CONTINUE                                                       LE1B1300
         IF (P .EQ. ZERO) GO TO 135                                     LE1B1310
         XL(I,NLC1) = ONE/P                                             LE1B1320
         IF (I .EQ. JEND) GO TO 37                                      LE1B1330
         IF (I .LT. JEND) GO TO 40                                      LE1B1340
         K = NN+1                                                       LE1B1350
         DO 35 J = K,NC                                                 LE1B1360
            A(I,J) = ZERO                                               LE1B1370
   35    CONTINUE                                                       LE1B1380
   37    NN = NN-1                                                      LE1B1390
   40 CONTINUE                                                          LE1B1400
      L = NLC                                                           LE1B1410
C                                L-U DECOMPOSITION                      LE1B1420
      DO 75 K = 1,N                                                     LE1B1430
         P =  DABS(A(K,1))*XL(K,NLC1)                                   LE1B1440
         I = K                                                          LE1B1450
         IF (L .LT. N) L = L+1                                          LE1B1460
         K1 = K+1                                                       LE1B1470
         IF (K1 .GT. L) GO TO 50                                        LE1B1480
         DO 45 J = K1,L                                                 LE1B1490
            Q = DABS(A(J,1))*XL(J,NLC1)                                 LE1B1500
            IF (Q .LE. P) GO TO 45                                      LE1B1510
            P = Q                                                       LE1B1520
            I = J                                                       LE1B1530
   45    CONTINUE                                                       LE1B1540
   50    XL(I,NLC1) = XL(K,NLC1)                                        LE1B1550
         XL(K,NLC1) = I                                                 LE1B1560
C                                SINGULARITY FOUND                      LE1B1570
         Q = RN+P                                                       LE1B1580
         IF (Q .EQ. RN) GO TO 135                                       LE1B1590
C                                INTERCHANGE ROWS I AND K               LE1B1600
         IF (K .EQ. I) GO TO 60                                         LE1B1610
         DO 55 J = 1,NC                                                 LE1B1620
            P = A(K,J)                                                  LE1B1630
            A(K,J) = A(I,J)                                             LE1B1640
            A(I,J) = P                                                  LE1B1650
   55    CONTINUE                                                       LE1B1660
   60    IF (K1 .GT. L) GO TO 75                                        LE1B1670
         DO 70 I = K1,L                                                 LE1B1680
            P = A(I,1)/A(K,1)                                           LE1B1690
            IK = I-K                                                    LE1B1700
            XL(K1,IK) = P                                               LE1B1710
            DO 65 J = 2,NC                                              LE1B1720
               A(I,J-1) = A(I,J)-P*A(K,J)                               LE1B1730
   65    CONTINUE                                                       LE1B1740
         A(I,NC) = ZERO                                                 LE1B1750
   70    CONTINUE                                                       LE1B1760
   75 CONTINUE                                                          LE1B1770
      IF (IJOB .EQ. 1) GO TO 9005                                       LE1B1780
C                                FORWARD SUBSTITUTION                   LE1B1790
   80 L = NLC                                                           LE1B1800
      DO 105 K = 1,N                                                    LE1B1810
         I = XL(K,NLC1)                                                 LE1B1820
         IF (I .EQ. K) GO TO 90                                         LE1B1830
         DO 85 J = 1,M                                                  LE1B1840
            P = B(K,J)                                                  LE1B1850
            B(K,J) = B(I,J)                                             LE1B1860
```

```
            B(I,J) = P                                                  LE1B1870
   85    CONTINUE                                                       LE1B1880
   90    IF (L .LT. N) L = L+1                                          LE1B1890
         K1 = K+1                                                       LE1B1900
         IF (K1 .GT. L) GO TO 105                                       LE1B1910
         DO 100 I = K1,L                                                LE1B1920
            IK = I-K                                                    LE1B1930
            P = XL(K1,IK)                                               LE1B1940
            DO 95 J = 1,M                                               LE1B1950
               B(I,J) = B(I,J)-P*B(K,J)                                 LE1B1960
   95       CONTINUE                                                    LE1B1970
  100    CONTINUE                                                       LE1B1980
  105 CONTINUE                                                          LE1B1990
C                                 BACKWARD SUBSTITUTION                 LE1B2000
      JBEG = NUC+NLC                                                    LE1B2010
      DO 125 J = 1,M                                                    LE1B2020
         L = 1                                                          LE1B2030
         K1 = N+1                                                       LE1B2040
         DO 120 I = 1,N                                                 LE1B2050
            K = K1-I                                                    LE1B2060
            P = B(K,J)                                                  LE1B2070
            IF (L .EQ. 1) GO TO 115                                     LE1B2080
            DO 110 KK = 2,L                                             LE1B2090
               IK = KK+K                                                LE1B2100
               P = P-A(K,KK)*B(IK-1,J)                                  LE1B2110
  110       CONTINUE                                                    LE1B2120
  115       B(K,J) = P/A(K,1)                                           LE1B2130
            IF (L .LE. JBEG) L = L+1                                    LE1B2140
  120    CONTINUE                                                       LE1B2150
  125 CONTINUE                                                          LE1B2160
      GO TO 9005                                                        LE1B2170
  135 IER = 129                                                         LE1B2180
 9000 CONTINUE                                                          LE1B2190
      CALL UERTST(IER,6HLEQT1B)                                         LE1B2200
 9005 RETURN                                                            LE1B2210
      END                                                               LE1B2220
```

```
C   IMSL ROUTINE NAME   - UERTST
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JUNE 1, 1982
C
C   PURPOSE             - PRINT A MESSAGE REFLECTING AN ERROR CONDITION
C
C   USAGE               - CALL UERTST (IER,NAME)
C
C   ARGUMENTS    IER    - ERROR PARAMETER. (INPUT)
C                           IER = I+J WHERE
C                             I = 128 IMPLIES TERMINAL ERROR MESSAGE,
C                             I =  64 IMPLIES WARNING WITH FIX MESSAGE,
C                             I =  32 IMPLIES WARNING MESSAGE.
C                             J = ERROR CODE RELEVANT TO CALLING
C                                 ROUTINE.
C                NAME   - A CHARACTER STRING OF LENGTH SIX PROVIDING
C                           THE NAME OF THE CALLING ROUTINE. (INPUT)
C
C   PRECISION/HARDWARE  - SINGLE/ALL
C
C   REQD. IMSL ROUTINES - UGETIO,USPKD
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      THE ERROR MESSAGE PRODUCED BY UERTST IS WRITTEN
C                TO THE STANDARD OUTPUT UNIT. THE OUTPUT UNIT
C                NUMBER CAN BE DETERMINED BY CALLING UGETIO AS
C                FOLLOWS..   CALL UGETIO(1,NIN,NOUT).
C                THE OUTPUT UNIT NUMBER CAN BE CHANGED BY CALLING
C                UGETIO AS FOLLOWS..
C                                NIN = 0
C                                NOUT = NEW OUTPUT UNIT NUMBER
C                                CALL UGETIO(3,NIN,NOUT)
C                SEE THE UGETIO DOCUMENT FOR MORE DETAILS.
C
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C
C-----------------------------------------------------------------------
C
      SUBROUTINE UERTST (IER,NAME)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER            IER
      INTEGER            NAME(1)
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER            I,IEQ,IEQDF,IOUNIT,LEVEL,LEVOLD,NAMEQ(6),
     *                   NAMSET(6),NAMUPK(6),NIN,NMTB
      DATA               NAMSET/1HU,1HE,1HR,1HS,1HE,1HT/
      DATA               NAMEQ/6*1H /
      DATA               LEVEL/4/,IEQDF/0/,IEQ/1H=/
C                                  UNPACK NAME INTO NAMUPK
C                                  FIRST EXECUTABLE STATEMENT
      CALL USPKD (NAME,6,NAMUPK,NMTB)
```

```
C                                 GET OUTPUT UNIT NUMBER
      CALL UGETIO(1,NIN,IOUNIT)
C                                 CHECK IER
      IF (IER.GT.999) GO TO 25
      IF (IER.LT.-32) GO TO 55
      IF (IER.LE.128) GO TO 5
      IF (LEVEL.LT.1) GO TO 30
C                                 PRINT TERMINAL MESSAGE
      IF (IEQDF.EQ.1) WRITE(IOUNIT,35) IER,NAMEQ,IEQ,NAMUPK
      IF (IEQDF.EQ.0) WRITE(IOUNIT,35) IER,NAMUPK
      GO TO 30
    5 IF (IER.LE.64) GO TO 10
      IF (LEVEL.LT.2) GO TO 30
C                                 PRINT WARNING WITH FIX MESSAGE
      IF (IEQDF.EQ.1) WRITE(IOUNIT,40) IER,NAMEQ,IEQ,NAMUPK
      IF (IEQDF.EQ.0) WRITE(IOUNIT,40) IER,NAMUPK
      GO TO 30
   10 IF (IER.LE.32) GO TO 15
C                                 PRINT WARNING MESSAGE
      IF (LEVEL.LT.3) GO TO 30
      IF (IEQDF.EQ.1) WRITE(IOUNIT,45) IER,NAMEQ,IEQ,NAMUPK
      IF (IEQDF.EQ.0) WRITE(IOUNIT,45) IER,NAMUPK
      GO TO 30
   15 CONTINUE
C                                 CHECK FOR UERSET CALL
      DO 20 I=1,6
         IF (NAMUPK(I).NE.NAMSET(I)) GO TO 25
   20 CONTINUE
      LEVOLD = LEVEL
      LEVEL = IER
      IER = LEVOLD
      IF (LEVEL.LT.0) LEVEL = 4
      IF (LEVEL.GT.4) LEVEL = 4
      GO TO 30
   25 CONTINUE
      IF (LEVEL.LT.4) GO TO 30
C                                 PRINT NON-DEFINED MESSAGE
      IF (IEQDF.EQ.1) WRITE(IOUNIT,50) IER,NAMEQ,IEQ,NAMUPK
      IF (IEQDF.EQ.0) WRITE(IOUNIT,50) IER,NAMUPK
   30 IEQDF = 0
      RETURN
   35 FORMAT(19H *** TERMINAL ERROR,10X,7H(IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
   40 FORMAT(27H *** WARNING WITH FIX ERROR,2X,7H(IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
   45 FORMAT(18H *** WARNING ERROR,11X,7H(IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
   50 FORMAT(20H *** UNDEFINED ERROR,9X,7H(IER = ,I5,
     1       20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
C
C                                 SAVE P FOR P = R CASE
C                                   P IS THE PAGE NAMUPK
C                                   R IS THE ROUTINE NAMUPK
   55 IEQDF = 1
      DO 60 I=1,6
   60 NAMEQ(I) = NAMUPK(I)
   65 RETURN
      END
```

```
C   IMSL ROUTINE NAME   - UGETIO
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JUNE 1, 1981
C
C   PURPOSE             - TO RETRIEVE CURRENT VALUES AND TO SET NEW
C                           VALUES FOR INPUT AND OUTPUT UNIT
C                           IDENTIFIERS.
C
C   USAGE               - CALL UGETIO(IOPT,NIN,NOUT)
C
C   ARGUMENTS    IOPT   - OPTION PARAMETER. (INPUT)
C                           IF IOPT=1, THE CURRENT INPUT AND OUTPUT
C                           UNIT IDENTIFIER VALUES ARE RETURNED IN NIN
C                           AND NOUT, RESPECTIVELY.
C                           IF IOPT=2, THE INTERNAL VALUE OF NIN IS
C                           RESET FOR SUBSEQUENT USE.
C                           IF IOPT=3, THE INTERNAL VALUE OF NOUT IS
C                           RESET FOR SUBSEQUENT USE.
C                NIN    - INPUT UNIT IDENTIFIER.
C                           OUTPUT IF IOPT=1, INPUT IF IOPT=2.
C                NOUT   - OUTPUT UNIT IDENTIFIER.
C                           OUTPUT IF IOPT=1, INPUT IF IOPT=3.
C
C   PRECISION/HARDWARE  - SINGLE/ALL
C
C   REQD. IMSL ROUTINES - NONE REQUIRED
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      EACH IMSL ROUTINE THAT PERFORMS INPUT AND/OR OUTPUT
C                OPERATIONS CALLS UGETIO TO OBTAIN THE CURRENT UNIT
C                IDENTIFIER VALUES. IF UGETIO IS CALLED WITH IOPT=2 OR
C                IOPT=3, NEW UNIT IDENTIFIER VALUES ARE ESTABLISHED.
C                SUBSEQUENT INPUT/OUTPUT IS PERFORMED ON THE NEW UNITS.
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C
C-----------------------------------------------------------------------
C
      SUBROUTINE UGETIO(IOPT,NIN,NOUT)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER            IOPT,NIN,NOUT
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER            NIND,NOUTD
      DATA               NIND/5/,NOUTD/6/
C                                  FIRST EXECUTABLE STATEMENT
      IF (IOPT.EQ.3) GO TO 10
      IF (IOPT.EQ.2) GO TO 5
      IF (IOPT.NE.1) GO TO 9005
      NIN = NIND
      NOUT = NOUTD
      GO TO 9005
```

```
    5 NINDD = NIN                                                           UGET0630
      GO TO 9005                                                            UGET0640
   10 NOUTD = NOUT                                                          UGET0650
 9005 RETURN                                                                UGET0660
      END                                                                   UGET0670
```

```
C   IMSL ROUTINE NAME   - USPKD
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - NOVEMBER 1, 1984
C
C   PURPOSE             - NUCLEUS CALLED BY IMSL ROUTINES THAT HAVE
C                           CHARACTER STRING ARGUMENTS
C
C   USAGE               - CALL USPKD  (PACKED,NCHARS,UNPAKD,NCHMTB)
C
C   ARGUMENTS    PACKED - CHARACTER STRING TO BE UNPACKED.(INPUT)
C                NCHARS - LENGTH OF PACKED. (INPUT)  SEE REMARKS.
C                UNPAKD - INTEGER ARRAY TO RECEIVE THE UNPACKED
C                         REPRESENTATION OF THE STRING. (OUTPUT)
C              . NCHMTB - NCHARS MINUS TRAILING BLANKS. (OUTPUT)
C
C   PRECISION/HARDWARE  - SINGLE/ALL
C
C   REQD. IMSL ROUTINES - NONE
C
C   REMARKS  1.  USPKD UNPACKS A CHARACTER STRING INTO AN INTEGER ARRAY
C                IN (A1) FORMAT.
C            2.  UP TO 129 CHARACTERS MAY BE USED.  ANY IN EXCESS OF
C                THAT ARE IGNORED.
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C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
      SUBROUTINE USPKD  (PACKED,NCHARS,UNPAKD,NCHMTB)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER            NC,NCHARS,NCHMTB
C
      LOGICAL*1          UNPAKD(1),PACKED(1),LBYTE,LBLANK
      INTEGER*2          IBYTE,IBLANK
      EQUIVALENCE (LBYTE,IBYTE)
      DATA               LBLANK /1H /
      DATA               IBYTE /1H /
      DATA               IBLANK /1H /
C                                  INITIALIZE NCHMTB
      NCHMTB = 0
C                                  RETURN IF NCHARS IS LE ZERO
      IF(NCHARS.LE.0) RETURN
C                                  SET NC=NUMBER OF CHARS TO BE DECODED
      NC = MIN0 (129,NCHARS)
      NWORDS = NC*4
      J = 1
      DO 110 I = 1,NWORDS,4
      UNPAKD(I) = PACKED(J)
      UNPAKD(I+1) = LBLANK
      UNPAKD(I+2) = LBLANK
      UNPAKD(I+3) = LBLANK
  110 J = J+1
C                                  CHECK UNPAKD ARRAY AND SET NCHMTB
C                                  BASED ON TRAILING BLANKS FOUND
      DO 200 N = 1,NWORDS,4
```

```
      NN = NWORDS - N - 2                                               USPK0630
      LBYTE = UNPAKD(NN)                                                USPK0640
      IF(IBYTE .NE. IBLANK) GO TO 210                                   USPK0650
 200 CONTINUE                                                           USPK0660
     NN = 0                                                             USPK0670
 210 NCHMTB = (NN + 3) / 4                                              USPK0680
     RETURN                                                             USPK0690
     END                                                                USPK0700
```

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