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Final Report

THEORETICAL INVESTIGATION OF NUCLEAR BURST PHENOMENA

(22 April 1965 To 31 December 1969)

By

P. Gordon
B. B. Hamel
J. Kulander
R. T. Liner, Jr.
D. H. Sampson
S. M. Scala
M. P. Sherman
R. B. Thomas, Jr.

Prepared Under Contract N60921-7166
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NAVAL ORDNANCE LABORATORY
WHITE OAK
SILVER SPRING, MARYLAND 20910

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Environmental Sciences Laboratory
Re-entry and Environmental Systems Division
General Electric Company
P.O. Box 8555
Philadelphia, Pennsylvania 19101

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I. GENERAL INTRODUCTION

I. GENERAL INTRODUCTION

A major deficiency of most methods used in the prediction of the effects of a nuclear burst on bodies passing through them at hypersonic velocities is that they have been based on a relatively crude knowledge of both the disturbed flow field about the body and the dynamic behavior of the plasma originating from the burst. In this study we have been concerned with developing improvements in the physics and in the numerical treatment of the equations governing the dynamics of the plasma produced by a nuclear burst. In such a self-consistent treatment of the radiation and the flow, one calculates all parameters, such as temperature, pressure, flow velocity, and radiation intensity that are significant in determining the time-dependent variation of the incident flux experienced by a body in the atmosphere. Our point of departure in undertaking this investigation has been the use of new analytical and numerical techniques developed at the General Electric Space Sciences Laboratory for treating the time dependent Navier-Stokes equations for compressible, viscous, thermally conducting flows. Herein, the new methods are applied to the nuclear burst plasma itself. Once the dynamic behavior of the plasma is known, the initial environment for the entering body is also known. The more complicated interaction problem of the hypersonic entry of a solid body into the plasma can, in principle, then be treated by a further extension of the same methods.

This report presents the results of an investigation which was carried out under the sponsorship of the Naval Ordnance Laboratory and includes the analytical and numerical results obtained in a number of interrelated areas of the physics and mathematics of a nuclear explosion.

The central purpose of the research program was the development of digital computer programs for solving the complete system of governing equations which describe both the radiation field, the gas dynamic motion of the hot plasma and the coupling between the radiation and the expanding plasma, at any altitude. Accordingly, subtasks were defined in order to investigate the three major areas which would contribute to the development of an improved understanding of this extremely complex problem.

The first area of activity, reported on in Section II of this final report, deals with the derivation of the general governing equations for the time-dependent motion of the plasma and the development of numerical methods for the solution of model sets of these equations, both at low altitude where continuum mechanics is applicable, and at high altitude where rarefied gas dynamics (Kinetic theory) is applicable. At low altitude, we have employed the general Navier-Stokes equations in an appropriate coordinate system, whereas for the rarefied regime we have used the Boltzmann equation as a point of departure.

Radiative properties and radiative transfer are presented in Sections III and IV. In general, radiation can be divided roughly into five categories:

1. Determination of appropriate absorption coefficients for the species present in the radiating plasma

2. Determination of the emission coefficient or source function

3. Determination of the specific radiation intensity

4. Determination of the monochromatic mean intensity, flux, pressure or higher moments

5. Determination of total mean intensities, fluxes, pressures and moments for all frequencies.

Concerning category 1, a discussion is given in Section III-B and it is noted that we have adapted the Burgess and Seaton method (1-1) for the calculation of the bound-free absorption cross sections in order to calculate the equilibrium absorption coefficients for O, N and air.

Concerning category 2, the equilibrium source function is simply the Planck function, and hence research in this area is equivalent to the consideration of non-LTE conditions.

Category 3 is concerned with the integration of absorption coefficients and source functions over spatial coordinates. While integrations in plane parallel geometries are relatively straightforward, integrations for spherical geometries are not.

In category 4, some work was done concerning the accuracy of the Eddington approximation in calculating the mean intensity J as opposed to using the exact expression. The results indicate that as long as the total optical thickness of the region is greater than unity, the error will seldom amount to more than 20 percent. Even when the radiating region is optically thin, the error seldom exceeds a factor of two. Since J is a necessary quantity in determining the non-LTE source function, the error in its calculation is of considerable interest.

In relationship to category 5, it should be pointed out that one can simplify the calculations enormously by approximating the energetics by utilizing spectrally averaged properties in relating theoretical calculations to field measurements. However, it is also important to have multi-spectral calculations, since the observables will not only be a continuum but also probably have high intensity discrete spectral regions, usually associated with the presence of other than air species.

Finally, time-dependent numerical techniques were developed for both the Navier-Stokes equations (in the absence of radiation effects) and a suitable form of the radiation equation (in the absence of hydrodynamic effects). After separate computer programs

were developed and checked out for each of these problems, the two programs were then combined. As a sample calculation, results were then obtained for early time (before the gas is actually in motion) when the temperature and radiation fields are adjusting toward a quasi-steady equilibrium.

II. FLOW FIELD STUDIES

II.A INTRODUCTION

In this part of the study, the general equations of motion for a chemically reacting plasma are derived. Numerical solutions are then obtained for the formation of the spherically-symmetric flow field corresponding to a simulated nuclear burst. Numerical studies were carried out for particular flow models including the Euler nonviscous flow limit and the fully-viscous Navier-Stokes equations. Comparisons were made with related calculations at NOL and LASL. Detailed descriptions of the new computer programs are also provided.

II.B FLOW EQUATIONS FOR CHEMICALLY REACTING PLASMA

by

R.B. Thomas, Jr.

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II.B FLOW EQUATIONS FOR CHEMICALLY REACTING PLASMA

II.B.1 INTRODUCTION

In the past, a certain broad class of fluid dynamic problems involving the flow of a chemically reacting gas in contact with a solid surface has been studied extensively. The solution of such problems obviously has very wide and important technical application. Experience already gained in this area is now being used to undertake a considerably more ambitious program in the field of fluid dynamics. Until now, Reference II.B-1 has provided the principal guidance in formulating our approach to gas dynamic problems. However, one cannot long neglect the presence of charged and excited components in a chemical reaction, especially when the chemical reaction takes place at an elevated temperature, a condition so often encountered in most applications of the theory. It is one purpose of this section to make the necessary modifications of the fluid dynamic equations. In doing so, the opportunity has presented itself for undertaking a more critical and detailed discussion of the underlying general theoretical approach to this class of problems. It is hoped this will serve the additional end of providing other investigators with a reasonable introduction to the theoretical methods and concepts of transport theory in gases.

II.B.2 GENERAL CONSIDERATIONS, KINETIC THEORY

When can a system of N interacting particles in a volume V be treated classically, that is, when can we neglect a part of the quantum mechanical interaction between the particles? Quantum mechanical states that matter has both particle and wave properties. The characteristic wave length of a particle of momentum p = mV is given, according to deBroglie, by $\lambda = h/p$, where h is Plank's constant, equal to $6.62 \cdot 10^{-27}$ erg sec. This wave length can be taken as a measure of the physical extension of the particle. In order to treat a particle classically in a gas, the average interparticle separation must be considerably greater than λ. At a temperature T, this condition takes the form

$$\frac{h}{\sqrt{3mkT}} \Big/ \left(\frac{V}{N}\right)^{1/3} << 1, \qquad \text{(II.B-1)}$$

where 3mkT is the average momentum of a particle of mass m and k is Boltzmann's constant, having the value $1.38 \cdot 10^{-16}$ erg/degree. A simple calculation will show that Eq. (II.B-1) is well satisfied for most gases; so that they can be treated classically. Nonetheless, there are systems, for example, high density stellar matter, where Eq. (II.B-1) is not satisfied. The entire system must be treated by quantum mechanics from the beginning. Where then do quantum mechanical effects enter in gases which do satisfy Eq. (II.B-1)? They enter in the collision process itself. Here the average density is sufficiently high to violate the condition Eq. (II.B-1). The close approach of two or more particles must in general be treated by quantum mechanics. It will be shown that a collision between two particles is completely characterized by the differential cross section, $\sigma(\theta, \phi)$. All of the quantum mechanical effects are contained in this parameter, and the gross motion of the gas can be completely formulated in terms of it using classical principles.

In general, we are not interested in the motion of each molecule in detail; rather we are interested in the distribution function $f(\vec{r}, \vec{v}, t)$, so defined that

$$f(\vec{r}, \vec{v}, t)\, dr^3\, d^3V \qquad \text{(II.B-2)}$$

is the number of molecules which, at time t, have positions lying within a volume element d^3r about $\vec{r}$ and velocities lying within a velocity space element d^3V about $\vec{V}$. Here we assume that only one type of molecule is present; later the results will be generalized to include several chemically interacting molecules.

Having defined the distribution function, we can express the information that there are N molecules in the volume V through the normalization condition

$$\int_V f(\vec{r}, \vec{v}, t)\, d^3r\, d^3V = N. \qquad \text{(II.B-3)}$$

The aim of kinetic theory is to find the distribution function $f(\vec{r}, \vec{v}, t)$ for a given form of molecular interaction, that is, for a known scattering cross section σ. Once f has been determined, all physically interesting properties of the system can be calculated from it. A knowledge of the function $f(\vec{r}, \vec{v}, t)$ gives the most detailed knowledge we can reasonably hope to have about a given molecular system, short of following each individual molecule, which is certainly impractical if not impossible. All transport properties of the system, such as energy, momentum, etc., can be expressed as integral over the distribution function. The limiting form of $f(\vec{r}, \vec{v}, t)$ as $t \to \infty$ would contain all of the equilibrium properties of the system. Kinetic theory therefore includes the derivation of the thermodynamics of the system in question.

Our first task is to find an equation of motion satisfied by the distribution function. The distribution function changes with time, because molecules constantly enter and leave a given volume element in μ - space, the six dimensional space made up of the components of velocity and coordinates. Suppose there are no molecular collisions, $\sigma = 0$. Then a molecule with the coordinates $(\vec{r}, \vec{v})$ at the instant t will have the coordinates $(\vec{r} + \vec{v}\ t,\ \vec{V} + \vec{F}/m\mathcal{L}t)$ at the later instant $t + \mathcal{L}t$, where F is the external force acting on the molecule. Thus, all molecules contained in $d^3r\ d^3V$, at $(\vec{r}, \vec{v})$ at time t, will all be found in $d^3r'\ d^3V'$ at $(\vec{r} + \vec{V}\mathcal{L}t,\ \vec{V} + \vec{F}/m\mathcal{L}t)$ at time $t + \mathcal{L}t$. Hence, in the absence of collisions we must have the equality

$$f(\vec{r} + \vec{V}\mathcal{L}t,\ \vec{V} + \vec{F}/m\mathcal{L}t,\ t + dt)\ d^3r'\ d^3V' = f(r, v, t)\ d^3r\ d^3V$$

which reduces to

$$f(\vec{r} + \vec{V}\ dt,\ \vec{V} + F/m\mathcal{L}t,\ t + dt) = f(\vec{r}, \vec{v}, t) \qquad \text{(II.B-4)}$$

because $d^3r\ d^3V = d^3r'\ d^3V'$. This volume equality is not self-evident, but can be shown by using the generalized system of coordinates connecting two points in μ - space.

When there are collisions, Eq. (II.B-4) must be modified. The difference between the two terms is the net contribution of collisions. We write

$$f(\vec{r} + \vec{V}\mathcal{L}t,\ \vec{V} + F/m\mathcal{L}t,\ t + \mathcal{L}t) = f(\vec{r}, \vec{v}, t) + (\mathcal{L}f/\mathcal{L}t)_{coll.}\ dt. \qquad \text{(II.B-5)}$$

This can be taken as the definition of $(\mathcal{L}f/\mathcal{L}t)_{coll}$, the collision contribution to the time rate of change of f. As $t \to 0$, the left-hand side can be expanded, and we obtain

$$(\mathcal{L}/\mathcal{L}t + \vec{V} \cdot \nabla_r + \vec{F}/m \cdot \nabla_v)\ f(\vec{r}, \vec{v}, t) = (\mathcal{L}f/\mathcal{L}t)_{coll} \qquad \text{(II.B-6)}$$

where ∇_r and ∇_v are respectively the gradient operators with respect to $\vec{r}$ and $\vec{V}$. This equation is not meaningful until we explicitly specify $(\mathcal{L}f/\mathcal{L}t)_{coll}$. The limiting process used to obtain Eq. (II.B-6) from Eq. (II.B-5) is not an approximation; since

dt is a true infinitesimal, unlike d^3r and d^3V, which are limited by the density of the gas. (When the density of the gas is so low that the volume element $d^3r\, d^3V$ must be taken to be large relative to macroscopic dimensions in order to contain a large number of molecules, then the theory no longer holds; $f(\vec{r}, \vec{v}, t)$ cannot be considered a continuous function.) Finally, it might be well to point out that the F appearing in Eq. (II.B-6) represents all possible external forces acting on the molecule except those due to force fields having their sources in other molecules: such forces are contained in the collision term. F will contain, however, all externally applied electric, magnetic and gravitational forces.

An explicit form of $(\mathcal{L}f/\mathcal{L}t)_{coll}$ can be obtained by going back to its defining equation, (II.B-6). Consider two elements of μ - space, six-dimensional volumes essentially, slightly displaced. Let A and B represent the volume elements at the respective points $\{\vec{r}, \vec{v}, t\}$ and $\{\vec{r} + \vec{V}\,t, \vec{V} + \vec{F}/m\mathcal{L}t, t + \mathcal{L}t\}$, where $\mathcal{L}t$ will tend to zero. During the time $\mathcal{L}t$, some molecules in A will be removed from A by collisions. We regard A as so small that any collision that a molecule in A suffers will knock it out of A. Such a molecule will not reach B because B is nearly coincident with A. On the other hand, there are molecules outside A which, through collisions, will be sent into A during $\mathcal{L}t$. These will be in B as $\mathcal{L}t \to 0$. Therefore, the number of molecules in B at $t + \mathcal{L}t$ as $\mathcal{L}t \to 0$, equals the original number of molecules in A at time t plus the net gain of molecules in A due to collisions during the time $\mathcal{L}t$. This statement is the content of Eq. (II.B-6) and may be expressed in the form

$$\left(\frac{\mathcal{L}f}{\mathcal{L}t}\right)_{coll} \mathcal{L}t = (R_I - R_o)\, \mathcal{L}t, \qquad \text{(II.B-7)}$$

where $R_I \mathcal{L}t\, d^3r\, d^3V$ is the number of collisions occurring during $\mathcal{L}t$ in which one of the initial molecules is in $d^3r\, d^3V$ at $(\vec{r}, \vec{v})$ and $R_o\, t\, d^3r\, d^3V$ is the number of collisions occurring during $\mathcal{L}t$ in which one of the final molecules is in $d^3r\, d^3V$ at $(\vec{r}, \vec{v})$. This holds in the limit as $\mathcal{L}t \to 0$. Still, a small error has been made here. We are implicitly assuming that if one molecule qualifies under the description, none of the partners in the collision qualifies for the purpose of counting in Eq. (II.B-7). This error is negligible provided d^3V is sufficiently small. It does indicate, however, that Eq. (II.B-7) probably would not hold for certain distributions. Still another assumption will be made. We assume that the gas is sufficiently dilute so that we need only consider binary collisions: the possibility of triple or higher order collisions is ignored.

II.B.3 BINARY COLLISIONS

It is useful to examine in some detail an elastic collision in free space between molecules of equal mass. The results for more complicated collisions will be indicated later. The molecules, as we have assumed are sufficiently well-defined in position and velocity so that we can describe the initial and final states of the collision classically.

Let the velocities of the incoming molecules be $\vec{v}_1$ and $\vec{v}_2$ and the velocities of the outgoing molecules be $\vec{v}_1'$, $\vec{v}_2'$. From conservation of energy and momentum we have

$$\vec{v}_1 + \vec{v}_2 = \vec{v}_1' + \vec{v}_2' \quad ,$$

$$\vec{v}_1^{\,2} + \vec{v}_2^{\,2} = \vec{v}_1'^{\,2} + \vec{v}_2'^{\,2} \qquad \text{(II.B-8)}$$

Now introduce the new variables

$$\vec{V} = 1/2\ (\vec{v}_1 + \vec{v}_2)$$

$$\vec{u} = \vec{V}_2 - \vec{V}_1 \qquad \text{(II.B-9)}$$

and the variables $\vec{V}'$ and $\vec{u}'$. $\vec{V}$ is essentially the average velocity of the system and $\vec{u}$ is the relative velocity of the two particles making up the system. This is a reasonable way to view such a physical system. If Eqs. (II.B-8) are rewritten in terms of these new variables, we obtain the simple result

$$\vec{V} = \vec{V}' \quad ,$$

$$\vec{u} = u' \quad . \qquad \text{(II.B-10)}$$

This shows that $\vec{V}$ remains unchanged by the collision; while $\vec{u}$ is at most rotated by the collision without changing its magnitude. This makes it possible to specify the collision completely by giving $\vec{V}$, $\vec{u}$, and the angles $\vec{u}'$ makes with u, say θ, ϕ are just the sperical coordinates of the vector u′ relative to u and are called the scattering angles. (It might be pointed out that here they are given in the center of mass system, and that these are not the same as those observed in the laboratory. It is, however, easy to construct a transformation between the two sets.)

Image $\vec{V}$ and $\vec{u}$ slightly changed, to $\vec{V} + d\vec{V}$ and $\vec{u} + d\vec{u}$ respectively, with θ, ϕ kept fixed. That is, consider a collision where the initial state is slightly different from the original one. Then $\vec{V}'$ and $\vec{u}'$ change respectively to $\vec{V}' + d\vec{V}'$ and $\vec{u}' + d\vec{u}'$. Since $\vec{V} = \vec{V}'$, we have $d\vec{V} = d\vec{V}'$. Since θ is fixed, we also have $d\vec{u} = d\vec{V}'$. Since θ is fixed, we also have $du = du'$. Therefore, we have

$$d^3V\, d^3u = d^3V'\, d^3u' \,, \qquad \text{(II.B-11)}$$

where $d^3V = dV_x dV_y dV_z$, etc. From Eq. (II.B-9) it can be shown that $d^3V\, d^3u = d^3V_1\, d^3V_2$, with a similar equality for the primed quantities. Therefore, we have the important result that if we change $\vec{V}_1$ and $\vec{V}_2$ slightly, keeping the scattering angles fixed, then $\vec{V}'_1$ and $\vec{V}_2'$ change in such a way that

$$d^3V_1\, d^3V_2 = d^3V_1'\, d^3V_2' \qquad \text{(II.B-12)}$$

The total velocity $\vec{V}$ is not a very interesting quantity: it is just the velocity of the center-of-mass. In the center-of-mass system it suffices to focus our attention on one of the molecules, because its partner always moves oppositely. Thus, the problem reduces to the equivalent problem of the scattering of a molecule by a fixed center of force. This molecule approaches the center of force along a path whose perpendicular distance to this center is b, the impact parameter. If the initial path is chosen along the z-axis, it is evident that the angles, θ, ϕ are sufficient to determine the scattering since $|\vec{u}| = |\vec{u}'|$ as we have seen.

The dynamical aspects of the collision are contained in the differential cross-section $\sigma(\theta, \phi) \equiv \sigma(\Omega)$, which will now be defined. The initial velocities V_1, V_2 do not uniquely determine the collision; because they do not determine the relative spatial position of the particle paths, that is, the impact parameter b. Specifying V_1 and V_2 specifies a class of collisions all having the same center-of-mass system. It is useful to imagine a steady uniform flux of particles spread over all space incident on the center of force with velocity $\vec{u}$.

Let I be the number of molecules in the incident beam crossing a unit area normal to the beam in one second. I is called the incident flux. The differential cross-section $\sigma(\Omega)$ is so defined that $I\sigma(\Omega)\, d\Omega$ is equal to the number of molecules deflected per second in a direction (θ, ϕ) lying within a solid angle element $d\Omega \equiv \sin\theta\, d\theta\, d\phi$. It is then evident that

$$I\,\sigma(\Omega)\, d\Omega = I\, b\, db\, d\phi. \qquad \text{(II.B-13)}$$

This simply states that all molecules scattered into a given solid angle have their origin in one section of a cylindrical annulus of incident particles. This is apparent from a physical point of view. ϕ and b determine the incident path relative to the scattering center. For a given potential interaction the outgoing path must then be completely determined, at least classically. $\sigma(\Omega)$ actually does have the dimensions of length squared. The total cross-section is the integral of $\sigma(\Omega)$ over all solid angle: this gives all the particles that are deflected from their incident path for the infinite plane uniform incident beam. Then the total cross-section

$$\sigma_T = \int \sigma(\Omega)\, d\Omega \qquad \text{(II.B-14)}$$

can be looked upon as a geometric section of area σ_T removed from the beam.

The differential cross-section can be measured, and it can be calculated if the intermolecular potential is known. It must, as has already been pointed out, be calculated using quantum mechanics; since in the region of collision the wave-lengths of the particles are of the order of the classical separation of the particles so that the system cannot be regarded as classical. For ourppresent purpose we regard $\sigma(\Omega)$ as a known property of the gas: it must be given before we can actually carry out any numerical calculations.

$\sigma(\Omega)$ of course depends on the initial and final velocities of the interacting particles and it is useful to write it as

$$\sigma(\Omega) = \sigma(\vec{v}_1, \vec{v}_2\ \vec{v}_1', \vec{v}_2'). \qquad \text{(II.B-15)}$$

This is possible since (θ, ϕ) are really the angles between $\vec{v}_2 - \vec{v}_1$ and $\vec{v}_2' - \vec{v}_1'$. σ has certain symmetry properties that do not depend in detail on the exact form of the interaction are electromagnetic in nature. First σ is invariant under time reversal,

$$\sigma(\vec{v}_1, \vec{v}_2\ \vec{v}_1', \vec{v}_2' = \sigma(-\mathbf{v}_1, -\mathbf{v}_2 - v_1', -v_2') \qquad \text{(II.B-16)}$$

which expresses the property that if we reverse the sense of time each particle will retrace its original path. σ is also invariant under rotation and reflection. This means that σ is the same after performing a given rotation of the v_s in space or a reflection of the v_s with respect to a given plane, or a combination of both.

Let the inverse collision be defined as the collision that differs from a given collision by interchanging the initial and final states, that is, the velocities of the particles. As a consequence of the symmetries Eq. (II.B-15) and (II.B-16), the inverse collision has the same cross section as the collision:

$$\sigma(v_1\ v_2, v_1', v_2') = \sigma(v_1', v_2', v_1, v_2) \quad . \qquad \text{(II.B-17)}$$

To show this is essentially a geometric problem, we will not give the details here. The problem is more complicated if spin is included, but nonetheless we arrive as nearly the same result except that $\sigma(\Omega)$ is then a sum over all spin quantum numbers in the initial and final state.

II.B.4 THE BOLTZMANN TRANSPORT EQUATION

We now wish to conclude the basic theory of collision scattering in a gas by obtaining a reasonably rigorous expression for $(\partial f/\partial t)_{coll}$ contained in Eq. (II.B-6). The result will be the well-known Boltzmann transport equation, which is the basis for the treatment of almost all collective collision processes. This will be one of our central results, and most of the preceding work was carried out for the purpose of presenting a logical discussion of the collision term in the Boltzmann equation.

In order to derive an explicit expression for $(\partial f/\partial t)_{coll}$, the following approximations will be (and are usually) made:

a. Only binary collisions are taken into account. This is only valid if the gas is sufficiently dilute.

b. The walls of the container are ignored.

c. The effect of the external force on the collision cross-section is ignored.*

d. The velocity of a molecule is uncorrelated with its position.

Assumption (d) is known as the hypothesis of molecular chaos. In more precise terms it states that in a spatial volume element d^3r the number of pairs of molecules with velocities lying in the volume elements d^3v_1 about $\vec{v}_1$ and d^3v_2 about $\vec{v}_2$ is

$$(f(\vec{r}, \vec{v}_1, t)\, d^3r\, d^3v)\ (f(\vec{r}, \vec{v}_2, t)\, d^3r\, d^3v_2). \qquad \text{(II.B-18)}$$

This assumption is introduced as a mathematical convenience. It is certainly a possible condition of the gas, but it is not clear whether it is a general condition. Certainly one can imagine situations in which the velocity is highly correlated with its position in space. It is possible to develop an equation, or rather a set of coupled equations describing the scattering process in terms of correlation functions, that does not require the assumption of molecular chaos. This approach might be the most appropriate in a treatment of gases at high temperature and vanishing density.

We now turn to the problem of finding an explicit expression for $(\partial f/\partial t)_{coll}$ valid under the conditions set down above. The rate of decrease of $f(\vec{r}, \vec{v}_1, t)$ due to collisions, denoted by R_o in (2.7), can be obtained by considering a molecule whose

*At present the problem of magnetic corrections to the scattering cross-section is being investigated. Because no true radial wave exists, it appears that the ordinary concept of a differential cross-section must be re-examined when a magnetic field is present.

velocity lies in d^3v_1 about $\vec{v}_1$, in the spatial volume d^3r about $\vec{r}$. In the same spatial volume there are molecules of any velocity $\vec{v}_2$ that may collide with a molecule of velocity $\vec{v}_1$. The flux of this incident beam is

$$I_o = (f(\vec{r}, \vec{v}_2, t)\ d^3V_2)\ \left|\vec{v}_1 - \vec{v}_2\right|, \qquad \text{(II.B-19)}$$

by assumption d. The number of collisions taking place in d^3r during $\mathcal{L}t$ of the type $\{\vec{v}_1, \vec{v}_2\} \rightarrow \{\vec{v}_1', \vec{v}_2'\}$ is given, according to Eq. (II.B-13) by

$$I\sigma(\Omega)d\Omega\,\mathcal{L}t = f(\vec{r}, \vec{v}_2, t)\ d^3v_2\ \left|v_2 - v_1\right|\ \sigma(\Omega)\,d\Omega\,\mathcal{L}t. \qquad \text{(II.B-20)}$$

The rate R_o is obtained by summing Eq. (II.B-20) over all possible initial velocities of molecule two multiplying the result by the spatial density of molecules in d^3v_1:

$$R_o = f(\vec{r}, \vec{v}_1, t)\int d^3V_2 \int d\Omega\sigma(\Omega)\ \left|v_1 - v_2\right|\ f(\vec{r}, \vec{v}_2, t). \qquad \text{(II.B-21)}$$

The integration over Ω can be immediately carried out here to yield the total cross section. We prefer, however, to leave it in its present form. The reason will appear shortly.

In a similar way we can calculate R_I, defined as the number of collisions per unit time that send molecules into the element $d^3v_1\ d^3r$ about $(\vec{r}, \vec{v}_1)$. We are, therefore, interested in collisions of the type $\{\vec{v}_1', \vec{v}_2'\} \rightarrow \{\vec{v}_1, \vec{v}_2\}$, where $\vec{v}_1$ is fixed. Consider molecule v_1' is fixed. Consider molecule v_1' with a beam of molecules $\vec{v}_2'$ incident upon it. The incident flux is now

$$I_I = f(\vec{r}, \vec{v}_2', t)\ d^3V_2'\ \left|v_2' - v_1'\right|. \qquad \text{(II.B-22)}$$

The number of collisions of this type in $\mathcal{L}t$ is

$$f(r, v_2' t)\ d^3V_2'\ \left|v_2' - v_1'\right|\ \sigma'(\Omega)\,d\Omega\,\mathcal{L}t. \qquad \text{(II.B-23)}$$

The rate R_I is then just

$$R_I d^3v_1 = \int d^3v_2' \int d\Omega\sigma'(\Omega)\ \ v_2' - v_1'\ \ f(r, v', t)\ d^3V_1'\ \ f(\vec{r}, \vec{v}_2', t). \qquad \text{(II.B-24)}$$

Now the vectors v_1, v_2, v_1', v_2' refer to collisions that are inverses of each other; hence $\sigma'(\Omega) = \sigma(\Omega)$ according to the result (3.9). If we also make use of Eq. (II.B-10) and (II.B-12) to transform the velocity space coordinates, Eq. (II.B-24) can be rewritten

$$R_I = \int d^3V_2 \int d\Omega\, \sigma(\Omega) \quad V_1 - V_2 \quad f(\vec{r}, \vec{V}_1', t)\, f(\vec{r}, \vec{V}_2', t). \qquad \text{(II.B-25)}$$

It must be understood that V_1 is fixed while V_1' and V_2' are functions of V_1, V_2, and Ω; so the integration over Ω cannot be so readily carried out in (Eq. II.B-25) as in Eq. (II.B-21). In order to see how the integration in Eq. (II.B-25) is to be carried out we imagine that we are in the center of mass system. The $\vec{V}_1 - \vec{V}_2$ and $\vec{V}_1' - \vec{V}_2'$ are vectors specified relative to one another by the scattering angles $(\theta, \varphi) = \Omega$. Choose a scattering cross section and a set of initial velocities. Then the orientation of $\vec{V}_1' - \vec{V}_2'$ is known in terms of (θ, φ). Its length is the same as that of $V_1 - V_2$ according to Eq. (II.B-10). This enables us to write V_1', V_2' completely in terms of V_1, V_2 and (θ, φ). After this has been done, the integration can in principle be carried out.

Combining the results for R_o and R_I we obtain for the collision contribution to the Boltzmann equation

$$\left(\frac{\partial f(v_1, r, t)}{\partial t}\right)_{coll} = R_I - R_o$$
$$= \int d^3v_2 \int d\Omega\, \sigma(\Omega)\, |\vec{V}_1 - \vec{V}_2|\, (f_1' f_2' - f_1 f_2), \qquad \text{(II.B-26)}$$

where $\sigma(\Omega)$ is the differential cross section for the collision $\{V_1, V_2\} \rightarrow \{V_1', V_2'\}$ $f_1' = f(\vec{r}, \vec{V}_1', t)$ etc. Substituting Eq. (II.B-26) into Eq. (II.B-6), we obtain the Boltzmann transport equation

$$\left(\frac{\partial}{\partial t} + \vec{V}_1 \cdot \nabla_r + \frac{\vec{F}}{M} \cdot \nabla_{V_1}\right) f_1 = \int d\Omega \int d^3V_2 \sigma(\Omega) \left|\vec{V}_1 - \vec{V}_2\right| \qquad \text{(II.B-27)}$$
$$(f_2' f_1' - f_2 f_1).$$

The most important characteristic of this equation is that of being non-linear. It is also an integral equation, which adds to the complexities of solving it, which is the basic problem of kinetic theory.

II.B.5 EQUILIBRIUM SOLUTION

It is interesting to note that if we did not make use of the assumption of molecular chaos, the quantity $(\partial f/\partial t)_{coll}$ would not be expressible in terms of f itself. Instead, it would involve a two-particle correlation function which is independent of f. In place of Eq. (II.B-27), therefore, we would not have an equation for f but an equation relating f to a two-particle correlation function. In general, we can obtain equations relating an n-particle correlation function to a (n + 1) - particle correlation function. In the general case, Eq. (II.B-27) is replaced by a set of N coupled equations.

It is useful to examine Eq. (II.B-27) under very simple conditions. By definition, equilibrium can be taken as the condition where the distribution function does not depend explicitly on the time. Then $(\partial f/\partial t) = 0$. We will also assume there is no external force present and that f does not depend on r. Then the collision term in Eq. (II.B-27) must vanish. A sufficient condition for this is that

$$f_o(\vec{V}_2')\, f_o(\vec{V}_1') - f_o(\vec{V}_2)\, f_o(\vec{V}_1) = 0. \qquad \text{(II.B-28)}$$

A subscript zero has been placed on f to indicate equilibrium. It can be shown that Eq. (II.B-28) is also a necessary condition for equilibrium. It is interesting to note that $f_o(V)$ is independent of the cross section, so long as it does not actually vanish. From Eq. (II.B-28) we can easily show that $f_o(V)$ is expected Maxwell-Boltzmann distribution. To do this, take the logarithm of (5.1) and write it as

$$\ell n f_o(\vec{V}_1) + \ell n f_o(\vec{V}_o) = \ell n f_o(\vec{V}_1') + \ell n f_o(\vec{V}_2'). \qquad \text{(II.B-29)}$$

Since $\{\vec{V}_1, \vec{V}_2\}$ and $\{\vec{V}_1', \vec{V}_2'\}$ refer respectively, to the initial and final velocities of any possible collision, Eq. (II.B-29) is seen to have the form of a conservation law If X(V) is any quantity associated with a molecule of velocity V, such that $X(V_1) + X(V_2)$ is conserved in a collision between molecules having velocities V_1 and V_2, a solution of Eq. (II.B-29) is just

$$\ell n f_o(V) = X(V). \qquad \text{(II.B-30)}$$

The most general solution of Eq. (II.B-29) is then

$$\ell n f_o(V) = X_1(V) + X_2(V) + \cdots, \qquad \text{(II.B-31)}$$

where X_1, X_2, -- exhausts all independently conserved quantities for the collision. For spinless molecules these are energy, momentum, and of course a constant. Hence, $\ell n f$ is a linear combination of V^2 and the three components $\vec{V}$ plus an arbitrary constant:

$$\ell n f_o(V) = -A(V - V_o)^2 + \ell n C, \tag{II.B-32}$$

or

$$f_o(V) = Ce^{-A(V - V_o)^2} \tag{II.B-33}$$

where C, A, and the three components of $\vec{V}_0$ are five arbitrary constants. This can be determined in terms of physical properties of the system.

Applying the condition Eq. (II.B-3) and denoting the particle density N/V by n shows that $C = (A/\pi)^{3/2} n$.

Let the average velocity of the gas be defined by

$$< V > = \frac{\int d^3V f_o(V) V}{\int d^3V f_o(V)} . \tag{II.B-34}$$

Then we find that $V_o = < V >$.

Next calculate the average energy of a molecule, defined by

$$\epsilon = \frac{\int d^3V f_o(V)\ 1/2\ mV^2}{\int d^3V f_o(V)} . \tag{II.B-35}$$

We then have, setting $V_0 = 0$, $\epsilon = 3m/4A$.

Finally, use f_o to determine the pressure P of the gas, defined as the rate of change of momentum at a wall. This shows that $P = (2/3) n_\epsilon$. This is the equation of state. Experimentally we know P = nKT, where K is Boltzmann's constant. Comparing

these equations shows that $\epsilon = \frac{3}{2} KT$. Then in terms of the temperature T, the average velocity V_o, and the particle density n, the equilibrium distribution function for a dilute gas in the absence of external forces is

$$f_o(V) = n\left(\frac{m}{2\pi KT}\right)^{3/2} e^{\frac{m}{2KT}(\vec{V}-\vec{V}_o)^2} . \qquad \text{(II.B-36)}$$

This is the Maxwell-Boltzmann distribution, the probability of finding a molecule with velocity V in the gas under equilibrium conditions.

II.B.6 THE CONSERVATION LAWS

In order to treat non-equilibrium phenomena, we must solve the Boltzmann equation. In general this is difficult to do. However, there are some rigorous properties of any solution to the Boltzmann equation that may be obtained from the fact that in any molecular collision there are dynamical quantities that are rigorously conserved.

To keep the treatment as simple as possible, we will continue to consider only elastic collisions between molecules. It will then be clear how the results can be extended to more general types of collisions. Let $X(\vec{r}, \vec{V})$ by any quantity associated with a molecule of velocity $\vec{V}$ located at $\vec{r}$, such that in any collision $\{V_1, V_2\} \rightarrow \{\vec{V}_1', \vec{V}_2'\}$ taking place at $\vec{r}$, we have

$$X_1 + X_2 = X_1' + X_2' \quad , \tag{II.B-37}$$

where $X_1 = X(r_1, V_1)$ etc. We call X a conserved property. Then

$$\int d^3V X(r, V) \left[\frac{\partial f(r, V, t)}{\partial t}\right]_{coll} = 0, \tag{II.B-38}$$

where $(\partial f/\partial t)_{coll}$ is the collision term in the Boltzmann equation. In order to show this, we note that by definition the left-hand side of Eq. (II.B-37) can be written

$$\int d^3V X \left(\frac{\partial f}{\partial t}\right)_{coll} = \int d^3V_1 \int d^3V_2 \int d\Omega\, \sigma(\Omega)\, x \left|\vec{V}_2 - \vec{V}_1\right| X_1 (f_1' f_2' - f_1 f_2). \tag{II.B-39}$$

Rewrite this by making use of the properties of $\sigma(\Omega)$ discussed in Section II.B.3 and making the following interchanges of variables:

First, $V_1 \rightleftarrows V_2$

Second, $V_1 \rightleftarrows V_1'$ and $V_2 \rightleftarrows V_2'$

Third, $V_1 \rightleftarrows V_2'$ and $V_2 \rightleftarrows V_1'$.

In each case we obtain a different but equivalent expression for the same integral. Adding the three new formulas so obtained to Eq. (II.B-38) and dividing the result by 4 shows that

$$\int d^3VX \left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{1}{4} \int d^3V_1 \int d^3V_2 \int d\Omega\, \sigma(\Omega)\, |V_1 - V_2| \times ,$$

$$(f_2' f_1' - f_2 f_1)\,(X_1 + X_2 - X_1' - X_2') \equiv 0 \qquad \text{(II.B-40)}$$

by using Eq. (II.B-37), which proves Eq. (II.B-38).

The conservation theorem relevant to the Boltzmann equation is obtained by multiplying the Boltzmann equation on both sides by X and integrating over V. The collision term vanishes by Eq. (II.B-38) and we have

$$\int d^3VX(\vec{r}, \vec{V}) \left(\frac{\partial}{\partial t} + \vec{V} \cdot \nabla_r + \frac{\vec{F}}{M} \cdot \nabla_V\right) f(r, V, t) = 0, \qquad \text{(II.B-41)}$$

We may write Eq. (II.B-41) in the form

$$\frac{\partial}{\partial t} \int d^3VXf + \frac{\partial}{\partial X_i} \int d^3VXV_i f - \int d^3V \frac{\partial X}{\partial X_i} V_i f$$

$$+ \frac{1}{m} \int d^3V \frac{\partial}{\partial V_i} (XF_i f) - \frac{1}{m} \int d^3V \frac{\partial X}{\partial V_i} F_i f - \frac{1}{m} \int d^3VX \frac{\partial F_i}{\partial V_i} f = 0 . \qquad \text{(II.B-42)}$$

The fourth term vanishes if f (r, V, t) is assumed to vanish when $V \to \infty$. Defining the average value (A) by

$$\langle A \rangle = \frac{\int d^3VAf}{\int d^3Vf} = \frac{1}{n} \int d^3VAf ,$$

we can rewrite Eq. (II.B-42) in the form

$$\frac{\partial}{\partial t} \langle nX \rangle + \frac{\partial}{\partial X_i} \langle nV_i X \rangle - n \left\langle V_i \frac{\partial X}{\partial X_i} \right\rangle$$

$$- \frac{n}{m} \left\langle F_i \frac{\partial X}{\partial V_i} \right\rangle - \frac{n}{m} \left\langle \frac{\partial F_i}{\partial V_i} \right\rangle , \qquad \text{(II.B-43)}$$

which is the conservation theorem.

For simple molecules the independently conserved properties are mass, momentum, and energy. For charged molecules we also include the charge, but this extension is trivial. Accordingly, we set successively

$X = m$, (mass)

$X = mV_i$, $i = 1, 2, 3$, (momentum)

$X = 1/2m\,[\,V-u(r,t)\,]^2$, (Thermal energy)

where $u(r, t) \equiv \langle u \rangle$, the average velocity. We should then have three independent conservation theorems.

For $X = m$ we have immediately from Eq. (II.B-43), the result

$$\frac{\partial}{\partial t}(mn) + \frac{\partial}{\partial X_i} \langle mnv_i \rangle = 0, \qquad \text{(II.B-44)}$$

or on introducing the mass density $\rho(r, t) \equiv mn\,(r, t)$, we obtain the familiar result

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \qquad \text{(II.B-45)}$$

the equation of continuity.

Next we put $X = m V_i$, obtaining

$$\frac{\partial}{\partial t} \langle \rho V_i \rangle + \frac{\partial}{\partial X_j} \langle \rho V_i V_j \rangle - \frac{1}{m} \rho F_i = 0 . \qquad \text{(II.B-46)}$$

To reduce this further we write

$$\langle V_i V_j \rangle = \langle (V_i - u_i)(V_j - u_j) \rangle + \langle V_i \rangle u_j + \langle V_j \rangle u_i$$

$$- u_i u_j$$

$$= \langle (V_i - u_i)(V_j - u_j) \rangle + u_i u_j .$$

Substituting this into Eq. (II.B-46) shows that

$$\rho\left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial X_j}\right) = \frac{1}{m}\rho F_i - \frac{\partial}{\partial X_j}<\rho (V_i - u_i)(V_j - u_j)>. \qquad \text{(II.B-47)}$$

Now introduce the abbreviation

$$P_{ij} \equiv \rho <(V_i - u_i)(V_j - u_j)> .$$

This is called the pressure tensor. Use this to write Eq. (II.B-47) as

$$\left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial X_j}\right) u_i = \frac{1}{m} F_i - \frac{1}{\rho} \frac{\partial}{\partial X_j} P_{ij} . \qquad \text{(II.B-48)}$$

Finally, we set $X = \frac{1}{2} m (\vec{V} - \vec{U})^2$. Then

$$\frac{1}{2} \frac{\partial}{\partial t} <\rho(\vec{V}-\vec{u})^2> + \frac{1}{2} \frac{\partial}{\partial X_i} <\rho V_i (\vec{V}-\vec{u})^2>$$

$$- \frac{1}{2} \rho <V_i \frac{\partial}{\partial X_i} (\vec{V}-\vec{u})^2> = 0 . \qquad \text{(II.B-49)}$$

We define the temperature by

$$KT = \frac{1}{3} m (\vec{V}-\vec{U})^2 \qquad \text{(II.B-50)}$$

and the heat flux by

$$q = \frac{1}{2} m\rho <(\vec{V}-\vec{U})(V-U)^2> .$$

Then it is evident that

$$\frac{1}{2}\, m\rho < V_i(V-u)^2 > = \frac{1}{2}\, m\rho < (V_i-u_i)\,(\vec{V}-\vec{u})^2 >$$

$$+ \frac{1}{2}\, m\rho u_i <(V-u)^2>$$

$$= q_i + \frac{3}{2}\, \rho K T u_i$$

and

$$\rho <v_i(V_j-u_j)> = \rho<(V_i-u_i)\,(v_j-u_j)>$$

$$+ \rho u_i <v_j-u_j> = P_{ij} \quad .$$

Using these results, Eq. (II.B-49 can be rewritten

$$\frac{3}{2}\, \frac{\partial}{\partial t}(\rho K T) + \frac{\partial q_i}{\partial X_i} + \frac{3}{2}\, \frac{\partial}{\partial X_i}(\rho K T u_i) + M P_{ij}\, \frac{\partial u_j}{\partial X_i} = 0.$$

Now since P_{ij} is symmetric, i.e., $P_{ij} = P_{ji}$

$$M P_{ij}\, \frac{\partial u_i}{\partial X_i} = P_{ij}\, \frac{m}{2} \left(\frac{\partial u_j}{\partial X_i} + \frac{\partial u_i}{\partial X_j} \right) \equiv P_{ij} \Phi_{ij} .$$

Then it is easily shown that

$$\rho \left(\frac{\partial}{\partial t} + u_i\, \frac{\partial}{\partial X_i} \right) KT + \frac{2}{3}\, \frac{\partial}{\partial X_i} q_i = - \frac{2}{3}\, \Phi_{ij} P_{ij} . \qquad \text{(II.B-51)}$$

The three conservation theorems in vector notation are then

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad , \qquad \text{(II.B-52)}$$

$$\rho \left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \right) \vec{u} = \frac{\rho}{m}\, \vec{F} - \nabla \cdot \vec{P} \quad , \qquad \text{(II.B-53)}$$

$$\rho K \left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \right) T = - \frac{2}{3} \quad \cdot \vec{q} - \frac{2}{3} \vec{\vec{P}} \cdot \vec{\vec{\Phi}} \ , \qquad \text{(II.B-54)}$$

where $\vec{\vec{P}}$ is a dyadic whose components are P_{ij}. $\nabla \cdot \vec{\vec{P}}$ is a vector whose i^{th} component is $\partial P_{ij}/\partial X_j$, and $\vec{\vec{P}} : \vec{\vec{\Phi}}_{ij}$. The auxiliary quantities are defined as follows:

$$\rho(\vec{r}, t) = M \int d^3V f(\vec{r}, \vec{V}, t) \ , \qquad \text{(II.B-55)}$$

$$U(\vec{r}, t) = \langle \vec{U} \rangle \ , \qquad \text{(II.B-56)}$$

$$KT(\vec{r}, t) = \frac{1}{3} M \langle (V-U)^2 \rangle \ , \qquad \text{(II.B-57)}$$

$$\vec{q}(\vec{r}, t) = \frac{1}{2} M \rho \langle (V-U) (V-U)^2 \rangle \ , \qquad \text{(II.B-58)}$$

$$P_{ij} = \rho \langle (V_i - U_i) (V_j - U_j) \rangle \ , \qquad \text{(II.B-59)}$$

$$\Phi_{ij} = \frac{1}{2} M \left(\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i} \right) . \qquad \text{(II.B-60)}$$

Although the conservation theorems are exact (within the limitations of the model so far developed), they still have no practical value unless we can actually solve the Boltzmann transport equation and use the distribution function so obtained to evaluate the quantities Eq. (II.B-55) to (II.B-60). Despite the fact that these quantities have been given rather suggestive names, their physical meaning can only be ascertained after the distribution function is known. It will now be shown that when it is known these conservation theorems become the physically meaningful equation of hydrodynamics.

II.B.7 THE ZERO ORDER APPROXIMATION

Assume that we are dealing with a gas that, although not strictly in equilibrium, is not far from it. In particular, we assume that in the neighborhood of any point in the gas, the distribution function is locally Maxwell-Boltzmann, and that the density, temperature, and average velocity vary only slowly in space and time. For such a gas it is natural that we try the approximation

$$f(\vec{r},\ \vec{V},\ t) \approx f^{(o)}(r,\ V,\ t)\ , \qquad \text{(II. B-61)}$$

where

$$f^{(o)}(\vec{r},\ \vec{V},\ t) = n\left(\frac{M}{2\pi KT}\right)^{3/2} e^{-\frac{M}{2KT}(V-u)^2}\ . \qquad \text{(II. B-62)}$$

Here n, T, and $\vec{u}$ are all assumed to be slowly varying functions of $\vec{r}$ and t. It is obvious that Eq. (II. B-61) cannot be an exact solution of the Boltzmann transport equation. However, it is obvious that

$$\left(\frac{\partial f^{(o)}}{\partial t}\right)_{coll} = 0\ ; \qquad \text{(II. B-63)}$$

because n, T, and $\vec{u}$ do not depend on $\vec{V}$, but it is also clear that in general

$$\left(\frac{\partial}{\partial t} + V\cdot\nabla_r + \frac{\vec{F}}{M}\cdot\nabla_v\right) f^{(o)}(\vec{r},\ \vec{\nu},\ t) \neq 0\ . \qquad \text{(II. B-64)}$$

In any case if the space-time variation is sufficiently small (this should be shown explicitly), Eq. (II. B-61) will turn out to be a very good first approximation.

If Eq. (II. B-61) is a good approximation, the left-hand side of Eq. (II. B-64) must be approximately equal to zero. This in turn would mean that n, T, and $\vec{u}$ are such that the conservation theorems Eq. (II. B-52) to (II. B-54) are approximately satisfied. The conservation theorems then become the equations governing the behavior of n, T, and $\vec{u}$. To see what they are, we must calculate $\vec{q}$ and P_{ij} to the lowest order. The results are denoted respectively by $\vec{q}^{(o)}$ and $P^{(o)}_{ij}$. Let $C(r,t) = n\,(M/2\pi KT)^{3/2}$ and $A(r,t) = M/2KT$. Then it is a simple matter to show that

$$\vec{q}^{(o)} = \frac{1}{2}\frac{m\rho}{n}\int d^3v(\vec{v}-\vec{u})\,(\vec{v}-\vec{u})^2\,C(\vec{r},\ t)e^{-A(\vec{v}-\vec{u})^2}$$

$$= \frac{1}{2}m^2C(r,\ t)\int d^2V\vec{V}V^2e^{-AU^2} = 0 \qquad \text{(II. B-65)}$$

and

$$P^{(o)}_{ij} = \frac{\rho}{n} C \int d^3v (v_i - u_i)(v_j - u_j) e^{-A(\vec{v}-\vec{u})^2}$$
$$= mC \int d^3U U_i U_j e^{-AU^2} = S_{ij} P \quad , \tag{II. B-66}$$

where

$$P = \frac{1}{3} \rho \left(\frac{M}{2\pi KT} \right)^{3/2} \int d^3u U^2 e^{-AU^2} = nKT, \tag{II. B-67}$$

just the local hydrostatic pressure.

Substituting these results into Eq. (II. B-53) and (II. B-54) and noting that

$$\nabla \cdot \vec{P} = P \ ,$$

$$\vec{P}^{(o)} \Phi = P \sum_{i=1}^{3} \Phi_{ii} = mP \cdot \vec{u} \ ,$$

we obtain the equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad , \tag{II. B-68}$$

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla \right) \vec{u} + \frac{1}{\rho} P = \frac{\vec{F}}{M} \quad , \tag{II. B-69}$$

$$K \left(\frac{\partial}{\partial t} + u \cdot \nabla \right) T + \frac{2}{3} (\nabla \cdot u) T = 0. \tag{II. B-70}$$

These are the hydrodynamic equations for the non-viscous flow of a gas. They contain no dissipative mechanism and hence they possess solutions describing flow patterns that persist indefinitely. Thus, in this approximation, the local Maxwell-Boltzmann distribution never decays to the true Maxwell-Boltzmann distribution, that is, to a state of equilibrium common to the entire mass of gas. This, it might be said, is in rough accord with experience, for we know that a hydrodynamic flow left to itself takes a long time to die out.

It is interesting to point out that although derived for dilute gases, Eqs. (II. B-68 to (II. B-70) are also used for liquids, because these equations can also be derived through heuristic arguments (forces on an element of fluid plus Newton's Law, etc.), which indicate that they are of a more general validity.

We will not treat the solution of Eqs. (II. B-68) to (II. B-70). This is a subject with a vast existing literature; our purpose is only the logical development of the equations themselves together with the limitations resulting from the method of derivation. In order to include a dissipative mechanism, i.e., viscosity, we now turn to the next approximation.

II.B.8 THE FIRST-ORDER APPROXIMATION

It is useful to make an estimate of the error incurred in the zero-order approximation Eq. (II. B-61) before proceeding with the first order approximation. Let $f(\vec{r}, \vec{V}, t)$ be the exact distribution function, and let

$$g(r, v, t) = f(r, v, t) - f^{(o)}(r, v, t). \qquad \text{(II. B-71)}$$

We are interested in the magnitude of g compared to $f^{(o)}$. First estimate the order of magnitude of $(\partial f/\partial t)_{coll}$. By definition we have

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \int d^3v_2 \int d\Omega\, \sigma(\Omega)\, |\vec{v}_2 - \vec{v}_1|\, (f_2' f_1' - f_2 f_1)$$

$$= \int d^3v_2 \int d\Omega\, \sigma(\Omega)\, |v_2 - v_1|\, (f_2^{(o)} g_1' - f_2^{(o)} g_1 + \qquad \text{(II. B. -72)}$$

$$g_2' f_1^{(o)\prime} - g_2 f_1^{(o)}),$$

where use has been made of Eq. (II. B-71), the fact that $(\partial f^{(o)}/\partial t)_{coll} = 0$, and the assumption that g is a small quantity whose square can be neglected. An order-of-magnitude estimate of Eq. (II. B-72) may be obtained by calculating the second term of the right-hand side of Eq. (II. B-72), which is

$$-g(\vec{r}, \vec{v}_1, t) \int d^3v_2 \sigma_T |v_2 - v_1| f_2^{(o)} = -\frac{g(r, v_1, t)}{\tau}, \qquad \text{(II. B-73)}$$

where τ is a number of the order of magnitude of the collision time. This can be easily seen; since the integral is essentially the particle density multiplied by the product of the velocity and total cross section σ_T. In simple kinetic theory this is just the number of collisions per second. Thus, if we put

$$\left(\frac{\partial f}{\partial t}\right)_{coll} \simeq -\frac{f - f^{(o)}}{\tau}, \qquad \text{(II. B-74)}$$

the results are qualitatively correct. With Eq. (II. B-74) the Boltzmann equation becomes

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla_r + \frac{F}{M} \cdot \nabla_v\right)(f^{(o)} + g) \simeq -\frac{g}{\tau}. \qquad \text{(II. B-75)}$$

Assuming $g \ll f^{(o)}$, we can neglect g on the left-hand side of Eq. (II. B-75). Assume further that $f^{(o)}$ varies by a significant amount (i.e., of the order of itself) only when $\vec{r}$ varies by a distance L. Then Eq. (II. B-75) furnishes the estimate

$$\vec{v} f^{(o)}/L \cong - \frac{g}{\tau}$$

or

$$\frac{g}{f^{(o)}} \cong - \frac{\lambda}{L} , \qquad \text{(II. B-76)}$$

where λ is a length of the order of the mean free path, such that $\lambda/\tau \cong \vec{V}$. From these conclusions we infer that $f^{(o)}$ is a good approximation if the local density, temperature, and velocity have characteristic wavelengths L much larger than the mean free path λ. The corrections to $f^{(o)}$ would then be of the order of λ/L.

A systematic expansion of f in powers of λ/L has been developed by Chapman and Enskog and is known by their names. It is interesting and instructive but rather complicated. It is much easier to develop the first order approximation on the basis of an assumed relaxation time τ. The precise value of τ cannot be ascertained, of course, but the method is sufficiently good to provide the main physical features of the theory. Even with this simplified version, the calculations required are rather extensive and we will only outline the procedure and present the main results.

Place

$$f = f^{(o)} + g \; ; \qquad \text{(II. B-77)}$$

then making use of Eq. (II. B-75) and neglecting g compared with $f^{(o)}$ we obtain for g

$$g = -\tau \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla_r + \frac{\vec{F}}{M} \cdot \nabla_v \right) f^{(o)} \qquad \text{(II. B-78)}$$

in terms of the assumed relaxation time τ. Since $f^{(o)}$ is given by Eq. (II. B-62), g can be readily calculated. The first order corrections to the density, average velocity, temperature, etc. according to Eqs. (II. B-55) to (II. B-60) can also be calculated. Now the heat flux vector does not vanish. In terms of the coefficient of thermal conductivity and the coefficient of viscosity, defined by

$$K = \frac{m^2 \tau}{6KT} \int d^3U U^4 \left(\frac{m}{2KT} U^2 - \frac{5}{2} \right) f^{(o)}$$

$$= \frac{5}{2} \tau k T n \qquad \text{(II. B-79)}$$

and

$$\mu = \frac{\tau m^2}{KT} \int d^3U U_1{}^2 U^2 f^{(o)} = \tau nkT \qquad \text{(II. B-80)}$$

respectively, and keeping only quantities of first order, we obtain from the conservation laws Eq. (II. B-52) to (II. B-54), the equations of hydrodynamics to first order:

$$\frac{\partial}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad , \qquad \text{(II. B-81)}$$

$$\left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \right) \vec{u} = \frac{\vec{F}}{M} - \frac{1}{\rho} \left(P - \frac{\mu}{3} \nabla \cdot \vec{u} \right) + \frac{\mu}{\rho} \nabla^2 \vec{u} \quad , \qquad \text{(II. B-82)}$$

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla \right) T = -\frac{2}{3} (\nabla \cdot \vec{u}) T + \frac{2K}{3\rho} \nabla^2 T \qquad \text{(II. B-83)}$$

The first equation is the equation of continuity, and this is not changed by including first order corrections in the system. The second equation is called the Navier-Stokes equation: here two added terms appear which are linear in the viscosity. If u is set equal to zero it reduces to Euler's equation. The third equation is the heat conduction equation. The Navier-Stokes equation can also be (and was initially) derived on an intuitive basis, provided we take the meaning of viscosity from experiments. This is done in most elementary texts on fluid mechanics.

II.B.9 CHARACTER OF THE TIME DEPENDENCE

The purpose of the Chapman-Enskog method is to solve the Boltzmann transport equation Eq. (II. B-27) by successive approximation. While it is not our purpose to undertake a presentation of this method of solution, it is well to point out this method will not yield the most general solutions to the Boltzmann equation, namely those that depend on the time implicitly through the local density, velocity and temperature. In Section II. B. 8 the simplifying assumption is that $(\partial f/\partial t)_{coll} \cong -(f-f^{(o)})/\tau$. It is useful, in view of our interest in equations (II. B-81) to (II. B-83) to point out the special importance attached to this type of solution. Its importance lies in the fact that a solution initially not of this type will become one of this type in a time of the order of a collision time. Since the collision time for ordinary gases is of the order of 10^{-11} sec, solutions of the type mentioned are the relevant ones in most physical applications. The claim may be justified as follows. Let f be a solution to the Boltzmann transport equation. It may depend on the time explicitly as well as implicitly through the time dependence of the local density, velocity, and temperature. Thus we may decompose the time derivative of f into two terms

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{explicit} + \left(\frac{\partial f}{\partial t}\right)_{implicit} . \qquad \text{(II. B-84)}$$

By making use of the approximate expression Eq. (II. B-74) for $(\partial f/\partial t)_{coll}$, we may write the Boltzmann equation in the form

$$\left(\frac{\partial f}{\partial t}\right)_{explicit} \quad L(f) = -\frac{f-f^{(o)}}{\tau} , \qquad \text{(II. B-85)}$$

where

$$L(f) = \left(\frac{\partial f}{\partial t}\right)_{implicit} + \left(\vec{v}\cdot\nabla_r + \frac{F}{M}\cdot\nabla_v\right)f . \qquad \text{(II. B-86)}$$

Now define f_1 to be the solution of the equation

$$L(f_1) = -\frac{f_1-f^{(o)}}{\tau} . \qquad \text{(II. B-87)}$$

Then f_1 has no explicit dependence on the time. Defining f_2 by

$$f = f_1 + f_2 , \qquad \text{(II. B-88)}$$

it is easily shown that f_2 satisfies the equation

$$\left(\frac{\partial f_2}{\partial t}\right)_{\text{explicit}} + L(f_2) = \left(\frac{\partial f_2}{\partial t}\right)_{\text{coll}} . \qquad \text{(II. B-89)}$$

If L $(f)_2$ can be neglected, this becomes

$$\frac{\partial f_2}{\partial t} = - f_2/\tau , \qquad \text{(II. B-90)}$$

which leads immediately to

$$f_2 \propto e^{-t/\tau} . \qquad \text{(II. B-91)}$$

Therefore, after a time τ, the solution essentially reduces to f_1, which has no explicit dependence on the time.

II.B.10 CHEMICAL REACTIONS

Thus far, we have limited the discussion to elastic collisions between identical particles. We now wish to extend the formalism to include the possibility of chemical reactions, that is, inelastic collisions between unlike particles. There are basically two mechanisms by means of which a chemical reaction can be brought about. The first is by means of a photon, a quantum of radiation incident on a molecule. The photon may simply excite the molecule (or atom) i.e., raise it to a higher quantized energy state, or it may separate some combination of atoms from the molecule. The photon may not necessarily impart all of its energy; it may even absorb energy if it happens to strike an excited molecule. There are obviously many possibilities open. The second and most common mechanism for producing chemical reactions is by means of collisions. The collection of molecules is heated and the increased kinetic energy of one molecule finally becomes sufficient to cause a chemical interaction when it strikes a second molecule. Here some of the translational energy is diverted to supply the necessary energy, and the products of the reaction move away with relatively smaller kinetic energies. Multiple collisions can also occur, and the products of the reaction need not necessarily consist of only two new molecules, but may be several in number. Low energy photons may also result (or be absorbed). Here again there are many possibilities open.

In general, photo-chemical reactions are not as important as reactions caused by heat; since the relatively high energy photons are usually not available. Here we will limit outselves to the consideration of collision-produced reactions, and these in turn will be further restricted to two-body interactions, i.e., two incident molecules and two product molecules. This is not a serious limitation, since at the densities ordinarily encountered three or more body collisions are rare.

It might be thought that there is still a third class of chemical reactions, those where molecules simply split into two or more smaller components when the temperature reaches a certain level. This is not the case, however, such reactions are in reality caused by collision with another atom or molecule which is left unchanged except for a reduced translational kinetic energy, the excess of which is used to supply the necessary energy for the reaction. The reactions are then contained in the class already discussed so long as they are only two-body collisions.

In order to obtain the most general set of equations within the set of restrictions already stated, we will designate each distinct particle by a subscript on the physical quantities corresponding to them, counting important excited states, charged combinations and electrons as well as the various molecules in the ground state (lowest internal energy state) as different and distinct. Thus $n_i(\vec{r},t)$ is the number of the ith type of particle or molecule, as the case may be, per unit volume at the position $\vec{r}$ at a time τ.

For the moment assume that the collisions between the various chemical species are still elastic. Then in addition to collisions between identical particles we have collisions between each species and all others. There will exist a cross-section for each such collision, and in general it will be different for each interacting pair of particles.

Let $f_i(r, v_i, t)$ be the distribution function of the ith species. Then for each of the N species existing in the system, we will have a Boltzmann equation determining the distribution function for the species in question. The contribution to the collision term $(\partial f_i / \partial t)_{coll}$ will, however, be made up of expressions like Eq. (II. B-26) resulting from collisions between the ith species and all other species. The derivation of such added contributions is exactly analogous to that presented in Section IV for collisions between identical particles. We obtain, in fact, N equations of the form*

$$\left(\frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla_r + \frac{F_i}{m_i} \cdot \nabla_{v_i} \right) f_i =$$

$$\sum_j \int d\Omega_{ij} \int d^3 v_j'' \, \sigma_{ij}(\Omega) \left| v_i - v_j'' \right| \times \qquad \text{(II. B-92)}$$

$$(f_j' f_i' - f_j f_i), \quad i = 1, 2 \cdots N$$

for i running from 1 to N. An i has been added to the force vector; since it may depend on the species, for example, because of differences in charge. Here again the single primes indicate the velocities after the collision and are connected to the initial or incident velocities by the equations of conservation of energy and momentum:

$$\frac{1}{2} m_i v_i^2 + \frac{1}{2} m_j v_j^2 = \frac{1}{2} m_i v_i'^2 + \frac{1}{2} m_j v_j'^2$$

$$m_i v_i + m_j v_j = m_i v_i' + m_j v_j' . \qquad \text{(II. B-93)}$$

It is of course understood that the primed velocities must be eliminated, using these relations, before the set of equations Eq. (II. B-92) can be integrated. In addition, the scattering angles on which the various cross sections $\sigma_{ij}(\Omega)$ depend must be determined in terms of these velocity vectors. Finally, note that in Eq. (10.1) it is necessary to add a double prime to the variable of integration in order to differentiate between the velocities of identical particles, which occur when i is placed equal to j.

We are again interested in the conservation theorems for this mixture of particles. In order to obtain such equations we assume that x_i, is a quantity that is conserved in a collision between particles i and j, such that

$$x_i + x_j = x_i' + x_j' , \qquad \text{(II. B-94)}$$

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*In some texts, for example Hirschfelder and Curtiss, this equation appears with 2π bdb replacing $\sigma(\Omega)\, d\Omega$, where b is the impact parameter. These are equivalent if we neglect the φ dependence of the scattering cross section.

where the primes indicate the conserved quantities after the collision, i.e., for velocities $\vec{v}_i'$ and $\vec{v}_j'$, respectively. Here again x_i may be mass momentum, or kinetic energy. Multiply Eq. (II. B-92) by x_i and integrate over $\vec{v}_i$. By exactly the same arguments used in Section VI, it can be shown that the general conservation law for the ith species is just

$$\frac{\partial}{\partial t} \langle n_i x_i \rangle + \nabla \langle n_i \vec{v}_i x_i \rangle$$

$$- n_i \langle \vec{v}_i \cdot \nabla_r x_i \rangle - \frac{n_i}{m_i} \langle \vec{F}_i \cdot \nabla_v x_i \rangle$$

$$- \frac{n_i}{m_i} \langle (\nabla_v \vec{F}_i) x_i \rangle = \int x_i \left(\frac{\partial f_i}{\partial t} \right)_{coll} d \vec{v}_i \ . \qquad \text{(II. B-95)}$$

$$i = 1, 2, \text{---} N,$$

where the angular brackets again mean an average over the respective quantities using the ith distribution function, and $(\partial f_i / \partial t)_{coll}$ is the sum of collision terms in Eq. (II. B-92). If we again substitute for x_i the mass m_i, the momentum $m_i \vec{v}_i$, or the kinetic energy $\frac{1}{2} m_i \vec{v}_i^{\,2}$, we obtain a set of equations similar to Eq. (II. B-43), except that the collision integral on the right-hand side does not in general vanish. If no chemical reaction takes place, the out-going masses are the same as the incident masses; so that for $x_i = m_i$ the collision integral does in fact vanish and Eq. (II. B-95) reduces to the equation of continuity for the ith species:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}_i) = 0 \ , \qquad \text{(II. B-96)}$$

where u_i is just the average velocity of the ith species given by $\langle v_i \rangle$ and ρ_i is the mass density of the ith species equal to $n_i m_i$.

Before going on, it is useful to define a few relationships between various velocities and related quantities that will be needed in the further course of the development. The absolute velocity of a particle of the ith species is just $\vec{v}_i$. The average of this,

$$\vec{u}_i (r,t) = \langle v_i \rangle = \frac{1}{n_i} \int \vec{v}_i f_i (\vec{r}, \vec{v}_i, t) \, d \vec{v}_i \ , \qquad \text{(II. B-97)}$$

is just the average flow velocity of the ith species at the point $\vec{r}$. Then we logically define the average mass velocity for the system as a whole by

$$\vec{u}(r, t) = \frac{1}{\rho} \sum_{i=1}^{N} \rho_i \vec{u}_i \ , \qquad \text{(II. B-98)}$$

where

$$\rho_i = n_i m_i \qquad \text{(II. B-99)}$$

and

$$\rho = \sum_{i=1}^{N} \rho_i = \sum_{i=1}^{N} n_i m_i \ . \qquad \text{(II. B-100)}$$

The difference between $\vec{u}_i$ and $\vec{u}$ at the point $\vec{r}$ is also an interesting quantity; it is just the rate of diffusion of the species i. We set it equal to $\vec{W}_i$; so that

$$\vec{W}_i = \vec{u}_i - \vec{u} \ . \qquad \text{(II. B-101)}$$

It is then possible to write the absolute velocity of the ith species as

$$\vec{v}_i = \vec{u} + \vec{W}_i + \vec{C}_i \ , \qquad \text{(II. B-102)}$$

where $\vec{C}_i$ is the random or thermal velocity of the ith species. $\vec{C}_i$ is a velocity having a zero average relative to a frame moving with velocity $\vec{u} + \vec{w}_i$. Hence,

$$\langle \vec{v}_i \rangle = \langle \vec{u} \rangle + \langle \vec{W}_i \rangle + \langle \vec{C}_i \rangle$$

$$= \vec{u} + \vec{W}_i = u_i \ . \qquad \text{(II. B-103)}$$

after using Eq. (II. B-101) in the last line, $\vec{C}_i$ determines the temperature of the ith species in a frame moving with velocity $\vec{u} + \vec{w}_i$.

If Eq. (II. B-96) is summed over i and use is made of Eq. (II. B-98) and (II. B-100) we obtain

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \qquad \text{(II. B-104)}$$

which has the same form as that for one species only. However, even in the absence of chemical reactions between the various species there does not exist equations exactly analogous to the momentum and energy equation where only one species is present. This is because the collision integral does not vanish except when x_i is a constant, i.e., independent of velocity, as in the case of $x_i = m_i$. In general the various species can interchange momentum and energy even in the absence of a chemical reaction so that the collision integrals make important contributions to equations derived from Eq. (II. B-95). The collision integral can be looked upon as a source of particles, momentum or energy as the case may be, for the ith species, which are contributed by all other species in the system.

If chemical reactions are included the collision integral in Eq. (II. B-95) becomes a mass source and it can be shown that

$$\left(\frac{\partial f_i}{\partial t} \right)_{coll.} d \vec{v}_i \qquad \text{(II. B-105)}$$

is just equal to the rate of increase of particles of mass m_i at the point r. This is obviously true, since $\left(\frac{\partial f_i}{\partial t} \right)_{coll}$ is by definition the total rate of change of the number of molecules of species i at r having the velocity v_i. Eq. (II. B-105) is just the sum over all velocities at the point $\vec{r}$. Hence, if a chemical reaction takes place, we obtain not Eq. (II. B-96) but

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}_i) = K_i m_i \, , \qquad \text{(II. B-106)}$$

where k_i is the rate of increase (or decrease if it is negative) of the number of molecules of species i at the point $\vec{r}$. Since total mass is always conserved we must have

$$\Sigma_i \; K_i \; m_i = 0 \, . \qquad \text{(II. B-107)}$$

If chemical reactions take place, the derivation of expressions for the collision terms in the Boltzmann equation can still be carried out in much the same way. Momentum is still conserved, and the relationship implied by this conservation remains the same. Energy is also conserved, however, we must now include a term describing the internal energy as well as the kinetic energy. Since the internal energy terms, or at least the difference between them for the initial and final states are presumed known (heats of reaction, etc.), we still obtain a definite relationship between the velocities. These four equations can then be used to reduce the number of variables in the collision terms so that a definite functional relationship exists and the integration can be carried out. The terms appear the same as those contained in Eq. (II. B-92).

Since momentum is conserved in a chemical reaction, the momentum equation obtained from Eq. (II. B-95) is not altered at all, except for the implicit relationships between the initial and final velocities already discussed. Here the collision integral on the right-hand side with $x_i = m_i v_i$ is simply the rate of gain of momentum of the ith species having velocity $\vec{v}_i$ at the point $\vec{r}$. For the momentum equation, it is not a simple matter to evaluate the collision integral. However, Burgers has shown that

$$\int m_i \vec{v}_i \left(\frac{\partial f_i}{\partial t} \right)_{coll} d\vec{v}_i = - \sum_{j=1}^{N} K_{ij} (W_i - W_j) . \qquad \text{(II. B-108)}$$

where k_{ij} is a very complicated function of the collision cross section. This is exactly what we might expect. The transfer of momentum from one species to another is proportional to the difference between their diffusion velocities. The total transfer to the ith species is the sum over all species.

If we set the force on the ith species equal to

$$\vec{F}_i = m_i \vec{G} + e_i \left[\vec{E} + (\vec{v}_i \times B) \right] , \qquad \text{(II. B-109)}$$

where $\vec{G}$ is the gravitational acceleration per unit mass, then equation of motion obtained from the conservation theorem Eq. (II. B-95) by setting $x_i = m_i (\vec{v}_i - \vec{u})$* is just

$$\rho_i \left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla_r \right) \vec{u} + \left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla_r \right) (\rho_i \vec{W}_i)$$

$$+ \rho_i \vec{W}_i \nabla \cdot \vec{u} + \rho_i \vec{W}_i \cdot \nabla_r \vec{u} + \nabla_r \cdot \vec{\vec{P}}_i$$

$$- \rho_i \vec{G} - \rho_{ei} \vec{E}_u - (\vec{J}_i \times \vec{B}) =$$

$$- \sum_{j=1}^{N} K_{ij} (\vec{W}_i - \vec{W}_j) , \qquad \text{(II. B-110)}$$

where we have replaced the collision integral on the right-hand side, using the approximate value given by Eq. (II. B-108). Here we have defined the effective electric field $\vec{E}_u$ equal to

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*Here a frame of reference moving with the average mass velocity $\vec{u}$ is used. If some other frame is used, the equations we obtain will be different. Care must be taken to determine the velocity relationships used in a particular set of equations.

$$\vec{E}_u = \vec{E} + \vec{u} \times \vec{B} \ . \qquad \text{(II. B-111)}$$

The current density resulting from the flow of the ith species is just

$$\vec{J} = \rho_{es} \vec{u}_i \ , \qquad \text{(II. B-112)}$$

where

$$\rho_{es} = n_i e_i \ , \qquad \text{(II. B-113)}$$

and e_i is the charge of the ith species. The pressure tensor of the ith species is

$$\vec{\vec{P}} = m_i n_i \langle(\vec{u} - \vec{v}_i)(u - \vec{v}_i)\rangle \ . \qquad \text{(II. B-114)}$$

The pressure of the ith species is the sum of the diagonal elements of this tensor times 1/3:

$$P_i = \frac{1}{3} (P_{xx} + P_{yy} + P_{zz}) . \qquad \text{(II. B-115)}$$

Finally, the viscous stress tensor for the ith species is equal to

$$\vec{\vec{\tau}}_i = - \vec{\vec{P}}_i + I \, p_i \ , \qquad \text{(II. B-116)}$$

where I is the unit dyadic.

Equation (II. B-110) can be considerably simplified by using the relationship obtained from it by summing over i:

$$\left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla_r\right)\vec{u} + \nabla_r \cdot \vec{\vec{P}} - \rho\vec{G} - \rho_e \vec{E}_u - (\vec{J} \times B) = 0 \ , \qquad \text{(II. B-117)}$$

where

$$\rho_e = \sum_i \rho_{ei} \quad ,$$

$$p = \Sigma\, p_i \quad , \qquad \text{(II. B-118)}$$

$$\vec{P} = \sum_i \vec{P}_i \quad .$$

The collision term vanishes when we sum over i: this is physically reasonable and easy to show. With the help of Eq. (II. B-117), Eq. (II. B-110) can be rewritten in the form

$$\left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla_r\right)(\rho_i \vec{W}_i) + \rho_i \vec{W}_i \nabla_r \cdot \vec{u} + \rho_i \vec{W}_i \cdot \nabla_r \vec{u}$$

$$- \nabla_r \cdot \vec{\tau}_i - \frac{\rho_i}{\rho} \nabla \cdot \vec{\tau} +$$

$$\nabla p_i - \frac{\rho_i}{\rho} \nabla p - \left(\rho_{ei} - \frac{\rho_i \rho_e}{\rho}\right) E_u^i \qquad \text{(II. B-119)}$$

$$- \left\{\left(\vec{J}_i - \frac{\rho_i}{\rho} J\right) \times B\right\} = - \sum_{j=1}^{N} K_{ij} (\vec{W}_i - \vec{W}_j).$$

This is the general equation of motion for the ith species.

The equation of the internal energy of the ith species can be obtained from the conservation theorem by setting

$$x_i = 1/2\, m_i (v_i - u)^2. \qquad \text{(II. B-120)}$$

We then find that

$$\left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla_r\right)\left(\frac{3}{2} p_i\right) + \frac{5}{2} p_i \nabla_r \cdot \vec{u} - \frac{1}{2} \vec{\tau}_i : \vec{\varepsilon}$$

$$+ \nabla_r \cdot \vec{Q}_{ci} + \rho_i \left[\left(\frac{\partial}{\partial t} + u \cdot \nabla_r\right) \vec{u}\right] \cdot \vec{W}_i \qquad \text{(II. B-121)}$$

$$- \rho_i \vec{G} \cdot \vec{W}_i - \vec{E}_u \cdot J_i = I(E)_{coll} \quad ,$$

where $I(E)_{coll}$ is the collision integral for the kinetic energy. It is the net rate of transfer of energy to the ith species due to collisions with other species. Using the same approximation as we did in obtaining Eq. (II. B-108), it can be shown that

$$I(E)_{coll} = - \sum_{j=1}^{N} 2\, n_i n_j \frac{m_i m_j}{(m_i+m_j)^2} \alpha\, Z_{ij}^{(11)} k(T_i - T_j) ,$$

where

$$\alpha = (2\, k\, T/\eta)^{\frac{1}{2}} ,$$

$$\eta = (m_i m_j / m_i + m_j) ,$$

and $Z_{ij}^{(11)}$ is a very complicated integral depending on the collision cross-section. Again, we see that, to this lowest order approximation, the kinetic energy transfer (heat transfer) is proportional to the temperature difference between the two species. In Eq. (II. B-118) we have also used the definition

$$e^{lm} = \frac{\partial u^m}{\partial x^l} + \frac{\partial u^l}{\partial x^m} - \frac{2}{3} \delta^{lm} \frac{\partial u^l}{\partial x^l} , \qquad \text{(II. B-122)}$$

and set the heat flux equal to

$$\vec{Q}_{ci} = m_i n_i < (\vec{v}_i - u)\ (\vec{v}_i - u)^2 > . \qquad \text{(II. B-123)}$$

To obtain the general equation for the second moment, the viscous stress equation, we set

$$x_i = m_i\ (\vec{v}_i - \vec{u})\ (\vec{v}_i - \vec{u}) . \qquad \text{(II. B-124)}$$

Placing this dyadic in the general conservation equation (II. B-95) gives, after some considerable manipulation, the result:

$$\left[\frac{D}{Dt} P_i^{lj} + P_i^{lj} \nabla \cdot u + \frac{\partial}{\partial x^k} (S_i^{ljk}) + \rho_i \{ W_i^{l} \frac{Du^l}{Dt} + W_i^{l} \frac{Du^j}{Dt} \} + P_i^{kl} \frac{\partial u^j}{\partial x^k} \right] .$$

$$+ P_i^{kj} \frac{\partial u^l}{\partial x^k} - \rho_i (G^l \cdot W_i^l + G^j W_i^l)$$

$$- (E_u^l J_i^j + E_u^j J_i^l) - (M_i^{(2)})^{lj} = I^{lj}_{coll} , \qquad \text{(II. B-125)}$$

where $(M_i^{(2)})^{\ell j}$ is a tensor expression depending on the viscous stresses and the magnetic field and

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u \cdot \nabla_r . \qquad \text{(II. B-126)}$$

In equation (II. B-125), we have used the usual summation conventions rather than vecor and dyadic notation, in order to simplify the equation. The collision integral indicated by $I^{\ell j}_{coll}$ is a complicated expression involving sums and differences of the viscous tensor.

Many of the terms in these equations can be neglected under certain conditions. They have been presented here in full (actually some approximations have already been made) in order to give a proper perspective on the scope of the problem of treating a chemically reacting plasma. Some of the terms contained in these equations, while not negligible, can be rewritten in simpler form, using a phenomenological approach in terms of the coefficients of thermal conductivity and viscosity. Here no further reduction will be attempted, because of the limitations of time and space. However, it should not be thought that this work is by any means complete. Considerable additional work in this area should be carried out. For example, the usual procedure is to next combine the moment equations of each species and obtain equations describing the gross motion of the plasma. It is then possible to express the equations in dimensionless form, this, in turn, defines ratios of various constants that provide us with convenient ways of specifying the important terms in the equations and processes corresponding to them. Such an analysis can also be performed on the species equations themselves. This would be very useful and should be carried out before any serious attempt is made to solve these equations.

II.B.11 EQUATIONS FOR THE ELECTROMAGNETIC FIELD

The force on the ith species is of course given by

$$\vec{F}_i = - \nabla \phi + n_i q_i (\vec{E} + \vec{v}_i X \vec{B}), \qquad \text{(II. B-127)}$$

where ϕ is the external potential, usually negligible in most problems of interest, but not negligible when we must consider hydrodynamic and magnetic buoyancy, and $\vec{E}$ and $\vec{B}$ and are the true local electric and magnetic field vectors, having their sources in external charges and currents together with sources in the plasma itself. $\vec{E}$ and $\vec{F}$ must at the same time satisfy Maxwell's equation (e.m units, i.e., Gaussian):

$$\nabla \cdot \vec{E} = 4\pi C^2 \rho_c , \qquad \text{(II. B-128)}$$

$$\nabla \cdot \vec{B} = 0 , \qquad \text{(II. B-129)}$$

$$\nabla X \vec{E} = - \frac{\partial \vec{B}}{\partial t} , \qquad \text{(II. B-130)}$$

$$\nabla X \vec{B} = \frac{1}{C^2} \frac{\partial \vec{E}}{\partial t} + 4\pi \vec{j} \qquad \text{(II. B-131)}$$

where ρ_c is the true charge density and $\vec{j}$ is the true current density. These quantities can be written

$$\rho_c = \frac{e}{c} \sum_i n_i z_i , \qquad \text{(II. B-132)}$$

$$\vec{j} = \frac{e}{c} \sum_i n_i z_i \vec{v}_i , \qquad \text{(II. B-133)}$$

where z_i for the electrons themselves is of course equal to unity.

Maxwell's equationsa are sometimes written in terms of the electric displacement vector $\vec{D}$ and the magnetic intensity $\vec{H}$. These are actually derived quantities, and depend on having some knowledge of the electric and magnetic susceptibilities of the plasma. To obtain such information, further assumptions must be made about the plasma. For this reason, the equations have been written in terms of the most fundamental electrical quantities: the electric intensity $\vec{E}$ and the magnetic induction $\vec{B}$.

There now exists a sufficient number of equations to provide a unique determination of the unknowns: temperature, species density, species velocity etc., together with the electromagnetic field vectors. It should be pointed out, however, that the treatment has not been sufficiently refined to describe the process of radiation absorption and emission by the various species. In order to include such elementary processes, one would need a detailed knowledge of the quantum mechanics of each species, along with the spectral intensity and polorization of the radiation at each point in the plasma.

Upon including such considerations, one would automatically obtain the correct values of the radiation intensity at each point and hence the total radiation loss at the surface of the system, which can be very important at high temperatures. As our equations stand, the energy loss through radiation would be independent of the density of the plasma and would be simply computed from the Poynting vector integrated over the surface. This would neglect completely any reabsorption of radiation by the plasma. In order to include such an effect, we require the radiation intensity I_ν, to satisfy one further equation, the radiative transport equation.

$$\frac{\partial I_\nu (\vec{s})}{c \partial t} + \vec{s} \cdot \nabla I_\nu (\vec{s}) = K_\nu [B_\nu (T) - I_\nu (\vec{s})] , \qquad \text{(II.B-134)}$$

where $\vec{s}$ is the unit vector in the direction of propagation.

To obtain this equation, the approximation of local thermodynamic equilibrium is made and scattering is neglected, i.e., radiation is either absorbed or emitted but not simply changed in its direction of propagation. This is obviously a good approximation for most simple systems. In Eq. (II.B-134), K_ν is the absorption coefficient defined by the equation.

$$K_\nu = \sum_i n_i \sigma_i (\nu) [1 - e^{-h\nu / kT}] . \qquad \text{(II.B-135)}$$

Here $n_i \nu$ is the number of absorbers of the ith species per unit volume (either electrons or atomic species), and has the value characteristic of thermal equilibrium at the local matter temperature T. $\sigma_i (\nu)$ is the cross-section for absorption of photons of frequency ν by these absorbers. The factor $1 - \exp(-h\nu/kT)$ has the effect of including emission with true absorption. $I_\nu(\vec{s})\, d\nu\, d\Omega$ is the amount of radiative energy with frequencies between ν and $\nu + d\nu$ traveling within the element of solid angle $d\Omega$ about the direction of the unit vector $\vec{s}$ and crossing unit area perpendicular to $\vec{s}$ per unit time. $I_\nu (\vec{s})$ is then simply related to Fourier components of the Poynting vector and hence to $\vec{F}$ and $\vec{B}$. $B_\nu (T)$ in Eq. (II.B-134) is the termal equilibrium value of $I_\nu (s)$. This is just the Planck intensity, of course.

Further approximations can be made in order to handle equation (II.B-134). These have been discussed at length by Sampson. In any case, it is clear that the physical properties of the species making up the plasma determine the absorption coefficient K_ν. Once this is known, we can (in principle at least) solve the problem of chemically reacting radiative flow with absorption limiting the radiation loss.

II.C THE CALCULATION OF THE FORMATION OF DISCONTINUITIES IN PLANAR AND SPHERICALLY-SYMMETRIC NONISENTROPIC INVISCID FLOWS

by

P. Gordon and S. M. Scala

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II C.1 INTRODUCTION

In attempting to solve the full Navier-Stokes equations by numerical methods, it has become evident to us, as well as to other investigators (II. C-1 to 8) that it is important to utilize difference equations that remain well-behaved in the special case where the viscous terms are identically zero. Although our continuing interest is still directed toward solving the full Navier-Stokes equations, this paper is concerned only with physical and mathematical problems associated with the inviscid equations, the goal being to obtain a better understanding of our numerical approximation to the Euler subsystem of the full Navier-Stokes equations. The major problem associated with the numerical solution of the Euler equations is the discontinuities that these equations can produce. If the mathematical problem under consideration does not produce a discontinuity, a variety of suitable numerical methods is available.

Some of the earliest treatments of flows in which discontinuities appeared were the studies of the propagation of waves of finite amplitude due to Earnshaw and Riemann, which are discussed in the later work of Rayleigh (II. C-9). In these studies the equations of fluid motion utilized were in their linearized form, and it was shown that with the passage of time, partial derivatives of the field variables with respect to distance can become infinite and then the method of analysis yields no information as to the subsequent course of the fluid motion.

In discussing discontinuities, we distinguish between gasdynamic discontinuities, which can "form", and mathematical discontinuities, which "appear"; since once the latter manifest themselves, the solution, by definition, is no longer continuous and cannot be followed in time without introducing additional information. (We will come back to this point.)

Here, we note that Hayes (II. C-10) has utilized the following definition: "a gasdynamic discontinuity is a surface in a fluid field across which various properties of the fluid appear to change discontinuously and across which there is some flow of fluid". He also observes that gasdynamic discontinuities are not discontinuities in the strict mathematical sense, since, for example, a shock wave has a finite thickness across which the physical properties actually change continuously.

Generally, mathematical discontinuities tend to occur in the Euler equations at the same location that gasdynamic discontinuities occur in the complete Navier-Stokes equations; therefore, one tends to associate these two different types of discontinuities rather closely in one's mind. Moreover, since an effect of the viscous terms (real or artificial) is to prevent a mathematical discontinuity from appearing, it has now become a common numerical approach to introduce an artificial viscosity when

the appearance of mathematical discontinuities is anticipated (II. C-11 to 13). Although such an artificial viscosity techniques have been highly successful, to incorporate them into a solution of the full Navier-Stokes equations would not be completely satisfactory, since by definition one would then be distorting the true viscous effects in ar unknown manner.

Another problem occurs because of the fact that questions still remain regarding the true behavior of the Euler equations, and this, of course, complicates the evaluation of a particular set of difference equations. Although many aspects of inviscid flow have received careful and thorough analysis (e.g. II. C-14 and 15), the area of mixed nonisentropic flow with shock waves, which is of particular interest to us since it occurs in so many of the problems which we are investigating with the full Navier-Stokes equations, is relatively unknown.

A preliminary exposition of some of these difficulties was presented at the International Symposium on High Speed Computing in Fluid Dynamics, in Monterey, California, August 1968. The purpose of this paper is to look at these difficulties more closely. Our major objectives are the following:

a. To present for consideration two solutions which remain continuous in regions of varying entropy, although at later times a discontinuity develops in an isentropic region of the flow. The apparent speed of propagation of the discontinuity will also be discussed.

b. To indicate that the difference equations used herein to solve the Euler equations are suitable for inclusion into a solution of the full Navier-Stokes equations. We will demonstrate with numerical results that for the particular problems investigated the difference equations we have utilized exhibited the following properties.

    1. If a particular solution to the Euler equations is continuously differentiable, then the functions defined by the difference equations will converge to this solution.

    2. If a particular solution breaks down because of the appearance of a mathematical discontinuity then the functions defined by the difference equations will at the appropriate point produce this discontinuity, and will also remain stable on either side of the discontinuity. In addition, no artificial viscosity effect is discernible.

As observed by Friedrichs (II. C-16), one question concerning discontinuities has been answered completely. Suppose that at the time $t = 0$, functions $V(0,X)$, $P(0,X)$, $S(0,X)$ are given which possess a discontinuity at a particular point $X = X_0$, but satisfy the Rankine-Hugoniot jump conditions across the discontinuity, then the question is

whether or not a solution of the Euler equations exists which possesses discontinuities at a certain curve F (t,X) which passes through the point F $(0,\lambda) = X_0$, at which the Rankine-Hugoniot jump conditions continue to be satisfied. The answer is affirmative for shocks. Thus, if in a given problem, we specified the additional information that the motion of the curve F (t,X) was given by the shock velocity compatible with the Rankine-hugoniot jump conditions, we would, in effect, have a recipe for continuing the solution in the presence of a mathematical discontinuity.

In general, of course, when one uses the Euler equations and a mathematical discontinuity appears, then since the initial value problem is not uniquely determined from that point on, it can therefore not be expected that a given numerical technique should automatically select that solution which satisfies the Rankine-Hugoniot conditions across the discontinuity, In particular, one should not expect to be able to compute the speed of propagation of the discontinuity without specifying additional conditions.

It should be emphasized, however, that when using the Euler equations, the ideal difference equations would be such that they converge properly to the correct solution in the continuous case, and in the presence of a discontinuity would be such that they "correctly" give the motion of the discontinuity as well as the distribution of the variables on either side. Lax and Wendroff (II. C-17, 18, 19)have suggested the possibility of such difference equations, and have demonstrated that their scheme can produce, at least in some cases, physically acceptable solutions (solutions which satisfy the Rankine-Hugoniot conditions). Since these methods do not introduce the Rankine-Hugoniot conditions specifically into the solution, and since these conditions are indeed satisfied in the case of a steady state wave whenever viscosity effects are introduced into the governing equations, one concludes that their difference equation includes an artificial viscosity. In our case, it is important that we demonstrate that our finite difference equations which represent the Euler equations do not contain an artificial viscosity which would act to mask the molecular viscosity effects which are given by the complete Navier-Stokes equations.

II.C.2 THE DIFFERENTIAL EQUATIONS AND THE DIFFERENCE EQUATIONS

The one-dimensional time-dependent Euler equations in cartesian coordinates are

$$\frac{\partial \rho}{\partial t} = - V \frac{\partial \rho}{\partial X} - \rho \frac{\partial V}{\partial X} \quad , \tag{II. C-1}$$

$$\rho \frac{\partial V}{\partial t} = - \rho V \frac{\partial V}{\partial X} - \frac{\partial P}{\partial X} \quad , \tag{II. C-2}$$

and

$$\rho C_v \frac{\partial T}{\partial t} = - \rho C_v V \frac{\partial T}{\partial X} - P \frac{\partial V}{\partial X} \quad , \tag{II. C-3}$$

where ρ is the density, V is the velocity, T is the temperature, P is the pressure, and C_v is the specific heat at constant volume.

The equation of state for a perfect gas is

$$P = \rho RT \quad , \tag{II. C-4}$$

where, as in earlier work (II. C-1), we utilize for convenience the properties of molecular nitrogen:

$$R = 55.2 \text{ ft-lb/lb}^{\circ}\text{R} \quad ,$$

$$C_v = 138 \text{ ft-lb/lb}^{\circ}\text{R}.$$

In spherically-symmetric coordinates, the Euler equations becomes

$$\frac{\partial \rho}{\partial t} = - V \frac{\partial \rho}{\partial r} - \rho \frac{\partial V}{\partial r} - \frac{2 \rho V}{r} \quad , \tag{II. C-5}$$

$$\rho \frac{\partial V}{\partial t} = - \rho V \frac{\partial V}{\partial r} - \frac{\partial P}{\partial r} \quad , \tag{II. C-6}$$

and

$$\rho C_v \frac{\partial T}{\partial t} = - \rho C_v V \frac{\partial T}{\partial r} - P \frac{\partial V}{\partial r} - \frac{2PV}{r} . \qquad \text{(II. C-7)}$$

Note that the assumptions of zero viscosity and zero thermal conductivity (i.e., $\mu = k = 0$) in the Navier-Stokes equations not only lead to the Euler equations, but also to the result

$$\frac{dS}{dt} = \frac{C_v}{T} \frac{dT}{dt} - \frac{R}{\rho} \frac{d\rho}{dt} = 0 , \qquad \text{(II. C-8)}$$

where S is the entropy.

The final form of the difference equation, as well as a summary of its derivation, is given in Appendix A. Full details, including the extension to more than two independent variables, can be found in Section II. D. Briefly, the method is modelled after the one proposed by Courant, Isaacson, and Rees (II. C-21), but falls more into the format discussed by Anucina (II. C-22), and Lees (II. C-23). Essentially, the equations are reduced locally (that is, by a linear transformation) to diagonal form, the resulting equations are differenced according to the sign of the characteristics, and these difference equations are transformed back. For the case of two independent variables convergence has been established for a well-posed initial value problem, even in the nonlinear case (Section II. D).

Note that the differential equations were left in dimensional forms. Several aspects of the scaling possibilities are discussed in Appendix B.

II.C.3 THE PHYSICAL PROBLEM AND POSSIBLE STEADY-STATE SOLUTIONS

We will study three physical problems. These are (a) a planar piston moving into a stationary gas, (b) mass injection into a stationary gas, and (c) a spherically-symmetric explosion.

II.C.3.1 PLANAR PISTON

In this piston problem, it is assumed that at time = 0 the piston and gas are stationary and that the initial density and temperature are everywhere constant ($\rho = \rho_0$ and $T = T_0$). The piston is then accelerated continuously up to some terminal velocity. Since the piston is planar, Eqs. (II. C-1) to (II. C-4) are utilized, except that an additional simple transformation is imposed:

$$\eta = \frac{X - X_P(t)}{X_1} \quad , \qquad \text{(II. C-9)}$$

where $X_P(t)$ denotes the location of the piston and X_1 is some arbitrarily chosen length. The region of computation is $0 \leq \eta \leq 1$ or $X_P \leq X \leq X_P + X_1$. This then is a moving coordinate system with all points moving with the same velocity as the piston.

In this moving coordinate system, the three characteristics are defined by

$$\frac{dt}{d\eta} = - \frac{1}{\lambda_i} \quad , \qquad \text{(II. C-10)}$$

$$\begin{aligned} \lambda_1 &= -(V - V_P) \, , \\ \lambda_2 &= -(V - V_P) + c_s \, , \\ \lambda_3 &= -(V - V_P) - c_s \, , \end{aligned} \qquad \text{(II. C-11)}$$

where V_P is the piston velocity = dX_P/dt and c_s is the local speed of sound.

At the piston surface, we impose the non-slip condition that $V = V_P$. Thus at the piston the characteristics given by λ_1 and λ_2 do not enter the region of computation (at this point $\eta = 0$ and $dt/d\eta$ is not negative) while the third characteristic enters. This means that only one boundary condition is needed at the piston (namely $V = V_P$), while the characteristic equations corresponding to λ_1 and λ_2 are used to determine T and ρ (II. C-24, 25). It is important to note that the equation corresponding to λ_1 is equivalent to $dS/dt = 0$, where S is entropy.

At $X = X_P + X_1$ the far boundary which is taken within the stationary gas, we impose the condition that $V = 0$. This implies that X_1 is taken so large that in the time of interest no effect reaches the point $X = X_P + X_1$. Although in this case nothing significant occurs at the far boundary, the precise general boundary conditions are given as follows. If $V_P \leq c_s$, the characteristics corresponding to λ_1 and λ_2 enter the region, while the characteristic corresponding to λ_3 does not enter. Consequently, one further boundary condition is needed, say $T = T_o$. If $V_P > c_s$, boundary conditions are specified for all variables.

II.C.3.2 MASS INJECTION

In the mass injection problem, mass is injected from a wall into a stationary gas. The time histories of ρ and V at the wall are specified as a function of time. That is, we are given

$$\rho\,(t,0) = f_1(t),$$
$$V\,(t,0) = f_2(t). \qquad \text{(II.C-12)}$$

At time zero, it is assumed that the flow is uniform and stationary:

$$V \equiv 0,\ \rho \equiv \rho_o,\ T \equiv T_o. \qquad \text{(II.C-13)}$$

This again is a cartesian problem and Eqs. (II.C-1) to (II.C-4) are utilized. The λ_i are

$$\lambda_1 = -V,\ \lambda_2 = -V + c_s,\ \lambda_3 = -V - c_s, \qquad \text{(II.C-14)}$$

where, as before, the characteristics are given by $dt/dX = -1/\lambda_i$. The wall is denoted as $X = 0$, and the region of computation is $0 \leq X \leq X_1$, where X_1 is chosen so large that no effect reaches that point during the time period of computation.

The boundary conditions at $X = 0$ depend on the sign of $(V-c_s)$ at $X = 0$. Suppose first that the flow is subsonic, that is $V_i < c_s$, where $V_i = V\,(t, 0)$ is the velocity of the injected gas. In this case, the characteristics corresponding to λ_1 and λ_3 enter the region, while the one corresponding to λ_2 leaves. Thus, the characteristic equation corresponding to λ_2 can be used to calculate T at the wall. If, as in our case, the flow becomes supersonic, that is $V > c_s$, λ_2 goes through zero and becomes negative, and then none of the characteristic equations can be used; consequently, an additional boundary condition is required for T. In order to maintain continuity of T, we simply chose to use for the additional boundary condition the equation that results when λ_2 is set equal to zero in the second characteristic equation.

At the downstream point, $X = X_1$, boundary conditions are specified as in the piston problem.

It is important to note that $\partial S/\partial t$ is not zero at $X = 0$, and consequently the gas is injected with an entropy which differs from the stationary fluid.

II.C.3.3 SPHERICALLY-SYMMETRIC EXPLOSION

In the spherically-symmetric explosion problem, Eqs. (II.C-4) to (II.C-7) are used. In this problem, a sphere of high pressure gas is surrounded by a region of low pressure gas. At time zero the envelope containing the high pressure gas ruptures. In order to have a continuous problem we impose the following initial conditions at $t = 0$.

$$\rho(0,r) = \rho_0 = \text{constant},$$
$$V(0,r) = 0. \tag{II.C-15}$$

$$T(0,r) = \begin{cases} T_1: \ 0 \le r \le r_1 \\ T_1 + \left(\dfrac{r - r_1}{r_2 - r_1} \right) (T_o - T_1): \ r_1 \le r \le r_2 \\ T_o: \ r_2 \le r \le \infty \end{cases} \tag{II.C-16}$$

This simply connects the high temperature and the low temperature regions with a linear variation in temperature.

The λ_1 have the following form:

$$\lambda_1 = -V, \ \lambda_2 = -V + c_s, \ \lambda_3 = -V - c_s \ . \tag{II.C-17}$$

The region of computation is $0 \le r \le R_1$ where, as before, R_1 is chosen so large that nothing occurs there during the time period of interest.

At $r = 0$ due to spherical symmetry, the velocity at the center is $V = 0$. This means that the characteristics corresponding to λ_1 and λ_2 do not enter the region, while the one corresponding to λ_3 does enter the region, and the characteristic equations corresponding to λ_1 and λ_2 can be used to calculate T and ρ. It should be noted that the characteristic equation corresponding to λ_1 is equivalent to $\partial S/\partial t = 0$.

At $r = R_1$, precise boundary conditions are specified as in the previous cases, although nothing occurs at this point during the time period of computation.

An important aspect of this problem is that the flow is non-isentropic at $t = 0$.

II.C.3.4 POSSIBLE STEADY-STATE SOLUTIONS

Let us now discuss the possible steady-state configurations that can be obtained in the cartesian case, that is, with Eqs. (II.C-1) to (II.C-4). First, perform the transformation

$$\xi = X - X_s \quad , \tag{II.C-18}$$

where

$$X_s = X_s(t),$$

and define a new relative velocity

$$W = V - \frac{dX_s}{dt} \quad . \tag{II.C-19}$$

Then, after eliminating P by the equation of state, Eq. (II.C-4), Eqs. (II.C-1) to (II.C-3) become

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= - W \frac{\partial \rho}{\partial \xi} - \rho \frac{\partial W}{\partial \xi} \quad , \\
\rho \left(\frac{\partial W}{\partial t} + \frac{\partial^2 X_s}{\partial t^2} \right) &= - \rho W \frac{\partial W}{\partial \xi} - RT \frac{\partial \rho}{\partial \xi} - R\rho \frac{\partial T}{\partial \xi} \quad , \\
\rho C_v \frac{\partial T}{\partial t} &= - \rho C_v W \frac{\partial T}{\partial \xi} - \rho R T \frac{\partial W}{\partial \xi} \quad .
\end{aligned} \tag{II.C-20}$$

Let us now assume the existence of a steady-state wave having the following properties:

(a) For t large enough, say $t \geq t_o$, $d^2X_s/dt^2 \equiv 0$ or dX_s/dt is the steady wave velocity.

(b) There exists a value of ξ, say $\xi = \xi_o$, such that in some neighborhood of ξ_o,

$$\frac{\partial \rho}{\partial t} \equiv \frac{\partial T}{\partial t} \equiv \frac{\partial V}{\partial t} \equiv 0, \text{ for } t \geq t_o \quad .$$

Define the vector Y and the matrix A as

$$Y = \begin{pmatrix} \frac{\partial \rho}{\partial \xi} \\ \frac{\partial W}{\partial \xi} \\ \frac{\partial T}{\partial \xi} \end{pmatrix} , \qquad A = \begin{pmatrix} W & \rho & 0 \\ RT & \rho W & R\rho \\ 0 & \rho RT & \rho C_v W \end{pmatrix} . \tag{II.C-21}$$

Then Eqs. (II.C-1) to (II.C-4) become

$$A\,Y = 0. \tag{II.C-22}$$

If Y is not the trivial solution, that is $Y \neq 0$, then we must have $|A|$ = determinant A = 0 :

$$|A| = C_v \rho^2 W \left[W^2 - RT \left(1 + \frac{R}{C_v} \right) \right] . \tag{II.C-23}$$

Thus, there are two cases:

Case 1: W = 0.

This implies that $\partial P/\partial \xi \equiv 0$, or $P = P_0$ = constant. Consequently, there can be a steady state stationary fluid having a varying temperature and density.

Case 2:

$$W^2 \equiv RT \left(1 + \frac{R}{C_v} \right) .$$

This implies that W is identically equal to the local speed of sound. Differentiating,

$$2W \frac{\partial W}{\partial \xi} \equiv R \left(1 + \frac{R}{C_v} \right) \frac{\partial T}{\partial \xi} . \tag{II.C-24}$$

But Eq. (II.C-24) is incompatible with Eq. (II.C-3), except for the trivial solution.

Summarizing, the only possible continuously differentiable steady-state solutions of Eqs. (II.C-1) to (II.C-4) are

(1) V = constant, ρ = constant, T = constant (this is the trivial solution),

(2) $V = dX_s/dt$, P = constant (this gives a varying entropy wave).

It is of interest to contrast this result with the steady, continuously differentiable solutions of the viscous one-dimensional cartesian Navier-Stokes equations. In this case, suppose the steady wave moves at the constant velocity V_W, let the driving velocity (for example, the piston velocity) be V_D, and suppose that sufficiently far downstream the flow is stationary. If we now let the value of W sufficiently far downstream be V_1, then $V_1 = - V_W$. Likewise, the upstream value of W is $V_2 = V_D - V_W$. In addition, we have the well-known Prandtl relationship

$$(c^*)^2 = V_1 V_2. \qquad \text{(II.C-25)}$$

Then, the family of continuously differentiable solutions can be graphed as in Figure II.C-1. Note that in this diagram c* is considered a parameter. As can be seen from the figure, V_2 is always negative, i.e., $V_W > V_D$. Also, these results are independent of the expressions utilized for viscosity and conductivity (varying these expressions can only change the shape of the wave connecting the upstream and downstream points).

Finally, we consider briefly the steady-state configuration in the spherically-symmetric case. Introducing as before $\xi = r - r_s$, $W = V - dr_s/dt$, then the steady-state form of Eqs. (II.C-22) become

$$A\,Y = B, \qquad \text{(II.C-26)}$$

where A and Y are as in Eq. (II.C-21), and

$$B = \begin{pmatrix} -2\rho\alpha \\ 0 \\ -2P\alpha \end{pmatrix}, \quad \alpha = \frac{V}{r} = \frac{W + \dfrac{dr_s}{dt}}{\xi + r_s}$$

If we want α to be independent of t, then V/r = constant. But then, if V is to be bounded, V = 0 or $W = - dr_s/dt$. Thus, the only possible steady-state solution to Eqs. (II.C-4) to (II.C-7) under our requirements is the trivial solution

$$V = 0, \quad P = \text{constant}. \qquad \text{(II.C-27)}$$

In our particular problem, described in Section II.C.3.3, a stationary condition exists at r = 0, that is, $V(t, 0) \equiv 0$. If we assume also that the final value of P obtained is the value ahead of the shock, $P = P_0 = \rho_0 R T_0$, then the final value of ρ and T at the center can be calculated as follows:

$$S(t, r) = C_v \ln\left(\frac{T}{T_0}\right) - R \ln\left(\frac{\rho}{\rho_0}\right), \qquad \text{(II.C-28)}$$

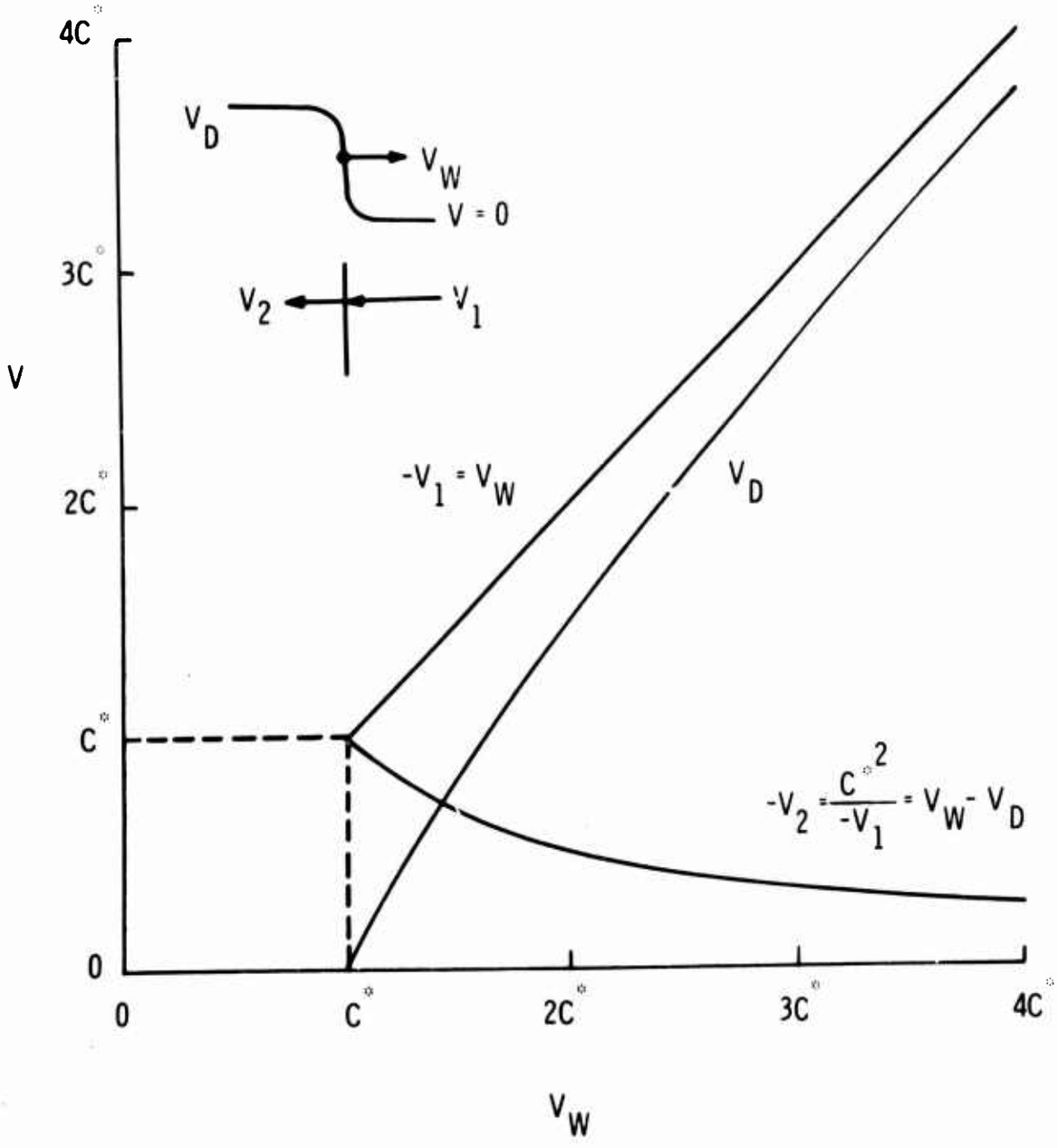


Figure II.C-1. Steady State Shock Velocity Relationships

This follows since C_v and R are constants. Noting also that

$$S(t, r) = S(t, 0) = C_v \ln\left(\frac{T_1}{T_o}\right), \qquad \text{(II.C-29)}$$

we obtain

$$\left[T(t, 0)\right]^{(R + C_v)} = T_1^{C_v} T_o^{R},$$

and

$$\rho(t, 0) = \rho_o T_o / T(t, 0). \qquad \text{(II.C-30)}$$

II.C.4 DISCUSSION OF RESULTS

II.C.4.1 THE PISTON PROBLEM

In Figure II.C-2, we have reproduced an earlier solution[II.C-26] of the complete time-dependent Navier-Stokes equations for the case of a planar piston moving into a stationary gas. One notes that in a relatively short time an apparent steady-state wave structure is achieved in that a steep but continuous gradient of the field variables propagates away from the piston at constant wave velocity. In this earlier work convergence was established by performing a sequence of calculations, each with a suitably reduced mesh size, until agreement to the desired accuracy was achieved. The question we now want to pursue is the following:

> Given any choice of mesh size, are the calculated structure and motion of the shock due to real viscosity and conductivity effects, or has an "artificial viscosity" been introduced by the approximation to the Euler inviscid subsystem of the Navier-Stokes equations?

The most direct test is to run the same or a similar problem without viscosity and thermal conductivity. In addition to setting all terms involving molecular transport coefficients equal to zero, this requires only a change in the boundary conditions at the piston surface. In the viscous case, one must specify a boundary condition for the temperature and one calculates the density at the piston surface, (in the case shown in Figure II.C-2, we chose $\partial T/\partial X=0$). For the inviscid case, one must calculate both the temperature and the density at the piston surface.

For the first test case, the piston was accelerated at a constant rate from rest to a final velocity of 1500 ft/sec., as given by

$$V_P = \begin{cases} \left[0.75 \times 10^{10}\right] t: \quad 0 \le t \le 2 \times 10^{-7} \text{ sec} \\ 1500: \quad t \ge 2 \times 10^{-7} \text{ sec} \end{cases} , \qquad \text{(II.C-31)}$$

which is less than the terminal piston velocity shown in Figure II.C-2, but is in the supersonic regime which suffices for our purposes.

The initial conditions in the stationary gas were taken as

$$\left.\begin{aligned} \rho_o &= 10^{-5} \text{ lb/ft}^3 , \\ T_o &= 400^\circ\text{R}, \end{aligned}\right\} \qquad \text{(II.C-32)}$$

while the mesh size selected for the computation was (see Table II.C-1).

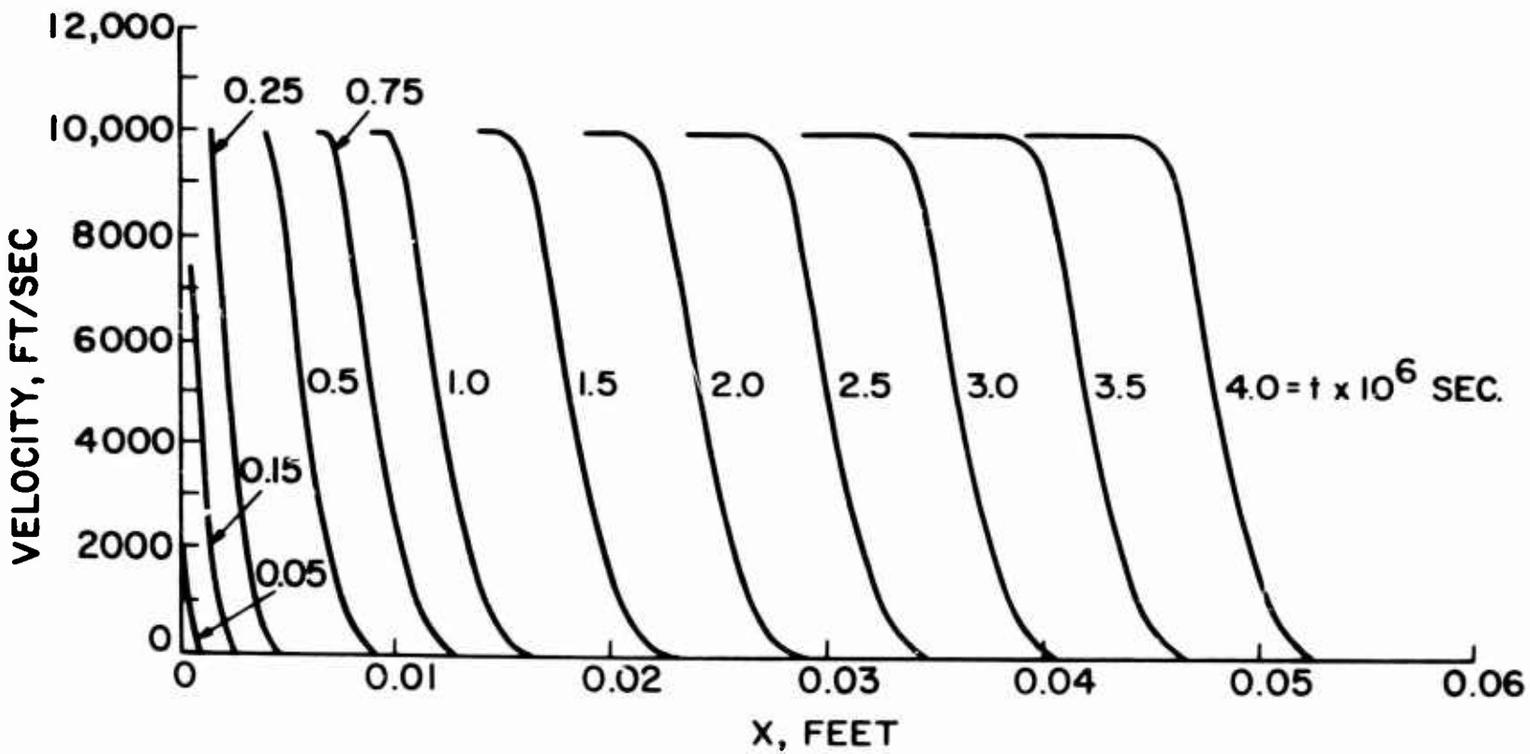


Figure II.C-2. Accelerating Supersonic Piston (Viscous Solution)

TABLE II.C-1. SUMMARY OF INITIAL AND BOUNDARY CONDITIONS

Problem	Initial Conditions (t = o)			Boundary Conditions (η = 0)			Boundary Conditions (η = 1)			Mesh Size	
	V	ρ	T	V	ρ	T	V	ρ	T	Δt	Δx
1) Supersonic piston (viscous; Fig. II-C-2)	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = V_p$	--	$\frac{\partial T}{\partial \eta} = 0$	0	ρ_o	T_o	$2. \times 10^{-8}$	4.166×10^{-4}
2) Supersonic piston (inviscid; Fig. II.C-3, -4, -5	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = V_p$ (Eq. II.C-31)	--	--	0	ρ_o	T_o	2.5×10^{-10}	2.68×10^{-6}
3) Supersonic piston (inviscid; Fig. II.C-6)	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = V_p$ (Eq. II.C-31)	--	--	0	ρ_o	T_o	$5. \times 10^{-10}$	5.36×10^{-6}
4) Subsonic piston (inviscid; Fig. II.C-7)	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = V_p$ (Eq. II.C-34)	--	--	0	ρ_o	T_o	$5. \times 10^{-10}$	$6. \times 10^{-6}$
5) Mass injection (inviscid; Fig. II.C-8, -9, -11)	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = f_1(t)$ (Eq. II.C-38)	$\rho = f_2(t)$ (Eq. II.C-37)	*	0	ρ_o	T_o	5.5×10^{-12}	3.34×10^{-8}
6) Mass injection (inviscid; Fig. II.C-10)	0	$\rho_o = 10^{-5}$	$T_o = 400$	$V = f_1(t)$ (Eq. II.C-38)	$\rho = f_2(t)$ (Eq. II.C-37)	*	0	ρ_o	T_o	2.5×10^{-10}	3.125×10^{-6}
7) Spherically-Symmetric Explosion (inviscid; (Fig. II.C-12,-13,-14)	0	$\rho_o = .0765$	$T = f(r)$ (Eq. II.C-16)	$V = 0$	--	--	0	ρ_o	T_o (Eq. II.C-16)	$1. \times 10^{-12}$	$.855 \times 10^{-6}$

*In this case, no boundary condition is needed when the flow is subsonic. When the flow becomes supersonic, a boundary condition is needed; in order to maintain continuity we chose to maintain the appropriate characteristic variable constant (at the value it had achieved when the flow reached the speed of sound).

$$\Delta X = 2.68 \times 10^{-6} \text{ ft},$$

and

$$\Delta t = 2.5 \times 10^{-10} \text{ sec.}$$

The results for this computation are shown in Figures II.C-3 to II.C-6. In Figure II.C-3, one notes that at later times the velocity curves appear to come to an abrupt end. This does not mean that the velocities were not calculated beyond this point (further to the right), but only that such velocities are so small that they are not visible on the plot. For example, at $t = 2 \times 10^{-7}$ sec, the computed value of the velocity $V = 7.35$ ft/sec, at the nodal point given by $X - X_p = 0.725 \times 10^{-4}$ ft. It is also important to state that the computed velocities on the right continue to decrease smoothly to zero. For example, at $t = 2.5 \times 10^{-7}$ sec this same node has a velocity $V = 0.12$ ft/sec and at $t = 3. \times 10^{-7}$ sec, $V = 9.9 \times 10^{-4}$ ft/sec. The corresponding profiles for temperature and density are shown in Figures II.C-4 and II.C-5.

It is well-known that the true solution to this problem, which is isentropic, does indeed contain a discontinuity(II.C-14). Consequently, it was not surprising to see a discontinuity occur in the numerical solution. However, to see this discontinuity develop in the smooth fashion that was computed here was unexpected. That is, there was a complete absence of the Gibbs' phenomenon which one comes to expect in these situations. For example, the use of artificial viscosity or of the Lax-Wendroff method will often produce bounded oscillations on either side of the discontinuity, with some kind of a connecting ramp.

In this first test problem, the piston was accelerated to supersonic speed corresponding to a Mach number of 1.53. Because of the moving coordinate system, the relative velocity becomes supersonic at the points to the right of the discontinuity, while the relative velocity is subsonic at the points on the left of the discontinuity. The characteristics (Section II.C.3.1) are such that the supersonic points obtain no information about the piston or the discontinuity. Since the difference equation has precisely this behavior also, this accounts for the fact that the downstream points go so smoothly to zero. On the other hand the subsonic points will have both forward and backward characteristics, in particular the point sitting on the piston side of the discontinuity will use information on both sides of the discontinuity. Such a procedure cannot be expected to produce physically meaningful results, and in fact we claim no physical or mathematical significance for the results after the formation of the discontinuity.

It is perhaps worthwhile to make several further comments concerning the meaning of the numerical results after the appearance of a discontinuity. Lax (II.C-17) has noted that such problems may have a variety of "weak" solutions. This means that mathematically it is necessary to impose further conditions in order to provide uniqueness in the presence of a discontinuity. For example, one can impose the Rankine-Hugoniot conditions (some such techniques have been referred to as "shock fitting", Moretti (II.C-27) seems to use this approach), or one can utilize an artificial viscosity technique which is intended, in fact, to automatically satisfy the Rankine-Hugoniot conditions. Lax(II.C-17) also notes that the form of a weak solution may depend on the form of the

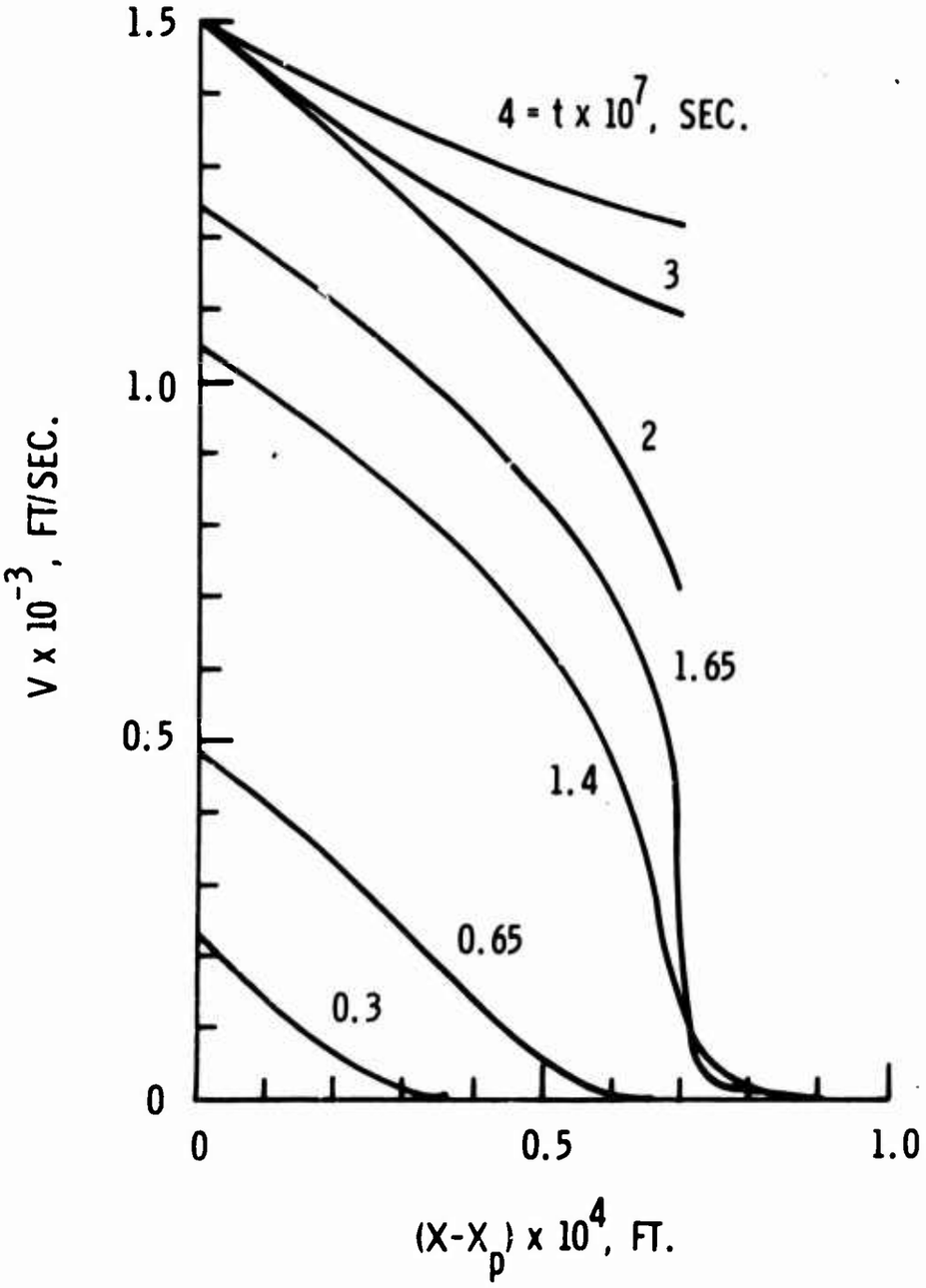


Figure II.C-3. Accelerating Supersonic Piston, Velocity Profiles

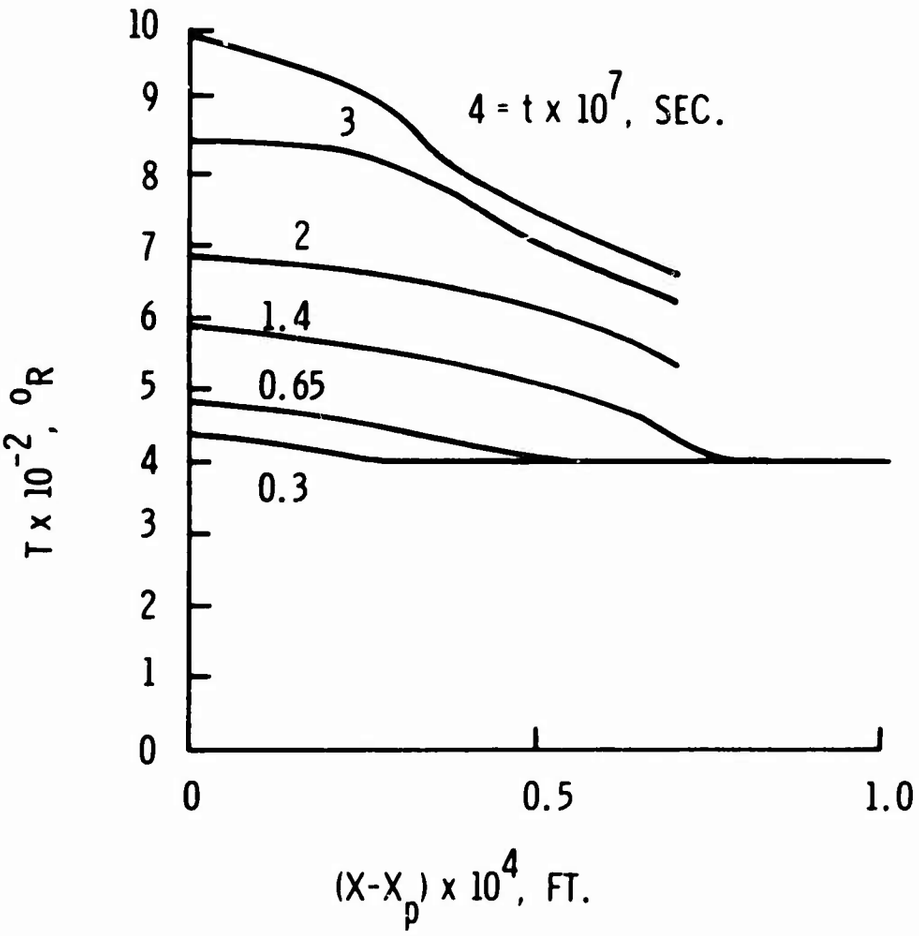


Figure II.C-4. Accelerating Supersonic Piston, Temperature Profiles

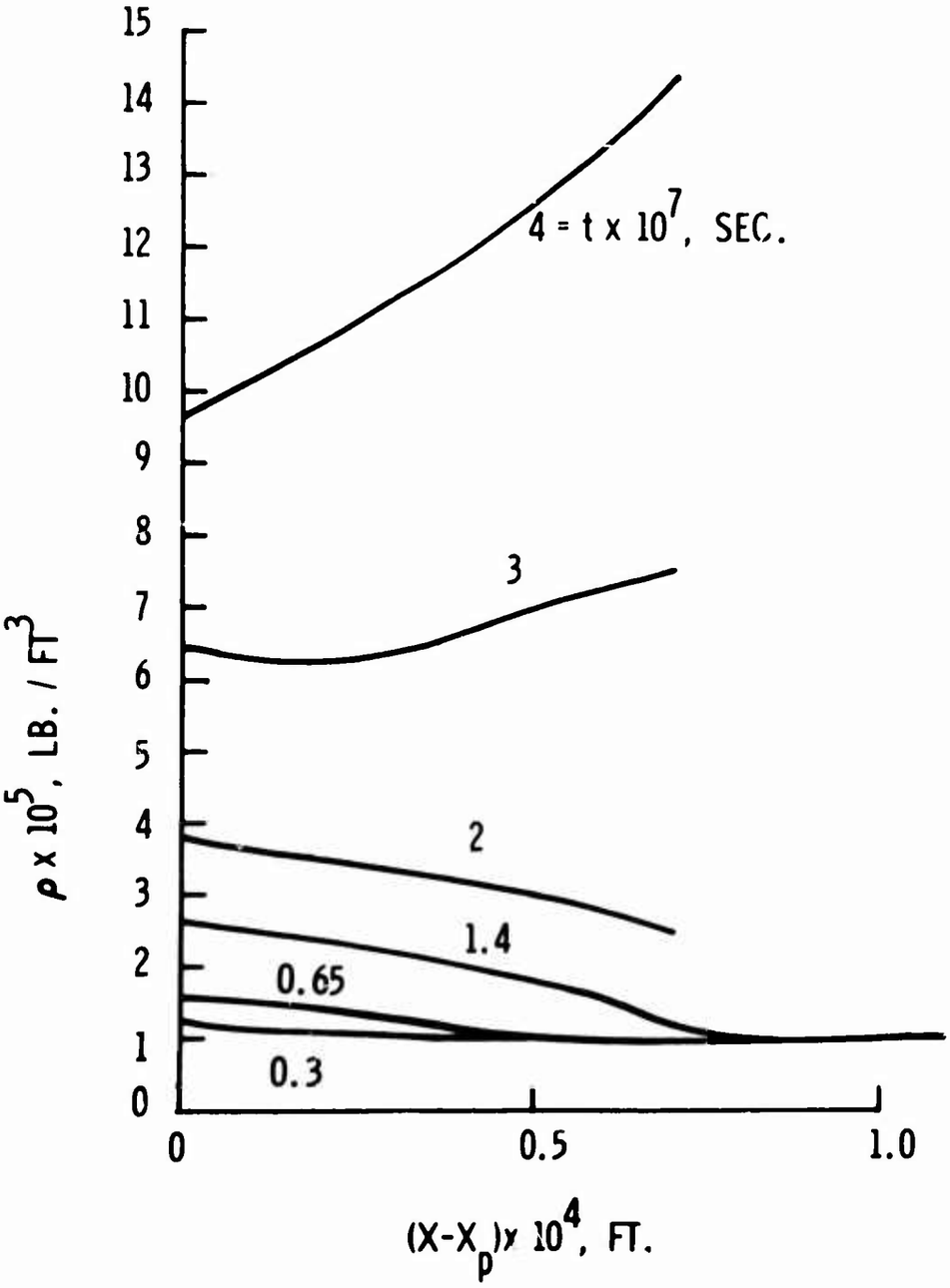


Figure II.C-5. Accelerating Supersonic Piston, Density Profile

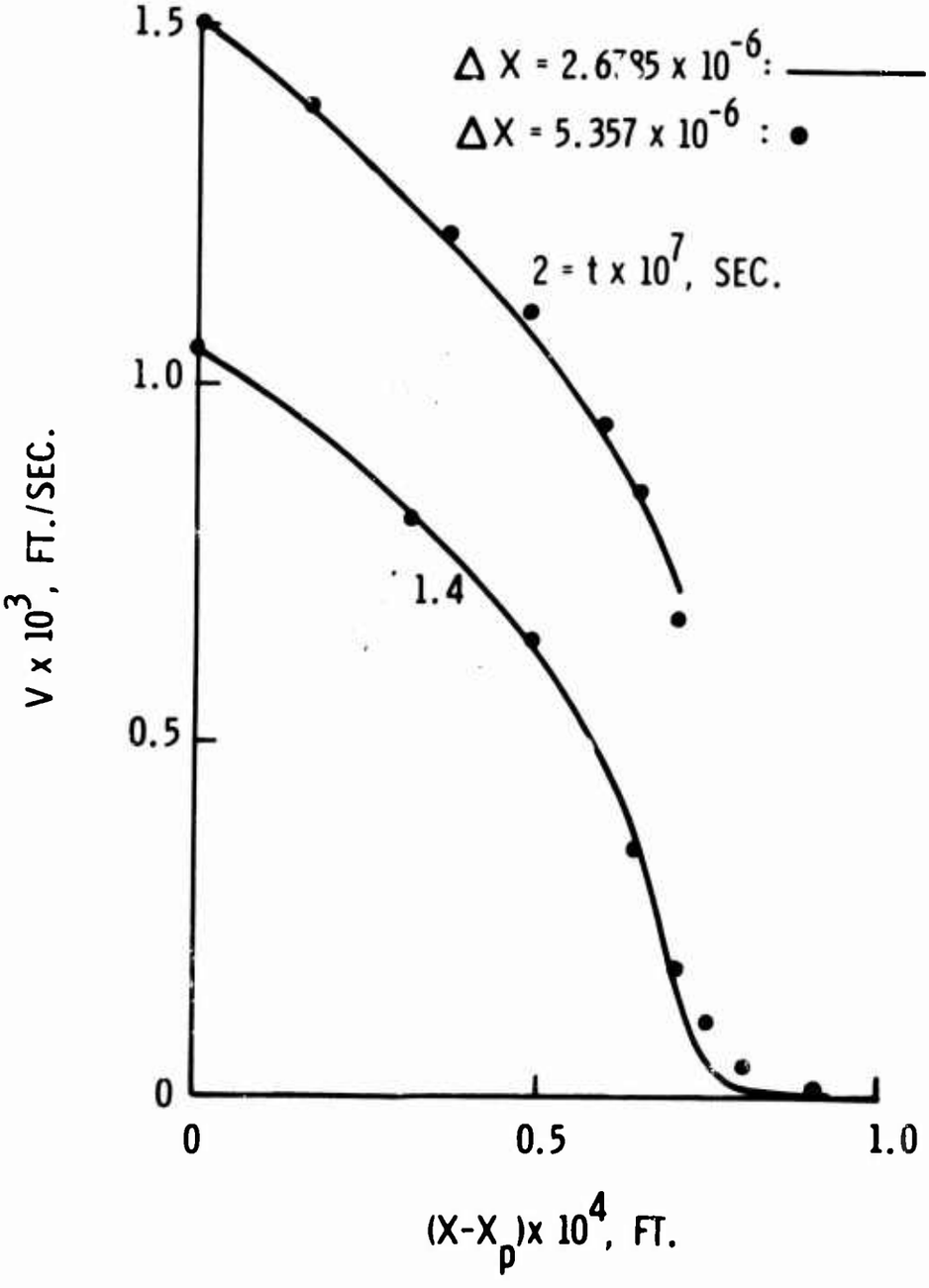


Figure II.C-6. Accelerating Supersonic Piston, Velocity Profile for Several Mesh Sizes

differential equations. Our results can also be interpreted from his point of view. For example, we have already noted that since the points to the right of the discontinuity are moving supersonically there is no way for them to obtain information about the shock. Consequently, the shock can never move any further away from the piston. Suppose, however, that we slow the downstream points to a velocity that is supersonic (greater than 998 ft/sec) but less than the piston velocity. These points can again obtain no information about the discontinuity. Thus, the result here is that the piston would eventually wipe out everything. The point to be made is that when the calculation is carried on beyond that time, when a discontinuity is formed, it is only for the purpose of obtaining information concerning the behavior of the numerical scheme and does not necessarily yield physically meaningful results.

This same problem was run with various mesh sizes. In all cases the discontinuity occurred initially at the same distance from the piston and at the same point in time, and always had a width of one node. One such comparison of the effect of mesh size is shown in Figure II.C-6, where the initial ΔX was doubled to 5.357×10^{-6} ft and $\Delta t = 5. \times 10^{-10}$ sec. It should also be noted that prior to the formation of the discontinuity, (i.e., when a unique, continuously differentiable solution is expected) our numerical results do indicate convergence.

Finally, a subsonic problem was run. In this case, it is convenient to modify the space transformation as follows

$$\eta = \frac{X - X_P(t)}{X_1(t)}, \quad 0 \le \eta \le 1 \text{ or } X_P \le X \le X_P + X_1, \qquad \text{(II.C-33)}$$

where X_1 is now allowed to vary with time also. The following velocity distributions were chosen:

$$V_P = \begin{cases} \left[3.75 \times 10^{9}\right] t: \ 0 \le t \le 2 \times 10^{-7} \text{ sec} \\ 7.50 \times 10^{2}: \ t \ge 2 \times 10^{-7} \text{ sec} \end{cases}, \qquad \text{(II.C-34)}$$

and

$$\frac{dX_1}{dt} = \begin{cases} \left[3.75 \times 10^{9}\right] t: \ 0 \le t \le 2 \times 10^{-7} \text{ sec} \\ \left[9 \times 10^{9}\right] t: \ 2 \times 10^{-7} \le t \le 2.5 \times 10^{-7} \text{ sec} \\ 1.2 \times 10^{3}: \ t \ge 2.5 \times 10^{-7} \text{ sec} \end{cases}. \qquad \text{(II.C-35)}$$

Since the piston velocity is subsonic, the wave that forms, which travels at sonic speed, must now run away from the piston; therefore, dX_1/dt was eventually taken to be greater than V_p.

The velocity distribution for this case is shown in Figure II. C-7. The maximum value of the Mach number at the piston occurs at $t = 2 \times 10^{-7}$ sec when its value is 0.15. At $t = 3.6 \times 10^{-7}$ sec, the discontinuity, which again is predicted theoretically(II. C-14), has clearly formed at $X - X_p = 1.79 \times 10^{-4}$ ft, or at $X = 3.65 \times 10^{-4}$ ft; and this distance (to within the accuracy of the computation, $\Delta X = 6 \times 10^{-6}$) is the distance traveled by a point starting at the piston surface at $t = 0$ and moving at the upstream speed of sound (998 ft/sec). At later times, when the numerical discontinuity is well-formed, the discontinuity continues to move at the speed of sound and does not become supersonic.

Note, that it may readily be calculated, using the method of characteristics, that the mathematical discontinuity should form much earlier, at approximately $t = 2. \times 10^{-7}$ sec and $X - X_p = 1.25 \times 10^{-4}$ ft. Although not evident in the data of Figure II. C-7, the formation of this discontinuity is indeed observed to occur at this point in time and space when one compares a sequence of computer runs (with suitably decreasing mesh sizes). This aspect of the numerical problem is discussed in more detail below (the mass-injection problem).

It should be emphasized again that no physical or mathematical significance is to be attached to these results after the formation of a discontinuity. The calculations are continued past this time only to aid in understanding the behavior of the difference equations. From these results the following assessment can be made:

(1) The difference equations that have been used (Section II. C. 2) do not exhibit, at least for this class of piston problems, an artificial viscosity, for if there were such an effect the waves must eventually move supersonically away from the piston. Figure II. C-1 demonstrates that when viscosity and thermal conductivity are present the steady-state wave motion is supersonic and is greater than the driving velocity.

(2) The discontinuity that exists in these problems is exhibited by the numerical results, without any instabilities or oscillations on either side of the discontinuity for both subsonic and supersonic piston motion.

(3) The shock speed and shock structure shown in Figure II. C-2 are indeed due entirely to the real effects of viscosity and conductivity, and not to an artificial viscosity related to the finite difference equations we have used to represent the inviscid subsystem in Ref. II. C-26, which are precisely the same as those studied herein.

II. C. 4. 2 THE MASS-INJECTION PROBLEM

The initial conditions for this case were chosen as follows (Section II. C. 3. 3):

$$T_o = 400°F,\ \rho_o = 10^{-5}\ \text{lb/ft}^3,\ V \equiv 0. \qquad \text{(II. C-36)}$$

The boundary conditions at $X = 0$ were taken as follows:

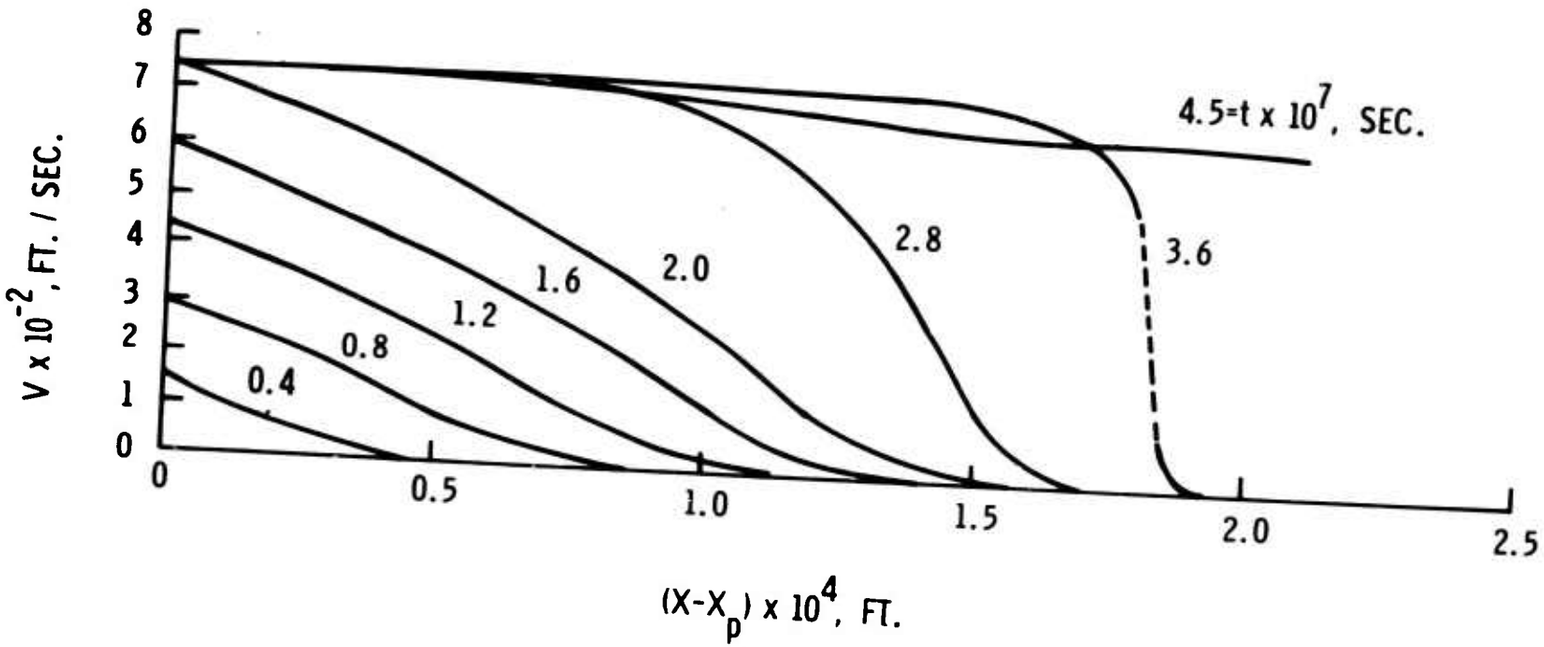


Figure II.C-7. Accelerating Subsonic Piston, Velocity Profiles

$$\rho(t,0) = \begin{cases} 10^{-5} + 10^{4}\ t:\ 0 \le t \le 5 \times 10^{-9}\ \text{sec.} \\ 6 \times 10^{-5}:\ t \ge 5 \times 10^{-9}\ \text{sec} \end{cases}, \qquad \text{(II. C-37)}$$

$$V(t,0) = \begin{cases} 4 \times 10^{11}\ t:\ 0 \le t \le 5 \times 10^{-9}\ \text{sec} \\ 2 \times 10^{3}:\ t \ge 5 \times 10^{-9}\ \text{sec.} \end{cases} . \qquad \text{(II. C-38)}$$

At time zero, the entropy is taken as constant everywhere S_0. However, because of the boundary conditions, an entropy distribution is introduced at the wall, as a variable entropy fluid is injected. When the Euler equations are utilized, the equation governing the entropy takes the form $dS/dt = 0$. Hence, the variable entropy distribution which tags the injected gas particles must remain permanently in this problem. The results of this set of computations are shown in Figures II. C-8 to II. C-11.

Figure II. C-8 displays the entropy distribution, first at the wall as a function of time, and then for several early times as a function of distance. In this calculation the mesh size utilized was $\Delta X = 3.344 \times 10^{-8}$ ft, and $\Delta t = 5.5 \times 10^{-12}$ sec. The velocity profile for a much longer time history is shown in Figure II. C-9. (Here the mesh size utilized was coarser, namely $\Delta X = 3.125 \times 10^{-6}$ ft and $\Delta t = 2.5 \times 10^{-10}$ sec) One notes that an apparent continuous steady-state solution exists. Yet from our discussion in Section II. C. 3. 4 we know that a continuous steady-state solution is not possible; the wave must become discontinuous or flatten out. Further computations were made with decreasing mesh sizes, and some of these results are shown in Figure II. C-10. If one estimates the steepness of the discontinuity by calculating dV/dX near the midpoint of the velocity curve, say V = 1,000 ft/sec one obtains

$$\Delta X = \delta:\ \frac{\partial V}{\partial X} = -\frac{900}{\delta} ,$$

$$\Delta X = \frac{\delta}{2}:\ \frac{\partial V}{\partial X} = -\frac{1800}{\delta} ,$$

$$\Delta X = \frac{\delta}{4}:\ \frac{\partial V}{\partial X} = -\frac{3600}{\delta} .$$

(These values are actually more easily obtained from the computer print out rather than the plotted values.) In any case, it becomes clear that we are calculating a discontinuity, for the steepness of the shock is inversely proportional to the node size, and in the limit of $\Delta X = 0$ will presumably have zero thickness.

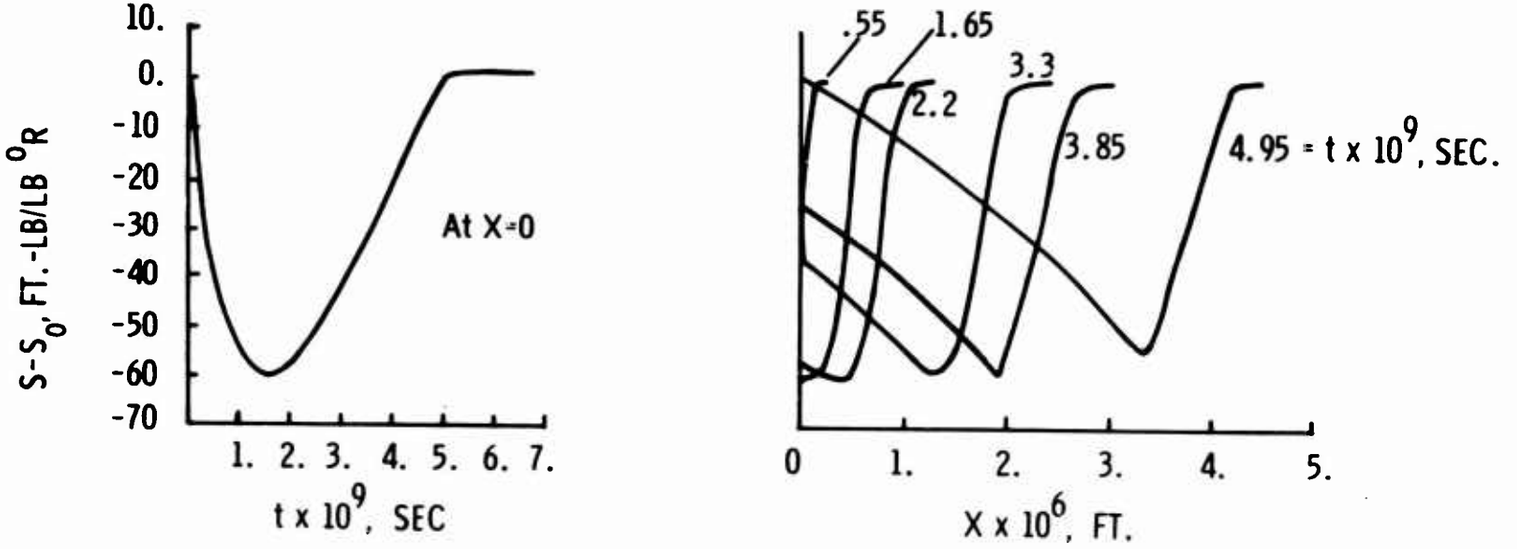


Figure II.C-8. Mass Injection, Entropy Profiles

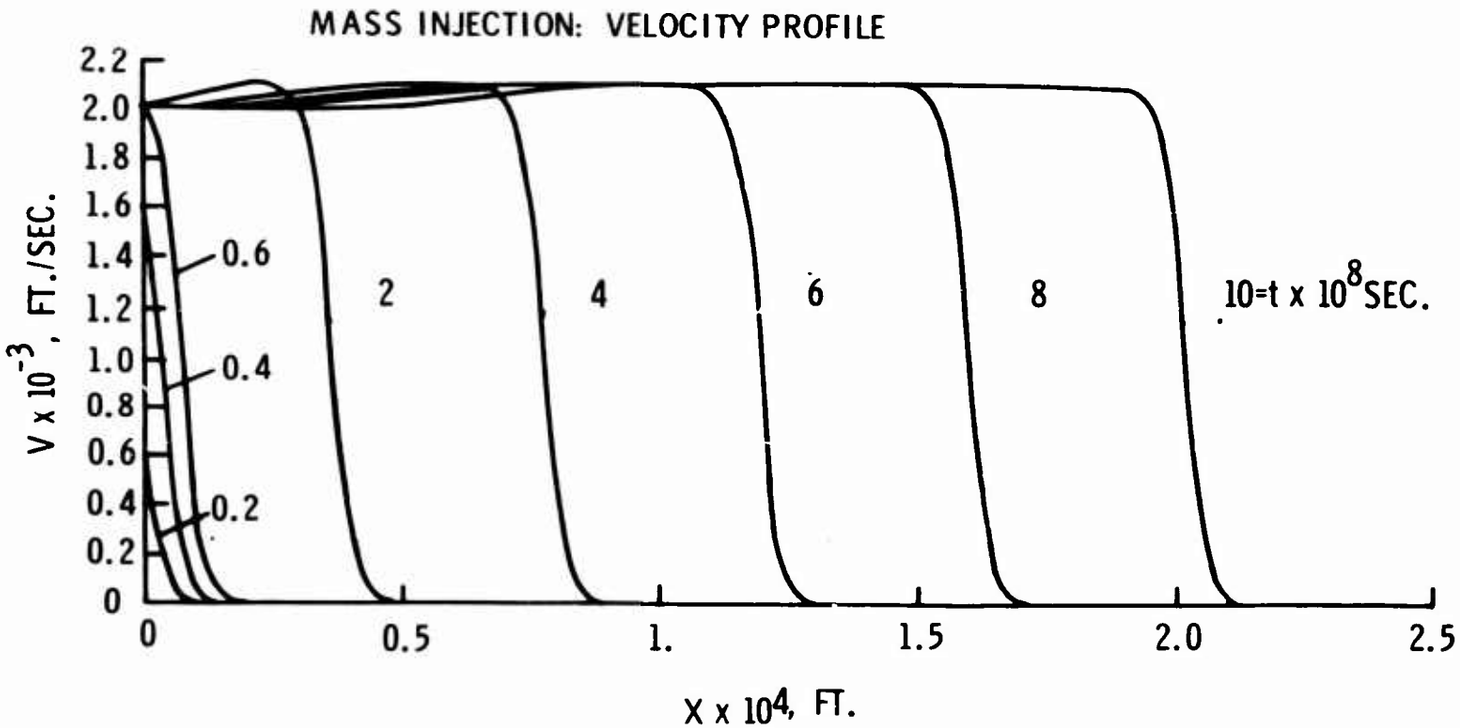


Figure II.C-9. Mass Injection, Velocity Profiles

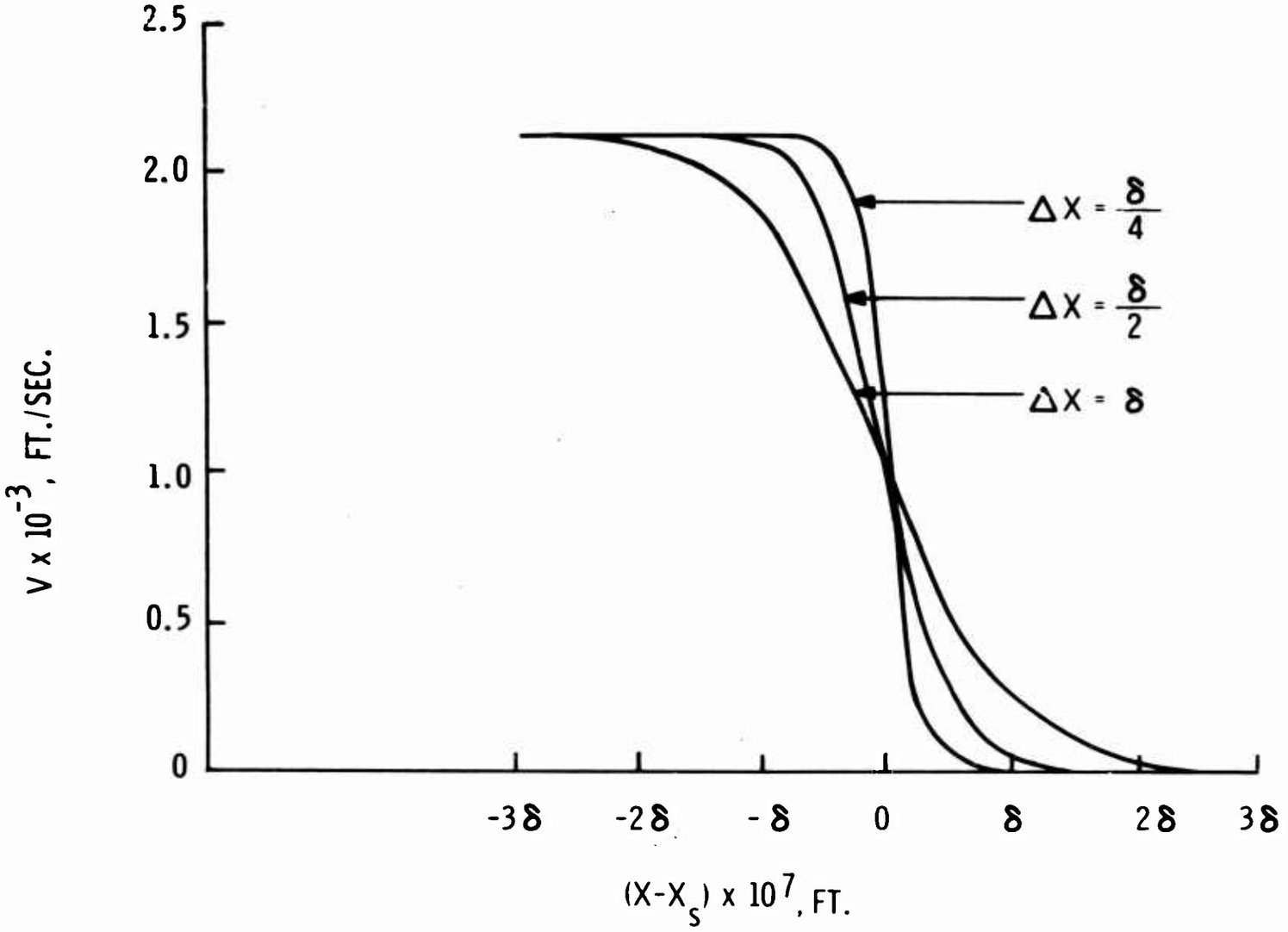


Figure II.C-10. Mass Injection, Shock Thickness Versus Mesh Size

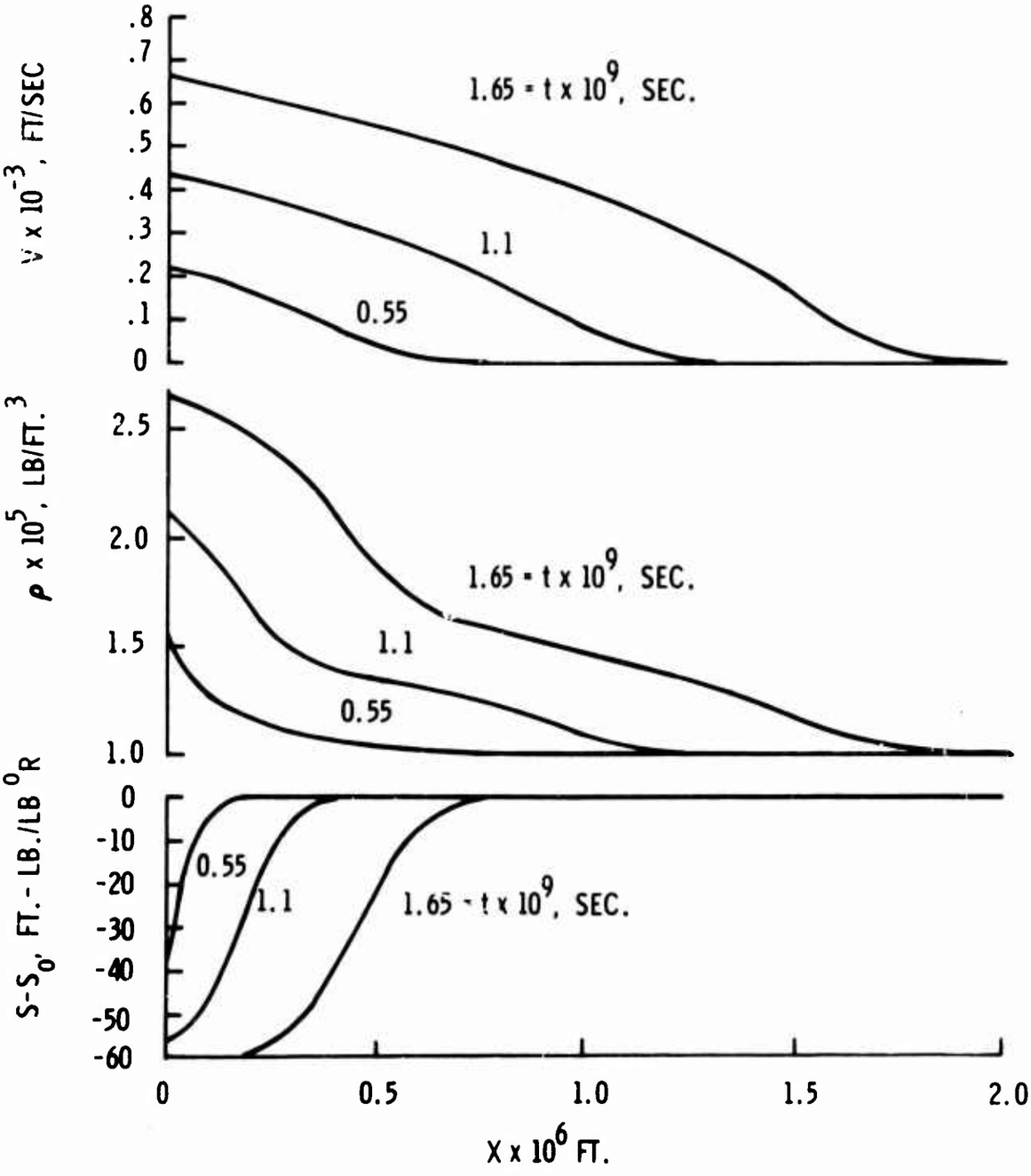


Figure II.C-11. Mass Injection; Velocity, Density and Entropy Waves

Two questions now arise: (1) Is the discontinuity a true occurrence in the mathematical problem, and (2) Is the "smoothing" that has occurred over the discontinuity an artificial viscosity effect?

The shock velocity was calculated from the data of Figure II.C-9 and is approximately 2,000 ft/sec. Calculations with smaller mesh sizes indicate this same result. Thus, since the wave is moving at the speed of the driving (gas-injection) velocity, we conclude from Figure II.C-1 again that this smoothing effect, introduced by the difference equations, does not behave as an artificial viscosity.

It is perhaps of interest to discuss briefly why the difference equations exhibited more smoothing in the mass injection problem than in the piston problem. One could resort to the second order truncation error terms (II.C-20) in an attempt to exhibit a "viscous" smoothing. However, because these truncation error terms exist in both problems and because of the shock velocity result just discussed, this would not seem to be a reasonable explanation. More insight can be obtained by looking at the characteristics of the two problems. As noted in the discussion of the piston results, the upstream points are supersonic and can receive no information about the advancing discontinuity. However, the downstream points are subsonic, so the point next to the discontinuity receives upstream information. In the mass-injection problem this situation is exactly reversed, the upstream points are subsonic while the downstream points are supersonic. The greater smoothing in the mass-injection case would simply indicate, then, that the numerical effect of downstream points on upstream points (mass injection) is much greater than the effect of upstream points on the downstream points (piston problem).

Let us now discuss the question of the discontinuity. If the entropy were not variable, there would obviously need to be a discontinuity, since the traveling wave front would simulate a piston. In Figure II.C-11 we have plotted entropy, density, and velocity for several early times where the problem is clearly still continuous (all data shown here are reproduced to within one percent when the mesh size is halved). The important point is that the density and velocity waves outdistance the entropy wave. This follows because the wave motion propagates at the speed of sound (in our case the downstream speed of sound is 998 ft/sec), while (since $dS/dt = 0$) entropy is transported at the gas particle velocity. In a short time, then, the advancing wave front outdistances the region of variable entropy and the flow then simulates a piston moving into a constant entropy fluid. Accordingly, a discontinuity must form.

It should be emphasized again that no physical or mathematical significance is to be attached to the numerical results computed after the formation of the discontinuity. For example, the propagation velocity of the discontinuity is indeterminate. To see this, suppose that we had chosen a moving coordinate system with the property that the wall (where $X = 0$) was stationary, while the last point in the computation moved at a speed of 1,000 ft/sec (slightly above the speed of sound). Then mathematically, this last point could never receive any information from the downstream points. This would be reflected in our numerical results, also; consequently, the calculated shock speed would not have been greater than 998 ft/sec.

The results of this computation that we want to emphasize are the following:

1. The solution remains continuous in the region of varying entropy.

2. A discontinuity forms, as it should, in a region of constant entropy. The difference equations produce this discontinuity without any indication of instabilities or oscillations.

3. There is no evidence of an artificial viscosity effect, for even though the calculations is continued long after the formation of the discontinuity, the velocity of this discontinuity never achieves a speed greater than the driving velocity (see Figure II.C-1).

II.C.4.3 SPHERICALLY-SYMMETRIC EXPLOSION

As a final case, we considered the problem of a spherically-symmetric explosion. The following initial conditions were chosen (Section II.C.3.2):

$$\rho_0 = .0755 \text{ lb/ft}^3, T_0 = 518^\circ R, T_1 = 2.5 \times 10^7 {}^\circ R,$$

$$r_1 = 7.36 \times 10^{-5} \text{ ft}, r_2 = 1.26 \times 10^{-4} \text{ft}.$$

We also took as our computation mesh $\Delta r = .855 \times 10^{-6}$ ft and $\Delta t = 1 \times 10^{-12}$ sec.

This problem has a variable entropy, but unlike the mass-injection problem, this non-constant entropy distribution exists in the fluid at $t = 0$, and remains unchanged at the boundaries of the computational region for all time.

Figure II.C-12 shows the entropy distribution for several points in time. Although the entropy wave steepens with time, it remains continuous. The slight dip in the curve is due to the inward motion of the inner wave (which remains continuous for some time), which has been reflected from the outer, outwardly-propagating discontinuity. Figure II.C-13 shows the formation of the two discontinuities that appear, the outer one progresses to the right, while the inner one (visible at $t = 7.2 \times 10^{-10}$ sec) moves to the left. Figure II.C-14 shows the corresponding velocity profiles.

As in the mass injection problem, repeating the calculation with a finer mesh reveals that these two steep waves are indeed numerical discontinuities (the width of the region of discontinuity is proportional to the computational mesh Δr). It is also of interest to note that both these discontinuities form in a region of constant entropy. The outer discontinuity forms almost immediately after the wave reaches the region of constant entropy. The inner discontinuity, which is a result of a wave reflection from the outer discontinuity, moves back through the region of varying entropy quite smoothly; the discontinuity appearing only after the wave reaches the inside plateau of constant entropy. To summarize, since it is known that discontinuities must be

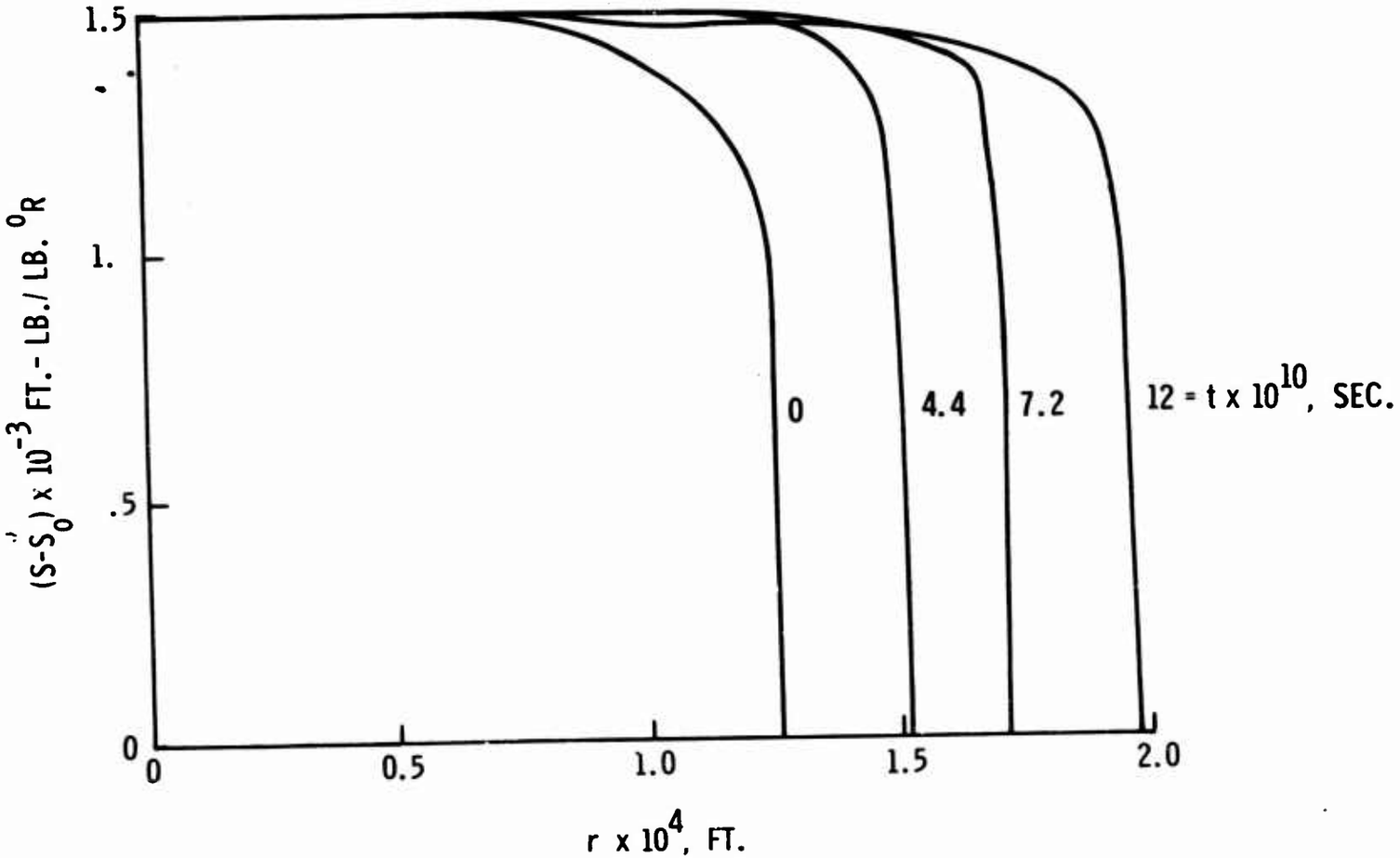


Figure II.C-12. Spherically-Symmetric Explosion, Entropy Profiles

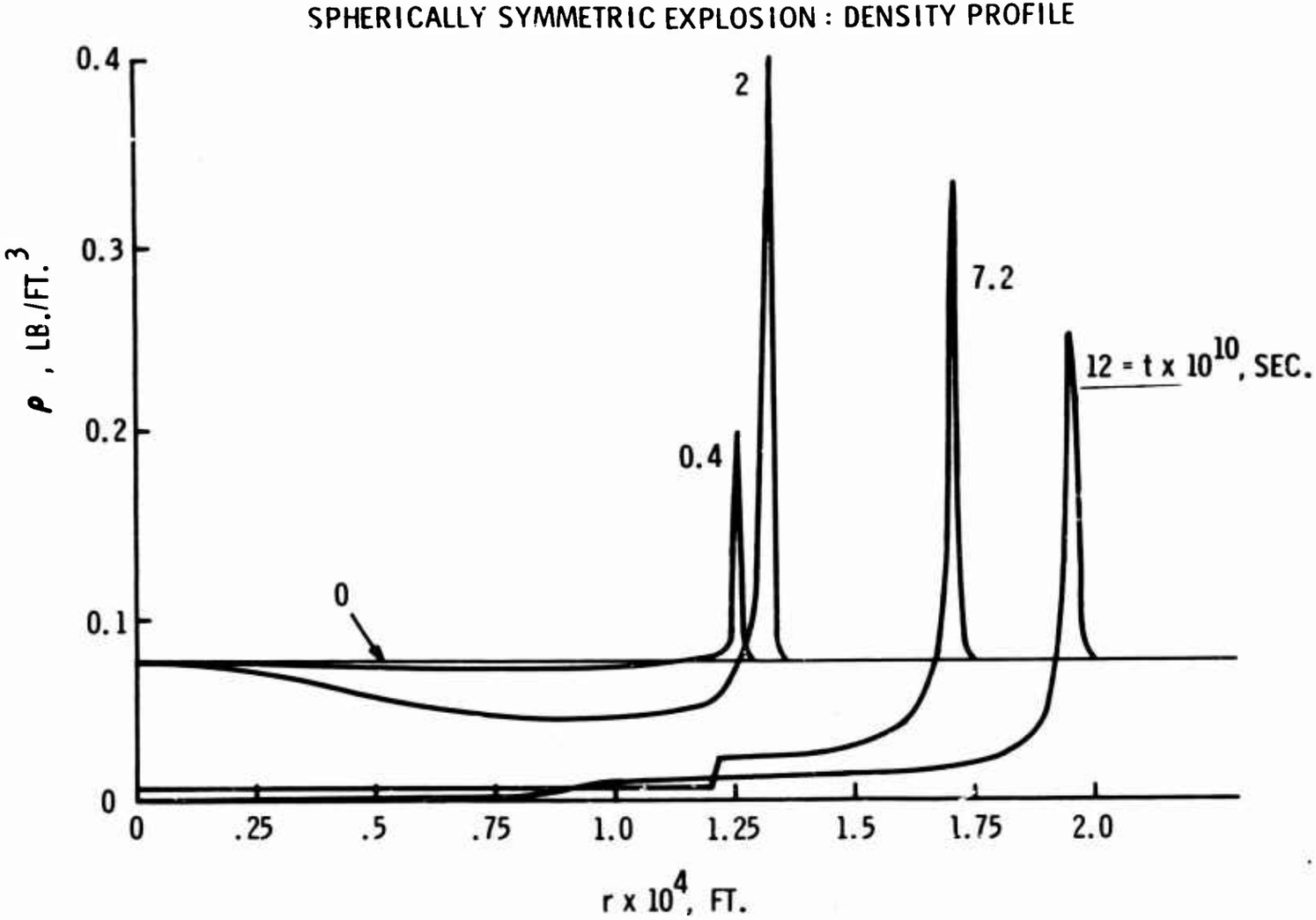


Figure II C-13 Spherically-Symmetric Explosion, Density Profiles

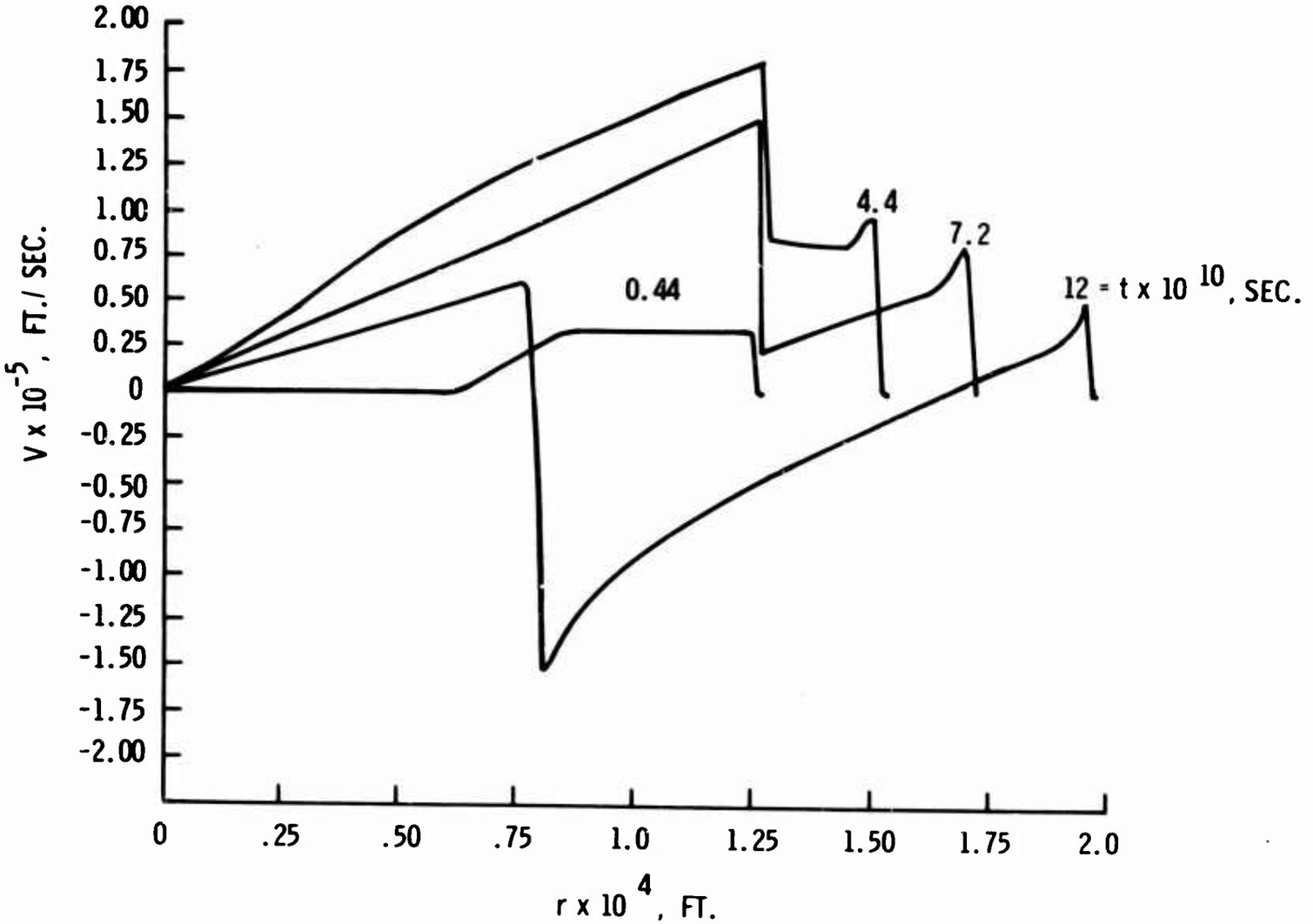


Figure II.C-14. Spherically-Symmetric Explosion, Velocity Profiles

produced by isentropic compression waves, it is not surprising that the two discontinuities are produced in the regions of constant entropy in this problem.

Finally, let us discuss the propagation velocities of the two discontinuities as indicated by the calculated results. The situation is not now nearly as clear-cut as in the previous two problems that have been discussed, for in both those problems (the accelerating piston and mass injection) a steady-state situation was quite evident; consequently, the information in Figure II.C-1 was applicable. However, in this spherically-symmetric explosion, no steady-state plateau is evident on the driving side of the discontinuity, nor are we close to satisfying the steady-state values discussed in Section II.C.3.4. Nevertheless, it is interesting to examine the behavior of the outer discontinuity. Accordingly, in Figure II.C-15 we have displayed as a function of time the position of the discontinuity, the velocity of the discontinuity, and the "driving velocity". Here, we have defined the driving velocity as the maximum velocity behind the discontinuity. The velocity of the discontinuity was calculated by differentiating the curve giving the position of the discontinuity. The interesting fact is that the driving velocity always remains greater than the velocity of the discontinuity, which would not be the expected result if an artificial viscosity effect were present. The same result holds true also for the inner discontinuity. Let us emphasize again that these numerical calculations have been continued in time beyond the formation of a discontinuity, therefore no physical or mathematical significance can be attached to the results.

The results of the spherically-symmetric explosion problem that we want to emphasize are the same as those for the mass-injection problem:

(1) The solution remains continuous in the region of varying entropy.

(2) The difference equations predict accurately the location of discontinuites, as well as the time of their occurrence, without any evidence of numerical instabilities or oscillations.

(3) There is no evidence of an artificial viscosity effect.

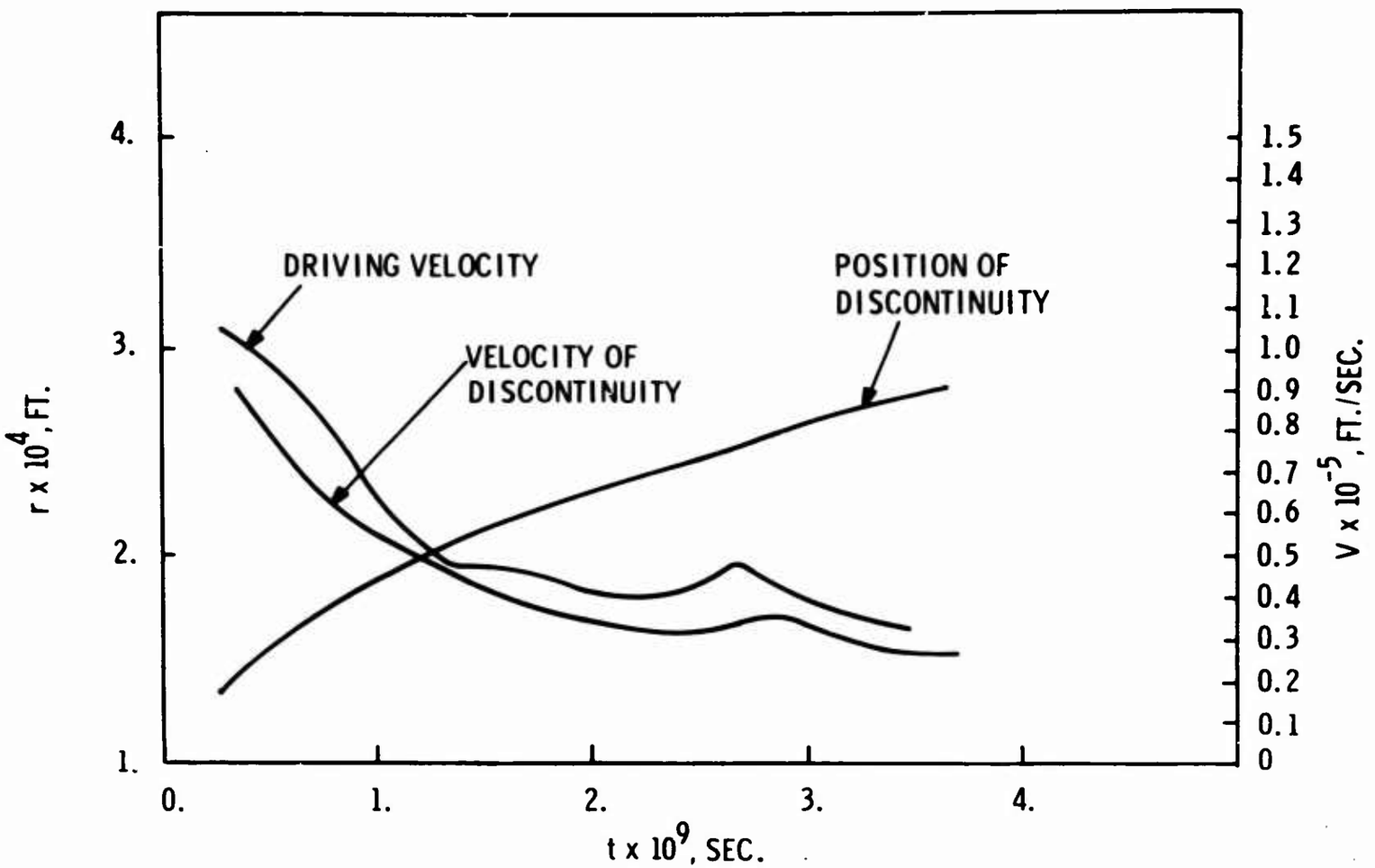


Figure II.C-15. Spherically-Symmetric Explosion, Outer Discontinuity

II.C.5 CONCLUSIONS

In this paper we have investigated the conditions under which discontinuities arise when one utilizes the Euler equations for the solution of problems involving one-dimensional planar and spherically-symmetric wave motion in compressible gases for both subsonic and supersonic flow. We have demonstrated that the finite difference equations which we employ for the Euler subsystem of the complete Navier-Stokes equations are well-behaved in the sense that at no time have we observed instabilities or oscillations, even in the presence of discontinuities.

We have shown that the finite difference equations we have utilized do not exhibit the effects which are associated with the concept of an artificial viscosity. In particular, the numerical discontinuities that appear do not satisfy the Rankine-Hugoniot conditions. We have also observed in the calculations presented here that the flow remains continuous in regions of variable entropy and that discontinuities are formed only when compression waves propagate into regions of constant entropy.

II.D THE DIAGONAL FORM OF QUASI-LINEAR HYPERBOLIC SYSTEMS AS A BASIS FOR DIFFERENCE EQUATIONS

by

P. Gordon

II.D THE DIAGONAL FORM OF QUASI-LINEAR HYPERBOLIC SYSTEMS AS A BASIS FOR DIFFERENCE EQUATIONS

II.D.1 INTRODUCTION

In this section we will consider two explicit difference approximations to the following system of first order quasi-linear partial differential equations:

$$\frac{\partial u}{\partial t} = \sum_{i=1}^{N} A_i \frac{\partial u}{\partial x_i} + F \qquad \text{(II. D-1)}$$

where $A_i = A_i(t,x,u)$ are m x m matrices,

$$x = \begin{pmatrix} x_1 \\ \\ x_N \end{pmatrix}, \quad u = \begin{pmatrix} u_1 \\ \\ u_m \end{pmatrix}, \quad F = \begin{pmatrix} f_1 \\ \\ f_m \end{pmatrix}, \text{ and } f_i = f_i(t,x,u).$$

(x denotes a point in euclidean N-space E^N and u is a point in E^m).

The two-dimensional semi-linear version of Eq. (II. D-1) is obtained by setting N = 1 and by assuming that the A_i are independent of u. For this case, there are two commonly used normal forms (II. D-2, p. 424-7). One of these normal forms replaces the original system with one in which each equation differentiates the variables along a common direction. In numerical work, this leads to the method of characteristics and to such difference equations as that proposed by Courant, Isaacson, and Rees (II. D-3). The second normal form replaces the system with a much simpler form, one in which the matrix corresponding to A_1 is diagonal. For quasi-linear cases, the first method can still be applied, but the transformation for the second form no longer produces a diagonal system. However, one can consider difference equations based on the diagonal form, without attempting to reduce the system to such a form.

For the case that the A_i are symmetric and independent of u, the diagonal form has been used by Anucina (II. D-1) as the basis for his difference equations. In fact, the first equation we will discuss can be considered a generalization of his first method to quasi-linear systems. This reduces to the same equation as that studied by Lees (II. D-14) for the case that the A_i are positive-definite symmetric and independent of u. (This latter case was also studied by Friedrichs (II. D-5).

Keller and Thomee (II. D-8-9) have utilized the diagonal form in their study of two-dimensional problems. However, they assume the system is diagonal (that is, A_1 is diagonal). Lax (II. D-10, p. 97) has shown that any m-order quasi-linear two-dimensional system can be replaced by a 2m-order diagonal system. Although this seems to be a good theoretical tool, it is not clear that the method can be reasonably applied to specific problems.

The two difference equations to be studied here are the extension of Anucina's first method (II. D-1) and Lax's proposed method for systems of conservation equations (II. D-11). The basic assumptions and form of the difference equations are described in Section II. D. 2. In Section II. D. 3, these two equations will be discussed for the case of a single equation in two dimensions. We will first consider them as interpolation formulas (Wendroff (II. D-20) introduced this kind of a discussion, and it does give some insight into the structure of the difference equation), and then relate them to the characteristic equations. In Section II. D. 4, convergence of the first difference equation is established for the quasi-linear two-dimensional version of Eq. II. D-1. In Section II. D. 5, the same problem is solved with respect to Lax's equation. In addition, Lax's difference equation is shown to be convergent when applied to the conservation form of Eq. II. D-1.

In the proofs, a unique solution to the differential equation will be assumed to exist. A maximum type norm (not the usual maximum norm) will be employed. An essential ingredient in the proofs will be to show that the solution of the difference equation satisfies a Lipschitz condition at the computed points.

It was our specific intent to use a maximum norm, rather than an L_2 norm. It was felt that this procedure, when possible, has these two advantages: a difference equation convergent in the maximum norm is more likely to produce a suitable numerical technique than one convergent in the L_2 norm, and a real understanding of the difference equation is more likely obtained by working with the maximum norm. However, in the N-dimensional case, which is discussed in Section II. D. 6, we were unable to establish convergence with respect to a maximum norm. Theorem 3 allows the use of an arbitrary norm, but still we are not able to establish convergence of our difference equations in full generality. An application is displayed in which convergence is established with respect to the L_2-norm.

II.D.2 BASIC ASSUMPTIONS AND DIFFERENCE EQUATIONS

Only the Cauchy problem will be considered here, and so it is assumed that initial conditions u (0, x) are given at t=0 in some region R of Euclidean N-space E^N. For any $\tilde{x}$ in R and for any $\delta > 0$ let I_δ be the interval $(0, \delta)$ in t-space, let $R_{\tilde{x},\delta}$ be a δ - neighborhood of $\tilde{x}$, and let $U_{\tilde{x},\delta}$ be a δ - neighborhood of u (0, x). Let the maximum norm of the matrix $Q = (q_{ij})$ be defined as follows:

$$\|Q\| = \max |q_{ij}| \qquad \text{(II. D-2)}$$

Let the maximum norm of a vector $v = \begin{pmatrix} v_1 \\ v_r \end{pmatrix}$ be defined as follows:

$$\|v\| = \max |v_i| \qquad \text{(II. D-3)}$$

Our basic assumptions, insofar as the difference equations are concerned, are given in the following statement.

For every $\tilde{x}$ in R there exists a $\delta > 0$ such that the following conditions are satisfied in $S_{\tilde{x},\delta} = I_\delta \times R_{\tilde{x},\delta} \times U_{\tilde{x},\delta}$:

1. At every point in $S_{\tilde{x},\delta}$ each A_i can be diagonalized, that is, there exists non-singular P_i such that $P_i A_i P_i^{-1} = D_i$ where the D_i are diagonal matrices. (II. D-4)

2. At every point in $S_{\tilde{x},\delta}$ P_i, A_i, and f_i have continuous first derivatives with respect to all variables. In particular, there exists a number C_1 (depending only on $\tilde{x}$) such that the following is true at any two points (t, x, u) and (t_1, x_1, u_1) in $S_{\tilde{x},\delta}$:

$$\|Q(t,x,u) - Q(t_1,x_1,u_1)\| \leq C_1 [\, |t-t_1| + \|x - x_1\| + \|u - u_1\| \,] \qquad \text{(II. D-5)}$$

   where Q can be any of the A_i, P_i, or f_i .

3. There exists a unique function $\omega(t, x)$ that satisfies Eq. (II. D-1) in $S_{\tilde{x},\delta}$ and that in $R_{\tilde{x},\delta}$ assumes the initial data u (0, x). Also, the Jacobian matrices $\frac{\partial \omega}{\partial x}$ and $\frac{\partial u}{\partial x}$ satisfy the following Lipschitz condition for any two points (t, x_1) and (t, x_2) in $I_\epsilon \times R_{\tilde{x},\delta}$:

$$\left\| \frac{\partial \omega}{\partial x}(t, x_1) - \frac{\partial \omega}{\partial x}(t, x_2) \right\| \leq C_1 \| x_1 - x_2 \|$$

$$\left\| \frac{\partial u}{\partial x}(0, x_1) - \frac{\partial u}{\partial x}(0, x_2) \right\| \leq C_1 \| x_1 - x_2 \| \qquad \text{(II. D-6)}$$

Remark 1: Mixed problems (those involving boundary conditions) will not be considered here. Thus, it will be assumed that the difference operators are employed only at points which depend on the initial data. It will be obvious from the choice of the difference equations that such points exist.

Remark 2: We have assumed the existence of $\omega(t, x)$ without going into any detail concerning the necessary requirements. See, for example Reference II. D-2, p. 448 and 593 and Reference II. D-10, p. 122.

We now describe the difference equations. Since the vector F in Eq. (II. D-1) adds no conceptual difficulties (it succeeds only in complicating the calculations), we assume $F \equiv 0$. Then, by assumption 2.3 the differential equations take the following form:

$$\frac{\partial u}{\partial t} = \sum_{i=1}^{N} (P_i^{-1} D_i P_i) \frac{\partial u}{\partial x_i} \qquad \text{(II. D-7)}$$

$$D_i = \text{diag} [d_i^1, \ldots, d_i^m]$$

The first difference equation is formed by differencing each component of the vector $P_i \frac{\partial u}{\partial x_i}$ according to the sign of d_i^ν. Forward differences are used if d_i^ν is positive and backward differences are used if d_i^ν is negative. This notation will be used. Let K represent the vector $\begin{pmatrix} n_1 \Delta x_1 \\ \\ n_m \Delta x_m \end{pmatrix}$. Then, for any function $f(t, x_1, \ldots, x_m)$,

$$f_K^n = f(n \Delta t, n_1 \Delta x_1, \ldots, n_m \Delta x_m)$$

$$f_{K \pm \Delta x_i}^n = f(n \Delta t, n_1 \Delta x_1, \ldots, n_{i-1} \Delta x_{i-1}, (n_i \pm 1) \Delta x_i, n_{i+1} \Delta x_{i+1}$$

$$\ldots, n_m \Delta x_m). \qquad \text{(II. D-8)}$$

Let

$$\Gamma_i = \max_\nu |d_i^\nu|.$$

Assume the following condition is satisfied:

$$\sum_i \Gamma_i \frac{\Delta t}{\Delta x_i} \leq 1 \qquad \text{(II. D-9)}$$

Letting $\frac{\partial u}{\partial t} \approx \frac{1}{\Delta t} (u_K^{n+1} - u_K^n)$, the difference equation can be put in the following form:

$$u_K^{n+1} = \sum_{i=1}^{N} (P_i^{-1})_K^n \left\{ (D_i^1 P_i)_K^n \; u_{K-\Delta x_i}^n + \right.$$

$$\left. + (D_i^2 P_i)_K^n \; u_K^n + (D_i^3 P_i)_K^n \; u_{K+\Delta x_i}^n \right\} \qquad \text{(II. D-10)}$$

where

$$D_i^1 = \text{diag} \left[(\alpha_i^1)_K^n, \ldots, (\alpha_i^m)_K^n \right]$$

$$D_i^2 = \text{diag} \left[(\beta_i^1 + c_i)_K^n, \ldots, (\beta_i^m + c_i)_K^n \right]$$

$$D_i^3 = \text{diag} \left[(\gamma_i^1)_K^n, \ldots, (\gamma_i^m)_K^n \right]$$

$$\gamma_i^\nu = (|d_i| \epsilon_i^\nu)_K^n \frac{\Delta t}{\Delta x_i}$$

$$\beta_i = - |d_i^\nu|_K^n \left(\frac{\Delta t}{\Delta x_i} \right)$$

$$\gamma_i = \left[|d_i^\nu| (1 - \epsilon_i) \right]_K^n \frac{\Delta t}{\Delta x_i}$$

$$\epsilon_i^\nu = \begin{cases} 1 : d_i^\nu \leq 0 \\ 0 : d_i > 0 \end{cases}$$

$$0 \leq c_i \leq 1 \text{ and } \sum_{i=1}^{N} c_i = 1.$$

It is assumed that the c_i are chosen so that all D_i are non-negative matrices. By condition 2.8, this can always be done.

Lax's approximation to Eq. (II. D-7) is obtained as follows. Use central differences for the "space" derivatives and let $\frac{\partial u}{\partial t} \approx \frac{1}{\Delta t}\left[u_K^{n+1} - \frac{1}{2N}\sum_{i=1}^{N}\left(u^n_{K+\Delta x_i} + u^n_{K-\Delta x_i}\right)\right]$.

Assume the following condition is satisfied:

$$\Gamma_i \frac{\Delta t}{\Delta x_i} < \frac{1}{N} \qquad \text{(II. D-11)}$$

The difference equation takes the following form:

$$u_K^{n+1} = \sum_{i=1}^{N} \left(P_i^{-1}\right)^n_K \left\{\left(D_i^1 P_i\right)^n_K u^n_{K-\Delta x_i} + \left(D_i^2 P_i\right)^n_K u^n_{K+\Delta x_i}\right\} \qquad \text{(II. D-12)}$$

where

$$D_i^1 = \frac{1}{2}\ \text{diag}\left[\frac{1}{N} - \frac{d_i \Delta t}{\Delta x_i}, \ldots, \frac{1}{N} - \frac{d_i^m \Delta t}{\Delta x_i}\right]^n_K$$

$$D_i^2 = \frac{1}{2}\ \text{diag}\left[\frac{1}{N} + \frac{d_i^1 \Delta t}{\Delta x_i}, \ldots, \frac{1}{N} + \frac{d_i^m \Delta t}{\Delta x_i}\right]^n_K$$

Lax's approximation as applied to the "conservation form" of the differential equations will be discussed later.

Remark: Condition 2.10 is more restrictive than condition 2.8, except for the case N=1. However, the greater ease in applying Eq. (II. D-12) might more than compensate for this in actual practice. No numerical results will be included here, but Eq. (II. D-10) has been used in several problems (II. D-16, 17).

II.D.3 A SINGLE EQUATION IN TWO-DIMENSIONS

Consider the equation

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial u}{\partial x} \text{ , where } \sigma \text{ is a positive constant.} \qquad \text{(II. D-13)}$$

Let u(o, x) be given. Let u_j^n represent the solution to the difference equation at $n\Delta t$ and $j\Delta x$.

The first equation, Eq. (II. D-10), takes the following form:

$$u_j^n = \beta \; u_j^{n-1} + \alpha \; u_{j+1}^{n-1}$$

$$0 \leq \alpha = \frac{\Delta t}{\Delta x} \; \sigma \leq 1, \; \beta = 1 - \alpha \qquad \text{(II. D-14)}$$

One can verify by induction that:

$$u_j^n = \sum_{\nu=0}^{n} \binom{n}{\nu} \; u_{j+\nu}^o \qquad \text{(II. D-15)}$$

Thus, Eq. (II. D-14) can be considered an interpolation formula for u (see Wendroff (II. D-20). Suppose now that j is fixed, that Δt and Δx are refined so that α is constant, and that $n = \frac{t_1}{\Delta t}$ where t_1 is given. Then, for all Δt and Δx we use data in the interval $\left[x_j, \; x_j + \frac{t_1 \; \Delta x}{\Delta t} \right]$. If we suppose this interval to be the unit interval, then Eq. (II. D-15) can be interpreted as the nth Bernstein Polynomial approximation to u (o, x). This is well known (II. D-21, p. 152) to converge to $u_{j+\alpha}^o$, which is of course the correct solution.

Eq. (II. D-12) takes the following form:

$$u_j^n = \frac{\sigma \Delta t}{2 \Delta x} \left(u_{j+1}^{n-1} - u_{j-1}^{n-1} \right) + \frac{1}{2} \left(u_{j+1}^{n-1} + u_{j-1}^{n-1} \right) \qquad \text{(II. D-16)}$$

again by induction, one obtains

$$u_j^n = \sum_{\nu=0}^{n} \binom{n}{\nu} \gamma^{n-\nu} \; \delta^{\nu} \; u_{j-n+2\nu}^o \qquad \text{(II. D-17)}$$

where $\gamma = \frac{1+\alpha}{2}$, $\delta = \frac{1-\alpha}{2}$.

Thus, we see that Eq. (II. D-14) and Eq. (II. D-16) represent the same approximation, but the approximation is applied to different intervals.

Further insight into the mechanics of these equations is obtained by looking at another proof of convergence. Consider u_j^n as a continuous function of x in some region of interest, and let this function be $u^n(x)$. In this region, suppose $\frac{d^\nu (u^o(x))}{dx^\nu}$ are uniformly bounded for $\nu = 1, 2$ and 3. Since α is constant, the same estimates clearly hold for $u^n(x)$ for all n. A series expansion of Eq. (II. D-14) produces the following:

$$u^{n+1}(x) = u^n (x + \alpha \Delta x) + \epsilon^n(x) \qquad \text{(II. D-18)}$$

where $|\epsilon^n(x)| \leq C \Delta x^2$ for some constant C.

The solution to Eq. (II. D-13) is also given by the following characteristic equations (II. D-2, p. 63 or 70).

$$\frac{du}{ds} = 0 , \quad \frac{dt}{ds} = 1, \quad \frac{dx}{ds} = -\sigma \qquad \text{(II. D-19)}$$

The Euler difference approximation to Eqs. (II. D-19) gives the following:

$$u^{i+1}(x) = u^i (x + \alpha \Delta x)$$

This is known to be a convergent approximation (II. D-8, p. 113). Henrici also shows that "arbitrary" second order errors will not disturb convergence (II. D-8, p. 28). $\epsilon_n(x)$ of Eq. (II. D-18) is such a perturbation.

The same analysis can be made for Eq. (II. D-16). Thus, we see that Eq. (II. D-14) are simply first approximations to the characteristic equations, Eq. II. D-19).

Remark: We have assumed here that the computed function is differentiable: If one hopes to use the method for computation, this is hardly a recommended procedure. This assumption will not be used in the general proof of the next section.

II.D.4 THE TWO-DIMENSIONAL CASE: DIFFERENCE EQUATION 1

We consider now Eq. (II. D-1) for the case N=1. The differential equation takes the following form:

$$\frac{\partial u}{\partial t} = P^{-1} D P \frac{\partial u}{\partial x} \quad , \quad D = \text{diag}\,(d^1, \ldots, d^m) \tag{II. D-20}$$

If in Eq. (II. D-10) the extra subscript is dropped and if K is replaced by j, the difference equation takes the following form:

$$u_j^{n+1} = (P^{-1})_j^n \left[(D^1 P)_j^n \; u_{j-1}^n + (D^2 P)_j^n \; u_j^n + (D^3 P)_j^n \; u_{j+1}^n \right] \tag{II. D-21}$$

$$\text{Let} \quad \frac{\Delta t}{\Delta x} = M, \tag{II. D-22}$$

Where M is a constant independent of any refinements of the mesh.

Theorem 1:

Suppose that conditions (II. D-9) and (II. D-22) and assumptions (II. D-4), (II. D-5) and (II. D-6) are satisfied.

Then, for every $\tilde{x}$ in R there exists a $\delta_1 > 0$ such that in $S_{\tilde{x},\,\delta_1} = I_{\delta_1} \times R_{\tilde{x},\,\delta_1} \times U_{x,\,\delta_1}$ u_j^n computed from Eq. (II. D-21) converges uniformly to the solution $\omega(t, x)$.

Proof: We proceed in the following manner:

1. Define an appropriate norm to be used in the calculation.
2. Establish a boundedness property and a Lipschitz condition for u_j^n.
3. Calculate the truncation error when Eq. (II. D-21) is applied to $\omega(t, x)$
4. Demonstrate convergence.

(1) For any non-singular matrix P, define the P-norm of a vector V as follows:

$$\| V \|_P = \| P V \| \tag{II. D-23}$$

where $\| P V \|$ is defined by Eq. (II. D-3).

The P-norm has the following geometric interpretation. The locus of points for which $\|V\|$ is a constant is given by the boundary of an "m-cube" centered at the origin. The locus of points for which $\|V\|_P$ is a constant in the image under P^{-1} of this boundary. This image is of course some skewed closed polygon containing the origin.

Motivation for the P-norm comes from the following simple result, which is stated without proof.

Lemma 1:

Let D_i be non-negative diagonal matrices such that $\sum_{i=1}^{\ell} D_i = I$. Let

$$V = \sum_{i=1}^{\ell} P^{-1} D_i P V_i.$$

Then, $\|V\|_P \leq \max_i [\|V_i\|_P]$.

We also need this result.

Lemma 2:

For any matrix B, $\|BV\|_P \leq \|PBP^{-1}\| \cdot \|V\|_P$

Finally, note that for any V in a given bounded set of vectors, $\|V\| \leq C_p \|V\|_P$, where C_p is a constant depending on P. Thus, we can assume that the Lipschitz conditions (II. D-5) and (II. D-6) hold with respect to a P-norm, where P is evaluated anywhere in $S_{\tilde{x}, \delta}$.

(2) We now look for a quantity L_n such that at all points in the computed region

$$\|u_{j+1}^n - u_j^n\|_{p_j^n} \leq L_n \Delta x \qquad \text{(II. D-24)}$$

L certainly exists since the initial data must satisfy assumption (II. D-6).

From Eq. (II. D-21) we obtain

$$P_j^n (u_j^{n+1} - u_j^n) = (D_1 P)_j^n (u_{j-1}^n - u_j^n) + (D_3 P)_j^n (u_{j+1}^n - u_j^n).$$

Thus,

$$\|u_j^{n+1} - u_j^n\|_{p_j^n} \leq L_n \Delta x \qquad \text{(II. D-25)}$$

Let

$$Q_j^n = (P^{-1} D_1 P)_j^n , \; R_j^n = (P^{-1} D_2 P)_j^n , \; S_j^n = (P^{-1} D_3 P)_j^n \qquad \text{(II. D-26)}$$

Then, from Eq. (II. D-21),

$$u_j^{n+1} - u_{j-1}^{n+1} = Q_j^n (u_{j-1}^n - u_{j-2}^n) + R_j^n (u_j^n - u_{j-1}^n) + S_j^n (u_{j+1}^n - u_j^n)$$

$$+ (Q_j^n - Q_{j-1}^n) (u_{j-2}^n - u_{j-1}^n) + (S_j^n - S_{j-1}^n) (u_j^n - u_{j-1}^n)$$

From Eq. (II. D-24), assumption (II. D-5), and lemma 1, we obtain:

$$\| u_j^{n+1} - u_{j-1}^{n+1} \|_{p_j^n} \leq L_n \Delta x + 2 C_1 \Delta x (1+L_n) L_n \Delta x \qquad \text{(II. D-27)}$$

Note also that from Eq. (II. D-22) and assumption (II. D-5), we can find a constant C_2, depending only on $\tilde{x}$, such that for any vector V:

$$\| V \|_{p_j^{n+1}} \leq \| V \|_{p_j^n} [1 + C_2 \Delta x (1 + L_n)] \qquad \text{(II. D-28)}$$

Substituting Eq. (II. D-28) into Eq. (II. D-27),

$$\| u_j^{n+1} - u_{j-1}^{n+1} \|_{p_j^{n+1}} \leq L_n \Delta x [1+2 C_1 \Delta x (1+L_n)] [1 + C_2 \Delta x (1+L_n)]$$

Thus, L_{n+1} can be chosen to satisfy this equation.

$$L_{n+1} = L_n + C_3 \Delta t L_n (1+L_n) + C_4 \Delta t^2 L_n (1+L_n)^2 \qquad \text{(II. D-29)}$$

where $C_3 = (2 C_1 + C_2)/M$ and $C_4 = 2 C_1 C_2 / M^2$.

But Eq. (II. D-29) is a convergent approximation to the following equation (Reference II. D-8, p. 113 and 28):

$$\frac{dL}{dt} = C_3 L (1+L) \qquad \text{(II. D-30)}$$

The solution to Eq. (II. D-30) is given by

$$L = C_5 \, e^{C_3 t} / (1 - C_5 e^{C_3 t}) \qquad \text{(II. D-31)}$$

where $C_5 = \dfrac{L_o}{1 + L_o} < 1.$

Thus, L is finite for $t < \dfrac{1}{C_3} \ln \left(\dfrac{1}{C_5} \right)$.

Remark: In a certain sense, this is the best result possible. That is, cases exist (II. D-12) in which the solution to the differential equation breaks down for this value of t.

We conclude that there exists a constant L, a $\delta_1 > 0$, and a region $S_{\tilde{x}, \delta 1}$ such that the following inequalities hold for all refinements of the mesh and for all P evaluated at points of $S_{\tilde{x}, \delta}$.

$$\left.\begin{aligned} &\text{a)} \quad \| u_{j+1}^{n+1} - u_j^{n+1} \|_p \leq L \Delta x \\ &\text{b)} \quad \| u_j^{n+1} - u_j^n \|_p \leq L \Delta x \\ &\text{c)} \quad \| u_j^n - u_j^o \|_p \leq L \end{aligned}\right\} \qquad \text{(II. D-32)}$$

(3) After some manipulation, Eq. (II. D-21) can be put in the following form:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = A \, \frac{u_j^n - u_{j-1}^n}{\Delta x} + P^{-1} D D^* P \, \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x}, \qquad \text{(II. D-33)}$$

$$= A \, \frac{u_{j+1}^n - u_{j-1}^n}{2 \Delta x} + P^{-1} D^{**} P \, \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{2 \Delta x} \qquad \text{(II. D-34)}$$

where $D^* = \text{diag} \left[(1-\epsilon_1), \ldots, (1-\epsilon_m) \right]$, $A = P^{-1} D P$,

$D^{**} = \text{diag} \left[|d_1|, \ldots, |d_m| \right]$.

Note that if for all i $d_i \leq 0$, then $D^* \equiv 0$ and the difference equation is obtained by simply replacing u_x with backward differences. Likewise, if the eigenvalues are all positive, the difference equation is obtained by using forward differences. Thus, for positive definite symmetric matrices (which necessarily have all positive eigenvalues) Eq. (II. D-21) is equivalent to the difference equation used by Lees (II. D-14).

Remark: It is not uncommon to hear one refer to the last term in Eqs. (II. D-33) and (II. D-34) as a "second order viscous" term, or more simply as an "artificial viscosity" (II. D-6). This can help to bring intuitive ideas into the picture, as for example in Eq. (II. D-34) which is unstable if one neglects the second order term. However, this analogy between the second order terms in Eqs. (II. D-33) and (II. D-34) and the classical artificial viscosity term of Von Neumann and Richtmyer should not be carried too far, the latter having been introduced for different reasons (II. D-14).

At any rate, substituting the true solution $\omega(t,x)$ into Eq. (II. D-33) and referring to assumption (II. D-6), we obtain:

$$\omega_{n+1,j} = (P^{-1})_{n,j} \left[(D_1 P)_{n,j}\, \omega_{n,j-1} + (D_2 P)_{n,j}\, \omega_{n,j} + (D_3 P)_{n,j}\, \omega_{n,j+1} \right] + O(\Delta t^2) \qquad \text{(II. D-35)}$$

Remark: The subscripts n, j indicate that the quantity is evaluated at n Δt, j Δx, $\omega(n\Delta t, j\Delta x)$. Also, $O(\Delta t^2)$ indicates a term of the form $C\Delta t^2$.

(4) Let

$$\epsilon_j^n = u_j^n - \omega_{n,j}$$

$$\epsilon^n = \max_j \left[\| \epsilon_j^n \|_{p_j^n} \right] \qquad \text{(II. D-36)}$$

Referring to equations (II. D-21), (II. D-26) and (II. D-35), we obtain:

$$\epsilon_j^{n+1} = Q_j^n\, \epsilon_{j-1}^n + R_j^n\, \epsilon_j^n + S_j^n\, \epsilon_{j+1}^n + O(\Delta t^2)$$

$$+ (Q_j^n - Q_{n,j})(\omega_{n,j-1} - \omega_{n,j}) + (S_j^n - S_{n,j})(\omega_{n,j+1} - \omega_{n,j}) \qquad \text{(II. D-37)}$$

From assumptions (II. D-5) and (II. D-6) and from lemma 2, there exists a constant C_3 such that

$$\left.\begin{aligned} \| S_j^n - S_{n,j} \|_{p_j^n} &\le C_3 \| \epsilon_j^n \|_{p_j^n} \\ \| Q_j^n - Q_{n,j} \|_{p_j^n} &\le C_3 \| \epsilon_j^n \|_{p_j^n} \\ \| \omega_{n,j} - \omega_{n,j\pm1} \|_{p_j^n} &\le C_3 \Delta t \end{aligned}\right\} \qquad \text{(II. D-38)}$$

Substituting Eq. (II. D-38), Eq. (II. D-28), and Eq. (II. D-32) into Eq. (II. D-37), we obtain the following expression as an upper bound for ϵ^{n+1}:

$$\epsilon^{n+1} = [\epsilon^n + 2 C_3^2 \epsilon^n \Delta t + O(\Delta t^2)][1 + \frac{C_2(1+L)}{M} \Delta t]$$

or

$$\epsilon^{n+1} = \epsilon^n + C_4 \epsilon^n \Delta t + C_5 \Delta t^2 \qquad \text{(II. D-39)}$$

As before, this is a convergent approximation to the differential equation $d\epsilon/dt = C_4 \epsilon$. For any bounded region in t the solution goes to zero as ϵ^0 goes to zero.

Remark: Condition 4.3 could be relaxed. It would be enough to know that positive constants M_1 and M_2 existed such that for all refinements of the mesh $M_1 < \Delta t/\Delta x < M_2$. However, we still assume that for a given computation Δt and Δx are fixed.

II.D.5 THE TWO-DIMENSIONAL CASE: DIFFERENCE EQUATION 2

When applied to Eq. (II. D-20), difference equation (II. D-12) takes the following form:

$$u_j^{n+1} = (P^{-1} D^1 P)_j^n \; u_{j-1}^n + (P^{-1} D^2 P)_j^n \; u_{j+1}^n$$

$$D^1 = \frac{1}{2} \text{ diag } (1 - \frac{\Delta t}{\Delta x} d^1, \ldots, 1 - \frac{\Delta t}{\Delta x} d^m) \qquad \text{(II. D-40)}$$

$$D^2 = \frac{1}{2} \text{ diag } (1 + \frac{\Delta t}{\Delta x} d^1, \ldots, 1 + \frac{\Delta t}{\Delta x} d^m)$$

Theorem 2:

Suppose that conditions (II. D-11) and (II. D-23) and assumptions (II. D-4), (II. D-5) and (II. D-6) are satisfied.

Then, for every $\tilde{x}$ in R there exists a $\delta_1 > 0$ such that in $S_{\tilde{x}, \delta_1} = I_{\delta_1} \text{ X } R_{\tilde{x}, \delta_1}$ X $U_{\tilde{x}, \delta_1}$ u_j^n computed from Eq. (II. D-40) converges uniformly to the solution $\omega(t, x)$.

Proof:

In terms of a norm, Eq. (II. D-40) behaves precisely as Eq. (II. D-21). Thus, the proof of Theorem 2 follows precisely the pattern of the proof of Theorem 1.

Corollary 1:

Let Eq. (II. D-40) be modified in the following fashion.

Let

$$(\bar{u}_i)_j^n = \min [(u_i)_{j-1}^n , (u_i)_{j+1}^n]$$

$$(\bar{\bar{u}}_i)_j^n = \max [(u_i)_{j-1}^n , (u_i)_{j+1}^n] \qquad \text{(II. D-41)}$$

Suppose each element of $A = P^{-1} D P$ is evaluated at an arbitrary point (that is, a different point for each element) in the range $x - \Delta x \le x \le x + \Delta x$,
$(\bar{u}_1)_j^n \le u_1 \le (\bar{\bar{u}}_1)_j^n, \ldots, (\bar{u}_m)_j^n \le u_m \le (\bar{\bar{u}}_m)_j^n$.

Then, Theorem 2 remains valid when applied to the modified difference equation.

Proof:

The only change that occurs in the proof is with respect to the coefficient of the truncation error term.

We consider now the conservation form of Eq. (II. D-20) which, when it exists, is as follows:

$$\frac{\partial u}{\partial t} = \frac{\partial g}{\partial x} = A \frac{\partial u}{\partial x}$$

$$A = P^{-1} D P, \; g = \begin{pmatrix} g_1 \\ \\ g_m \end{pmatrix}, \; g_r = g_r (t, x, u) \qquad \text{(II. D-42)}$$

Lax's approximation to Eq. (II. D-42) takes this form:

$$\frac{1}{\Delta t} \left[u_j^{n+1} - \frac{1}{2} \left(u_{j+1}^n + u_{j-1}^n \right) \right] = \frac{1}{2\Delta x} \left(g_{j+1}^n - g_{j-1}^n \right) \qquad \text{(II. D-43)}$$

Corollary 2:

Theorem 2 remains valid when applied to difference equation (II. D-43).

Proof:

Considering each element of g separately, note that:

$$\frac{1}{2\Delta x} \left[(g_i)_{j+1}^n - (g_i)_{j-1}^n \right] = \lambda_o + \sum_{\nu=1}^{m} \lambda_\nu \qquad \text{(II. D-44)}$$

where

$$(2\Delta x) \lambda_o = g_i (t, x+\Delta x, u_{j+1}^n) - g_i (t, x-\Delta x, u_{j+1}^n)$$

$$(2\Delta x) \lambda_\nu = g_i \left[t, x-\Delta x, (u_1)_{j-1}^n, \ldots, (u_{\nu-1})_{j-1}^n, (u_\nu)_{j+1}^n, \ldots, (u_m)_{j+1}^n \right]$$

$$- g_i \left[t, x-\Delta x, (u_1)_{j-1}^n, \ldots, (u_\nu)_{j-1}^n, (u_{\nu+1})_{j+1}^n, \ldots, (u_m)_{j+1}^n \right]$$

Thus, $\lambda_o = \frac{\partial g_i}{\partial x}$ and $\lambda_\nu = \frac{\partial g_i}{\partial u_\nu} \left[\frac{(u_\nu)^n_{j+1} - (u_\nu)^n_{j+1}}{2\Delta x} \right]$, where $\frac{\partial g_i}{\partial x}$ and $\frac{\partial g_i}{\partial u_\nu}$

are evaluated at points in the range $x-\Delta x \le x \le x + \Delta x$, $(\bar{u}_i)^n_j \le u_i \le (\bar{\bar{u}}_i)^n_j$ for $i = 1, 2, \ldots m$. This means that Eq. (II. D-43) applied to the conservation form is the same as Eq. (II. D-43) applied to the non-conservation form, with the exception that the elements of A are evaluated at different points. The result then follows from Theorem 2, corollary 1.

Remark: λ_o produces the vector F of Eq. (II. D-1).

II.D.6 THE MULTI-DIMENSIONAL CASE

Consider now Eq. (II. D-1) for N>1. One might conjecture that for this case difference Eqs. (II. D-10) and (II. D-11) should represent convergent approximations to Eq. (II. D-1). (For the case that all the A_i are semi-linear and symmetric this is precisely the result of Lees (II. D-13) and Anucina (II. D-1) if convergence is taken with respect to the L_2 - norm). However, we are unable to obtain this result in full generality. The difficulty lies in finding a function which can serve as a bound (in the sense of lemma 1) for all the A_i simultaneously. And the problem here may be simply a lack of understanding of what the conditions for hyperbolicity really mean or perhaps even what they should be. For example, if the A_i of Eq. (II. D-1) are pairwise commuting normal matrices, then they can be simultaneously diagonalized (II. D-7, p. 291, Theorem (11). The matrix P, which performs the diagonalization, would serve as a simultaneous bound for all the A_i.

More generally, the difference equations would be convergent if one could find a matrix Q that satisfied the following condition with respect to each matrix P_i of Eq. (II. D-1), where $A_i = P_i^{-1} D_i P_i$.

Let $\{D^\nu\}$ be non-negative diagonal matrices such that $\sum_{\nu=1}^{k} D^\nu = I$. Then, if U_ν are arbitrary vectors, and $u = \sum_{\nu=1}^{k} P_i^{-1} D^\nu P_i U_\nu$, then $\|u\|_Q \le \max_\nu \|u_\nu\|_Q$.

Having searched unsuccessfully for such a matrix Q, one is tempted to conjecture that it does not exist! Be this as it may, we can obtain some further results by relaxing the choice of a norm.

Theorem 3:

Suppose norms are given for a matrix A and a vector V, denoted by $\|A\|_*$ and $\|A\|_*$. Suppose that these norms satisfy the equation: $\|AV\|_* \le \|A\|_* \|V\|_*$

Suppose that assumptions (II. D-4), (II. D-5) and (II. D-6) are satisfied relative to these norms.

Suppose that a consistent difference equation is specified for Eq. (II. D-7) and suppose it has the following form:

$$u_K^{n+1} = \sum_{i=1}^{N} \sum_{\nu=-\alpha_i^1}^{\alpha_i^2} (Q_\nu^i)^n_{K+\nu\Delta\chi_i} + \Delta t\,(G)_K^n , \qquad \text{(II. D-45)}$$

where $K = (n_1 \Delta X_1, \ldots, n_N \Delta X_N)$, the Q^i_ν are m X m matrices, and G is a vector. Suppose that the Q^1_ν and G satisfy the Lipshitz condition (II. D-5) relative to the given norms.

Remark: By "consistent" we mean that Eq. (II. D-45) represents Eq. (II. D-7) to at least first order accuracy. This implies that $\sum_{i=1}^{N} \sum_{\nu=-\alpha_i^1}^{\alpha_i^2} Q^i_\nu = I$.

Suppose that Δx_i are specified by functions: $\Delta x_i = f_i(\Delta t)$, i=1, . . . , N such that $\Delta x_i \to 0$ as $\Delta t \to 0$. Suppose also that there exists a Δt^* such that for all $0 < \Delta t < \Delta t^*$ Eq. (II. D-45) satisfies the following stability condition:

$$\| u_K^{n+1} \|^* \leq (1 + c\,\Delta t) \max_n \| u^n \|^* \qquad \text{(II. D-46)}$$

where c is a constant dependent only on the region given by assumptions (II. D-4) - (II. D-5).

Then, for every $\tilde{x}$ in R there exists a $\delta_1 > 0$ such that in $S_{\tilde{X}, \delta_1} = I_{\delta_1} \times R_{\tilde{x}, \delta_1} \times U_{\tilde{x}, \delta_1}$, u_K^n converges uniformly to the solution $u(t,x)$, where convergence of course is with respect to the norm $\| \ \|^*$.

Proof:

The proof follows exactly the pattern of Theorem 1, except that the complication of the p-matrix is not there, and we omit the details. Again, the major task is to establish a Lipschitz condition similar to Eq. (II. D-24). It is understood that the difference is to be taken relative to any Δx_i, and that L_n is to be valid for all Δx_i.

Theorem 4:

Suppose again that norms $\|A\|^*$ and $\|V\|^*$ are given and that they satisfy $\|AV\|^* \leq \|A\|^* \|V\|^*$

Suppose that Eq. (2.6) is modified in the following fashion:

$$\frac{\partial u}{\partial t} = P^{-1} \sum_{i=1}^{N} (P_i^{-1} D_i P_i) P \frac{\partial u}{\partial x_i}, \text{ where} \qquad \text{(II. D-47)}$$

P is non-singular in the region and satisfies the Lipschitz condition (II. D-5) relative to the given norm.

Suppose that the assumptions of Theorem 3 are satisfied, so that Eq. (II. D-45) is a convergent approximate to Eq. (II. D-7).

Suppose that Eq. (II. D-45) is modified as follows:

$$u_K^{n+1} = P^{-1} \sum_{i=1}^{N} \sum_{r=-\alpha_i}^{\alpha_i^2} Q_\nu^i \; P \, U^n_{K+\bar{\nu}\Delta_i}) + \Delta t \, G^*, \qquad \text{(II. D-48)}$$

where G* again satisfies the Lipschitz condition (II. D-5).

Then, in a region defined as in Theorem 3, Eq. (II. D-48) is a convergent approximation to Eq. (II. D-47).

Proof: The proof now follows exactly the pattern of Theorem 1 and will not be repeated.

Remark 1: If Eq. (II. D-47) were linear, then the matrix P could be simply transformed away. The effect of Theorem 4 is that even in the quasi-linear case, where such a transformation cannot be applied, the corresponding difference equation is still valid.

Remark 2: Theorem 1 is a direct consequence of Theorems 3 and 4.

Remark 3: The use of the P-norm here is similar to the technique used by Lax (II. D-14, p. 514).

Remark 4: It is perhaps appropriate to compare our results with those of Strang (II. D-18) and Veidinger (II. D-19). Both their results employ the L_2-norm. Strang's results can be applied to methods of higher order accuracy, and so in this sense it is stronger than our Theorems 3 and 4. Veidinger's result is interesting in that he obtains convergence relative to the maximum norm although stability is defined relative to the L_2-norm. Our approach is similar to Veidinger's in that the first step is to establish boundedness of the computed function. However, Veidinger's proof is subject to the criticism that it involves differentiation of the computed function. The results of Strang and Veidinger as well as our Theorem 3 would establish convergence of difference Eqs. (II. D-10) and (II. D-12) for the symmetric case (employing the L_2-norm). Theorem 4, however, can also be applied to the case where the A_i of Eq. (II. D-1) can be simultaneously symmetrized by some matrix P.

Remark 5: Modifications of Theorem 4, similar to corollary 2 of Theorem 2, can be made so as to allow application of difference Eq. (II. D-12) to the conservation form of Eq. (II. D-1).

As noted earlier, we were not able to obtain general results with respect to difference Eqs. (II. D-10) and (II. D-12). However, we present now on application where the assumption of Theorem 4 can be applied. We consider one form of the

two-dimensional, time-dependent, non-viscous Navier-Stokes equations. These equations in cylindrical coordinates can be written as follows:

$$\frac{\partial u}{\partial t} = A_1 \frac{\partial u}{\partial r} + A_2 \frac{\partial u}{\partial \theta} + F \qquad \text{(II. D-49)}$$

where u is a 4-component vector, and the A_i are 4 x 4 matrices. The precise definition of these quantities can be found in Reference II. D-16. For our purposes, it is enough to note that A_1 and A_2 can be diagonalized so that Eq. (II. D-47) can be put in this form:

$$\frac{\partial u}{\partial t} = (P_1^{-1} D_1 P_1) \frac{\partial u}{\partial r} + (P_1^{-1} Q^{-1} D_2 Q P_1) \frac{\partial u}{\partial \theta} \qquad \text{(II. D-50)}$$

where

$$Q = \begin{pmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 & 1/2 \end{pmatrix} \quad Q^{-1} = Q^T = \begin{pmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 & -1/2 \\ 1/2 & -1/2 & 1/2 & -1/2 \\ -1/2 & 1/2 & 1/2 & -1/2 \end{pmatrix} \qquad \text{(II. D-51)}$$

Relative to the reduced equation

$$\frac{\partial u}{\partial t} = D_1 \frac{\partial u}{\partial r} + Q^{-1} D_2 Q \frac{\partial u}{\partial \theta} \qquad \text{(II. D-52)}$$

difference Eqs. (II. D-10) and (II. D-12) are both convergent relative to the L_2-norm. (Since the matrices are symmetric, the stability condition (II. D-46) follows from the results of Anucina (II. D-1), and convergence follows from Theorem 3. Thus, by Theorem 4, Eqs. (II. D-10) and (II. D-12) are convergent approximations to Eq. (II. D-49).

II.E. NUMERICAL ANALYSIS OF THE NAVI-I DIGITAL COMPUTER PROGRAM

by

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II.E. NUMERICAL ANALYSIS OF THE NAVI-I DIGITAL COMPUTER PROGRAM

This section contains a description of the mathematical and numerical analysis that is involved in the NAVY-I computer program. This program has the capability of solving various forms of the one-dimensional Navier-Stokes equation. Section II.E.1 defines the differential equations. The system of differential equations consists of the following four equations: conservation of mass, energy, momentum, and species. Since the problem is one-dimensional, there is one momentum equation, and since we have thus far included only a two-component gas, there is one species equation. The equations are first written with respect to an arbitrary orthogonal curvilinear coordinate system. Three special forms are then retained; these are the one-dimensional cartesian, cylindrical, and spherical forms. In order to allow for unequal spacing of nodal points, an additional space transformation is introduced. Finally, all versions of the differential equations are combined into one general form, and it is with this form that the remainder of the report is concerned.

Section II.E.2 describes several forms of the spacing parameter that can be used. These allow capability to "squeeze" points toward either boundary (of the finite region of computation), or toward some point in the interior.

Section II.E.3 contains a discussion of the boundary conditions. In particular, boundary conditions for four specific problems are defined. These problems are: a piston moving into a stationary gas; reflection from a solid surface; the burst problem; and mass injection.

The difference equations are derived in Section II.E.4. The inviscid hyperbolic subsystem is differenced according to the diagonal form, and the remaining parabolic portion is differenced according to the explicit-implicit difference equation. Convergence of both these difference equations has been established elsewhere, but partial proofs are reproduced here.

Finally, Section II.E.5 discusses the problem of including radiation in the calculations. A new "time-scale" now appears and its significance and effect on the calculations is described.

Appendix C describes the iteration scheme which is used in the program.

II.E.1 THE MATHEMATICAL SYSTEM

The equations are first written in an arbitrary orthogonal curvilinear coordinate system.(II.E-17) Let u_1, u_2, u_3 represent the spatial coordinates and let t represent the time coordinates. Let $\underset{\rightharpoonup}{u}_1$, $\underset{\rightharpoonup}{u}_2$, and $\underset{\rightharpoonup}{u}_3$ represent unit vectors in the respective directions. Let h_1, h_2, h_3 be the corresponding components of the metric tensor. That is,

$$ds = h_1^2\, du_1 + h_2^2\, du_2 + h_3^2\, du_3 \,. \qquad \text{(II.E-1)}$$

The velocity vector is written as follows

$$\underset{\rightharpoonup}{V} = V_1 \underset{\rightharpoonup}{u}_1 + V_2 \underset{\rightharpoonup}{u}_2 + V_3 \underset{\rightharpoonup}{u}_3 \,. \qquad \text{(II.E-2)}$$

The notation for the remaining flow variables is

$$\left.\begin{aligned} \rho &= \text{density,} \\ T &= \text{temperature,} \\ P &= \text{pressure,} \\ C &= \text{mass fraction.} \end{aligned}\right\} \qquad \text{(II.E-3)}$$

The problem is assumed to be one-dimensional. Thus, the following assumptions are made:

$$\left.\begin{aligned} &\frac{\partial f}{\partial u_2} = \frac{\partial f}{\partial u_3} = 0, \\ &\text{where f is any of the flow variables} \\ &V_2 = V_3 = 0. \end{aligned}\right\} \qquad \text{(II.E-4)}$$

Conservation of Mass:

$$\frac{\partial \rho}{\partial t} + \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} (h_2 h_3 \rho V_1) = 0 \,. \qquad \text{(II.E-5)}$$

Conservation of Species:

$$\rho \left(\frac{\partial C}{\partial t} + \frac{V_1}{h_1} \frac{\partial C}{\partial u_1} \right) = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \rho \mathcal{D} \frac{\partial C}{\partial u_1} \right) + \dot{w}_1 \,. \qquad \text{(II.E-6)}$$

(This applies to a binary mixture and includes concentration diffusion, but neglects thermal diffusion, pressure diffusion and external forces.

Conservation of Energy:

$$\rho \bar{C}_v \left(\frac{\partial T}{\partial t} + \frac{V_1}{h_1} \frac{\partial T}{\partial u_1} \right) = \frac{-P}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} (h_2 h_3 V_1)$$

$$+ \mu \left\{ 2 \left(\frac{1}{h_1} \frac{\partial V_1}{\partial u_1} \right)^2 + 2 \left(\frac{V_1}{h_1 h_2} \frac{\partial h_2}{\partial u_1} \right)^2 + 2 \left(\frac{V_1}{h_1 h_3} \frac{\partial h_3}{\partial u_1} \right)^2 \right.$$

$$\left. + \left(\frac{V_1}{h_1 h_3} \frac{\partial h_1}{\partial u_3} \right)^2 + \left(\frac{V_1}{h_1 h_2} \frac{\partial h_1}{\partial u_2} \right)^2 \right\}$$

$$+ \lambda \left[\frac{1}{h_1} \frac{\partial V_1}{\partial u_1} + \frac{V_1}{h_1 h_2} \frac{\partial h_2}{\partial u_1} + \frac{V_1}{h_1 h_3} \frac{\partial h_3}{\partial u_1} \right]^2$$

$$+ \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} K \frac{\partial T}{\partial u_1} \right)$$

$$+ \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} \left[\frac{h_2 h_3}{h_1} \rho \mathcal{D} (h_i - h_j) \frac{\partial C}{\partial u_1} \right]$$

$$- (e_i - e_j) \dot{w}_1 - \frac{e_i - e_j}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \rho \mathcal{D} \frac{\partial C}{\partial u_1} \right) . \qquad \text{(II.E-7)}$$

Conservation of Momentum (u_1):

$$\rho \frac{\partial V_1}{\partial t} + \frac{\rho V_1}{h_1} \frac{\partial V_1}{\partial u_1} + \frac{1}{h_1} \frac{\partial P}{\partial u_1} = \frac{\lambda V_1}{h_1} \frac{\partial}{\partial u_1} \left[\frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} (h_2 h_3) \right]$$

$$- \frac{\mu V_1}{h_2} \frac{\partial}{\partial u_2} \left[\frac{1}{h_1 h_2} \frac{\partial h_1}{\partial u_2} \right] - \frac{\mu V_1}{h_3} \frac{\partial}{\partial u_3} \left[\frac{1}{h_1 h_3} \frac{\partial h_1}{\partial u_3} \right]$$

$$- \frac{\mu V_1}{h_1 h_3} \frac{\partial h_1}{\partial u_3} \left[\frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_3} (h_1 h_2) + \frac{1}{h_1 h_3} \frac{\partial h_1}{\partial u_3} \right]$$

$$- \frac{\mu V_1}{h_1 h_2} \frac{\partial h_1}{\partial u_2} \left[\frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_2} (h_1 h_3) + \frac{1}{h_1 h_2} \frac{\partial h_1}{\partial u_2} \right]$$

$$- 2\mu V_1 \left[\left(\frac{1}{h_1 h_2} \frac{\partial h_2}{\partial u_1} \right)^2 + \left(\frac{1}{h_1 h_3} \frac{\partial h_3}{\partial u_1} \right)^2 \right] + \left(\frac{2\mu + \lambda}{h_1^2} \right) \frac{\partial^2 V_1}{\partial u_1^2}$$

$$+ \frac{\partial V_1}{\partial u_1} \left(\frac{2\mu + \lambda}{h_1} \right) \left[\frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1} (h_2 h_3) - \frac{1}{h_1^2} \frac{\partial h_1}{\partial u_1} \right]$$

$$+ \frac{2}{h_1^2} \frac{\partial \mu}{\partial u_1} \frac{\partial V_1}{\partial u_1} + \frac{1}{h_1^2} \frac{\partial \lambda}{\partial u_1} \frac{\partial V_1}{\partial u_1}$$

$$+ \left(\frac{1}{h_1} \frac{\partial \lambda}{\partial u_1} \right) \left(\frac{V_1}{h_1 h_2 h_3} \right) \frac{\partial}{\partial u_1} (h_2 h_3) . \qquad \text{(II.E-8)}$$

In the cartesian coordinate system, we can let $u_1 = x$ and $h_1 \equiv h_2 \equiv h_3 \equiv 1$. We then have

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho V_1) = 0 , \qquad \text{(II.E-9)}$$

$$\rho \left(\frac{\partial C}{\partial t} + V_1 \frac{\partial C}{\partial x} \right) = \frac{\partial}{\partial x} \left(\rho \mathcal{D} \frac{\partial C}{\partial x} \right) = \dot{w}_1 , \qquad \text{(II.E-10)}$$

$$\rho \bar{C}_v \left(\frac{\partial T}{\partial t} + V_1 \frac{\partial T}{\partial x} \right) = - P \frac{\partial V_1}{\partial x} + 2\mu \left(\frac{\partial V_1}{\partial x} \right)^2 + \lambda \left(\frac{\partial V_1}{\partial x} \right)^2$$

$$+ \frac{\partial}{\partial x} \left(K \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial x} \left[\rho \mathcal{D} (h_i - h_j) \frac{\partial C}{\partial x} \right]$$

$$- (e_i - e_j) \dot{w}_1 - (e_i - e_j) \frac{\partial}{\partial x} \left(\rho \mathcal{D} \frac{\partial C}{\partial x} \right) , \qquad \text{(II.E-11)}$$

$$\rho \left(\frac{\partial V_1}{\partial t} + V_1 \frac{\partial V_1}{\partial x} \right) + \frac{\partial P}{\partial x} = (2\mu + \lambda) \frac{\partial^2 V_1}{\partial x^2}$$

$$+ \left[\frac{\partial}{\partial x} (2\mu + \lambda) \right] \frac{\partial V_1}{\partial x} . \qquad \text{(II.E-12)}$$

In the cylindrical coordinate system, we have the following coordinates:

$$u_1 = r = \sqrt{x^2 + y^2} ,$$

$$u_2 = z ,$$

$$\tan u_3 = \frac{z}{x} .$$

It turns out that $h_1 \equiv h_2 \equiv 1$, and $h_3 = r$. We then have

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r \rho V_1) = 0 , \qquad \text{(II.E-13)}$$

$$\rho \left(\frac{\partial C}{\partial t} + V_1 \frac{\partial C}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho \mathcal{D} \frac{\partial C}{\partial r} \right) + \dot{w}_1 , \qquad \text{(II.E-14)}$$

$$\begin{aligned} \rho \bar{C}_v \left(\frac{\partial T}{\partial t} + V_1 \frac{\partial T}{\partial r} \right) &= - \frac{P}{r} \frac{\partial}{\partial r} (r V_1) \\ &+ 2\mu \left[\left(\frac{\partial V_1}{\partial r} \right)^2 + \left(\frac{V_1}{r} \right)^2 \right] + \lambda \left[\frac{\partial V_1}{\partial r} + \frac{V_1}{r} \right]^2 \\ &+ \frac{1}{r} \frac{\partial}{\partial r} \left(r K \frac{\partial T}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left[r \rho \mathcal{D} (h_i - h_j) \frac{\partial C}{\partial r} \right] \\ &- (e_i - e_j) \dot{w}_1 - \left(\frac{e_i - e_j}{r} \right) \frac{\partial}{\partial r} \left(r \rho \mathcal{D} \frac{\partial C}{\partial r} \right) , \end{aligned} \qquad \text{(II.E-15)}$$

$$\begin{aligned} \rho \left(\frac{\partial V_1}{\partial t} + V_1 \frac{\partial V_1}{\partial r} \right) + \frac{\partial P}{\partial r} &= - \frac{\lambda V_1}{r^2} - \frac{2\mu V_1}{r^2} \\ &+ (2\mu + \lambda) \frac{\partial^2 V_1}{\partial r^2} + \left(\frac{2\mu + \lambda}{r} \right) \frac{\partial V_1}{\partial r} \\ &+ \left[\frac{\partial}{\partial r} (2\mu + \lambda) \right] \frac{\partial V_1}{\partial r} + \frac{V_1}{r} \frac{\partial \lambda}{\partial r} . \end{aligned} \qquad \text{(II.E-16)}$$

In the spherical coordinate system, we have the following coordinates:

$$u_1 = r = \sqrt{x^2 + y^2 + z^2} ,$$

$$\tan u_2 = \frac{z}{y} ,$$

$$\tan u_3 = \sqrt{y^2 + z^2}/x .$$

It turns out that $h_1 \equiv 1$, $h_2 = r \sin u_3$, and $h_3 = r$. We then have

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho V_1) = 0 , \qquad \text{(II.E-17)}$$

$$\rho \left(\frac{\partial C}{\partial t} + V_1 \frac{\partial C}{\partial r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho \mathcal{D} \frac{\partial C}{\partial r} \right) + \dot{w}_1 , \qquad \text{(II.E-18)}$$

$$\begin{aligned} \rho \bar{C}_v \left(\frac{\partial T}{\partial t} + V_1 \frac{\partial T}{\partial r} \right) &= - \frac{P}{r^2} \frac{\partial}{\partial r} (r^2 V_1) \\ &+ 2\mu \left[\left(\frac{\partial V_1}{\partial r} \right)^2 + 2 \left(\frac{V_1}{r} \right)^2 \right] + \lambda \left[\frac{\partial V_1}{\partial r} + \frac{2V_1}{r} \right]^2 \\ &+ \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 K \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \rho \mathcal{D} (h_i - h_j) \frac{\partial C}{\partial r} \right] \\ &- (e_i - e_j) \dot{w}_1 - \frac{e_i - e_j}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho \mathcal{D} \frac{\partial C}{\partial r} \right) , \end{aligned} \qquad \text{(II.E-19)}$$

$$\begin{aligned} \rho \left(\frac{\partial V_1}{\partial t} + V_1 \frac{\partial V_1}{\partial r} \right) + \frac{\partial P}{\partial r} &= - \frac{2\lambda V_1}{r^2} - \frac{4\mu V_1}{r^2} \\ &+ (2\mu + \lambda) \frac{\partial^2 V_1}{\partial r^2} + \frac{2}{r} (2\mu + \lambda) \frac{\partial V_1}{\partial r} \\ &+ \frac{\partial}{\partial r} (2\mu + \lambda) \frac{\partial V_1}{\partial r} + \frac{2V_1}{r} \frac{\partial \lambda}{\partial r} . \end{aligned} \qquad \text{(II.E-20)}$$

By defining a new quantity, δ, we can combine these three sets of equations into one set. Let

$$\delta = \begin{cases} 0 : & \text{cartesian coordinate system} \\ 1 : & \text{cylindrical coordinate system (radial direction)} \\ 2 : & \text{spherical coordinate system (radial direction).} \end{cases}$$

We have then the following equations where we let r represent the spatial coordinate in all cases:

$$\frac{\partial \rho}{\partial t} + V\frac{\partial \rho}{\partial r} + \rho\frac{\partial V}{\partial r} = -\frac{\delta}{r}\rho V , \qquad \text{(II. E-21)}$$

$$\rho\left(\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial r}\right) = \frac{\partial}{\partial r}\left(\rho \mathcal{D}\frac{\partial C}{\partial r}\right) + \frac{\delta}{r}\left(\rho \mathcal{D}\frac{\partial C}{\partial r}\right) + \dot{w}_1 , \qquad \text{(II. E-22)}$$

$$\begin{aligned}\partial \bar{C}_v\left(\frac{\partial T}{\partial t} + V\frac{\partial T}{\partial r}\right) &= -P\frac{\partial V}{\partial r} - \frac{\delta}{r}PV - (e_i - e_j)\dot{w}_1 \\ &+ 2\mu\left[\left(\frac{\partial V}{\partial r}\right)^2 + \delta\left(\frac{V}{r}\right)^2\right] + \lambda\left[\frac{\partial V}{\partial r} + \frac{\delta V}{r}\right]^2 \\ &+ \frac{\partial}{\partial r}\left(K\frac{\partial T}{\partial r}\right) + \frac{\delta}{r}K\frac{\partial T}{\partial r} \\ &+ \frac{\partial}{\partial r}\left[\rho \mathcal{D}(h_i - h_j)\frac{\partial C}{\partial r}\right] + \frac{\delta}{r}\rho \mathcal{D}(h_i - h_j)\frac{\partial C}{\partial r} \\ &- (e_i - e_j)\frac{\partial}{\partial r}\left(\rho \mathcal{D}\frac{\partial C}{\partial r}\right) - \frac{\delta}{r}(e_i - e_j)\rho \mathcal{D}\frac{\partial C}{\partial r} ,\end{aligned} \qquad \text{(II. E-23)}$$

$$\begin{aligned}\rho\left(\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial r}\right) + \frac{\partial P}{\partial r} &= -\frac{\delta}{r^2}(2\mu + \lambda)V \\ &+ (2\mu + \lambda)\frac{\partial^2 V}{\partial r^2} + \frac{\delta}{r}(2\mu + \lambda)\frac{\partial V}{\partial r} \\ &+ \frac{\partial}{\partial r}(2\mu + \lambda)\frac{\partial V}{\partial r} + \frac{\delta}{r}V\frac{\partial \lambda}{\partial r} .\end{aligned} \qquad \text{(II. E-24)}$$

We will also employ the following auxilliary relation in our problems:

$$P = \rho \bar{R} T ,$$

$$\mu = a T^{1/2} ,$$

$$K = b T^{1/2} ,$$

$$\lambda = -\frac{2}{3}\mu ,$$

$$\rho \mathcal{D} = C T^{1/2} / \bar{R} ,$$

$$\bar{C}_v = C_{v_2} + C (C_{v_1} - C_{v_2}) ,$$

$$\bar{R} = R_2 + C (R_1 - R_2) ,$$

$$e_i - e_j = (C_{v_1} - C_{v_2}) (T - T_{ref}) + (\Delta e_{f_1} - \Delta e_{f_2}) ,$$

$$h_i - h_j = (C_{p_1} - C_{p_2}) (T - T_{ref}) + (\Delta h_{f_1} - \Delta h_{f_2}) , \qquad \text{(II.E-25)}$$

where a, b, c, c_{v1}, c_{v2}, R_1, R_2, T_{ref}, Δe_{f_1}, Δe_{f_2}, c_{p1}, c_{p2}, Δh_{f_1}, Δh_{f_2} are constants.

Also,

$$\dot{w}_1 = \frac{2M_n}{A} (62.5) \left[k_{f_{N_2}} n_{N_2}^2 - k_{r_{N_2}} n_N^2 n_{N_2} + k_{f_N} n_{N_2} n_N - k_{r_N} n_N^3 \right] = \text{lbm/ft}^3\text{-sec.} \qquad \text{(II.E-26)}$$

$$M_n = 14 = \text{gr/gr mole} ,$$

$$A = 6.023 \times 10^{23} = \text{part/mole},$$

$$n_{N_1} = 2.127 \times 10^{19} \frac{C\rho}{14} = \text{part./cm}^3 ,$$

$$n_{N_2} = 2.127 \times 10^{19} \frac{(1-C)\rho}{28} = \text{part./cm}^3 ,$$

$$k_{f_{N_2}} = 7.9 \times 10^{-7} \times T_K^{(-.5)} e^{-113,000/T_K} ,$$

$$k_{f_N} = 6.9 \times 10^{-2} \times T_K^{(-1.5)} e^{-113,000/T_K} ,$$

$$k_{r_{N_2}} = 1.25 \times 10^{-31} \times T_k^{(-.57)} ,$$

$$k_{r_N} = 1.09 \times 10^{-26} \times T_k^{(-1.5)} ,$$

T_K = temperature - ^{o} kelvin .

Let "′" denote differentiation. This notation will be used (hopefully) when there is no ambiguity. Let

$$\left.\begin{aligned} f_1 &= (h_i - h_j) - (e_i - e_j) , \\ f_2 &= e_i - e_j . \end{aligned}\right\} \qquad \text{(II.E-27)}$$

Then, the equations can be written as

$$\frac{\partial \rho}{\partial t} + V \frac{\partial \rho}{\partial r} + \rho \frac{\partial V}{\partial r} = - \frac{\delta}{r} \rho V , \qquad \text{(II.E-28)}$$

$$\rho \left(\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial r} \right) = \rho \mathcal{D} \frac{\partial^2 C}{\partial r^2} + \left[\frac{\partial}{\partial r} (\rho \mathcal{D}) + \frac{\delta}{r} \rho \mathcal{D} \right] \frac{\partial C}{\partial r} + \dot{w}_1 , \qquad \text{(II.E-29)}$$

$$\begin{aligned} \rho \bar{C}_v \left(\frac{\partial T}{\partial t} + V \frac{\partial T}{\partial r} \right) &= - p \frac{\partial V}{\partial r} - \frac{\delta}{r} pV - f_2 \dot{w}_1 \\ &+ \frac{4}{3} \mu \left(\frac{\partial V}{\partial r} \right)^2 + 2 \mu \left(\frac{V}{r} \right)^2 \left[\delta \left(1 - \frac{\delta}{3} \right) \right] - \frac{4}{3} \mu \left(\frac{V}{r} \right) \frac{\partial V}{\partial r} \delta \\ &+ K \frac{\partial^2 T}{\partial r^2} + \left(K' \frac{\partial T}{\partial r} + \frac{\delta}{r} K \right) \frac{\partial T}{\partial r} + \rho \mathcal{D} f_1 \frac{\partial^2 C}{\partial r^2} \\ &+ f_1 \frac{\partial (\rho \mathcal{D})}{\partial r} \frac{\partial C}{\partial r} + \rho \mathcal{D} \frac{\partial}{\partial r} (h_i - h_j) \frac{\partial C}{\partial r} + \frac{\delta}{r} \rho \mathcal{D} f_1 \frac{\partial C}{\partial r} , \end{aligned} \qquad \text{(II.E-30)}$$

$$\rho\left(\frac{\partial V}{\partial t}+V\frac{\partial V}{\partial r}\right)+\frac{\partial P}{\partial r}=-\frac{\delta}{r^2}\left(\frac{4\mu}{3}\right)V+\frac{4\mu}{3}\frac{\partial^2 V}{\partial r^2}+\frac{4\mu}{3}\left(\frac{\delta}{r}\right)\frac{\partial V}{\partial r}$$

$$+\frac{4}{3}\mu'\frac{\partial T}{\partial r}\frac{\partial V}{\partial r}-\frac{2\delta}{3r}V\mu'\frac{\partial T}{\partial r}\ . \qquad \text{(II.E-31)}$$

Suppose we now introduce a transformation of the form

$$\eta = f(r,t)\ ,$$
$$\tau = t\ . \qquad \text{(II.E-32)}$$

(Several forms of f(r,t) are discussed in Section II.E.2).

Let

$$\eta_r=\frac{\partial f}{\partial r}\ ,\qquad \eta_t=\frac{\partial f}{\partial t}\ ,$$

$$\eta_{rr}=\frac{d^2 f}{dr^2}\ .$$

Then, for any quantity $\varphi(t,r)$ we have

$$\frac{\partial\varphi}{\partial r}=\frac{\partial\varphi}{\partial\eta}\frac{\partial\eta}{\partial r}+\frac{\partial\varphi}{\partial\tau}\frac{\partial\tau}{\partial r}=\frac{\partial\varphi}{\partial\eta}\eta_r\ ,$$

$$\frac{\partial^2\varphi}{\partial r^2}=\eta_{rr}\frac{\partial\varphi}{\partial\eta}+\eta_r\left[\frac{\partial^2\varphi}{\partial\eta^2}\eta_r+\frac{\partial^2\varphi}{\partial\eta\partial\tau}\frac{\partial\tau}{\partial r}\right]\ ,$$

$$=(\eta_r)^2\frac{\partial^2\varphi}{\partial\eta^2}+\eta_{rr}\frac{\partial\varphi}{\partial\eta}\ ,$$

$$\frac{\partial\varphi}{\partial t}=\frac{\partial\varphi}{\partial\eta}\frac{\partial\eta}{\partial t}+\frac{\partial\varphi}{\partial\tau}\frac{\partial\tau}{\partial t}\ ,$$

$$=\frac{\partial\varphi}{\partial\tau}+\eta_t\frac{\partial\varphi}{\partial\eta}\ .$$

The equations then take the following form, where t is still used instead of τ. Note that the unbarred terms represent the inviscid system, while the barred terms represent the viscous terms.

Conservation of Mass:

$$\frac{\partial \rho}{\partial t} + \eta_t \frac{\partial \rho}{\partial \eta} + V \eta_r \frac{\partial \rho}{\partial \eta} + \rho \eta_r \frac{\partial V}{\partial \eta} = - \frac{\delta}{r} \rho V ,$$

or

$$\frac{\partial \rho}{\partial t} = - a_1 \frac{\partial \rho}{\partial \eta} - a_2 \frac{\partial V}{\partial \eta} - a_3 , \qquad \text{(II.E-33)}$$

$$a_1 = V \eta_r + \eta_t ,$$

$$a_2 = \rho \eta_r ,$$

$$a_3 = \frac{\delta}{r} \rho V .$$

Conservation of Momentum:

$$\rho \left(\frac{\partial V}{\partial t} + \eta_t \frac{\partial V}{\partial \eta} + V \frac{\partial V}{\partial \eta} \eta_r \right) + \eta_r \left(\frac{\partial P}{\partial \rho} \frac{\partial \rho}{\partial \eta} + \frac{\partial P}{\partial T} \frac{\partial T}{\partial \eta} + \frac{\partial P}{\partial C} \frac{\partial C}{\partial \eta} \right)$$

$$= - \frac{\delta}{r^2} \left(\frac{4\mu}{3} \right) V + \frac{4\mu}{3} \left[\eta_r^2 \frac{\partial^2 V}{\partial \eta^2} + \eta_{rr} \frac{\partial V}{\partial \eta} \right]$$

$$+ \left(\frac{4\mu}{3} \right) \left(\frac{\delta}{r} \right) \eta_r \frac{\partial V}{\partial r} + \frac{4}{3} \mu' \eta_r^2 \frac{\partial T}{\partial \eta} \frac{\partial V}{\partial \eta}$$

$$- \frac{2\delta}{3r} V \mu' \eta_r \frac{\partial T}{\partial \eta} ,$$

or

$$\frac{\partial V}{\partial t} = \bar{b}_1 \frac{\partial^2 V}{\partial \eta^2} + \bar{b}_2 \frac{\partial V}{\partial \eta} - \bar{b}_3 V - b_1 \frac{\partial V}{\partial \eta} - b_2 \frac{\partial \rho}{\partial \eta}$$

$$- b_3 \frac{\partial T}{\partial \eta} - b_4 \frac{\partial C}{\partial \eta} , \qquad \text{(II.E-34)}$$

$$\bar{b}_1 = \frac{4\mu}{3\rho} \eta_r^2 ,$$

$$\bar{b}_2 = \frac{4\mu}{3\rho} \left[\eta_{rr} + \eta_r \frac{\delta}{r} + \frac{\mu'}{\mu} \eta_r^2 \frac{\partial T}{\partial \eta} \right] ,$$

$$\bar{b}_3 = \frac{4\mu}{3\rho}\left(\frac{\delta}{r^2}\right) + \frac{2\delta}{3r}\,\frac{\mu'\eta_r}{\rho}\,\frac{\partial T}{\partial r}\,,$$

$$b_1 = \eta_t + V\eta_r\,,$$

$$b_2 = \frac{1}{\rho}\,\eta_r\frac{\partial p}{\partial \rho} = \frac{\eta_r \bar{R}\,T}{\rho}\,,$$

$$b_3 = \frac{1}{\rho}\,\eta_r\frac{\partial P}{\partial T} = \eta_r \bar{R}\,,$$

$$b_4 = \frac{1}{\rho}\,\eta_r\frac{\partial P}{\partial C} = \eta_r\, T\bar{R}'\,.$$

Conservation of Energy:

$$\rho\bar{C}_v\left(\frac{\partial T}{\partial t} + \eta_t\frac{\partial T}{\partial \eta} + V\eta_r\frac{\partial T}{\partial \eta}\right) = -P\eta_r\frac{\partial V}{\partial \eta} - \frac{\delta}{r}PV - f_2\dot{w}_1$$

$$+\frac{4}{3}\mu\eta_r^2\left(\frac{\partial V}{\partial \eta}\right)^2 + \frac{2\delta(3-\delta)}{3r^2}\mu V^2 - \frac{4}{3}\mu\left(\frac{\delta}{r}\right)V\eta_r\,\frac{\partial V}{\partial \eta}$$

$$+K\left[\eta_r^2\frac{\partial^2 T}{\partial \eta^2} + \eta_{rr}\frac{\partial T}{\partial \eta}\right] + K'\eta_r^2\left(\frac{\partial T}{\partial \eta}\right)^2 + \frac{\delta}{r}K\eta_r\frac{\partial T}{\partial \eta}$$

$$+\rho\mathcal{D}f_1\left[\eta_r^2\frac{\partial^2 C}{\partial \eta^2} + \eta_{rr}\frac{\partial C}{\partial \eta}\right] + f_1\eta_r^2\frac{\partial}{\partial \eta}(\rho\mathcal{D})\frac{\partial C}{\partial \eta}$$

$$+\rho\mathcal{D}\eta_r^2\frac{\partial}{\partial \eta}(h_i - h_j)\frac{\partial C}{\partial \eta} + \frac{\delta}{r}\rho\mathcal{D}f_1\eta_r\frac{\partial C}{\partial \eta}\,,$$

or

$$\frac{\partial T}{\partial t} = \bar{C}_1\frac{\partial^2 T}{\partial \eta^2} + \bar{C}_2\frac{\partial T}{\partial \eta} + \bar{C}_3\left(\frac{\partial T}{\partial \eta}\right)^2 + \bar{C}_4 + \bar{C}_5\frac{\partial C}{\partial \eta}\,\frac{\partial T}{\partial \eta}$$

$$-\bar{C}_6\left(\frac{\partial C}{\partial \eta}\right)^2 + \bar{C}_7\frac{\partial^2 C}{\partial \eta^2} + \bar{C}_8\frac{\partial C}{\partial \eta} - C_1\frac{\partial T}{\partial \eta} - C_2\frac{\partial V}{\partial \eta} - C_3 T,$$

(II. E-35)

$$\bar{c}_1 = \eta_r^2 \frac{K}{\rho \bar{C}_v} ,$$

$$\bar{c}_2 = \frac{K}{\rho \bar{C}_v} \left(\eta_n + \frac{\delta}{r} \eta_r \right) ,$$

$$\bar{c}_3 = \frac{K'}{\rho \bar{C}_v} \eta_r^2 ,$$

$$\bar{c}_4 = \frac{4\mu}{3\rho \bar{C}_v} \left[\eta_r^2 \left(\frac{\partial V}{\partial \eta} \right)^2 + \frac{\delta(3-\delta)}{2r^2} V^2 - \frac{\delta V \eta_r}{r} \frac{dV}{d\eta} \right]$$

$$- \dot{w}_1 f_2 / \rho \bar{C}_v ,$$

$$\bar{c}_5 = \frac{f_1 \eta_r^2}{\rho \bar{C}_v} \frac{\partial}{\partial T} (\rho \mathcal{D}) + \frac{\rho \mathcal{D} \eta_r^2}{\rho \bar{C}_v} \frac{\partial}{\partial T} (h_i - h_j) ,$$

$$\bar{c}_6 = - \frac{f_1 \eta_r^2}{\rho \bar{C}_v} \frac{\partial}{\partial C} (\rho \mathcal{D}) ,$$

$$\bar{c}_7 = \rho \mathcal{D} f_1 \eta_r^2 / \rho \bar{C}_v ,$$

$$\bar{c}_8 = \frac{\rho \mathcal{D} f_1}{\rho \bar{C}_v} \left(\eta_{rr} + \frac{\delta}{r} \eta_r \right) ,$$

$$a_1 = \eta_t + V \eta_r ,$$

$$c_2 = \frac{\bar{R} T \eta_r}{\bar{C}_v} ,$$

$$c_3 = \frac{\delta \bar{R} V}{r \bar{C}_v} .$$

Conservation of Species:

$$\rho\left(\frac{\partial C}{\partial t} + \eta_t \frac{\partial C}{\partial \eta} + V\eta_r \frac{\partial C}{\partial \eta}\right) = \rho\mathcal{D}\left(\eta_r^2 \frac{\partial^2 C}{\partial \eta^2} + \eta_{rr} \frac{\partial C}{\partial \eta}\right)$$

$$+\left[\eta_r \frac{\partial}{\partial C}(\rho\mathcal{D}) \frac{\partial C}{\partial \eta} + \eta_r \frac{\partial}{\partial T}(\rho\mathcal{D}) \frac{\partial T}{\partial \eta} + \frac{\delta \rho\mathcal{D}}{r}\right] \eta_r \frac{\partial C}{\partial \eta} + \dot{w}_1$$

or

$$\frac{\partial C}{\partial t} = \bar{d}_1 \frac{\partial^2 C}{\partial \eta^2} - \bar{d}_2 \left(\frac{\partial C}{\partial \eta}\right)^2 + \bar{d}_3 \frac{\partial C}{\partial \eta} + \bar{d}_4 \frac{\partial C}{\partial \eta} \frac{\partial T}{\partial \eta} + \bar{d}_5 - d_1 \frac{\partial C}{\partial \eta}, \quad \text{(II.E-36)}$$

$$\bar{d}_1 = -\frac{\rho\mathcal{D}}{\rho} \eta_r^2 ,$$

$$\bar{d}_2 = -\frac{\eta_r^2}{\rho} \frac{\partial}{\partial C}(\rho\mathcal{D}) ,$$

$$\bar{d}_3 = \frac{\rho\mathcal{D}}{\rho}\left(\eta_{rr} + \frac{\delta}{r}\eta_r\right) ,$$

$$\bar{d}_4 = \frac{\eta_r^2}{\rho} \frac{\partial}{\partial T}(\rho\mathcal{D}) ,$$

$$\bar{d}_5 = \dot{w}_1/\rho ,$$

$$d_1 = \eta_t + V\eta_r .$$

≡

If we define the vector $X = \begin{pmatrix} \rho \\ V \\ T \\ C \end{pmatrix}$, we can put the equations in the following matrix form:

$$\frac{\partial X}{\partial t} = A \frac{\partial X}{\partial \eta} + B, \quad \text{(II.E-37)}$$

$$A = \begin{pmatrix} -a_1 & -a_2 & 0 & 0 \\ -b_2 & -a_1 & -b_3 & -b_4 \\ 0 & -c_2 & -a_1 & 0 \\ 0 & 0 & 0 & -a_1 \end{pmatrix}, \qquad B = \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{pmatrix},$$

$$B_1 = - a_3 ,$$

$$B_2 = \bar{b}_1 \frac{\partial^2 V}{\partial \eta^2} + \bar{b}_2 \frac{\partial V}{\partial \eta} - \bar{b}_3 V ,$$

$$B_3 = \bar{c}_1 \frac{\partial^2 T}{\partial \eta^2} + \bar{c}_2 \frac{\partial T}{\partial \eta} + \bar{c}_3 \left(\frac{\partial T}{\partial \eta} \right)^2 + \bar{c}_4 + \bar{c}_5 \frac{\partial C}{\partial \eta} \frac{\partial T}{\partial \eta}$$

$$- \bar{c}_6 \left(\frac{\partial C}{\partial \eta} \right)^2 + \bar{c}_7 \frac{\partial^2 C}{\partial \eta^2} + \bar{c}_8 \frac{\partial C}{\partial \eta} - c_3 T,$$

$$B_4 = \bar{d}_1 \frac{\partial^2 C}{\partial \eta^2} - \bar{d}_2 \left(\frac{\partial C}{\partial \eta} \right)^2 + \bar{d}_3 \frac{\partial C}{\partial \eta} + \bar{d}_4 \frac{\partial C}{\partial \eta} \frac{\partial T}{\partial \eta} + \bar{d}_5 .$$

II.E.2 SPACE TRANSFORMATIONS

The space transformations are imposed in order to allow the following possibilities:

1. A moving coordinate system (moving with time).

2. Unequal spacing of nodal points.

These goals will be accomplished in two steps. The first transformation $r \to \xi$ allows for the moving coordinate system, and the second $\xi \to \eta$ allows for unequal spacing. In Part A the transformations will be defined, in Part B arithmetic problems will be discussed, and in Part C the squeezing setup for the burst problem is described.

PART A.

We assume that the region of computation is defined as input to the problem

$$r_o(t) \leqq r \leqq r_1(t), \tag{II.E-38}$$

where $r_0(t)$ and $r_1(t)$ are given.

We then define the transformation

$$\xi = \frac{r - r_o(t)}{r_1(t) - r_o(t)}. \tag{II.E-39}$$

Thus

$$r = r_o(t) \to \xi = 0$$

$$r = r_1(t) \to \xi = 1$$

If $r_0(t)$ and $r_1(t)$ are constant, then Eq. (II.E-39) serves merely to normalize the space variable in (0,1)

$$\frac{\partial \xi}{\partial r} = \frac{1}{r_1 - r_o} \tag{II.E-40}$$

Thus, this is a valid transformation:

$$\frac{\partial \xi}{\partial r} > 0 \quad \text{as long as } r_1 > r_o.$$

$$\frac{\partial^2 \xi}{\partial r^2} \equiv 0 \tag{II.E-41}$$

$$\frac{\partial \xi}{\partial t} = \frac{-(r_1 - r_o)\dfrac{dr_o}{dt} - (r - r_o)\left(\dfrac{dr_1}{dt} - \dfrac{dr_o}{dt}\right)}{(r_1 - r_o)^2},$$

$$= \frac{dr_o}{dt}\left[\frac{r - r_1}{(r_1 - r_o)^2}\right] - \frac{dr_1}{dt}\left[\frac{r - r_o}{(r_1 - r_o)^2}\right].$$

Note that $\dfrac{r - r_1}{r_1 - r_o} = \xi - 1$,

or

$$\frac{\partial \xi}{\partial t} = \frac{\xi - 1}{(r_1 - r_o)}\frac{dr_o}{dt} - \frac{\xi}{(r_1 - r_o)}\frac{dr_1}{dt}. \qquad \text{(II.E-42)}$$

Now we define the following transformation:

$$\eta = \left(\frac{e^{-s\xi_o} + e^{-s}}{1 - e^{-s}}\right)\left(\frac{1 - e^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}}\right), \qquad \text{(II.E-43)}$$

where $s = s(t)$ and $\xi_o = \xi_o(t)$.

Various properties of this transformation will be pointed out as we proceed. We want now to calculate $\dfrac{\partial \eta}{\partial \xi}$, $\dfrac{\partial^2 \eta}{\partial \xi^2}$, $\dfrac{\partial \eta}{\partial \xi_o}$ and $\dfrac{\partial \eta}{\partial s}$.

$$\ell n\eta = \ell n\,(e^{-s\xi_o} + e^{-s}) - \ell n\,(1 - e^{-s}) + \ell n(1 - e^{-s\xi}) - \ell n(e^{-s\xi_o} + e^{-s\xi}),$$

$$\left(\frac{1}{\eta}\right)\frac{\partial \eta}{\partial \xi} = \frac{se^{-s\xi}}{1 - e^{-s\xi}} + \frac{se^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}},$$

$$= \frac{se^{-s\xi}(e^{-s\xi_o} + e^{-s\xi} + 1 - e^{-s\xi})}{(1 - e^{-s\xi})(e^{-s\xi_o} + e^{-s\xi})},$$

$$\frac{\partial \eta}{\partial \xi} = \frac{\eta s e^{-s\xi}(1 + e^{-s\xi_o})}{(1 - e^{-s\xi})(e^{-s\xi_o} + e^{-s\xi})}, \qquad \text{(II.E-44)}$$

$$\left(\frac{1}{\eta}\right)\frac{\partial \eta}{\partial \xi_o} = \frac{-se^{-s\xi_o}}{e^{-s\xi_o} + e^{-s}} + \frac{se^{-s\xi_o}}{e^{-s\xi_o} + e^{-s\xi}},$$

$$= \frac{se^{-s\xi_o}(e^{-s\xi_o} + e^{-s} - e^{-s\xi_o} - e^{-s\xi})}{(e^{-s\xi_o} + e^{-s})(e^{-s\xi_o} + e^{-s\xi})},$$

and

$$\frac{\partial \eta}{\partial \xi_o} = \frac{e^{-s\xi_o}(e^{-s} - e^{-s\xi})(s\eta)}{(e^{-s\xi_o} + e^{-s})(e^{-s\xi_o} + e^{-s\xi})} , \qquad \text{(II.E-45)}$$

$$\left(\frac{1}{\eta}\right)\frac{\partial \eta}{\partial s} = -\frac{\xi_o e^{-s\xi_o} + e^{-s}}{e^{-s\xi_o} + e^{-s}} - \frac{e^{-s}}{1 - e^{-s}} + \frac{\xi e^{-s\xi}}{1 - e^{-s\xi}}$$

$$+ \frac{\xi_o e^{-s\xi_o} + \xi e^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}} .$$

$$\left(\frac{1}{\eta}\right)\frac{\partial \eta}{\partial s} = \frac{\xi_o e^{-s\xi_o} + \xi e^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}} - \frac{\xi_o e^{-s\xi_o} + e^{-s}}{e^{-s\xi_o} + e^{-s}} - \frac{e^{-s}}{1-e^{-s}}$$

$$+ \frac{\xi e^{-s}(e^{-s\xi_o} + e^{-s})}{\eta(1 - e^{-s})(e^{-s\xi_o} + e^{-s\xi})} ,$$

and

$$\frac{\partial \eta}{\partial s} = \eta\left(\frac{\xi_o e^{-s\xi_o} + \xi e^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}} - \frac{\xi_o e^{-s\xi_o} + e^{-s}}{e^{-s\xi_o} + e^{-s}} - \frac{e^{-s}}{1-e^{-s}}\right)$$

$$+ \xi \frac{e^{-s\xi}(e^{-s\xi_o} + e^{-s})}{(1-e^{-s})(e^{-s\xi_o} + e^{-s})} . \qquad \text{(II.E-46)}$$

From Eq. (II.E-44) and Eq. (II.E-43)

$$\frac{\partial \eta}{\partial \xi} = s e^{-s\xi} \frac{(1 + e^{-s\xi_o})(e^{-s\xi_o} + e^{-s})}{(1-e^{-s})(e^{-s\xi_o} + e^{-s\xi})^2} , \qquad \text{(II.E-47)}$$

$$\ell n \frac{\partial \eta}{\partial \xi} = \ell n \left(\frac{s(e^{-s\xi_o} + e^{-s})(1 + e^{-s\xi_o})}{(1-e^{-s})}\right)$$

$$-2\ell n(e^{-s\xi_o} + e^{-s\xi}) - s\xi ,$$

$$\frac{1}{\left(\frac{\partial \eta}{\partial \xi}\right)} \frac{\partial^2 \eta}{\partial \xi^2} = -s + \frac{2se^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}} ,$$

$$= s\left(\frac{2e^{-s\xi} - e^{-s\xi_o} - e^{-s\xi}}{e^{-s\xi_o} + e^{-s\xi}}\right) ,$$

and

$$\frac{\partial^2 \eta}{\partial \xi^2} = s\frac{\partial \eta}{\partial \xi}\left(\frac{e^{-s\xi} - e^{-s\xi_o}}{e^{-s\xi_o} + e^{-s\xi}}\right) . \qquad \text{(II.E-48)}$$

Let us now obtain $\frac{\partial \eta}{\partial r}$, $\frac{\partial^2 \eta}{\partial r^2}$ and $\frac{\partial \eta}{\partial t}$:

$$\frac{\partial \eta}{\partial r} = \frac{\partial \eta}{\partial \xi}\frac{\partial \xi}{\partial r} , \qquad \text{(II.E-49)}$$

$$\frac{\partial^2 \eta}{\partial r^2} = \frac{\partial \eta}{\partial \xi}\frac{\partial^2 \xi}{\partial r^2} + \frac{\partial^2 \eta}{\partial \xi^2}\left(\frac{\partial \xi}{\partial r}\right)^2 \qquad \text{(II.E-50)}$$

$$\frac{\partial \eta}{\partial t} = \frac{\partial \eta}{\partial \xi}\frac{\partial \xi}{\partial t} + \frac{\partial \eta}{\partial s}\frac{\partial s}{\partial t} + \frac{\partial \eta}{\partial \xi_o}\frac{\partial \xi_o}{\partial t} ,$$

where

$$r = \xi(r_1 - r_o) + r_o , \qquad \text{(II.E-51)}$$

$$\xi = -\frac{1}{s}\ln\left\{\frac{1 - \left(\frac{\eta e^{-s\xi_o}(1-e^{-s})}{e^{-s\xi_o} + e^{-s}}\right)}{1 + \left(\frac{\eta(1-e^{-s})}{e^{-s\xi_o} + e^{-s}}\right)}\right\} . \qquad \text{(II.E-52)}$$

Finally, let us summarize some of the properties of the η transformation, Eq. (II.E-43).

a) $\eta(o) = o$: From Eq. (II.E-43).

b) $\eta(1) = 1$: from Eq. (II.E-43).

c) $\frac{\partial \eta}{\partial \xi} > 0$: this follows from Eq. (II.E-47) if one notes that $\frac{s}{1 - e^{-s}}$ is always positive.

d) $\frac{\partial^2 \eta}{\partial \xi^2}(\xi o) = 0$: from Eq. (II.E-48).

e) $\frac{\partial \eta}{\partial \xi}$ has a maximum at $\xi = \xi o$. By substituting into Eq. (II.E-47) we can calculate this max.

$$\max \frac{\partial \eta}{\partial \xi} = \frac{s\, e^{-\xi_o}(1 + e^{-s\xi_o})(e^{-s\xi_o} + e^{-s})}{(1 - e^{s})\, 4\, e^{-2s\xi_o}} ,$$

$$= \frac{s(1 + e^{-s\xi_o})(e^{-s\xi_o})(e^{-s\xi_o} + e^{-s})}{(1 - e^{-s})\, 4\, e^{-s\xi_o}} ,$$

$$= \frac{s(e^{s\xi_o} + 1)(e^{-s\xi_o} + e^{-s})}{4(1 - e^{-s})} ,$$

$$= \left(\frac{s}{1 - e^{-s}}\right) \frac{1 + e^{-s\xi_o} + e^{s(\xi_o - 1)} + e^{-s}}{4} .$$

Thus, for large $|s|$,

$$\max \frac{\partial \eta}{\partial \xi} \to \frac{s}{4} .$$

f) $\max \frac{\partial \eta}{\partial \xi}$ has a minimum at $\xi_o = \frac{1}{2}$ and is symmetric about $\xi_o = \frac{1}{2}$:

$$\frac{\partial}{\partial \xi_o}\left(\max \frac{\partial \eta}{\partial \xi}\right) = \frac{-s\, e^{-s\xi_o} + s\, e^{s(\xi_o + 1)}}{4} \frac{s}{1 - e^{-s}} ,$$

$$= \frac{s^2}{4(1 - e^{-s})}\left(e^{s(\xi_o - 1)} - e^{-s\xi_o}\right) = 0 \to \xi_o = \frac{1}{2} .$$

Since

$$\frac{\partial^2}{\partial \xi_o^2}\left(\max \frac{\partial \eta}{\partial \xi}\right) = \frac{s^3}{4(1 - e^{-s})}\left(e^{s(\xi_o - 1)} + e^{-s\xi_o}\right) > 0,$$

$\max \frac{\partial \eta}{\partial \xi}$ has a minimum at $\xi_o = \frac{1}{2}$. In fact,

$$\min_{\xi_o}(\max \frac{\partial \eta}{\partial \xi}) = \left(\frac{s}{1 - e^{-s}}\right)\left(\frac{1 + e^{-s/2}}{2}\right)^2 .$$

Also,

$$\max_{\xi_o}(\max \frac{\partial \eta}{\partial \xi} = \left(\frac{s}{1 - e^{-s}}\right)\left(\frac{1 - e^{-s}}{2}\right)$$

g) $\eta(s) = \eta(-s)$:

$$\eta(-s) = \left(\frac{e^{s\xi_o} + e^{s}}{1 - e^{s}}\right)\left(\frac{1 - e^{s\xi}}{e^{s\xi_o} + e^{s\xi}}\right),$$

$$= \left(\frac{e^{s\xi_o - s} + 1}{e^{-s} - 1}\right)\left(\frac{e^{-s\xi} - 1}{e^{+s\xi_o - s\xi} + 1}\right) ,$$

$$= \frac{e^{-s} + e^{-s\xi_o}}{1 - e^{-s}} \quad \frac{1 - e^{-s\xi}}{e^{-s\xi} + e^{-s\xi_o}} = \eta(s) .$$

$\equiv$

(There are computational difficulties near s = 0 in Eqs. (II.E-49, II.E-52). These will be discussed in Part B.

PART B.

Several of the operations developed in the previous section exhibit computational difficulties at s = 0. In order to handle these, we will obtain an expansion for η about s = 0. We will use the following formulas.

For any f(x), let $g(x) = \frac{1}{f(x)}$,

$$\frac{d(g)}{d(x)} = g'(x) = \frac{-f'}{(f)^2} ,$$

$$g''(x) = -\frac{(f)^2 f'' - 2f(f')^2}{(f)^4} = \frac{2(f')^2 - f\,f''}{(f)^3} ,$$

$$g'''(x) = \frac{(f)^3\left(4f'f'' - f'f'' - f\,f'''\right) - \left(2(f')^2 - f\,f''\right)3(f)^2 f'}{(f)^6} ,$$

$$= \frac{f(3f'f'' - f\,f''') - 6(f')^3 + 3f\,f'f''}{(f)^4} ,$$

$$= \frac{6f\,f'f'' - (f)^2 f''' - 6(f')^3}{(f)^4} ,$$

$$g''''(x) = \Big[(f)^4\left(6\,f\,f'f''' + 6\,(f')^2 f'' + 6\,f\,(f'')^2 - 2\,f\,f'\,f''' - (f)^2 f'''' - 18(f')^2 f''\right) - \left(6\,f\,f'\,f'' - (f)^2 f''' - 6\,(f')^3\right)4\,(f)^3 f'\Big] \Big/ (f)^8 ,$$

$$= \Big[6(f)^2 f'\,f''' + 6(f)^2(f'')^2 + 6f(f')^2 f'' - 2(f)^2 f'\,f''' - (f)^3 f'''' - 18f(f')^2 f'' - 24f(f')^2 f'' + 4(f)^2 f'\,f''' + 24(f')^4\Big] \Big/ (f)^5 ,$$

$$= \frac{\left[-36f(f')^2 f'' + 8(f)^2 f'f''' + 24(f')^4 + 6(f)^2(f'')^2 - (f)^3 f''''\right]}{(f)^5} ,$$

and

$$g(x) = g(0) + \frac{g'(0)}{1}x + \frac{g''(0)}{2}x^2 + \frac{g'''(0)}{6}x^3 + \frac{g''''(0)}{24}x^4 + \cdots \qquad \text{(II.E-53)}$$

Now let

$$\eta = g_1 g_2 g_3 g_4, \qquad \text{(II.E-54)}$$

where

$$g_1 = e^{-s\xi_o} + e^{-s},$$

$$g_2 = \frac{1}{e^{-s\xi_o} + e^{-s\xi}},$$

$$g_3 = (1 - e^{-s\xi})/s,$$

$$g_4 = s/(1 - e^{-s}).$$

We now obtain expansions for all the g_i.

1) g_1:

$$g_1' = -\xi_o e^{-s\xi_o} - e^{-s},$$

$$g_1'' = \xi_o^2 e^{-s\xi_o} + e^{-s},$$

$$g_1''' = -\xi_o^3 e^{-s\xi_o} - e^{-s},$$

$$g_1'''' = \xi_o^4 e^{-s\xi_o} + e^{-s},$$

$$g_1(0) = 2,$$

$$g_1'(0) = -(1 + \xi_o),$$

$$g_1''(0) = (1 + \xi_o^2),$$

$$g_1'''(0) = -(1 + \xi_o^3),$$

$$g_1''''(0) = (1 + \xi_o^4).$$

Thus,

$$g_1 = g_{10} + g_{11}s + g_{12}s^2 + g_{13}s^3 + g_{14}s^4 \cdots, \qquad \text{(II.E-55)}$$

$$g_{10} = 2,$$

$$g_{11} = -(1 + \xi_o),$$

$$g_{12} = (1 + \xi_o^2)/2,$$

$$g_{13} = -(1 + \xi_o^3)/6,$$

$$g_{14} = (1 + \xi_o^4)/24.$$

2) g_2:

$$f(s) = e^{-s\xi_o} + e^{-s\xi} ,$$

$$f'(s) = -\xi_o e^{-s\xi_o} - \xi e^{-s\xi} ,$$

$$f'' = \xi_o^2 e^{-s\xi_o} + \xi^2 e^{-s\xi} ,$$

$$f''' = -\xi_o^3 e^{-s\xi_o} - \xi^3 e^{-s\xi} ,$$

$$f'''' = \xi_o^4 e^{-s\xi_o} + \xi^4 e^{-s\xi} ,$$

$$f(0) = 2, \quad f'(0) = -(\xi_o + \xi), \quad f''(0) = (\xi_o^2 + \xi^2), \quad f'''(0) = -(\xi_o^3 + \xi^3),$$

$$f''''(0) = (\xi_o^4 + \xi^4) ,$$

$$g_2(0) = 1/2$$

$$g_2'(0) = +(\xi_o + \xi)/4$$

$$g_2''(0) = \frac{2(\xi_o + \xi)^2 - 2(\xi_o^2 + \xi)}{8} = \frac{\xi_o \xi}{2},$$

$$g_2'''(0) = \left(-12(\xi_o + \xi)(\xi_o^2 + \xi^2) + 4(\xi_o^3 + \xi^3) + 6(\xi_o + \xi)^3\right)/16$$

$$= \left(-6\,(\xi_o^3 + \xi_o\xi^2 + \xi\xi_o^2 + \xi^3) + 2\xi_o^3 + 2\xi^2 \right.$$

$$\left. + 3\,(\xi_o^3 + 3\xi_o^2\xi + 3\xi_o\xi^2 + \xi^3)\right)/8 ,$$

$$= (-\xi_o^3 + 3\xi_o^2\xi + 3\xi_o\xi^2 - \xi^3)/8 ,$$

$$g_2''''(0) = \left(-72(\xi_o + \xi)^2(\xi_o^2 + \xi^2) + 32(\xi_o + \xi)(\xi_o^3 + \xi^3)\right.$$

$$\left. + 24(\xi_o + \xi)^4 + 24(\xi_o^2 + \xi^2)^2 - 8(\xi_o^4 + \xi^4)\right)/32 ,$$

$$= \left(-9(\xi_o^2 + 2\xi_o\xi + \xi^2)(\xi_o^2 + \xi^2) + 4(\xi_o + \xi)(\xi_o^3 + \xi)\right.$$

$$\left. + 3(\xi_o + \xi)^4 + 3(\xi_o^2 + \xi^2)^2 - (\xi_o^4 + \xi^4)\right)/4 ,$$

$$= (-9\xi_o^4 - 18\xi_o^2\xi^2 - 18\xi_o\xi^3 - 9\xi^4 - 18\xi_o^3\xi$$

$$+ 4\xi_o^4 + 4\xi\xi_o^3 + 4\xi_o\xi^3 + 4\xi^4$$

$$+ 3\xi_o^4 + 12\xi_o^3\xi + 18\xi_o^2\xi^2 + 12\xi_o\xi^3 + 3\xi^4$$

$$+ 3\xi_o^4 + 6\xi_o^2\xi^2 + 3\xi^4 - \xi_o^4 - \xi^4)/4 ,$$

$$= \frac{1}{4}\left(-2\xi_o^3\xi - 2\xi_o\xi^3 + 6\xi_o^2\xi^2\right),$$

$$= -\frac{\xi_o\xi}{2}(\xi_o^2 + \xi^2 - 3\xi_o\xi) ,$$

and

$$g_2 = g_{20} + g_{21}s + g_{22}s^2 + g_{23}s^3 + g_{24}s^4 + \ldots , \qquad \text{(II.E-56)}$$

$$g_{20} = \frac{1}{2} ,$$

$$g_{21} = (\xi_o + \xi)/4 ,$$

$$g_{22} = \xi_o\xi/4 ,$$

$$g_{23} = (-\xi_o^3 + 3\xi_o^2\xi + 3\xi_o\xi^2 - \xi^2)/48 ,$$

$$g_{24} = -\xi_o\xi(\xi_o^2 - 3\xi_o\xi + \xi^2)/48 .$$

3)

$$g_3 = \frac{1 - e^{-s\xi}}{s} = \frac{1 - \left(1 - s\xi + \frac{s^2\xi^2}{2} - \frac{s^3\xi^3}{6} + \frac{s^4\xi^4}{24} - \frac{s^5\xi^5}{120}\right)}{s},$$

$$= \frac{s\xi - \frac{s^2\xi^2}{2} + \frac{s^3\xi^3}{6} - \frac{s^4\xi^4}{24} + \frac{s^5\xi^5}{120}}{s} ,$$

$$= \xi\left(1 - \frac{1}{2}s\xi + \frac{s^2\xi^2}{6} - \frac{s^3\xi^3}{24} + \frac{s^4\xi^4}{120}\right),$$

or

$$g_3 = g_{30} + g_{31}s + g_{32}s^2 + g_{33}s^3 + g_{34}s^4 \cdots , \qquad \text{(II.E-57)}$$

$$g_{30} = \xi ,$$

$$g_{31} = -\xi^2/2 ,$$

$$g_{32} = \xi^3/6 ,$$

$$g_{33} = -\xi^4/24 ,$$

$$g_{34} = \xi^5/120 .$$

4) $$g_4 = s \Big/ \left(s - \frac{s^2}{2} + \frac{s^3}{6} - \frac{s^4}{24} + \frac{s^5}{120} \right) ,$$

$$= 1 \Big/ \left(1 - \frac{s}{2} + \frac{s^2}{6} - \frac{s^3}{24} + \frac{s^4}{120} \right) ,$$

$$f(s) = 1 - \frac{s}{2} + \frac{s^2}{6} - \frac{s^3}{24} + \frac{s^4}{120} ,$$

$$f' = -\frac{1}{2} + \frac{s}{3} - \frac{s^2}{8} + \frac{s^3}{30} ,$$

$$f'' = \frac{1}{3} - \frac{s}{4} + \frac{s^2}{10} ,$$

$$f''' = -\frac{1}{4} + \frac{s}{5} ,$$

$$f'''' = \frac{1}{5} .$$

Thus,

$$f(0) = 1,\ f'(0) = -\frac{1}{2},\ f''(0) = \frac{1}{3},\ f'''(0) = -\frac{1}{4},\ f''''(0) = \frac{1}{5} ,$$

$$g_4(0) = 1 ,$$

$$g_4'(0) = +\frac{1}{2} ,$$

$$g_4''(0) = \frac{1}{2} - \frac{1}{3} = \frac{1}{6} ,$$

$$g_4'''(0) = -1 + \frac{1}{4} + \frac{6}{8} = -\frac{3}{4} + \frac{3}{4} = 0 ,$$

$$g_4''''(0) = -3 + 1 + \frac{3}{2} + \frac{2}{3} - \frac{1}{5} = -\frac{1}{30} ,$$

and

$$g_4 = g_{40} + g_{41}s + g_{42}s^2 + g_{44}s^3 \quad , \qquad \text{(II.E-58)}$$

$$g_{40} = 1 \ ,$$

$$g_{41} = 1/2 \ ,$$

$$g_{42} = 1/12 \ ,$$

$$g_{44} = -1/720 \ ,$$

$$g_1 g_2 = (g_{10} + g_{11}s + g_{12}s^2 + g_{13}s^3 + g_{14}s^4) + (g_{20} + g_{21}s + g_{22}s^2 + g_{23}s^3 + g_{24}s^4) =$$

$$= g_{10}g_{20} + (g_{11}g_{20} + g_{10}g_{21})s + (g_{10}g_{22} + g_{11}g_{21} + g_{12}g_{20})s^2 + (g_{10}g_{23} + g_{11}g_{22} + g_{12}g_{21} + g_{13}g_{20})s^3 + (g_{10}g_{24} + g_{11}g_{23} + g_{12}g_{22} + g_{13}g_{21} + g_{14}g_{20})s^4 \ ,$$

$$g_1 g_2 = b_o + b_1 s + b_2 s^2 + b_3 s^3 + b_4 s^4 \quad , \qquad \text{(II.E-59)}$$

$$b_o = 1 \ ,$$

$$b_1 = -\frac{1}{2}(1 + \xi_o) + \left(\frac{\xi_o + \xi}{2}\right) = -\frac{1}{2} + \frac{\xi}{2} = \frac{\xi - 1}{2} = -\frac{1}{2}(1 - \xi) \ ,$$

$$b_2 = \frac{\xi_o \xi}{2} - \frac{(1 + \xi_o)(\xi_o + \xi)}{4} + \frac{1 + \xi_o^2}{4} \ ,$$

$$= \frac{\xi_o \xi}{2} - \frac{\xi_o}{4} - \frac{\xi}{4} - \frac{\xi_o^2}{4} - \frac{\xi_o \xi}{4} + \frac{1}{4} + \frac{\xi_o^2}{4} \ ,$$

$$= \frac{1}{4} - \frac{(\xi_o + \xi)}{4} + \frac{\xi_o \xi}{4} = \frac{1}{4}(1 - \xi_o - \xi + \xi_o \xi)$$

$$= \left(\frac{1 - \xi}{4}\right)(1 - \xi_o) \ ,$$

$$b_3 = \frac{1}{24}(-\xi_o^2 + 3\xi_o^2 \xi + 3\xi_o \xi^2 - \xi^3) - \frac{\xi_o \xi}{4}(1 + \xi_o) + \frac{1}{8}(1 + \xi_o^2)(\xi_o + \xi) - \frac{1}{12}(1 + \xi_o^3) \ ,$$

$$= \frac{1}{24}(-\xi_o^3 + 3\xi_o^2\xi + 3\xi_o\xi^2 - \xi^3) - \frac{\xi_o\xi}{4} - \frac{\xi_o^2\xi}{4} + \frac{1}{8}(\xi_o + \xi + \xi_o^3 + \xi_o^2\xi)$$

$$- \frac{1}{12}(1 + \xi_o^3) ,$$

$$= \frac{1}{8}\xi_o\xi^2 - \frac{\xi_o\xi}{4} + \frac{\xi_o}{8} + \frac{\xi}{8} - \frac{\xi^3}{24} - \frac{1}{12} ,$$

$$= \frac{1}{24}(3\xi_o\xi^2 - 6\xi_o\xi + 3\xi_o) - (\xi^3 - 3\xi + 2)\frac{1}{24} ,$$

$$= \frac{\xi_o}{8}(\xi - 1)^2 - \frac{\xi - 1}{24}(\xi^2 + \xi - 2) ,$$

$$= \frac{\xi_o}{8}(\xi - 1)^2 - \frac{(\xi - 1)^2}{24}(\xi + 2) ,$$

$$= -\frac{(1 - \xi)^2}{24}(2 + \xi - 3\xi_o) ,$$

$$b_4 = -\frac{\xi_o\xi}{24}(\xi_o^2 - 3\xi_o\xi + \xi^2) - \frac{1 + \xi_o}{48}(-\xi_o^3 + 3\xi_o^2\xi + 3\xi_o\xi^2 - \xi^3)$$

$$+ \frac{\xi_o\xi}{8}(1 + \xi_o^2) - \frac{\xi_o + \xi}{24}(1 + \xi_o^3) + \frac{1}{48}(1 + \xi_o^4) ,$$

$$= \frac{1}{48}(-2\xi_o^3\xi + 6\xi_o^2\xi - 2\xi_o\xi^3 + \xi_o^3 - 3\xi_o^2\xi - 3\xi_o\xi^2 + \xi^3 + \xi_o^4 - 3\xi_o^3\xi$$

$$-3\xi_o^2\xi + \xi_o\xi^3 + 6\xi_o\xi + 6\xi_o^3\xi - 2\xi_o - 2\xi_o^4 - 2\xi - 2\xi\xi_o^3 + 1 + \xi_o^4)$$

$$= \frac{1}{48}\Big(\xi_o(1 - 4\xi + 6\xi - 3\xi) + \xi_o^2(6\xi^2 - 3\xi - 3\xi^2)$$

$$+ \xi_o(-2\xi^3 - 3\xi^2 + \xi^3 + 6\xi - 2) + (\xi^3 - 2\xi + 1)\Big) ,$$

$$= \frac{1}{48}\Big(\xi_o^3(1-\xi) + 3\xi_o^2(\xi^2 - \xi) + \xi_o(-\xi^3 - 3\xi^2 + 6\xi - 2) + (\xi^3 - 2\xi + 1)\Big),$$

$$= \frac{1}{48}\Big(\xi_o^3(1 - \xi) + 3\xi\xi_o^2(\xi - 1) + \xi_o(\xi - 1)(-\xi^2 - 4\xi + 2) + (\xi - 1)(\xi^2 + \xi - 1)\Big) ,$$

$$= \frac{1 - \xi}{48}\Big(\xi_o^3 - 3\xi\xi_o^2 + (\xi^2 + 4\xi - 2)\xi_o + (1 - \xi - \xi^2)\Big) ,$$

$$= \frac{1-\xi}{48}\left((1 - 2\xi_o + \xi_o^3) + \xi(-3\xi_o^2 + 4\xi_o - 1) + \xi^2(\xi_o - 1)\right),$$

$$= \frac{1-\xi}{48}\left((1-\xi_o)(1 - \xi_o - \xi_o^2) + \xi(1-\xi_o)(-1 + 3\xi_o) + \xi^2(\xi_o - 1)\right),$$

$$= \frac{(1-\xi)(1-\xi_o)}{48}\left((1 - \xi_o - \xi_o^2) + \xi(3\xi_o - 1) - \xi^2\right),$$

$$g_3 g_4 = c_o + c_1 s + c_2 s^2 + c_3 s^3 + c_4 s^4 , \qquad \text{(II.E-60)}$$

$$c_o = g_{30} g_{40} = \xi ,$$

$$c_1 = g_{31} g_{40} + g_{30} g_{41} ,$$

$$= \left(\frac{-\xi}{2} + \frac{1}{2}\right)\xi = \frac{\xi}{2}(1 - \xi) ,$$

$$c_2 = g_{30} g_{42} + g_{31} g_{41} + g_{32} g_{40} ,$$

$$= \xi\left(\frac{1}{12} - \frac{\xi}{4} + \frac{\xi^2}{6}\right) = \frac{\xi}{12}(1 - 3\xi + 2\xi^2) = \frac{\xi(1-\xi)}{12}(1 - 2\xi) ,$$

$$c_3 = g_{30} g_{43} + g_{31} g_{42} + g_{32} g_{41} + g_{33} g_{40} ,$$

$$= \xi\left(-\frac{\xi}{24} + \frac{\xi^2}{12} - \frac{\xi^3}{24}\right) = -\frac{\xi^2}{24}(1 - 2\xi + \xi^2) = \frac{-\xi^2(1-\xi)^2}{24} ,$$

$$c_4 = g_{30} g_{44} + g_{31} g_{43} + g_{32} g_{42} + g_{33} g_{41} + g_{34} g_{40} ,$$

$$= \xi\left(-\frac{1}{720} + \frac{\xi^2}{72} - \frac{\xi^3}{48} + \frac{\xi^4}{120}\right) ,$$

$$= -\frac{\xi}{720}(1 - 10\xi^2 + 15\xi^3 - 6\xi^4) ,$$

$$= \frac{-\xi(1-\xi)}{720}(1 + \xi - 9\xi^2 + 6\xi^3) ,$$

$$g_1 g_2 g_3 g_4 = d_o + d_1 s + d_2 s^2 + d_3 s^3 + d_4 s^4 , \qquad \text{(II.E-61)}$$

$$d_o = c_o b_o = \xi ,$$

$$d_1 = c_o b_1 + c_1 b_o = \frac{-\xi(1-\xi)}{2} + \frac{\xi(1-\xi)}{2} = 0 !!!!$$

$$d_2 = c_o b_2 + c_1 b_1 + c_2 b_o ,$$

$$= \frac{\xi(1-\xi)(1-\xi_o)}{4} - \frac{(1-\xi)(1-\xi)}{2}\xi + \frac{\xi(1-\xi)}{12}(1-2\xi) ,$$

$$= \frac{\xi(1-\xi)}{4}\left(1 - \xi_o - 1 + \xi + \frac{1-2\xi}{3}\right)$$

$$= \frac{\xi(1-\xi)}{4}\left(\xi - \xi_o + \frac{1-2\xi}{3}\right),$$

$$= \frac{\xi(1-\xi)}{12}(\xi - 3\xi_o + 1) ,$$

$$d_3 = c_o b_3 + c_1 b_2 + c_2 b_1 + c_3 b_o ,$$

$$= \frac{-\xi(1-\xi)^2}{24}(2 + \xi - 3\xi_o) + \frac{\xi}{2}(1-\xi)\left(\frac{1-\xi}{4}\right)(1 - \xi_o$$

$$- \frac{\xi(1-\xi)}{12}(1-\xi)\frac{(1-\xi)}{2} - \frac{\xi^2(1-\xi)^2}{24} ,$$

$$= -\frac{\xi(1-\xi)^2}{24}(2 + \xi - 3\xi_o - 3 + 3\xi_o + 1 - 2\xi + \xi) = 0 !!!!$$

$$d_4 = c_o b_4 + c_1 b_3 + c_2 b_2 + c_3 b_1 + c_4 b_o ,$$

$$= \frac{\xi(1-\xi)(1-\xi_o)}{48}\left((1 - \xi_o - \xi_o^2) + \xi(3\xi_o - 1) - \xi^2\right)$$

$$- \frac{\xi}{2}(1-\xi)\frac{(1-\xi)^2}{24}(2 + \xi - 3\xi_o)$$

$$+ \frac{\xi(1-\xi)}{12}(1-2\xi)\frac{(1-\xi)}{4}(1-\xi_o) + \frac{\xi^2(1-\xi)^2}{24}\frac{(1-\xi)}{2}$$

$$- \frac{\xi(1-\xi)}{720}(1 + \xi - 9\xi^2 + 6\xi^3) ,$$

$$= \frac{\xi(1-\xi)}{720}15\left[\left(1 - \xi_o - \xi_o^2 + 3\xi\xi_o - \xi - \xi^2 - \xi_o + \xi_o^2 + \xi_o^3 - 3\xi\xi_o^2\right.\right.$$

$$+\xi\xi_o + \xi_o\xi^2\Big) - 15\Big(2 + \xi - 3\xi_o - 4\xi - 2\xi^2 + 6\xi\xi_o + 2\xi^2 + \xi^3 - 3\xi^2\xi_o\Big)$$

$$+ 15\Big(1 - 3\xi + 2\xi^2 - \xi_o + 3\xi_o\xi - 2\xi_o\xi^2\Big)$$

$$+ 15\Big(\xi - 2\xi^2 + \xi^3\Big)\Big(1 + \xi - 9\xi^2 + 6\xi^3\Big)\Big],$$

$$= \frac{\xi(1-\xi)}{720}\Big(-1 - \xi - 6\xi^2 - 6\xi^3 + 15\xi_o^3 + 15\xi\xi_o - 45\xi\xi_o^2 + 30\xi_o\xi^2\Big) .$$

Summarizing,

$$\eta = \xi + \frac{\xi(1-\xi)}{12}\Big(f_1 s^2 + f_2 s^4\Big) = \text{for small } s , \qquad \text{(II.E-62)}$$

$$f_1 = 1 + \xi - 3\xi_o ,$$

$$f_2 = \frac{1}{60}(-1 - \xi - 6\xi^2 - 6\xi^3 + 15\xi_o^3 + 15\xi\xi_o$$

$$-45\xi\xi_o^2 + 30\xi_o\xi^2)$$

As a small check on Eq. (II.E-63), we note

(a) $\eta(s) = \eta(-s)$,

(b) $\eta(o) = o$, $\eta(1) = 1$,

(c) We know that at $\xi = \xi_o$ $\eta_{\xi\xi} = 0$,

$$\eta_\xi = 1 + \frac{1-2\xi}{12}(f_1 s^2 + f_2 s^4) + \frac{\xi - \xi^2}{12}\Big(f_{1_\xi} s^2 + f_{2_\xi} s^4\Big),$$

$$\eta_{\xi\xi} = -\frac{2}{12}(f_1 s^2 + f_2 s^4) + \frac{2(1-2\xi)}{12}(f_{1_\xi} s^2 + f_{2_\xi} s^4) + \frac{\xi - \xi^2}{12}(f_{1_{\xi\xi}} s^2 + f_{2_{\xi\xi}} s^4) ,$$

$$\eta_{\xi\xi} = as^2 + bs^4 ,$$

$$a = +\frac{2}{12}\Big(-f_1 + (1-2\xi)f_{1_\xi} + \frac{\xi - \xi^2}{2} f_{1_{\xi\xi}}\Big) ,$$

$$b = \frac{2}{12}\Big(-f_2 + (1-2\xi)(f_2)_\xi + \frac{\xi - \xi^2}{2}(f_2)_{\xi\xi}\Big)$$

At $\xi = \xi_o$, $f_1 = 1 - 2\xi$, $f_{1_\xi} = 1$, $f_{1_{\xi\xi}} = 0$:

$$a = \frac{1}{6}\left(-(1 - 2\xi) + 1 - 2\xi\right) = 0 \ .$$

At $\xi = \xi_o$, $f_2 = \frac{1}{60}(-1 - \xi + 9\xi^2 - 6\xi^3)$,

$$f_{2_\xi} = \frac{1}{60}(-1 - 12\xi - 18\xi^2 + 15\xi_o - 45\xi_o^2 + 60\xi_o\xi) \ ,$$

$$= \frac{1}{60}(-1 + 3\xi - 3\xi^2) \text{ at } \xi = \xi_o \ ,$$

$$f_{2_{\xi\xi}} = \frac{1}{60}(-12 - 36\xi + 60\xi_o) = \frac{1}{60}(-12 + 24\xi) \text{ at } \xi = \xi_o \ ,$$

$$b = \frac{1}{360}\left(1 + \xi - 9\xi^2 + 6\xi^3 + (1 - 2\xi)(-1 + 3\xi - 3\xi^2) + (\xi - \xi^2)(-6 + 12\xi)\right)$$

$$= \frac{1}{360}\left(1 + \xi - 9\xi^2 + 6\xi^3 - 1 + 3\xi - 3\xi^2 + 2\xi - 6\xi^2 + 6\xi^3 - 6\xi + 12\xi^2 + 6\xi^2 - 12\xi^3\right) = 0 \ ,$$

(d) at $\xi_o = \frac{1}{2}$, $\eta_\xi(\frac{1}{2} + \epsilon) = \eta_\xi(\frac{1}{2} - \epsilon)$,

$$\eta_\xi = 1 + as^2 + bs^4 \ ,$$

$$a = \frac{1}{12}\left((1 - 2\xi)f_1 + (\xi - \xi^2)(f_1)_\xi\right).$$

At $\xi_o = \frac{1}{2}$, $f_1 = \xi - \frac{1}{2}$, $f_{1_\xi} = 1$,

$$a = \frac{1}{12}\left((1 - 2\xi)(\xi - \tfrac{1}{2}) + \xi(1 - \xi)\right) \ ,$$

$$= \frac{1}{12}\left(-2(\xi - \tfrac{1}{2})^2 - (\xi - \tfrac{1}{2})^2 + \tfrac{1}{4}\right),$$

$$b = \frac{1}{12}\left((1 - 2\xi) f_2 + (\xi - \xi^2)(f_2)_\xi\right)$$

At $\xi_o = \frac{1}{2}$, $f_2 = \frac{1}{480}(7 - 38\xi + 72\xi^2 - 48\xi^3)$,

$$= \frac{2\xi - 1}{480}\left(-6(2\xi - 1)^2 - 1\right).$$

At $\xi_o = \frac{1}{2}$, $(f_2)_\xi = \frac{1}{240}(-19 + 72\xi - 72\xi^2)$,

$$= \frac{1}{240}\left(-18(2\xi - 1)^2 - 1\right).$$

Thus,

$$12b = \frac{(1-2\xi)^2}{480}\left(1 + 6(1-2\xi)^2\right) - \left((\xi - \tfrac{1}{2})^2 - \tfrac{1}{4}\right)\left(\frac{1 + 18(2\xi - 1)^2}{240}\right).$$

The range of validity of Eq. (II.E-62) still needs to be defined. However we proceeded experimentally - in the case to be described in Part C. Eq. (II.E-62) was used for $|s| < .01$. In this case we also used

$$\frac{\partial \eta}{\partial \xi} = 1 + \frac{1-2\xi}{12}(f_1 s^2 + f_2 s^4) + \frac{\xi(1-\xi)}{12}(f_{1_\xi} s^2 + f_{2_\xi} s^4) , \qquad \text{(II.E-62.1)}$$

$$\frac{\partial^2 \eta}{\partial \xi^2} = -\frac{1}{6}(f_1 s^2 + f_2 s^4) + \frac{1-2\xi}{6}(f_{1_\xi} s^2 + f_{2_\xi} s^4) \qquad \text{(II.E-62.2)}$$

$$+ \frac{\xi(1-\xi)}{12}(f_{1_{\xi\xi}} s^2 + f_{2_{\xi\xi}} s^4) ,$$

$$\frac{\partial \eta}{\partial \xi_o} = \frac{\xi(1-\xi)}{12}(f_{1_{\xi_o}} s^2 + f_{2_{\xi_o}} s^4) , \qquad \text{(II.E-62.3)}$$

$$\frac{\partial \eta}{\partial s} = \frac{\xi(1-\xi)}{6}(f_1 s + 2 f_2 s^3). \qquad \text{(II.E-62.4)}$$

$$f_{1_\xi} = 1 ,$$

$$f_{1_{\xi\xi}} = 0 ,$$

$$f_{1_{\xi_o}} = -3 ,$$

$$f_{2_\xi} = \frac{1}{60}(-1 - 12\xi - 18\xi^3 + 15\xi_o - 45\xi_o^2 + 60\xi_o\xi) ,$$

$$f_{2_{\xi\xi}} = \frac{1}{60}(-12 - 36\xi + 60\xi_o) ,$$

$$f_{2_{\xi o}} = \frac{1}{60}\left(45\xi_o^2 + 15\xi - 90\xi\xi_o + 30\xi^2\right).$$

PART C.

In the burst problem, which will be discussed in detail in Section II.E.3, the initial flow is constant and only the presence of a very steep gradient in temperature (which occurs over a small region) causes flow to occur. Thus initially it is desired to keep all nodes in this region. As the flow moved out, it is necessary to expand the region of computation also. However, the shock front remains quite narrow and it would seem advantageous to keep smaller nodes in the vicinity of the shock. Thus, we attempted the following:

Let $\xi o = \xi o(t)$ be the position of the shock front, and suppose it is specified.

We want to satisfy

$$\left(\frac{\eta_\xi(\xi o)}{r_1 - r_o}\right)(t) = \left(\frac{\eta_\xi(\xi o)}{r_1 - r_o}\right)(t=o) \ ,$$

where $\eta_\xi = \frac{\partial \eta}{\partial \xi}$.

That is, the actual Δr at $\xi = \xi_o$ should be maintained at its initial value. If we let

$$A = \frac{\eta_\xi(\xi o)}{r_1 - r_o} \quad \text{at } t = o \ ,$$

$$\eta_\xi(\xi o) = A(r_1 - r_o) \ , \qquad \text{(II.E-63)}$$

$$\eta_\xi(\xi_o) = \frac{se^{-s\xi o}(1 + e^{-s\xi o})(e^{-s\xi o} + e^{-s})}{(1 - e^{-s})\, 4e^{-2\xi_o}} \ ,$$

$$= \frac{s(e^{s\xi o} + 1)(1 + e^{s(1 - \xi_o)})}{4(e^s - 1)} \ ,$$

$$= \frac{s}{4(e^{+s} - 1}\left(1 + e^{s\xi o} + e^s + e^{s(1 - \xi_o)}\right) .$$

At any time t, then, this equation is to be solved:

$$s = \frac{4(e^s - 1)A(r_1 - r_o)}{1 + e^{s\xi_o} + e^s + e^{s(1-\xi_o)}} = g(s) \quad A(r_1 - r_o) \qquad \text{(II.E-64)}$$

where A is given and ξ_o, r_o, r_1 are given functions of t.

$$\frac{g'(s)}{4} = \frac{\left(1 + e^{s\xi_o} + e^s + e^{s(1-\xi_o)}\right) e^s - (e^s - 1)\left(\xi_o e^{s\xi_o} + e^s + (1-\xi_o)e^{s(1-\xi_o)}\right)}{(\quad)^2},$$

$$= e^s + e^{s(1+\xi_o)} + e^{2s} + e^{s(2-\xi_o)} + \xi_o e^{s\xi_o} + e^s + (1 - \xi_o)e^{s(1-\xi_o)}$$

$$- \frac{\xi_o e^{s(1+\xi_o)} - e^{2s} - (1 - \xi_o)e^{s(2-\xi_o)}}{(\quad)^2}$$

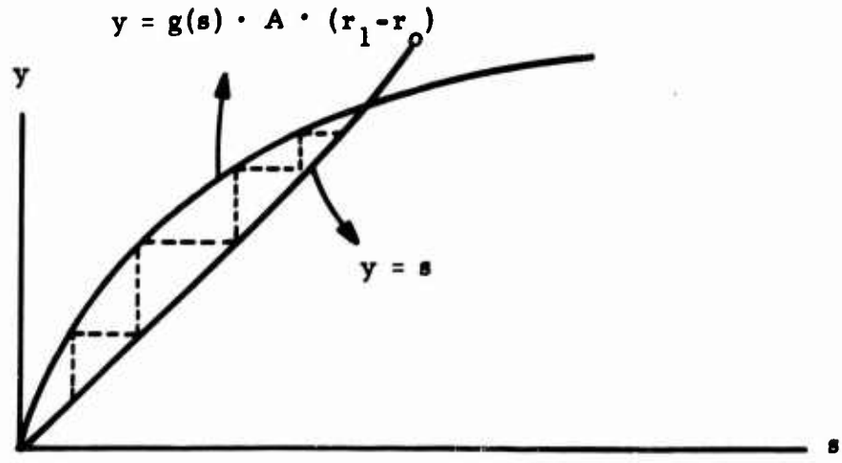
$$= \frac{e^s + (1 - \xi_o)e^{s(1+\xi_o)} + \xi_o e^{s(2-\xi)} + \xi_o e^{s\xi_o} + e^s + (1 - \xi_o)e^{s(1-\xi_o)}}{(\quad)^2}$$

or

$$g'(s) > 0$$

$$g'(0) = \frac{4\left(1 + (1 - \xi_o) + \xi_o + \xi_o + 1 + 1 - \xi_o\right)}{16} = 1 \ .$$

Thus, if $r_1 - r_o$ is increasing (as is the case in our particular problem) and if $A \geq 1$ (as it is in our case), then $g'(s)\, A\, (r_1 - r_o) > 0$ and $g'(0) \cdot A \cdot (r_1 - r_o) > 1$. We have then



and successive iterations, as indicated, can be used to solve the equation.

We also need to determine $\frac{ds}{dt} = s'$ from Eq. (II.E-64)

$$s'(1 + e^{s\xi_o} + e^{s} + e^{s(1-\xi_o)} + s\,s'(\xi_o e^{s\xi_o} + e^{s} + (1-\xi_o)e^{s(1-\xi_o)} + s\xi_o'\left(se^{s\xi_o} - se^{s(1-\xi_o)}\right) =$$

$$4Ae^{s}(r_1 - r_o)s' + 4A(e^{s} - 1)(r_1' - r_o') \quad .$$

Let

$$g_1 = 1 + e^{s\xi_o} + e^{s} + e^{s(1-\xi_o)} - 4e^{s}(r_1 - r_o) + s\left(\xi_o e^{s\xi_o} + e^{s} + (1-\xi_o)e^{s(1-\xi_o)}\right) \quad ,$$

$$g_2 = 4A(e^{s} - 1)(r_1' - r_o') - s^2\xi_o'\left(e^{s\xi_o} - e^{s(1-\xi)}\right).$$

Then

$$s' = \frac{g_2}{g_1} \quad . \qquad \text{(II.E-65)}$$

Clearly, there is a difficulty with eq. (II.E-65) at s = 0. For small s, from Eq. (II.E-62)

$$\frac{d\eta}{d\xi} = 1 + \left(\frac{1 - 2\xi}{12}\right)\left(f_1 s^2 + f_2 s^4\right) + \frac{\xi - \xi^2}{12}\left(f_{1_\xi} s^2 + f_{2_\xi} s^4\right) ,$$

$$f_1(\xi_o) = 1 - 2\xi_o ,$$

$$f_2(\xi_o) = \frac{1}{60}(-1 - \xi_o + 9\xi_o^2 - 6\xi_o^3) ,$$

$$f_{1_\xi}(\xi_o) = 1 ,$$

$$f_{2_\xi}(\xi_o) = \frac{1}{60}(-1 + 3\xi_o - 3\xi_o^2) .$$

Then, from Eq. (II.E-63)

$$1 + \left(\frac{(1 - 2\xi_o)}{12}\right)\left(f_1 s^2 + f_2 s^4\right) + \frac{(\xi_o - \xi_o^2)}{12}\left(f_{1_\xi} s^2 + f_{2_\xi} s\right) =$$

$$A(r_1 - r_o) . \qquad \text{(II.E-65)}$$

Let

$$f_1' = \frac{df_1(\xi_o)}{d\xi_o} , \left(f_{1_\xi}\right)' = \frac{d}{d\xi_o}\left(\frac{\partial f_1}{\partial \xi}(\xi = \xi_o)\right) , \text{ etc.}$$

Then,

$$\left(\frac{(1 - 2\xi_o)}{12}\left(2f_1 s + 4f_2 s^3\right)\right) + \frac{(\xi_o - \xi_o^2)}{12}\left(2f_{1_\xi} s + 4f_{2_\xi} s^3\right) s'$$

$$+\left(-\frac{1}{6}\left(f_1 s^2 + f_2 s^4\right) + \frac{(1 - 2\xi_o)}{12}\left(f_1' s + f_2' s^4\right)\right.$$

$$\left. + \frac{(1 - 2\xi_o)}{12}\left(f_{1_\xi} s^2 + f_{2_\xi} s^4\right) + \frac{(\xi_o - \xi_o^2)}{12}\left(f_{1_\xi}' s^2 + f_{2_\xi}' s^4\right)\right)\xi_o'$$

$$= A(r_1' - r_o') .$$

Let

$$g_1 = s\left(f_1\frac{(1-2\xi_o)}{6} + f_{1_\xi}\frac{(\xi_o - \xi_o^2)}{6}\right) + s^3\left(\frac{f_2(1-2\xi_o)}{3} + f_{2_\xi}\frac{(\xi_o - \xi_o^2)}{3}\right),$$

$$g_2 = A(r_1' - r_o') - \left(-\frac{1}{6}(f_1 s^2 + f_2 s^4) + \frac{(1-2\xi_o)}{12}(f_1' s^2 + f_2' s^4)\right.$$

$$+\frac{(1-2\xi_o)}{12}(f_{1_\xi} s^2 + f_{2_\xi} s^4)$$

$$\left. + \frac{(\xi_o - \xi_o^2)}{12}(f_{1_\xi}' s^2 + f_{2_\xi}' s^4)\right)\xi_o' .$$

Then,

$$s' = \frac{g_2}{g_1} \qquad \text{(II.E-66)}$$

Eq. (II.E-66) need not be well-behaved at s = 0. However, in the differential equations, the quantity that is needed is $\eta_s s'$. From Eq. (II.E-66) and Eq. (II.E-62.4), it is seen that $\eta_s s'$ is well-behaved at s = 0.

Finally, it is of some interest to comment on the effectiveness of the transformation. The fact is that in the case of the burst problem it proved to be practically useless. The transformation worked as expected. However, it turned out that the region of the shock was not the only area where fine spacing was required. A strong shock reflecting to and from the center of the sphere occurred in this problem, and consequently fine spacing was required at every point at some time or another. It is possible that a different spacing transformation would have been more effective. However, it is possible that unequal spacing of points can only be a "second order" improvement during the early part of the burst problem.

II.E.3 BOUNDARY CONDITIONS

The question now arises as to the existence and uniqueness of a solution to Eqs. (II.E-37). In particular, one would like boundary conditions such that these boundary conditions, together with initial conditions, determine a unique solution to Eqs. (II.E-37). In such generality, this is still an unsolved problem. As a first step in determining proper boundary conditions, we shall first investigate the Cauchy problem for a pure initial value problem. The goal here is to apply the Cauchy-Kowalewsky Theorem (II.E-2, p. 39-50). Roughly, this theorem says the following:

> If in Eqs. (II.E-37) all elements of the matrix A and the vector B are analytic in all arguments; and if the initial data are analytic; and if, after eqs. (II.E-37) are reduced to a first order quasilinear system, none of the corresponding characteristics lie in the surface of the initial data (in our case this surface would be the $t = 0$ plane); then there is a unique solution to Eqs. (II.E-37) which is valid in some region of $t = 0$ and which assumes the initial data for $t = 0$.

Note, then, that in this situation no additional boundary conditions will be needed. Since in our problems we do not expect this to be the case (that is, we expect that additional boundary conditions will be needed), we do not expect to be able to satisfy the hypotheses of this theorem. Nevertheless, an investigation of the characteristics and of the initial data will enable us to proceed at least intuitively to the specification of boundary conditions. In Part A, we will apply this kind of analysis to Eq. (II.E-37) and to two special subcases. In Part B, we will apply the results of this work to four specific physical problems.

PART A

In general, the characteristics are calculated by inquiring along what curves the partial derivatives in the direction orthogonal to the curve cannot be calculated. (Intuitively, one expects then that initial data on such a curve will not determine a unique solution.) Courant and Hilbert (II.E-2, p. 173-175) have introduced techniques which considerably reduce the labor involved in the calculation of these characteristics. Rather than becoming involved in the details of this work, we shall proceed in a simpler fashion. Since our problem is only two-dimensional, this can be done without an extreme amount of unnecessary labor.

The first step is to reduce the equations to first order. This is accomplished by introducing the following definitions:

$$p = \frac{\partial V}{\partial \eta} ,$$

$$q = \frac{\partial T}{\partial \eta} , \qquad \text{(II.E-67)}$$

$$r = \frac{\partial C}{\partial \eta} .$$

Equations (II.E-37) can now be written as

$$\frac{\partial \rho}{\partial t} = - a_1 \frac{\partial \rho}{\partial \eta} - a_2 p - a_3 , \qquad \text{(II.E-68)}$$

$$\frac{\partial V}{\partial t} = \bar{b}_1 \frac{\partial p}{\partial \eta} + \bar{b}_2 p - \bar{b}_3 V - b_1 p - b_2 \frac{\partial \rho}{\partial \eta} - b_3 q - b_4 r , \qquad \text{(II.E-69)}$$

$$\frac{\partial T}{\partial t} = \bar{c}_1 \frac{\partial q}{\partial \eta} + \bar{c}_2 q + \bar{c}_3 q^2 + \bar{c}_4 + \bar{c}_5 qr - \bar{c}_6 r^2 \qquad \text{(II.E-70)}$$

$$+ \bar{c}_7 \frac{\partial r}{\partial \eta} + \bar{c}_8 r - c_1 q - c_2 p - c_3 T ,$$

$$\frac{\partial C}{\partial t} = \bar{d}_1 \frac{\partial r}{\partial \eta} - \bar{d}_2 r^2 + \bar{d}_3 r + \bar{d}_4 qr + \bar{d}_5 - \bar{d}_1 r . \qquad \text{(II.E-71)}$$

If we now define the vector $X = \begin{pmatrix} p \\ q \\ r \\ \rho \\ V \\ T \\ C \end{pmatrix}$, Eqs. (II.E-67 - II.E-71) can be written as

$$A_1 \frac{\partial X}{\partial t} + A_2 \frac{\partial X}{\partial \eta} = A_3 \qquad \text{(II.E-72)}$$

$$A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad \text{(II.E-73)}$$

$$A_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & a_1 & 0 & 0 & 0 \\ -\bar{b}_1 & 0 & 0 & b_2 & 0 & 0 & 0 \\ 0 & -\bar{c}_1 & -\bar{c}_7 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\bar{d}_1 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(II.E-74)}$$

$$A_3 = \begin{pmatrix} p \\ q \\ r \\ -a_2 p - a_3 \\ \bar{b}_2 p - \bar{b}_3 V - b_1 p - b_3 q - b_4 r \\ \bar{c}_2 q + \bar{c}_3 q^2 + \bar{c}_4 + \bar{c}_5 qr - \bar{c}_6 r^2 + \bar{c}_8 r \\ \qquad\qquad - c_1 q - c_2 p - c_3 T \\ -\bar{d}_2 r^2 + \bar{d}_3 r + \bar{d}_4 qr + \bar{d}_5 - \bar{d}_1 r \end{pmatrix} \qquad \text{(II.E-75)}$$

Note that all elements of the matrices A_1 and A_2 and of the vector A_3 are functions only of t, η, and of the elements of the vector X. Thus, the system (II.E-72) is a quasi-linear.

We now consider a transformation of the t, η plane at some point in the t, η plane. Since we are interested only in this particular point, we may consider the transformation to be linear:

$$\left.\begin{aligned} t &= \alpha_1\theta + \alpha_2\zeta \\ \eta &= \alpha_3\theta + \alpha_4\zeta \end{aligned}\right\} \quad (\theta, \zeta) \rightarrow (t, \eta) . \qquad \text{(II.E-76)}$$

By definition, t, η are taken to be orthogonal. On t - constant $\frac{d\theta}{d\zeta} = -\frac{\alpha_2}{\alpha_1}$ and on η = constant $\frac{d\theta}{d\zeta} = -\frac{\alpha_4}{\alpha_3}$. By orthogonality we must have $-\frac{\alpha_2}{\alpha_1} = -1/(-\alpha_4/\alpha_3)$, or

$$\alpha_1\alpha_3 + \alpha_2\alpha_4 = 0. \qquad \text{(II.E-77)}$$

The inverted transformation is the following:

$$\begin{aligned} \theta &= \beta_1 t + \beta_2\eta , \\ \zeta &= \beta_3 t + \beta_4\eta , \end{aligned} \qquad \text{(II.E-78)}$$

where

$$\begin{aligned} \beta_1 &= \alpha_4/(\alpha_1\alpha_4 - \alpha_3\alpha_2) , \\ \beta_2 &= -\alpha_2/(\alpha_1\alpha_4 - \alpha_3\alpha_2) , \\ \beta_3 &= -\alpha_3/(\alpha_1\alpha_4 - \alpha_3\alpha_2) , \\ \beta_4 &= \alpha_1/(\alpha_1\alpha_4 - \alpha_3\alpha_2) . \end{aligned} \qquad \text{(II.E-79)}$$

We require that θ, ζ be orthogonal also, or that $\beta_1\beta_3 + \beta_2\beta_4 = 0$. From Eqs. (II.E-79) this becomes

$$\alpha_1\alpha_2 + \alpha_3\alpha_4 = 0. \qquad \text{(II.E-80)}$$

As a final condition on the transformation we require that the determinant be positive (this preserves orientation):

$$\alpha_1\alpha_4 - \alpha_3\alpha_2 > 0 \,. \qquad \text{(II.E-81)}$$

Under this transformation, Eq. (II.E-72) becomes

$$A_1(\alpha_1 X_\theta + \alpha_2 X_\zeta) + A_2(\alpha_3 X_\theta + \alpha_4 X_\zeta) = A_3 \,,$$

or

$$(\alpha_1 A_1 + \alpha_3 A_2) X_\theta + (\alpha_2 A_1 + \alpha_4 A_2) X_\zeta = A_3 \,. \qquad \text{(II.E-82)}$$

Assume now that data is given in a θ = constant plane. In order for this plane to be characteristic at the point in question, it must not be possible to obtain X_θ; that is, we must have det $|\alpha_1 A_1 + \alpha_3 A_2| = 0$. (Note that the definition of ζ is quite unnecessary in terms of finding the characteristics. The technique given by Courant and Hilbert (II.E-2, p. 173-175) does not require the introduction of the superfluous coordinates.) Let $A_4 = \alpha_1 A_1 + \alpha_3 A_2$. Then,

$$A_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & \alpha_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \alpha_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \alpha_3 \\ 0 & 0 & 0 & (\alpha_1 + a_1\alpha_3) & 0 & 0 & 0 \\ -\bar{b}_1\alpha_3 & 0 & 0 & b_2\alpha_3 & \alpha_1 & 0 & 0 \\ 0 & -\bar{c}_1\alpha_3 & -\bar{c}_7\alpha_3 & 0 & 0 & \alpha_1 & 0 \\ 0 & 0 & -\bar{d}_1\alpha_3 & 0 & 0 & 0 & \alpha_1 \end{pmatrix} , \qquad \text{(II.E-83)}$$

$$|A_4| = \alpha_3^6 (\alpha_1 + a_1\alpha_3) \bar{b}_1 \bar{c}_1 \bar{d}_1 \,.$$

Therefore, $|A_4| = 0$ requires $\alpha_3 = 0$ or $\alpha_1 + a_1\alpha_3 = 0$.

Consider first $\alpha_3 = 0$. From Eq. (II.E-77) either α_2 or $\alpha_4 = 0$. But from Eq. (II.E-81) α_3 and α_4 cannot both be zero. Thus, $\alpha_2 = 0$ and from Eq. (II.E-79) $\beta_2 = 0$. But then from Eq. (II.E-78) θ = constant corresponds to a t = constant plane. This means that six characteristics correspond to t = constant planes. Intuitively, this is the expected result. The last three equations of (II.E-67) are "individually" parabolic (that is, if each of these three equations is considered independently as a function only of its dominant variable, it is parabolic) and each would be expected to produce two t = constant characteristics.

Consider now $\alpha_1 + a_1\alpha_3 = 0$, or $\alpha_1 = -a_1\alpha_3$. Note that $\alpha_3 \neq 0$. For then $\alpha_1 = 0$ and this violates Eq. (II.E-81). From Eq. (II.E-80), $-a_1\alpha_2\alpha_3 + \alpha_3\alpha_4 = 0$, or $\alpha_4 = a_1\alpha_2$. From Eq. (II.E-77), $-a_1\alpha_3^2 + a_1\alpha_2^2 = 0$, or $\alpha_2 = \pm\alpha_3$. At this point, then, we have $\alpha_1 = -a_1\alpha_3$, $\alpha_2 = \pm\alpha_3$, $\alpha_4 = \pm a_1\alpha_3$. Substituting into Eq. (II.E-81), $\pm a_1^2\alpha_3^2 \pm \alpha_3^2 = \pm\alpha_3^2(1 + a_1^2) > 0$, or we must choose the plus sign. Thus, $\alpha_1 = -a_1\alpha_3$ and $\alpha_2 = \alpha_3$. From Eq. (II.E-78), on θ = constant, $\frac{dt}{d\eta} = -\frac{\beta_2}{\beta_1} = \frac{\alpha_3}{a_1\alpha_3}$, or $\frac{dt}{d\eta} = \frac{1}{a_1}$. Again this is intuitively as expected. Equation (II.E-68), considered only as an equation in ζ, produces precisely this characteristic.

Summarizing, the characteristics of Eq. (II.E-37) are

$$\frac{dt}{d\eta} = 0: \text{ six characteristics,}$$

$$\frac{dt}{d\eta} = \frac{1}{a_1} . \qquad \text{(II.E-84)}$$

As noted earlier, the question of existence and uniqueness of a solution to Eq. (II.E-37) represents an unsolved problem. However, theory is very well developed for equations of the form (II.E-72) when the initial data curve is not characteristic. Let us now briefly and roughly state a result of this theory. We will follow Lax (II.E-72, p. 107). See also Courant and Hilbert (II.E-2, p/ 471).

If t = 0 is not characteristic, then A_1 is not singular, or Eq. (II.E-72) can be written as

$$\frac{\partial X}{\partial t} = A\frac{\partial X}{\partial \eta} + C. \qquad \text{(II.E-85)}$$

Suppose that X represents an n-vector, and that the region of interest is $t \geq 0$, $0 \leq \eta \leq 1$. The following assumptions are needed.

1) Suppose the matrix is diagonalizable; that is, there exists a matrix M such that $MAM^{-1} = D = \text{diagonal}\ (\lambda_1, \ldots, \lambda_n)$.

2) Suppose that at $\eta = 0$ m_1 of the $\{\lambda_1\}$ are negative and that at $\eta = 1$ m_2 of the λ_1 are positive, while none of the remaining characteristics are zero at any point of $\eta = 0$ and $\eta = 1$. (This statement needs to be made more precise, since, in general, for $t > 0$ the λ_i depend on the unknown solution X, as does the matrix P. Also, the restriction that none of the λ_j be zero can probably be suppressed for the special case that one of the λ_i is identically zero - this does occur in some of our problems.)

3) Suppose that at $\eta = 0$ we specify m_1 additional functions with the following property:

Suppose P to be a constant matrix and perform the transformation $Y = MX$.

Then locally Eq. (II.E-56) becomes $\dfrac{\partial Y}{\partial t} = D\dfrac{\partial Y}{\partial x} + C_1$.

Let $\left\{\lambda_{i_1}, \ldots, \lambda_{i_{m_1}}\right\}$ denote the negative eigenvalues. Then $\left\{y_{i_1}, \ldots, y_{i_{m_1}}\right\}$

must be uniquely determined by these m_1 functions and the remaining y_j.

4) Suppose that at $\eta = 1$ m_2 functions with the comparable property are specified.

Then, there is a unique solution to Eq. (II.E-56) which assumes given data at $t = 0$ and is valid in $0 \leq t \leq t_1$, $0 \leq \eta \leq 1$ for some $t_1 > 0$.

Remark: The above statement of the theorem is obviously not very precise. For example, the differentiability properties are not stated. See Lax (II.E-12, p. 107) for a thorough discussion.

Let us now return to the characteristics of Eq. (II.E-37) as given by Eq. (II.E-84). We want to intuitively apply the information given by these characteristics. Consider first the six characteristics given by $\frac{dt}{d\eta} = 0$. As noted earlier this is in line with the idea that the last three equations of (II.E-37) (that is, Eqs. (II.E-34), (II.E-35), (II.E-36) are individually parabolic. Thus, at $\eta = 0$ we expect to specify (with additional boundary conditions) V or $\frac{\partial V}{\partial \eta}$, T $\frac{\partial T}{\partial \eta}$, C or $\frac{\partial C}{\partial \eta}$. The same situation for V, T, and C holds at $\eta = 1$. Now consider the characteristic given by $\frac{dt}{dx} = \frac{1}{a_1}$. As noted earlier this is the same characteristic as is obtained by considering Eq. (II.E-33) individually. It turns out that the corresponding eigenvalue of the matrix M, Eq. (II.E-35, $= -a_1$.

Applying our results for quasi-linear systems, we specify boundary conditions for ρ as follows: at $\eta = 0$, a boundary condition is given for ρ if $a_1 > 0$, while the differential equation (II.E-33) is used if $a_1 = 0$ ($a_1 = 0$ implies that $a_1 = 0$ for all t); at $\eta = 1$ the situation is reversed. Summarizing, then, the boundary conditions for Eq. (II.E-37) are

1) $\eta = 0$:

   a) a function for V or $\frac{\partial V}{\partial \eta}$,

   b) a function for T or $\frac{\partial T}{\partial \eta}$, (II.E-86)

   c) a function for C or $\frac{\partial C}{\partial \eta}$,

   d) a function for ρ if $a_1 > 0$; otherwise no boundary condition is given (eq. 1.33 is used)

2) $\eta = 1$:

   a) a function for V or $\frac{\partial V}{\partial \eta}$,

   b) a function for T or $\frac{\partial T}{\partial \eta}$, (II.E-87)

   c) a function for C or $\frac{\partial C}{\partial \eta}$,

   d) a function for ρ if $a_1 < 0$; otherwise no boundary condition is given (Eq. II.E-33 is used).

Consider now the subset of Eq. (II.E-37) obtained by suppressing C. That is, assume C is identically a constant, thereby reducing the vector X to a three vector $\begin{pmatrix} \rho \\ V \\ T \end{pmatrix}$. The equations simplify in a straight-forward fashion. The result is that boundary conditions for this case are precisely the same as those given by Eqs. (II.E-86) and (II.E-87) (except that the quantity C is ignored).

We now consider the case obtained by suppressing all the viscous terms. Eq. (II.E-37) then becomes

$$\frac{\partial X}{\partial t} = A \frac{\partial X}{\partial \eta} + B^* , \qquad \text{(II.E-88)}$$

where A is as defined in Eq. (II.E-37) and

$$B^* = \begin{pmatrix} -a_3 \\ 0 \\ -c_3 T \\ 0 \end{pmatrix} \qquad X = \begin{pmatrix} \rho \\ V \\ T \\ C \end{pmatrix}. \tag{II.E-89}$$

Eq. (II.E-88) is a two-dimensional quasi-linear system and we could now apply directly the theory which was quoted earlier*. However, it is also of interest to relate the characteristics of Eq. (II.E-88) to the eigenvalues of A_1 and we shall do this now. To find the characteristics we proceed as before. The transformation (II.E-76) produces this system:

$$\alpha_1 \frac{\partial X}{\partial \theta} + \alpha_2 \frac{\partial X}{\partial \zeta} = A \left(\alpha_3 \frac{\partial X}{\partial \theta} + \alpha_4 \frac{\partial X}{\partial \zeta} \right) + B^* ,$$

$$\text{or} \qquad (\alpha_1 I - \alpha_3 A) \frac{\partial X}{\partial \theta} = (\alpha_4 A - \alpha_2 I) \frac{\partial X}{\partial \zeta} + B^* . \tag{II.E-90}$$

The characteristics are given by values for which $\det A_1 = 0$, where

$A_1 = \alpha_1 I - \alpha_3 A,$

$$\det A = \begin{vmatrix} (\alpha_1 + \alpha_3 a_1) & \alpha_3 a_2 & 0 & 0 \\ \alpha_3 b_2 & (\alpha_1 + \alpha_3 a_1) & \alpha_3 b_3 & \alpha_3 b_4 \\ 0 & \alpha_3 c_2 & (\alpha_1 + \alpha_3 a_1) & 0 \\ 0 & 0 & 0 & (\alpha_1 + \alpha_3 a_1) \end{vmatrix} = 0. \tag{II.E-91}$$

Note that if $\alpha_3 = 0$, Eq. (II.E-91) requires also that $\alpha_1 = 0$, and this violates Eq. (II.E-81). Thus, $\alpha_3 \neq 0$. and we have:

$$\det A_1 = \begin{vmatrix} \left(\frac{\alpha_1}{\alpha_3} + a_1\right) & a_2 & 0 & 0 \\ b_2 & \left(\frac{\alpha_1}{\alpha_3} + a_1\right) & b_3 & b_4 \\ 0 & c_2 & \left(\frac{\alpha_1}{\alpha_3} + a_1\right) & 0 \\ 0 & 0 & 0 & \left(\frac{\alpha_1}{\alpha_3} + a_1\right) \end{vmatrix} = \det \left(\frac{\alpha_1}{\alpha_2} I - A \right) = 0 . \tag{II.E-92}$$

Let $\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$ be the eigenvalues of the matrix A. Then, $\frac{\alpha_1}{\alpha_3} = +\lambda_i$ produces the four characteristics. From Eq. (II.E-80), $+\lambda_i\alpha_3\alpha_2 + \alpha_3\alpha_4 = 0$, or $\alpha_4 = -\lambda_i\alpha_2$. From Eq. (II.E-77), $+\lambda_i\alpha_3^2 - \lambda_i\alpha_2^2 = 0 \rightarrow \alpha_2 = \pm\alpha_3$. Substituting into Eq. (II.E-81), we find that the plus sign is to be used. Thus, we have $\alpha_1 = \lambda_i\alpha_3$, $\alpha_2 = \alpha_3$, $\alpha_4 = -\lambda_i\alpha_3$. From Eq. (II.E-78) θ = constant $\rightarrow \frac{dt}{d\eta} = -\frac{\beta_2}{\beta_1}$, and from Eq. (II.E-79) $\frac{dt}{d\eta} = \frac{\alpha_2}{\alpha_4} = \frac{\alpha_3}{-\lambda_i\alpha_3} = -\frac{1}{\lambda_i}$. Thus, the characteristics of Eq. (II.E-88) are the negative reciprocals of the eigenvalues of A.

Let us now find the eigenvalues of A.

$$\det |A-\lambda I| = \begin{vmatrix} (-a_1-\lambda) & -a_2 & 0 & 0 \\ -b_2 & (-a_1-\lambda) & -b_3 & -b_4 \\ 0 & -c_2 & (-a_1-\lambda) & 0 \\ 0 & 0 & 0 & (-a_1-\lambda) \end{vmatrix} = (-a_1-\lambda) \begin{vmatrix} (-a_1-\lambda) & -a_2 & 0 \\ -b_2 & (-a_1-\lambda) & -b_3 \\ 0 & -c_2 & (-a_1-\lambda) \end{vmatrix},$$

$$= (-a_1-\lambda)\left\{ (-a_1-\lambda)\left[(a_1+\lambda)^2 - b_3 c_2 \right] + b_2 a_2 (a_1+\lambda) \right\},$$

$$= -(a_1+\lambda)^2 \left[(a_1+\lambda)^2 - b_3 c_2 - b_2 a_2 \right],$$

$$= (a_1+\lambda)^2 \left[(a_1+\lambda)^2 - (b_3 c_2 + b_2 a_2) \right].$$

Let

$$c_s^2 = b_3 b_2 + b_2 a_2 = \text{speed of sound}, \qquad \text{(II.E-93)}$$

$$= \eta_r \bar{R}\bar{R}T\,\eta_r/\bar{C}_v + (\eta_r \bar{R}T/\rho)(\rho\eta_r) = \eta_r^2 \bar{R}T\left(1 + \frac{\bar{R}}{\bar{C}_v}\right) > 0.$$

Then

$$\det |A-\lambda I| = (a_1+\lambda)^2 \left[(a_1+\lambda)^2 - c_s^2 \right],$$

and the eigenvalues of A are

$$\{\lambda_i\} = \{ -a_1, -a_1 + c_s, -a_1 - c_s, -a_1 \} \qquad \text{(II.E-94)}$$

We now need to find the matrix M such that $MAM^{-1} = \text{diag}\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} = D$. It is of interest also to characterize all such M. In order to do this, let B_i be the class of matrices such that $BAB^{-1} = A$. (That is, B commutes with A.) Let M_1 be such that $M_1 A M_1^{-1} = D$. Then, for any other M_2 satisfying $M_2 A M_2^{-1} = D$ there exists a B in $\{B_\alpha\}$ such that $M_2 = M_1 B^{-1} = M_1 B \left[B \in B_\alpha \rightarrow B^{-1} \in B_\alpha\right]$.

Proof:

$$M_1 A M_1^{-1} = D = M_2 A M_2^{-1},$$

$$M_2^{-1} M_1 A M_1^{-1} M_2 = A \rightarrow M_2^{-1} M_1 = B^{-1} \text{ in } \{B_\alpha\}.$$

Thus, there is considerable freedom in the choice of M. (However, this freedom does not affect the eigenvalues nor the difference equation (Section II-D).

The above equation can also be written as MA = DM. Let $M = (m_{ij})$ and let $MA = C = (i_{ij})$. We need then to satisfy the following equations.

$$c_{11} = -m_{11}a_1 - m_{12}b_2 = -a_1 m_{11},$$

$$c_{12} = -m_{11}a_2 - m_{12}a_1 - m_{13}c_2 = -a_1 m_{12},$$

$$c_{13} = -m_{12}b_3 - m_{13}a_1 = -a_1 m_{13},$$

$$c_{14} = -m_{12}b_4 - a_1 m_{14} = -a_1 m_{14}.$$

From the c_{11} equation, we must have $m_{12} = 0$. From the c_{12} equation, $m_{11}a_2 + m_{13}c_2 = 0$. c_{13} and c_{14} are already satisfied. Thus, let $m_{11} = c_2$, $m_{12} = 0$, $m_{13} = -a_2$, $m_{14} = 0$.

$$c_{21} = -m_{21}a_1 - m_{22}b_2 = (-a_1 + c_s)\, m_{21},$$

$$c_{22} = -m_{22}a_2 - m_{22}a_1 - m_{23}c_2 = (-a_1 + c_s)\, m_{22},$$

$$c_{23} = -m_{22}b_3 - m_{23}a_1 = (-a_1 + c_s)\, m_{23},$$

$$c_{24} = -m_{22}b_4 - m_{24}a_1 = (-a_1 + c_s)\, m_{24}.$$

From the c_{21} equation, $c_s m_{21} + b_2 m_{22} = 0$, or we can choose $m_{21} = -b_2$, $m_{22} = c_s$. Then, from the c_{22} equation, $m_{23} = \dfrac{b_2 a_2 - c_s^2}{c_2} = -b_3$. The c_{23} equation is now automatically satisfied. From the c_{24} equation, $m_{24} = -b_4$. Thus, $m_{21} = -b_2$, $m_{22} = c_s$, $m_{23} = -b_3$, $m_{24} = -b_4$.

$$c_{31} = -m_{31}a_1 - m_{32}b_2 = -(a_1 + c_s)\, m_{31} ,$$

$$c_{32} = -m_{31}a_2 - m_{32}a_1 - m_{33}c_2 = -(a_1 + c_s)\, m_{32} ,$$

$$c_{33} = -m_{32}b_3 - m_{33}a_1 = -(a_1 + c_s)\, m_{33} ,$$

$$c_{34} = -m_{32}b_4 - m_{34}a_1 = -(a_1 + c_s)\, m_{34} .$$

From the c_{31} equation, $c_s m_{31} - b_2 m_{32} = 0$, or we can choose $m_{31} = b_2$, $m_{32} = c_s$. From the c_{32} equation, $m_{33} = -\dfrac{a_2 b_2 + c_s^2}{c_2} = b_3$. The c_{33} equation is already satisfied, and from the c_{34} equation, $c_{34} = b_4$. Thus, $m_{31} = b_2$, $m_{32} = c_s$, $m_{33} = b_3$, $m_{34} = b_4$,

$$c_{41} = -m_{41}a_1 - m_{42}b_2 = -a_1 m_{41} ,$$

$$c_{42} = -m_{41}a_2 - m_{42}a_1 - m_{43}c_2 = -a_1 m_{42} ,$$

$$c_{43} = -b_3 m_{42} - a_1 m_{43} = -a_1 m_{43} ,$$

$$c_{44} = -m_{42}b_4 - a_1 m_{44} = -a_1 m_{44} .$$

We now choose $m_{41} = m_{42} = m_{43} = 0$ and $m_{44} = 1$.

Summarizing,

$$MAM^{-1} = D = \text{diag}\{-a_1, -a_1 + c_s, -a_1 - c_s, -a_1\} , \qquad \text{(II.E-95)}$$

where

$$M = \begin{pmatrix} c_2 & 0 & -a_2 & 0 \\ -b_2 & c_s & -b_3 & -b_4 \\ b_2 & c_s & b_3 & b_4 \\ 0 & 0 & 0 & 1 \end{pmatrix} .$$

We need to verify that M is nonsingular:

$$\det M = \begin{vmatrix} c_2 & 0 & -a_2 \\ 0 & 2c_s & 0 \\ b_2 & c_s & b_3 \end{vmatrix} = 2c_s(c_2 b_3 + a_2 b_2) = 2c_s^3 .$$

In discussing the difference equation (Section II.E.4), we will need M^{-1}. We digress somewhat in order to perform this calculation. Let $M^{-1} = (m_{ij}^{-1})$,

$$m_{11}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_s & -b_3 & -b_4 \\ c_s & b_3 & b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{2c_s b_3}{2c_s^3} = \frac{2b_3}{2c_s^2} ,$$

$$m_{12}^{-1} = \frac{-1}{2c_s^3} \begin{vmatrix} 0 & -a_2 & 0 \\ c_s & b_3 & b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{-a_2 c_s}{2c_s^3} = -\frac{a_2}{2c_s^2} ,$$

$$m_{13}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} 0 & -a_2 & 0 \\ c_s & -b_3 & -b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{a_2 c_s}{2c_s^3} = \frac{a_2}{2c_s^2} ,$$

$$m_{14}^{-1} = \frac{-1}{2c_s^3} \begin{vmatrix} 0 & -a_2 & 0 \\ c_s & -b_3 & -b_4 \\ c_s & b_3 & b_4 \end{vmatrix} = \frac{-a_2 2c_s b_4}{2c_s^3} = \frac{-2a_2 b_4}{2c_s^2} ,$$

$$m_{21}^{-1} = \frac{-1}{2c_s^3} \begin{vmatrix} -b_2 & -b_3 & -b_4 \\ b_2 & b_3 & b_4 \\ 0 & 0 & 1 \end{vmatrix} = 0 ,$$

$$m_{22}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & -a_2 & 0 \\ b_2 & b_3 & b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{c_2 b_3 + a_2 b_2}{2c_s^3} = \frac{c_s^3}{2c_s^3} = \frac{c_s}{2c_s^2} ,$$

$$m_{23}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & -a_2 & 0 \\ -b_2 & -b_3 & -b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{c_2 b_3 + a_2 b_2}{2c_s^3} = \frac{c_s}{2c_s^2} ,$$

$$m_{24}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & -a_2 & 0 \\ -b_2 & -b_3 & -b_4 \\ b_2 & b_3 & b_4 \end{vmatrix} = 0 ,$$

$$m_{31}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} -b_2 & c_s & -b_4 \\ b_2 & c_s & b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{-2b_2 c_s}{2c_s^3} = \frac{-2b_2}{2c_s^2} ,$$

$$m_{32}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & 0 & 0 \\ b_2 & c_s & b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{-c_2 c_s}{2c_s^3} = \frac{-c_2}{2c_s^2} ,$$

$$m_{33}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & 0 & 0 \\ -b_2 & c_s & -b_4 \\ 0 & 0 & 1 \end{vmatrix} = \frac{c_2 c_s}{2c_s^3} = \frac{c_2}{2c_s^2} ,$$

$$m_{34}^{-1} = \frac{1}{2c_s^3} \begin{vmatrix} c_2 & 0 & 0 \\ -b_2 & c_s & -b_4 \\ b_2 & c_s & b_4 \end{vmatrix} = \frac{2c_s b_4 c_2}{2c_s^3} = \frac{-2c_2 b_4}{2c_s^2},$$

Thus,

$$M_{41}^{-1} = M_{42}^{-1} = m_{43}^{-1} = 0 \text{ and } m_{44}^{-1} = 1.$$

$$M^{-1} = \frac{1}{2c_s^2} \begin{pmatrix} 2b_3 & -a_2 & a_2 & -2a_2 b_4 \\ 0 & c_s & c_s & 0 \\ -2b_2 & -c_2 & c_2 & -2c_2 b_4 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \qquad \text{(II.E-96)}$$

We now find the components of the vector Y = MX:

$$\begin{aligned} y_1 &= c_2\rho - a_2 T, \\ y_2 &= -b_2\rho + c_s V - b_3 T - b_4 C, \\ y_3 &= {}_2\rho + c_s V + b_3 T + b_4 C, \\ y_4 &= C. \end{aligned} \qquad \text{(II.E-97)}$$

The boundary conditions are now specified as follows. Locally, then, the transformation Y = MX reduces Eq. (II.E-88) to the form

$$\frac{\partial Y}{\partial t} = D\frac{\partial Y}{\partial \eta} + C_1,$$

where

$$C_1 = MB^* = \begin{pmatrix} -c_2 a_3 + a_2 c_3 T \\ b_2 a_3 + b_3 c_3 T \\ -b_2 a_3 - b_3 c_3 T \\ 0 \end{pmatrix},$$

$$a_2c_3T - c_2a_3 = \frac{\rho\eta_r\delta\bar{R}VT}{r\bar{C}_v} - \frac{\bar{R}T\eta_r\delta\rho V}{r\bar{C}_v} = 0 ,$$

$$b_2a_3 + b_3c_3T = \frac{\eta_r\bar{R}T}{\rho}a_3 + \eta_r\bar{R}\frac{a_3}{\rho}\frac{\bar{R}}{\bar{C}_v}T ,$$

$$= \frac{a_3}{\rho}\eta_r\bar{R}\bar{T}\left(1+\frac{\bar{R}}{\bar{C}_v}\right) = \frac{a_3}{\rho\eta_r}c_s^2 : \text{ from Eq. (II.E-93)}$$

$$-b_2a_3 - b_3c_3T = -\frac{a_3}{\rho\eta_r}c_s^2 .$$

Thus, we have these equations

$$\left.\begin{aligned}
\frac{\partial y_1}{\partial t} &= -a_1\frac{\partial y_1}{\partial \eta} , \\
\frac{\partial y_2}{\partial t} &= (-a_1+c_s)\frac{\partial y_2}{\partial \eta} + \frac{a_3c_s^2}{a_2} , \\
\frac{\partial y_3}{\partial t} &= (-a_1-c_s)\frac{\partial y_3}{\partial \eta} - \frac{a_3}{a_2}c_s^2 , \\
\frac{\partial y_4}{\partial t} &= -a_1\frac{\partial y_4}{\partial \eta} .
\end{aligned}\right\} \qquad \text{(II.E-98)}$$

1) $\eta = 0$: (II.E-99)

For each negative eigenvalue λ_ν, a function must be specified such that y_ν can be determined. (It may be necessary to solve the set of functions simultaneously). Note that this implies that if for some ν λ_ν is positive, then y_ν is to be obtained from the corresponding member of Eq. (II.E-98).

2) $\eta = 1$: (II.E-100)

For each positive eigenvalue λ_ν, a function must be specified such that y_ν can be determined.

In the case that C is suppressed the situation is again as expected. The vector Y is now

$$\left.\begin{aligned} y_1 &= c_2\rho - a_2 T\,, \\ y_2 &= -b_2\rho + c_s V - b_3 T, \\ y_3 &= b_2\rho + c_s V + b_3 T\,. \end{aligned}\right\} \quad \text{(II. E-101)}$$

The eigenvalues in this case are

$$\{\lambda_\nu\} = \{-a_1,\ -a_1 + c_s,\ -a_1 - c_s\}\,. \qquad \text{(II. E-102)}$$

Boundary conditions are specified as above.

PART B

We consider now the boundary conditions for several specific physical problems. In all cases it will be important to evaluate the coefficient a_1 at $\eta = 0$ and $\eta = 1$. From Eq. (II. E-33),

$$a_1 = V\eta_r + \eta_t. \qquad \text{(II. E-103.1)}$$

From Eq. (II. E-46),

$$\eta_s = 0 \text{ at } \eta = 0 \text{ and } \eta = 1.$$

From Eq. (II. E-42) and (II. E-40),

$$\xi_t = \begin{cases} -\xi_r r'_o\colon\ \eta = 0 \\ -\xi_r r'_1\colon\ \eta = 1 \end{cases}$$

From Eq. (II. E-45),

$$\eta_{\xi_o} = 0 \text{ at } \eta = 0 \text{ and } \eta = 1.$$

Combining these statements with Eq. (II. E-51),

$$\eta_t = \begin{cases} -\eta_r r'_o\colon\ \eta = 0 \\ -\eta_r r'_1\colon\ \eta = 1\,, \end{cases} \qquad \text{(II. E-103.2)}$$

or

$$a_1 = \begin{cases} \eta_r (V - r'_o)\colon\ \eta = 0 \\ \eta_r (V - r'_1)\colon\ \eta = 1\,, \end{cases} \qquad \text{(II. E-104)}$$

where $\eta_r > 0$.

In the following discussion, one is not to assume that the boundary conditions given are the only ones possible. They are simply the ones that were chosen for these problems.

1) The Piston Problem

It is assumed that a piston is moved into a stationary gas. In our applications this has been a planar piston moving in the direction orthogonal to the piston. However, it could be a solid sphere expanding in a spherically symmetric fashion or a cylindrical sphere expanding symmetrically with respect to the axis of the cylinder. Suppose we are considering a one-component gas; thus, the variable C is ignored in the following. Suppose also that the velocity of the piston is specified, and let it be denoted by $v_p(t)$. In order to have $\eta = 0$ correspond to the piston surface we let $r_o' = v_p(t)$.

Case 1: Consider the full set of equations, Eq. (II.E-37). At the piston surface we assume that gas moves with the velocity of the piston, or that $V(t,0), = v(t)$. We also assume that $\eta = 1$ is always so far ahead of the piston that $V(t,1) \equiv 0$. The initial conditions were

a) $V(0,\eta) \equiv 0$,

b) $T(0,\eta) \equiv T_o = \text{constant}$,

c) $\rho(0,\eta) \equiv \rho_o = \text{constant}$.

The boundary conditions at $\eta = 0$ were

a) $V(t,0) = v_p(t)$,

b) $\frac{\partial T}{\partial \eta}(t,0) = 0$: adiabatic case,

or

$T(t,0) = T_o$: isothermal case,

c) From Eq. (II.E-104) $a_1 = \eta_r \left[V_p(t) - v_p(t) \right] = 0$, or from Eq. (II.E-86) no boundary condition is given for ρ.

The boundary conditions at $\eta = 1$ were

a) $V(t,1) \equiv 0$,

b) $T(t,0) = T_o$,

c) If $r_1' = 0$, $a_1' = 0$ from Eq. (II.E-104) and so from Eq. (II.E-87) no boundary condition is given. If $r_1' > 0$, $a_1 < 0$ and ρ must be specified: $\rho(t,1) = \rho_o$.

Some results for this problem are reported in Reference (II.E-18).

Case 2: Consider the case obtained by suppressing all the viscous terms, that is Eq. (II. E-88). The initial conditions are as in case 1. The boundary conditions at $\eta = 0$ are as follows.

From Eq. (II. E-92) the eigenvalues are:

$$\lambda_1 = -a_1, \lambda_2 = -a_1 + c_s, \lambda_3 = -a_1 - c_s,$$

where the 4th eigenvalue is ignored since we are suppressing C and where c_s is the speed of sound (Eq. II. E-93). In case 1 we saw that $a_1 \equiv 0$ at $\eta = 0$. Thus, $\lambda_1 \equiv 0$, $\lambda_2 > 0$, $\lambda_3 < 0$. From Eq. (II. E-99) we must specify a boundary condition corresponding to λ_3: we choose this to be $V(t, 0) \equiv 0$. Thus, ρ and T, or y_1 and y_2 see Eq. (II. E-101) must be obtained from the differential system. This will be discussed further in Section II. E. 4.

The boundary conditions at $\eta = 1$ are as follows.

We saw in case 1 that $a_1 \equiv 0$ or $a_1 < 0$. If $a_1 \equiv 0$, the situation is precisely as just discussed for $\eta = 0$, except that the y_1 and y_2 components must be obtained from the differential equations. If $a_1 < 0$, then λ_1 and λ_2 are positive while λ_3 may be positive or negative; if λ_3 is positive all variables must be specified ($V = 0$, $\rho = \rho_0$, $T = T_0$), while if λ_3 is negative only two variables are specified and y_3 is obtained from the differential system.

2) Reflection from a Solid Surface

This problem is generated, as in problem 1, by a piston moving into a stationary gas. The wave thus formed is allowed to reflect from a far surface. Again, $r_0(t) = v_p(t)$. However, $r_1(t) \equiv 0$. Again, we assume only one component, and thus ignore the variable C.

Case 1: Consider the full set of equations, Eq. (II. E-37). The initial conditions are

a) $V(0, \eta) \equiv 0$,

b) $T(0, \eta) \equiv T_0$,

c) $\rho(0, \eta) \equiv \rho_0$,

The boundary conditions at $\eta = 0$ were

a) $V(t, 0) = v_p(t)$,

b) $\frac{\partial T}{\partial \eta}(t, 0) \equiv 0$,

c) Since $a_1(t, 0) \equiv 0$, no boundary condition is given for ρ. Note that this is valid even after the piston is brought back to rest. In fact, this situation would be

valid even if the motion of the piston were reversed, thereby creating an expansion wave.

The boundary conditions at $\eta = 1$ were

a) $V(t,1) \equiv 0$,

b) $\frac{\partial T}{\partial \eta}(t,1) \equiv 0$,

or

$T(t,1) \equiv T_o$,

c) Since $a_1(t,1) \equiv 0$, no boundary condition is given for ρ.

Case 2: Consider the inviscid case, Eqs. (II. E-88). The initial conditions are as in case 1. The boundary conditions are as follows.

At $\eta = 0$ since λ_1 and λ_2 are non-negative, while λ_3 is negative, we need one boundary condition, $V(t,0) \equiv 0$. y_1 and y_2 see Eq. (II. E-101) are obtained from the differential system. At $\eta = 1$, since λ_1 and λ_3 are non-positive, while λ_2 is positive, we again need one boundary condition, $V(t,1) \equiv 0$. y_1 and y_3 are obtained from the differential system.

Some results for this problem are reported in Reference II. E-19.

3) The Burst Problem

This problem has been handled only in spherical coordinates. The problem as originally defined was as follows: one postulates a sphere of stationary gas such that the gas inside the sphere is at a higher pressure than the gas outside; at time zero the "casing" for the sphere (or the solid boundary) is instantaneously removed, thus producing a flow. However, in order to avoid the discontinuity that results, we postulated a continuous distribution of all variables at $t = 0$. In particular, our initial conditions were

a) $V(0,\eta) \equiv 0$,

b) $\rho(0,\eta) \equiv \rho_o$,

c) $$T(0,\eta) = \begin{cases} T_1: \ 0 \le \eta \le \eta_1 \\ T_1 + \left(\frac{T_2 - T_1}{\eta_2 - \eta_1}\right)(\eta - \eta_1): \ \eta_1 \le \eta \le \eta_2 \\ T_2: \ \eta_2 \le \eta \le 1 \end{cases}$$

In our case $T_1 > T_2$, and $\eta_2 - \eta_1$ was taken as very small so as to produce a steel ramp.

Initially, r_o and r_1 could be chosen close to $r(\eta_1)$ and $r(\eta_2)$. They could then move as the shock moves, $r_o' < 0$ and $r_1' > 0$. Of course, when r_o reached the center of the sphere, that is $r_o = 0$, then $r_o' = 0$, then $r_o' \equiv 0$.

Case 1: Consider the full set of equations, Eq. (II.E-37)

The boundary conditions at $\eta = 0$ were

a) $V(t,0) \equiv 0$,

b) $\frac{\partial T}{\partial \eta}(t,0) \equiv 0$,

c) If $r_o' < 0$, then $a_1 > 0$ and from Eq. (II.E-87)

a boundary condition for ρ is needed; we use $\rho(t,0) \equiv \rho_o$. If $r_o' \equiv 0$, ρ is calculated from the differential system.

The boundary conditions at $\eta = 1$ were

a) $V(t,1) \equiv 0$,

b) $T(t,1) \equiv T_2$,

c) If $r_1' > 0$, then $a_1 < 0$ and from Eq. (II.E-87)

a boundary condition for ρ is needed; we use $\rho(t,0) \equiv \rho_o$. If $r_1' \equiv 0$, ρ is calculated from the differential system.

Case 2: Consider the inviscid case, Eqs. (II.E-88)

The boundary conditions at $\eta = 0$ are,

If $r_o' = 0$, $a_1 = 0$ and $\lambda_1 = 0$, $\lambda_2 > 0$, $\lambda_3 < 0$; thus from Eq. (II.E-99) one boundary condition is needed ($V = 0$) while y_1 and y_2 are obtained from the differential system. If $r_o' < 0$, $a_1 > 0$ and there are two possibilities:

1) $\lambda_1 < 0$, $\lambda_2 < 0$, $\lambda_3 < 0$: then boundary conditions are needed for all variables ($V = 0$, $\rho = \rho_o$, $\frac{\partial T}{\partial \eta} = 0$).

2) $\lambda_1 < 0$, $\lambda_2 > 0$, $\lambda_3 < 0$: then two boundary conditions are needed ($V = 0$, $\frac{\partial T}{\partial \eta} = 0$) and y_2 is calculated from the differential system.

The boundary conditions at $\eta = 1$ are,

If $r_1' = 0$, $a_1 = 0$ and $\lambda_1 = 0$, $\lambda_2 > 0$, $\lambda_3 < 0$; thus, one boundary condition is needed ($V = 0$), while y_1 and y_3 are obtained from the differential system. If $r_1' > 0$, there are two possibilities:

1) $\lambda_1 > 0$, $\lambda_2 > 0$, $\lambda_3 > 0$: then boundary conditions are needed for all variables ($V = 0$, $\rho = \rho_o$, $\frac{\partial T}{\partial \eta} = 0$).

2) $\lambda_1 > 0$, $\lambda_2 > 0$, $\lambda_3 < 0$: then two boundary conditions are needed ($V = 0$, $T = T_2$), while y_3 is obtained from the differential system.

Results for this problem are discussed in Section II.G.

4) The Mass Injection Problem

The assumption here is that mass is being injected into the region at the point $\eta = 0$. Likewise, one could suppose that somehow mass were being withdrawn at $\eta = 0$. Also, one could interpret this to be a point in the flow for which the flow conditions were known.

The initial conditions are

a) $V(0, \eta) \equiv 0$,

b) $T(0, \eta) \equiv T_o$,

c) $\rho(0, \eta) \equiv \rho_o$,

d) $C(0, \eta) \equiv 0$.

Let ρ_1 be the density of the injected gas and V_1 the velocity of the injected gas. Thus, $\rho_1(t)$ and $V_1(t)$ are assumed given. We can also assume that r_o and r_1 are not moving, $r_o' \equiv r_1' \equiv 0$.

Case 1: Consider the full set of equations, Eq. (II.E-37)

The boundary conditions at $\eta = 0$ were

a) $V(t, 0) = C\, V_1(t)$,

b) $t(T, 0) = T_1(t)$: input,

c) $(1-C)\, \dot{m}_w = - \rho \mathcal{D} \eta_r \frac{\partial C}{\partial \eta}$,
where $\dot{m}_w = \rho_1 V_1$,

d) If $V(t,0) > 0$, $a_1 > 0$ and a boundary condition is needed for ρ: $\rho(t,0) = C\rho(t)$. If $V(t,0) \leq 0$, $a_1 \leq 0$ and ρ must be calculated from the differential system [see Eq. (II.E-87)].

The boundary conditions at $\eta = 1$ were

a) $V(t,1) \equiv 0$,

b) $T(t,1) \equiv T_o$,

c) $C(t,1) \equiv 0$,

d) Since a_1 is zero, ρ is calculated from the differential system.

Case 2: Consider the inviscid case, Eq. (II.E-88)

The boundary conditions at $\eta = 0$ were;

If $V(t,0) = 0$, $a_1 = 0$ and $\lambda_1 = 0$, $\lambda_2 > 0$, $\lambda_3 < 0$, $\lambda_4 = 0$ See Eq. (II.E-94). Then, from Eq. (II.E-99) one boundary condition is needed (we use $V = CV_1$), while y_1, y_2, and y_4 are calculated from the differential system, Eq. (II.E-98). If $V(t,0) > 0$, there are two possibilities:

a) $\lambda_1 < 0$, $\lambda_2 < 0$, $\lambda_3 < 0$, $\lambda_4 < 0$: then from Eq. (II.E-99) boundary conditions must be specified for all variables (these would be the same as those used in Case 1).

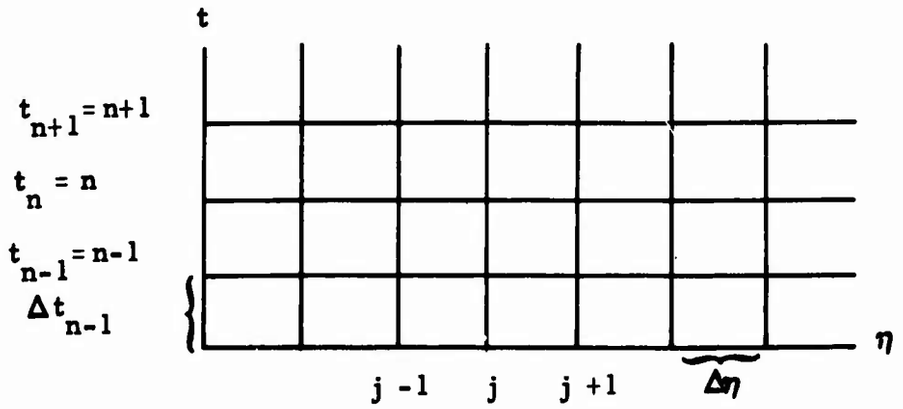
b) $\lambda_1 < 0$, $\lambda_2 > 0$, $\lambda_3 < 0$, $\lambda_4 < 0$: then three boundary conditions must be specified (these would be the same as those used for V, T, and C in Case 1), and y_2 would be obtained from the differential system.

The boundary conditions at $\eta = 1$ were,

Since $V(t,1) \equiv 0$, $a_1 \equiv 0$ and $\lambda_1 = 0$, $\lambda_2 > 0$, $\lambda_3 < 0$, and $\lambda_4 = 0$. Thus, from Eq. (II.E-100) one boundary condition must be given (namely $V = 0$), while y_1, y_3, and y_4 are obtained from the differential system.

II.E.4 DIFFERENCE EQUATIONS

In this section we discuss the difference equations employed to solve Eq. (II. E-37). Stability theory in the sense of Richtmyer(II. E-14) reveals that stability is unaffected by low order terms. In practice we have indeed found this to be the case. However, we have also found that the rate of convergence is greatly affected, that is, a poor choice of approximation to these low order terms can force the introduction of an unreasonable number of nodes in order to obtain required accuracy. Our approach then is as follows. The system is split into two parts, as indicated by Eq. (II. E-37). The viscous system, contains all the parabolic terms (the barred quantities), and the nonviscous system, contains all the inviscid terms (the unbarred quantities). In Part A, the difference equations for the viscous terms will be described, while in Part B, the difference equations for the hyperbolic inviscid system will be described. Finally, in Part C, the two will be combined and the final form of the difference equations will be derived. Boundary equations will be discussed in Part D, and stability criteria will be outlined in Part E. The following notation will be used in regard to the difference equations:



$$u_j^n = u\,(t_n,\ j\Delta\eta)$$

PART A: The Parabolic (Viscous) Case

Consider first the parabolic equation

$$\frac{\partial u}{\partial t} = \beta \frac{\partial^2 u}{\partial \eta^2} , \qquad \text{(II. E-105)}$$

where β is a positive constant.

There seems to be three difference equations commonly used for Eq. (II. E-105).

These are as follows, where $q = \frac{\Delta t \beta}{\Delta \eta^2}$.

1) Explicit: (II. E-14)

$$u_j^{n+1} = (1-2q)\, u_j^n + q\,(u_{j+1}^n + u_{j-1}^n)$$

This equation is handicapped by the restriction that $q \leq \frac{1}{2}$. Although there are many cases where Δt must be chosen small because of other considerations, it seems unduly restrictive to write any kind of a general computer program with this stability criterion.

2) Implicit: (II. E-14)

$$(1+2q)\, u_j^{n+1} = u_j^n + q\,(u_{j+1}^{n+1} + u_{j-1}^{n+1})$$

This equation is of course always stable. However, practical applications require linerization of the coefficients. Since it is precisely the nonlinear terms which produce a shock, it does not seem advisable in our case to use this equation.

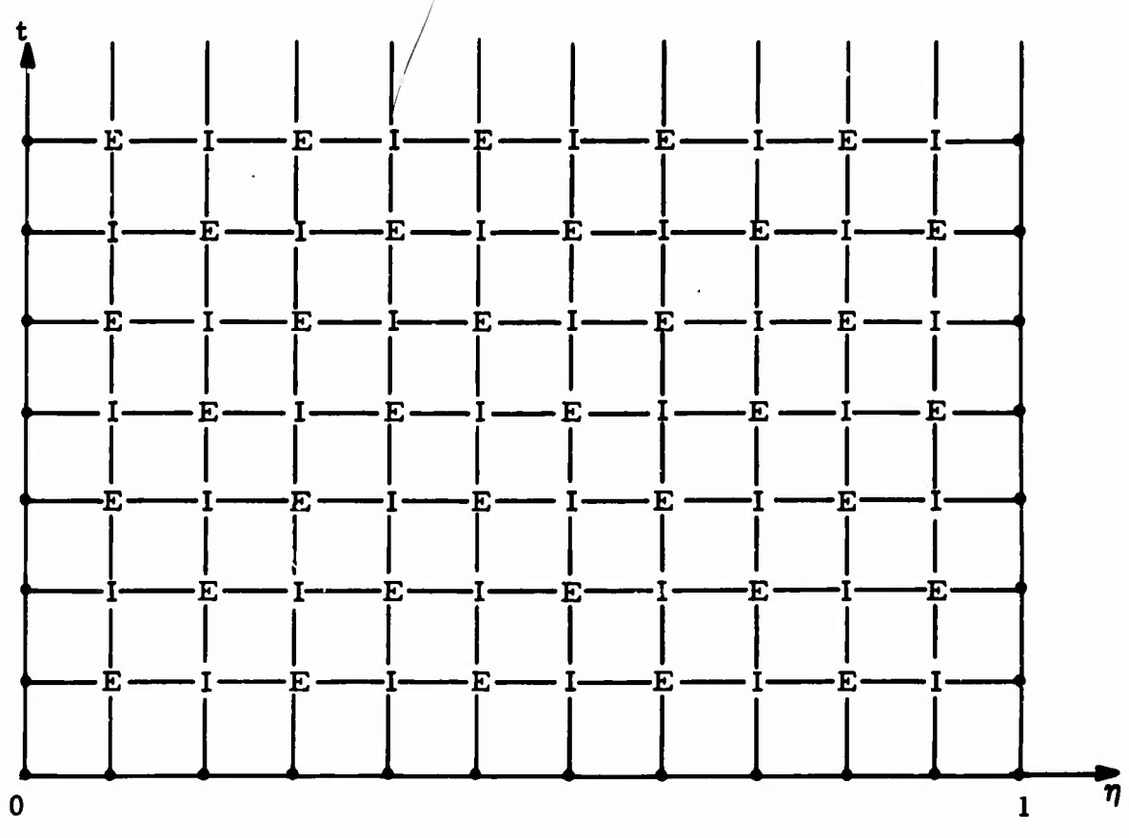
3) Dufort-Frankel: (II. E-5)

$$(1+2q)\, u_j^{n+1} = (1-2q)\, u_j^{n-1} + 2q\,(u_{j+1}^{n-1} + u_{j-1}^{n-1})$$

It can be argued that this is one of the best equations available for nonlinear cases. Although intended for parabolic equations, consistent versions can be obtained for hyperbolic equations. It is explicit, although point-by-point iterations are required

for nonlinear cases. The convergence criterion is $\frac{\Delta t}{\Delta \eta} \to 0$, which is the best possible for explicit difference equations for Eq. (II.E-105). Fromm[II.E-7] seems to have used this equation successfully. The major disadvantage is the poor truncation error term, which can cause slow convergence. In using this equation to reproduce the steady-state results of Crocco[II.E-4], we found this convergence problem clearly indicated.

Recently, we have devised another difference equation, and this is the one we have used in our computer program. Essentially the explicit and implicit equations are alternated. The following diagram indicates the procedure.



Points marked with an "E" are computed by the explicit scheme. Points marked with an "I" are computed by the implicit scheme. (Points marked "•" are assumed known either through direct data or additional boundary conditions.) One notes that if, at any time level, the explicit points are computed first, then the I points can be obtained individually. Thus, the difference equation is an explicit one, although point-by-point iterations are required for nonlinear cases.

Convergence and stability of this explicit-implicit approximation to Eq. (II. E-105) has been established. For convergence in the L^2 norm see Ref. II. E-9. For convergence in the maximum norm see Ref. II. E-8 and Ref. II. E-11.

This explicit-implicit equation turns out to resemble very closely the Dufort-Frankel scheme, and the convergence criterion turns out to be the same, $\frac{\Delta t}{\Delta \eta} \to 0$. Two advantages of this new equation over the Dufort-Frankel equation were found.

1) The explicit-implicit scheme requires half the computer time for calculating the interior points. This is because the explicit points, after the first time step, are simply a direct extrapolation from the previously calculated implicit points. This also holds for nonlinear cases.

2) In our applications, convergence was faster (although still slower than either the explicit or implicit schemes). It is not entirely clear why this occurs. Apparently, however, it comes about because of the fact that the behavior of the explicit-implicit scheme deviates greatly from the Dufort-Frankel scheme near the boundaries, and for a parabolic equation this conceivably could be quite crucial.

In applying this difference equation to a system of equations, new problems, of course, appear. It is, first, not clear as to what approximations should be used in the low order viscous terms in the individual equations. These terms will be discussed individually as we proceed. In addition, there is interaction of the high order terms. Consider the following subsystem of Eq. (II. E-37):

$$\left.\begin{aligned} \frac{\partial T}{\partial t} &= \bar{c}_1 \frac{\partial^2 T}{\partial \eta^2} + \bar{c}_7 \frac{\partial^2 C}{\partial \eta^2}, \\ \frac{\partial C}{\partial t} &= \bar{d}_1 \frac{\partial^2 C}{\partial \eta^2}. \end{aligned}\right\} \quad \text{(II. E-106)}$$

As noted in Ref. II. E-9, for linear cases stability in L_2 for the explicit-implicit scheme follows from stability of the Dufort-Frankel. Let us, then, assume

$\bar{c}_1$, $\bar{c}_7$, and $\bar{d}_1$ are constant, and let us consider the Dufort-Frankel approximation to Eq. (II.E-106). This is

$$\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = \frac{\bar{c}_1}{\Delta\eta^2}\left[T_{j+1}^n + T_{j-1}^n - T_j^{n+1} - T_j^{n-1}\right]$$

$$+ \frac{\bar{c}_7}{\Delta\eta^2}\left[C_{j+1}^n + C_{j-1}^n - C_j^{n+1} - C_j^{n-1}\right],$$

$$\frac{C_j^{n+1} - C_j^{n-1}}{2\Delta t} = \frac{\bar{d}_1}{\Delta\eta^2}\left[C_{j+1}^n + C_{j-1}^n - C_j^{n+1} - C_j^{n-1}\right].$$

Let

$$\alpha_1 = \frac{2\bar{c}_1\,\Delta t}{\Delta\eta^2},$$

$$\alpha_2 = \frac{2\bar{c}_7\,\Delta t}{\Delta\eta^2},$$

$$\beta_1 = 2\bar{d}_1\,\Delta t/\Delta\eta^2,$$

$$T_j^{n+1} - T_j^{n-1} = \alpha_1\left(T_{j+1}^n + T_{j-1}^n - T_j^{n+1} - T_j^{n-1}\right) + \alpha_2\left(C_{j+1}^n + C_{j-1}^n - C_j^{n+1} - C_j^{n-1}\right),$$

$$C_j^{n+1} - C_j^{n-1} = \beta_1\left(C_{j+1}^n + C_{j-1}^n - C_j^{n+1} - C_j^{n-1}\right)$$

or

$$(1+\alpha_1)\,T_j^{n+1} + \alpha_2\,C_j^{n+1} = \alpha_1\left(T_{j+1}^n + T_{j-1}^n\right) + (1-\alpha_1)\,T_j^{n-1}$$

$$+ \alpha_2\left(C_{j+1}^n + C_{j-1}^n\right) - \alpha_2\,C_j^{n-1},$$

$$(1+\beta_1)\,C_j^{n+1} = \beta_1\left(C_{j+1}^n + C_{j-1}^n\right) + (1-\beta_1)\,C_j^{n-1}.$$

Following Richtmyer(II. E-14), we reduce this to a two level equation by the following substitutions

$$u_j^{n+1} = T_j^n ,$$

$$V_j^{n+1} = C_j^n .$$

Then, we have

$$(1+\alpha_1)\, T_j^{n+1} + \alpha_2\, C_j^{n+1} = \alpha_1\, (T_{j+1}^n + T_{j-1}^n) + (1-\alpha_1)\, u_j^n$$

$$+ \alpha_2\, (C_{j+1}^n + C_{j-1}^n) - \alpha_2 V_j^n ,$$

$$(1+\beta_1)\, C_j^{n+1} = \beta_1\, (C_{j+1}^n + C_{j-1}^n) + (1-\beta_1)\, V_j^n ,$$

or, if we define

$$W_j^n = \begin{pmatrix} T_j^n \\ u_j^n \\ C_j^n \\ V_j^n \end{pmatrix} ,$$

we obtain

$$A_1 W_j^{n+1} + A_2 W_j^n + A_3 (W_{j+1}^n + W_{j-1}^n) = 0$$

$$A_1 = \begin{pmatrix} (1+\alpha_1) & 0 & \alpha_2 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & (1+\beta_1) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} ,$$

$$A_2 = \begin{pmatrix} 0 & -(1-\alpha_1) & 0 & \alpha_2 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -(1-\beta_1) \\ 0 & 0 & -1 & 0 \end{pmatrix} ,$$

$$A_3 = \begin{pmatrix} -\alpha_1 & 0 & -\alpha_2 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\beta_1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} .$$

Substituting the typical Fourier term

$$W_j^n = W_n e^{(ik\Delta\eta)j} ,$$

$$A_1 W_{n+1} + A_2 W_n + A_3 (e^{i\theta} + e^{-i\theta}) W_n = 0.$$

Letting $q = \cos\theta$, the last equation becomes

$$A_1 W_{n+1} + (A_2 + 2q A_3) W_n = 0 ,$$

$$A_2 + 2q A_3 = \begin{pmatrix} -2q\alpha_1 & (\alpha_1 - 1) & -2q\alpha_2 & \alpha_2 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -2q\beta_1 & (\beta_1 - 1) \\ 0 & 0 & -1 & 0 \end{pmatrix} .$$

Let $A_1 = D = (1 + \alpha_1)(1 + \beta_1)$.

Then A_1^{-1} is

$$A_1^{-1} = \begin{pmatrix} \frac{1}{(1+\alpha_1)} & 0 & \frac{-\alpha_2}{D} & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{(1+\beta_1)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} .$$

$W_{n+1} = A_5 W_n$,

where $A_5 = -A_1^{-1}(A_2+2qA_3)$,

$$A_5 = \begin{pmatrix} \frac{2q\alpha_1}{1+\alpha_1} & \frac{1-\alpha_1}{1+\alpha_1} & \left(\frac{2q\alpha_2}{1+\alpha_1} + \frac{2q\beta_1\alpha_2}{D}\right) & \left(\frac{-\alpha_2}{1+\alpha_1} + \frac{\alpha_2(\beta_1-1)}{D}\right) \\ +1 & 0 & 0 & 0 \\ 0 & 0 & \frac{2q\beta_1}{1+\beta_1} & \frac{1-\beta_1}{1+\beta_1} \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

The eigenvalues of A_5 are those of the subsystems

$$\begin{pmatrix} \frac{2q\alpha_1}{1+\alpha_1} & \frac{1-\alpha_1}{1+\alpha_1} \\ 1 & 0 \end{pmatrix} , \quad \begin{pmatrix} \frac{2q\beta_1}{1+\beta_1} & \frac{1-\beta_1}{1+\beta_1} \\ 1 & 0 \end{pmatrix} .$$

These matrices are identical to that obtained for the Dufort-Frankel equation when applied to an equation of the form Eq. (II.E-105) (II.E-14). Thus, we conclude that our difference equation is stable when applied to a system of the form (II.E-106).

Let us now consider the individual equations of (II. E-37). In defining the difference equations the following notation will be used:

$$\left.\begin{aligned} f^n_\eta &= \frac{f^n_{j+1} - f^n_{j-1}}{2\Delta\eta}, \\ f^n_{\eta\eta} &= \frac{f^n_{j+1} + f^n_{j-1} - 2f^n_j}{\Delta\eta^2} \end{aligned}\right\} \quad \text{(II. E-107)}$$

The first component of Eq. (II. E-37), the ρ equation, has no viscous terms. The second component is as follows, where nonviscous terms are suppressed

$$\frac{\partial V}{\partial t} = \bar{b}_1 \frac{\partial^2 V}{\partial \eta^2} + \bar{b}_2 \frac{\partial V}{\partial \eta} - \bar{b}_3 V.$$

For the high order term we use

$$\frac{\partial^2 V}{\partial \eta^2} = V_{\eta\eta}.$$

The subscript, the time level, will be specified later. The low order term is treated as though it were a separate hyperbolic equation. Our difference equation for this is as follows: use a forward difference if $\bar{b}_2 > 0$ and use a backward difference if $\bar{b}_2 < 0$. This will be discussed more thoroughly in Part B, where we show that this is equivalent to

$$\bar{b}_2 \frac{\partial V}{\partial \eta} = \bar{b}_2 V_\eta + |\bar{b}_2| \left(\frac{\Delta\eta}{2}\right) V_{\eta\eta}.$$

We have then

$$\frac{\partial V}{\partial t} = \left(\bar{b}_1 + \frac{\Delta\eta}{2}|\bar{b}_2|\right) V_{\eta\eta} + \bar{b}_2 V_\eta - \bar{b}_3 V, \quad \text{(II. E-108.1)}$$

where $\frac{\partial V}{\partial t}$ will be defined later.

The third and fourth components of Eq. (II.E-37) have coupling which, as noted earlier, presents some problems. For the second order terms we will use the explicit-implicit approximation (We have noted earlier that this is stable for the linear problem.). The term $\frac{\partial C}{\partial \eta}\ \frac{\partial T}{\partial \eta}$, which appears in both these equations, is an engima at the present time, since we know of no theoretical basis for specifying differences. Our approach is to treat $\frac{\partial C}{\partial \eta}$ as a coefficient in the T equation and to treat $\frac{\partial T}{\partial \eta}$ as a coefficient in the C equation. The term $\left(\frac{\partial T}{\partial \eta}\right)^2$ is treated as follows: $\frac{\partial T}{\partial \eta}$ is considered as a coefficient, or $\left(\frac{\partial T}{\partial \eta}\right)^2$ takes the form a $\frac{\partial T}{\partial \eta}$. The other low order terms are treated as in the V equation above.

The T equation is

$$\frac{\partial T}{\partial t} = \bar{c}_1 \frac{\partial^2 T}{\partial \eta^2} + \bar{c}_2 \frac{\partial T}{\partial \eta} + \bar{c}_3 \left(\frac{\partial T}{\partial \eta}\right)^2 + \bar{c}_4 + \bar{c}_5 \frac{\partial C}{\partial \eta}\ \frac{\partial T}{\partial \eta}$$

$$- \bar{c}_6 \left(\frac{\partial C}{\partial \eta}\right)^2 + \bar{c}_7 \frac{\partial^2 C}{\partial \eta^2} + \bar{c}_8 \frac{\partial C}{\partial \eta} .$$

Let

$$\bar{c}_9 = \bar{c}_2 + \bar{c}_3 T_\eta ,$$
$$\bar{c}_{10} = \bar{c}_5 C_\eta ,$$
$$\bar{c}_{11} = - \bar{c}_6 C_\eta .$$

Then,

$$\frac{\partial T}{\partial t} = \bar{c}_1 T_{\eta\eta} + \bar{c}_9 T_\eta + |\bar{c}_9| \frac{\Delta\eta}{2} T_{\eta\eta} + \bar{c}_4 + \bar{c}_{10} T_\eta$$
$$+ |\bar{c}_{10}| \frac{\Delta\eta}{2} T_{\eta\eta} + \bar{c}_{11} C_\eta + |\bar{c}_{11}| \frac{\Delta\eta}{2} C_{\eta\eta} + \bar{c}_7 C_{\eta\eta}$$
$$+ \bar{c}_8 C_\eta + |c_8| \frac{\Delta\eta}{2} C_{\eta\eta} ,$$

or

$$\frac{\partial T}{\partial t} = \left[\bar{c}_1 + \frac{\Delta\eta}{2} |\bar{c}_9| + \frac{\Delta\eta}{2} |\bar{c}_{10}| \right] T_{\eta\eta} + (\bar{c}_9 + \bar{c}_{10}) T_\eta + \bar{c}_4 \qquad \text{(II. E-108. 2)}$$

$$+ \left(\bar{c}_7 + \frac{\Delta\eta}{2} |\bar{c}_{11}| + \frac{\Delta\eta}{2} |\bar{c}_8| \right) C_{\eta\eta} + (\bar{c}_8 + \bar{c}_4) C_\eta \ .$$

The C equation is

$$\frac{\partial C}{\partial t} = \bar{d}_1 \frac{\partial^2 C}{\partial \eta^2} - \bar{d}_2 \left(\frac{\partial C}{\partial \eta} \right)^2 + \bar{d}_3 \frac{\partial C}{\partial \eta} + \bar{d}_4 \frac{\partial C}{\partial \eta} \frac{\partial T}{\partial \eta} + \bar{d}_5 \ .$$

Let

$$\bar{d}_6 = - \bar{d}_2 C_\eta \ ,$$

$$\bar{d}_7 = \bar{d}_4 T_\eta \ .$$

Then,

$$\frac{\partial C}{\partial t} = \bar{d}_1 C_{\eta\eta} + \bar{d}_6 C_\eta + |\bar{d}_6| \frac{\Delta\eta}{2} C_{\eta\eta} + \bar{d}_3 C_\eta + |\bar{d}_3| \frac{\Delta\eta}{2} C_{\eta\eta}$$

$$+ \bar{d}_7 C_\eta + |\bar{d}_7| \frac{\Delta\eta}{2} C_{\eta\eta} + \bar{d}_5 \ ,$$

or

$$\frac{\partial C}{\partial t} = \left[\bar{d}_1 + \frac{\Delta\eta}{2} (|\bar{d}_6| + |\bar{d}_3| + |\bar{d}_7|) \right] C_{\eta\eta} + (\bar{d}_6 + \bar{d}_3 + \bar{d}_7) C_\eta \qquad \text{(II. E-108. 3)}$$

$$+ \bar{d}_5 \ .$$

PART B: The Hyperbolic (Inviscid) System

Two classes of methods are generally available for solving first-order hyperbolic partial differential equations. One of these, methods of characteristics, rely heavily on the characteristics of the system (see, for example, Sauerwein (II.E-16)). The other, finite difference methods, in principle allows much more flexibility. However, in reality there is no difference in the two approaches, since ultimately both result in difference equations. Since the behavior of the system is so strongly governed by the characteristics, one can hardly believe that a difference equation could be unrelated to the characteristics of the system and still be reasonably successful.

We chose to adopt what most commonly would be called a finite difference equation. Various methods are available (II.E-15). We chose as our guide the method of Courant, Isaacson & Rees (II.E-3), although our final equation is an extension of a method proposed by Anucina (II.E-1). Details of this difference equation, as well as its stability and convergence properties, have been written up elsewhere (See Section II.E).

The differential equation is

$$\frac{\partial X}{\partial t} = A \frac{\partial X}{\partial \eta} \quad \text{from Eq. (II.E-37)}$$

We know there exists a matrix M such that $MAM^{-1} = D$, where $D = \text{diag}(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$: Eq. (II.E-95). The difference equation can then be written as

$$X_t = AX_\eta + A^* \left(\frac{\Delta\eta}{2}\right) X_{\eta\eta}, \qquad \text{(II.E-109)}$$

where

1) $X_t = \left(X_j^{n+1} - X_j^n\right)/\Delta t$,

2) $|D| = \text{diag}(|\lambda_1|, |\lambda_2|, |\lambda_3|, |\lambda_4|)$,

3) X_η, $X_{\eta\eta}$: see eq. (II.E-107),

4) $A^* = M^{-1}\,|D|\,M = (a^*_{ij})$,

5) $\lambda_1 = -a_1$, $\lambda_2 = -a_1 + c_s$, $\lambda_3 = -a_1 - c_s$, $\lambda_4 = -a_1$.

Remark: It was found in earlier work (II.E-8) that if the explicit-implicit scheme was used for the parabolic terms, then a corresponding scheme should be used for the hyperbolic terms. Otherwise, in highly nonlinear cases we encountered instability. Note that the subscripts, the time level, are not indicated in Eq. (II.E-109). These will be supplied later. We will actually alternate the explicit and implicit versions of Eq. (II.E-109) in the same way as indicated for the parabolic terms (see Part A). Convergence of Eq. (II.E-109), when applied in this alternating form, has not been established in full generality. However, as indicated in Ref. II.E-9, it appears that the same methods used in Ref. II.E-10 could be used to establish convergence of the explicit-implicit form of Eq. (II.E-109).

We will need the following quantities:

$$\left.\begin{aligned} \alpha_1 &= \frac{|a_1 + c_s| + |a_1 - c_s| - 2|a_1|}{2c_s} \quad , \\ \alpha_2 &= \frac{|a_1 + c_s| - |a_1 - c_s|}{2c_s} \quad . \end{aligned}\right\} \qquad \text{(II.E-110)}$$

One verifies

$$\left.\begin{aligned} \alpha_1 &= \begin{cases} 0: \ |a_1| > c_s \\ 1 - \dfrac{|a_1|}{c_s} : \ |a_1| < c_s \end{cases} , \\ \alpha_2 &= \begin{cases} 1: \ a_1 > c_s \\ \dfrac{a_1}{c_s} : \ |a_1| < c_s \\ -1 : \ a_1 < -c_s \end{cases} , \end{aligned}\right\} \qquad \text{(II.E-111)}$$

$$|D|M = \begin{pmatrix} c_2|\lambda_1| & 0 & -a_2|\lambda_1| & 0 \\ -b_2|\lambda_2| & c_s|\lambda_2| & -b_3|\lambda_2| & -b_4|\lambda_2| \\ b_2|\lambda_3| & c_s|\lambda_3| & b_3|\lambda_3| & b_4|\lambda_3| \\ 0 & 0 & 0 & |\lambda_4| \end{pmatrix}$$

From Eq. (II. E-97) we obtain

$$a_{11}^{*} = \frac{1}{2c_s^2}\left[2b_3c_2|\lambda_1| + a_2b_2\left(|\lambda_2| + |\lambda_3|\right)\right],$$

$$= \frac{1}{2c_s^2}\left[2c_s^2|\lambda_1| + a_2b_2\left(|\lambda_2| + |\lambda_3| - 2|\lambda_1|\right)\right],$$

$$= |a_1| + \left(\frac{a_2b_2}{c_s}\right)\alpha_1$$

$$a_{12}^{*} = \frac{1}{2c_s^2}\left[a_2c_s\left(|\lambda_3| - |\lambda_2|\right)\right] = a_2\alpha_2,$$

$$a_{13}^{*} = \frac{1}{2c_s^2}\left[-2b_3a_2|\lambda_1| + a_2b_3\left(|\lambda_3| + |\lambda_2|\right)\right],$$

$$= \frac{a_2b_3}{2c_s^2}\left(|\lambda_2| + |\lambda_3| - 2|\lambda_1|\right) = \frac{a_2b_3}{c_s}\alpha_1,$$

$$a_{14}^{*} = \frac{a_2b_4}{2c_s^2}\left(|\lambda_3| + |\lambda_2| - 2|\lambda_1|\right) = \frac{a_2b_4}{c_s}\alpha_1,$$

$$a_{21}^{*} = \frac{1}{2c_s^2}\left[c_sb_2\left(|\lambda_3| - |\lambda_2|\right)\right] = b_2\alpha_2,$$

$$a_{22}^{*} = \frac{1}{2c_s^2}\left[c_s^2\left(|\lambda_3| + |\lambda_2|\right)\right] = \frac{|\lambda_2| + |\lambda_3|}{2} = |a_1| + \alpha_1c_s,$$

$$a_{23}^{*} = \frac{1}{2c_s^2}\left[c_sb_3|\lambda_3| - |\lambda_2|\right] = b_3\alpha_2,$$

$$a_{24}^{*} = \frac{1}{2c_s^2}\left[c_sb_4|\lambda_3| - |\lambda_2|\right] = b_4\alpha_2,$$

$$a^*_{31} = \frac{1}{2c_s^2}\left[-2b_2c_2|\lambda_1| + c_2b_2|\lambda_2| + c_2b_2|\lambda_3|\right],$$

$$= \frac{c_2b_2}{c_s}\alpha_1 ,$$

$$a^*_{32} = \frac{c_2c_s\,|\lambda_3| - |\lambda_2|}{2c_s^2} = c_2\alpha_2 ,$$

$$a^*_{33} = \frac{1}{2c_s^2}\left[2a_2b_2|\lambda_1| + c_2b_3\left(|\lambda_2| + |\lambda_3|\right)\right],$$

$$= |a_1| + \frac{c_2b_3}{c_s}\alpha_1 ,$$

$$a^*_{34} = \frac{c_2b_4}{2c_s^2}\left[|\lambda_2| + |\lambda_3| - 2|\lambda_1|\right] = \frac{c_2b_4}{c_s}\alpha_1 ,$$

$$a^*_{41} = a^*_{42} = a^*_{43} = 0 , \quad a^*_{44} = |\lambda_1| = |a_1| .$$

We thus obtain

$$\frac{\partial \rho}{\partial t} = -a_1\rho_\eta - a_2V_\eta + \frac{\Delta\eta}{2}\left[a^*_{11}\rho_{\eta\eta} + a^*_{12}V_{\eta\eta} + a^*_{13}T_{\eta\eta} + a^*_{14}C_{\eta\eta}\right], \tag{II.E-112.1}$$

$$\frac{\partial V}{\partial t} = -b_2\rho_\eta - a_1V_\eta - b_3T_\eta - b_4C_\eta + \frac{\Delta\eta}{2}\left[a^*_{21}\rho_{\eta\eta} + a^*_{22}V_{\eta\eta} + a^*_{23}T_{\eta\eta} + a^*_{24}C_{\eta\eta}\right], \tag{II.E-112.2}$$

$$\frac{\partial T}{\partial t} = -c_2V_\eta - a_1T_\eta + \frac{\Delta\eta}{2}\left[a^*_{31}\rho_{\eta\eta} + a^*_{32}V_{\eta\eta} + a^*_{33}T_{\eta\eta} + a^*_{34}C_{\eta\eta}\right], \tag{II.E-112.3}$$

$$\frac{\partial C}{\partial t} = -a_1C_\eta + \frac{\Delta\eta}{2}|a_1|C_{\eta\eta} . \tag{II.E-112.4}$$

PART C: Final Form of the Difference Equation

We now combine the difference Equations (II.E-108.1) and (II.E-112.1), add in the "zero order" terms of Eq. (II.E-37), and put them in final form.

1) The ρ equation:

There are no viscous terms, so the Eq. is (II. E-111)

$$\frac{\partial \rho}{\partial t} = -a_1 \rho_\eta - a_2 V_\eta + \frac{\Delta\eta}{2}\left[a^*_{11}\rho_{\eta\eta} + a^*_{12}V_{\eta\eta} + a^*_{13}T_{\eta\eta} + a^*_{14}C_{\eta\eta}\right] - a_3 .$$

We will want to solve this equation for ρ, assuming that T, V, and C are known (actually, all equations will be solved simultaneously). Thus, we can use

$$\frac{\partial \rho}{\partial t} = -a_1\rho_\eta - \rho\eta_r V_\eta + \frac{\Delta\eta}{2}\left[a^*_{11}\rho_{\eta\eta} + \rho\eta_r V_{\eta\eta} + \frac{\rho\eta_r b_3\alpha_1}{c_s}T_{\eta\eta} + \frac{\rho\eta_r b_4\alpha_1}{c_s}C_{\eta\eta}\right] - \frac{\delta}{r}\rho V . \qquad \text{(II. E-113.1)}$$

Note that the coefficients a_1, a^*_{11}, $\frac{b_3\alpha_1}{c_s}$, $\frac{4\alpha_1}{c_s}$ have no explicit dependence on ρ.

Let

$$\left.\begin{aligned} A_4 &= -a_1\rho_\eta + \frac{\Delta\eta}{2}\left[a^*_{11}\frac{(\rho_{i+1}+\rho_{i-1})}{\Delta\eta^2}\right] = -a_1\rho_\eta + a^*_{11}\frac{(\rho_{i+1}+\rho_{i-1})}{2\Delta\eta}, \\ A_5 &= \eta_r V_\eta + \frac{a^*_{11}}{\Delta\eta} - \frac{\Delta\eta}{2}\left[\eta_r V_{\eta\eta} + \frac{\eta_r b_3\alpha_1}{c_s}T_{\eta\eta} + \frac{\eta_r b_4\alpha_i}{c_s}C_{\eta\eta}\right] + \frac{\delta}{r}V , \end{aligned}\right\}$$

$$\frac{\partial \rho}{\partial t} = A_4 - \rho A_5 . \qquad \text{(II. E-113.2)}$$

Letting

$$\frac{\partial \rho}{\partial t} = \frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} ,$$

$$\rho_i^{n+1} = \rho_i^n + \Delta t_n A_4 - \rho \Delta t_n A_5 .$$

For the explicit scheme, we have

$$\rho_i^{n+1} = \rho_i^n (1-\Delta t_n A_5) + \Delta t_n A_4. \qquad \text{(II. E-113.3)}$$

For the implicit scheme, we have

$$\rho_i^{n+1} = \left(\rho_i^n + \Delta t_n A_4\right) / (1+\Delta t_n A_5) . \qquad \text{(II. E-113.4)}$$

After the first time, the explicit scheme simplifies to the following extrapolation formula:

$$\rho_i^{n+1} = \left(1 + \frac{\Delta t_n}{\Delta t_{n-1}}\right)\rho_i^n - \frac{\Delta t_n}{\Delta t_{n-1}} \rho_i^{n-1}. \qquad \text{(II. E-113.5)}$$

Remark: as noted earlier, Eq. (II. E-113.4) needs no iteration.

The right side is independent of ρ_i^{n+1}.

2) The V-equation:

$$\frac{\partial V}{\partial t} = - b_2\rho_\eta - a_1 V_\eta - b_3 T_\eta - b_4 C_\eta$$

$$+ \frac{\Delta\eta}{2}\left[b_2\alpha_2\rho_{\eta\eta} + \left(|a_1| + \alpha_1 c_s\right)V_{\eta\eta} + b_3\alpha_2 T_{\eta\eta} + b_4\alpha_2 C_{\eta\eta}\right] \qquad \text{(II. E-114.1)}$$

$$+ \left(\bar{b}_1 + \frac{\Delta\eta}{2}|\bar{b}_2|\right)V_{\eta\eta} + \bar{b}_2 V_\eta - \bar{b}_3 V .$$

Let

$$B_4 = -b_2\rho_\eta - b_3 T_\eta - b_4 C_\eta - \eta_t V_\eta$$

$$+\left(\bar{b}_1 + \frac{\Delta\eta}{2}\,|\bar{b}_2|\right)\left(\frac{V_{i+1} + V_{i-1}}{\Delta\eta^2}\right) + \bar{b}_2 V_\eta \,,$$

$$B_5 = +\eta_r V_\eta + \left(\bar{b}_1 + \frac{\Delta\eta}{2}\,|\bar{b}_2|\right)\frac{2}{\Delta\eta^2} + \bar{b}_3 \,, \qquad \text{(II.E-114.2)}$$

$$B_6 = \frac{\Delta\eta}{2}\,(b_2\rho_{\eta\eta} + b_3 T_{\eta\eta} + b_4 C_{\eta\eta}) \,,$$

$$\frac{\partial V}{\partial t} = B_4 - B_5 V + \alpha_2 B_6 + \frac{\Delta\eta}{2}\left(|a_1| + \alpha_1 c_s\right) V_{\eta\eta}$$

Let

$$\delta_1 = \operatorname{sgn} a_1 \rightarrow |a_1| = a_1\delta_1 \,,$$

$$\alpha_2 = \begin{cases} \delta_1 : & |a_1| > c_s \\ \dfrac{a_1}{c_s} : & |a_1| < c_s \end{cases} \,, \qquad \text{(II.E-114.3)}$$

$$\alpha_1 c_s + |a_1| = \begin{cases} |a_1| = a_1\delta_1 : & |a_1| > c_s \\ c_s : & |a_1| < c_s \,. \end{cases}$$

Let

$$\delta_2 = \begin{cases} 0 : & |a_1| > c_s \\ 1 : & |a_1| < c_s \,. \end{cases} \qquad \text{(II.E-114.4)}$$

Then,

$$\left.\begin{aligned} &\alpha_2 = \delta_1 (1-\delta_2) + \delta_2 \frac{a_1}{c_s} \quad , \\ &\alpha_1 c_s + |a_1| = \delta_2 c_s + (1-\delta_2)\,\delta_1 a_1 \quad , \end{aligned}\right\} \text{(II. E-114.5)}$$

$$\frac{\partial V}{\partial t} = B_4 - B_5 V + \left[\delta_1(1-\delta_2) + \delta_2 \frac{a_1}{c_s}\right] B_6 + \frac{\Delta\eta}{2}\left[\delta_2 c_s + (1-\delta_2)\,\delta_1 a_1\right] V_{\eta\eta} \quad ,$$

$$V_i^{n+1} - V_i^n = B_4 \Delta t_n - B_5 V_i \Delta t_n + \left[\delta_1(1-\delta_2) + \delta_2 \frac{\eta_t}{c_s}\right] B_6 \Delta t_n + \frac{\delta_2 V_i \eta_r}{c_s} B_6 \Delta t_n$$

$$+ \left[\delta_2 c_s + (1-\delta_2)\,\delta_1 \eta_t\right]\left(\frac{\Delta t_n}{2\Delta\eta}\right)\left(V_{i+1} + V_{i-1} - 2V_i\right) \quad ,$$

$$+ \left[(1-\delta_2)\,\delta_1 V_i \eta_r\right]\left(\frac{\Delta t_n}{2\Delta\eta}\right)\left(V_{i+1} + V_{i-1} - 2V_i\right) \quad .$$

Let

$$\left.\begin{aligned} B_7 &= V_i^n + B_4 \Delta t_n + \left[\delta_1(1-\delta_2) + \delta_2 \frac{\eta_t}{c_s}\right] B_6 \Delta t_n \\ &\quad + \left[\delta_2 c_s + (1-\delta_2)\,\delta_1 \eta_t\right]\left(\frac{\Delta t_n}{2\Delta\eta}\right)\left(V_{i+1} + V_{i-1}\right) , \\ B_8 &= B_5 \Delta t_n - \frac{\delta_2 \eta_r}{c_s} B_6 \Delta t_n + \left[\delta_2 c_s + (1-\delta_2)\,\delta_1 \eta_t\right] \frac{\Delta t_n}{\Delta\eta} \\ &\quad - \left[(1-\delta_2)\,\delta_1 \eta_r\right]\left(\frac{\Delta t_n}{2\Delta\eta}\right)\left(V_{i+1} + V_{i-1}\right) , \\ B_9 &= (1-\delta_2)\,(\delta_1 \eta_r)\left(\frac{\Delta t_n}{\Delta\eta}\right) . \end{aligned}\right\} \text{(II. E-114.6)}$$

Then,

$$V_i^{n+1} = B_7 - B_8 V_i - B_9 (V_i)^2 \quad . \qquad \text{(II. E-114.7)}$$

For the explicit scheme

$$V_i^{n+1} = B_7 - B_8 V_i^n - B_9 (V_i^n)^2 . \qquad \text{(II. E-114. 8)}$$

After the first time step the explicit scheme reduces to the following extrapolation formula.

$$V_i^{n+1} = \left(1 + \frac{\Delta t_n}{\Delta t_{n-1}}\right) V_i^n - \left(\frac{\Delta t_n}{\Delta t_{n-1}}\right) V_i^{n-1} . \qquad \text{(II. E-114. 9)}$$

The implicit scheme becomes

$$B_9 (V_i^{n+1})^2 + (1+B_8) V_i^{n+1} - B_7 = 0. \qquad \text{(II. E-114. 10)}$$

If $B_9 = 0$, Eq. (II. E-114. 10) becomes

$$V_i^n = B_7/(1+B_8) . \qquad \text{(II. E-114. 11)}$$

If $B_9 \neq 0$, we proceed to solve the quadratic

$$V_i^{n+1} = - \frac{(1+B_8) \pm \sqrt{(1+B_8)^2 + 4B_7B_9}}{2B_9} .$$

To determine the sign let $\Delta t \rightarrow 0$

$$B_7 \rightarrow V_i^n , \; B_8 \rightarrow 0, \; B_9 \rightarrow 0 ,$$

$$V_i^{n+1} \rightarrow \frac{-1 \pm \sqrt{1 + 4 B_7 B_9}}{2B_9} .$$

If we choose the + sign:

$$V_i^{n+1} = \frac{-1 + 1 + 2B_7B_9}{2B_i} = B_7, \text{ which is what we want.}$$

Thus,

$$V_i^{n+1} = \frac{-(1+B_8) + \sqrt{(1+B_8)^2 + 4B_7B_9}}{2B_9} ,$$

$$= \frac{-(1+B_8) + |1+B_8|\sqrt{1 + \frac{4B_7B_9}{(1+B_8)^2}}}{2B_9} , \qquad \text{(II. E-114. 12)}$$

$$V_i^{n+1} = + \left(\frac{1+B_8}{2B_9}\right)\left[-1 + \epsilon\sqrt{1 + B_{10}}\right] ,$$

where

$$\epsilon = \text{sgn}\,(1+B_8) ,$$

$$B_{10} = \frac{4B_7B_9}{(1+B_8)^2} .$$

Remark: Note that Eq. (II. E-114. 12) is continuous as $1+B_8$ goes through zero.

$$\lim_{1+B_8 \to \pm 0} V_i^{n+1} = \frac{1+B_8}{2B_9}\left[-1+\epsilon\,\frac{2\sqrt{B_7B_9}}{|1+B_8|}\right]$$

$$\to \frac{\epsilon\,(1+B_8)}{|1+B_8|}\sqrt{\frac{B_7}{B_9}} = \sqrt{\frac{B_7}{B_9}} .$$

Equation (II. E-114. 12) can be solved directly for V_i^{n+1}, almost! Actually, we need to guess at ζ_1 and δ_2. In practice Eq. (II. E-114. 12) requires iteration only as a_1 and $a_1 \pm c_s$ go through zero, and actually the general procedure, which will be discussed later, handled these situations as part of the normal routine.

If B_{10} is small, $B_{10} < .02$, we use,

$$-1 + \sqrt{B_{10}} = \frac{B_{10}}{2}\left[1 - \frac{B_{10}}{4} + \frac{B_{10}^2}{8} - \frac{5}{64}B_{10}^3\right] . \quad \text{(II. E-114.13)}$$

Iteration problems have occurred in the V equation for some values of V. For example, if a significant V is in the order of 10^4, then $V = 10^{-3}$ cannot be obtained with any significant digits. In fact, a situation occurred where a change in ρ in the 8th digit affected V in the 4th digit and consequently convergence was not obtained. However, this value of V was insignificant. Two corrective devices are used here:

1) If $|V| < \delta$, where δ is input, set $V = 0$.
2) If V does not converge, but if $\left|\frac{V}{V_{max}}\right| < \delta$, where V_{max} is max V, then accept the result.

3) The T equation:

$$\frac{\partial T}{\partial t} = -c_2 V_\eta - a_1 T_\eta + \frac{\Delta\eta}{2}\left[\frac{c_2 b_2 \alpha_1}{c_s}\rho_{\eta\eta} + c_2\alpha_2 V_{\eta\eta} + \left(|a_1| + \frac{c_2 b_3}{c_s}\alpha_1\right)T_{\eta\eta} + \frac{c_2 b_4}{c_s}\alpha_1 C_{\eta\eta}\right] - c_3 T$$
$$+ \left(\bar{c}_1 + \frac{\Delta\eta}{2}|\bar{c}_9| + \frac{\Delta\eta}{2}|\bar{c}_{10}|\right)T_{\eta\eta} + (\bar{c}_9 + \bar{c}_{10})T_\eta \quad \text{(II. E-115.1)}$$
$$+ \bar{c}_4 + \left(\bar{c}_7 + \frac{\Delta\eta}{2}|\bar{c}_{11}| + \frac{\Delta\eta}{2}|\bar{c}_8|\right)C_{\eta\eta} + (\bar{c}_8 + \bar{c}_{11})C_\eta .$$

Because of the various coefficients which are a function of T, it is not possible to solve this equation explicitly for T. However, we will "extract" as much T dependence as possible.

a) c_2 has a factor of T; . ˙ ., let $c_2 = \left(\frac{c_2}{T}\right)T$,
b) a_1: independent of T,
c) c_s: $T^{1/2}$ (see Eq. II.E-93); . ˙ ., let $c_s = \left(\frac{c_s}{T^{1/2}}\right)T^{1/2}$,
d) b_2 and b_4: factor of T.

$$\frac{\partial T}{\partial t} = -T\left\{ -\left(\frac{c_2}{T}\right)V_\eta + \frac{\Delta\eta}{2}\left[\left(\frac{b_2\alpha_1}{c_s}\right)\rho_{\eta\eta} + \alpha_2 V_{\eta\eta} + \left(\frac{b_4\alpha_1}{c_s}\right)C_{\eta\eta}\right]\left(\frac{C_2}{T}\right) - c_3\right\} - a_1 T_\eta + \left(\frac{\Delta\eta}{2}\right)\left[|a_1| + \frac{c_2 b_3}{c_s}\alpha_1\right] T_{\eta\eta}$$

$$+\left(\bar{c}_1 + \frac{\Delta\eta}{2}|\bar{c}_9| + \frac{\Delta\eta}{2}|\bar{c}_{10}|\right)T_{\eta\eta} + (\bar{c}_9 + \bar{c}_{10})\,T_\eta + \bar{c}_4$$

$$+\left(\bar{c}_7 + \frac{\Delta\eta}{2}|\bar{c}_{11}| + \frac{\Delta\eta}{2}|\bar{c}_8|\right)C_{\eta\eta} + (\bar{c}_8 + \bar{c}_{11})\,C_\eta .$$

Note that $\frac{b_2}{c_s}$ has a factor of $T^{1/2}$, as does $\frac{b_4}{c_s}$. Also, α_1 and α_2 may or may not have a T dependence.

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = T\left\{ -\left(\frac{c_2}{T}\right)V_\eta + \frac{\Delta\eta}{2}\left(\frac{b_2\alpha_1}{c_s}\rho_{\eta\eta} + \alpha_2 V_{\eta\eta} + \frac{b_4\alpha_1}{c_s}C_{\eta\eta}\right)\frac{c_2}{T} - c_3\right\}$$

$$- a_1 T_\eta + \left[|a_1| + \frac{c_2 b_3 \alpha_1}{c_s}\right]\left(\frac{T_{i+1} + T_{i-1} - 2T_i}{2\Delta\eta}\right)$$

$$+\left[\bar{c}_1 + \frac{\Delta\eta}{2}\left(|\bar{c}_9| + |\bar{c}_{10}|\right)\right]\left(\frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta\eta\, 2}\right) + (\bar{c}_9 + \bar{c}_{10})\,T_\eta + \bar{c}_4$$

$$+\left(\bar{c}_7 + \frac{\Delta\eta}{2}|\bar{c}_{11}| + \frac{\Delta\eta}{2}|\bar{c}_8|\right)C_{\eta\eta} + (\bar{c}_8 + \bar{c}_{11})\,C_\eta .$$

Let

$$-a_1 T_\eta + \left(\frac{T_{i+1} + T_{i-1}}{2\Delta\eta}\right)\left[|a_1| + \frac{c_2 b_3 \alpha_1}{c_s} + \frac{2\bar{c}_1}{\Delta\eta} + |\bar{c}_9| + |\bar{c}_{10}|\right]$$

$$+ (\bar{c}_9 + \bar{c}_{10})\,T_\eta + \bar{c}_4 + \left(\bar{c}_7 + \frac{\Delta\eta}{2}|\bar{c}_{11}| + \frac{\Delta\eta}{2}|\bar{c}_8|\right)C_{\eta\eta}$$

$$+ (\bar{c}_8 + \bar{c}_4)\,C_\eta ,$$

$$c_5 = -\left(\frac{c_2}{T}\right) V_\eta + \left(\frac{\Delta\eta\, c_2}{2T}\right)\left(\frac{b_2\alpha_1}{c_s}\rho_{\eta\eta} + \alpha_2 V_{\eta\eta} + \frac{b_4\alpha_1}{c_s} C_{\eta\eta}\right) - c_3$$

$$- \frac{1}{\Delta\eta}\left(|a_1| + \frac{c_2 b_3 \alpha_1}{c_s}\right) - \frac{2\bar{c}_1}{\Delta\eta^2} - \frac{1}{\Delta\eta}\left(|\bar{c}_9| + |\bar{c}_{10}|\right) .$$

Then,

$$T_i^{n+1} - T_i^n = c_4 \Delta t_n + c_5 \Delta t_n T_i .$$

For the explicit scheme,

$$T_i^{n+1} = (1 + c_5 \Delta t_n)\, T_i^n + c_4 \Delta t_n . \qquad \text{(II.E-115.2)}$$

After the first time step the explicit scheme becomes:

$$T_i^{n+1} = \left(1 + \frac{\Delta t_n}{\Delta t_{n-1}}\right) T_i^n - \frac{\Delta t_n}{\Delta t_{n-1}} T_i^{n-1} . \qquad \text{(II.E-115.3)}$$

The implicit scheme is

$$T_i^{n+1} = (T_i^n + c_4 \Delta t_n)/(1 - c_5 \Delta t_n) . \qquad \text{(II.E-115.4)}$$

4) The C equation:

$$\frac{\partial C}{\partial t} = -a_1 C_\eta + |a_1|\left(\frac{\Delta\eta}{2}\right) C_{\eta\eta} + \left[\bar{d}_1 + \frac{\Delta\eta}{2}\left(|d_6| + |\bar{d}_3| + |\bar{d}_7|\right)\right] C_{\eta\eta} \qquad \text{(II.E-116.1)}$$

$$+ (\bar{d}_6 + \bar{d}_3 + \bar{d}_7)\, C_\eta .$$

Let

$$d_2 = -a_1 C_\eta + \left(\frac{C_{i+1} + C_{i-1}}{2\Delta\eta}\right)\left[|a_1| + |\bar{d}_6| + |\bar{d}_3| + |\bar{d}_7| + \frac{2\bar{d}_1}{\Delta\eta}\right]$$

$$+ (\bar{d}_6 + \bar{d}_3 + \bar{d}_7)\, C_\eta ,$$

$$d_3 = \frac{2\bar{d}_1}{\Delta\eta^2} + \frac{1}{\Delta\eta}\left(|\bar{d}_6| + |d_3| + |\bar{d}_7| + |a_1|\right) .$$

Then,

$$C_i^{n+1} - C_i^n = d_2 \Delta t_n - d_3 C_i \Delta t_n .$$

For the explicit scheme,

$$C_i^{n+1} = d_2 \Delta t + C_i^n\,(1 - d_3 \Delta t_n) . \qquad \text{(II.E-116.2)}$$

After the first time step, the explicit scheme becomes

$$C_i^{n+1} = \left(1 + \frac{\Delta t_n}{\Delta t_{n-1}}\right) C_i^n - \left(\frac{\Delta t_n}{\Delta t_{n-1}}\right) C_i^{n-1} . \qquad \text{(II.E-116.3)}$$

The implicit scheme becomes

$$C_i^{n+1} = (C_i^n + d_2 \Delta t_n) \;/\; (1 + d_3 \Delta t_n) . \qquad \text{(II.E-116.4)}$$

≡

When using the implicit scheme, the following four equations must be solved simultaneously for the variables C_i^{n+1}, T_i^{n+1}, V_i^{n+1}, ρ_i^{n+1}: Eq. (II.E-116.4), Eq. (II.E-115.4), Eq. (II.E-114.10), and Eq. (II.E-113.4). Note that in these equations it is intended that the coefficients are evaluated with the variables at $n+1$; for example, in Eq. (II.E-113.4) A_4 and A_5 are evaluated at $(t_{n+1}, i\Delta\eta)$. Thus, the system of equations is highly nonlinear. The method of iteration will be discussed in Appendix C. Effectively, this scheme goes as follows.

Let Problem A be the problem of solving Eq. (II.E-113.4) and Eq. (II.E-114.10) simultaneously for ρ_i^{n+1}, V_i^{n+1}.

Let Problem B be the problem of solving Eq. (II. E-113.4), Eq. (II. E-114.10), and Eq. (II. E-116.4) for ρ_i^{n+1}, V_i^{n+1}, C_i^{n+1}.

The procedure is as follows:

a) Guess at T_i^{n+1} and solve problem B. Calculate T_i^{n+1} from Eq. (II. E-115.4) and get a new guess for T_i^{n+1}. Solve problem B, etc.

b) In order to solve Problem B, guess at C_i^{n+1} and solve problem A. Calculate C_i^{n+1} from Eq. (II. E-116.4) and get a new guess at T_i^{n+1}. Solve Problem A again, etc.

c) Problem A is solved in the indicated fashion.

When the implicit point is next to $\eta = 0$ or $\eta = 1$, the situation can be further complicated. In this case, the four variables at the boundary may need to be solved simultaneously with the four variables at the interior point. This could result in a system of eight simultaneous equations. These would be set up as indicated above. (The Boundary conditions will be discussed further in Part D).

PART D: Boundary Conditions Equations

We will now outline the approximations that have been used at the boundary. As noted in the discussion of boundary conditions, any new physical problem could require a new set of boundary conditions. We will first present general formulas that are used, and then go through the four physical problems that were outlined in Section II. E. 3.2).

For any function f,

$$\frac{\partial f}{\partial \eta}(\eta=0)=\begin{cases} \frac{1}{2\Delta\eta}(-3f_o + 4f_1 - f_2): \text{ 3-point formula} \\ \frac{1}{\Delta\eta}(f_1 - f_o): \text{ 2-point formula,} \end{cases} \quad \text{(II. E-117)}$$

$$\frac{\partial f}{\partial \eta}(\eta=1)=\begin{cases} \frac{1}{2\Delta\eta}(3f_N - 4f_{N-1} + f_{N-2}): \text{ 3-pt. formula} \\ \frac{1}{\Delta\eta}(f_N - f_{N-1}): \text{ 2-point formula.} \end{cases} \quad \text{(II. E-118)}$$

It is necessary in some cases to approximate the ρ-equation on the boundary

$$\frac{\partial \rho}{\partial t} = - a_1 \frac{\partial \rho}{\partial \eta} - a_2 \frac{\partial V}{\partial \eta} - a_3 .$$

At $\eta = 0$ we use a forward difference and at $\eta = 1$ a backward difference is used. Note that in so far as $\frac{\partial \rho}{\partial \eta}$ is concerned, this is consistent with our difference equation.

$$-a_1 \frac{\partial \rho}{\partial \eta} = - a_1 \rho_\eta + |a_1| \left(\frac{\Delta \eta}{2}\right) \rho_{\eta\eta} ,$$

$$= |a_1| \rho_\eta + |a_1| \frac{\Delta \eta}{2} \rho_{\eta\eta} : \text{ at } \eta = 0 \quad (a_1 \leq 0 \text{ from Eq. (II. E-86)},$$

$$= \frac{|a_1|}{2\Delta \eta} (\rho_{i+1} - \rho_{i-1} + \rho_{i+1} + \rho_{i-1} - 2\rho_i) = \frac{|a_1|}{\Delta \eta} (\rho_{i+1} - \rho_i)$$

$$= - \frac{a_1}{\Delta \eta} (\rho_{i+1} - \rho_i) .$$

At $\eta = 1$, where $a_1 \geq 0$ (from Eq. (II. E-87))

$$-a_1 \frac{\partial \rho}{\partial \eta} = - a_1 \rho_\eta + a_1 \frac{\Delta \eta}{2} \rho_{\eta\eta} ,$$

$$= - \frac{a_1}{2\Delta \eta} (\rho_{i+1} - \rho_{i-1} - \rho_{i+1} - \rho_{i-1} + 2\rho_i) = - \frac{a_1}{\Delta \eta} (\rho_i - \rho_{i-1}) .$$

The difference equation is

$$\frac{\rho_o^{n+1} - \rho_o^n}{\Delta t} = - \frac{a_1}{\Delta \eta} \left(\rho_1^{n+1} - \rho_o^{n+1}\right) - a_2 \left(\frac{\partial V}{\partial \eta}\right) - a_3 ,$$

where $\frac{\partial V}{\partial \eta}$ is evaluated by Eq. (II. E-117).

$$\rho_o^{n+1} - \rho_o^n = - \frac{a_1 \Delta t}{\Delta \eta} \left(\rho_1^{n+1} - \rho_o^{n+1}\right) - \rho_o^{n+1} \left(\eta_r \frac{\partial V}{\partial \eta} + \frac{\delta V}{r}\right) \Delta t .$$

Let

$$A_4 = \frac{+|a_1|\Delta t}{\Delta\eta} + \Delta t\left(\eta_r \frac{\partial V}{\partial \eta} + \frac{\delta V}{r}\right),$$

$$A_5 = \rho_o^n - \frac{a_1 \Delta t}{\Delta \eta}\,\rho_1^{n+1},$$

$$\rho_o^{n+1} = A_5/(1+A_4): \text{ at } \eta = 0. \qquad \text{(II.E-119)}$$

$$\equiv$$

$$\frac{\rho_N^{n+1} - \rho_N^n}{\Delta t} = -\frac{a_1}{\Delta\eta}\left(\rho_N^{n+1} - \rho_{N-1}^{n+1}\right) - a_2 \frac{\partial V}{\partial \eta} - a_3,$$

where $\frac{\partial V}{\partial \eta}$ is evaluated by Eq. (II.E-118).

$$\rho_N^{n+1} - \rho_N^n = -\frac{a_1 \Delta t}{\Delta \eta}\left(\rho_N^{n+1} - \rho_{N-1}^{n+1}\right) - \left(\eta_r \frac{\partial V}{\partial \eta} + \frac{\delta V}{r}\right)\rho_N^{n+1}\,\Delta t.$$

Let

$$A_4 = \frac{a_1 \Delta t}{\Delta \eta} + \left(\eta_r \frac{\partial V}{\partial \eta} + \frac{\delta V}{r}\right)\Delta t,$$

Then,

$$A_5 = \rho_N^n + \frac{a_1 \Delta t}{\Delta \eta}\,\rho_{N-1}^{n+1}.$$

$$\rho_N^{n+1} = A_5/(1+A_4): \text{ at } \eta = 1. \qquad \text{(II.E-120)}$$

Note that Eq. (II.E-119) and (II.E-120) are both implicit, the quantities are evaluated at t_{n+1}. Thus, Equations (II.E-119) and (II.E-120) at alternate time steps may need to be solved simultaneously with the values at the neighboring node.

We now discuss the problems which were specifically treated in Section II.E.3.2.

1) The Piston Problem

For the full set of equations (the viscous equations) $\frac{\partial T}{\partial \eta}$ is obtained from Eqs. (II.E-117) or (II.E-118), while ρ is obtained from Eqs. (II.E-119) and (II.E-120).

For the nonviscous system, we have:

a) $\eta = 0$: V was given as the piston velocity, resulting in the condition that $a_1 = 0$. The first two components of Eq. (II. E-98) were to be used for the remaining variables. The first gives

$$\frac{\partial y_1}{\partial t} = 0,$$

or

$$\left(\frac{\partial \rho}{\partial t}\right)_{\eta=0} = \left(\frac{a_2}{c_2}\right)\left(\frac{\partial T}{\partial t}\right)_{\eta=0} . \qquad \text{(II. E-121. 1)}$$

The second gives

$$\frac{\partial y_2}{\partial t} = c_s \frac{\partial y_2}{\partial \eta} + \frac{a_3}{\rho \eta_r} c_s^2 ,$$

or

$$-b_2 \frac{\partial \rho}{\partial t} + c_s \frac{\partial V}{\partial t} - b_3 \frac{\partial T}{\partial t} = c_s \left[-b_2 \frac{\partial \rho}{\partial \eta} + c_s \frac{\partial V}{\partial \eta} - b_3 \frac{\partial T}{\partial \eta} \right] + \frac{a_3}{a_2} c_s^2 ,$$

$$- \left(\frac{\partial \rho}{\partial t}\right)\left(b_2 + b_3 \frac{c_2}{a_2}\right) + c_s \frac{\partial V}{\partial t} = - \frac{c_s^2}{a_2} \frac{\partial \rho}{\partial t} + c_s \frac{\partial V}{\partial t} ,$$

$\therefore$

$$- \frac{\partial \rho}{\partial t} + \frac{a_2}{c_s} \frac{\partial V}{\partial t} = \frac{a_2}{c_s} \left[-b_2 \frac{\partial \rho}{\partial \eta} + c_s \frac{\partial V}{\partial \eta} - b_3 \frac{\partial T}{\partial \eta} \right] + a_3 ,$$

or

$$\frac{\partial \rho}{\partial t} = + \frac{a_2}{c_s} \left[\frac{\partial V}{\partial t} + b_2 \frac{\partial \rho}{\partial \eta} - c_s \frac{\partial V}{\partial \eta} + b_3 \frac{\partial T}{\partial \eta} \right] - a_3 . \qquad \text{(II. E-121. 2)}$$

In Eq. (II. E-121.2) $\frac{\partial V}{\partial t}$ is known and forward differences are used for the space derivatives. We obtain then

$$\rho_o^{n+1} - \rho_o^n = \frac{a_2}{c_2} (T_o^{n+1} - T_o^n) , \qquad \text{(II. E-122.1)}$$

$$\rho_o^{n+1} - \rho_o^n = \frac{a_2 \Delta t}{\Delta \eta c_s} \left[\left(\frac{\Delta \eta}{\Delta t} \right) \frac{\partial V}{\partial t} + b_2 (\rho_1 - \rho_o) - c_s (V_1 - V_o) \right.$$

$$\left. + b_3 (T_1 - T_o) \right] - a_3 \Delta t \ .$$

The explicit form of the previous equation is

$$\rho_o^{n+1} = \rho_o^n + \frac{a_2 \Delta t}{c_s \Delta \eta} \left[b_2 (\rho_1^n - \rho_o^n) - c_s (V_1^n - V_o^n) \right.$$

$$\left. + b_3 (T_1^n - T_o^n) \right] - a_3 \Delta t + \frac{a_2 \Delta t}{c_s} \frac{\partial V}{\partial t} \ . \qquad \text{(II. E-122.2)}$$

The implicit form is

$$\left(1 + \frac{a_2 b_2 \Delta t}{\Delta \eta c_s} \right) \rho_o^{n+1} - \frac{a_2 b_2 \Delta t}{\Delta \eta c_s} \rho_1^{n+1} + \frac{a_2 \Delta t}{\Delta \eta} V_1^{n+1}$$

$$+ \frac{a_2 b_3 \Delta t}{\Delta \eta c_s} T_o^{n+1} - \frac{a_2 b_3 \Delta t}{\Delta \eta c_s} T_1^{n+1} =$$

$$\frac{\Delta t a_2}{c_s} \frac{\partial V}{\partial t} + \frac{a_2 \Delta t}{\Delta \eta} V_o^{n+1} - a_3 \Delta t \ . \qquad \text{(II. E-122.3)}$$

Thus, if the explicit equation is needed, Eq. (II. E-122.3) and (II. E-122.2) are used, while in the implicit scheme Eq. (II. E-122.1) and (II. E-122.3) are used. Note that in the implicit scheme, these equations must be solved simultaneously with the interior point (if it is implicit). Also, in the implicit scheme the coefficients must be evaluated with the unknown values at time t_{n+1}.

b) $\eta = 1$: There are two cases here. The first is $a_1 = 0$. In this case the first and third components of Eq. (II. E-98) are used:

$$\frac{\partial y_1}{\partial t} = 0, \text{ or } \left(\frac{\partial \rho}{\partial t}\right)_{\eta = 1} = \left(\frac{a_2}{c_2}\right)\left(\frac{\partial T}{\partial t}\right)_{\eta = 1},$$

$$\frac{\partial y_3}{\partial t} = - c_s \frac{\partial y_3}{\partial \eta} - \frac{a_3}{a_2} c_s^2 .$$

Proceeding as before,

$$\frac{\partial \rho}{\partial t}\left(\frac{c_s^2}{a_2}\right) + c_s \frac{\partial V}{\partial t} = - c_s \left[b_2 \frac{\partial \rho}{\partial \eta} + c_s \frac{\partial V}{\partial \eta} + b_3 \frac{\partial T}{\partial \eta}\right] - \frac{a_3 c_s^2}{a_2},$$

or

$$\frac{\partial \rho}{\partial t} = - \frac{a_2}{c_s}\left[\frac{\partial V}{\partial t} + b_2 \frac{\partial \rho}{\partial \eta} + c_s \frac{\partial V}{\partial \eta} + b_3 \frac{\partial T}{\partial \eta}\right] - a_3 .$$

Substituting differences,

$$\left(\rho_N^{n+1} - \rho_N^n\right) = \frac{a_2}{c_2}\left(T_N^{n+1} - T_N^n\right), \qquad \text{(II. E-123. 1)}$$

and the second equation becomes

$$\rho_N^{n+1} - \rho_N^n = - \frac{a_2}{c_s}\frac{\partial V}{\partial t} - \frac{a_2 \Delta t}{c_s \Delta \eta}\left[b_2 (\rho_N - \rho_{N-1}) + c_s (V_N - V_{N-1}) + b_3 (T_N - T_{N-1})\right] - a_3 \Delta t .$$

The explicit scheme produces

$$\rho_N^{n+1} = \rho_N^n \frac{-\Delta t a_2}{c_s} \frac{\partial V}{\partial t} - \frac{a_2 \Delta t}{c_s \Delta \eta} \left[b_2 \left(\rho_N^n - \rho_{N-1}^n \right) + c_s \left(V_N^n - V_{N-1}^n \right) + b_3 \left(T_N^n - T_{N-1}^n \right) \right] - a_3 \Delta t. \quad \text{(II. E-123. 2)}$$

The implicit scheme produces

$$\rho_N^{n+1} \left(1 + \frac{a_2 b_2 \Delta t}{c_s \Delta \eta} \right) - \frac{a_2 b_2 \Delta t}{c_s \Delta \eta} \rho_{N-1}^{n+1} - \frac{a_2 \Delta t}{\Delta \eta} V_{N-1}^{n+1} + \frac{a_2 b_3 \Delta t}{c_s \Delta \eta} \left(T_N^{n+1} - T_{N-1}^{n+1} \right) = - \frac{a_2 \Delta t}{c_s} \frac{\partial V}{\partial t} - a_3 \Delta t . \quad \text{(II. E-123. 3)}$$

The second case at $\eta = 1$ is $a_1 < 0$. If $\lambda_3 > 0$, then all variables are specified with boundary conditions (and none of the equations in (II. E-98) are used). If $\lambda_3 > 0$, two boundary conditions are specified and the third Equation of (II. E-98) is used. This is differenced as before, producing

$$b_2 \frac{\partial \rho}{\partial t} + c_s \frac{\partial V}{\partial t} + b_3 \frac{\partial T}{\partial t} = (-a_1 - c_s) \left(b_2 \frac{\partial \rho}{\partial \eta} + c_s \frac{\partial V}{\partial t} + b_3 \frac{\partial T}{\partial t} \right) - \frac{a_3}{a_2} c_s^2$$

$$b_2 \left(\rho_N^{n+1} - \rho_N^n \right) + c_s \left(V_N^{n+1} - V_N^n \right) + b_3 \left(T_N^{n+1} - T_N^n \right) =$$

$$- (a_1 + c_s) \left(\frac{\Delta t}{\Delta \eta} \right) \left[b_2 (\rho_N - \rho_{N-1}) + c_s (V_N - V_{N-1}) + b_3 (T_N - T_{N-1}) \right] - \frac{a_3}{a_2} c_s^2 \Delta t .$$

Explicit:

$$b_2 \rho_N^{n+1} + c_s V_N^{n+1} + b_3 T_N^{n+1} = b_2 \rho_N^n + c_s V_N^n + b_3 T_N^n$$

$$-(a_1 + c_s)\left(\frac{\Delta t}{\Delta \eta}\right)\left[b_2\left(\rho_N^n - \rho_{N-1}^n\right) + c_s\left(V_N^n - V_{N-1}^n\right)\right.$$

$$\left. + b_3 \left(T_N^n - T_{N-1}^n\right)\right] - \frac{a_3 c_s^2 \Delta t}{a_2} \quad . \qquad \text{(II. E-124. 1)}$$

Implicit:

$$\left[1 + \frac{\Delta t}{\Delta \eta}(a_1 + c_s)\right]\left[b_2 \rho_N^{n+1} + c_s V_N^{n+1} + b_3 T_N^{n+1}\right]$$

$$- \frac{\Delta t}{\Delta \eta}(a_1 + c_s)\left[b_2 \rho_{N-1}^{n+1} + c_s V_{N-1}^{n+1} + b_3 T_{N-1}^{n+1}\right]$$

$$= b_2 \rho_N^n + c_s V_N^n + b_3 T_N^n - \frac{a_3}{a_2} c_s^2 \Delta t \, . \qquad \text{(II. E-124. 2)}$$

2) Reflection from a Solid Surface:

The situation here is identical to that already treated in the piston problem.

3) The Burst Problem:

This again is almost identical to the previous cases, and so no further discussion is given here.

4) Mass Injection

For the full viscous case, the necessary equations have been developed in the earlier discussion of the piston problem, except for the new equation for C. This equation is set up as

$$\left(1 - C_o^{n+1}\right)\dot{m}_w = - \frac{\rho \Delta \eta_r}{2\Delta \eta}\left(-3 C_o^{n+1} + 4 C_1^{n+1} - C_2^{n+1}\right) ,$$

$$\left(\dot{m}_w + \frac{3\rho \Delta \eta_r}{2\Delta \eta}\right) C_o^{n+1} - \frac{4\rho \Delta \eta_r}{2\Delta \eta} C_1^{n+1} + \frac{\rho \Delta \eta_r}{2\Delta \eta} C_2^{n+1} = \dot{m}_w \, .$$

(II. E-125)

The inviscid system is again the same, where obvious modifications for the C equation are made wherever necessary.

PART E: Stability Conditions

The difference equation for the nonviscous hyperbolic subsystem has the following stability condition:(II. E-10)

$$\Delta t = \frac{\Delta \eta}{|a_1| + c_s} = M_1 . \qquad \text{(II. E-126)}$$

The explicit-implicit scheme has no stability criterion (II.E-9), and so when the explicit-implicit scheme is used for the viscous terms Eq. (II.E-126) is the only stability criterion.

The program has the option of using the purely explicit scheme, rather than the combination. In this case, the parabolic terms in the viscous portion of the equations produces this condition.

$$\Delta t \leq \min \left[\frac{(\Delta \eta)^2}{2\bar{b}_1} , \frac{(\Delta \eta)^2}{2\bar{c}_1} , \frac{\Delta \eta^2}{2\bar{d}_1} \right] = M_2 . \qquad \text{(II.E-27)}$$

The two previous conditions are then "added" so as to produce the following condition for the explicit scheme:

$$\Delta t \leq \frac{1}{\frac{1}{M_1} + \frac{1}{M_2}} . \qquad \text{(II.E-28)}$$

Remark: The low-order viscous terms were differenced as though they formed a separate hyperbolic subsystem. However, the corresponding stability conditions have not been included in the program. This may be necessary for a new case. Also, as noted in the discussion of the difference equations, certain mixed derivative quantities were handled without any real theoretical basis. These may cause some problems at some time.

II.E.5 SPHERICALLY SYMMETRIC RADIATION

It is desired now to add radiation effects to the equations. The basic equations (II. E-37) remain the same except that a term is added to the energy equation. That is, the following term is added to $\bar{c}_4$:

$$-\frac{1}{\rho \bar{C}_v}\left\{\frac{1}{c}\frac{\partial}{\partial t}\left[\int_{-1}^{+1} I\, d\mu\right] + \nabla \cdot F\right\}, \qquad \text{(II. E-129)}$$

where F is the radiative flux vector.

The basic equation is as follows (see Sections IV. C and IV. D for a discussion of the assumptions and derivation related to this equation):

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial r} + \left(\frac{1-\mu^2}{r}\right)\frac{\partial I}{\partial \mu} = K\,(B-I), \qquad \text{(II. E-130)}$$

where

$$F = \int_{-1}^{+1} I\mu\, d\mu$$

I = Intensity

K = Absorption coefficient

B = Planck function

c = Speed of light

$\mu = \cos\theta$, where θ is the polar angle from the radius vector.

Note first that Eq. (II. E-130) applies only to spherically symmetric problems.

Also, note that Eq. (II. E-130) has three independent variables. In principle, Eq. (II. E-37) are also a function of μ, but by assumption the flow variables are constant for fixed r.

Next, note that Eq. (II. E-130) contains the $\frac{\partial}{\partial t}$ term. This has been the source of quite a bit of discussion. As will be noted later, the solution of this equation by difference equations will require a very small time step (on the order of $\frac{1}{c}$). Generally, in this short time period the hydrodynamic equations exhibit no appreciable change in the flow variables. Our point of view here is as follows:

1) If the $\nabla \cdot F$ term is large, so that changes in T occur in time scales comparable to $\frac{1}{c}$, then nothing is lost by retaining the time term. In fact, it should be retained in this case.

2) If $\nabla \cdot F$ is comparable to the other hydrodynamic terms, so that significant changes in the flow variables occur in a time scale comparable to $\frac{1}{c_s}$ (where c_s is the speed of sound), then we look for a quasi-steady state solution of Eq. (II.E-130). That is, for a fixed time we look for a solution of Eq. (II.E-130) for which $\frac{\partial I}{\partial t} \equiv 0$. In this case, one interprets the time scale in Eq. (II.E-130) as meaningless. Successive time steps are simply successive iterations as a means toward solving the steady-state version of Eq. (II.E-130). This will be discussed further after we define the difference equation.

We first transform the equation to the η-system (see Eq. (II.E-32). We obtain

$$\begin{aligned} \frac{\partial I}{\partial t} &= e_1 \frac{\partial I}{\partial \eta} + e_2 \frac{\partial I}{\partial \mu} + e_3, \\ e_1 &= -(\eta_t + c_\mu \eta_r), \\ e_2 &= -\frac{c}{r}(1-\mu^2), \\ e_3 &= cK(B-I). \end{aligned} \qquad \text{(II.E-131)}$$

We now use the same difference equation as discussed in Section II.E.4 for first order hyperbolic systems (see also Ref. II.E-10). This takes the following form:

$$e_1 \frac{\partial I}{\partial \eta} = e_1 I_\eta + |e_1| \frac{\Delta \eta}{2} I_{\eta\eta}, \qquad \text{see Eq. (II.E-107)}$$

$$\begin{aligned} e_2 \frac{\partial I}{\partial \mu} &= e_2 I_\mu + |e_2| \frac{\Delta \mu}{2} I_{\mu\mu} \\ &= e_2 I_\mu - e_2 \frac{\Delta \mu}{2} I_{\mu\mu}, \qquad \text{since } e_2 \le 0. \end{aligned}$$

Substituting into Eq. (II.E-131),

$$\frac{\partial I}{\partial t} = e_1 I_\eta + \frac{|e_1|}{2\Delta\eta}\left(I_{i+1,j} + I_{i-1,j}\right)$$

$$+ e_2 I_\mu - \frac{e_2}{2\Delta\mu}\left(I_{i,j+1} + I_{i,j-1}\right)$$

$$- \frac{|e_1|}{\Delta\eta} I_{i,j} + \frac{e_2}{\Delta\mu} I_{i,j} + e_3 ,$$

where

$$I^n_{i,j} = I\left(t_n, i\Delta\eta, j\Delta\mu\right)$$

$$\frac{\partial I}{\partial t} = \left(\frac{e_1 + |e_1|}{2\Delta\eta}\right) I_{i+1,j} + \left(\frac{|e_1| - e_1}{2\Delta\eta}\right) I_{i-1,j} - \frac{e_2}{\Delta\mu} I_{i,j-1}$$

$$- \left(\frac{|e_1|}{\Delta\eta} + \frac{|e_2|}{\Delta\mu}\right) I_{i,j} + cK\,(B-I).$$

Let

$$e_4 = \left(\frac{e_1 + |e_1|}{2\Delta\eta}\right) I_{i+1,j} + \left(\frac{|e_1| - e_1}{2\Delta\eta}\right) I_{i-1,j} - \frac{e_2}{\Delta\mu} I_{i,j-1} + cKB$$

$$e_5 = \frac{|e_1|}{\Delta\eta} + \frac{|e_2|}{\Delta\mu} + cK ,$$

then,

$$I^{n+1}_{i,j} - I^n_{i,j} = \Delta t\, e_4 - \Delta t\, e_5 I_{i,j} .$$

For the explicit scheme we have

$$I^{n+1}_{i,j} = \Delta t\, e_4 + (1 - \Delta t\, e_5) I^n_{i,j} . \qquad \text{(II.E-132.1)}$$

For the implicit scheme we have

$$I^{n+1}_{i,j} = (I^n_{i,j} + \Delta t\, e_4)/(1 + \Delta t\, e_5). \qquad \text{(II.E-132.2)}$$

The stability criterion for the difference equation is

$$\Delta t \leq \frac{1}{\frac{|e_1|}{\Delta \eta} + \frac{|e_2|}{\Delta \mu}} \qquad \text{(II. E-133. 1)}$$

Also, a complication arises from the cK term. Suppose e_1, e_2, and B = 0. Then, from Eq. (II. E-132. 1)

$$I^{n+1} = I^n (1 - \Delta t\, cK) ,$$

and from Eq. (II. E-132.2)

$$I^{n+2} = I^{n+1}/(1+\Delta t\, ck).$$

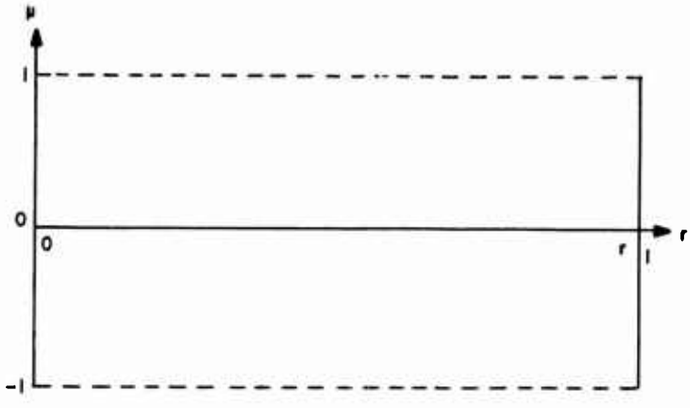
Combining the two equations,

$$I^{n+2} \; I^n \left(\frac{1-\Delta t\, cK}{1+\Delta t\, cK}\right) .$$

This makes sense only if we impose the following condition:

$$\Delta \leq \frac{1}{cK} \qquad \text{(II. E-133.2)}$$

We consider now the question of boundary conditions.



a) $\eta = 1$, or $r = r_1$.

If $e_1 \leq 0$, we do not need a boundary condition. From Eq. (II. E-103.2), $\eta_t \leq 0$ at $\eta = 1$; this assumes the forward point is not moving in. $e_1 = 0 \rightarrow \mu = -\eta_t / r\eta_r = \mu^*$. Thus, we do not need a boundary condition for $\mu < \mu^*$.

The boundary condition we use is

$$I(\eta, \mu) = 0 \text{ for } \mu < \mu^* \text{ and } \eta = 1 \qquad \text{(II. E-134)}$$

(This says there is no incident radiation from outside the sphere).

b. $\mu = -1$.

$e_2 = 0$, therefore no boundary condition is needed. However, note that $I(\eta = 1, \mu = -1) \equiv 0$ (see Eq. (II. E-134). Since $e_1 > 0$ at $\mu = -1$ (actually this could be violated at some interior values of η), a forward difference is used for $\frac{\partial I}{\partial \eta}$. Thus, I at $\mu = -1$ can be obtained by starting at $\eta = 1$. When using the explicit-implicit scheme, there is no problem, since the alternating procedure takes place at the boundary also.

c. $\eta = 0$, or $r = r_o = 0$.

The assumption at $\eta = 0$ is that $\frac{1}{r}\frac{\partial I}{\partial \mu}$ is finite, or that $\frac{\partial I}{\partial \mu} \equiv 0$. Thus, if we know I at some value of μ, we know it everywhere. Consequently, we set $\mu = -1$ and use the normal difference equation.

d. $\mu = +1$.

$e_2 = 0$, therefore no boundary condition is needed. However, we now expect that $e_1 < 0$, or that a backward difference is used for $\frac{\partial I}{\partial \eta}$. Thus I at $\mu = +1$ can be obtained by starting at $\eta = \Delta\eta$ ($\eta = 0$ was obtained from part c above).

It remains now to specify the quantity given by Eq. (II. E-129) to be added to the energy equation. From Eq. (II. E-130),

$$\int_{-1}^{+1} K(B-I)d\mu = \int_{-1}^{+1} \left[\frac{1}{c}\frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial r} + \left(\frac{1-\mu^2}{r}\right)\frac{\partial I}{\partial \mu} \right] d\mu$$

$$= \frac{1}{c}\frac{\partial}{\partial t}\int_{-1}^{+1} I d\mu + \frac{\partial F}{\partial r} + \left(\frac{1-\mu^2}{r}\right) I \Big|_{-1}^{+1} + \frac{1}{r}\int_{-1}^{+1} 2\mu I d\mu$$

$$= \frac{1}{c}\frac{\partial}{\partial t}\int_{-1}^{+1} I d\mu + \frac{\partial F}{\partial r} + \frac{2}{r}F: \text{ in spherical coordinates}$$

$$= \frac{1}{c} \frac{\partial}{\partial t} \int_{-1}^{+1} I d\mu + \nabla \cdot F .$$

Thus, the following quantity is added to the energy equation.

$$- \frac{1}{\rho \overline{C}_v} K \int_{-1}^{+1} I d\mu \quad -2BK . \qquad \text{(II. E-135)}$$

II.F CONSIDERATIONS ON THE EXPANSION OF A HIGH TEMPERATURE GAS INTO A VACUUM

by

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II.F CONSIDERATIONS ON THE EXPANSION OF A HIGH TEMPERATURE GAS INTO A VACUUM

In order to predict the dynamics of a nuclear burst at high altitudes, it is necessary to utilize the Maxwell-Boltzmann transport equation. The hydrodynamic theory, which is appropriate for lower altitude bursts is inappropriate at high altitude because the collisional mean free path between particles becomes large compared to the distance over which the fluid variables experience significant changes. To analyze this problem, a dual point of view has been adopted. We first are interested in constructing progressively more complete models of the plasma expansion into vacuum which results from a nuclear burst at high altitude, and secondly, we are concerned with developing a large scale numerical capability for calculating the expansion directly from the Boltzmann equation. The models for expansion into vacuum will first be discussed.

The point of view we adopt in constructing models for the expansion into a vacuum of a high temperature plasma is that we should first isolate those physical phenomena which describe the expansion and then include them selectively in progressively more complete models of the physical processes. In discussing the time-dependent expansion of a plasma into vacuum, the key features that must be considered are the transition from collision-dominated flow in the core of the burst sphere to collision-free flow at the edge of the expansion, and in addition, the consideration of electrostatic charge separation effects due to the difference in thermal velocity between electrons and ions. To consider these effects in a systematic way we chose to first illuminate the transition from collision-dominated to collision-free flow in a steady state source flow model. That is to say, we consider the steady-state expansion of a charge-free plasma from a high-temperature source. The problem of the source flow of a neutral, monatomic gas has been considered by Hamel and Willis (II.F-1). In their work, a systematic approximation was constructed for the moment equations of kinetic theory which describe source flow expansion. For small source Knudsen number, the moments were expanded and solutions obtained near the source. These solutions are non-uniformly valid far from the source, breaking down when transition flow is encountered. To analyze the rarefied regime, the equations are rescaled taking account that the flow is hypersonic in the transition regime. This allowed them to apply a hypersonic approximation to the moment equations in the rarefied regime and subsequently match this to the inviscid solution. For spherical expansions, the problem was resolved to a relaxation process with two translational temperatures, one along streamlines, $T_{||}$, and the other transverse to streamlines, $T_{\perp}$. An expression for the terminal Mach number in terms of source Knudsen number and intermolecular force law was found, and a simple rarefaction criteria proposed

which states that transition flow is encountered with $T_{||} - T_{\perp} \cong T_{isentropic}$.

To extend this work to the case of a charge-free plasma is difficult because for the neutral gas the implicit assumption was that the $[\text{Prandtl No. x (Mach No.)}^2]^{-1}$ is small compared to one. For a neutral expansion this is realized; however, in a plasma, thermal conduction is quite important and rather small Prandtl numbers are obtained. We must therefore modify the Hamel and Willis theory to account for thermal conduction. We have been able to do this, although in an ad-hoc manner. The approach has been to include a Fourier heat conduction term in the moment equations both in the collision-dominated and collision free regime. The rationale for this procedure is that close to the source, thermal conduction effects dominate over viscous effects and one must consider a set of inviscid, thermal conduction moment equations. Far from the source, the flow is hypersonic and thermal conduction becomes less important. We therefore need not be concerned with the presence of the thermal conduction in the transition regime since it will be small; it will, however, permit the smooth matching of the inner, inviscid region with the outer transition flow. The results obtained from this theory are a transition to rarefied flow at some distance from the source, with the attendant interplay between a temperature parallel to streamlines, $T_{||}$, which becomes a constant and a temperature transverse to streamlines, $T_{\perp}$, which continues to decrease to zero.

Having successfully considered the transition from collision dominated to collision free flow for a steady plasma expansion, the direction of future research should be to consider the above problem in the framework of an unsteady source flow. In this way one can begin to consider problems that have progressively more of the burst physics in them.

The second line of endeavor has been to perform large scale numerical computations with the complete Maxwell-Boltzmann equation. The guiding principle here is to make approximations only in the sense of numerical truncation rather than attempt ad-hoc physical assumptions.

At the Fourth International Rarefied Gas Dynamics Symposium in 1964, Hamel and Wachman (II.F-2) presented a paper which discussed in detail a method for obtaining numerical solutions to the linearized Boltzmann equation. The point of view adopted was that approximations to the Boltzmann equation be made only in the sense of numerical truncation. The numerical method developed was one of discrete ordinates and involved analyzing the linearized Boltzmann equation for hard-sphere molecules at discrete points in velocity space, with the collision integral considered as a finite sum through the use of Gauss quadrature formulas. With this method, the problem of linearized Couette flow was satisfactorily handled. In the intervening two years, this numerical method has been extended to treat the nonlinear Boltzmann equation.

In scope, the numerical computation of the nonlinear Boltzmann equation is significantly more difficult than for a comparable linearized problem. These complications stem from the fact that linearization of the collision integral reduces the order of integration

from five to three. In the linear case, it is possible to explicitly perform the angular integrations since a particle will scatter from a known Maxwellian background. This decrease in the order of the integrations allows one to set up a discrete ordinate grid in velocity space for which the number of differential equations is equal to the number of dependent variables, $f(v_i, x, t)$, and no interpolation is necessary. For the non-linear Boltzmann equation, there can be no reduction in the order of integration and a straight forward discrete ordinate grid in velocity space is no longer possible. This is because a particle which may have a velocity v_i (on the grid) before collision will after collision be scattered onto v_k, which may not necessarily be on the grid. To circumvent this, an elaborate method of interpolation in velocity space is necessary. Therefore, for the nonlinear Boltzmann equation we must, in addition to utilizing Gauss quadrature formulas, utilize an interpolation scheme, and must choose a grid with this in mind.

An outline of our numerical method follows:

If we define the function $\psi(\underline{v})$ through the relation $e^{-v^2}\psi(\underline{v}) = f(\underline{v})$ where $f(\underline{v})$ is the molecular distribution, we can then write the Boltzmann Equation in the form:

$$\frac{d\psi(\underline{v})}{dt} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\pi/2}\int_{0}^{2\pi} e^{-\xi^2}\left[\psi(\underline{v})\psi(\underline{\xi}) - \psi(\underline{v}+\underline{\chi})\psi(\underline{\xi}-\underline{\chi})\right]|\underline{\xi}-\underline{v}|$$

$$\sin\theta\cos\theta\, d\theta d\epsilon d\xi$$

where the components of $\underline{\chi}$ are defined as:

$$\chi_i = 1/2\left\{2(\xi_i - v_i)\cos^2\theta + \left[|\underline{\xi}-\underline{v}| - (\xi_i - v_i)^2\right]^{1/2}\sin(2\theta)\cos(\epsilon-\omega_i)\right\}$$

$(i = x, y, z)$ and where:

$$\omega_x = 0,\quad \cos\omega_y = \frac{-(\xi_x - v_x)(\xi_y - v_y)}{\left[|\underline{\xi}-\underline{v}|^2 - (\xi_x - v_x)^2\right]^{1/2}\left[|\underline{\xi}-\underline{v}|^2 - (\xi_y - v_y)^2\right]^{1/2}}$$

$$\cos\omega_z = \frac{-(\xi_x - v_x)(\xi_z - v_z)}{\left[|\underline{\xi}-\underline{v}|^2 - (\xi_x - v_x)^2\right]^{1/2}\left[|\underline{\xi}-\underline{v}|^2 - (\xi_z - v_z)^2\right]^{1/2}}$$

In the first step of our numerical scheme, we evaluate $\frac{d\psi(\underline{v})}{dt}$. To this end we use a Gauss quadrature formula on the fifth fold integral in Eq. (II.F-1). We perform a Gauss-Legendre quadrature (after an appropriate coordinate transformation) on the angular integrations and a Gauss-Hermite quadrature on the three-dimensional velocity integrations. In this manner, we evaluate $\frac{d\psi(\underline{v})}{dt}$, provided that we know the values of ψ at $\underline{v}$, and at the various points $\underline{\xi}$, $\underline{v} + \underline{\chi}$, $\underline{\xi} - \underline{\chi}$, which will result from the substitution of the quadrature roots. Initially we encounter no problems at these points because we start with a known function ψ. At the time $t_0 + \Delta t$, however, all we get are the values of ψ at the points $\underline{v}$ because we solve the differential equation $\frac{d\psi(\underline{v})}{dt}$ with the initial conditions of the known function $\psi(\underline{v})$. In order to be able to perpetuate the procedure, we will have to evaluate equation (2.1) at $t_0 + \Delta t$ and therefore need to again know ψ on the same grid points $\underline{\xi}$, $\underline{v} + \underline{\chi}$, $\underline{\xi} - \underline{\chi}$. To solve this dilemma, we choose the $\underline{v}$ in such a manner that it will provide an adequate interpolation grid for the region of greatest importance in velocity space.

Each particular case (defined by given initial conditions) will require a different grid of $\underline{v}$. Since we have a relaxation problem, and $f(\underline{v}) = e^{-v^2}\psi(\underline{v})$ eventually becomes Maxwellian, if a proper coordinate axis is chosen, we assume that $\psi(\underline{v})$ will be most difficult to interpolate initially. Therefore, if we choose a well placed and large enough grid initially, it should suffice as we increase t. Thus far Wachman and Hamel (II.F-3) have considered the problem of nonlinear, homogenous, pseudo-shock relaxation. That is to say, we consider a gas of hard-sphere molecules at $t = 0$ with $f_0(\underline{v})$ for all $\underline{r}$ and then solve for the subsequent $f(\underline{v}, t)$ as it relaxes to a Maxwellian. The adjective, pseudo-shock is injected above to indicate the class of $f_0(\underline{v})$ that we consider - that is to say, $f_0(\underline{v})$ will consist of two Maxwellian distributions centered about ordered velocities in the x direction of $-\underline{\xi}$ and $+\underline{\xi}$ respectively. In velocity space, as these distributions interact through collisions, their ordered velocities will be thermalized, and as $t \to \infty$, we will have a single Maxwellian distribution centered about $v_x = 0$. We can therefore think of this as a shock in velocity space and so we use the adjective pseudo-shock. In the future we plan to utilize these techniques for the solution of a gas dynamic problem in which a shock wave occurs. The ability to perform large scale computations with the Maxwell-Boltzmann equation for flows with shock waves should enable us to study numerically the nuclear burst shock wave formation and expansion in the higher altitude regime without restrictive ad-hoc assumptions.

II.G SPHERICALLY-SYMMETRIC SHOCK FORMATION ACCORDING TO THE NAVIER-STOKES EQUATIONS

by

S. M. Scala and P. Gordon

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II.G SPHERICALLY-SYMMETRIC SHOCK FORMATION ACCORDING TO THE NAVIER-STOKES EQUATIONS

II.G.1 INTRODUCTION

This section consists of two parts. The first describes the results of the numerical solutions to the Navier-Stokes equations for the burst problem, while the second describes the radiation program.

II.G.2 NUMERICAL SOLUTIONS

The physical problem considered in this investigation was defined as follows:

a. The flow was spherically-symmetric so that the one-dimensional form of the Navier-Stokes equations in spherical coordinates governed the flow. The perfect gas equation of state was employed (see Section II. E).

b. The precise values of the various coefficients are as follows:

$$R = 55.2 \text{ ft-lb/lb°R}$$

$$C_V = 138 \text{ ft-lb/lb°R}$$

$$\mu = 1.28 \times 10^{-6} \sqrt{T(°R)} \text{ lb/ft}^2\text{sec}$$

$$K = 3.49 \times 10^{-4} \sqrt{T(°R)} \text{ Btu-ft/ft}^2\text{sec}$$

$$\lambda = -\frac{2}{3}\mu$$

c. The physical problem studied was that of a sphere of high pressure gas. At time zero, the "envelope" containing the high pressure gas ruptures. Since the density is assumed constant at time zero throughout the region, this instantaneous rupture would provide a discontinuity in temperature. In order to have a continuous initial-value problem, the temperature was chosen to vary linearly between the high and low values over some small, but arbitrary, distance.

Precisely, the initial conditions at time zero were chosen to model the conditions shown in Figure II. G-1:

1. $V \equiv 0$

2. $\rho \equiv \rho_o = \text{constant}$

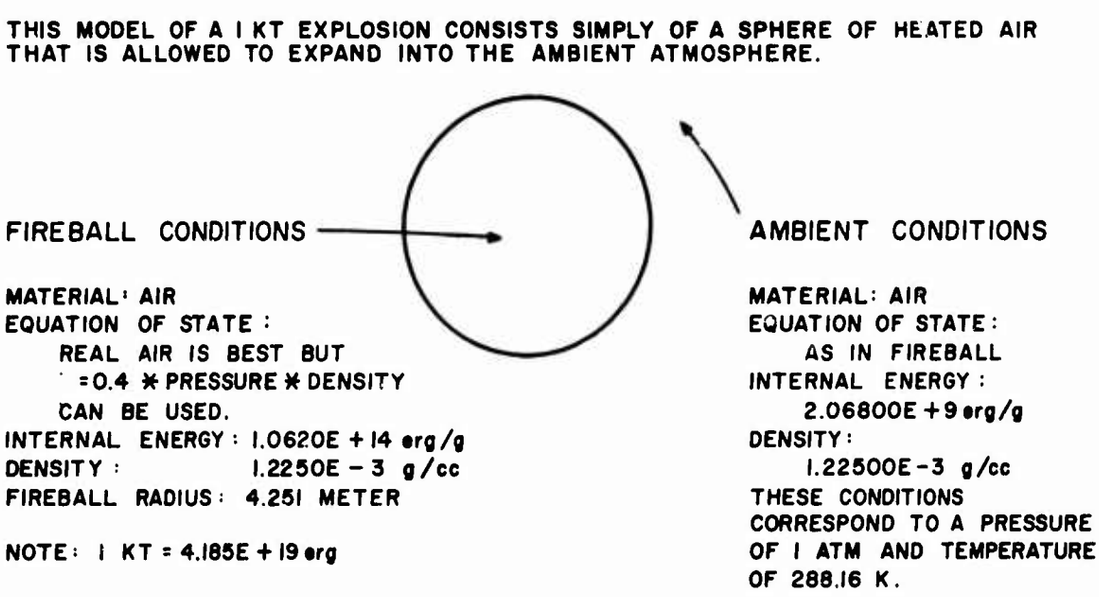


Figure II.G-1. "Standard" 1 KT at Sea Level Problem as Used at NOL

This model of a 1 KT explosion consists simply of a sphere of heated air that is allowed to expand into the ambient atmosphere.

3. $T_1: 0 \leq r \leq r^*$

$$T = T_o + \left(\frac{T_1 - T_o}{r^* - r^{**}}\right) (r - r^{**}): r^* \leq r \leq **$$

$$T_o: r^{**} \leq r \leq r_1$$

d. The boundary conditions are as follows:

1. at $r = 0$, $V \equiv 0$ and $\frac{\partial T}{\partial r} = 0$. Note that the density at the center is calculated and no further boundary condition is imposed.

2. at $r = r_1(t)$, $V \equiv 0$, $\rho = \rho_o$, $T \equiv T_o$ (i.e., it is assumed that r_1 varies with time so as to stay ahead of the propagating shock.)

The major numerical difficulty as one might suspect, revolved around the mesh size. Since this was to be a viscous solution, it was clear that in the neighborhood of the shock (whose thickness is usually of the order of several mean-free paths) the mesh size had to be on the order of the mean-free path. However, in other regions it was expected that a mesh size mush larger than the mean-free path could be employed. Thus, one is led to the concept of a moving coordinate system with variable spacing, whose motion and spacing is related to the position of the shock. In a problem with one stationary shock, given the position of the shock, one can devise a spacing which behaves as desired (maximum spacing about the shock). Further, if the shock is moving and the motion of the shock were known "a priori," the problem is still relatively simple. However, when the motion of the shock is to be calculated indirectly, by watching the flow profiles vary with time, and when this information is to be coupled with the spacing, and when one has as a goal the calculation of accurate and reproducible results, then the specification of an appropriate coordinate system becomes very difficult. We experimented with a variety of ideas. The coordinate system that was most successful is described in Section II.E and has the following form.

$$\eta = \left(\frac{e^{-s\zeta_o} + e^{-s}}{1-e^{-s}}\right)\left(\frac{1-e^{-s\zeta}}{e^{-s\zeta_o} + e^{-s\zeta}}\right)$$

$$\zeta = \frac{r}{r_1}$$

$$r_1 = r_1(t),\ \zeta_o = \zeta_o(t),\ s = s(t)$$

ζ normalizes the radial component of the spherical coordinate system between 0 and 1. The intent is to have a fixed number of equally spaced points in the η coordinate. r_1 defines the length of the computational region, and is allowed to vary so as to accommodate the larger computational region that is required as the shock moves out. ζ_o (t) is the point of maximum squeezing (minimum Δr), and, of course, the objective is to keep ζ_o situated on or about the shock. s(t) defines the amount of squeezing at ζ_o. Full details of this transformation, including all required equations, can be found in Section II.E.

This transformation showed some promise, although it was far from a complete success. In general, we were not able to keep ζ_o to within more than a 20% deviation (where the deviation here denotes a measure of its position as related to the position of the shock). When, furthermore, it turned out that in the neighborhood of the weaker secondary shock a fine spacing was also required, it became clear that analytic transformations of this type would not be successful.

At this point in time, we think we understand the spacing problem more clearly. In Reference II.G-1, which appeared recently, the following conjecture was stated:

> It it is desirable to allow for the presence of viscous effects in the solution of the complete Navier-Stokes equations, whether or not such effects actually appear in the solution, then the spatial mesh size must be comparable to the local mean-free path.

This restriction is in no way related to the time step (and is not a stability criterion) and seems to be simply a manifestation of the existence of both first order terms (inviscid) and second order terms (viscous) in the Navier-Stokes equations. We believe this conjecture to be valid, and, if so, this accounts for the lack of success of the various spatial transformations we attempted. Although these transformations behaved essentially as required, we were in effect imposing insufficient requirements on them.

Some typical results of our calculations will now be described. In all the following results, equally spaced nodes were utilized.

The first set of calculations was for sea level conditions:

$$\rho_o = 0.0765 \text{ lb/ft}^3$$

$$T_o = 518°R$$

The outer radius was kept fixed, i.e.:

$$r_1 = 2 \text{ ft.}$$

Comparisons were made with the results of the WUNDY code (Ref. II.G-2). The time step utilized varied, but for the case of 50 pts,

$$\Delta t \approx 5 \times 10^{-8} \text{ sec}$$

For the case of 100 points, Δt was decreased by a factor of 3 (see Section II.E):

$$\Delta t \approx 1.6 \times 10^{-8} \text{ sec}$$

For 200 points, Δt was again reduced,

$$\Delta t \approx 5 \times 10^{-9} \text{ sec}$$

Figures II. G-2 to II. G-4 show a comparison at a fixed time for the three different cases and for the NOL results. We see that in the vicinity of the shock, convergence is clearly not indicated for all three calculations. In addition, it is clear that after the inward reflection, results are far different in terms of behavior of the inward shock (Figure II. G-3). However, propagation of the outward shock remains qualitatively similar to the NOL results. This was also the case for longer times.

In Figure II. G-5 we have shown all three calculations for the time at which the maximum positive velocity occurs. Again, convergence is clearly not adequate. Figures II. G-6 to II. G-9 show similar comparisons. Figure II. G-6 shows velocity profiles at a later time. Figure II. G-7 displays the pressure profiles. Note that all results do not tend in the direction of the NOL results. Figures II. G-8 and II. G-9 display density and temperature variations. It is of interest to note that none of our results contained any of the oscillatory behavior that one normally associates with the use of an artificial viscosity technique.

Note that for this problem the initial mean-free path is approximately 2×10^{-7} ft. Thus, we see that in the case of 200 points, Δr, which was 0.02, was five orders of magnitude greater than the mean-free path.

The next calculation was for a much smaller initial radius:

$$r_1 = 0.01 \text{ ft.}$$

We chose

$$\Delta r = 0.00001 \text{ ft.}$$

and

$$\Delta t \approx 2 \times 10^{-11} \text{ sec}$$

This run used over six hours of CDC 6600 computer time.

Figure II. G-10 shows the velocity profiles at two early times. Figure II. G-11 shows the pressure distribution for selected times through the entire calculation. Figure II. G-12 shows the pressure oscillations at the center due to the series of inward moving reflections. From this data one can calculate the position of the shock and the shock velocity. This is tabulated in Table II. G-1. This data agreed quite well with the NOL results. For this calculation Δr is still several orders of magnitude greater than the mean-free path, and it is clear that we had still not obtained sufficient resolution at the shock. From an earlier calculation on one-dimensional cartesian problems, we knew that with a sufficiently fine mesh resolution at the shock could be obtained. Calculations with a fine mesh verified that this was also the case in spherical coordinates. However, the number of nodes required for such a calculation, and the

corresponding small time step, make the cost of such calculations prohibitively high. It is concluded that the spacing problem must be solved efficiently in order to allow viscous calculations.

TABLE II. G-1. POSITION OF SHOCK AND SHOCK VELOCITY

t	r_s (ft)	V_s (ft/sec)
8.0×10^{-9}	2.603×10^{-3}	6.51×10^{4}
1.2×10^{-8}	2.864×10^{-3}	5.25×10^{4}
1.6×10^{-8}	3.074×10^{-3}	4.5×10^{4}
2.0×10^{-8}	3.254×10^{-3}	3.662×10^{4}
2.355×10^{-8}	3.384×10^{-3}	3.275×10^{4}
2.755×10^{-8}	3.515×10^{-3}	3.0×10^{4}
3.155×10^{-8}	3.635×10^{-3}	2.75×10^{4}
3.555×10^{-8}	3.745×10^{-3}	2.75×10^{4}
3.955×10^{-8}	3.855×10^{-3}	2.5×10^{4}
4.355×10^{-8}	3.955×10^{-3}	

r_s = position of the shock

V_s = velocity of the shock

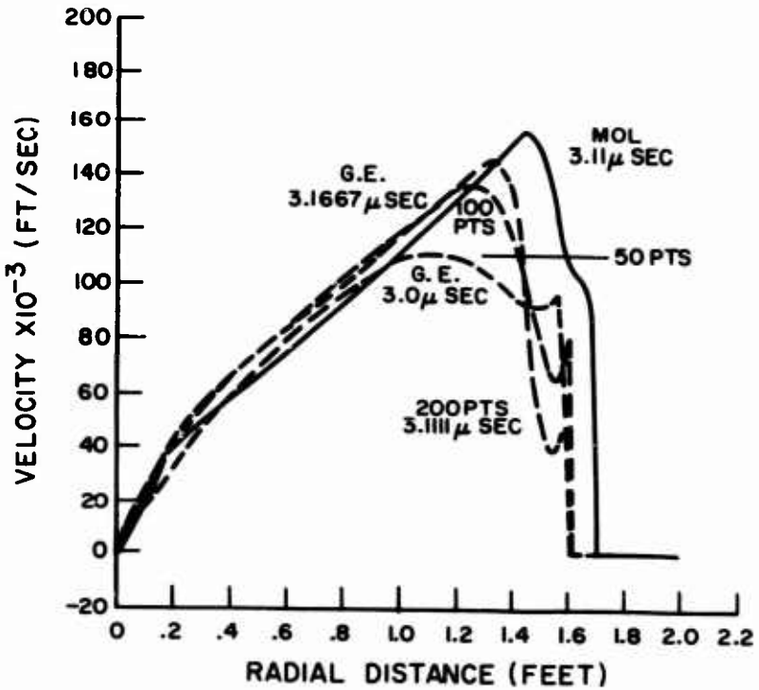


Figure II.G-2. Radial Distance vs. Velocity

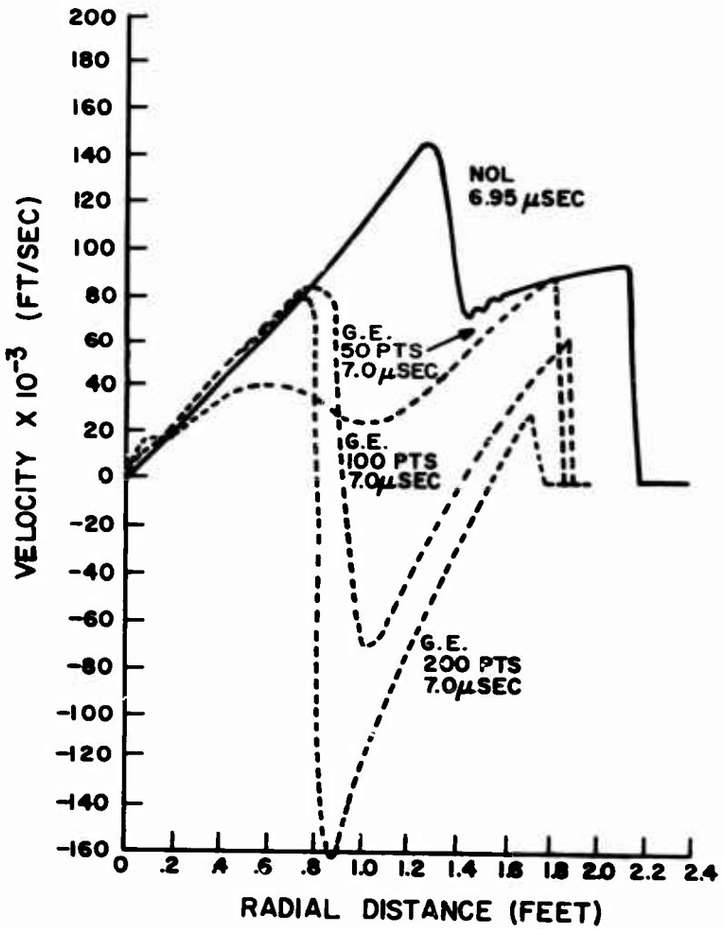


Figure II.G-3. Radial Distance vs. Velocity

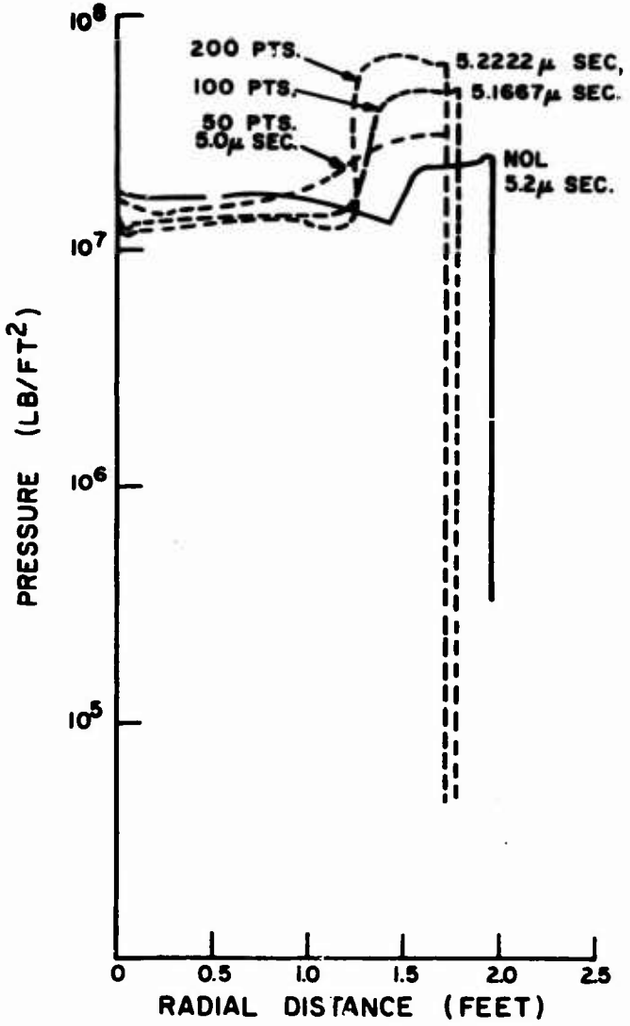


Figure II.G-4. Radial Distance Vs. Pressure

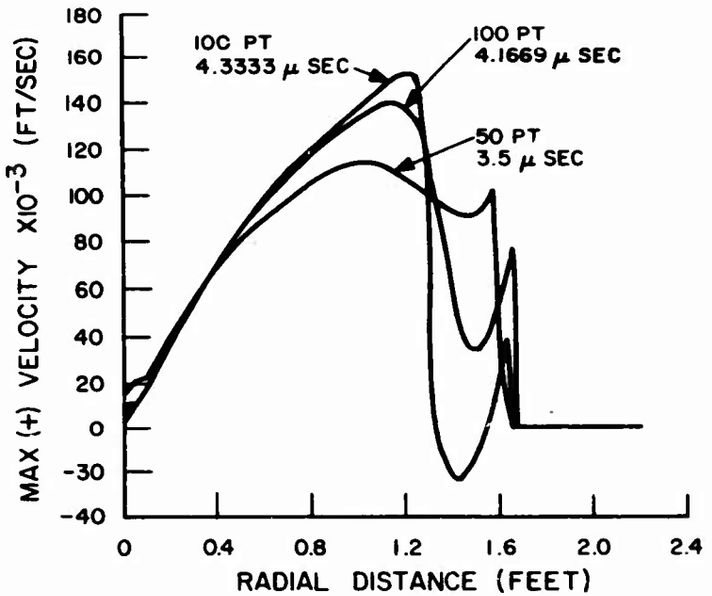


Figure II.G-5. Radial Distance vs. Maximum Positive Velocity

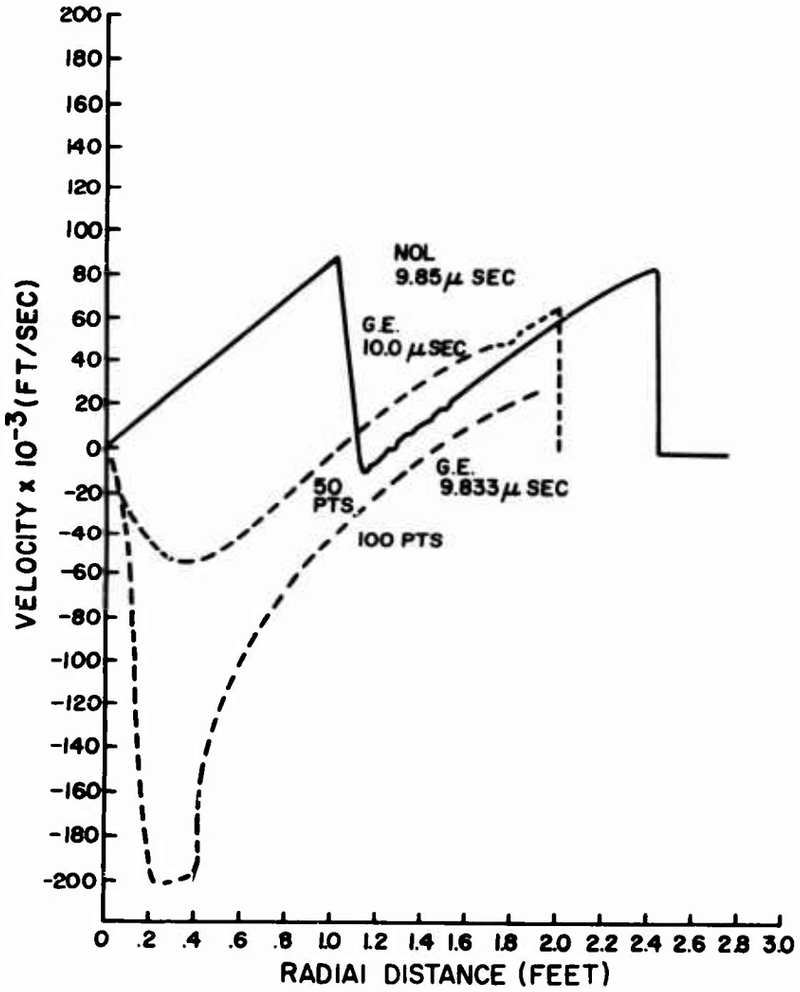


Figure II.G-6. Velocity Profiles

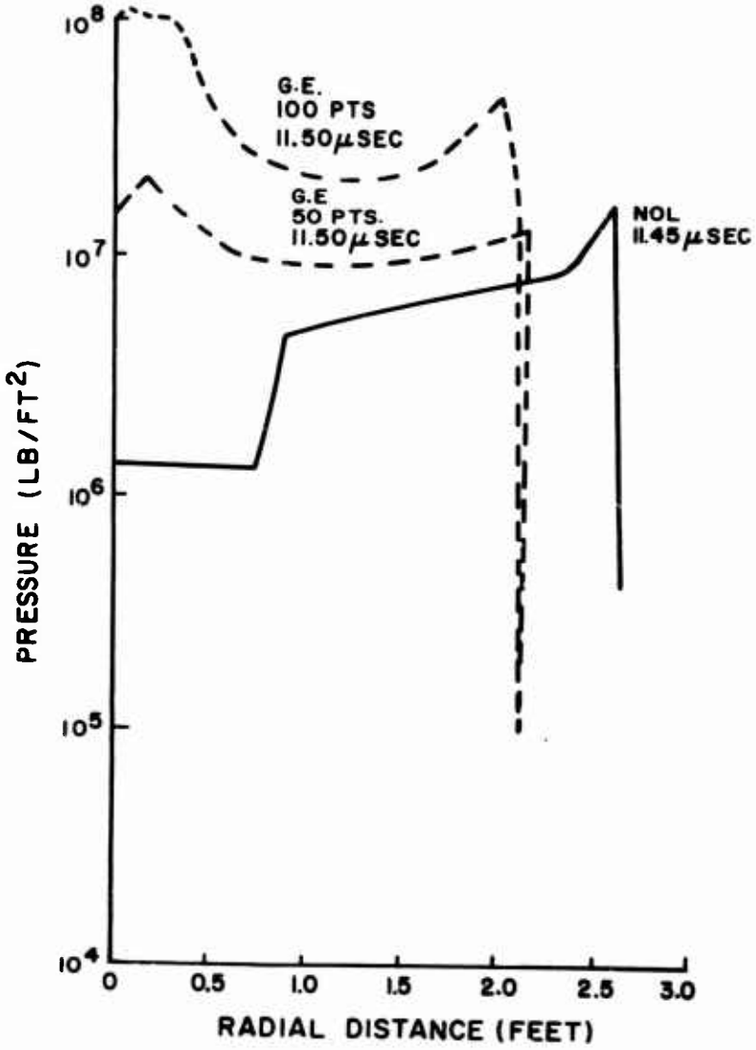


Figure II.G-7. Pressure Profiles

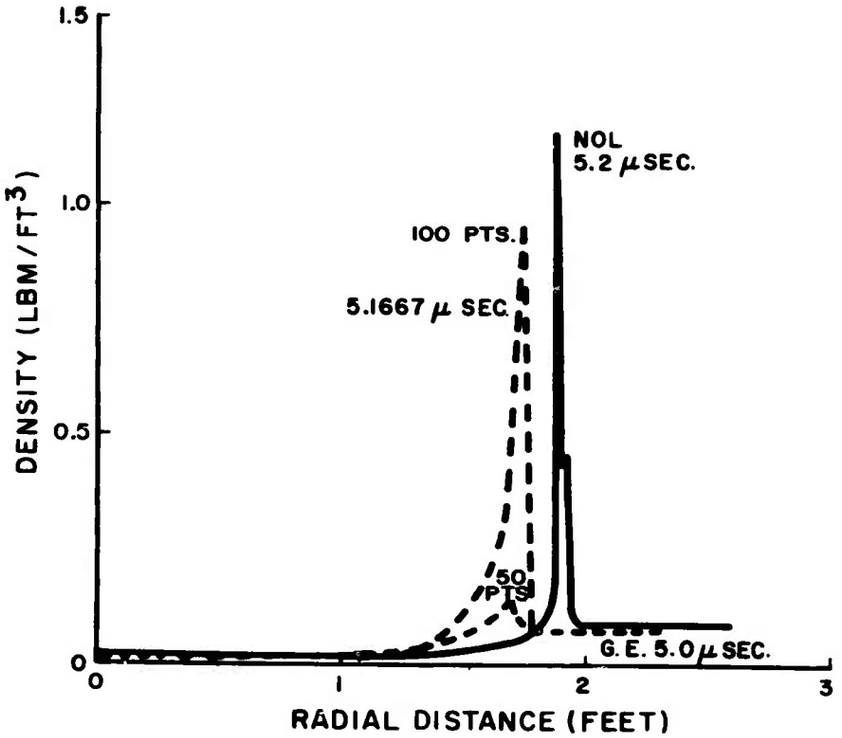


Figure II.G-8. Density Variations

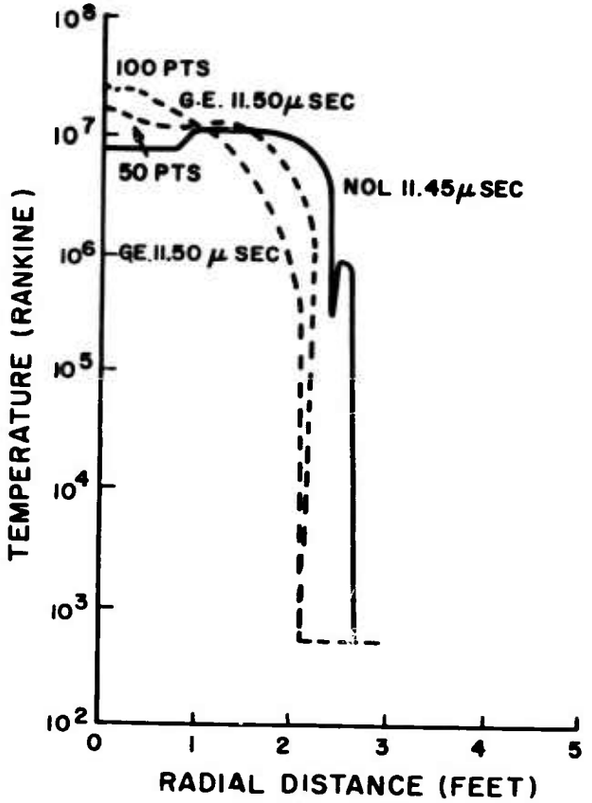


Figure II.G-9. Temperature Variations

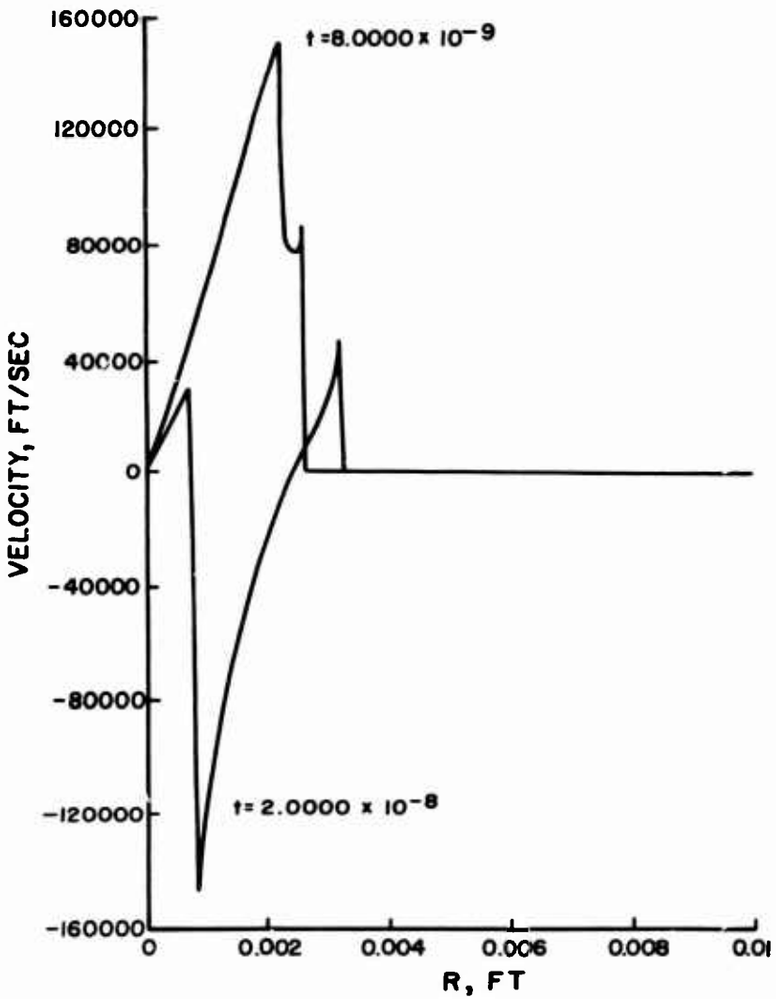


Figure II.G-10. Velocity Profiles

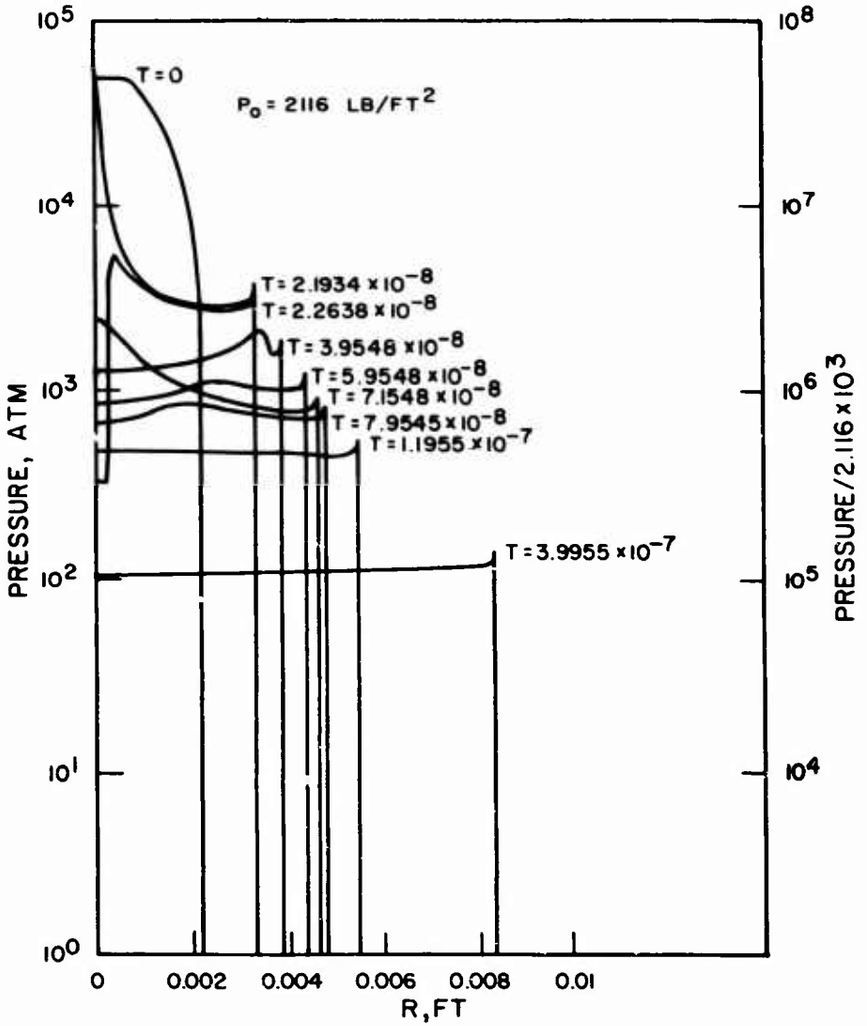


Figure II.G-11. Pressure Distribution for Selected Times

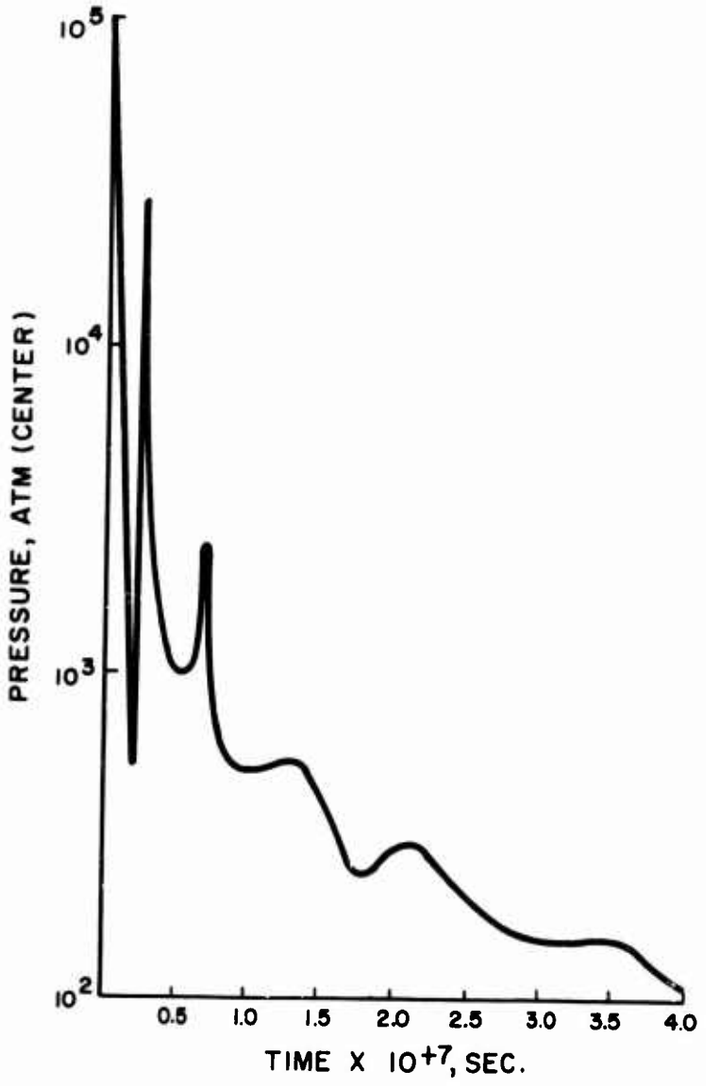


Figure II.G-12. Pressure Oscillations

II.G.3 DESCRIPTION AND USE OF RADIATION CODE

The program solves simultaneously the time dependent radiation intensity equation (see Section IV. C with a time dependent energy equation. We have obtained preliminary results for two specific cases. The first is a comparison with the results described in Ref. II. G-3. The second case is the temperature ramp case which is described below. Both cases utilize the following time dependent radiation intensity equation:

$$\frac{1}{C}\frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial r} + \left(\frac{1-\mu^2}{r}\right)\frac{\partial I}{\partial \mu} = K\,(B-I)$$

where

$$B = \sigma T^4/\pi$$

and

$$-1 \leq \mu \leq +1$$

This equation is solved simultaneously with a time dependent energy equation by means of an alternating explicit-implicit finite difference scheme.

The comparison case utilized the following energy equation:

$$\frac{\partial I}{\partial t} = \frac{2\pi K}{\rho C_V}\left[\int_{-1}^{+1} I\,d\mu - 2B\right]$$

where

$$K/\rho = \text{constant} = 0.488 \text{ ft.}^2/\text{lbm.}$$

and

$$C_V = 4600 \text{ ft.-lbf./lbm.-°R}$$

The density is variable in r, but fixed in time. The density is eliminated from the energy equation, but is needed in the intensity equation. The density profile and the initial temperature profile are obtained from Spillman (II. G-3). Initially, I is set equal to B (black-body radiation).

After Ref. II. G-3 we considered r from 10^{-7} ft. to 0.3608 ft. We used 56 r-wise nodes and 11 μ- wise nodes. $\Delta t = 7.5 \times 10^{-13}$ sec. as from the stability criteria. Two runs were made and they are compared with Spillman's results on an enclosed plot, Figure II. G-13. The first run used the table given by Spillman to obtain the initial temperature profile. The comparison with Spillman is not very satisfactory. However, we noticed that Spillman's table did not agree with the initial temperature profile given on Spillman's plot. Out second run used Spillman's plot ot obtain our initial temperature profile. The results of this run compare more favorably. We can not fully explain the discrepancy between Spillman's tabulated initial temperature profile and his plotted initial temperature profile. We speculate that perhaps the density profile which we also obtained from a table given by Spillman might not be precisely the same density profile which was used to obtain the results plotted by Spillman. Perhaps this might explain the remaining difference between our results and his. Each of our runs stopped when $t = 4 \times 10^{-10}$ sec. and they used about 8 minutes on the IBM 7079. To make a complete comparison with Spillman a run must be made to $t = 50 \times 10^{-10}$ sec. which would take about 100 minutes on the 7094.

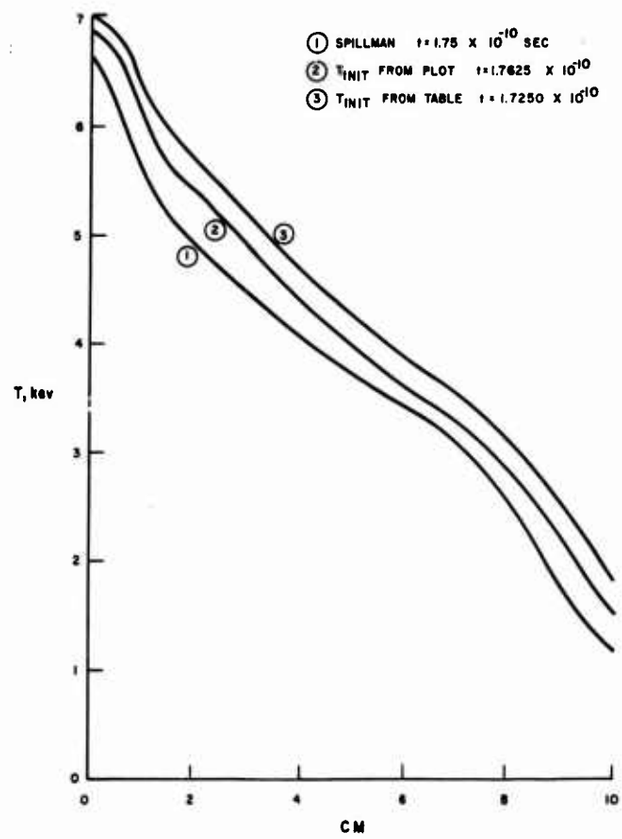


Figure II. G-13. Comparison of Two Runs with Spellman's Results

The ramp case utilized the following energy equation.

$$\frac{\partial T}{\partial t} = \frac{-\nabla \cdot F}{\rho C_V} \text{ , where } \nabla \cdot F_i^N = \frac{F_i^N - F_i^N}{\Delta r} + \frac{2 F_i^N}{r}$$

and

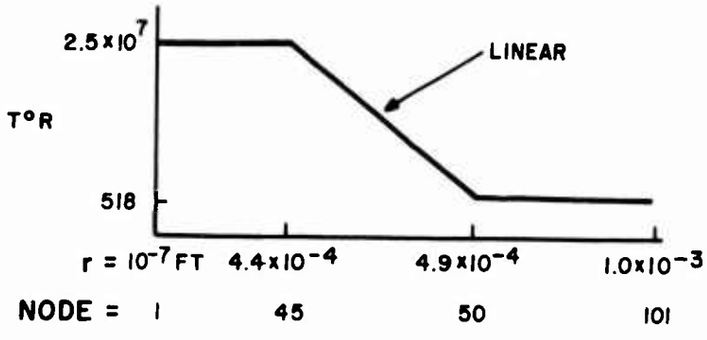
$$F_i^N = 2\pi \int_{-1}^{+1} I(r_i, \mu, t^N)\, \mu \, d\mu, \quad \begin{cases} i - \text{Node} \\ N - \text{time step} \end{cases}$$

$$\rho = \text{constant} = 7.65 \times 10^{-2} \text{ lbm./ft.}^3$$

$$C_V = 138 \text{ ft.-lbf./lbm.-°R}$$

This energy equation is equivalent to that used in the comparison case. We became dissatisfied with this form of the energy equation because the difference needed to obtain V·F caused numerical problems. In the last runs we made of the ramp case (which were made earlier than the comparison case) we actually held T fixed in time ($\partial T/\partial t = 0$). These last runs checked the convergence of I for the initial T ramp. These runs also checked the effect of the initial (t = 0) evaluation of I on the rate of convergence of I. A formula devised by R. T. Liner of the General Electric Space Sciences Laboratory was found to be the most desirable for the ramp case.

The last runs of the ramp case utilized the following temperature ramp.



We used 101 r-wise nodes and 11 μ - wise nodes. With $\Delta t = 8 \times 10^{-16}$ sec. we ran to 2.4×10^{-13} sec. ($\frac{2.4 \times 10^{-13}}{8 \times 10^{-16}}$ = 300 steps) which took 6 minutes on the IBM 7094. K was taken in a tabular form from the curve provided by Liner ($\eta = 1$).

The various formulations which are either included in the program or are easily added to the program are as follows:

a. Three energy equations

1) $\frac{\partial T}{\partial t} = \frac{2\pi K}{\rho C_V} \left[\int_{-1}^{+1} I \, d\mu - 2B \right]$, set input parameter NERGY = 1 (ISOTEE = 0)

2) $\frac{\partial T}{\partial t} = - \frac{\nabla \cdot F}{\rho C_V}$, set input parameter NERGY = 2 (ISOTEE = 0)

3) $\frac{\partial T}{\partial t} = 0$, set input parameter ISOTEE = 1

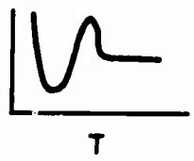
b. Two density formulations

1) ρ fixed in the time but variable in r, set input parameter KASE = 1

2) ρ fixed in time and r, set input parameter KASE = 2

c. Three formulations of the absorption coefficient.

1) $K = K_\rho$, set input parameter KASE = 1

2) 

, this is tabulated from Liner's plot in subroutine KRAD, set input parameter KASE = 2 (see Figure II.G-14).

3) K = f (T) , this option can be placed in the program simply by changing subroutine KRAD to any f (T), set input parameter KASE = 2

d. Three formulations of the initial intensity distribution

1) I = 0 , this option can be placed in the program by obvious changes to the beginning of subroutine MAIN

2) I = B , set input parameter KASE = 1

3) I = (Liner's formulation) , set input parameter KASE = 2

The comparison case, then, consists of A1, B1, C1 and D2 (NERGY = 1 and KASE = 1); the ramp case consists of A3, B2, C2, and D3 (ISOTEE = 1 and KASE = 2). Data decks and sample runs for both cases are available. The ramp case was also run using A2 (KASE = 2, NERGY = 2 and ISOTEE = 0), but the results were unsatisfactory as discussed previously. It would be interesting to run the ramp case using A1 (KASE = 2, NERGY = 1 and ISOTEE = 0); the program has been hastily altered to allow this, but it has not been tested.

The following is a description of the data input. NUMX is the number of r-wise nodes, NUMMU is the number of μ-wise nodes. The independent variable r has the limits RSTART and RSTART + RLENTH. The initial temperature profile is entered in tabular form. RTINIT is the table of nodal positions and TINIT is the table of the temperatures at the corresponding nodes. NTINIT is the number of entries in both the RTINIT array and the TINIT array. When the density varies with r, a similar pair of arrays is used to enter the ρ variation in tabular form. However, RRINIT is not a table of nodal position. But rather, it is a table of r positions. RINIT is the table of the densities at the corresponding r positions. NRINIT is the number of entries in RRINIT and RINIT. When the density is constant, NRINIT, RRINIT and RINIT are not used; instead, RHO is used. CSUBV is C_V. The manner of entering the time increment, Δt, is best described by an example: NUMDT = 2, DTTAB (1,1) = 7.5E-13, 9.0E-13, DTTAB (1,2) = 7.5E-12,1.

This means that Δt will have a maximum value (it could be cut by the stability criteria) of 7.5×10^{-13} until $t = 7.5 \times 10^{-12}$ after which Δt will be increased (by the factor 1.333 each time step) to a maximum value of 9.0×10^{-13}; Δt will remain at this value until t = 1. sec. NUMDT, the number of entries in the table (first subscript) can have any value up to 20. The print frequency table, PRINTB, works the same as DTTAB. For example: NPRINT = 3, PRINTB (1,1) = 2., 5., 1., PRINTB (1,2) = 8.E-12, 5.E-11,1., means that output will be printed every second time step until $t = 8 \times 10^{-12}$ sec., after which output will be printed every fifth time step until $t = 5 \times 10^{-11}$, after which output will be printed every time step until t = 1. sec. The run will be terminated when t = TIMEND. If MYDUMP = 0, the run will be terminated after executing for CLOCK minutes. If MYDUMP $\neq$ 0, a file of binary information will be written onto tape 16 every CLOCK minutes; the run will not terminate. Each file produced has an identification number, the first file produced by the run has its identification number equal to MYDUMP. Each subsequent file has its identification number incremented by one. After each file is written, a message is printed; for instance, a run with input parameter MYDUMP = 3 will, after the fifth file is written, print the message MYDUMP No. 7 SUCCESSFULLY COMPLETED. These files may be used to restart a fun. After perusing the output from a run, one may decide that valuable information would be obtained by continuing the run (increasing TIMEND). This may be effected by using the data on the tape file (INTAPE = 1) to start the continuation run instead of the time zero values (INTAPE = 0). The data is read from tape 15 when INTAPE = 1 and

the proper file is selected by using a skip file control card. For example, to continue the above case using the last file (fifth file), one would skip 4 files, set INTAPE = 1, increase TIMEND and set MYDUMP = 8. Setting MYDUMP = 8 will cause files to be written up on tape 16, the first file will have its identification number equal to 8; these files may then be used for subsequent continuation runs. Notice in the beginning of the MAIN subroutine the appearance of the subroutines SETTIM and LAPSED. LAPSED determines the real time (in seconds) which has elapsed since SETTIM was last called. A different computer installation may have a different set-up and some program conversion may be necessary. If there is no equivalent to the pair, SETTIM and LAPSED, I suggest creating dummy subroutines named SETTIM and LAPSED, each with one executable statement, TIEM = 0. And the program may be changed to have a file written when t = TIMEND.

At each time step for which data is outputted the following information is printed at each r-wise node (I): the radius at I, R (I); the temperature at I, T(I); the μ - wise average of the radiation intensity at I, SUMJ = $\sum_{j} I_{ij}/N\mu$, the radiative flux at I, RFLUX = $2\pi \int_{-1}^{+1} I\mu \, d\mu$; and the radiation intensity at each μ - wise node at I, RADI (I, J) where J is the μ - wise node. Units are as follows: r, ft.; T, °R; SUMJ, RFLUX and RADI, ft. - lbf./ft.^{2}-sec. Incidently, note that I, the program variable name for the r-wise nodes, is to be differentiated from I, the radiation intensity, which assumes the program variable name RADI.

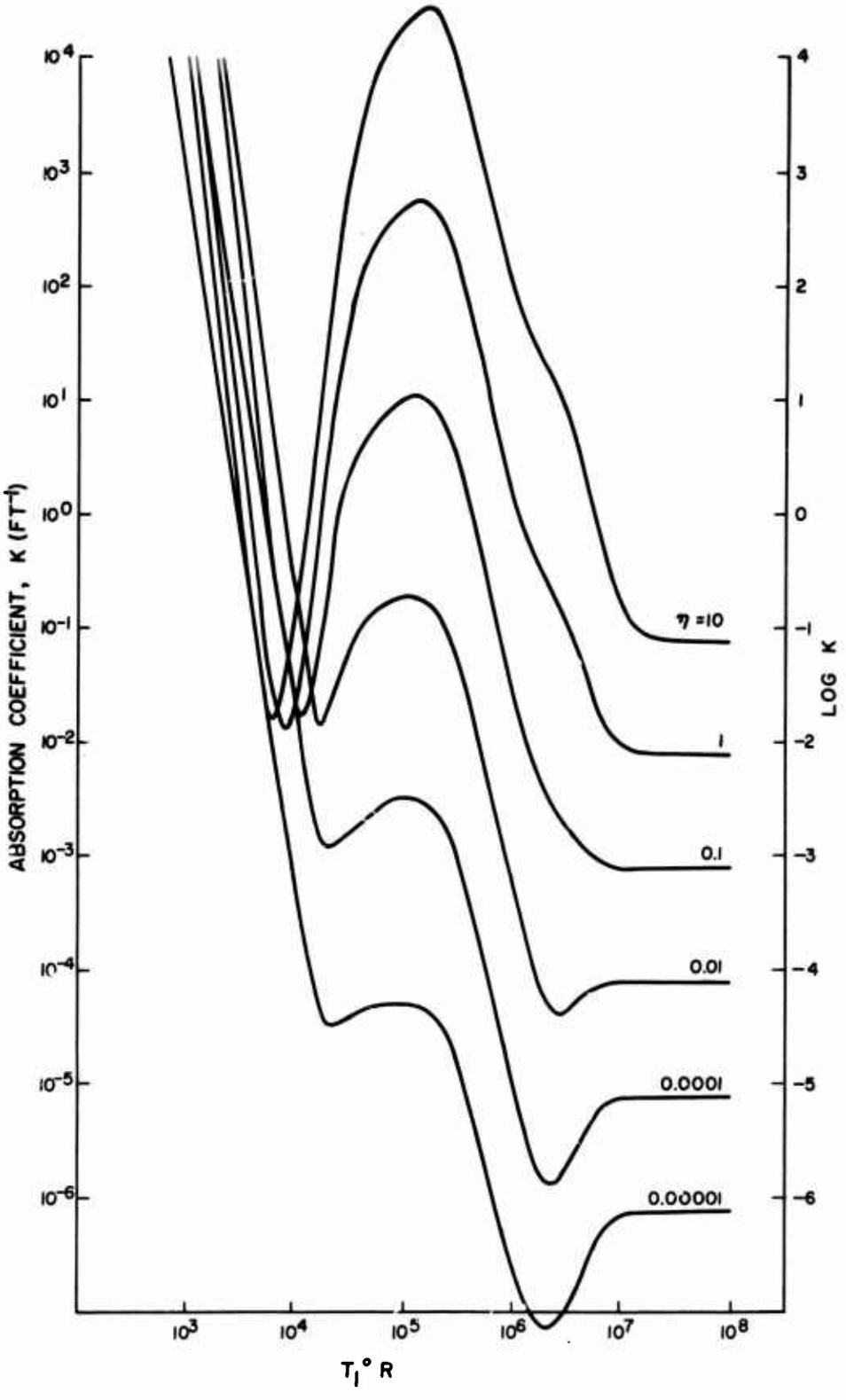


Figure II.G-14. Temperature vs. Absorption Coefficient

III. RADIATIVE PROPERTIES

III.A INTRODUCTION

III.A INTRODUCTION

This part of the study consists of four sections which deal with the subject of the thermal and radiative properties of high temperature air and specific metallic contaminants. A description is also given of a suggested approach to the calculation of a mean absorption coefficient which lies between the Planck and Rosseland limits and hence is appropriate for use in the general gray gas radiative energy transfer equation.

III.B A BRIEF INTRODUCTION TO HIGH TEMPERATURE AIR RADIATION

by

M.P. Sherman

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III.B A BRIEF INTRODUCTION TO HIGH TEMPERATURE AIR RADIATION

III. B.1 INTRODUCTION

The following section is intended to give a brief qualitative introduction to the subject of the radiation from high temperature air. References are given to enable one to explore in detail. Some comments are made on the results presented by various workers. In neither respect is this work comprehensive.

Radiation problems can be divided into two parts, radiative properties and radiative transfer. The basic radiative properties are the various photo cross sections and transition probabilities. If the gas is near equilibrium, the individual radiative properties can be summed to give absorption coefficients. This information becomes input into radiative transfer models. It is the result of the radiative transfer studies which is of engineering interest.

This section will deal mainly with radiative properties and only slightly with radiative transfer. Current work in these fields usually appears in the following Journals: Journal of Quantitative Spectroscopy and Radiative Transfer; Astrophysical Journal; and Optics and Spectroscopy (Russian).

III. B.2 CONTINUUM AND LINE RADIATION

When a system loses energy E by a radiative transition, radiation of frequency ν is emitted, where

$$E = h\nu$$

$$h = \text{Planck constant } 6.626 \times 10^{-27} \text{ erg-sec}$$

Conversely, if the system gains energy E by a radiative transition, radiation of frequency ν is absorbed. If the system has discrete energy levels, then radiative transitions will have distinct values of E, and the spectrum will consist of "lines." The bound states of atoms have fairly definite values and hence their spectra consist of lines. Such radiation is called bound-bound. When a free electron undergoes a radiative recombination, the lower energy level has a definite value but the electron can start with any value of kinetic energy, i.e., translational energy is not noticeably quantized. The spectrum of such a process will not consist of lines, but will be a continuum. Radiative recombination is an example of a bound-free process. If a free electron loses only part of its kinetic energy by a radiative process, the spectrum is a continuum and the process is called free-free.

III. B.3 ATOMIC LINE RADIATION

Atomic line radiation can only be important when there are many atoms present. For the purposes of this discussion, atomic ions will be considered as atoms. Atoms are present in significant amounts only at temperatures greater than about 3000°K. Oxygen dissociates first, and then the nitrogen.

The atomic bound-bound spectrum will consist of a series of lines. The shape and width of the lines is determined by the Doppler shift caused by the motion of the atoms in the direction of the observer, and lack of discreteness of the energy levels. This lack of discreteness is mainly due to the perturbation of the levels by the disturbing effects of other nearby particles, collision broadening. There is a "natural" width of atomic lines due to the uncertainty in the energy levels from the uncertainty principle, but this is usually orders of magnitude smaller than other effects. Assuming a Maxwellian distribution of emitters, the theory of Doppler broadening gives a Gaussian shape. The simple theory of collision broadening gives the "Lorentz shape" for the atomic line. The shape of the line will be determined by a suitable combination of the various effects. At low densities, the Doppler broadening dominates, while at higher densities, collision broadening dominates. The theory of atomic line shapes is a field of active interest. Suggested references include Griem (III. B-1) and Breene (III. B-2). More elementary discussions are found in References III. B-3 and III. B-4.

The subject of atomic line shapes is important to determine the radiant energy heat transfer caused by atomic line radiation. If conditions are such that the gas is optically thin, the shape of the line is immaterial. The intensity of radiation is determined only by the strength of the line, usually given by its "f number." However, the gas is usually not optically thin at frequencies near the center of strong lines. In this case, the radiant energy transmitted may strongly depend on the shape of the lines far from the center.

The atomic radiators in air will be O, O^+, etc., and N, N^+, etc. with small contributions due to the presence of argon and carbon. The known energy levels of these species can be found in the collection by Moore (III. B-5). Radiative "allowed transitions" are possible between some energy levels, and are "forbidden" between others. Forbidden transitions do occur with low probability and are not important here. The quantum rules for transitions and a general discussion of atomic radiation can be found in many books, e.g., Hertzberg (III. B-6), White (III. B-3), and Condon and Shortley (III. B-7).

Determining the strength or f number of the lines is a subject of current interest. There is some experimental data. Kelly (III. B-8) has computed large numbers of f numbers for nitrogen and oxygen atoms and ions using a method of modest accuracy. More exact calculations exist for a very limited numbers of lines. The agreement between various sources is often no better than a factor of two and sometimes worse.

III. B.4 MOLECULAR BAND RADIATION

This discussion will be limited to diatomic molecules. Diatomic molecules are homopolar, e.g., N_2, O_2, C_2, etc. or heteropolar, e.g., NO, CO, CN, etc. The radiation properties are very different. Diatomic molecules can have rotational, vibrational, and electronic internal energies. Homopolar molecules can only have radiant transitions between different electronic states.

The rotational levels differ by small energy differences. The corresponding radiation has low frequency and lies in the microwave region. The vibrational energy levels differ by a few tenths of an electron volt. The corresponding radiation will have higher frequency and lie in the near infrared. Vibrational transitions are accompanied by rotational transitions so instead of obtaining lines, we obtain a series of closely spaced lines called "bands." Nitric oxide vibration bands are important at temperatures below 4000K.

Electronic levels differ by energies of the order of electron volts. The corresponding radiation is in the visible and ultraviolet. Electronic transitions are accompanied by vibrational and rotational transitions so bands are obtained. The subject of the possible radiative transitions in diatomic molecules is perhaps best covered in Hertzberg "Spectra of Diatomic Molecules." (III. B-9.)

The weakest part of a molecular analysis is probably the calculation of the f numbers. The results of various workers is often in serious disagreement (III. B-10, 11, 12). The Doppler mechanism of line broadening is identical to that of atoms, but collision broadening at low temperatures where molecules are important is mainly by neutral collisions rather than by Coulombic interactions at high temperatures. Different approximate theories hold. Fortunately, if the lines are optically thin, the line shape is not needed, and this is often the case.

III. B.5 FREE-BOUND RADIATION

The principal free-bound processes will be the electronic recombination of nitrogen and oxygen ions. The models now in use to compute the free-bound continuum are the hydrogenic and the quantum defect. The hydrogenic method was used by the early work of Breene (III. B-10) and is still being used by Allen of AVCO. The quantum defect method of Burgess and Seaton (III. B-13) is far more sophisticated than the hydrogenic model. However, it too makes approximations and the reliability of the answers only partly known. The results given by the two methods tend to differ by about a factor of two, the hydrogenic being larger. Experimental data, which is still very rough, appears to give higher values than the quantum defect theory, but this may be due to atomic line contributions.

The use of the Burgess and Seaton theory is not quite straightforward. Results of various workers may differ. Sherman and Kulander (III. B-14) have made a quantum defect calculation at General Electric. More accurate quantum defect methods than those using the Burgess and Seaton approximations are being considered and doubtless more accurate theories will become available.

In addition to the recombination of positive ions, a continuum results when electrons combine with atoms to form negative ions. Breene (III. B-10) has included this effect for oxygen and shown it is a small contributor. Recently, there has been a flurry of interest in possible nitrogen negative ion contributions. Norman (III. B-15) indicated it could have a large effect. AVCO picked this up to explain some experimental results. The subject is controversial, but indications are that it is not important (III. B-16).

III. B.6 FREE-FREE RADIATION

The only significant free-free process is the radiative transitic of electrons in the field of ions, often called Bremsstrahlung. This process gives a continuum which falls off roughly as ν^{-3}, and hence, is most important in the infrared and red end of the visible. It will be dominated by free-bound processes in the ultraviolet and violet end of the visible. The integrated contribution of the spectrum is usually of the order of a tenth of the free-bound for temperatures in the range 10 - 20,000 K. The free-free is easily computed using the classical "Kramers" formula corrected by a quantum mechanical correction, the Gaunt factor. For conditions of interest, the Gaunt factor is about 1.2 - 1.3. Gaunt factors can be found in References III. B-17 and III. B-18.

III. B.7 CONTAMINANTS

A molecule which is present in trace amount but which is a very efficient radiator, such as CN, can dominate the radiation from air at temperatures up to about 7000 K. At high temperatures which processes involving singly ionized particles are dominant, the contribution of species tend to be proportional to their concentration and hence radiation from trace species becomes negligible.

III.C A SHORT NOTE ON THE OBSERVABLE LINE RADIATION FROM THREE ATOMIC SPECIES,

Na, Ca, Ca^+, Ba, and Ba^+

by

M.P. Sherman

III.C A SHORT NOTE ON THE OBSERVABLE LINE RADIATION FROM THREE ATOMIC SPECIES, Na, Ca, Ca^+, Ba, and Ba^+

In this section we will show that small amounts of the atomic impurities sodium, calcium, and barium can give rise to atomic line radiation which is more intense then the radiation from shock heated air. Therefore, if the threshold of a spectroscopic film is sufficiently high, one may see atomic lines from the impurities and not see the normal air molecular bands.

The spontaneous rate of emission of energy per unit volume in an atomic line is given by

$$I = \frac{NgA \exp(-E/kT)h\nu}{Q}$$

where N is the number of atoms or ions of the radiator per unit volume, g is the statistical weight of the upper level, E is the energy of the upper level above the ground state. T is the temperature, is the electronic partition function. A is the Einstein transition probability, ν is the frequency of the line, k and h are the Boltzmann and Planck constants. This energy is distributed over the apparent width of the atomic line. The broadening of the line caused by a low resolution spectroscope will far outweigh the true line width. We will assume all atomic lines are broadened to 10A. If they are narrower, the lines will be more intense and conversely. The transition probabilities were obtained from NBS Monograph 53, "Experimental Transition Probabilities for Spectral Lines of Seventy Elements". The energy levels and statistical weights ($g = 2J + 1$) were obtained from NBS Circular 467, "Atomic Energy Levels". The intensity of air radiation was taken from Breene and Nardone, "Radiant Emission from High Temperature Air". In this study, we take $\underline{T = 6000°K}$, and pressures of 26.32 Atm (density ratio of 1).

At 6000°K and 26.32 Atm., there are 0.3×10^{20} particles per cm^3. If the spectral widths are 10A and the impurities are in concentrations of 10^{11} (less than 1 part in 10 million), then the energy per unit volume per A, radiated by the atomic lines is obtained by multiplying the last column of the table by 10^{10}. We obtain numbers like 10^{-2} for the strongest lines to 10^{-4} for the lines not seen. Typical values of air molecular band radiation are 10^{-3} to 10^{-5} watts/cm^3 -A, with the Schumann-Runge about 10^{-2}.

Wave Length		g	$gA(x10^{-8})$	$\frac{g\ Exp(-E/kT)}{Q}$	$h\nu\ (x10^{-17})$ watt sec.	Watts - cm^3 $(x10^{-12})$
NaI	6161	2	0.56	0.010	3.226	0.090
	6154	2	0.28	0.010	3.224	0.045
	5890	4	1.80	0.137	3.374	1.93
	5896	2	0.90	0.069	3.371	1.04
CaI	4227	3	1.0	0.038	4.703	0.596
	7148	5	0.28	0.0156	2.780	0.024
CaII	3934	4	0.91	0.048	5.025	0.546
	3968	2	0.45	0.0246	5.009	0.276
	8662	2	0.025	0.0246	2.295	0.0071
	8542	4	0.047	0.0479	2.327	0.0013
BaI	7059	9	2.7	0.042	2.815	0.354
	7280	7	1.5	0.036	2.730	0.266
	7672	5	0.64	0.082	2.591	0.094
	6595	3	1.3	0.013	3.014	0.166
	5535	3	2.0	0.027	3.591	0.650
BaII	6496	2	0.15	0.024	3.060	0.055
	6141	4	0.38	0.039	3.236	0.120

III.D ON THE EQUATIONS OF STATE OF REAL GASES

by

R. B. Thomas, Jr.

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III.D ON THE EQUATIONS OF STATE OF REAL GASES

III.D.1 INTRODUCTION

A knowledge of real gases is useful for setting limits on the use of the perfect gas laws and for making the necessary corrections to these laws when it becomes necessary. For our present purposes, it will be assumed that sufficient knowledge of a gas is at hand when the equation of state is known. Thus our principal concern will be with the theory of the equations of state. As is well known, the equation of state of any substance is a relation between its pressure, volume, and temperature. (If there are other variables present, such as electric and magnetic fields, the equation of state will also involve these additional variables.) There always exists an equation of state for every homogeneous substance, solid liquid and gas. While it may not be possible to express this equation in any simple analytic form, a function of the type

$$F(p, v, T) = 0 \qquad \text{(III. D-1)}$$

exists for every substance, and the substance always knows how to solve the equation for v, when p and T are given, even if we do not.

The present discussion will be limited to gases, which is here meant to include ionized and excited molecules as well as simple neutral atoms in their lowest energy state. In order to put the subject in proper perspective, a brief discussion of the perfect gas will first be presented. With the understanding gained from this we will go on to consider real gases in Section III. D. 3. Finally, in Section III. D. 4, the added complications brought about by the existence of ions will be considered.

III.D.2 THE PERFECT GAS

Of central importance in the theory of gases is the concept of the so-called perfect gas. By this we mean a gas in which the interaction between the particles (molecules) composing the gas is so weak that it can be neglected. This approximation is physically justified either when the interaction is small, whatever the distance between the particles, or when the gas is sufficiently rarefied. In the latter, more important case, the molecules are almost always sufficiently far apart for the interaction forces to be negligible.

From a theoretical point of view, the equation of state is determined once the Helmholtz free energy F is known. F is defined by

$$F = E - ST \tag{III. D-2}$$

where E is the internal energy, S is the entropy, and T is the temperature of the system in question. Differentiating (III. D-2) gives

$$dF = dE - TdS - SdT. \tag{III. D-3}$$

combining this with the first law of thermodynamics,

$$dE = TdS - PdV \tag{III. D-4}$$

shows that

$$dF = -PdV - SdT. \tag{III. D-5}$$

Then

$$\left(\frac{\partial F}{\partial V}\right)_S = -P \tag{III. D-6}$$

which is the equation of state of the system. To obtain the equation of state, the Helmholtz free energy must some how be found. Quantum statistical mechanics states that this is given by

$$F = -kT \ell n \sum_n e^{-E_n/kt} \tag{III. D-7}$$

where the sum is over all states of the system independent of whether they are degenerate in energy. It makes it possible, in principle, to calculate the thermodynamic

functions of any system from its energy system. This is then an important result and it can at once be used as a criteria for judging the accuracy with which one might predict the equation of state of a given system. If the system is simple enough so that the energy levels (and their degree of degeneracy) can readily be found, then one can expect to have a reliable equation of state for the system. However, if the system is so complicated that the energy levels cannot be found with any degree of accuracy, then it is not possible to theoretically predict the equation of state. The complications can in general be divided into two categories; internal interactions, that is, interactions among the atoms within the molecule and external interactions, those which exist between the molecules. Depending on the strength of these interactions, they become progressively more important and at the same time more difficult to calculate. One can conclude at once from this that excited states of atoms and molecules, which fall into the group of involved internal structure, will be very difficult to treat since the interactions are strong and constitute a relatively large part of the internal energy of the system. If in addition to being excited an important fraction of the molecules are also ionized, which is certainly the case at elevated temperatures, then one must also deal with a very strong intermolecular interaction, the coulomb interaction. In the case of a plasma we are faced with both of these problems at once since at temperatures high enough to produce ionization, the molecular species are certainly highly excited.

So the problem of determining the equation of state for any substance from theory reduces to that of solving for the eigenvalues of the Hamiltonian of the system.

For the purpose of illustrating the procedures involved, we proceed with the ideal gas, which it will be recalled, is defined by the requirement that the intermolecular forces be negligible. Then the absence of these intermolecular interactions reduces the quantum mechanical problem of determining the energy levels E_n of the gas as a whole, to the determination of the energy levels of a single molecule. The energy E_n in Eq. (III. D-7) will then represent the sum of the energies of all the molecules.

It must be borne in mind, however, that even in the absence of any direct dynamic interaction between the molecules there exist certain peculiar quantum mechanical effects of the particles on one another which are connected with the identity of the particles (the so-called exchange effects). Thus if the particles obey Fermi statistics, then this effect appears in that no more than one particle can be in each quantum state at a given time; a similar effect acting in a different way takes place for particles obeying Bose statistics.

We denote by n_k the number of particles in a gas which are in the k th quantum state; the numbers n_k are sometimes called the occupation numbers of the different quantum states. Then the most important case to be considered is where the average of n_k, say $\overline{n}_k$, satisfies the inequality

$$\overline{n}_k << 1. \qquad \text{(III. D-8)}$$

Physically, this case corresponds to the gas being sufficiently rarefied. It is satisfied by all in practice for all the usual molecular and atomic gases. The condition would only be violated at densities which are so high that the substance could in no way be regarded as a gas.

The condition (III. D-8) for the mean occupation numbers means that, at any time, no more than one particle is in fact in each quantum state. As a result of this, one can neglect not only the direct forces of interaction between the particles, but also the quantum mechanical effects mentioned above. This fact, in turn, enables us to apply the Gibbs distribution to the separate molecules.

We now apply the general formula (III. D-7) to the calculation of the free energy of a gas obeying Boltzmann statistics. When we write the energy E_n as the sum of the energies ϵ_k we can reduce the summation over all states of gas to a summation over all states of a single molecule. Every state of the gas will be specified by a set of N (N being the number of molecules in the gas) of the quantities ϵ_k which, in the Boltzmann case, can be taken to be all different (no more than one molecule in each molecular state). Writing the exponential in (III. D-7) as the product of factors for each molecule and summing independently overall states of each molecule we obtain the equality

$$\sum_n e^{-E_n/kT} = \left(\sum_k e^{-\epsilon k/KT} \right)^N , \qquad \text{(III. D-9)}$$

which must hold for an ideal gas. The set of possible values of ϵ_k is the same for all the molecules since they are independent (definition of the ideal gas) and hence the sum over k in (III. D-9) is the same for all molecules.

It is necessary, however, to bear in mind the following fact. All the sets of ϵ_k differing only by a permutation of identical molecules of the gas among the levels ϵ_k correspond to the same quantum state of the gas, but in the partition function in (III. D-7) each of these states must be counted only once. Hence we must divide expression (III. D-9) on the right-hand side by the number of possible permutations of N molecules, i.e., by N!. This gives

$$\sum_n e^{-E_n/KT} = \frac{1}{N!} \left(\sum_k e^{-\epsilon k/KT} \right) \qquad \text{(III. D-10)}$$

as the correct expression for the partition function.

Substituting (III. D-10) in Eq. (III. D-7) we obtain

$$F = -KT \ln \sum_k e^{-\epsilon k/KT} + KT \ln N! \qquad \text{(III. D-11)}$$

Since N is a very large number one can use the formula

$$\ell n N! = N \ell n N \qquad \text{(III. D-12)}$$

and (III. D-11) then becomes

$$F = -NKT \ell n \left[\frac{1}{N} \sum_k e^{-\epsilon k/KT} \right] \qquad \text{(III. D-13)}$$

which allows us to calculate the free energy of any gas consisting of identical non-interacting molecules and obeying Boltzmann statistics.

For a free molecule the energy may be written in the form:

$$\epsilon_k (p_x, p_y, p_z) = \frac{1}{2m} (p_x^2 + p_y^2 + p_2^2) + \epsilon_k' , \qquad \text{(III. D-14)}$$

where the first term on the right is the kinetic energy of its translational motion and ϵ_k' are the energy levels corresponding to the rotation of the molecule and its internal motion; ϵ_k' depends neither on the velocity, nor the coordinates of the center of gravity of the molecule, assuming of course that there is no external field present. Placing (III. D-14) in Eq. (III. D-13) and carrying out the indicated integrations gives the result:

$$F = -NKT \ell n \left\{ \frac{V}{N} \left(\frac{MKT}{2\pi n^2} \right)^{3/2} \sum_k e^{-\epsilon' k/KT} \right\} \qquad \text{(III. D-15)}$$

where v is the volume of the gas.

The sum in (III. D-15) obviously cannot be calculated in general form without any assumption about the properties of the molecules. However, it is important to note that it is a function of temperature alone. Hence the way in which the free energy depends on the volume is completely determined by Eq. (III. D-15) as it stands, making it possible to obtain some very important results about the properties of a perfect gas in the absence of external fields without any further knowledge of the internal structure of the molecule.

Isolating the volume term in (III. D-15), we may write the free energy in the form

$$F = -NKT \ell n \frac{V}{N} + N f(T) \qquad \text{(III. D-16)}$$

where f(T) is some function of the temperature. Placing (III. D-16) in Eq. (III. D-6) gives the gas pressure

$$P = - \frac{\partial F}{\partial V} = \frac{NKT}{V}$$

or

$$PV = NKT - RT \qquad \text{(III. D-17)}$$

which is the well known equation of state for a perfect gas. We call attention to the important fact, that the molecular structure of a gas, no matter how complicated, does not enter the question as to whether or not it can be treated as a perfect gas; the absence of interactions among the molecules is all that is necessary to make the gas behave as a perfect gas, i.e., for its pressure, volume and temperature to satisfy Eq. (III. D-17).

Since the heat capacity of a gas is also of some interest for our purposes we will use the example of a perfect gas to show how this is calculated.

If the volume of a body remains constant during the process of adding heat to it, then from the first law (III. D-4) it is seen that $dQ = dE$, i.e., the quantity of heat gained by the body is equal to the change in its energy. If the process takes place at constant pressure then the quantity of heat can be written as the differential

$$dQ = d(E + PV) = dW \qquad \text{(III. D-18)}$$

of a certain quantity

$$W = E + PV, \qquad \text{(III. D-19)}$$

which is called the heat function or enthalpy of the body. The change in the heat function during a process at constant pressure is then equal to the heat gained by the body. The specific heat at constant volume, C_v, is just

$$C_v = \left(\frac{\partial E}{\partial T}\right)_v \qquad \text{(III. D-20)}$$

and that at constant pressure C_p, is equal to

$$C_v = \left(\frac{\partial W}{\partial T}\right)_P. \qquad \text{(III. D-21)}$$

Thus in order to calculate C_v we must know the energy of the system as a function of temperature; to find C_p the product P V as a function of temperature is required in addition.

From the first law (III. D-4) we see that C_v can also be written

$$C_v = T\left(\frac{\partial S}{\partial T}\right)_v \qquad \text{(III. D-22)}$$

while C_p takes the form

$$C_p = T\left(\frac{\partial S}{\partial T}\right)_P . \qquad \text{(III. D-23)}$$

This makes it clear that the entropy of the system as a function of temperature is needed to calculate either heat capacity. Now from (III. D-5) we have at once

$$S = -\left(\frac{\partial F}{\partial T}\right)_v , \qquad \text{(III. D-24)}$$

so that the entropy follows directly from the Helmholtz free energy. Thus F is the central quantity in any discussion of the properties of a gas (or any substance). For completeness we note that the energy can also be written in terms of the free energy:

$$E + F + TS + F - T\left(\frac{\partial F}{\partial T}\right) = -T^2\left(\frac{\partial}{\partial T}\frac{F}{T}\right)_v . \qquad \text{(III. D-25)}$$

In the case of a perfect gas F is given by (III. D-16) and we see from Eq. (III. D-24) that

$$S(T) = NK\,\ell n\,\frac{V}{N} - N\,\frac{\partial f}{\partial T} \qquad \text{(III. D-26)}$$

or, as a function of P and T

$$S(T) = -NK\,\ell n\,P - N\,\frac{\partial \chi(T)}{\partial T} \qquad \text{(III. D-27)}$$

where $\chi(T)$ is defined in terms of f (T) by

$$\chi(T) = f(T) - KT\,\ell n\,KT , \qquad \text{(III. D-28)}$$

From (III. D-25) the energy is just

$$E = F + TS = Nf(T) - NT \frac{\partial f(T)}{\partial T}. \qquad \text{(III. D-29)}$$

From this we see that the energy of a perfect gas is a function of temperature only (the same applies to $W = E + PV = E + NKT$). This must be true of course since the molecules of a perfect gas are by definition non-interacting and a change in the average distance between them as the volume changes cannot affect the energy. The energy does depend on the internal structure of the molecule, however, and for this reason the specific heats of different perfect gases are not necessarily the same. While neither C_v or C_p can be found without some further assumption of about the internal structure, their difference

$$C_p - C_v = NK = R \qquad \text{(III. D-30)}$$

for a perfect gas since here $W = E - NKT$.

III.D.3 REAL GASES

The equation of state of a perfect gas can in very many cases be applied to real gases with sufficient accuracy. This approximation may however be insufficient, and one must then take into account deviations of the behavior of a real gas from that of a perfect gas, connected with the interaction of the molecules which compose it.

To indicate the approach, which is about all that is possible with limited space and time, we shall consider the density of the gas to be so low that we may neglect triple, quadruple, etc. collisions of molecules and assume that they only interact by collisions of pairs of molecules.

To simplify the derivation of the formulae consider first a monatomic real gas. The motion of its particles may be considered classically so that its energy can be written in the form

$$E(p, q) = \sum_{a=1}^{N} \frac{p_a^2}{2m} + U \ , \qquad \text{(III. D-31)}$$

where the first term is the kinetic energy of the atoms of the gas and U is the energy of their interaction. For a monatomic gas, U is a function only of the distances between atoms. The partition function then splits up into the product of an integral over the momenta and an integral over the coordinates. The latter has the form

$$\int \cdots \int e^{-U/KT} \, dV_1 \, dV_2 \cdots dV_N \ , \qquad \text{(III. D-32)}$$

where the integration over each $dV_a = dX_a \, dy_a \, dZ_a$ is taken over the total volume V of the gas. For an ideal gas, U = 0 and this integral would simply be V^N. Hence it is clear that in calculating the free energy by the general formula

$$F = -KT \, \ell n \int e^{-E(p, q)/KT} \, d\Gamma \qquad \text{(III. D-33)}$$

where

$$d\Gamma = \frac{dp\,dq}{N!\,(2\pi h)^N}$$

is the appropriate differential over phase space (times the necessary factors), we obtain

$$F = F_p - KT \ln \frac{1}{V^N} \int \cdots \int e^{-U/KT} \, dV_1 \, dV_2 \cdots dV_N .$$

Here F_p is the free energy of a perfect gas.

Adding unity to the integrand and subtracting it and remembering that the integral over all volume elements gives V^N, we may rewrite (III.D-32) in the form

$$F = F_p - KT \ln \left\{ \frac{1}{V^N} \cdots \left(e^{-U/KT} - 1 \right) dV_1 \cdots dV_N + 1 \right\} \quad \text{(III. D-34)}$$

To carry out further calculations we shall make use of the following formal device. We will assume that the gas is not only of sufficiently low density but that there is a sufficiently small quantity of it for us to assume that not more than one pair of particles collide at the same time. Such an assumption in no way affects the general validity of the formulae thus obtained since, owing to the additively of the free energy, we know that it must be of the form

$$F = N f (T, \, V/N)$$

and hence formulae obtained for small quantities of the gas are automatically true for any quantity of it.

The interaction between the atoms is appreciable only when the two atoms in question are situated very near to each other, i.e., practically collide. Hence the integrand in Eq. (III.D-34) differs appreciably from zero only when some pairs of atoms are very close together. According to the assumption we have made, this condition can be satisfied by not more than one pair of atoms at the same time. This pair can be chosen from the N atoms in 1/2 N (N-1) ways.

Owing to this the integral in (III. D-33) may be written in the form

$$\frac{1}{2} N (N-1) \int \cdots \int \left(e^{-U_{12}/KT} - 1 \right) dV_1 \cdots dV_N , \quad \text{(III. D-35)}$$

where U_{12} is the interaction energy of two atoms. U_{12} already depends only on the coordinates of two atoms. Hence we can integrate over all the others, which will give a factor V^{N-2}. In addition, one can certainly replace $N(N-1)$ by N^2 since N is a very large number; substituting the resulting expression into (III. D-34) in place of the integral there and using the fact that $\ell n\,(1+x) \cong$ for $x << 1$ we have

$$F = F_p - \frac{KTN^2}{2V^2} \iint \left(e^{-U_{12}/KT} - 1 \right) dV_1\, dV_2 , \qquad \text{(III. D-36)}$$

where $dV_1\, dV_2$ is the product of the elements of the coordinates of the two atoms.

However, U_{12} is a function only of the distance between the two atoms, i.e., of the differences between their coordinates. Hence if one introduces, instead of the coordinates of each of the atoms, the coordinates of their common center of mass and their relative coordinates, then U_{12} will depend only on the latter. Thus one can integrate over the coordinates of the common center of mass giving again the volume V. In this way we finally obtain

$$F = F_p + \frac{N^2 KT\, B(T)}{V} , \qquad \text{(III. D-37)}$$

where

$$B(T) = \frac{1}{2} \int \left(1 - e^{-U_{12}/KT} \right) dV. \qquad \text{(III. D-38)}$$

Hence the pressure is given by

$$P = -\left(\frac{\partial F}{\partial X} \right)_T = \frac{NKT}{V} \left(1 + \frac{NB(T)}{V} \right), \qquad \text{(III. D-39)}$$

having used our previous result for the perfect gas. This is the equation of state of the gas in the approximation we are considering.

It was assumed in the beginning that we were dealing with a monatomic gas. Without giving the details, it will simply be stated that the results can also be applied to polyatomic gases as well if we interpret the integration over the relative coordinates as integrations over relative coordinates and relative orientations, a summation over spin is here also included if such refinements are of interest.

All the results here derived only make sense, clearly, if the integral (III. D-38) converges. A necessary condition for this is that the interaction between the molecules should decrease sufficiently rapidly with distance. If at large distances U_{12} decreases as $\sim r^{-n}$ then n must be greater than 3. If this condition is not satisfied, then a gas consisting of such particles cannot exist at all as a homogeneous body. In this case, each element of the substances will be acted on by very strong forces due to distance particles of the gas. Hence regions near to and far from the boundary of the volume occupied by the gas will be in very different conditions and as a result the homogeneity of the gas will be destroyed.

For monatomic gases the function $U_{12}(r)$ has a form such that for small distances it increases for a decrease in distance, corresponding to repulsive forces between the atoms. At large distances, it approaches the axis from below after having gone through a minimum at some point r near the origin.

For neutral atoms, these forces arise from multipole electric moment interaction between the atoms and is always attractive, even though it becomes very small at large distances. These multipole moments or small changes in the relative charge distribution on the individual atoms arise for two reasons. First, we may have a permanent asymmetry in the distribution of electric and positive charge on the atom resulting from the fact that the chemical bounds seek to take up the most advantageous positions from the point of view of energy. For example, water has a permanent electric dipole moment caused by the clustering of both hydrogen atoms on one side of the oxygen atom. The field produced by a permanent dipole can induce a redistribution of charge in an atom which has no electric moment of any order and they will attract one another.

The motion of electrons in atoms with no average electric moment may give rise to a momentary distribution of charge whose field can in turn induce an electric moment in another atom. The result is also an attractive force, though it is weaker than for a set of atoms with permanent dipole moments. An example is the force which exists between the atoms of the rare gases.

From what has been said one can conclude that the deviations from perfect gas behavior will become progressively less as the density is lowered, since the attractive forces fall off rapidly with distance. At a sufficiently low density every gas can be considered as perfect and the ideal gas law can be used to describe it, so far as the equation of state is concerned. If the atoms of the gas are excited, there may be a considerable enhancement of the electric multipole moment and the density at which the gas can be treated as ideal may be very much lower than for the unexcited state. Little work has been done in this area even through it is becoming increasingly important for treating systems operating with gases at elevated temperatures. The difficulty with making such calculations is that the wave functions of atoms in excited states are very difficult to calculate. Although approximate methods exist for the ground state, they are useless or difficult to apply to excited states.

In any case, no matter what the density of the gas, the heat capacity, which depends on the internal structure of the individual atoms is never a very simple quantity to calculate accurately. The difficulties inherent in such calculations would be considerably enhanced by exciting the atoms. Much useful work could be performed in determining the physical properties of gases in an excited state.

III.D.4 COMPLETELY IONIZED GAS

The method so far developed in the previous sections are not suitable for calculating thermodynamic quantities of real gases consisting of ionized particles with Coulomb interaction, since in this case the integrals entering the formulas diverge. (This is the difficulty which is always encountered in treating potentials going as one over the distance at large distances.) Thus, such a gas requires special consideration.

Consider a completely ionized gas and denote the charges on its particles by $Z_a^e \rightarrow Z_a e$ where the suffix a is used to distinguish different kinds of ions e is the elementary charge, and Z_a is a positive or negative integer. Let N_{ao} be the number of type a in unit volume of the gas. The gas as a whole is obviously electrically neutral, so that

$$\sum_a Z_a N_{ao} = 0 \ . \qquad \text{(III. D-40)}$$

We shall assume that the behavior of the gas deviates slightly from the perfect gas. To ensure this, it is necessary that the mean energy of the Coulomb interaction of two ions must be small compared with the mean kinetic energy of the ions ($\sim K T$). Thus we must have

$$(Z e)^2 N^{1/3} << K T$$

or

$$N << \left(\frac{K T}{2^2 e^2}\right)^3 \ , \qquad \text{(III. D-41)}$$

since $r \sim n^{-1/3}$.

To calculate thermodynamic quantities of such a gas one must begin by determining the increase E_c in its energy due to the Coulomb interaction of its particles compared with the energy of the corresponding perfect gas. It is well known from electrostatics that the energy of the electrical interaction of a system of charged particles can be written down as half the sum of the products of each charge with its potential in the field of all the other charges. Here this takes the form

$$E_c = V \frac{1}{2} \sum e Z_a N_{ao} \phi_a \ , \qquad \text{(III. D-42)}$$

where ϕ_a is the field potential acting on an ion of type a due to all the other charges. To calculate these potentials, we proceed in the following way.

Each of the ions creates around itself an inhomogeneously charge ion cloud. In other words, if one chooses some ion of the gas and considers the density of distribution of the other ions relative to the given one then this density will depend only on the distance r from its center, approximately, since it is on the average spherically symmetrical. We denote the density of distribution of ions of type a in the ion cloud by N_a. The potential energy of each ion of type a in the electric field surrounding it is $Z_a e \phi$ where ϕ is the potential of this field. Hence, in accordance with the Boltzmann formula we have

$$N_a = N_{ao} e^{-Z_a e \phi / KT} \qquad \text{(III. D-43)}$$

The constant coefficient is put equal to N_{ao} since at a great distance from the center, as $\phi \to 0$, the density of the ion cloud must become the mean ionic density of the gas.

The potential ϕ of the field in the ionic cloud is related to the charge density in it by Poisson's electrostatic equation

$$\nabla^2 \phi = -4 \pi e \sum_a Z_a N_a \, . \qquad \text{(III. D-44)}$$

Because of the assumption that was made about the relative weakness of the ionic interaction, the energy $e Z_a \phi$ is small compared with KT and Formula (III. D-42) may be written approximately in the form

$$N_a = N_{ao} - \frac{N_{ao} e Z_a}{KT} \qquad \text{(III. D-45)}$$

Substituting this expression into (III. D-45) and bearing in mind the condition (III. D-40) that the gas as a whole should be neutral, we obtain the equation

$$\nabla^2 \phi - k^2 \phi = 0 \, , \qquad \text{(III. D-46)}$$

where the notation

$$k^2 = \frac{4 \pi e^2}{KT} \sum_a N_{ao} Z_a^2 \qquad \text{(III. D-47)}$$

has been introduced. The quantity k has the dimensions of inverse length.

The spherically symmetric solution of Eq. (III. D-46) is just

$$\phi = \text{const} \ \frac{e^{-kr}}{r} \ .$$

In the immediate neighbourhood of the center, the field must become the pure Coulomb field of the given charge ($Z_b e$). In other words, for sufficiently small r we must have $\phi \cong e Z_b / r$; hence one can see that we must make the constant equal to $Z_b e$, so that the required potential distribution is given by

$$\phi = e Z_b \ \frac{e^{-kr}}{r} \ . \qquad \text{(III. D-48)}$$

Hence we can see that the field becomes very small for distances large compared to 1/k. Thus the length 1/k may be regarded as determining the size of the ion cloud produced by the given ion.

Expanding the potential (III. D-48) as a series we find that for small k r

$$\phi = \frac{e Z_b}{r} - e Z_b k + \text{---} \ .$$

The omitted terms vanish at r = 0. The first term is the Coulomb field of the given ion itself. The second is obviously the potential due to all other ions of the cloud at the position of the given ion; this is the quantity which must be substituted into (III. D-42): $\phi_a = - e Z_a k$.

Thus we obtain the following expression for the Coulomb part of the energy of the gas

$$E_c = - \frac{V}{2} k e^2 \sum_a N_{ao} Z_a^2$$

$$= - V e^3 \left(\frac{\pi}{KT}\right)^{1/2} \left(\sum_a N_{ao} Z_a^2\right)^{3/2} \qquad \text{(III. D-49)}$$

or, introducing the total number of different ions in the gas, $N_a = n_{ao} V$, we have

$$E_c = -e^3 \left(\frac{\pi}{KTV}\right)^{1/2} \left(\sum_a N_a Z_a^2\right)^{3/2} \qquad \text{(III. D-50)}$$

Thus the energy is inversely proportional to the temperature and the volume of the gas.

Integrating the thermodynamic relation

$$E / T^2 = - \left(\frac{\partial}{\partial T}\right) \left(F / T\right)$$

We can obtain from E_c the corresponding addition to the free energy,

$$F = F_p - \frac{2e^3}{3} \left(\frac{\pi}{KTV}\right)^{1/2} \left(\sum_a N_a Z_a^2\right)^{3/2} \qquad \text{(III. D-51)}$$

Here the constant of integration has been set equal to zero since $F \to F_p$ as $T \to \infty$. . Hence we obtain the pressure from Eq. (III. D-6)

$$P = \frac{KT}{V} \sum_a N_a - \frac{e^3}{3 V^{3/2}} \left(\frac{\pi}{KT}\right)^{1/2} \left(\sum_a N_a Z_a^2\right)^{3/2} \qquad \text{(III. D-52)}$$

Here we see that the equation of state is modified by the addition of a new term which depends on the volume as we expect. As the interaction becomes stronger, the pressure becomes a much more involved function of the volume.

In obtaining Eq. (III. D-52) we have made many simplifying assumptions which cannot be expected to hold at higher densities. None the less, for plasmas ordinarily encountered, the result obtained can be expected to hold reasonably well.

By a simple application of the formalism presented in Section III. D-2, we can also obtain the heat capacities. This will not be shown in detail.

We can conclude from what has been said that for sufficiently low densities, the perfect gas law can be expected to give a reasonable description of our plasma. If corrections are necessary, the theory given here is sufficient to allow an estimate of the conditions under which they do become necessary and also indicates how one should go about making such corrections.

III.E CHOICE OF AN APPROPRIATE MEAN ABSORPTION COEFFICIENT FOR USE IN THE GENERAL GREY GAS EQUATIONS

by

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III.E CHOICE OF AN APPROPRIATE MEAN ABSORPTION COEFFICIENT FOR USE IN THE GENERAL GREY GAS EQUATIONS

III.E.1 INTRODUCTION

The treatment of radiative transport problems is relatively easy in the limits that the gas under consideration is very optically thin or very optically thick. For in either of these cases the radiative energy flux vector $\underset{\sim}{F}$ is given by a simple well known expression involving the Planck mean absorption coefficient (optically thin limit) or the Rosseland mean absorption coefficient (optically thick limit). Also, even though the gas is neither optically thin nor optically thick, in the special case that it can be approximated by a plane parallel layer and the frequency dependence of the spectral absorption coefficient K_ν is so small that it can be neglected, the relatively simple general grey gas expression applies for $\underset{\sim}{F}$. However, in many problems none of these simple expressions are directly applicable. This results because usually K_ν depends quite strongly on the frequency ν. Then the grey gas approximation is not valid and also the gas is likely to be neither optically thick nor optically thin to the radiation of all important frequencies. (The important frequencies are those within about an order of magnitude of the peak of the Planck function at $\nu \simeq 2.8\ kT/h$.) In this case, even though the gas can be approximated by a plane-parallel layer, the expression for the flux involves rather complicated integrations over both space and frequency which must be performed numerically. Hence, an exact treatment involves a very large amount of computing machine time.

The purpose of this section is to describe and test numerically the reliability of an approximate method for handling this latter type situation which avoids the frequency integration in the expression for the flux. This is done by using the general grey gas expression for the flux, but choosing the mean absorption coefficient K_a to be a function of the Planck mean K_P, the Rosseland mean K_R, and the optical depth. That is, we take into account the fact that the proper mean over frequency of K_ν varies with optical depth. Our choice of this mean leads to exactly correct results in the limits of very optically thick and very optically thin gases and, of course, gives the correct result when the gas really is grey, $K_\nu = K_P = K_R = K_a$.

The method proposed is convenient because the general grey gas equations are fairly simple and also because many investigators have been using these equations in treating radiative transport problems and are familiar with their properties. As discussed in more detail in the text, use of these grey gas equations with a single mean over frequency absorption coefficient, such as K_P, for all optical thicknesses, as usually done, can easily lead to error in $\underset{\sim}{F}$ by a couple of orders of magnitude for a fairly wide range of optical depths. However, by choosing the average over frequency of K_ν to vary with optical depth, with essentially no more complication we obtain (for the cases studied) results for the flux and its divergence which are nearly always within a factor of 2 of the correct values.

A limitation of the method is that it is strictly applicable only when there is spatial dependence on one cartesian coordinate. However, perhaps the majority of problems dealing with the regime of intermediate optical thickness can at least be fairly well approximated by this geometry. By applying our approach directly to the radiative intensity rather than the flux the general approach could be extended to other geometries, as well. However, the accurate treatment of the intermediate regime of optical thickness for nonplane-parallel geometry, even with the frequency dependence eliminated, becomes very difficult.

III.E.2 GENERAL EQUATIONS AND DEVELOPMENT OF THE METHOD

We consider the radiation in a plane-parallel layer of gas (Figure III. E-1) located between y = 0 and y = L. The vector $\underset{\sim}{n}$ is a unit vector in the negative y direction. Complete homogeneity is assumed in the XZ plane. At position y in the gas the net radiative energy flux vector is then

$$\underset{\sim}{F}(y) = \underset{\sim}{n}\,[F^{+}(y) - F^{-}(y)]\ , \qquad \text{(III. E-1)}$$

where F^{+} and F^{-} are the radiative fluxes arising from photons traveling in directions with positive components along $\underset{\sim}{n}$ and negative components along $\underset{\sim}{n}$, respectively.

$$F^{+}(y) = \int_0^{\infty} d\nu\ F_{\nu}^{+}(y)\ ,\ F^{-}(y) = \int_0^{\infty} d\nu\ F_{\nu}^{-}(y) \qquad \text{(III. E-2)}$$

As is derived in most books dealing with radiative transport (III. E-1)

$$F_{\nu}^{+}(y) = 2\pi \int_{\tau_\nu}^{\tau_{\nu L}} B_{\nu}^{0}(\tau_{\nu 1}) E_2(\tau_{\nu 1} - \tau_{\nu}) d\tau_{\nu 1} + 2\, F_{\nu}^{+}(L) E_3(\tau_{\nu L} - \tau_{\nu}) \qquad \text{(III. E-3)}$$

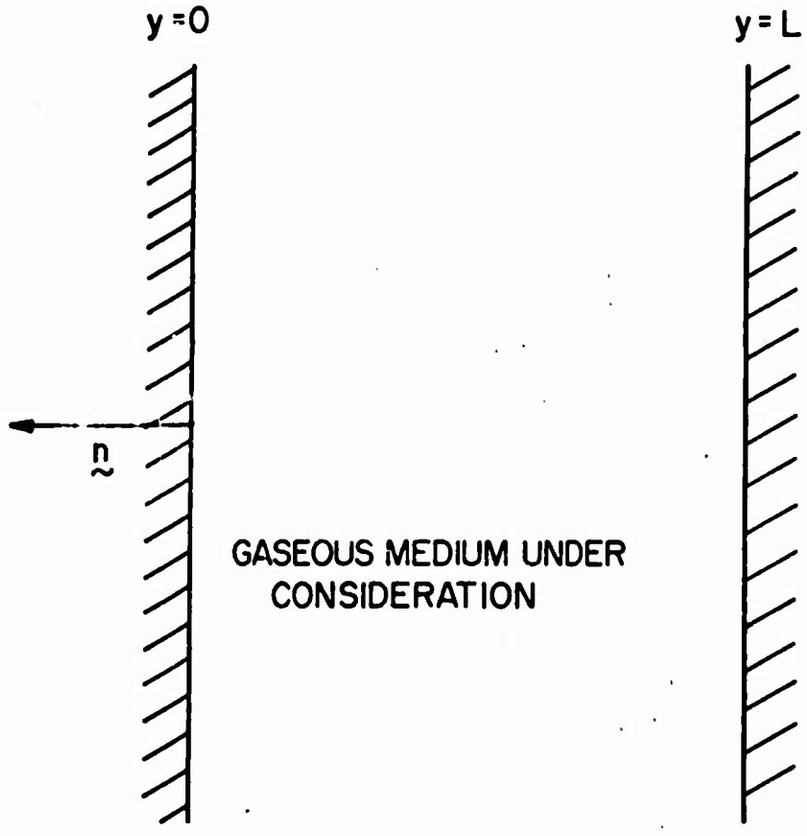


Figure III. E-1. Plane Parallel Layer of Gas

and

$$F_\nu^-(y) = 2\pi \int_0^{\tau_\nu} B_\nu^0(\tau_{\nu 1}) E_2(\tau_\nu - \tau_{\nu 1}) d\tau_{\nu 1} + 2 F_\nu^-(0) E_3(\tau_\nu) . \quad \text{(III. E-4)}$$

Here τ_ν is the optical depth of position y for radiation of frequency ν

$$\tau_\nu \equiv \tau_\nu(y) = \int_0^y K_\nu(y')dy' \; ; \; \tau_{\nu 1} \equiv \tau_\nu(y_1) = \int_0^{y_1} K_\nu(y')dy' . \quad \text{(III. E-5)}$$

K_ν is the spectral absorption coefficient defined to include the effect of induced emission (exponential factor in Eq. (III. E-6))

$$K_\nu = \sum_a N_a \sigma_a(\nu) \left[1 - e^{-h\nu/kT}\right] \quad \text{(III. E-6)}$$

where N_a is the density of absorbers "a" and $\sigma_a(\nu)$ is the cross section for absorption of a photon of frequency ν by these absorbers. $E_n(\tau)$ is the exponential integral

$$E_n(\tau) = \int_0^1 \mu^{n-2} e^{-\tau/\mu} d\mu . \quad \text{(III. E-7)}$$

Some of its properties are given in App. I of Ref. III. E-1. $B_\nu{}^0(\tau_\nu)$ is the Planck intensity

$$B_\nu{}^0(\tau_\nu) = B_\nu[T(y)] = \frac{2h\nu^3}{c^2} \left[e^{h\nu/kT(y)} - 1\right]^{-1} . \quad \text{(III. E-8)}$$

The first term in Eqs. (III. E-3) and (III. E-4) is valid only if the gas is in local thermodynamic equilibrium so that the source function is the Planck function. The boundary value contributions, the second terms in Eqs. (III. E-3) and (III. E-4), are strictly valid only when the intensities $I_\nu^-(0, \mu)$ and $I_\nu^+(L, \mu)$ are independent of direction, i.e., do not depend on μ, the direction cosine of the photon propagation vector along $\underset{\sim}{n}$.

We want to investigate the possibility of representing $F^+(y)$ and $F^-(y)$ by the approximate quantities $F_a{}^+(y)$ and $F_a{}^-(y)$ given by the equations analogous to Eqs. (III. E-3), (III. E-4), and (III. E-1)

$$F_a^+(y) = 2\pi \int_{\tau_a}^{\tau_{aL}} B^0(\tau_{a1}) E_2(\tau_{a1} - \tau_a) d\tau_{a1} + 2 F^+(L) E_3(\tau_{a1} - \tau_a) \quad \text{(III. E-9)}$$

$$F_a^-(y) = 2\pi \int_0^{\tau_a} B^0(\tau_{a1}) E_2(\tau_a - \tau_{a1}) d\tau_{a1} + 2 F^-(0) E_3(\tau_a) \quad \text{(III. E-10)}$$

and

$$\underset{\sim}{F}_a(y) = \underset{\sim}{n}\,[F_a^{+}(y) - F_a^{-}(y)] \ . \qquad \text{(III.E-11)}$$

Here

$$B^0(\tau_{a1}) \equiv B[T(y_1)] = \int_0^\infty B_\nu[T(y_1)]d\nu = \frac{\sigma}{\pi}\,T(y_1)^4 \ , \qquad \text{(III.E-12)}$$

where σ is the Stephan-Boltzmann constant. τ_a is a mean optical depth

$$\tau_{a1} \equiv \tau_a(y_1) = \int_0^{y_1} K_a(y')dy' \qquad \text{(III.E-13)}$$

in which K_a is a mean (over frequency) absorption coefficient.

Eqs. (III.E-9) and (III.E-10) are called the general grey gas equations for the flux. They are seen from Eqs. (III.E-2) to (III.E-5) and Eqs. (III.E-12) and (III.E-13) to be exactly correct when the spectral absorption coefficient is independent of frequency, $K_\nu = K_a$. It is easily shown that these equations also give the correct result in the optically thin limit if K_a is chosen equal to the Planck mean K_p. When $\tau \ll 1$

$$E_2(\tau) = 1 + \tau(\gamma - 1 + \ln\,\tau) - \frac{\tau^2}{2} + \frac{\tau^3}{12} - \ldots, \gamma = 0.577216 \qquad \text{(III.E-14)}$$

$$E_3(\tau) = \tfrac{1}{2} - \tau + \frac{\tau^2}{2}\,(-\gamma + 3/2 - \ln\,\tau) + \frac{\tau^3}{6} - \ldots \qquad \text{(III.E-15)}$$

Thus, when the gas is optically thin, $\tau_{\nu L} \ll 1$ for all important frequencies, we use the first term in Eqs. (III.E-14) and (III.E-15) together with Eqs. (III.E-2) to (III.E-5) and Eq. (III.E-12) to obtain

$$F^{+}(y) = 2\pi \int_0^\infty d\nu \int_y^L B_\nu\,[T(y')]K_\nu(y')dy' + F^{+}(L) \qquad \text{(III.E-16)}$$

$$= 2\pi \int_y^L B[T(y')]K_p(y')dy' + F^{+}(L) \ ; \ \tau_{PL} \ll 1$$

and similarly

$$F^{-}(y) = 2\pi \int_0^y B[T(y')]K_p(y')dy' + F^{-}(0) \ ; \ \tau_{PL} \ll 1 \ , \qquad \text{(III.E-17)}$$

where the Planck mean K_P is given by

$$K_P = \frac{\int_0^\infty K_\nu B_\nu(T)d\nu}{B(T)} \qquad \text{(III. E-18)}$$

Analogously, applying Eqs. (III. E-14) and (III. E-15) to the approximate Eqs. (III. E-9) and (III. E-10) we get

$$F_a^+(y) = 2\pi \int_y^L B[T(y')]K_a(y')dy' + F^+(L) \; ; \; \tau_{aL} << 1 \qquad \text{(III. E-19)}$$

and

$$F_a^-(y) = 2\pi \int_0^y B[T(y')]K_a(y')dy' + F^-(0) \; ; \; \tau_a << 1 \qquad \text{(III. E-20)}$$

Thus, if K_a were chosen equal to K_p, or equivalently τ_a chosen equal to τ_p given by

$$\tau_P \equiv \tau_P(y) = \int_0^y K_P\,(y')dy' \; , \qquad \text{(III. E-21)}$$

we see that the approximate Eqs. (III. E-9) and (III. E-10) would give the correct result in the limit of an optically thin gas.

It is also interesting to consider Eqs. (III. E-3), (III. E-4), (III. E-9), and (III. E-10) when the condition

$$\frac{d\,B_\nu{}^0\,(\tau_\nu)}{d\,\tau_\nu} << B_\nu{}^0\,(\tau_\nu) \qquad \text{(III. E-22)}$$

is satisfied for all important frequencies. Then we can make a Taylor series expansion of $B_\nu{}^0(\tau_{\nu 1})$ and $B^0(\tau_{a1})$ about $B_\nu{}^0(\tau_\nu)$ and $B^0(\tau_a)$, respectively

$$F_\nu{}^+(y) = 2\pi \int_{\tau_\nu}^{\tau_{\nu L}} [B_\nu{}^0(\tau_\nu) + (\tau_{\nu 1}-\tau_\nu)\frac{dB_\nu(\tau_\nu)}{d\,\tau_\nu} + \cdots]E_2(\tau_{\nu 1}-\tau_\nu)d\tau_{\nu 1}$$

$$+ 2\,F_\nu{}^+(L)E_3(\tau_{\nu L}-\tau_\nu) \quad . \qquad \text{(III. E-23)}$$

Making use of Eq. (III. E-7) one readily performs the integration and obtains

$$F_\nu^+(y) = \pi\, B_\nu^0(\tau_\nu)[1-2\,E_3(\tau_{\nu L}-\tau_\nu)] + \frac{2\pi}{3}\,\frac{dB_\nu^0(\tau_\nu)}{d\,\tau_\nu}\,[1-3(\tau_{\nu L}-\tau_\nu)E_3(\tau_{\nu L}-\tau_\nu)-3E_4(\tau_{\nu L}-\tau_\nu)] + 2F_\nu^+(L)E_3(\tau_{\nu L}-\tau_\nu);\quad \frac{dB_\nu^0(\tau_\nu)}{d\,\tau_\nu} \ll B_\nu^0(\tau_\nu). \quad \text{(III. E-24)}$$

Analogously one gets

$$F_\nu^-(y) = \pi\, B_\nu^0(\tau_\nu)[1-2E_3(\tau_\nu)] - \frac{2\pi}{3}\,\frac{dB_\nu^0(\tau_\nu)}{d\,\tau_\nu}\,[1-3\tau_\nu E_3(\tau_\nu)-3E_4(\tau_\nu)] + 2F_\nu^-(0)E_3(\tau_\nu)$$

(III. E-25)

and

$$F_a^-(y) = \pi B^0(\tau_a)[1-2E_3(\tau_a)] - \frac{2\pi}{3}\,\frac{dB^0(\tau_a)}{d\tau_a}\,[1-3\tau_a E_3(\tau_a)-3E_4(\tau_a)]+2F^-(0)E_3(\tau_a)\ , \quad \text{(III. E-26)}$$

when condition (III. E-22) is satisfied. An equation for $F_a^+(y)$ also results which is exactly like Eq. (III. E-24) in form, but with the subscript "ν" everywhere replaced with "a" except on B, i.e., $B^0(\tau_a)$ replaces $B_\nu^0(\tau_\nu)$.

For very large τ all the exponential integrals $E_n(\tau)$ approach zero. Thus, in the interior of an optically thick gas ($\tau_\nu \gg 1$), $\tau_{\nu L} \gg 1$ which satisfies condition (III. E-22), Eqs. (III. E-1), (III. E-2), (III. E-24), (III. E-25), and (III. E-5) lead to

$$\underset{\sim}{F}(y) \simeq \frac{4\pi}{3}\,\underset{\sim}{n}\int_0^\infty \frac{dB_\nu^0(\tau_\nu)}{d\,\tau_\nu}\,d\nu = \frac{4\pi}{3}\,\underset{\sim}{n}\int_0^\infty \frac{1}{K_\nu}\,\frac{dB_\nu[T(y)]}{dy}\,d\nu$$

$$= \frac{16\,\underset{\sim}{n}\,\sigma\,T(y)^3}{3\,K_R(y)}\,\frac{dT(y)}{dy}\ , \quad \text{(III. E-27)}$$

where use of Eq. (III. E-12) was made in obtaining the last form and K_R is the Rosseland mean absorption coefficient

$$K_R^{-1} = \frac{\int_0^\infty \frac{1}{K_\nu} \frac{dB_\nu(T)}{dT} d\nu}{\frac{dB(T)}{dT}} \quad . \qquad \text{(III. E-28)}$$

Similarly, Eqs. (III. E-11), (III. E-26), the analogue of Eq. (III. E-24), Eq. (III. E-12) and Eq. (III. E-13) lead to

$$\underset{\sim}{F}_a(y) = \frac{4\pi}{3} \frac{dB^0(\tau_a)}{d\tau_a} = \frac{16\sigma T(y)^3}{3K_a(y)} \frac{dT(y)}{dy} \; ; \; \tau_a >> 1; \; \tau_{aL} - \tau_a >> 1 \qquad \text{(III. E-29)}$$

From a comparison of Eqs. (III. E-27) and (III. E-29) it is seen that the grey gas equations, Eqs. (III. E-9) to (III. E-11), also give the correct answer for the flux in the interior of an optically thick gas satisfying condition (III. E-22) if $K_a = K_R$.

Usually K_P and K_R are quite different with K_P somewhat larger than K_R. This results principally from the fact that K_ν appears in the denominator in the average performed in Eq. (III. E-28), while it appears in the numerator in Eq. (III. E-18). Thus, it is apparent that Eqs. (III. E-9) to (III. E-11) can be a good approximation to Eqs. (III. E-1) to (III. E-4) for all optical thicknesses in a non-grey gas (one in which K_ν is not independent of frequency) only if the mean over frequency of K_ν is chosen to be a function of optical depth rather than a single mean such as K_P for all optical depths.

The large error that can result if only a single frequency mean is used in Eqs. (III. E-9) to (III. E-11) is shown more clearly by comparing the equation resulting when Eqs. (III. E-24) and (III. E-25) are used in Eqs. (III. E-1) and (III. E-2) with the equation resulting when Eq. (III. E-26) and the analogue of Eq. (III. E-24) are used in Eq. (III. E-11). One obtains, with the additional use of Eqs. (III. E-5), (III. E-8), (III. E-12) and (III. E-13),

$$\underset{\sim}{F}(y) = 2\pi\underset{\sim}{n}\int_0^\infty d\nu B_\nu[T(y)]\{E_3[\tau_\nu(y)]-E_3[\tau_\nu(L)-\tau_\nu(y)]\}$$

$$+\frac{2\pi\underset{\sim}{n}}{3}\int_0^\infty \frac{d\nu}{K_\nu(y)}\frac{dB_\nu[T(y)]}{dy}\Big(2-3\{[\tau_\nu(L)-\tau_\nu(y)E_3[\tau_\nu(L)-\tau_\nu(y)]+\tau_\nu(y)E_3[\tau_\nu(y)]\}$$

$$-3\{E_4[\tau_\nu(L)-\tau_\nu(y)]+E_4[\tau_\nu(y)]\}\Big) \qquad \text{(III. E-30)}$$

$$+2\underset{\sim}{n}\int_0^\infty d\nu\ \{F_\nu^+(L)E_3[\tau_\nu(L)-\tau_\nu(y)]-F^-(0)E_3[\tau_\nu(y)]\}$$

and

$$\underset{\sim}{F}_a(y) = 2\pi\underset{\sim}{n}\,B[T(y)]\{E_3[\tau_a(y)]-E_3[\tau_a(L)-\tau_a(y)]\}$$

$$+\frac{2\pi\underset{\sim}{n}}{3K_a(y)}\frac{dB[T(y)]}{dy}\Big(2-3\{[\tau_a(L)-\tau_a(y)]E_3[\tau_a(L)-\tau_a(y)]+\tau_a(y)E_3[\tau_a(y)]\} \qquad \text{(III. E-31)}$$

$$-3\{E_4[\tau_a(L)-\tau_a(y)]+E_4[\tau_a(y)]\}\Big)$$

$$+2\underset{\sim}{n}\{F^+(L)E_3[\tau_a(L)-\tau_a(y)]-F^-(0)E_3[\tau_a(y)]\}$$

which are applicable when condition (III. E-22) is satisfied. Now let us consider the case that K_a is set equal to K_P. In the limit of an optically thin gas, as noted above, $\underset{\sim}{F}_a$ will then give the correct result, but for the interior of an optically thick gas, where all the $E_n(\tau)$ integrals vanish and Eqs. (III. E-30) and (III. E-31) reduce to Eqs. (III. E-27) and (III. E-29), the result given by Eq. (III. E-31) is wrong by the ratio K_R/K_P. However, the error can be even considerably larger than this for part of the region of intermediate optical thickness. This results because (unless K_ν depends very slightly on frequency) in this region use of $\tau_a = \tau_P$, Eq. (III. E-21), overestimates the proper average τ and causes the terms in Eq. (III. E-31) involving the exponential E_n integrals to drop out and Eq. (III. E-31) to reduce to Eq. (III. E-29) for much smaller gas thicknesses than those for which the correct equation,

Eq. (III. E-30), reduces to Eq. (III. E-27). For small temperature gradients the magnitude of $\underset{\sim}{F}$ given by either Eq. (III. E-27) or Eq. (III. E-29) is very small. Thus, in the case of small temperature gradients use of $\tau_a = \tau_P$ will lead to very large error for the usually quite broad region in which τ_P is large while τ_R, Eq. (III. E-33) below, is not. In the case of free-free absorption where $\tau_P \simeq 30\ \tau_R$ we expect the maximum error in this region due to using $\tau_a = \tau_P$ to be several orders of magnitude for small temperature gradients. (The approximate method we propose greatly reduces, but does not completely eliminate this type error, as discussed further near the end of this section.) Of course, use of $\tau_a = \tau_R$ would also lead to large error for intermediate and small optical thickness.

The approximate method we propose is to use Eqs. (III. E-9) - (III. E-11), but with τ_a chosen to be a function of τ_R, τ_P and optical thickness such that it changes smoothly from the value τ_P at very small optical thickness to τ_R at very large optical thickness. In particular we have chosen to study the case in which τ_a is given by the equation

$$\tau_a(y) = \left[\frac{b + \tau_R(y)}{b + \tau_P(y)} \right] \tau_P(y) \quad , \qquad \text{(III. E-32)}$$

which is probably the most simple expression that has these properties. Here b is a parameter of order unity which can be adjusted on the basis of comparison between numerical results obtained with Eqs. (III. E-9) to (III. E-11) and the exact results obtained with Eqs. (III. E-1) to (III. E-4). $\tau_P(y)$ is given by Eq. (III. E-21) and $\tau_R(y)$ by the analogous expression

$$\tau_R(y) = \int_0^y K_R(y')dy' \quad . \qquad \text{(III. E-33)}$$

With τ_a given by Eq. (III. E-32) K_a has the value

$$K_a(y) = \frac{d\tau_a(y)}{dy} = \left[\frac{b}{b+\tau_P(y)} \right] \left[\frac{b+\tau_R(y)}{b+\tau_P(y)} \right] K_P(y) + \left[\frac{\tau_P(y)}{b+\tau_P(y)} \right] K_R(y) \qquad \text{(III. E-34)}$$

which changes smoothly from the value $K_p(y)$ for very small optical thickness, τ_R and $\tau_P \ll 1$ to $K_R(y)$ at very large optical thickness τ_R and $\tau_P \gg 1$.

We mention at this point that for strongly frequency dependent K_ν we can, of course, not expect to get an almost perfect fit to F for all optical thicknesses by our approximate method. Part of the reason for this is again seen by a comparison of Eqs. (III. E-30) and (III. E-31). One sees that more than one average K or τ would have to enter Eq. (III. E-31) if it were to give a perfect representation of Eq. (III. E-30). The most important of these averages are those occurring in the averages of the E_3 integrals over the Planck function and those occurring in the term proportional dB_ν/dy.

These tend usually to be important at different optical thicknesses. Thus, we can hope to approximate well the dominate terms for each region of optical thickness. However, for very small temperature gradients the E_3 terms in the first curly braces on the right-hand sides of Eqs. (III. E-30) and (III. E-31), although small, remain important relative to the terms proportional to the space derivatives of B_ν and B for quite large optical thicknesses. For large optical thickness the true effective average τ entering the exponentials becomes small relative even to τ_R. Thus, our approximate method makes the exponential terms in Eq. (III. E-31) become very small more quickly than the corresponding terms in Eq. (III. E-30) and gives erroneous results when this occurs before the gradient terms have become dominate in determining F. For the same reason in the case of very low temperature gradients the boundary value contributions (which are proportional to E_3 as well, as seen from the last terms in Eqs. (III. E-30) and (III. E-31)) will be significant for larger distances from the boundary than one would expect by using $\tau_a = \tau_R$.

Also for sufficiently large τ_P/τ_R ratios there will exist a range of y values for which $\tau_P \gg b$ while $\tau_R \ll b$. Then Eq. (III. E-32) yields for τ_a approximately the constant value b and will lead to erroneous results.[2] However, the large values of τ_P/τ_R required for this to strongly limit the accuracy of use of the method are probably not frequently encountered. Another choice for the relation between τ_a, τ_P and τ_R might make the method applicable for larger ratios of τ_P/τ_R.

III.E.3 RESULTS AND DISCUSSION

In testing our approximate method numerically we assumed that

$$K_\nu = \frac{a(kT_o/h)^{7/2}}{(kT/h)^{\frac{1}{2}}\,\nu^3}\left[1-e^{-h\nu/kT}\right] . \qquad \text{(III. E-35)}$$

This corresponds to the absorption coefficient due to free-free transitions with unit free-free Gaunt factor. The quantity "a" should be a function of density; however, we set a equal to unity. This is equivalent to putting K_ν and y in dimensionless form by dividing the former by a and multiplying the latter by a. Also in determining the divergence of the flux it means that we assume constant density. The temperature dependence studied was

$$T = T_o \left[1 - Ay\right] \qquad \text{(III. E-36)}$$

It was thought that if the method worked well for both small and large values of A it would very likely also work well for more complicated temperature dependence on y and in the case of a density gradient.

In carrying out our numerical work the Eqs. (III. E-4) and (III. E-25) (integrated over frequency) and Eqs. (III. E-10) and (III .E-26) were coded and evaluated on an IBM 7094 computer. The boundary value contributions, the terms proportional to $F_\nu^-(0)$ or $F^-(0)$ were omitted. However, a comparison of the terms $< E_3(\tau_\nu) >$ and $E_3(\tau_a)$, where

$$< E_3(\tau_\nu) > = \frac{\int_0^\infty d\nu\; B_\nu[T(y)]E_3(\tau_\nu)}{B[T(y)]} , \qquad \text{(III. E-37)}$$

indicates how well our approximate method would give the boundary contribution if $F_\nu^-(0) \simeq B_\nu[T(y)]$. The accurate test would be to compare $E_3(\tau_a)$ with the results given by Eq. (III. E-37) when $F_\nu^-(0)$ and $F^-(0)$ replace $B_\nu[T(y)]$ and $B[T(y)]$. However, this is not feasible in testing our method, since $F_\nu^-(0)$ and $F^-(0)$ can be anything.

The equations for $F_\nu^+(y)$ and $F_a^+(y)$ were not evaluated because $F_\nu^+(y)$ and $F_a^+(y)$ are also given by Eqs. (III. E-4), (III. E-25), (III. E-10), and (III. E-26) if we change our choice of coordinates and let the boundary at y = L instead pass through the origin and choose the positive y direction to be $\underline{n}$ rather than $-\underline{n}$. Thus, in order to obtain the total flux for a particular gas thickness L the values used for $F^+(y)$ and $F_a^+(y)$ are given by the results for $F^-(L-y)$ and $F_a^-(L-y)$ obtained when A has the opposite sign to that used in computing $F^-(y)$ and $F_a^-(y)$.

The value in computing results based on Eqs. (III. E-25) and (III. E-26) resulting from making a Taylor expansion of $B_\nu{}^0(\tau_{\nu 1})$ and $B^0(\tau_{a1})$ about $B_\nu{}^0(\tau_\nu)$ and $B^0(\tau_a)$ is that these equations give the same answer as Eqs. (III. E-4) and (III. E-10) when condition (III. E-22) is well satisfied and use much less computing machine time. Also the agreement for small temperature gradients of the results based on Eqs. (III. E-25) and (III. E-26) with those based on Eqs. (III. E-4) and (III. E-10), respectively, served as a test that we had made no coding errors. However, the program was, of course, hand checked in addition.

We note that the interval size Δy must be taken small enough in numerically integrating Eq. (III. E-4) over y that $\Delta\tau_\nu \simeq \Delta y\, K_\nu(y) \ll 1$. Since K_ν given by Eq. (III. E-35) becomes large for small ν, this means that for small ν we would have to use very small Δy in order to satisfy this condition. Thus, in our production runs we always used Eq. (III. E-25) rather than Eq. (III. E-4) to obtain F_ν^- for small frequencies $\nu < \nu_1$, where ν_1 was chosen such that condition (III. E-22) was well satisfied.

In integrating over frequency we changed to the dimensionless frequency $Z = h\nu/kT_0$. For small temperature gradients ($A = \pm 10^{-4}$ cases) an interval size $\Delta Z = 0.5$ was found to be sufficiently accurate and for large temperature gradients ($A = \pm 0.3$ cases) an interval size of $\Delta Z = 0.25$ was used. Usually we integrated up to $Z = 20$, but for $A = -0.3$ we integrated to $Z = 25$ which corresponds to $h\nu_{max}/kT_{max} \simeq 15$.

Values for $E_n(\tau_a)$ and $E_n(\tau_\nu)$ were obtained by interpolation on tables of $E_n(\tau)$ which had been placed on tape. $E_1(\tau)$ values were taken from Reference III. E-3 and the other $E_n(\tau)$ were generated from $E_1(\tau)$ by use of the relation III. E-4.

$$n\, E_{n+1}(\tau) = e^{-\tau} - \tau\, E_n(\tau). \qquad \text{(III. E-38)}$$

For small $\tau < 0.1$ we used in Eqs. (III. E-25) and (III. E-26) the approximate equations

$$[1-2\, E_3(\tau)] = 2\tau - \tau^2\left(-\gamma + \frac{3}{2} - \ln\tau\right) - \frac{\tau^3}{3} + \cdots \qquad \text{(III. E-39)}$$

and

$$[1-3\,\tau\, E_3(\tau) - 3\, E_4(\tau)] = \frac{3}{2}\tau^2 - \tau^3\left(-\gamma + \frac{4}{3} - \ln\tau\right) - \frac{9\tau^4}{24} + \cdots \qquad \text{(III. E-40)}$$

which are obtained by use of Eqs. (III. E-15) and (III. E-38).

Our numerical results are given in Tables III. E-1 to III. E-8. We studied cases in which the parameter b occurring in Eqs. (III. E-32) and (III. E-34) had the values 0.5 and 0.25 and cases in which the quantity A entering Eq. (III. E-36) had the values $A = \pm 0.3$ and $A = \pm 10^{-4}$. As discussed in this paragraph below the one containing Eq. (III. E-37), one can combine results for a given b and positive A with those for the same b and same magnitude of A but opposite sign of A to get results for the net flux or divergence of the flux. The tables should be self-explanatory except for the

TABLE III. E-1. MEAN OPTICAL DEPTHS AND MEAN ABSORPTION COEFFICIENTS[a] ($A = 10^{-4}$)

y	$\left(\frac{T}{T_o}\right)^4 = (1-Ay)^4$	τ_a, b=0.5	τ_a, b=0.25	τ_P	τ_R	K_a, b=0.5	K_a, b=0.25	K_P	K_R
.2	.9999	2.91 (-2)	2.75 (-2)	3.08 (-2)	1.02 (-3)	1.37 (-1)	1.23 (-1)	1.54 (-1)	5.09 (-3)
.5	.9998	6.71 (-2)	5.95 (-2)	7.70 (-2)	2.54 (-3)	1.17 (-1)	9.21 (-2)	1.54 (-1)	5.09 (-3)
1.0	.9996	1.19 (-1)	9.72 (-2)	1.54 (-1)	5.09 (-3)	9.21 (-2)	6.21 (-2)	1.54 (-1)	5.09 (-3)
4.0	.9984	2.87 (-1)	1.92 (-1)	6.16 (-1)	2.04 (-2)	3.50 (-2)	1.75 (-2)	1.54 (-1)	5.10 (-3)
10.0	.9960	4.16 (-1)	2.59 (-1)	1.54 (0)	5.10 (-2)	1.41 (-2)	8.01 (-3)	1.55 (-1)	5.11 (-3)
40.0	.9841	6.52 (-1)	4.37 (-1)	6.20 (0)	2.05 (-1)	6.00 (-3)	5.39 (-3)	1.56 (-1)	5.16 (-3)
120.0	.9529	1.09 (0)	8.62 (-1)	1.89 (1)	6.24 (-1)	5.41 (-3)	5.33 (-3)	1.61 (-1)	5.31 (-3)
280.0	.8926	1.98 (0)	1.74 (0)	4.53 (1)	1.50 (0)	5.64 (-3)	5.63 (-3)	1.70 (-1)	5.62 (-3)
440.0	.8353	2.90 (0)	2.66 (0)	7.33 (1)	2.42 (0)	5.96 (-3)	5.96 (-3)	1.80 (-1)	5.96 (-3)
600.0	.7807	3.89 (0)	3.65 (0)	1.03 (2)	3.41 (0)	6.32 (-3)	6.32 (-3)	1.91 (-1)	6.32 (-3)
760.0	.7289	4.93 (0)	4.69 (0)	1.35 (2)	4.45 (0)	6.71 (-3)	6.71 (-3)	2.03 (-1)	6.71 (-3)

[a] The numbers in the parenthesis are the powers of ten by which the adjacent entries should be multiplied.

TABLE III.E-2. COMPARISON BETWEEN EXACT AND APPROXIMATE VALUES FOR THE FLUX AND RELATED QUANTITIES ($A = 10^{-4}$)

y	$\frac{F^-}{\sigma T^4}$	$\frac{F_a^-}{F^-}$, b=0.5	$\frac{F_a^-}{F^-}$ b=0.25	$2\langle E_3(\tau_\nu)\rangle$	$\frac{E_3(\tau_a)}{\langle E_3(\tau_\nu)\rangle}$ b=0.5	$\frac{E_3(\tau_a)}{\langle E_3(\tau_\nu)\rangle}$ b=0.25	Q	$\frac{Q_a}{Q}$, b=0.5	$\frac{Q_a}{Q}$, b=0.25	$\frac{dF_o^{-*}}{dy}$	$\frac{dF_{oa}^{-*}/dy}{dF_o^{-*}/dy}$ b=0.5	$\frac{dF_{oa}^{-*}/dy}{dF_o^{-*}/dy}$ b=0.25
.2	3.64 (-2)	1.49	1.42	9.64 (-1)	.98	.98	6.60 (-7)	3.39	3.35	1.45 (-1)	1.68	1.52
.5	7.17 (-2)	1.64	1.47	9.29 (-1)	.95	.96	3.35 (-6)	3.86	3.93	1.01 (-1)	1.68	1.49
1.0	1.15 (-1)	1.69	1.42	8.85 (-1)	.91	.94	1.11 (-5)	4.25	4.37	7.55 (-2)	1.67	1.19
4.0	2.66 (-1)	1.46	1.08	7.34 (-1)	.83	.97	1.09 (-4)	5.14	5.28	4.02 (-2)	1.10	.71
10.0	4.17 (-1)	1.20	.87	5.83 (-1)	.86	1.10	4.35 (-4)	5.72	4.78	~1.8(-2)	~.56	~.45
40.0	6.85 (-1)	.96	.76	3.18 (-1)	1.12	1.53	2.73 (-3)	4.03	2.57	4.91 (-3)	.69	.86
120.0	8.69 (-1)	.95	.87	1.40 (-1)	1.38	1.89	8.96 (-3)	2.53	1.97	1.23 (-3)	1.29	1.71
280.0	9.65 (-1)	1.01	.98	5.35 (-2)	1.16	1.57	1.81 (-2)	1.99	1.83	2.91 (-4)	1.39	2.11
440.0	9.97 (-1)	1.02	1.02	2.68 (-2)	.75	1.00	2.39 (-2)	1.73	1.68	1.13 (-4)	1.13	1.58
600.0	1.01 (0)	1.02	1.02	1.51 (-2)	.42	.55	2.76 (-2)	1.55	1.53	5.02 (-5)	.50	1.23
760.0	1.02 (0)	1.02	1.02	9.00 (-3)	.21	.28	2.99 (-2)	1.41	1.41	2.18 (-5)	-.31	-.26

TABLE III. E-3. MEAN OPTICAL DEPTHS AND MEAN ABSORPTION COEFFICIENTS ($A = -10^{-4}$, $b = 0.25$)

y	$\left(\frac{T}{T_o}\right)^4 = (1-Ay)^4$	τ_a	τ_P	τ_R	K_a	K_P	K_R
.2	1.0001	2.75 (-2)	3.08 (-2)	1.02 (-3)	1.23 (-1)	1.54 (-1)	5.09 (-3)
.5	1.0002	5.95 (-2)	7.70 (-2)	2.54 (-3)	9.21 (-2)	1.54 (-1)	5.09 (-3)
1.0	1.0004	9.72 (-2)	1.54 (-1)	5.09 (-3)	6.21 (-2)	1.54 (-1)	5.09 (-3)
4.0	1.0016	1.92 (-1)	6.16 (-1)	2.03 (-2)	1.75 (-2)	1.54 (-1)	5.08 (-3)
10.0	1.0040	2.59 (-1)	1.54 (0)	5.08 (-2)	7.97 (-3)	1.53 (-1)	5.07 (-3)
40.0	1.0161	4.34 (-1)	6.12 (0)	2.02 (-1)	5.24 (-3)	1.52 (-1)	5.02 (-3)
120.0	1.0489	8.36 (-1)	1.81 (1)	5.98 (-1)	4.91 (-3)	1.48 (-1)	4.88 (-3)
280.0	1.1168	1.60 (0)	4.11 (1)	1.36 (0)	4.62 (-3)	1.40 (-1)	4.62 (-3)
440.0	1.1880	2.32 (0)	6.29 (1)	2.08 (0)	4.38 (-3)	1.32 (-1)	4.38 (-3)
600.0	1.2625	3.00 (0)	8.35 (1)	2.76 (0)	4.15 (-3)	1.26 (-1)	4.15 (-3)
760.0	1.3404	3.65 (0)	1.03 (2)	3.41 (0)	3.94 (-3)	1.19 (-1)	3.94 (-3)

TABLE III. E-4. COMPARISON BETWEEN EXACT AND APPROXIMATE VALUES FOR THE FLUX AND RELATED QUANTITIES ($A = -10^{-4}$, $b = 0.25$)

y	$\frac{F^-}{\sigma T^4}$	$\frac{F_a^-}{F^-}$	$2\langle E_3(\tau_\nu)\rangle$	$\frac{E_3(\tau_a)}{\langle E_3(\tau_\nu)\rangle}$	Q	$\frac{Q_a}{Q}$	$\frac{dF_o^{-*}}{dy}$	$\frac{dF_{oa}^{-*}/dy}{dF_o^{-*}/dy}$
.2	3.64 (-2)	1.42	9.64 (-1)	.98	-6.59 (-7)	3.35	1.44 (-1)	1.53
.5	7.17 (-2)	1.47	9.29 (-1)	.96	-3.34 (-6)	3.93	1.01 (-1)	1.47
1.0	1.15 (-1)	1.42	8.86 (-1)	.94	-1.11 (-5)	4.37	7.51 (-2)	1.21
4.0	2.66 (-1)	1.08	7.34 (-1)	.97	-1.09 (-4)	5.28	3.95 (-2)	.70
10.0	4.15 (-1)	.86	5.84 (-1)	1.10	-4.33 (-4)	4.80	~1.7 (-2)	~.45
40.0	6.75 (-1)	.75	3.23 (-1)	1.51	-2.71 (-3)	2.62	4.04 (-3)	.89
120.0	8.42 (-1)	.84	1.50 (-1)	1.83	-8.84 (-3)	2.05	1.03 (-3)	1.68
280.0	9.16 (-1)	.94	6.66 (-2)	1.50	-1.82 (-2)	1.96	1.96 (-4)	2.60
440.0	9.35 (-1)	.98	4.02 (-2)	1.01	-2.51 (-2)	1.88	5.26 (-5)	2.94
600.0	9.42 (-1)	.99	2.78 (-2)	.64	-3.05 (-2)	1.78	3.92 (-6)	7.96
760.0	9.44 (-1)	.99	2.09 (-2)	.40	-3.51 (-2)	1.69	-1.88 (-5)	.97

TABLE III.E-5. MEAN OPTICAL DEPTHS AND MEAN ABSORPTION COEFFICIENTS (A = -0.3)

y	$\left(\frac{T}{T_o}\right)^4 = (1-Ay)^4$	τ_a, b=0.5	τ_a, b=0.25	τ_P	τ_R	K_a, b=0.5	K_a, b=0.25	K_P	K_R
.2	1.2625	2.64 (-2)	2.51 (-2)	2.78 (-2)	9.20 (-4)	1.13 (-1)	1.02 (-1)	1.26 (-1)	4.15 (-3)
.4	1.5735	4.62 (-2)	4.24 (-2)	5.07 (-2)	1.67 (-3)	8.60 (-2)	7.27 (-2)	1.04 (-1)	3.42 (-3)
.6	1.9388	6.14 (-2)	5.49 (-2)	6.96 (-2)	2.30 (-3)	6.71 (-2)	5.39 (-2)	8.63 (-2)	2.85 (-3)
.8	2.3642	7.34 (-2)	6.44 (-2)	8.54 (-2)	2.82 (-3)	5.36 (-2)	4.14 (-2)	7.25 (-2)	2.40 (-3)
1.0	2.8561	8.30 (-2)	7.17 (-2)	9.88 (-2)	3.26 (-3)	4.34 (-2)	3.26 (-2)	6.15 (-2)	2.03 (-3)
1.2	3.4210	9.09 (-2)	7.76 (-2)	1.10 (-1)	3.64 (-3)	3.58 (-2)	2.62 (-2)	5.25 (-2)	1.73 (-3)
1.4	4.0659	9.75 (-2)	8.23 (-2)	1.20 (-1)	3.96 (-3)	2.99 (-2)	2.14 (-2)	4.51 (-2)	1.49 (-3)
1.6	4.7978	1.03 (-1)	8.62 (-2)	1.28 (-1)	4.23 (-3)	2.52 (-2)	1.78 (-2)	3.90 (-2)	1.29 (-3)
1.8	5.6245	1.08 (-1)	8.95 (-2)	1.36 (-1)	4.48 (-3)	2.15 (-2)	1.49 (-2)	3.40 (-2)	1.12 (-3)
2.0	6.5536	1.12 (-1)	9.22 (-2)	1.42 (-1)	4.69 (-3)	1.84 (-2)	1.27 (-2)	2.97 (-2)	9.82 (-4)

TABLE III. E-6. COMPARISON OF EXACT AND APPROXIMATE RESULTS FOR THE FLUX AND ITS DIVERGENCE (A = -0.3)

y	$\frac{F^-}{\sigma T^4}$	$\frac{F_a^-}{F^-}$, b=0.5	$\frac{F_a^-}{F^-}$, b=0.25	$\frac{dF_o^-}{dy}$	$\frac{dF_{oa}^-/dy}{dF_o^-/dy}$, b=0.5	$\frac{dF_{oa}^-/dy}{dF_o^-/dy}$, b=0.25
.2	2.89 (-2)	1.53	1.46	1.54 (-1)	1.68	1.53
.4	4.15 (-2)	1.61	1.48	1.39 (-1)	1.69	1.45
.6	4.76 (-2)	1.63	1.45	1.35 (-1)	1.65	1.34
.8	5.05 (-2)	1.63	1.42	1.35 (-1)	1.59	1.25
1.0	5.13 (-2)	1.61	1.38	1.37 (-1)	1.54	1.17
1.2	5.10 (-2)	1.60	1.34	1.41 (-1)	1.48	1.11
1.4	4.99 (-2)	1.58	1.30	1.45 (-1)	1.44	1.04
1.6	4.85 (-2)	1.56	1.27	1.50 (-1)	1.39	1.00
1.8	4.68 (-2)	1.53	1.24	1.55 (-1)	1.35	0.96
2.0	4.50 (-2)	1.51	1.20	1.61 (-1)	1.31	0.93

quantities Q, Q_a, F_0^-, F_0^{-*}, $F^-{}_{0a}$ and F_{0a}^{-*}. Q is the integral over frequency of the part of Eq. (III. E-25) proportional to $d B_\nu{}^0(\tau_\nu)/d\tau_\nu$ after it has been divided by $\sigma T(y)^4 = \pi B\,[T(y)]$. Q_a is the analogous quantity entering Eq. (III. E-26), i.e., it is the term proportional to $d B^0(\tau_a)/d\tau_a$ after division by $\pi B^0(\tau_a) = \sigma T(y)^4$. We notice that the ratio Q_a/Q is large for a wide range of y or τ; however, this occurs only for intermediate and small values of τ_a for which Q gives an insigificant contribution relative to $2 < E_3(\tau_\nu) >$, Eq. (III. E-37), and is unimportant in determining F^- or $\underline{F}$. The quantities F_0^- and F_{0a}^- are equal to $F^-/\sigma T_0{}^4$ and $F_a^-/\sigma T_0{}^4$, respectively, while F_0^{-*} is equal to $F_0^- - (T/T_0)^4$ and F_{0a}^{-*} is equal to $F_{0a}^- - (T/T_0)^4$.

We use $d F_0^{-*}/dy$ rather than $d F_0^-/dy$ in the small gradient case because it will usually be a better measure of the space derivative of the net normalized flux $d F_0/dy$ for the whole range of optical thicknesses. For small optical depth and small A, $d F_0^{-*}/dy$ is very nearly equal to $d F_0^-/dy$, but the interior of a medium with $\tau_a \gtrsim 1$ or 2 the part $(T/T_0)^4$ subtracted out of F_0^- to obtain F_0^{-*} is mostly cancelled out when the net normalized flux F_0 is obtained by subtracting F_0^- from F_0^+. Also for similar reasons it would perhaps be better for the small A cases to give F_{0a}^{-*}/F_{0a}^{-*} rather than F_a^-/F^- for $\tau_a \gtrsim 1$ or 2. However, $F/\sigma T^4$ is composed completely (when boundary contributions are neglected) of the $2 < E_3(\tau_\nu) >$ and Q terms we have tabulated, as seen from Eq. (III. E-30).

TABLE III.E-7. MEAN OPTICAL DEPTHS AND MEAN ABSORPTION COEFFICIENT (A = 0.3, b = 0.25)

y	$\left(\frac{T}{T_o}\right)^4 = (1-Ay)^4$	τ_a	τ_P	τ_R	K_a	K_P	K_R
.2	.7807	3.03 (-2)	3.43 (-2)	1.14 (-3)	1.49 (-1)	1.91 (-1)	6.32 (-3)
.4	.5997	5.97 (-2)	7.73 (-2)	2.55 (-3)	1.44 (-1)	2.41 (-1)	7.96 (-3)
.6	.4521	8.78 (-2)	1.32 (-1)	4.36 (-3)	1.38 (-1)	3.08 (-1)	1.02 (-2)
.8	.3336	1.15 (-1)	2.02 (-1)	6.69 (-3)	1.32 (-1)	4.02 (-1)	1.33 (-2)
1.0	.2401	1.41 (-1)	2.96 (-1)	9.76 (-3)	1.27 (-1)	5.37 (-1)	1.77 (-2)
1.2	.1678	1.66 (-1)	4.21 (-1)	1.39 (-2)	1.23 (-1)	7.34 (-1)	2.43 (-2)
1.4	.1132	1.90 (-1)	5.96 (-1)	1.97 (-2)	1.22 (-1)	1.04 (0)	3.42 (-2)
1.6	.0731	2.15 (-1)	8.48 (-1)	2.80 (-2)	1.26 (-1)	1.52 (0)	5.02 (-2)
1.8	.0448	2.41 (-1)	1.23 (0)	4.05 (-2)	1.42 (-1)	2.33 (0)	7.78 (-2)
2.0	.0256	2.73 (-1)	1.82 (0)	6.03 (-2)	1.79 (-1)	3.80 (0)	1.26 (-1)

TABLE III. E-8. COMPARISON OF EXACT AND APPROXIMATE RESULTS FOR THE FLUX AND ITS DIVERGENCE (A = 0.3, b = 0.25)

y	$\frac{F^-}{\sigma T^4}$	$\frac{F_a^-}{F^-}$	$\frac{dF_o^-}{dy}$	$\frac{dF_{oa}^-/dy}{dF_o^-/dy}$
.2	4.31 (-2)	1.49	1.25 (-1)	1.62
.4	9.01 (-2)	1.53	8.41 (-2)	1.55
.6	1.50 (-1)	1.53	5.57 (-2)	1.42
.8	2.30 (-1)	1.51	3.33 (-2)	1.29
1.0	3.39 (-1)	1.49	1.49 (-2)	1.19
1.2	4.93 (-1)	1.48	-3.57 (-4)	-2.65
1.4	7.19 (-1)	1.50	-1.30 (-2)	.79
1.6	1.06 (0)	1.53	-2.30 (-2)	.79
1.8	1.61 (0)	1.59	-3.06 (-2)	.83
2.0	2.56 (0)	1.66	-3.55 (-2)	.93

Results were obtained for somewhat more values of y then presented in the tables. However, since the principal interest is in the accuracy of the method, we give only sufficient values to indicate the approximate maximum deviation of quantities computed by our approximate method from the correct values for the range of y considered. The numerical results should be accurate to within $\sim 1\%$ except for the case of the entries involving derivatives of the fluxes, the last 3 or 4 entries in Tables III. E-2, -4, -6 and -8. These might be off by as much as 10% in some cases.

Although it would be desirable to test the method for additional forms of the frequency dependence of K_ν, it would appear on the basis of the fairly severe case tested here ($K_P/K_R \simeq 30$) that apart from a few exceptional situations we can obtain the net flux and divergence of the flux to within about a factor of two of the correct values for the entire range of optical thicknesses. The exceptions occur in the near vicinity of a point where either of these quantities changes sign, and for a range of fairly large optical depths when the type error discussed near the end of Section III. E-2 occurs if the temperature gradient is very small. (In terms of the quantities presented in the tables, this is the error arising when $E_3(\tau_a)/\langle E_3(\tau_\nu)\rangle$ becomes very small before $\langle E_3(\tau_\nu)\rangle$ is negligible relative to Q.) Of course, for very large optical depth our method again gives the correct result.

IV. RADIATIVE ENERGY TRANSFER

IV.A INTRODUCTION

This part of the investigation consists of four sections dealing with the derivation of the governing equations of radiative energy transfer and numerical techniques for their solution for various limiting cases.

IV.B MOMENT AND DISCRETE ORDINATE METHODS IN RADIATIVE TRANSFER PROBLEMS

by

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IV.B MOMENT AND DISCRETE ORDINATE METHODS IN RADIATIVE TRANSFER PROBLEMS

IV. B.1 INTRODUCTION

The reduction of the equation of radiative transfer to a finite set of differential equations for moments of the intensity is a well known procedure for obtaining approximate solutions to radiative transfer problems. The general procedure, usually referred to as the moments method, is outlined by Krook, [IV. B-1] who also shows the equivalence between the moments method, the spherical harmonics method and the discrete ordinates method. Although Krook considers only scattering media in radiative equilibrium, the essential features of his analysis relating to differential approximations apply also to the problem considered here, namely, that of a non-scattering medium.

Recently, a modified approach to the moments method was described by Sherman[IV. B-2] for the lower order approximations. Basically, this consisted of making a canonical transformation of the standard moment equations, which resulted in a set of uncoupled equations whose dependent variables represented linear combinations of the moments.

The purpose of this section is to examine the modified moments method in detail for the general N-th order approximation. This generality affords considerably more insight into the method than can be obtained from treating a specific order of approximation. In particular, it will be shown that the modified moments method is essentially identical to the discrete ordinates method, but considerably more cumbersome to apply. Nevertheless, the method is useful in a pedagogical sense in that it forms a connecting link between the moments method and the discrete ordinates method.

For purposes of illustration, the problem considered is that of a gray, semi-infinite plane-parallel radiating medium without scattering or polarization effects and with no radiation incident on the free surface. However, the methods discussed can be applied equally well to finite one-dimensional problems of a similar nature.

In Section IV. B. 2, a brief outline of the standard moments method is presented, both for completeness and as a convenient reference for the later sections. The canonical transformation is developed in Section IV. B. 3 and its relationship to the discrete ordinates method is described in Section IV. B. 4. The so-called half-range methods are discussed briefly in Section IV. B. 5.

IV. B.2 THE STANDARD MOMENT METHOD

The equation of transfer in a planar, radiating, non-scattering medium with no polarization is

$$\mu \frac{dI}{dx} = S - I \qquad \text{(IV.B-1)}$$

where $I(x, \mu)$ is the integrated intensity, $S(x)$ the integrated source function, x is the distance from the surface in photon mean free paths and μ is the direction cosine of the field direction with respect to the x-axis. Assuming no incident radiation on the free surface, the boundary condition there is

$$I(0, \mu) = 0, \quad \mu > 0. \qquad \text{(IV.B-2)}$$

The n-th moment of the intensity is defined as

$$M_n(x) = \frac{1}{2} \int_{-1}^{1} \mu^n I(x, \mu)\, d\mu. \qquad \text{(IV.B-3)}$$

Physically, the zeroth moment is equal to the mean (over angle) intensity and the first moment is equal to $1/4\pi$ times the radiative flux. Physically, these are the most important properties of the radiation field. One of the advantages of the moments method is that they appear explicitly in the equations. Knowledge of the intensity itself is usually of very little importance.

The standard moment equations are obtained by operating on Eq. (IV.B-1) with

$$\frac{1}{2} \int_{-1}^{1} \mu^n [\ ]\, d\mu.$$

This gives

$$\frac{dM_{n+1}}{dx} = \alpha_n S - M_n, \quad n = 0, 1, 2\ldots \qquad \text{(IV.B-4)}$$

where

$$\alpha_n \equiv \frac{1 + (-1)^n}{2(n+1)}. \qquad \text{(IV.B-5)}$$

In the N-th order approximation, the first N equations, involving the N + 1 moments $M_0, M_1, \ldots, M_N$, are retained. In order to make the set determinate, an additional equation is needed that expresses one of the moments in terms of the others. Such an expression is obtained as follows. Let the N-th Legendre polynomial be written as

$$P_N(\mu) = \sum_{j=0}^{N} C_j \mu^{N-j} \qquad \text{(IV.B-6)}$$

and let μ_i, $i = 1, 2, \ldots N$ be the zeros of $P_N(\mu)$. Express the moments in terms of a Gauss quadrature, viz.,

$$M_n(x) \equiv \frac{1}{2}\int_{-1}^{1} \mu^n I(x, \mu)\, d\mu \simeq \frac{1}{2}\sum_{j=1}^{N} \mu_j^n A_j I(x, \mu_j) \qquad \text{(IV.B-7)}$$

where the A_j's ($j = 1, 2, \ldots N$) are the uniquely determined Gaussian weight constants. It can be shown[IV.B-1] that for the N-th order approximation represented by Eq. (IV.B-7) the moments satisfy the relation

$$\sum_{j=0}^{N} C_j M_{N-j} = 0. \qquad \text{(IV.B-8)}$$

Equation (IV.B-8) is the desired expression. It is usually used to eliminate M_N from the moment equations.

In order to complete the formulation of the moments method, it is necessary to express the boundary condition given by Eq. (IV.B-2) in terms of the moments. We shall use the procedure described by Krook[IV.B-1]. This involves restricting the approximations to those of even order (i.e., N even) and setting the intensity equal to zero at $x = 0$ for each of the positive μ_i's, the latter having been defined above. This form of the boundary condition is actually taken from the discrete ordinates method[IV.B-3] and is equivalent to the Mark boundary condition of neutron transport theory.[IV.B-4]

Recall that the zeros of $P_N(\mu)$ when N is even are all distinct and occur in pairs of equal magnitude but opposite sign. For convenience let the even numbered μ_i's be positive and let $\mu_{i-1} = -\mu_i, -1 = 2, 4, \ldots N$. Then, evaluation of Eq. (IV.B-7) at $x = 0$ gives

$$M_n(0) = \frac{1}{2}\sum_{\substack{j=1 \\ \text{odd}}}^{N-1} \mu_j^n A_j I(0, \mu_j), \qquad n = 0, 1, 2, \ldots, N-1. \qquad \text{(IV.B-9)}$$

Recall that M_N is eliminated by means of Eq. (IV.B-8). Equation (IV.B-9) represents N equations in the N/2 unknowns $A_j I(0, \mu_j)/2$, $j = 1, 3, \ldots N-1$. Thus, the moments $M_{N/2}, M_{N/2+1}, \ldots, M_{N-1}$, can be expressed in terms of the moments $M_0, M_1, \ldots, M_{N/2-1}$. This provides N/2 boundary conditions at $x = 0$. In determinantal form, they can be written

$$\begin{vmatrix} M_0(0) & 1 & 1 & \cdots & 1 \\ M_1(0) & \mu_1 & \mu_3 & \cdots & \mu_{N-1} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ M_{N/2-1}(0) & \mu_1^{N/2-1} & \mu_3^{N/2-1} & \cdots & \mu_{N-1}^{N/2-1} \\ M_\ell(0) & \mu_1^\ell & \mu_3^\ell & \cdots & \mu_{N-1}^\ell \end{vmatrix} = 0, \quad \ell = \frac{N}{2}, \frac{N}{2}+1, \ldots N-1. \quad \text{(IV.B-10)}$$

The remaining N/2 boundary conditions required must be specified in terms of conditions at the other end of the layer. Since these are not important to the subsequent discussion, they will not be discussed here.

Although the moments method has the advantage of yielding the information required for most problems directly, it suffers from the fact that the moment equations, Eq. (IV.B-4), are coupled and from the complexity of the boundary conditions at the free surface. These difficulties, which also occur in the spherical harmonics method, become increasingly more serious as the order of approximation increases. The method presented in the following section represents an attempt to eliminate these difficulties.

IV. B.3 THE CANONICAL TRANSFORMATION

The essential feature of the method presented here is the canonicalization of the moment equations by means of linear algebra. To accomplish this, M_0 is first eliminated from Eq. (IV.B-4) by means of Eq. (IV.B-8). The resulting equations can be written in matrix form, viz.,

$$\frac{d}{dx}\tilde{M} = \tilde{\alpha}S - \tilde{A}\tilde{M} \qquad \text{(IV.B-11)}$$

where, for the N-th order approximation,

$$\tilde{M}=\begin{bmatrix} M_1 \\ M_2 \\ M_3 \\ \cdot \\ \cdot \\ \cdot \\ M_N \end{bmatrix}, \quad \tilde{\alpha}=\begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_{N-1} \end{bmatrix}, \quad \tilde{A}=\begin{bmatrix} 0 & -\frac{C_{N-2}}{C_N} & 0 & -\frac{C_{N-4}}{C_N} & 0 & \cdots & 0 & -\frac{C_0}{C_N} \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & & 1 & 0 \end{bmatrix}. \qquad \text{(IV.B-12)}$$

The α_n's are given by Eq. (IV.B-5) and the C_N's are the coefficients in Eq. (IV.B-6). The general procedure is as follows. First, find the eigenvalues λ_i, $i = 1, 2, \ldots, N$ and the corresponding eigenfunctions, u_i, of the matrix $\tilde{A}$. Then form the "modal matrix", $\tilde{Q}$, with elements defined as $Q_{i,j} = u_i(\lambda_j)$. With $\tilde{Q}$ defined in this manner, we have

$$(\tilde{Q}^{-1}\tilde{A}\tilde{Q}) = \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & \cdots & \lambda_N \end{bmatrix}. \qquad \text{(IV.B-13)}$$

Multiplying Eq. (IV.B-11) by $\tilde{Q}^{-1}$ gives

$$\frac{d}{dx}(\tilde{Q}^{-1}\tilde{M}) = \tilde{Q}^{-1}\tilde{\alpha}S - \tilde{Q}^{-1}\tilde{A}\tilde{M}. \qquad \text{(IV.B-14)}$$

Now define a vector $\tilde{Z}$ by

$$\tilde{Z} = \tilde{Q}^{-1}\tilde{M} \qquad \text{(IV.B-15)}$$

with the elements of $\tilde{Z}$ denoted by Z_n, n = 1, 2, . . . , N. Then,

$$\tilde{M} = \tilde{Q}\tilde{Z}. \qquad \text{(IV.B-16)}$$

Substitution of the last two equations in Eq. (IV.B-14) and the use of Eq. (IV.B-13) yields N uncoupled scalar equations, viz.,

$$\frac{dZ_i}{dx} = \gamma_i S - \lambda_i Z_i, \quad i = 1, 2, \ldots, N \qquad \text{(IV.B-17)}$$

where the γ_i are elements of the vector $\tilde{\Gamma}$, defined by

$$\tilde{\Gamma} \equiv \tilde{Q}^{-1}\tilde{\alpha}. \qquad \text{(IV.B-18)}$$

Equation (IV.B-17) represents the modified moment equations for the canonical variables, Z_i, i = 1, 2, . . . , N.

It is shown in Appendix A that the eigenvalues of $\tilde{A}$ are the roots of $\lambda^N P_N(1/\lambda)$, i.e.,

$$\lambda_i^N P_N\left(\frac{1}{\lambda_i}\right) = 0, \qquad i = 1, 2, \ldots, N. \qquad \text{(IV.B-19)}$$

If quantities μ_i are defined as $\mu_i = 1/\lambda_i$, then we also have

$$P_N(\mu_i) = 0, \qquad i = 1, 2, \ldots, N. \qquad \text{(IV.B-20)}$$

It is also shown in Appendix D that if the eigenfunctions are normalized by letting $u_N = 1$, they are given by

$$u_i(\lambda) = \lambda^{N-i}, \qquad i = 1, 2, \ldots, N. \qquad \text{(IV.B-21)}$$

Thus, the elements of $\tilde{Q}$ are

$$Q_{i,j} = \lambda_j^{N-i}. \qquad \text{(IV.B-22)}$$

Sherman [IV.B-2] applied this method for N = 2 and N = 4 (referred to as the first and second full-moment approximations, respectively) by computing the elements of $\tilde{Q}^{-1}$ specifically for each approximation. He then used Eqs. (IV.B-16) and (IV.B-10) to obtain the appropriate boundary conditions on the Z_n's at the free surface. While

this can also be done for the general N-th order approximation, a less direct but simpler and more revealing procedure is available.

If the elements of $\tilde{Q}^{-1}$ are denoted by $\tilde{Q}_{i,j}$ and the identity matrix by $\tilde{I}$, the system of equations represented by the matrix equation $\tilde{Q}^{-1}\,\tilde{Q}=\tilde{I}$ can be written

$$\sum_{i=1}^{N} \mu_j^i \tilde{Q}_{\ell,i} = \mu_j^N \delta_{\ell j}, \quad j,\ell = 1,2,\ldots,N \qquad \text{(IV.B-23)}$$

where $\delta_{\ell j}$ is the Kronecker delta function. This relation will be useful later.

Approximating the moments by a Gauss quadrature as in Eq. (IV.B-7), we have

$$M_i(x) \simeq \frac{1}{2} \sum_{j=1}^{N} \mu_j^i A_j I(x, \mu_j). \qquad \text{(IV.B-24)}$$

Note that, because of Eq. (IV.B-20), the reciprocals of the eigenvalues of $\tilde{A}$ are identical to the points of division in the Gauss quadrature. From Eq. (IV.B-15), it is evident that

$$Z_n(x) = \sum_{i=1}^{N} \tilde{Q}_{n,i} M_i, \quad n=1,2,\ldots,N. \qquad \text{(IV.B-25)}$$

Substituting Eq. (IV.B-24) in Eq. (IV.B-25) and interchanging the order of summation gives

$$Z_n(x) = \frac{1}{2} \sum_{j=1}^{N} \left(\sum_{i=1}^{N} \tilde{Q}_{n,i} \mu_j^i \right) A_j I(x, \mu_j). \qquad \text{(IV.B-26)}$$

But by Eq. (IV.B-23), the interior sum is equal to $\mu_j^N \delta_{nj}$. Therefore, Eq. (IV.B-26) reduces to

$$Z_n(x) = \frac{1}{2} \mu_n^N A_n I(x, \mu_n), \quad n=1,2,\ldots,N. \qquad \text{(IV.B-27)}$$

Equation (IV.B-27) reveals immediately that the Z_n's are each proportional to the intensity in specific directions, namely, those corresponding to the points of division of the Gauss quadrature. This implies that the canonical transformation procedure is essentially identical to the discrete ordinates method. The relationship between the two methods will be examined more closely in the next section.

Equation (IV.B-27) makes the formulation of boundary conditions on the Z_n at the free surface a trivial matter. Evaluating Eq. (IV.B-27) at $x = 0$ and recalling that $I(0, \mu_n) = 0$ for $\mu_n > 0$, we have

$$Z_n(0) = 0 \qquad n \text{ even.} \tag{IV.B-28}$$

The odd numbered Z_n's, corresponding to $\mu_n < 0$, are determined from conditions at infinity, or, in the case of a finite medium, by the conditions at the opposite surface.

The moments are obtained in terms of the canonical variables either directly from Eq. (IV.B-16) or by substituting Eq. (IV.B-27) into Eq. (IV.B-24). The result is

$$M_n(x) = \sum_{j=1}^{N} \lambda_j^{N-n} Z_j(x), \qquad n=1, 2, \ldots, N. \tag{IV.B-29}$$

This equation, which is the inverse of Eq. (IV.B-25), is also valid for $n = 0$, as can be shown by substituting it in Eq. (IV.B-8) and solving for M_0.

To complete the general formulation of the method, the elements of $\tilde{Q}^{-1}$ must be obtained. For the sake of completeness, these quantities are derived in Appendix F. However, it will be demonstrated conclusively in the next section that the canonical transformation is not necessary in practice.

IV. B.4 COMPARISON WITH THE DISCRETE ORDINATES METHOD

In problems of the type under consideration, in which the source function is not an explicit function of the intensity, the discrete ordinates method is especially straightforward. The method essentially consists of choosing an appropriate quadrature formula for approximating the moments and then solving the equation of transfer, Eq. (IV. B-1), separately for each point of division of the quadrature interval. The simplicity in this case results from the fact that μ occurs in Eq. (IV. B-1) as a simple parameter.

The Gauss quadrature is often used because of its high degree of accuracy. (IV. B-3) Although other quadrature formulas may also be used, (IV. B-5) the Gauss formula will be used here for consistency with the previous discussion.

Dividing Eq. (IV. B-1) by μ and then setting μ equal to each of the zeros of $P_N(\mu)$ gives

$$\frac{dI(x, \mu_i)}{dx} = \frac{1}{\mu_i} S(x) - \frac{1}{\mu_i} I(x, \mu_i), \quad i=1,2,\ldots,N. \qquad \text{(IV. B-30)}$$

This represents N equations in the N unknowns $I(x, \mu_i)$, $i=1,2,\ldots,N$. The boundary condition at the surface is simply

$$I(0, \mu_i) = 0, \quad i \text{ even} \qquad \text{(IV. B-31)}$$

where the same numbering system is used for the μ_i's as in the previous section. In practice, one simply solves Eq. (IV. B-30) for each value of μ_i, subject to the boundary condition given by Eq. (IV. B-31) and utilizes the results in a quadrature formula such as Eq. (IV. B-7) to evaluate the desired moments. Our purpose here, however, is to show that Eq. (IV. B-30) is essentially identical to the modified moment equation, Eq. (IV. B-17).

Multiplying Eq. (IV. B-30) by $A_i \mu_i^{N}/2$ and utilizing Eq. (IV. B-27), the former becomes

$$\frac{dZ_i}{dx} = \frac{1}{2} A_i \mu_i^{N-1} S - \lambda_i Z_i, \quad i = 1,2,\ldots, N. \qquad \text{(IV. B-32)}$$

The system represented by Eq. (IV. B-32) is seen to be precisely identical to Eq. (IV. B-17) provided only that

$$\gamma_i = \frac{1}{2} A_i \mu_i^{N-1}. \qquad \text{(IV. B-33)}$$

This equation is verified in Appendix E. Thus, for a given characteristic direction μ_i, it is clear that the equations of the discrete ordinate method, Eq. (IV.B-31), and the modified moment method, Eq. (IV.B-17), differ only by a constant factor.

The relationship between Eq. (IV.B-30) and the standard moment equations, Eq. (IV.B-4), is also readily demonstrated. Multiplying Eq. (IV.B-31) by $A_i \mu_i^{n+1}/2$ and summing over i gives

$$\frac{d}{dx}\left[\frac{1}{2}\sum_{i=1}^{N} A_i \mu_i^{n+1} I(x, \mu_i)\right] = \frac{1}{2}\left[\sum_{i=1}^{N} A_i \mu_i^{n}\right] S - \frac{1}{2}\sum_{i=1}^{N} A_i \mu_i^{n} I(x, \mu_i). \quad \text{(IV.B-34)}$$

Using Eq. (IV.B-24), this becomes

$$\frac{dM_{n+1}}{dx} = \frac{1}{2}\left[\sum_{i=1}^{N} A_i \mu_i^{n}\right] S - M_n. \quad \text{(IV.B-35)}$$

This is identical to Eq. (IV.B-4) since, as is shown in Appendix E,

$$\alpha_n = \frac{1}{2}\sum_{i=1}^{N} A_i \mu_i^{n}. \quad \text{(IV.B-36)}$$

Whereas in the discrete ordinates method the equations are solved for $I(x, \mu_i)$, $i = 1, 2, \ldots, N$, in the modified moments method the equations are solved for $A_i \mu_i N_I(x, \mu_i)$, $i = 1, 2, \ldots, N$. The significance of the constant factors relating the two sets of variables is trivial. Hence, in effect, the two methods are precisely identical. For this reason, it would obviously be preferrable in practice to use the discrete ordinates method in order to avoid the algebraic complexities involved in the canonical transformation.

It should be noted that the discrete ordinate equations, Eq. (IV.B-30), are uncoupled and, although finite in number, do not involve a truncation as do the moment equations. Therefore, Eq. (IV.B-30) represents an exact system of differential equations for $I(x, \mu_i)$, $i = 1, 2, \ldots, N$. The approximation enters only in the use of a finite order quadrature for evaluating the moments. Conversely, combining Eq. (IV.B-25) and (IV.B-27) and rearranging yields

$$I(x, \mu_n) = \frac{2}{\mu_n A_n^N} \sum_{i=1}^{N} \tilde{Q}_{n,i} M_i(x), \qquad n = 1, 2, \ldots N. \quad \text{(IV.B-37)}$$

This equation is also exact, even though the M_i are obtained from an approximate system of differential equations, namely, the N-th order moment equations. Actually, Eq. (IV.B-37) is the inverse of the quadrature formula, Eq. (IV.B-24). Thus, the errors involved in the truncation of the moment equations cancel out exactly in the above equation.

The preceding discussion demonstates the complete equivalence between the moments method and the discrete ordinates method. It is clear that the canonical transformation simply transforms the former into the latter. The key to both the equivalence and the transformation as presented here is the Gauss quadrature. As noted earlier, other quadrature formulas could be used in either method but the relationship between the two methods would have to be examined separately for each one. In any case, it is evident that the equivalence breaks down if the same quadrature formula is not used in both methods.

IV. B.5 HALF-RANGE METHODS

The so-called half-range methods are variations on the full-range methods already presented, in which the positive and negative portions of the range of μ are treated separately. For example, positive and negative half-moments are defined as

$$M_n^+(x) = \frac{1}{2}\int_0^1 \mu^n I(x, \mu)\, d\mu \qquad \text{(IV.B-38a)}$$

$$M_n^-(x) = \frac{1}{2}\int_{-1}^0 \mu^n I(x, \mu)\, d\mu . \qquad \text{(IV.B-38b)}$$

The advantage of the half-range methods is that they are well suited to handling the boundary condition given by Eq. (IV.B-2).

Half-range moment methods are discussed by Krook[IV.B-1] and by Sherman[IV.B-2]. Sykes [IV.B-6] introduced the half-range discrete ordinates method, which he referred to as the double-Gauss method. In either case, for the m-th order approximation, the characteristic directions, i.e., the μ_i's, are obtained from

$$P_m(2\mu_i - 1) = 0 \qquad \text{(IV.B-39a)}$$

$$P_m(2\mu_i + 1) = 0. \qquad \text{(IV.B-39b)}$$

Equation (IV.B-39a) gives the positive μ_i's while Eq. (IV.B-39b) gives the negative μ_i's. There are 2m discrete values of μ (m for each half-range) so that for purposes of comparison, the full-range approximation of order N should be compared with the half-range approximation of order m = N/2.

Suffice it to say here that the half-range methods are equivalent in the same sense that the full-range methods are equivalent and that an analogous transformation exists between the two half-range methods. This can be shown by an analysis which parallels precisely that given in the previous sections for the full-range methods.

IV. B-6 CONCLUSIONS

For radiative transfer problems in planar, radiating, non-scattering media, it has been shown that the modified moments method introduced by Sherman [IV.B-2] is essentially identical to the discrete ordinates method. Therefore, the algebraic complexities involved in the modified moments method can be eliminated in practice by utilizing the discrete ordinate method directly.

Nevertheless, the canonical transformation is useful in a pedagogical sense in that it helps to clarify the relationship between the moments method and the discrete ordinates method.

IV.C ON THE DIFFERENTIAL FORM OF THE TIME-DEPENDENT RADIATIVE TRANSPORT EQUATION

by

R.T. Liner and M. P. Sherman

IV.C ON THE DIFFERENTIAL FORM OF THE TIME-DEPENDENT RADIATIVE TRANSPORT EQUATION

IV.C.1 PHYSICAL PROBLEM

It is assumed that the flow field is specified by its composition, temperature and pressure, or composition, temperature and density, at each point and at the necessary times. The problem is to compute the radiative flux, $F(\vec{r}, t)$, or its divergence, $\nabla \cdot F$, the latter being the quantity which actually appears in the energy balance equation. The radiative flux, $F(\vec{r}, t)$, is a vector quantity which is defined as the net radiative energy per unit area crossing a plane passing through the field point $\vec{r}$ and normal to the direction of interest, at time t.

IV.C.2 EXACT MATHEMATICAL REPRESENTATION

The appropriate coordinate system is indicated in Figure IV.C-1. In general, the flux is defined in terms of the intensity, $I_\nu(\vec{r}, \hat{\Omega}, T)$, by

$$F(\vec{r}, t) = \int_0^\infty F_\nu(\vec{r}, t)\, d\nu \qquad \text{(IV.C-1)}$$

and

$$F_\nu(\vec{r}, t) = \int_{4\pi} I_\nu(\vec{r}, \hat{\Omega}, t)\, \hat{\Omega} \cdot n\, d\hat{\Omega} \qquad \text{(IV.C-2)}$$

where $\hat{n}$ is a unit vector in the direction of F.

The intensity, $I_\nu(\vec{r}, \hat{\Omega}, t)$, is a scalar quantity in a seven-dimensional phase space (frequency, three space coordinates, two angular coordinates, and time). It is determined by the equation

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu = -K_\nu(\vec{r})\left[I_\nu(\vec{r}, \hat{\Omega}, t) - S_\nu(\vec{r}, \hat{\Omega}, t)\right] \qquad \text{(IV.C-3)}$$

where I_ν is the spectral intensity, S_ν is the source function, $\vec{s}$ is a unit vector in the s direction, and K_ν is the absorption coefficient. Making the assumption of L.T.E., the source function becomes equal to the Planck function. The boundary conditions and formal solution of (IV.C-3) are given in reference IV.C-1. Also see Reference IV.C-2.

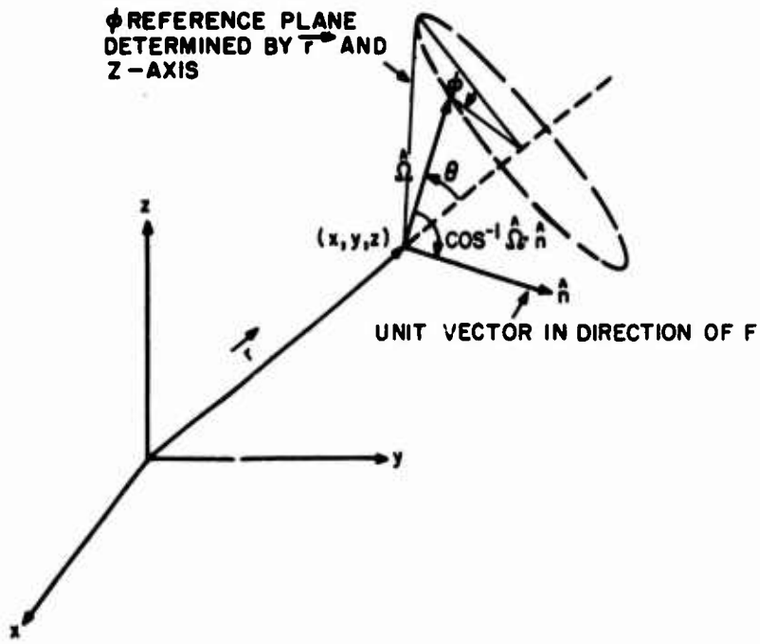


Figure IV. C-1. General Coordinate System

IV.C.3 PHYSICAL MODEL

Since it is not feasible to solve the problem in its most general form, it is necessary to make several simplifying assumptions. Those recommended are as follows:

1. Gray-gas

It is assumed that the absorption coefficient is not a function of ν, i.e., $K_\nu = K$. Equation (IV. C-3) can then be integrated over frequency, so that it is necessary to deal only with frequency-integrated quantities.

Since this assumption is far from being physically correct, it is necessary, if the assumption is to be retained in the ultimate solution, to devise an appropriate means of averaging K_ν over the entire spectrum.

The only practical alternative to the gray-gas approximation is to divide the spectrum into a finite number of intervals and assume that K_ν is constant in each interval. One then solves Eq. (IV. C-3) for each interval and evaluates Eq. (IV. C-1) by means of a quadrature. The gray-gas approximation is essentially the lowest order approximation for this type of procedure. It can, at least in principle, be easily generalized to higher order. With the gray gas assumption we can integrate the equation over frequency,

$$\frac{1}{c}\frac{\partial I}{\partial t} + \vec{s} \cdot \nabla I = K \left[B - I \right] \qquad \text{(IV. C-4)}$$

where

$$B = \frac{\sigma}{\pi} T^4 \qquad \text{(IV. C-5)}$$

$$I = \int_0^\infty I_\nu \, d_\nu \qquad \text{(IV. C-6)}$$

2. LTE, no scattering

The source function becomes

$$S(\vec{r}, \hat{\Omega}, t) = \int_0^\infty S_\nu (\vec{r}, \hat{\Omega}, t) \, d_\nu \qquad \text{(IV. C-7)}$$

3. Spherical symmetry

For spherically-symmetric problems, I_ν is not a function of φ. Only the radial flux is needed so $\Omega \cdot \hat{n} = \cos\theta \equiv \mu$.

For a problem with spherical symmetry the equation becomes

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial r} + \frac{(1-\mu^2)}{r}\frac{\partial I}{\partial \mu} = K\left[B - I\right] \qquad \text{(IV. C-8)}$$

with

$$\mu = \cos \theta \qquad \text{(IV. C-9)}$$

The angle θ is the polar angle from the radius vector. Note that

$$-1 \leq \mu \leq 1 \qquad \text{(IV. C-10)}$$

There are two complications in the solution of this equation, the optically thick limit, and the quasi-stationary limit. (See Sections IV. C. 5 and IV. C. 6) which follow).

IV.C.4 MATHEMATICAL MODEL

With the above three assumptions, i.e. gray gas, LTE and spherical symmetry, eq. (IV. C. 3) becomes

$$\frac{1}{c}\frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I = - K(r) \left[I(r, \mu, t) - B(r) \right] \qquad \text{(IV. C-11)}$$

or

$$\frac{dI}{ds}(s, t - s/c) = K(s, t) \left[B(s, t) - I\left(s, t - \frac{s}{c}\right) \right] \qquad \text{(IV. C-12)}$$

and F (r, t) becomes

$$F(r, t) = 2\pi \int_{-1}^{1} I(r, \mu, t)\, \mu \, d\mu \qquad \text{((V. C-13)}$$

It is convenient to write the term $\hat{\Omega} \cdot \nabla I$ in one of the two forms

$$\hat{\Omega} \cdot \nabla I = \mu \frac{\partial I}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I}{\partial \mu} \qquad \text{(IV. C-14)}$$

$$\hat{\Omega} \cdot \nabla I = \frac{\partial I}{\partial s} \qquad \text{(IV. C-15)}$$

where s is the coordinate along the line coincident with the vector $\hat{\Omega}$. (See Figure IV. C-2).

It is assumed that the radius of the sphere is large enough so that there is no incident radiation from outside the sphere. Thus, the boundary condition is

$$I(R, \mu) = 0, \quad \mu < 0 \qquad \text{(IV. C-16)}$$

The formal solution of (IV. C-11) is

$$I(r, \mu, t) = \int_{0}^{s(r,\mu)} K\left[s', t - \frac{s - s'}{c}\right] B\left[s', t - \frac{s - s'}{c}\right] e^{-\int_{s'}^{s} K(s'', t - \frac{s - s''}{c})\, ds''} ds' \qquad \text{(IV. C-17)}$$

The recommended procedure is to either solve Eq. (IV. C-11) or evaluate Eq. (IV. C-17) numerically, and then evaluate Eq. (IV. C-13) by means of an appropriate quadrature. This procedure should be satisfactory except in optically thick regions.

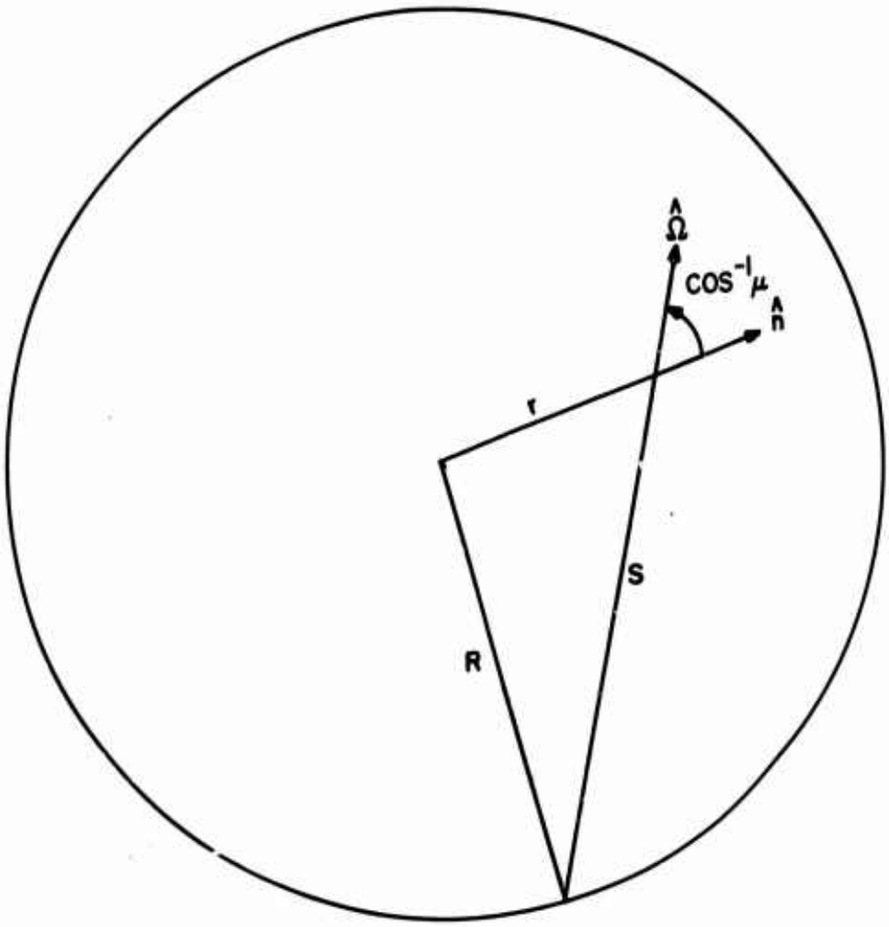


Figure IV.C-2. Coordinate System for the Spherically Symmetric Problem

IV.C.5 THE OPTICALLY THICK LIMIT

The formal definition of the "optically thick limit" is that the photon mean free path be much less than the characteristic lengths of the hydrodynamic change. Also

$$\frac{4}{cK}\ \frac{\partial\, \ell n\, T}{\partial t} << 1 \qquad \text{(IV. C-18)}$$

In this case, the intensity will be nearly isotropic. However, the slight anisotropy gives the flux, F.

$$F = 2\ \pi \int_{-1}^{1} I\ \mu\, d\,\mu \qquad \text{(IV. C-19)}$$

Therefore, a special procedure must be instituted if accurate values of the flux are to be obtained. Expanding B in a Taylor series we obtain

$$I(r,\mu,t) = B(r,t) - \frac{1}{K(r,t)}\left[\frac{1}{c}\frac{\partial}{\partial t} + \frac{\mu\partial}{\partial r}\right] B(r,t)$$

$$+ \frac{1}{K(r,t)}\left[\frac{1}{c}\frac{\partial}{\partial t} + \frac{\mu\partial}{\partial r}\right]\left\{\left[\frac{1}{K}\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{\partial}{\mu\partial r}\right)\right] B(r,t)\right\} + \ldots \qquad \text{(IV. C-20)}$$

Performing the integration of Equation (IV. C-19)

$$F = \frac{4\pi}{3K(r,t)}\left(\frac{\partial\ B(r,t)}{\partial r} + \frac{1}{c}\frac{\partial}{\partial t}\ \frac{1}{K(r,t)}\ \frac{\partial B}{\partial r}\right) + \ldots . \qquad \text{(IV. C-21)}$$

The first term is the usual optically thick result; the second term gives the first non-steady correction. The next correction could be obtained from the fourth term of the Taylor series, but this is not done usually.

IV.C.6 QUASI-STEADY LIMIT

The quasi-steady limit is the case

$$\frac{1}{c}\frac{\partial I}{\partial t} << \vec{s} \cdot \nabla I \qquad \text{(IV. C-22)}$$

Here we have the problem of an overly restrictive stability limit caused by the physically unimportant non-steady term. A perturbation solution is suggested. To the zeroth order

$$\mu \frac{\partial I^o}{\partial r} + \frac{(1-\mu^2)}{r}\frac{\partial I^o}{\partial \mu} = K\left[B-I^o\right] \qquad \text{(IV. C-23)}$$

and to the first order

$$\frac{1}{c}\frac{\partial I^o}{\partial t} + \mu \frac{\partial I^1}{\partial r} + \frac{(1-\mu^2)}{r}\frac{\partial I^1}{\partial r} = K I^1 \qquad \text{(IV. C-24)}$$

where

$$I = I^o + \epsilon I^1 \qquad \text{(IV. C-25)}$$

IV.D NONRELATIVISTIC DERIVATION OF RADIATION-GAS DYNAMIC CONSERVATION EQUATIONS

by

M. P. Sherman

NOMENCLATURE

c	=	speed of light, 2.99793×10^{10} cm/sec
e	=	material internal energy per unit mass
E	=	radiation energy per unit volume
f_ν	=	photon distribution function
$\vec{F}$	=	radiative flux
h	=	Planck constant, 6.6252×10^{-27} erg-sec
H	=	stagnation enthalpy
I_ν	=	radiative intensity
$\vec{M}$	=	momentum of radiation field per unit volume
p	=	hydrostatic pressure
$\vec{\vec{P}}_r$	=	radiative pressure tensor
$\vec{q}$	=	molecular diffusive flux of energy
t	=	time
$\vec{s}$	=	area
$\vec{V}$	=	mass average (usual) fluid velocity
ρ	=	fluid density
$\vec{\vec{\sigma}}$	=	viscous stress tensor
τ	=	volume
$\hat{\Omega}$	=	unit direction vector
Ω	=	solid angle
ν	=	frequency

IV.D NONRELATIVISTIC DERIVATION OF RADIATION-GAS DYNAMIC CONSERVATION EQUATIONS

For a photon of frequency ν

$$\text{photon energy} = h\nu \tag{IV.D-1.1}$$

$$\text{photon momentum} = h\nu\,\hat{\Omega}/c \tag{IV.D-1.2}$$

$$\text{photon (rest) mass} = 0 \tag{IV.D-1.3}$$

The photon distribution function in units of photons per unit volume and solid angle is related to the intensity by

$$I_\nu = h\nu\, c f_\nu \tag{IV.D-2}$$

The radiative energy per unit volume is

$$E = \int_0^\infty \int h\nu\, f_\nu\, d\Omega\, d\nu = \frac{1}{c} \int_0^\infty \int I_\nu\, d\Omega\, d\nu \tag{IV.D-3}$$

The radiative energy flux (energy/area-time) is

$$\vec{F} = \int_0^\infty \int h\nu\, f_\nu\, (c\,\hat{\Omega})\, d\Omega\, d\nu = \int_0^\infty \int I_\nu\, \hat{\Omega}\, d\Omega d\nu \tag{IV.D-4}$$

where $c\,\hat{\Omega}$ is the velocity of the photons.

The momentum of the radiation field per unit volume is

$$\vec{M} = \int_0^\infty \int \frac{h\nu\hat{\Omega}}{c}\, f_\nu\, d\Omega d\nu = \frac{1}{c^2} \int_0^\infty I_\nu\, \hat{\Omega}\, d\Omega d\nu \tag{IV.D-5}$$

$$= \frac{1}{c^2}\, \vec{F}$$

The momentum flux (momentum/area-time) is

$$\int_0^\infty \iint \left(\frac{h\nu\, \hat{\Omega}}{c} f_\nu \right) (c\, \hat{\Omega})\, d\Omega\, d\nu \qquad \text{(IV. D-6)}$$

$$= \frac{1}{c} \int_0^\infty \iint I_\nu\, \hat{\Omega}\, \hat{\Omega}\, d\Omega d\nu$$

$$= \vec{\vec{P}}_r, \text{ the definition of radiative pressure}$$

The radiation mass per unit area and mass flux are zero, and hence there is no change in the overall continuity equation. Using Equations (IV. D-3, -4, -5 and -6), the derivation of the momentum and energy equation parallels the nonradiative case. We start with the integral form of the momentum equation.

$$\iiint \frac{\partial}{\partial t} (\rho \vec{V} + \vec{M})\, d\tau + \iint \left[\vec{V}\, \rho \vec{V} + \vec{\vec{P}}r \right] \cdot d\vec{s} + \int\int p\, d\vec{s} - \iint \vec{\vec{\sigma}} \cdot d\vec{s} = 0 \qquad \text{(IV. D-7)}$$

The first term is the rate of change of momentum, the second the flux of momentum and the last two the pressure and viscous surface forces.

Using the divergence theorem, Equations (IV. D-6) and (IV. D-7) and going to the differential form

$$\frac{\partial}{\partial t} (\rho \vec{V}) + \frac{1}{c^2} \frac{\partial \vec{F}}{\partial t} + \nabla \cdot (\vec{V} \rho \vec{V}) + \nabla \cdot \vec{\vec{P}}r + \nabla p - \nabla \cdot \vec{\vec{\sigma}} = 0 \qquad \text{(IV. D-8)}$$

Expanding terms and subtracting the continuity equation

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

we get the final form

$$\rho \left\{ \frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} \right\} + \frac{1}{c^2} \frac{\partial \vec{F}}{\partial t} + \nabla \cdot \vec{\vec{P}}r + \nabla p - \nabla \cdot \vec{\vec{\sigma}} = 0 \qquad \text{(IV. D-9)}$$

The integral form of the energy equation is

$$\iiint \frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}V^2\right)+E\right]d\tau+\iint\left[\rho\vec{V}\left(e+\frac{1}{2}V^2\right)+\vec{F}\right]\cdot d\vec{s}$$

$$+\iint p\vec{V}\cdot d\vec{s}-\iint \vec{V}\cdot\vec{\vec{\sigma}}\cdot d\vec{s}+\iint\vec{q}\cdot d\vec{s}=0 \qquad \text{(IV.D-10)}$$

The first term is the rate of change of internal, kinetic and radiative energy. The second term is the flux of these quantities through the surface, while the last term is the molecular diffusion of energy (thermal conductivity, etc.) through the boundary. The other terms are pressure and viscous work at the surface. Using the divergence theorem and going to the differential form,

$$\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}V^2\right)+E\right]+\nabla\cdot\left[\rho\vec{V}\left(e+\frac{1}{2}V^2\right)+\vec{F}\right]+\nabla\cdot(p\vec{V})$$

$$-\nabla\cdot\left[\vec{V}\cdot\vec{\vec{\sigma}}\right]+\nabla\cdot\vec{q}=0 \qquad \text{(IV.D-11)}$$

Using the continuity equation as before, we obtain one possibly useful form of the energy equation

$$\rho\frac{\partial}{\partial t}\left(e+\frac{1}{2}V^2\right)+\frac{\partial E}{\partial t}+\rho\vec{V}\cdot\nabla\left(e+\frac{1}{2}V^2\right)+\nabla\cdot\vec{F}+\nabla\cdot(p\vec{V})$$

$$-\nabla\cdot(\vec{V}\cdot\vec{\vec{\sigma}})+\nabla\cdot\vec{q}=0 \qquad \text{(IV.D-12)}$$

The usual form is obtained by subtracting V · (IV.D-9) from Eq. (IV.D-12)

$$\rho\left(\frac{\partial e}{\partial t}+\vec{V}\cdot\nabla e\right)+\left\{\frac{\partial E}{\partial t}-\frac{\vec{V}}{c^2}\cdot\frac{\partial\vec{F}}{\partial t}+\nabla\cdot\vec{F}-\vec{V}\cdot\nabla\cdot\vec{\vec{P}}r\right\}+p\nabla\cdot\vec{V}$$

$$-\vec{\vec{\sigma}}:\nabla\vec{V}+\nabla\cdot q=0 \qquad \text{(IV.D-13)}$$

The four radiative terms are in the curly braces. After algebraic manipulation, we obtain from Eq. (IV.D-12) an alternate useful form

$$\rho\left[\frac{\partial H}{\partial t} + \vec{V}\cdot\nabla H\right] + \left\{\frac{\partial E}{\partial t} + \nabla\cdot\vec{F}\right\} - \frac{\partial p}{\partial t} - \nabla\cdot(\vec{V}\cdot\vec{\vec{\sigma}}) + \nabla\cdot\vec{q} = 0 \qquad \text{(IV.D-14)}$$

where H is the stagnation enthalpy

$$H = e + \frac{p}{\rho} + \frac{V^2}{2}$$

IV.E RADIATION EMITTED BY A NONEQUILIBRIUM NITROGEN PLASMA

by

J. L. Kulander

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IV.E RADIATION EMITTED BY A NONEQUILIBRIUM NITROGEN PLASMA

IV.E.1 INTRODUCTION

The nonequilibrium populations of a selected number of electronic levels in NI-VIII were previously determined[IV. E-1] for a uniform, low density, optically thin N plasma with electron temperature, T_e, between 10^4 and $10^{6\circ}$K. The gas was assumed to be in a statistically steady state but was not in local thermodynamic equilibrium (LTE) because it was neither collision dominated nor optically thick at all frequencies. Equilibrium population of the levels was found to occur with $n_e \sim 10^{18}$ e/cm^3 at $10^{4\circ}$K and $n_e \sim 10^{23}$ e/cm^3 at $10^{6\circ}$K. The requirement of an optically thin medium limited application of the results to situations where no more than 10^{12} - 10^{14} N particles were present in any path length through the medium.

The purpose of this section is to specify the spectrum of radiation emitted from a semi-infinite, plane-parallel layer of N under similar physical conditions. The plasma considered is irradiated by an external diluted Planckian field W B_ν (T_r) where T_r does not necessarily equal T_e. Results for various layer thickness are obtained in situations where one spectral line is no longer optically thin. The solution in this case is accomplished through simultaneous solution of the Eddington transfer equation and the population rate equations and allows extension of the previous results to higher total N concentrations. In a non-optically thin line, the internal emission of the gas itself tends to partially balance the downward radiative rate and hence increase the population of the upper level over the optically thin case. In the optically thin case, the occupation numbers are not functions of position within the layer. In the optically thick case, depending upon the degree of coupling between any general level and the upper and lower levels of the optically thick line, the emission coefficient at all frequencies may be a function of position within the gas.

IV.E.2 TRANSFER EQUATIONS

The specification of the radiation field requires knowledge of the radiative source function at all frequencies or in turn the populations of the excited and ionized states under consideration. We shall assume the 26 levels shown in Table IV. E-1 to be representative of the system of ions NI-VIII. The levels are labeled as q i where i refers to a particular bound level in the q state of ionization. Upper levels for electric dipole transitions are followed in parentheses by the corresponding lower levels.

In the statistically steady state, the rate equation describing the population n_i of the state i is,

$$\sum_{j \neq i} (n_j P_{ji} - n_i P_{ij}) = \sum_j n_j P_{ji} = 0$$

$$P_{ii} = - \sum_{j \neq i} P_{ij} \qquad \text{(IV. E-1)}$$

where P_{ij} is the total transition rate from i to j per second per particle in the i state. In general, $P_{ij} = \bar{A}_{ij} + C_{ij}$ where $\bar{A}_{ij}$ and C_{ij} represent the radiative and collision transition rates respectively. The detailed evaluation of the transition rates has been discussed previously (IV. E-1). We shall assume a Maxwellian distribution for the electrons and nitrogen particles and since we also assume a known external radiation field the transitions involving the continuum can be represented by a single term in Eq. (IV. E-1). The general solution of (IV. E-1) is (IV. E-2)

$$n_i = \lambda_m P^{mi} \quad ; \quad \lambda_m = \frac{N}{\sum_j P^{mj}} \qquad \text{(IV. E-2)}$$

where P^{mj} is the cofactor of the element P_{mj} in the coefficient matrix represented by the i equations of type (IV. E-1) and N is the total number of nitrogen particles per cm^3.

When the medium becomes optically non-thin for certain frequencies the radiation field producing internal excitation and ionization for these frequencies is no longer merely the external radiation field but is partly dependent on the internal properties of the gas and must be determined from the radiative transfer equation,

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu \qquad \text{(IV. E-3)}$$

TABLE IV.E-1. ASSUMED ENERGY LEVELS

Ion	Level	qi	Energy (ev)
NI	$2p^3\ ^4S^o$	11	0
	$2p^3\ ^2D^o$	12	2.38
	$2p^3\ ^2P^o$	13	3.57
	$2p^2 3s\ ^4P$	14 (11)	10.3
	$2p^2 3p\ (^4S^o,\ ^4P^o,\ ^4D^o)$	15 (14)	11.8
NII	$2p^2\ ^3P$	21	14.5
	$2p^2\ ^1D$	22	16.4
	$2p^2\ ^1S$	23	18.6
	$2p\ 3s\ ^3P^o$	24 (21)	33.0
	$2p\ 3s\ (^3S,\ ^3P,\ ^3D)$	25 (24)	35.4
NIII	$2s^2\ 2p\ ^2P^o$	31	44.1
	$2s\ 2p^2\ ^4P$	32	51.2
	$2s\ 2p^2\ (^2S,\ ^2P,\ ^2D)$	33 (31)	59.7
NIV	$2s^2\ ^1S$	41	91.5
	$2s\ 2p\ ^3P^o$	42	99.9
	$2s\ 2p\ ^1P^o$	43 (41)	107.7
	$2s\ 3s\ ^1S$	44 (43)	139.7
NV	$2s\ ^2S$	51	169.0
	$2p\ ^2P^o$	52 (51)	178.9
NVI	$1s^2\ ^1S$	61	266.8
	$1s\ 2s\ ^3S$	62	686.3
	$1s\ 2p\ ^3P^o$	63	692.8
	$1s\ 2p\ ^1P^o$	64 (61)	697.2
NVII	$1s\ ^2S$	71	818.5
	$2p\ ^2P^o$	72 (71)	1318.
NVIII		81	1485.

where cos μ represents the angle between the direction of propagation and the outward normal z and $\tau_\nu = \int \kappa_\nu dz$. S_ν is the source function, κ_ν is the linear absorption coefficient and I_ν is the specific intensity of the radiation. In LTE $S_\nu = B_\nu$; however, in the non-LTE case S_ν must be specified in terms of microscopic processes(IV. E-3, 4). In terms of such processes the transfer equation governing the spectral line between upper level u and lower level ℓ may be written as,

$$-4\pi\mu \frac{dI_\nu}{dz} = \left[n_\ell B_{\ell u} \Phi_\nu h\nu - n_u B_{u\ell} \psi_\nu h\nu + \kappa_c \right] I_\nu - n_u A_{u\ell} j_\nu h\nu - \kappa_c S_c (T_e)$$

(IV. E-4)

where κ_c represents the continuum absorption coefficient at frequency ν_0 and S_c is the continuum source function. $B_{\ell u}$, $B_{u\ell}$ and $A_{u\ell}$ are the Einstein transition probabilities for absorption, stimulated emission and spontaneous emission. j_ν, ψ_ν and Φ_ν are the normalized, emission, stimulated emission and absorption coefficients within the line defined such that $\int_0^\infty \Phi_\nu \, d\nu = \int_0^\infty \psi_\nu \, d\nu = \frac{1}{4\pi} \iint_{4\pi}^{\infty} j_\nu \, d\nu d\omega = 1$. The continuum absorption coefficient is generally very small compared with the line absorption coefficient and will be neglected in determining the source function within the line. Using the standard relations between the Einstein coefficients and assuming $j_\nu = \Phi_\nu = \psi_\nu$, the source function becomes:

$$S_{u\ell} = \frac{2h\nu^3}{c^2} \frac{1}{\frac{g_u}{g_\ell}\frac{n_\ell}{n_u} - 1}$$

(IV. E-5)

where g represents the statistical weight. The minus one term in the denominator represents stimulated emissions.

In evaluating the radiative excitation rate $\bar{A}_{ij}$ for transitions between bound levels, the line radiation field enters as $\int_0^\infty J_\nu(\tau) \Phi_\nu(\tau) \, d\nu$ where $J_\nu(\tau) = \frac{1}{4\pi} \int_{4\pi} I_\nu(\tau, \mu) \, d\omega$ is the mean intensity and $d\omega$ represents the solid angle. It is thus convenient to formulate the transfer equation in terms of J_ν rather than I_ν. We shall adopt the Eddington form of the transfer equation,

$$\frac{1}{3}\frac{d^2 J_\nu}{d \tau_\nu^2} = J_\nu - S_\nu \qquad \text{(IV. E-6)}$$

obtained by placing certain limitations (IV. E-5) on the form for the angular dependence of I_ν. Writing $d\tau_\nu = \varphi_\nu \, dt$ where dt is the opacity at the line center and φ_ν represents the frequency variation within the line and neglecting stimulated emission, Eq. (IV. E-6) becomes,

$$\frac{d^2 J_\nu}{dt^2} = x_\nu^2 \left[J_\nu - \rho_{u\ell} \frac{P^{\ell u}}{P^{u\ell}} \right] \qquad \text{(IV. E-7)}$$

where $x_\nu = \sqrt{3}\,\varphi_\nu$ and $\rho_{u\ell} = \frac{2h\nu^3}{c^2} \frac{g_\ell}{g_u}$. It is now convenient to separate those components involving the unknown radiation field, $J_{u\ell}$, from the co-factors. This is done by expanding the determinant P^{ij} in terms of its co-factors Q^{ij}.

Thus

$$P^{\ell u} = \sum_{k \neq \ell} P_{\ell k} Q^{k\ell} = P_{\ell u} Q^{u\ell} + \sum_{k \neq \ell \neq u} P_{\ell k} Q^{k\ell}$$

$$P^{u\ell} = \sum_{k \neq u} P_{uk} Q^{ku} = P_{u\ell} Q^{\ell u} + \sum_{k \neq u \neq \ell} P_{uk} Q^{ku} \,. \qquad \text{(IV. E-8)}$$

Since we retain the notation that a_{ij} is the ith row and j^{th} column matrix element, we have $P_{ij} = a_{ji}$ and hence the reverse order of the subscripts and superscripts in Eq. (IV. E-8).

Using the standard relationships between the Einstein coefficients, the source function may be written as

$$S_{u\ell} = \frac{\int_{u\ell} J_\nu \Phi_\nu \, d\nu + \epsilon B + \iota}{1 + \epsilon + \eta} \qquad \text{(IV. E-9)}$$

where B is the Planck function $B_{\nu_o}(T_e)$, $\epsilon = \frac{C_{u\ell}}{A_{u\ell}}$

$$\iota = \rho_{u\ell} \frac{1}{A_{u\ell} Q^{u\ell}} \sum_{k \neq u \neq \ell} P_{\ell k} Q^{k\ell}$$

$$\eta = \frac{1}{A_{u\ell} Q^{\ell u}} \sum_{k \neq u \neq \ell} P_{uk} Q^{ku} \quad . \qquad \text{(IV. E-10)}$$

Equations (IV. E-6) and (IV. E-9) are solved using a discrete ordinate method in which we assume

$$\int_0^\infty J_\nu \Phi_\nu d\nu = \sum_{i=1}^{n} a_i J_i \qquad \text{(IV. E-11)}$$

We shall assume Φ_ν to be Gaussian, i.e.,

$$\Phi_\nu = \frac{e^{-v^2}}{\sqrt{\pi}\, \Delta\nu_D} \quad ; v = \frac{\Delta\nu}{\Delta\nu_D} \quad . \qquad \text{(IV. E-12)}$$

$\Delta\nu_D$ is the Doppler half width given by

$$\frac{\nu_o}{c}\sqrt{\frac{2kT}{M}} \qquad \text{(IV. E-13)}$$

where M is the nitrogen particle mass. For this integration the frequency division points v_i and weighting factors a_i are characteristic of a Hermite-Gauss quadrature. In all cases considered, the convergence of (IV. E-11) with increasing n is rapid and n = 8 reproduces the exact result within a few percent. Since Φ_ν in an even function, the summation over half the line profile (i.e., n = 4) is merely doubled to obtain the total integral in (IV. E-11). The values of v_i and a_i are given in Table IV. E-2.

Equation (IV. E-7) may now be replaced by n equations of the form.

$$\frac{d^2 J_i}{dt^2} = x_i^2 \left[J_i - \varpi \sum_i a_i J_i - \lambda B - \varpi \iota \right] \qquad \text{(IV. E-14)}$$

where $\varpi = \frac{1}{1+\epsilon+\eta}$, $\lambda = \frac{\epsilon}{1+\epsilon+\eta}$.

TABLE IV. E-2. HERMITE - GAUSS WEIGHTING FACTORS AND DIVISION POINTS

a_1	= .7460	v_1	= .3812
a_2	= .2345	v_2	= 1.1572
a_3	= 1.927×10^{-2}	v_3	= 1.9817
a_4	= 2.252×10^{-4}	v_4	= 2.9306

Assuming a solution of the form $g_i e^{kt}$ the solution of Eq. (IV. E-14) with ϵ and η constant with depth (i.e., n_e and T_e constant with depth) is

$$\frac{J_i}{B} = \varpi \sum_{\alpha} \frac{L_\alpha e^{-k_\alpha t}}{1 - k_\alpha^2 / x_i^2} + \omega \sum_{\alpha} \frac{G_\alpha e^{k_\alpha t}}{i - k_\alpha^2 / x_i^2}$$

$$+ \frac{\lambda}{1 - \varpi} + \frac{\varpi}{1 - \omega} \frac{\iota}{B} \qquad \text{(IV. E-15)}$$

where the k are roots of the characteristic equation

$$\varpi \sum_i \frac{a_i}{1 - k^2 / x_i^2} = 1. \qquad \text{(IV. E-16)}$$

The integration constants are determined by the boundary conditions at the upper and lower surfaces of the layer. The Eddington boundary condition at t = 0 as modified by Krook, (IV. E-6) which requires no inward flux, is

$$x_\nu J_\nu = J'_\nu. \qquad \text{(IV. E-17)}$$

At $t = t_1$ we consider the radiation field WB (T_r) to be incident upon the layer. The boundary condition at this point is then,

$$x_\nu \left(J_\nu - W B_\nu (T_r) \right) = - J'_\nu \qquad \text{(IV. E-18)}$$

Letting $G_\alpha = L_\alpha e^{-k_\alpha t_1} + F_\alpha e^{-k_\alpha t_1}$, we find the following expressions for L_α and F_α,

$$\varpi \sum_\alpha \frac{L_\alpha}{1 - k_\alpha/x_i} \left[1 + \frac{(1 - k_\alpha/x_i)}{(1 + k_\alpha/x_i)} e^{-k t_1} + \varpi \sum_\alpha \frac{F_\alpha e^{-k_\alpha t_1}}{1 + k_\alpha/x_i} \right]$$

$$+ \frac{\lambda}{1 - \varpi} + \frac{\varpi}{1 - \varpi} \frac{\iota}{B} = 0 \qquad \text{(IV. E-19)}$$

$$\varpi \sum_\alpha \frac{L_\alpha e^{-k_\alpha t_1}}{1 + k_\alpha/x_i} \cdots + \varpi \sum_\alpha \frac{L_\alpha + F_\alpha}{1 - k_\alpha/x_i} + \frac{\lambda}{1 - \varpi} + \frac{\varpi}{1 - \varpi} \frac{\iota}{B}$$

$$- WB(T_r) / B = 0. \qquad \text{(IV. E-20)}$$

Once the mean intensity of the radiation field is determined at each point within the layer the total upward excitation rate in the line can be evaluated and hence all the coefficients in the rate equations become known. Figure IV. E-1 illustrates the mean intensity of the radiation field at the four quadrature frequencies in the non-thin line in cases where W = 0 and W = 1/2. In the figure, we consider the first resonance line of NII at electron and radiation temperatures of 2×10^4° K. Values of k_α, L_α, F_α for these cases are given in Table IV. E-3. It is noted that for W = 0, the optically non-thin line is the first resonance line of NII while for W = 0.5, it is the first resonance line of NIII.

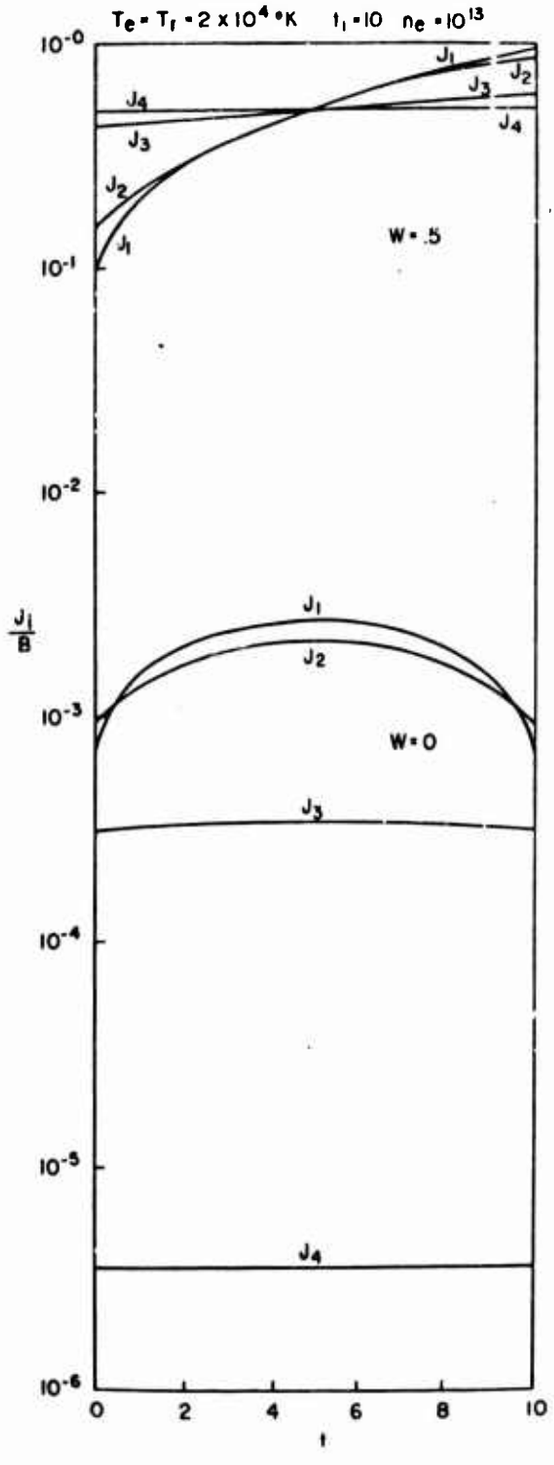


Figure IV. E-1. Mean Intensity at 4 Quadrature Points in Non-Thin Line vs. t
$T_e = T_r = 2 \times 10^4$ °K, $n_e = 10^{15}/cm^3$, $t_1 = 10$, W = 0, .5.

TABLE IV. E-3. CHARACTERISTIC VALUES OF k_α, L_α, F_α

$T_e = T_r = 2 \times 10^4$° K, $n_e = 10^{13}$, $t_1 = 10$

W = 0

$\epsilon = 8.860 \times 10^{-5}$ $\eta = 1.050 \times 10^{-4}$ $\iota = 3.367 \times 10^{-9}$

$k_1 = .8457$	$L_1 = -4.220 \times 10^{-4}$	$F_1 = 0$
$k_2 = .1175$	$L_2 = -5.944 \times 10^{-3}$	$F_2 = 0$
$k_3 = 4.785 \times 10^{-3}$	$L_3 = -.2437$	$F_3 = 0$
$k_4 = 2.191 \times 10^{-4}$	$L_4 = -.2847$	$F_4 = 0$

W = .5

$\epsilon = 1.464 \times 10^{-4}$ $\eta = 1.649 \times 10^{-5}$ $\iota = 1.364 \times 10^{-8}$

$k_1 = .8456$	$L_1 = -.0417$	$F_1 = .0825$
$k_2 = .1174$	$L_2 = -.3759$	$F_2 = .7393$
$k_3 = 4.610 \times 10^{-3}$	$L_3 = -2.414$	$F_3 = 4.280$
$k_4 = 2.087 \times 10^{-4}$	$L_4 = -.7382$	$F_4 = .7144$

IV.E.3 NON-EQUILIBRIUM POPULATIONS

Equations (IV. E-1) and (IV. E-7) have been solved for the relative level populations for the following ranges of T_e, T_r, W and t_1:

$$10^4\ ^oK \leq T_e,\ T_r \leq 10^6\ ^oK$$

$$0 \leq W \leq 1/2$$

$$.1 \leq t_1 \leq 100.$$

When $t_i << 1$ for all frequencies, only equation (IV. E-1) needs to be considered since J_ν is simply the external radiation field $W B_\nu (T_r)$ where W may vary between 0 and 1. W = 1 represents irradiation of the layer from all directions, W = 1/2, irridation from only one hemisphere, and W = 0, a completely isolated layer. As indicated by the boundary conditions applied to the transfer equation, we consider only irradiation over the lower hemisphere in the optically non-thin case.

Previous results (IV. E-1) for a completely optically thin gas with $T_e = T_r$ showed the anticipated decrease in excitation conditions as W went from 1 to 0. When $T_r < T_e$, a general lowering in excitation with respect to the $T_e = T_r$ case occurs, while for $T_r > T_e$, an increase in excitation is found. When $T_r << T_e$, the populations become constant at the W = 0 result since all radiative transitions become insignificant with respect to collisional transitions. These results are illustrated in Figures IV. E-2 - 9 where relative populations are shown for optically thin layers with various electron and radiation temperatures. The dotted curves refer to situations where $T_r < T_e$ while for the dashed curves $T_r > T_e$. As noted previously, the population changes are not always monotonic. When the equilibrium population is quite stable at one major species (i.e., the gradient of the population with respect to temperature and density is small), only a severe perturbation such as letting W approach very close to zero causes a change in population. The non-monotonic behavior of many populations as $W \rightarrow 0$ is enhanced when $T_r > T_e$.

Neglecting for the moment the absolute changes in population of the various species, let us consider the departure from equilibrium of the relative populations within each stage of ionization. We define

$$R_{qj} = \frac{n_j^q/n_1^q}{(n_j^q/n_1^q)_{eq.}}$$

to be the ratio of the relative population of n_j^q with respect to the ground state divided by the equilibrium relative population. Values of R_{qj} are given in Table IV. E-4 for $n_e = 10^{15}$, $T_e = 5x10^4$ °K and $T_r = 4x10^4$, $5x10^4$ and $6x10^4$ °K. When W - 1 at 5×10^5 °K, R_{qj} is of course 1. For W = 1, $T_r > T_e$ yields an increased population of the upper levels with respect to the ground state while for $T_r < T_e$ they are relatively less heavily populated. When W is decreased, even $T_r > T_e$ is not

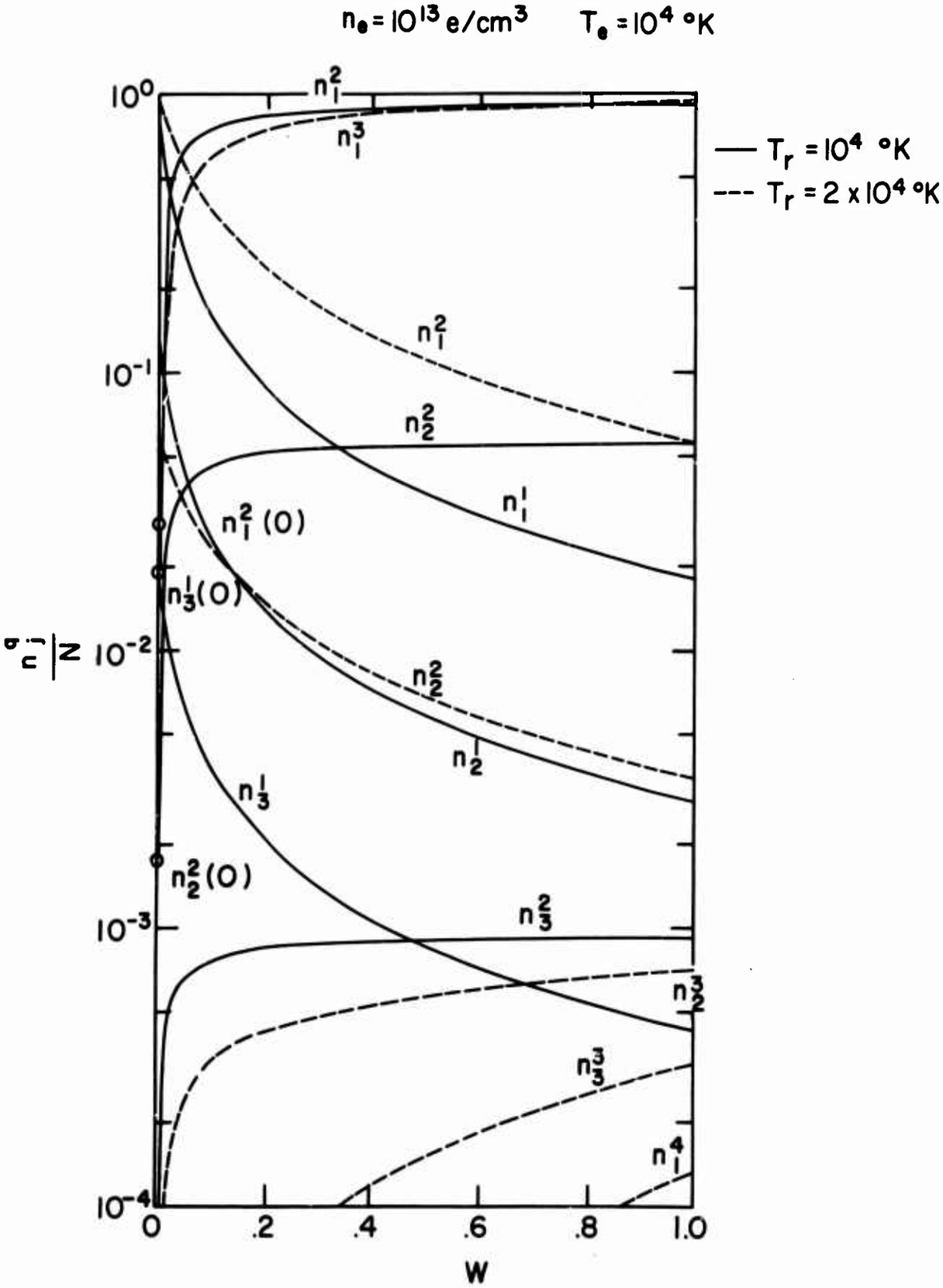


Figure IV. E-2. Relative Level Populations vs W

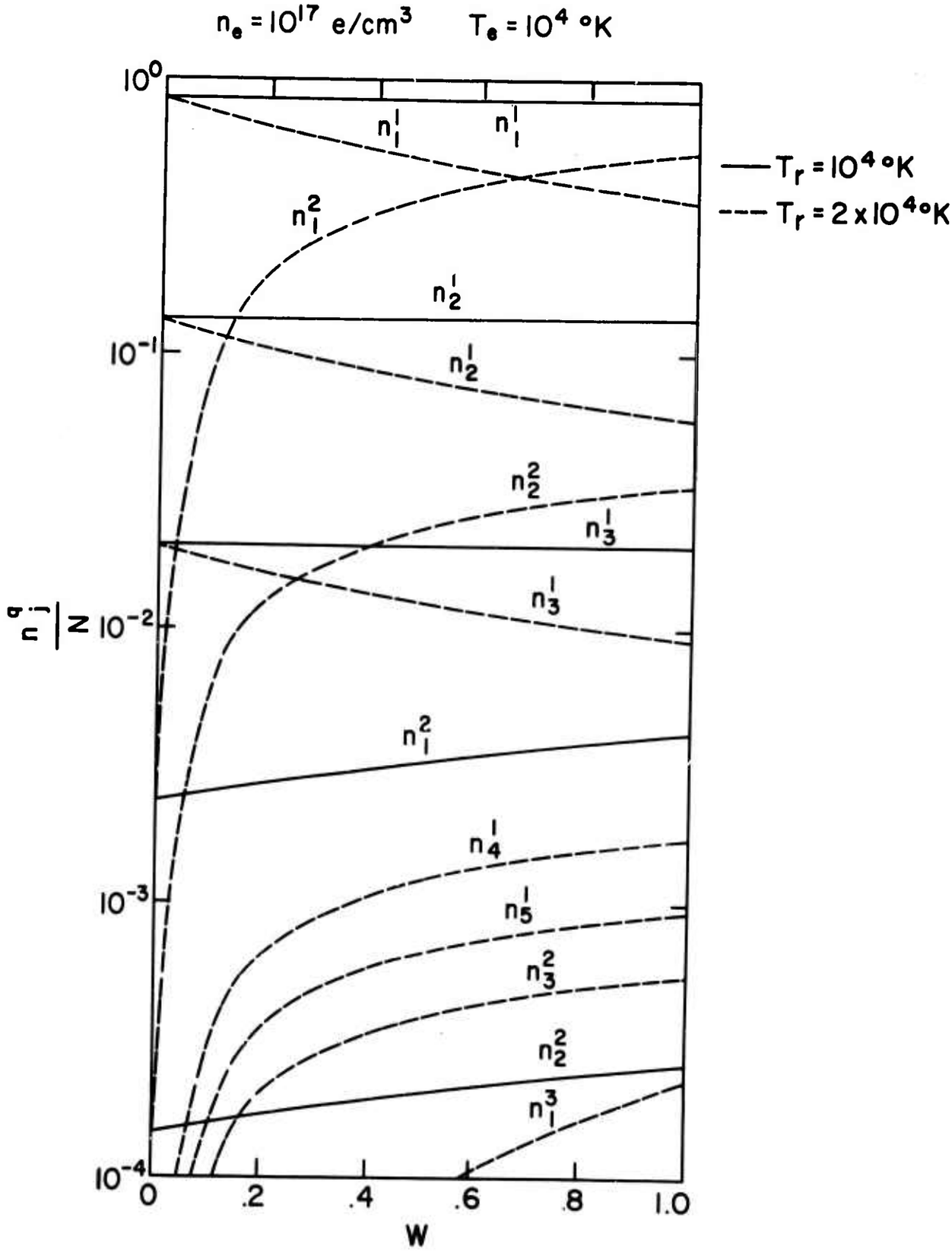


Figure IV. E-3. Relative Level Populations vs W

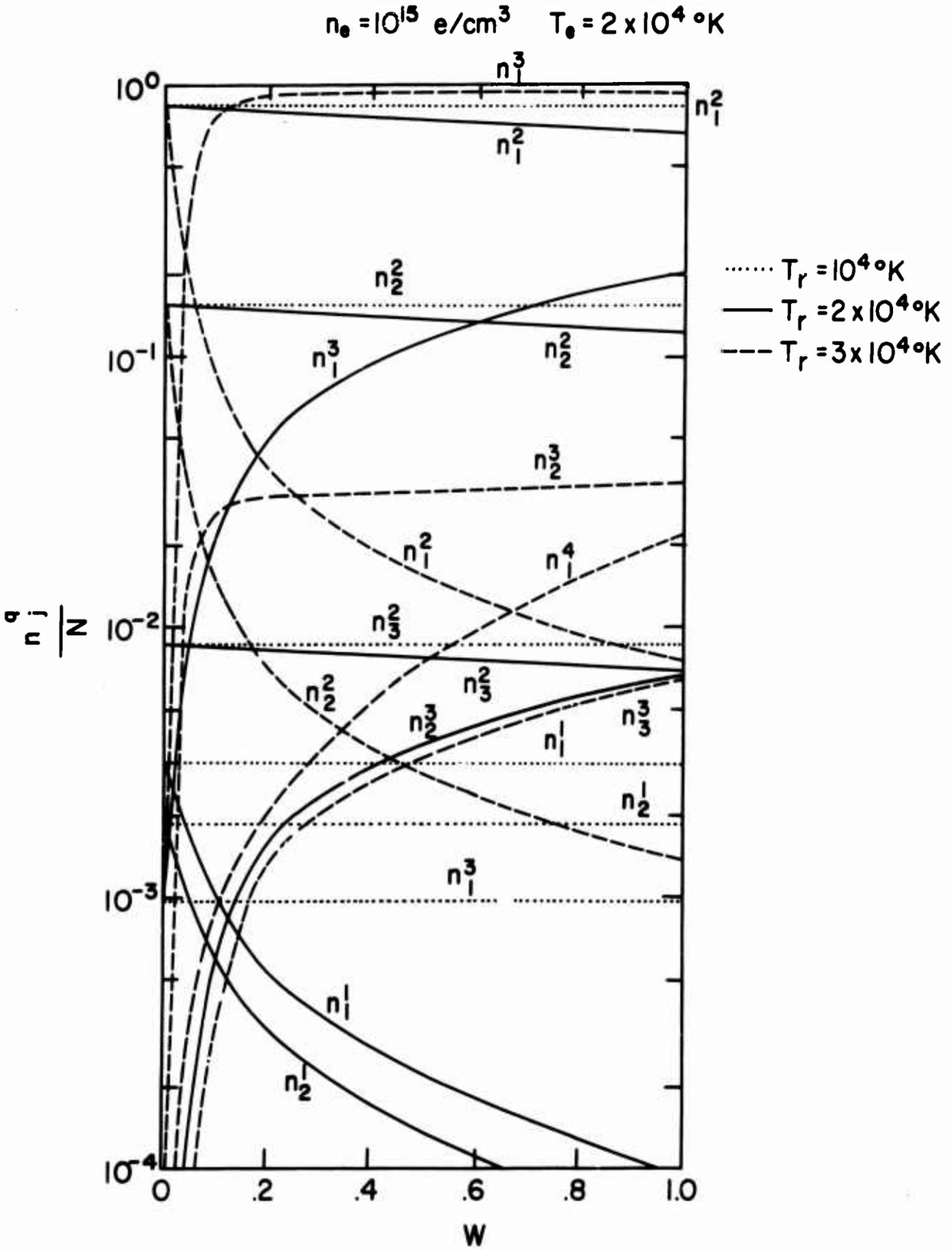


Figure IV. E-4. Relative Level Populations vs W

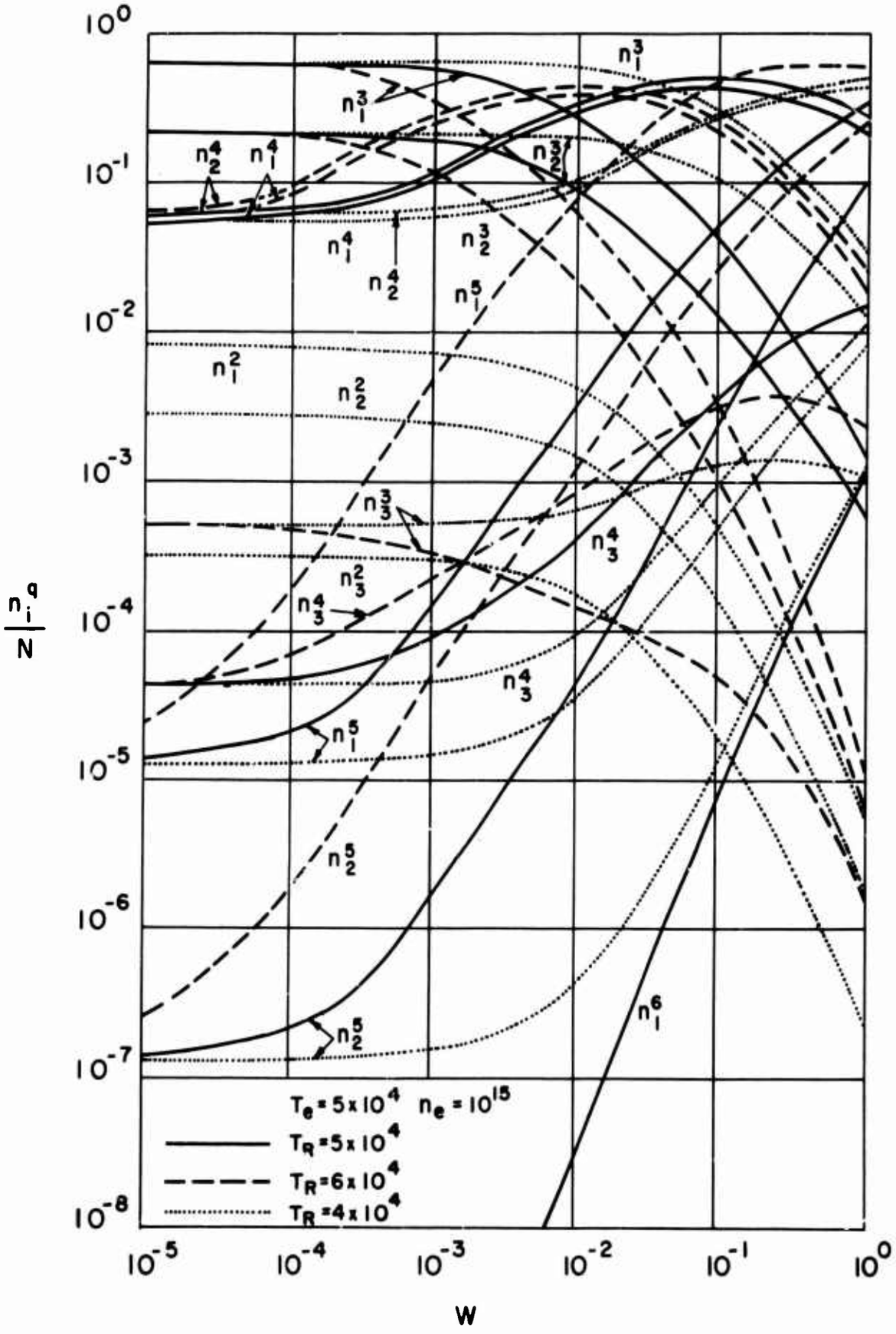


Figure IV.E-5. Relative Level Populations vs W

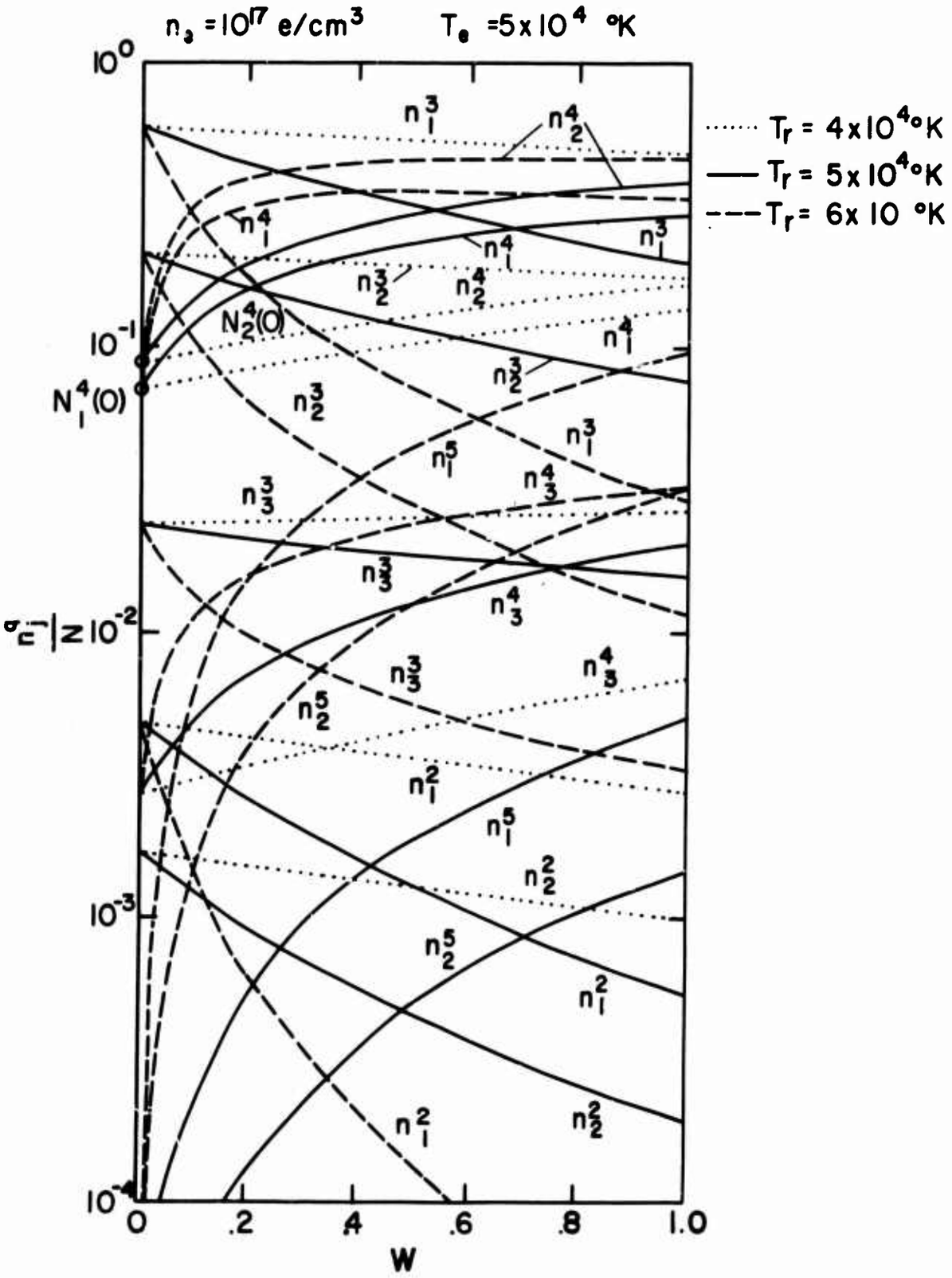


Figure IV. E-6. Relative Level Populations vs W

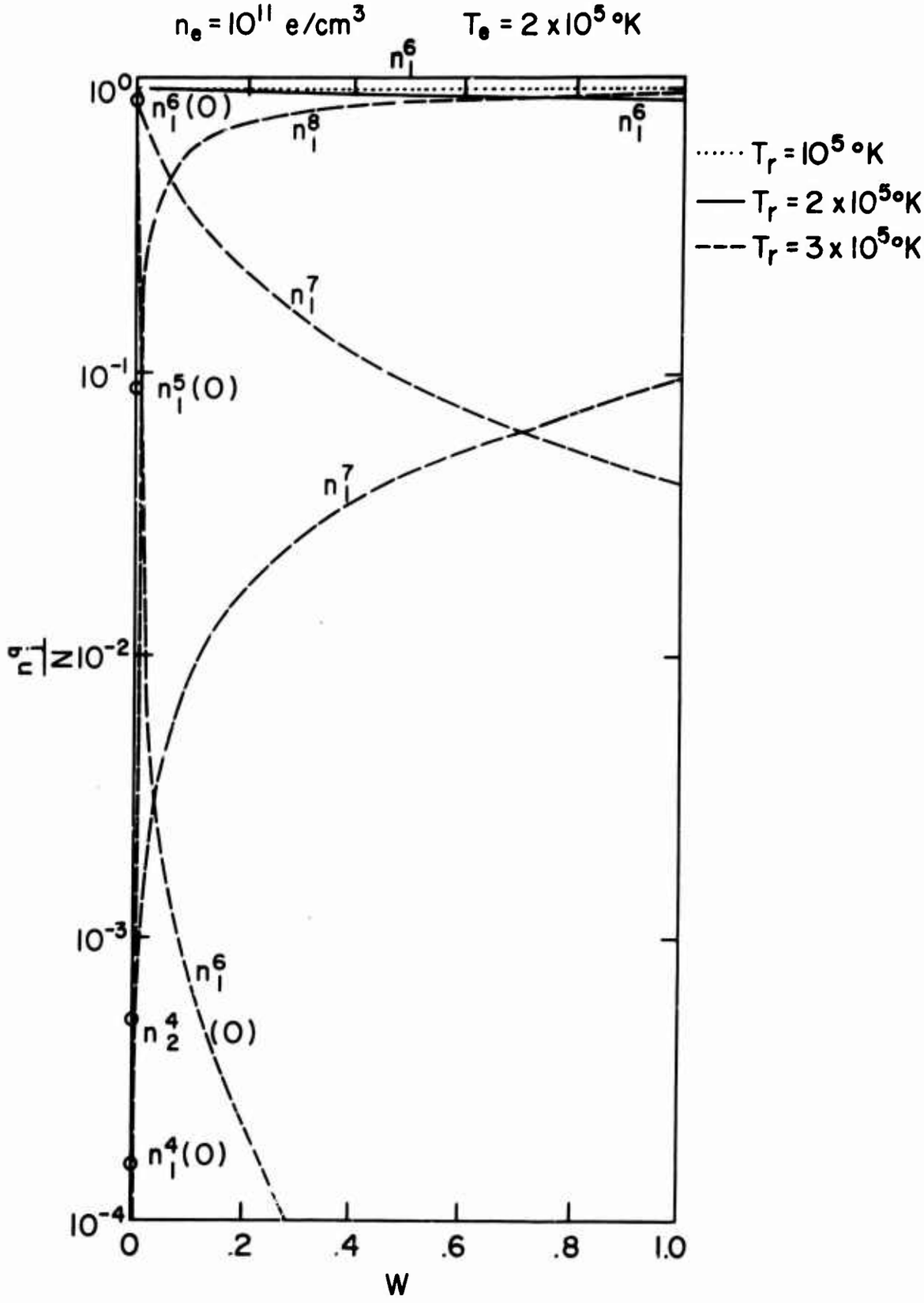


Figure IV. E-7. Relative Level Populations vs W

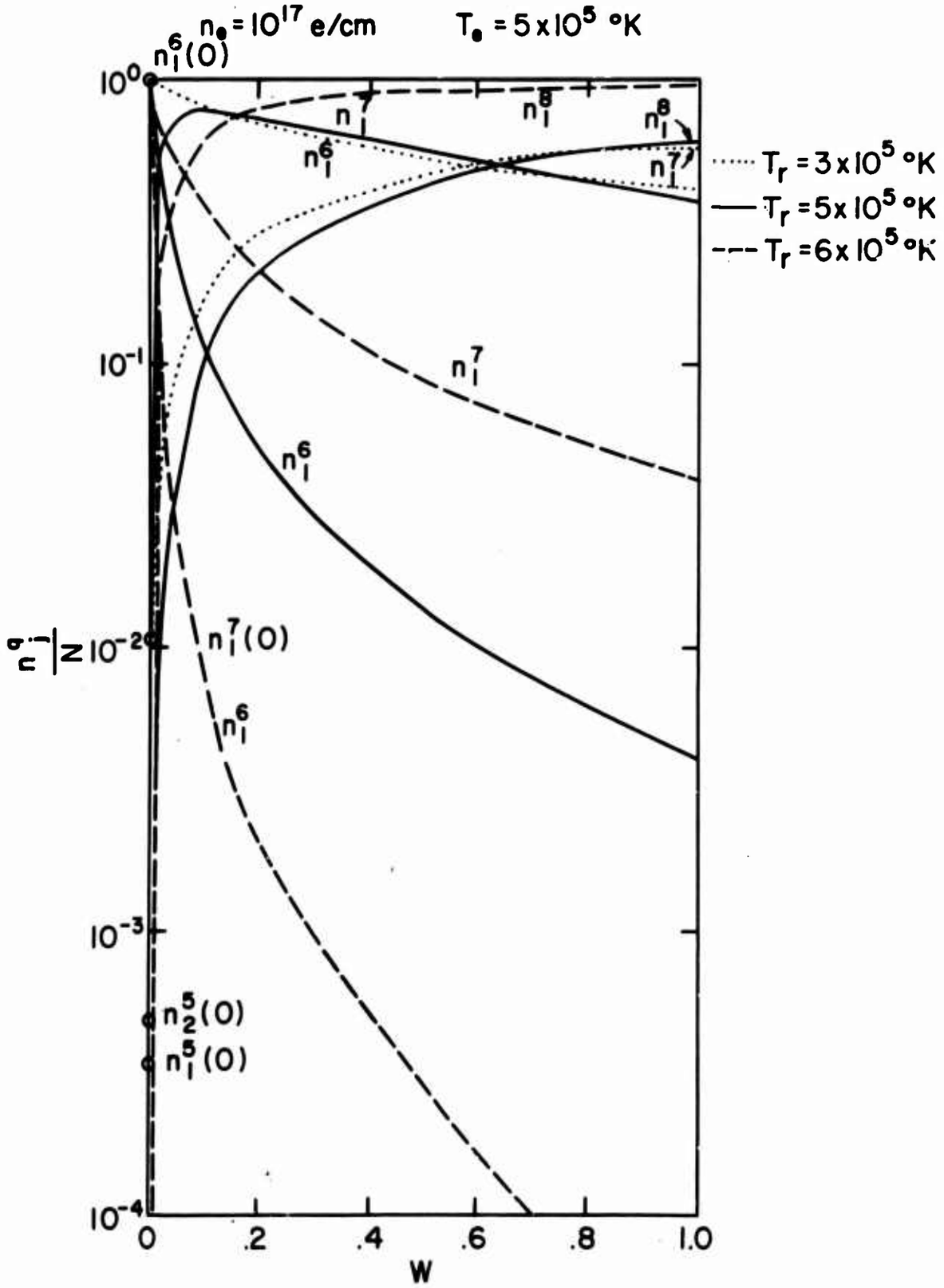


Figure IV. E-8. Relative Level Populations vs. W

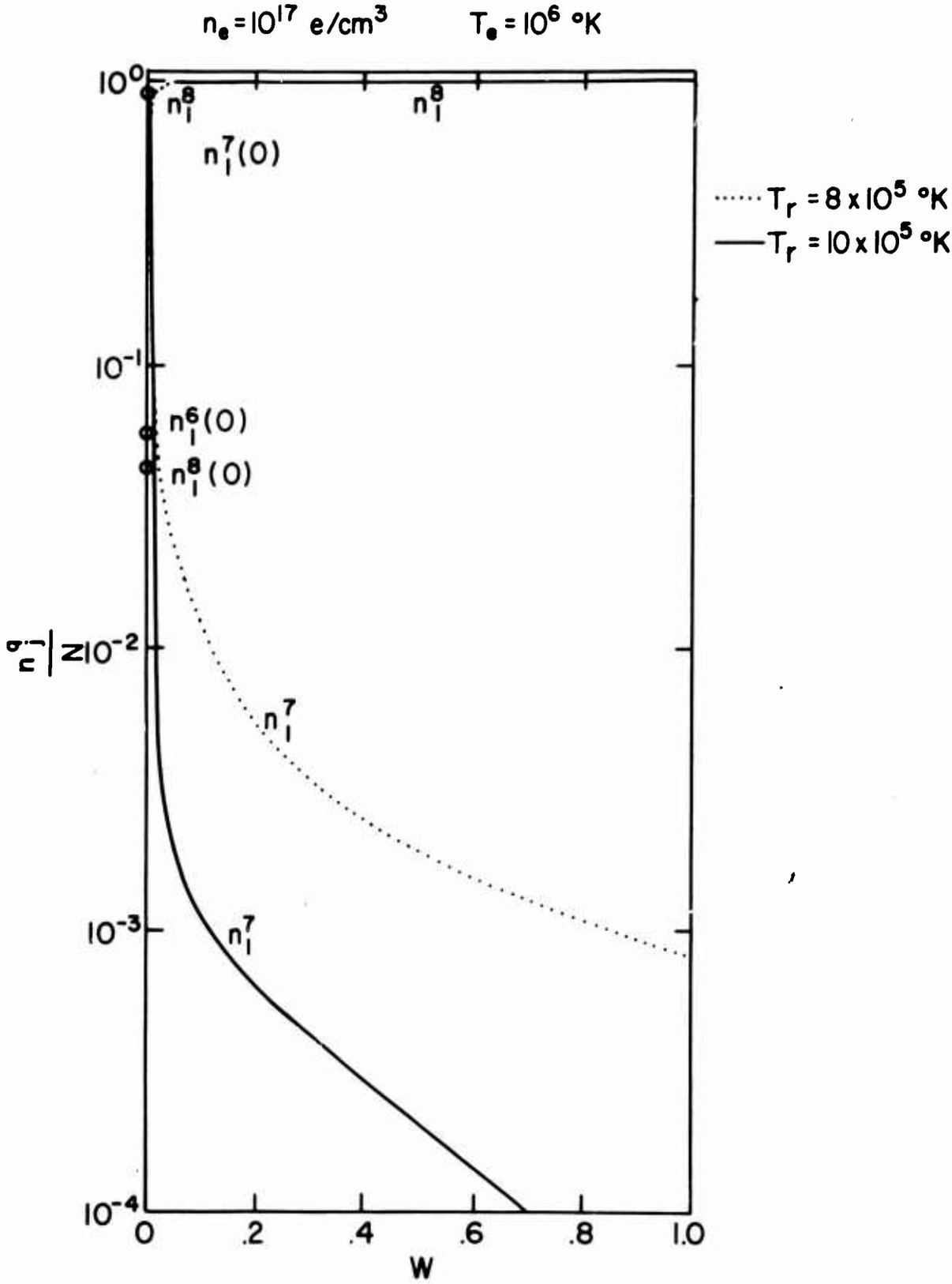


Figure IV. E-9. Relative Level Populations vs. W

TABLE IV.E-4. RATIO OF RELATIVE NONEQUILIBRIUM TO EQUILIBRIUM POPULATION

	$n_e = 10^{15}$		$T_e = 5 \times 10^4\ ^oK$			
	W = 1		W = .02			W = 0
	$T_r = 4 \times 10^4\ ^oK$	$T_r = 6 \times 10^4\ ^oK$	$T_r = 4 \times 10^4\ ^oK$	$T_r = 5 \times 10^4\ ^oK$	$T_r = 6 \times 10^4\ ^oK$	
R_{32}	.93	1.53	.88	.88	.88	.92
R_{33}	.41	1.81	.018	.031	.048	.011
R_{42}	.92	1.13	.87	.87	.87	.87
R_{43}	.40	1.86	.019	.032	.050	.012
R_{52}	.57	1.46	.046	.056	.067	.035

sufficient to maintain the upper level populations. Levels not involved in electric dipole transitions are very insensitive to changes in T_r as W decreases.

The results shown in Figures IV. E-2 - 9 are only valid when the total line of sight optical depth at all frequencies $<< 1$. Increasing the total number of nitrogen particles in the line of sight increases the upward radiative excitation rate in lines where $t \gtrsim 1$ and hence increases the population of the upper level of the line, providing the rate is not negligible in comparison with the corresponding collisional rate. A general enhancement of the populations of higher levels coupled with this upper level occurs. These populations are functions of optical depth while levels which are not coupled have constant populations within the medium. Many upper levels of electric dipole transitions never attain significant relative populations under any circumstances. Table IV. E-5 illustrates the populations for various t_1 by comparing the thin result with the non-thin result at $t = 0$ and $t = t_1/2$. As t_1 increases a Boltzmann distribution between upper and lower levels in the non-thin line is established. We note that although the upper levels of the allowed transitions do not become heavily populated, the continuum levels just above them do show a non-negligible increase in population. This results from the relatively strong collisional coupling between the higher levels and the continuum. Only levels whose relative populations are above 10^{-9} and change by more than 0.5% are shown in the table. For many purposes, such as computing the overall opacity of the plasma, the fact that one line has become optically thick will not alter the corresponding thin results significantly. The population of the upper level of the thick line and the higher levels coupled with it increase markedly, however, and since significant energy is emitted in the lines, these populations must be accurately specified.

The results obtained by allowing one spectral line to become optically non-thin are applicable providing the optical depth in another line does not become significant. We arbitrarily define an optically thin line to exist when t_1 at the line center $\lesssim 0.1$. Accepting this definition, we find that the maximum values of t_1 which are allowable for the optically non-thin line with $W = 0$ are those given in Figure IV. E-10. For many higher temperatures, this extension of the thin results only allows an increase in the total particle density some 2-8 times while for lower temperatures, it can be as much as 10^3. Illustrative corresponding total line of sight N densities are given in Table IV. E-6. We again emphasize that although the uppermost level populations are not correct for higher total densities, in general, the lower level populations are not affected by the thickening of one line. This is illustrated in Figure IV. E-11 where the populations are shown vs. t. The constant populations are the same as those obtained neglecting the non-thin line transfer problem.

TABLE IV.E-5. CHANGE IN RELATIVE POPULATION WITH OPTICAL THICKNESS

Level q_i	n_i^q/N (thin)	n_i^q/N (thick t = 0)	n_i^q/N (thick $t_1/2$)
	$T_e = 1 \times 10^4$, $n_e = 10^{15}$, W = 0, t_1 = 9, thick transition 14 → 11		
11	.828	.814	.786
12	.130 *	.128	.124
13	.196-1	.193-1	.186-1
14	.131-6	.251-5	.707-5
15	.153-6	.110-5	.291-5
21	.205-1	.364-1	.671-1
22	.125-2	.223-2	.411-2
23	.206-4	.367-4	.676-4
	$T_e = 2 \times 10^4$, $n_e = 10^{13}$, W = 0, t_1 = 10, thick transition 24 → 21		
24	.423-8	.182-7	.500-7
25	.253-7	.257-7	.265-7
31	.774-3	.775-3	.776-3
32	.250-4	.250-4	.251-4
	$T_e = 2 \times 10^4$, $n_e = 10^{13}$, W = 0, t_1 = 10, thick transition 24 → 21		
24	.411-6	.153-5	.396-5
25	.741-6	.136-5	.271-5
31	.970-3	.118-2	.165-2
32	.313-4	.382-4	.533-4
33	.540-8	.659-8	.918-8
	$T = 5 \times 10^4$, $n_e = 10^{15}$, W = 0, t_1 = .76, thick transition 33 → 31		
21	.803-2	.802-2	.802-2
22	.277-2	.277-2	.276-2
23	.333-3	.332-3	.332-3
25	.755-5	.754-5	.754-5

* The numbers following each entry represent the powers of 10 by which the entries should be multiplied.

TABLE IV. E-5. CHANGE IN RELATIVE POPULATION WITH OPTICAL THICKNESS (Continued)

Level q_i	n_i^q/N (thin)	n_i^q/N (thick t = 0)	n_i^q/N (thick $t_1/2$)
31	.651	.650	.650
32	.221	.220	.220
33	.525-3	.916-3	.102-2
41	.548-1	.553-1	.554-1
42	.616-1	.621-1	.622-1
43	.441-4	.444-4	.445-4
51	.135-4	.136-4	.136-4
52	.136-6	.137-6	.138-6
	$T = 5 \times 10^4$, $n_e = 10^{17}$, W = 0, $t_1 = .9$, thick transition 33 → 31		
21	.480-2	.464-2	.460-2
22	.169-2	.164-2	.162-2
23	.204-3	.197-3	.196-3
24	.347-4	.336-4	.332-4
25	.589-4	.569-4	.564-4
31	.592	.573	.567
32	.214	.212	.211
33	.239-1	.307-1	.327-1
41	.721-1	.789-1	.808-1
42	.879-1	.961-1	.984-1
43	.271-2	.296-2	.303-2
51	.272-4	.298-4	.305-4
52	.627-5	.685-5	.702-5
	$T_e = 1 \times 10^5$, $n_e = 10^{17}$, W = 0, $t_1 = .25$, thick transition 52 → 51		
31	.134-2	.132-2	.132-2
32	.100-2	.991-3	.990-3
33	.274-3	.271-3	.270-3
41	.769-1	.760-1	.759-1
42	.221	.218	.218
43	.156-1	.155-1	.154-1
44	.120-3	.118-3	.118-3
51	.393	.389	.388
52	.267	.275	.275
61	.239-1	.243-1	.244-1

TABLE IV. E-5. CHANGE IN RELATIVE POPULATION WITH OPTICAL THICKNESS (Continued)

Level qi	n_i^q/N (thin)	n_i^q/N (thick t = 0)	n_i^q/N (thick $t_1/2$)
$T = 5 \times 10\text{-}5$, $n_e = 10^{17}$, W = 0, $t_1 = 13.5$, thick transition 64 → 61			
51	.334-3	.334-3	.333-3
52	.488-3	.488-3	.487-3
61	.988	.988	.987
62	.959-4	.967-4	.990-4
63	.240-3	.243-3	.249-3
64	.371-7	.150-5	.565-5
71	.108-1	.111-1	.120-1
81	.898-7	.925-7	.100-6

TABLE IV. E-6. TOTAL PERMISSIBLE LINE OF SIGHT N DENSITY

T_e (^oK)	n_e (cm^{-3})	N (cm^{-2})
10^4	10^{15}	2.1×10^{14}
2×10^4	10^{13}	7.9×10^{14}
2×10^4	10^{15}	7.0×10^{14}
5×10^4	10^{15}	1.3×10^{13}
5×10^4	10^{17}	1.6×10^{13}
10^5	10^{17}	1.6×10^{13}
2×10^5	10^{15}	3.1×10^{15}
5×10^5	10^{13}	4.0×10^{15}
5×10^5	10^{17}	1.3×10^{16}

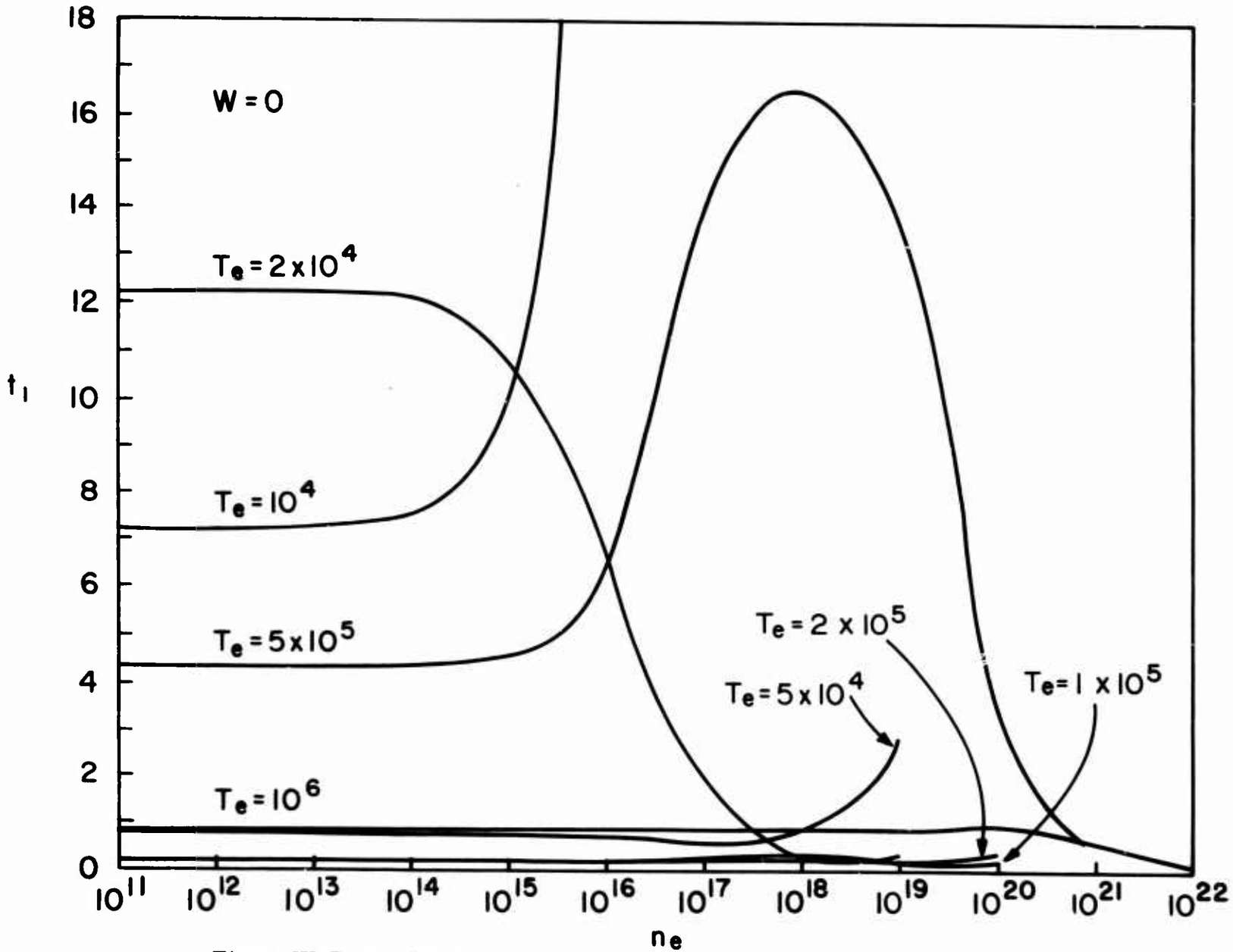


Figure IV. E-10. Maximum Layer Optical Thickness at Center of Non-Thin Line Permitting Only One Non-Thin Line

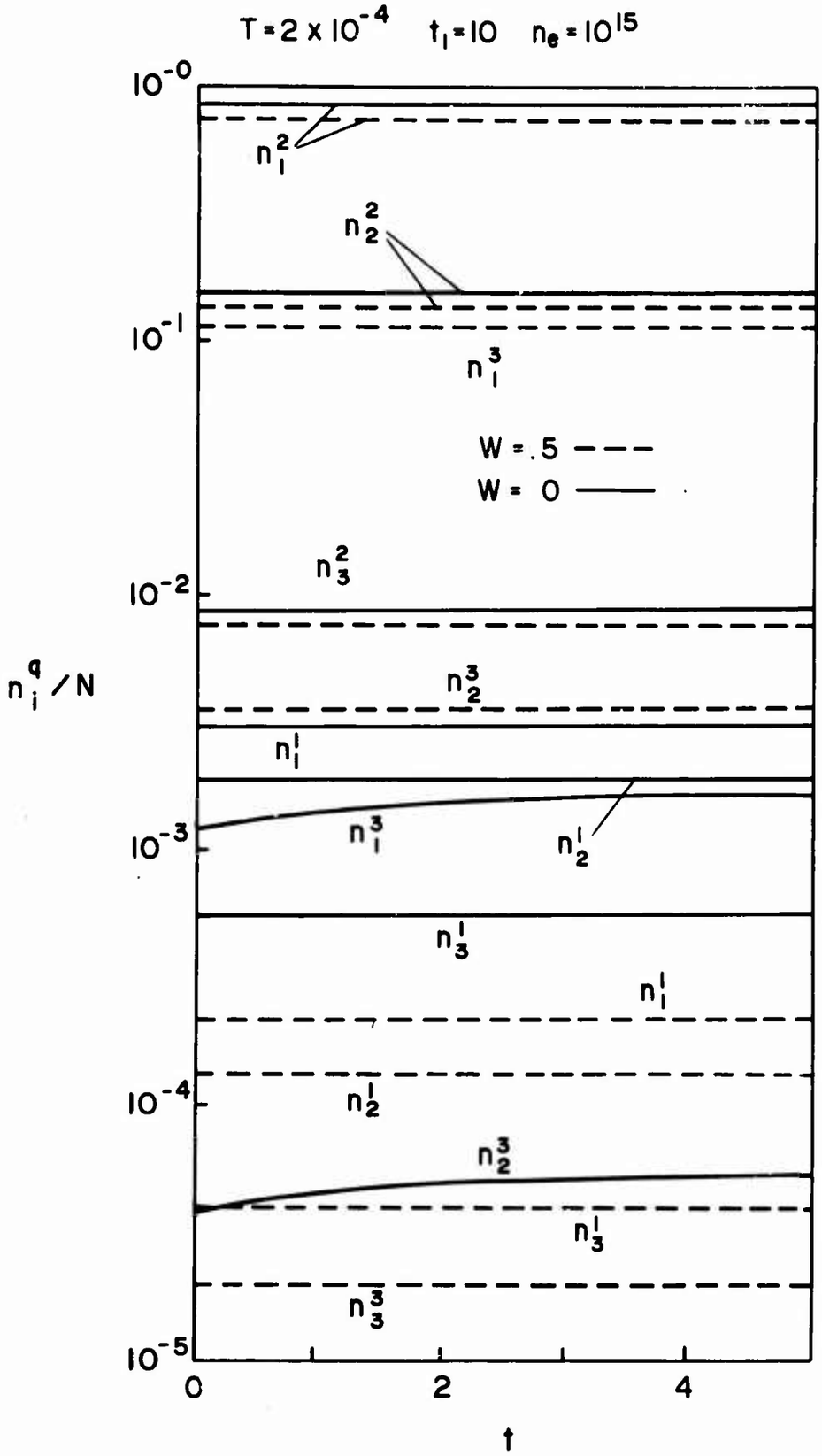


Figure IV. E-11. Relative Level Populations vs t. For W = 0 the Solutions are Symmetrical about $t_1/2$.

IV.E.4 EMITTED RADIATION

We shall characterize the radiation by the spectrum emitted perpendicular to the layer at the surface, I_ν (0, 1). For optically thin regions, this spectral distribution is usually very nearly the same as that of the volume emission coefficient. We consider separately the contributions from optically thin lines, optically thick lines, free-bound continua and free-free continua.

The thin line specific intensity is,

$$\frac{n_{uT} A_{u\ell} h\nu \Phi_\nu}{4\pi} \qquad \text{(IV. E-21)}$$

where n_{uT} is the total number of nitrogen particles in the upper state in a 1 cm. column in the line of sight. The values of $A_{u\ell}$ for the transitions in the model are given in Table IV. E-7. The total amount of energy emitted in the line/cm^2 sec. unit solid angle is independent of Φ_ν and is given by

$$\frac{n_{uT} A_{u\ell} h\nu}{4\pi} \qquad \text{(IV. E-22)}$$

while the central intensity for a Doppler profile is

$$\frac{n_{uT} A_{u\ell} h\nu}{4\pi^{3/2} \Delta\nu_D} \qquad \text{(IV. E-23)}$$

In the optically thick line (i.e., $t \gtrsim 1$) where κ_c and κ_o are the continuum and line center absorption coefficients respectively, the intensity is given by

$$\int_0^{t_1} (\varphi_\nu S_L + \epsilon_c/\kappa_o)\ e^{-(\varphi_\nu + r_o)t}\, dt. \qquad \text{(IV. E-24)}$$

ϵ_c is the continuum emission coefficient at the line center. In Section IV. E-2, we found expressions for the mean intensity J_ν in the non-thin line which were required to evaluate the upward excitation rates entering the population rate equations. We now use these expressions to explicitly evaluate equation (IV. E-9) for the line source function, yielding,

$$\frac{S_L}{B} = \frac{\epsilon}{\epsilon+\eta} + \frac{1}{1+\epsilon+\eta} \sum_\alpha L_\alpha e^{-k_\alpha t} + \frac{1}{\epsilon+\eta}\ \iota/B. \qquad \text{(IV. E-25)}$$

TABLE IV. E-7. ALLOWED BOUND-BOUND TRANSITION PROBABILITIES

Allowed Transition Upper q_i	Lower q_i	Designation	Einstein Coefficient A^q_{ij}	λ_o (Å)
14	11	a	1.92×10^8	1200
15	14	b	1.04×10^7	8121
24	21	c	1.31×10^9	671
25	24	d	3.47×10^7	5100
33	31	e	2.04×10^9	813
43	41	f	3.30×10^9	765
44	43	g	6.52×10^9	387
52	51	h	3.37×10^8	1240
64	61	i	1.70×10^{12}	28.8
72	71	j	1.46×10^{12}	24.8

Using Eq. (IV. E-25) in Eq. (IV. E-3), the line profile at t = 0 and $\mu = 1$ becomes

$$\frac{I_\nu(0,1)}{B} = \left(\frac{\epsilon + \iota/B}{\epsilon + \eta}\right)\left(1 - e^{-\varphi t_1}\right)$$

$$+ \sum_\alpha \frac{\varphi L'_\alpha}{(k_\alpha + \varphi)}\left[1 - e^{-(k_\alpha + \varphi)\, t_1}\right]$$

$$+ \sum_\alpha \frac{\varphi L'_\alpha}{(\varphi - k_\alpha)}\, e^{-k_\alpha t_1}\left[1 - e^{-(\varphi - k_\alpha)\, t_1}\right] \qquad \text{(IV. E-26)}$$

where $L'_\alpha = \dfrac{L_\alpha}{1 + \epsilon + \eta}$.

Line profiles for both thick and thin transitions are illustrated in Figure IV. E-12 for $T_e = T_r = 2 \times 10^{4°}$ K. The central minima observed in the thick lines indicate that the source function is increasing inward from the surface of the layer (as can be seen from Figure IV. E-1). The line profile, reflecting roughly the depth variation of the source function, increases outward from the line center and falls off only for frequencies where the layer becomes transparent. The central minimum becomes more pronounced as the amount of scattering increases (i.e., ϵ becomes small) and t_1 increases.

The intensity at wavelength λ due to free-bound continuum emission is the summation over all such continua with ionization thresholds $\lambda_j > \lambda$. Each continua has the intensity

$$n_{iT} n_e \frac{h^2 c}{4\pi m} Q_R f\left(\frac{1}{\lambda} - \frac{1}{\lambda_j}\right) \qquad \text{(IV. E-27)}$$

where n_{iT} is the total number of recombining ions in the line of sight and Q_R is the recombination cross section. f is the electron distribution function, assumed to be Maxwellian. Q_R is obtained from the photoionization cross-section which is determined using the quantum defect method

Finally, for the free-free emission Kramer's result yields (IV. E-7),

$$5.44 \times 10^{-39}\, Z^2 \exp\left(-h\nu/k T_e\right) T_e^{-1/2}\, n_e n_i \qquad \text{(IV. E-28)}$$

where we assume a unit gaunt factor.

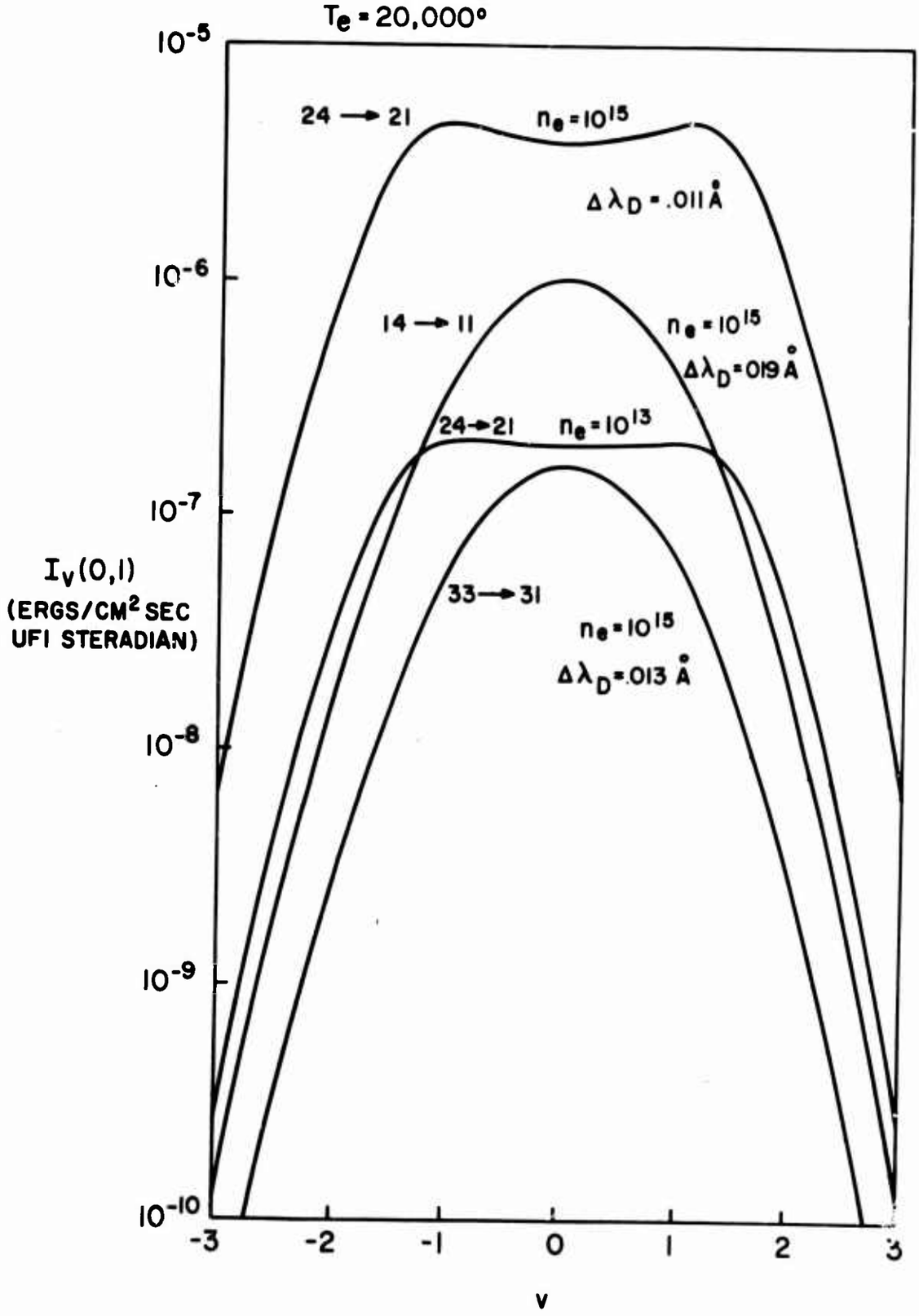


Figure IV. E-12. Line Profiles for Optically Thin and Non-Thin Lines vs. $v = \Delta v/\Delta v_o$

The emitted spectrum is illustrated in Figures IV. E-13-19 for various values of T_e, n_e and t_1 with W = 0. The intensity per unit frequency interval is given vs wavelength.

Since the layers considered are quite optically thin in the continuum, even a very small value of W yields a much larger background radiation field than the emission from the layer itself. (The three largest continuum optical depths for each case are given in Table IV. E-10). The wavelengths of the possible free-bound emission edges and the corresponding transitions are given in Table IV. E-8. The numbering of the edges in the table is followed in the figures. For comparison, the LTE result, $\kappa_\nu B_\nu$ is also given, by the dashed curves, for the f-b radiation. The f-f emission is generally very small except at longer wavelengths and then is only significant because we do not include many higher levels in our model. The region of maximum emission shifts in general to higher wavelengths in the non LTE case as a result of the shift of the more heavily populated species to lower stages of ionization. The optically thin emission lines have a Gaussian shape with half width $\frac{\lambda_o}{c} (1\ n\ 2) \sqrt{\frac{2kT}{M}}$ while the shape of the non-thin line is complex as seen in Figure IV. E-12. The position and central intensity of each line is noted on each figure. The lines are designated by the letters given in Table IV. E-7.

It is interesting to compare the total amount of energy radiated by the plasma in the various lines and in the continua. For each of the cases illustrated in Figures IV. E-13-19, Table IV. E-9 gives the relative contributions to the total energy emitted by the thick and thin lines and the b-f and f-f continua to 5000 Å. The contribution from each individual line is given in Table IV. E-10. Also given in Table IV. E-10 are the continuum optical depths of the layer at the three bound-free thresholds where the optical depth is the largest. In the free-bound continua, the total energy radiated is always less in the non-LTE than in the LTE case. In each case, more energy is radiated in the optically thick line than by all other processes. The total continuum equilibrium radiation is much less than the optically thick value of $\sigma/\pi\ T^4$ due to the very low average value of the continuum optical depth as illustrated in Table IV. E-10. The situation treated in these cases, where essentially one line is just becoming optically thick, probably maximizes the influence of the line radiation over the continuum radiation. It is clear that an accurate specification of the total radiated energy will require consideration of more energy levels thus involving simultaneous solution of several transfer equations.

We note that the amount of energy radiated is very sensitive to the small populations of the upper levels of the resonance lines. A closer inspection of the mechanisms involved in populating these levels is thus appropriate at this point. The terms entering the numerator of Eq. (IV. E-9) each represent a method of populating the upper level from the lower level. The first term represents direct radiative excitation, the second direct collisional excitation and the third any combination of radiative or collisional processes involving one or more intermediate levels in going from the lower to the upper level. The denominator, on the other hand, consists of

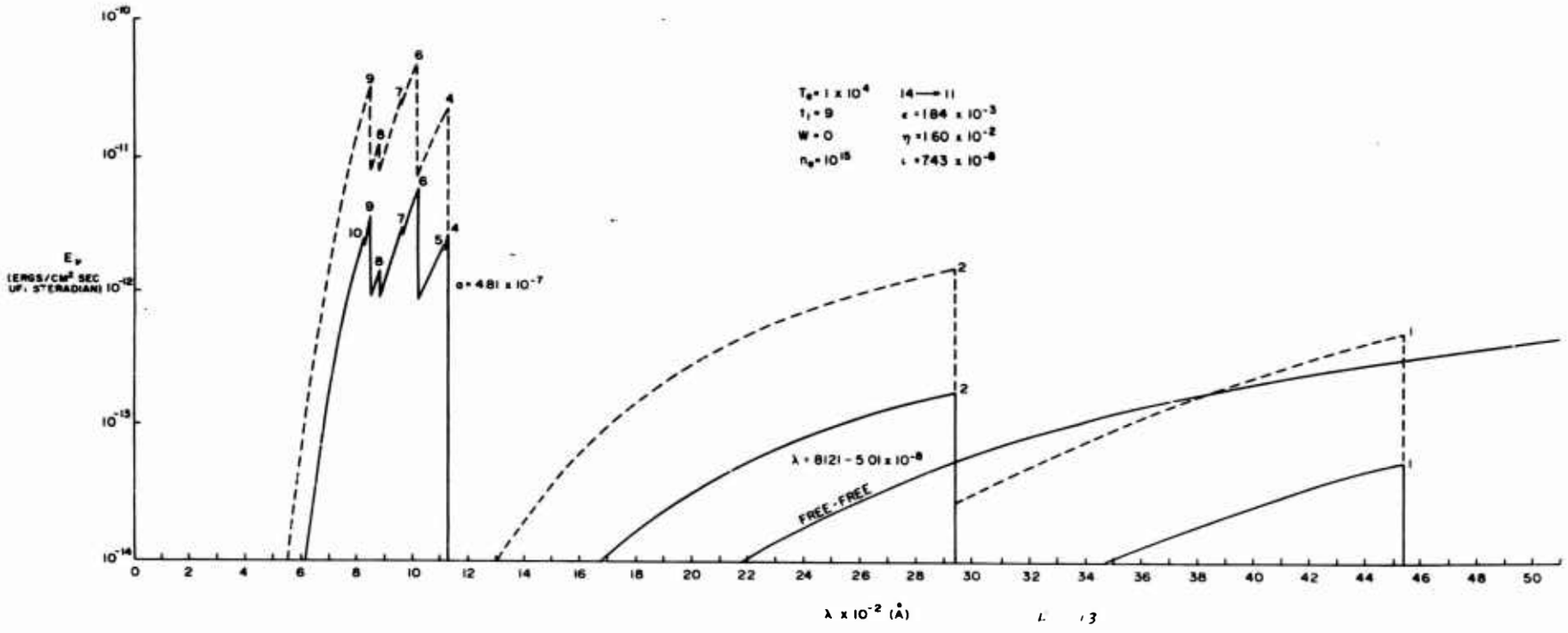


Figure IV. E-13. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

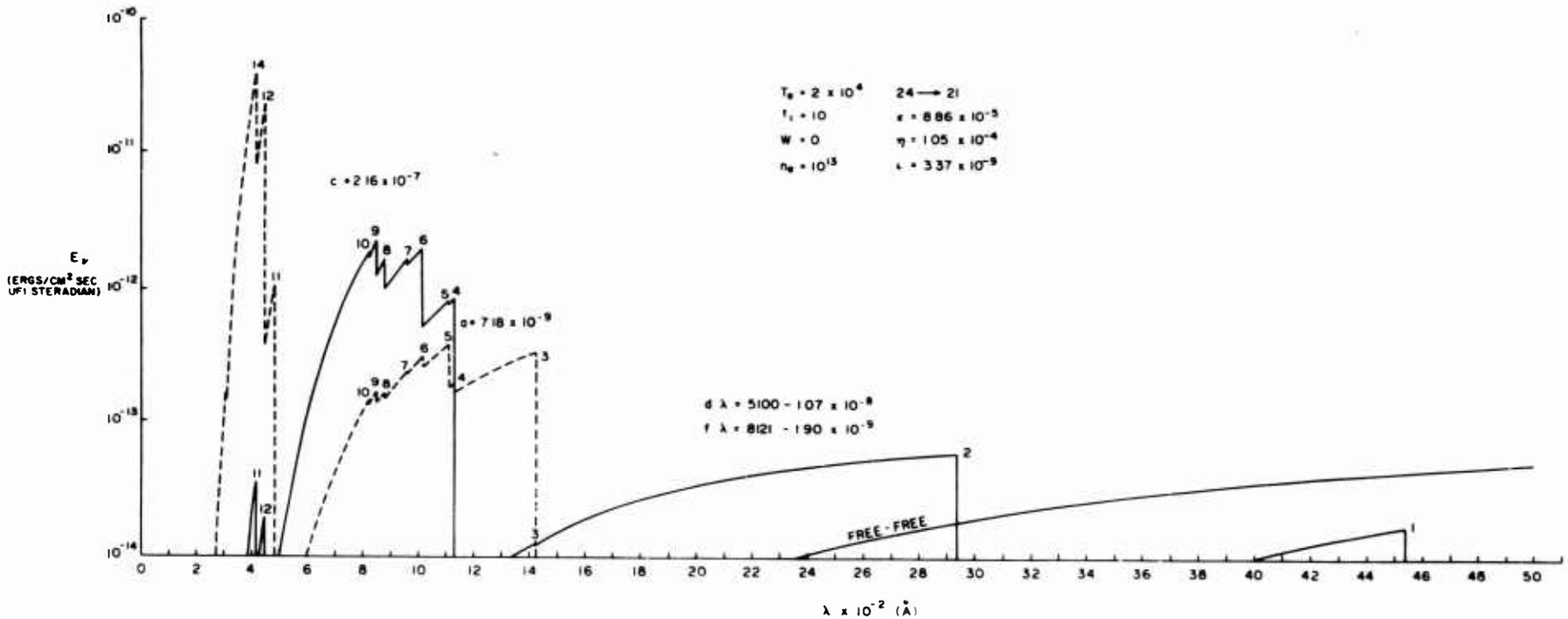


Figure IV. E-14. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

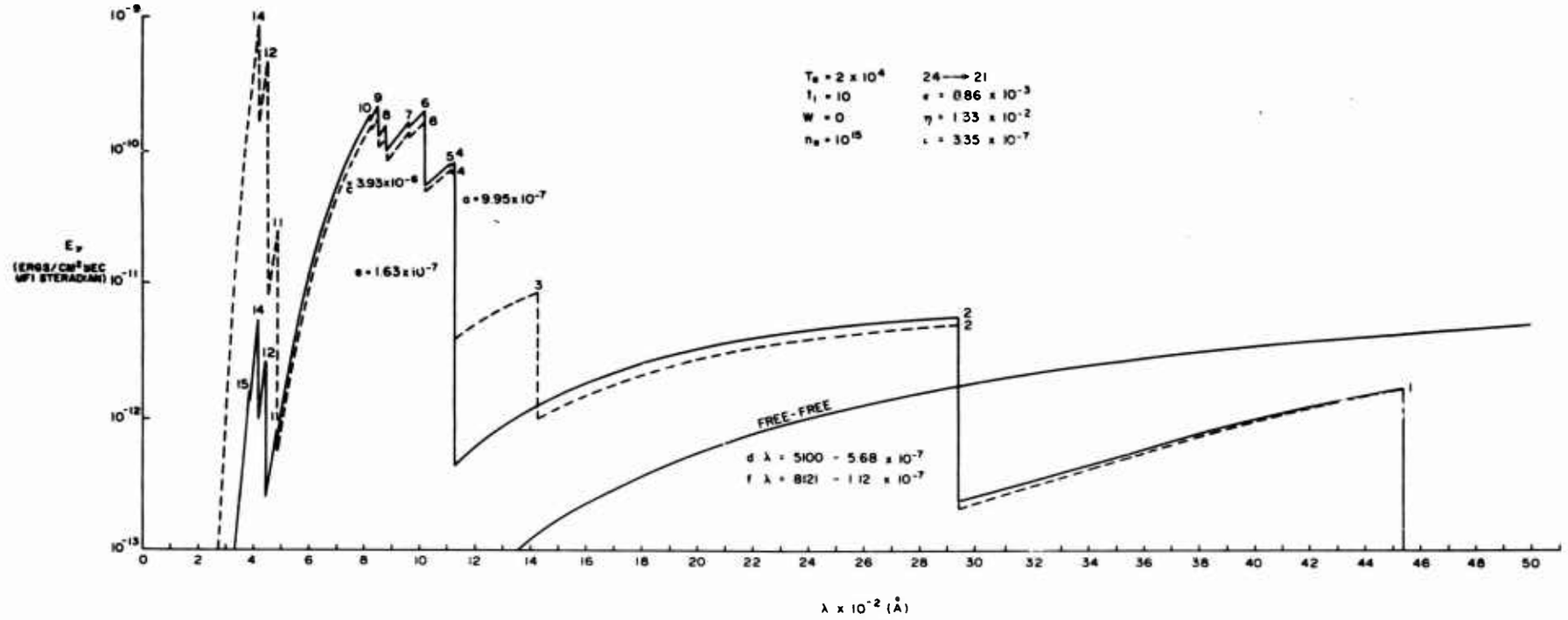


Figure IV. E-15. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

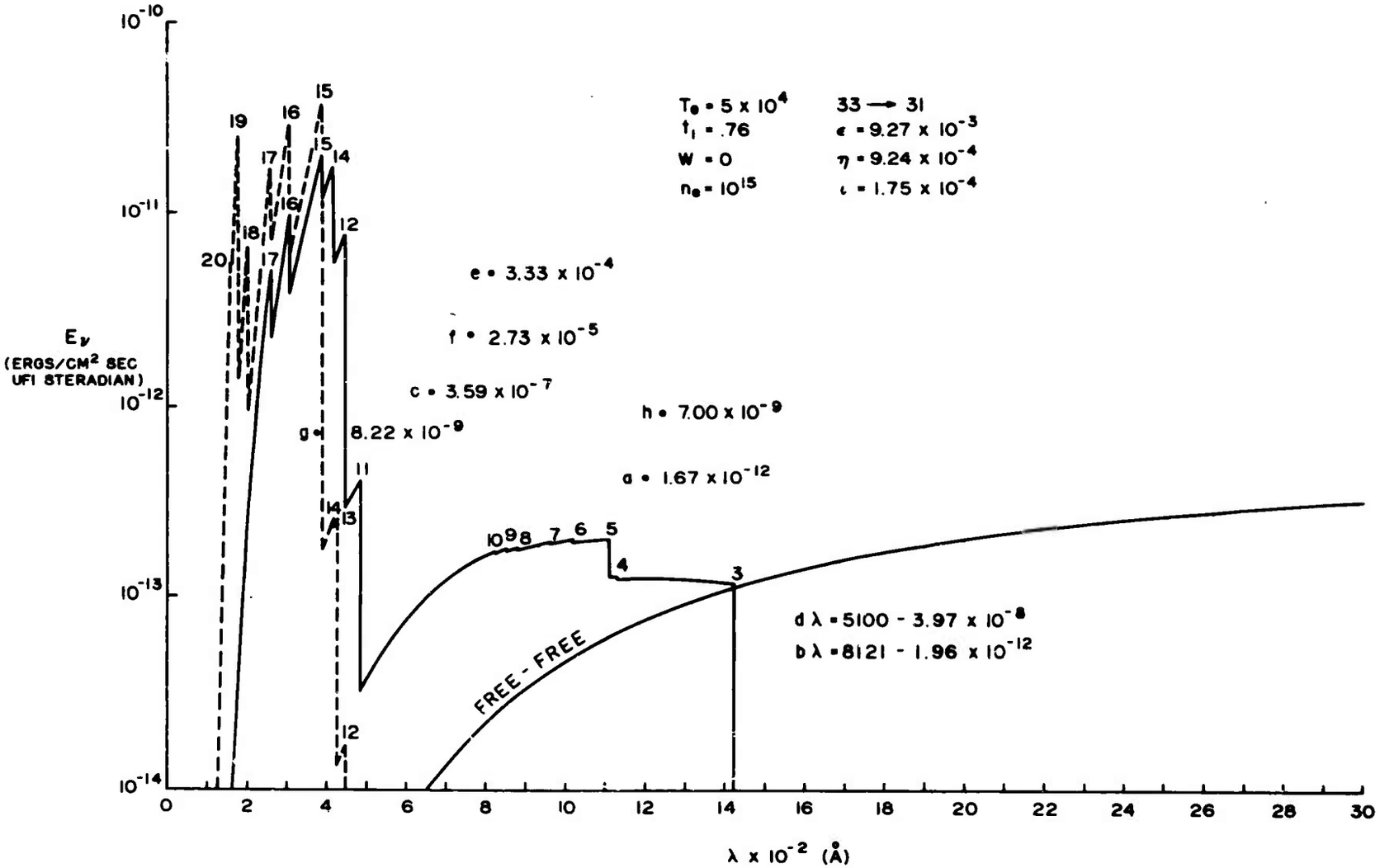


Figure IV. E-16. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

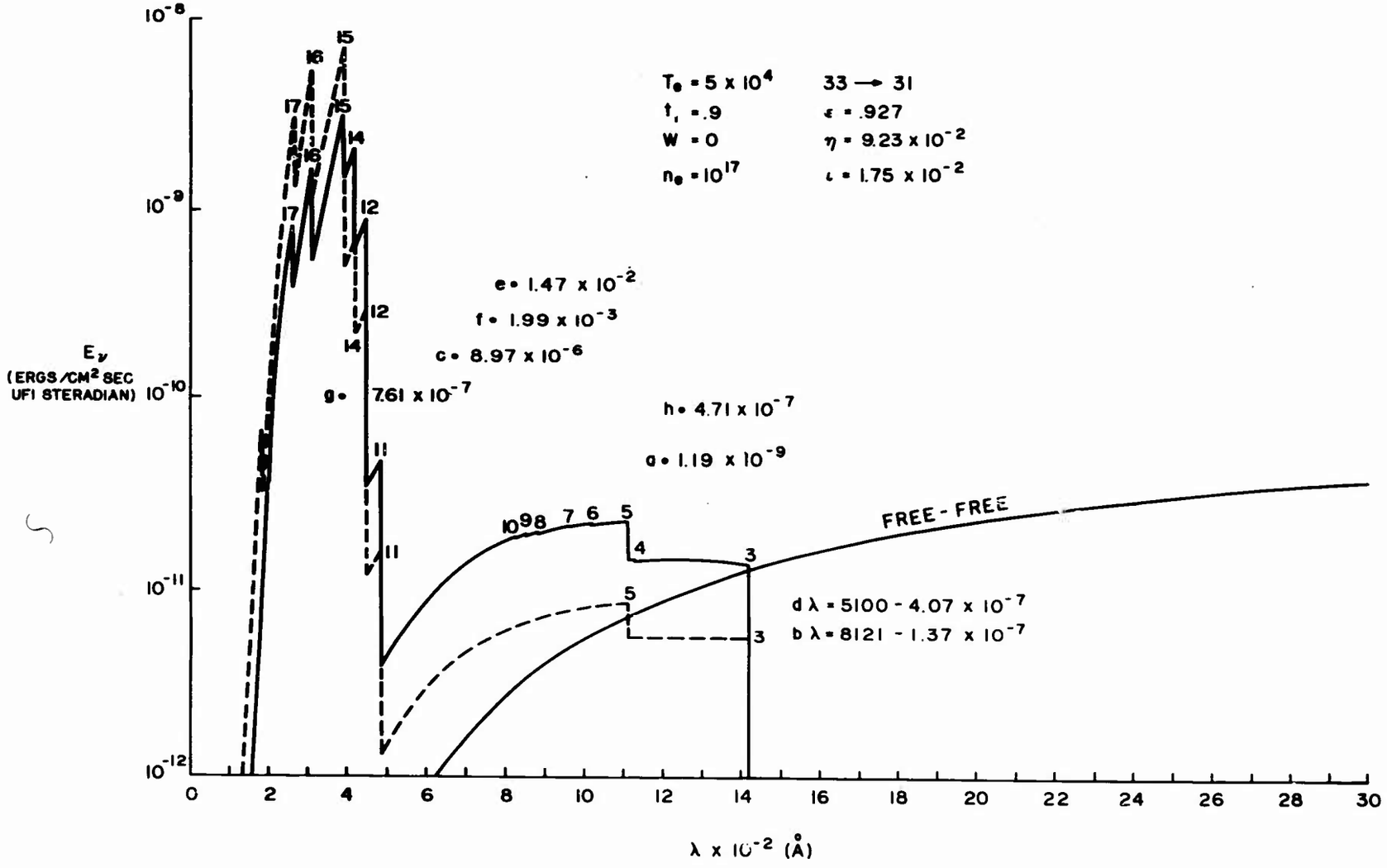


Figure IV. E-17. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

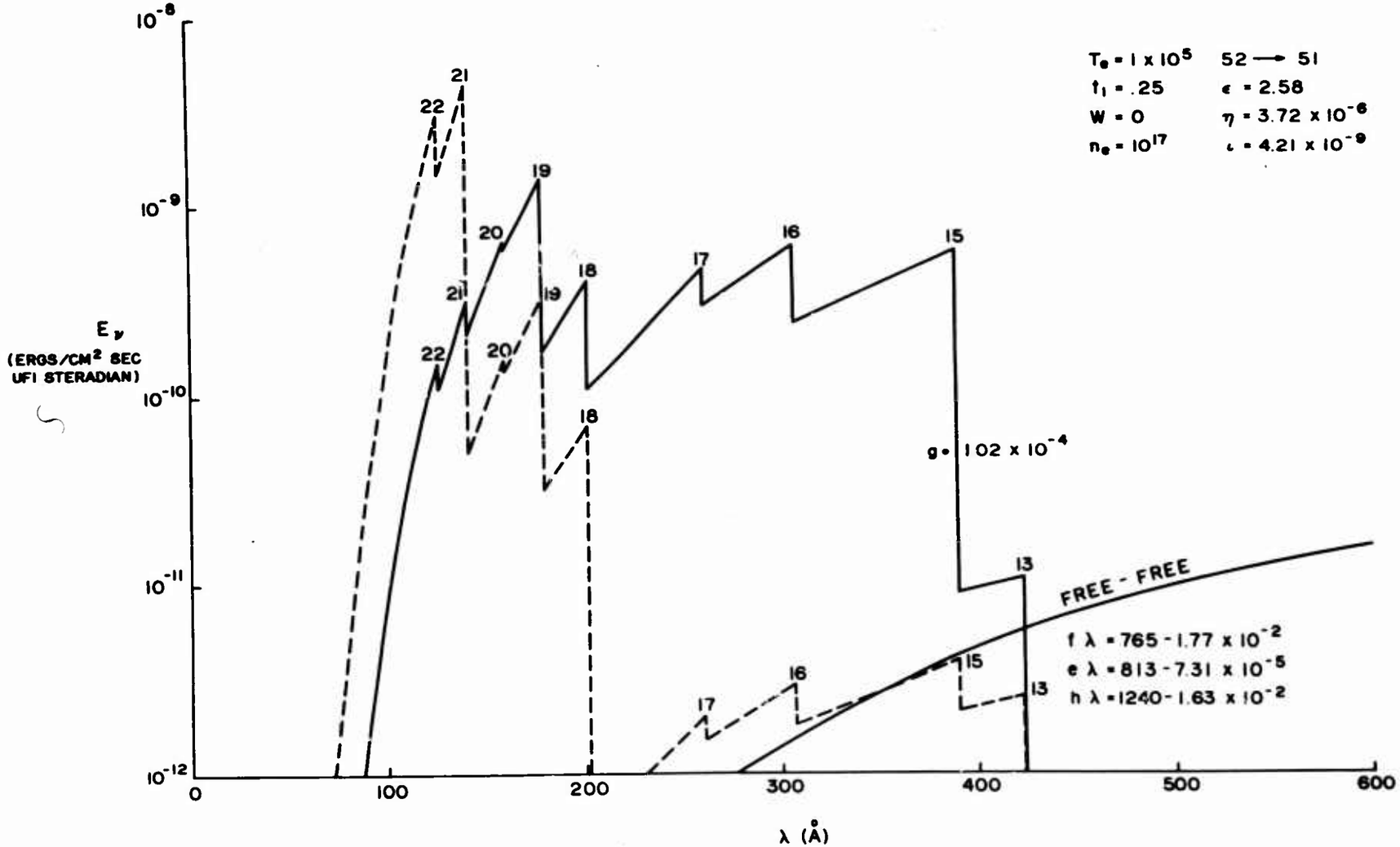


Figure IV. E-18. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

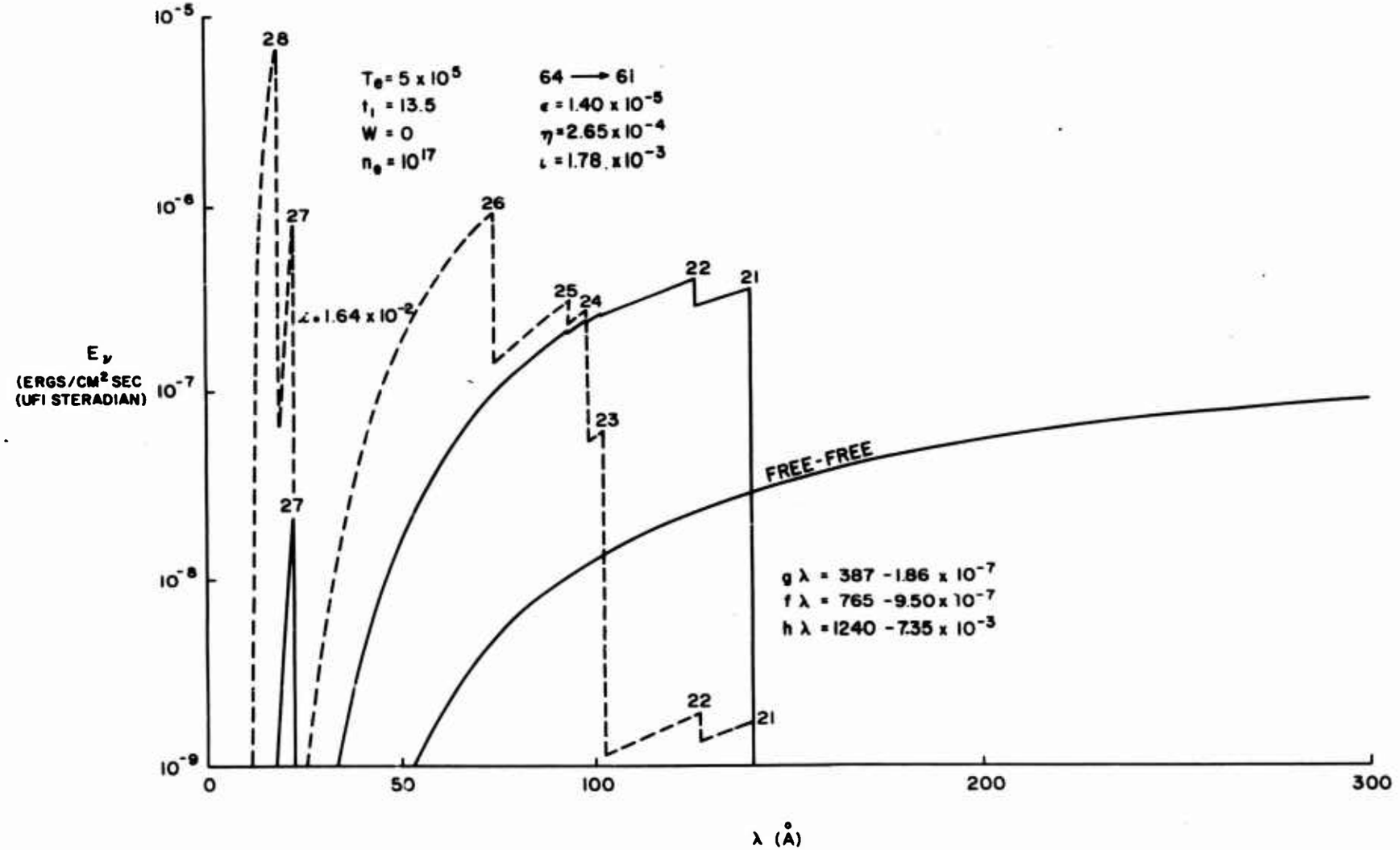


Figure IV. E-19. Radiated Energy Perpendicular to the Surface/sec cm^2 unit frequency interval (ufi) unit solid angle (usa). The dashed curves represent the equilibrium free-bound radiation at this same n_e and T_e. The thick line transition is indicated at the top of the figure.

TABLE IV. E-8. DESIGNATION OF FREE-BOUND RECOMBINATION THRESHOLDS

Designation	λ_o	Upper State qi		Lower State qi
1	4540	(2, 1)	→	(1, 5)
2	2939	(2, 1)	→	(1, 4)
3	1424.5	(3, 1)	→	(2, 5)
4	1130	(2, 1)	→	(1, 3)
5	1112.3	(3, 1)	→	(2, 4)
6	1019.2	(2, 1)	→	(1, 2)
7	963.2	(2, 2)	→	(1, 3)
8	881.6	(2, 2)	→	(1, 2)
9	852.2	(2, 1)	→	(1, 1)
10	825.1	(2, 3)	→	(1, 3)
11	485.1	(3, 1)	→	(2, 3)
12	447.4	(3, 1)	→	(2, 2)
13	423.7	(5, 1)	→	(4, 4)
14	418.7	(3, 1)	→	(2, 1)
15	389.6	(4, 1)	→	(3, 3)
16	307.3	(4, 1)	→	(3, 2)
17	261.4	(4, 1)	→	(3, 1)
18	202.4	(5, 1)	→	(4, 3)
19	179.3	(5, 1)	→	(4, 2)
20	160.0	(5, 1)	→	(4, 1)
21	141.06	(6, 1)	→	(5, 2)
22	126.7	(6, 1)	→	(5, 1)
23	102.14	(7, 1)	→	(6, 4)
24	98.57	(7, 1)	→	(6, 3)
25	93.73	(7, 1)	→	(6, 2)
26	74.36	(8, 1)	→	(7, 2)
27	22.46	(7, 1)	→	(6, 1)
28	18.59	(8, 1)	→	(7, 1)

TABLE IV.E-9. TOTAL EMISSION (E) AT ALL FREQUENCIES FOR VARIOUS PROCESSES E (ERGS/CM^2 SEC STERADIAN)

T_e (^oK)	n_e (cm^{-3})	Thick Transition	Free-Bound Continua	Equilibrium Free-Bound Continua	Free-Free Continua	Total Thin Line	Thick Line	$\frac{\sigma}{\pi} T_e^4$
10^4	10^{15}	14 → 11	3.02 + 3	2.56 + 4	6.85 + 1	3.78 + 2	5.07 + 4	1.82 + 11
2×10^4	10^{13}	24 → 21	2.39 + 3	3.70 + 4	1.82 + 1	8.99 + 1	4.94 + 4	2.92 + 12
2×10^4	10^{15}	24 → 21	2.34 + 5	1.01 + 6	1.82 + 3	9.91 + 4	1.07 + 6	2.92 + 12
5×10^4	10^{15}	33 → 31	4.74 + 4	1.42 + 5	4.60 + 2	4.05 + 6	2.35 + 7	1.14 + 14
5×10^4	10^{17}	33 → 31	7.44 + 6	1.86 + 7	5.46 + 4	3.56 + 8	2.58 + 9	1.14 + 14
10^5	10^{17}	52 → 51	6.86 + 6	1.50 + 7	1.19 + 4	1.78 + 9	2.52 + 9	1.82 + 15
5×10^5	10^{17}	64 → 61	5.87 + 9	2.69 + 11	1.18 + 9	2.56 + 9	5.95 + 11	1.14 + 18

TABLE IV. E-10. THIN LINE AND CONTINUUM OPTICAL DEPTHS

T_e (^oK)	n_e (cm^{-3})	Thin Transition	Energy Radiated ($ergs/cm^2$ sec steradian)	Optical Depth	Continuum Transition	Optical Depth
10^4	10^{15}	15 → 14	3.78 + 2	5.03-4	11 → 21	1.18-3
					12 → 21	1.97-4
					12 → 22	1.54-4
2×10^4	10^{13}	14 → 11	5.15 + 1	8.25-2	21 → 31	5.43-3
		15 → 14	2.02 + 1	1.71-6	22 → 31	1.28-3
		25 → 24	1.82 + 1	7.49-6	23 → 31	2.38-5
2×10^4	10^{15}	14 → 11	7.11 + 4	9.40-2	21 → 31	5.43-3
		15 → 14	1.19 + 3	2.36-4	22 → 31	1.28-3
		25 → 24	9.60 + 3	6.29-4	23 → 31	2.39-5
		33 → 31	1.72 + 4	.109		
5×10^4	10^{15}	14 → 11	1.90	3.14-8	31 → 41	1.35-5
		15 → 14	3.28-2	3.96-9	32 → 41	8.12-6
		24 → 21	7.30 + 4	1.22-3	21 → 31	1.04-6
		25 → 24	1.06 + 3	9.39-6		
		43 → 41	3.95 + 6	9.36-2		
		44 → 43	2.90 + 4	2.14-6		
		52 → 51	7.68 + 2	9.99-6		
5×10^4	10^{17}	24 → 21	1.82 + 6	9.46-4	31 → 41	1.59-5
		25 → 24	1.07 + 4	2.34-4	32 → 41	1.05-5
		43 → 41	3.58 + 8	.17	33 → 41	3.07-6
		44 → 43	2.68 + 5	1.92-4		
		52 → 51	5.18 + 4	2.95-4		
10^5	10^{17}	33 → 31	1.74 + 7	1.35-4	42 → 51	3.53-6
		43 → 41	1.74 + 9	.11	51 → 61	2.77-6
		44 → 43	5.09 + 7	6.50-4	52 → 61	2.65-6
5×10^5	10^{17}	43 → 41	5.35 + 5	4.79-6	61 → 71	1.99-3
		44 → 43	2.06 + 5	9.13-8	71 → 81	1.74-5
		52 → 51	2.56 + 9	7.25-2	52 → 61	3.56-6

terms indicating transition paths from the upper to the lower level. All the terms are normalized with respect to A_{21}. The first term represents direct radiative de-excitation, the second direct collisional de-excitation, and the third any indirect process going from the upper to the lower state. ϵ, η, ι /B, and $J_\nu \Phi_\nu \, d\nu = F$ for the cases illustrated in Figures IV. E-13-19 are given in Table IV. E-11. F varies with t and we give the values at t = 0 and $t = t_1/2$.

Two types of behavior are distinguished. When the upper resonance line level lies close to the continuum, indirect processes dominate direct collisional processes in depopulating the upper level. Hence for the lower temperatures $\eta > \epsilon$. In NI-NIV ions there are low lying levels between the upper and lower resonance levels which are not radiatively coupled with any other bound levels. The indirect depopulation of the upper level is roughly evenly divided between collisional ionization and radiative recombination, and two step collisional de-excitation involving one of these metastable levels. Since $\iota/B > \epsilon$ the indirect population also dominates direct collisional population for the lower temperatures. Since the collisional excitation or ionization rate decreases exponentially with energy separation, the indirect collisional population through the continuum is small. The indirect population is governed instead by two step collisional processes involving lower levels. We recall for W = 0 there are no radiative excitations or ionizations. Other types of behavior would be experienced for $W \neq 0$. When the upper level is quite close to the ground state, on the other hand, both forward and reverse indirect processes are less than the direct collisional rates (cf 10^5 °K case), i.e., $\epsilon > \iota/B$ and $\epsilon > \eta$.

TABLE IV. E-11. SOURCE FUNCTION PARAMETERS

T_e (^oK)	n_e (cm^{-3})	ϵ	η	ι / B	F ($t = 0$)	F ($t = t_1/2$)
10^4	10^{15}	1.84-3	1.60-2	5.22-2	.159	.496
2×10^4	10^{13}	8.86-5	1.05-4	1.16-4	7.57-4	2.48-3
2×10^4	10^{15}	8.86-3	1.33-2	1.16-2	6.18-2	.197
5×10^4	10^{15}	9.27-3	9.24-4	7.93-3	7.42-3	9.34-3
5×10^4	10^{17}	.927	9.23-2	.793	.334	.434
10^5	10^{17}	2.58	3.72-6	4.42-6	9.68-2	.105
5×10^5	10^{17}	1.40-5	2.65-4	2.34-3	1.08-2	4.61-2

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V. CONCLUSIONS

It has been shown herein that one can solve the complete time-dependent Navier-Stokes equations for a spherically-symmetric explosion. That is, it has been shown that it is possible to utilize the exact equation for the conservation of momentum (Navier-Stokes equation), such that no artificial viscosity effect is present to mask the true molecular viscosity effects on the structure of the strongly viscous regions, i.e., the inner and outer moving shocks for a spherically-symmetric explosion.

However, it has been found that in order to maintain desired accuracy, a new mesh size restriction must be imposed, namely that the local spatial mesh utilized in the computations must be of the order of the local mean free path in the gas. If one is utilizing a flow model in which the viscosity is assumed absent, this restriction does not appear. If, on the other hand, one utilizes the complete Navier-Stokes equations, the viscous effects are masked from the solution in those regions of the flow field where the local spatial mesh is considerably larger than the local mean free path. While, if the local spatial mesh utilized is orders of magnitude smaller than the local mean free path, the inviscid effects are masked. In the case of a spherically-symmetric burst, due to the very large drop in gas density near the center of the spherical region, the latter situation of obtaining a large local mean free path actually occurs and, hence, the choice of the computation mesh is crucial.

In this study, there has been a successful demonstration of the numerical solution of the time-dependent radiation transfer equation rather than the usual "steady state" formulation. Moreover, this time dependent equation has been solved simultaneously with the time-dependent energy equation, prior to the initiation of gas dynamic motion.

It is noted that in this new formulation, in spite of the spherical symmetry, there are three independent variables in the partial differential equation for the intensity of the radiation, i.e., angle, radius and time. In the case of spherical symmetry, the temperature distribution, however, depends only on two independent variables, i.e., radius and time.

Future applications and extensions of the methods derived herein should be concerned with:

1. The derivation of a suitable efficient coordinate transformation which scales the computation mesh directly as the local mean free path and not by means of an arbitrary geometric function.

2. The simultaneous solution of the complete set of time-dependent gas dynamic equations with the coupled radiative energy transfer equation.

3. The inclusion of flow asymmetries and departures from spherical symmetry.

4. The incorporation of the effects of charged particles and the Earth's magnetic field.

5. The incorporation of non-LTE effects into the overall model.

APPENDIX A. THE DIFFERENCE EQUATIONS

After the η-transformation is introduced, the equations can be put in the following form:

$$\frac{\partial Y}{\partial t} = A \frac{\partial Y}{\partial \eta} + B,$$

$$Y = \begin{pmatrix} \rho \\ V \\ T \end{pmatrix}, \quad A = \begin{pmatrix} -a_1 & -a_2 & 0 \\ -b_1 & -a_1 & -b_3 \\ 0 & -c_2 & -a_1 \end{pmatrix}, \quad B = \begin{pmatrix} -a_3 \\ 0 \\ -c_3 \end{pmatrix},$$

$$a_1 = V\eta_x + \eta_t, \quad a_2 = \rho \eta_x, \quad a_3 = \frac{\delta}{x} \rho V,$$

$$b_1 = \frac{RT\eta_x}{\rho}, \quad b_3 = \eta_x R,$$

$$c_2 = \frac{RT\eta_x}{C_v}, \quad c_3 = \frac{\delta RV}{xC_v},$$

$$\eta_x = \frac{\partial \eta}{\partial X}, \quad \eta_t = \frac{\partial \eta}{\partial t},$$

$$\delta = \begin{cases} 0: & \text{Cartesian coordinates} \\ 2: & \text{Spherically-symmetric coordinates (x=r)} \end{cases}$$

The matrix A is diagonalized by M. That is, $MAM^{-1} = D$

where

$D = \text{diag}\,(\lambda_1, \lambda_2, \lambda_3)$ - see for example, Eq. (II.C-11).

$$M = \begin{pmatrix} c_2 & o & -a_2 \\ -b_1 & c_s & -b_3 \\ b_1 & c_s & b_3 \end{pmatrix}, \quad c_s^2 = c_2 b_3 + a_2 b_1 .$$

The difference equation is obtained by differencing the ith component of the vector $M\,\partial Y/\partial\eta$ according to the sign of λ_i. Forward differences are used if λ_i is positive and backward differences are used if λ_i is negative. After some manipulation the difference equations can be written in the following form:

$$Y_t = AY_\eta + \frac{\Delta\eta}{2} A^* Y_{\eta\eta} \ ,$$

where

$$Y_t = Y_j^{n+1} - Y_j^n \ ,$$

$$Y_\eta = \frac{1}{2\Delta\eta} \left(Y_{j+1}^n - Y_{j-1}^n\right) \ ,$$

$$Y_{\eta\eta} = \frac{1}{\Delta\eta^2} \left(Y_{j+1}^n - 2Y_j^n + Y_{j-1}^n\right) \ ,$$

where

$$Y_j^n = Y(n\Delta t,\ j\Delta x).$$

$$A^* = M^{-1} |D| M,$$

$$|D| = \text{diag}\left(|\lambda_1|,\ |\lambda_2|,\ |\lambda_3|\right).$$

Letting $A^* = (a_{ij}^*)$,

$$a_{11}^* = |a_1| + \frac{a_2 b_1}{c_s} \alpha_1 \ ,$$

$$a_{12}^* = a_2 \alpha_2 \ ,$$

$$a_{13}^* = \frac{a_2 b_3}{c_s} \alpha_1 \ ,$$

$$a_{21}^* = b_1 \alpha_2 \ ,$$

$$a_{22}^* = |a_1| + c_s \alpha_1 \ ,$$

$$a_{23}^* = b_3 \alpha_2$$

$$a^*_{31} = \frac{c_2 b_1}{c_s} \alpha_1 \ ,$$

$$a^*_{32} = c_2 \alpha_2 \ ,$$

$$a^*_{33} = |a_1| + \frac{c_2 b_3}{c_s} \alpha_1 \ ,$$

where

$$\alpha_1 = \begin{cases} 0: \ |a_1| > c_s \\ 1 - \dfrac{|a_1|}{c_s} : \ |a_1| < c_s \end{cases} \ ,$$

$$\alpha_2 = \begin{cases} 1: \ a_1 > c_s \\ \dfrac{a_1}{c_s} : \ |a_1| < c_s \\ -1: \ a_1 < c_s \end{cases} \ ,$$

The stability criterion is,

$$\frac{\Delta t}{\Delta \eta} \leq \frac{1}{|a_1| + c_s}$$

APPENDIX B. SCALING THE DIFFERENTIAL EQUATIONS

A partial scaling of the differential equations can be achieved in the following manner. Introduce constants ρ_o, t_o, X_o. Define new variables:

$$\bar{\rho} = \rho/\rho_o \ ,$$

$$\bar{dx} = dX/X_o \ ,$$

$$\bar{dt} = dt/t_o \ .$$

Letting $c_o = t_o/X_o$, Eqs. (II.C-1) to (II.C-3) take the form

$$\frac{1}{c_o}\frac{\partial\bar{\rho}}{\partial\bar{t}} = -V\frac{\partial\bar{\rho}}{\partial\bar{x}} - \bar{\rho}\frac{\partial V}{\partial\bar{x}} \ ,$$

$$\frac{\bar{\rho}}{c_o}\frac{\partial V}{\partial\bar{t}} = -\bar{\rho}\,V\frac{\partial V}{\partial\bar{x}} - RT\frac{\partial\bar{\rho}}{\partial\bar{x}} - \bar{\rho}\,R\frac{\partial T}{\partial\bar{x}} \ ,$$

$$\frac{\bar{\rho}\,C_v}{c_o}\frac{\partial T}{\partial\bar{t}} = -\bar{\rho}\,C_v V\frac{\partial T}{\partial\bar{x}} - \bar{\rho}\,RT\frac{\partial V}{\partial\bar{x}} \ .$$

We note first that ρ_o does not affect the solution; that is, the density rise and not the density level is the significant quantity. (The value of ρ_o actually used in the calculation is simply a value that, from other considerations, was convenient at the time the calculation was made.)

Also, it is clear that if X_o and t_o are changed in the same ratio, so that c_o is constant, then the solution is unchanged. However, this is somewhat misleading, since the boundary and initial conditions are defined in terms of real X and t. For example, if the equations were solved in the $\bar{x}$, $\bar{t}$ form, then the solution can be extended to other values of X_o and t_o (where c_o remains constant) if, and only if, the real boundary and initial conditions are changed so as to remain unchanged in the $\bar{t}$, $\bar{x}$ form.

APPENDIX C. AN ITERATION PROCEDURE

Throughout the program many relationships are encountered which require iteration. Rather than have a separate procedure for each case, we found it advantageous to write one fairly general technique: it is then necessary to make each case conform to the specified format.

We assume that the equation can be intelligently written in the form:

$$x = f(x)$$

Note that any root problem can be put in this form:

Suppose we want a root of $g(x) = 0$. An equivalent problem is to solve:

$$x = f(x), \text{ where } f(x) = x + g(x)$$

A well-known method of iteration is that of successive approximations:

$$x_{n+1} = f(x_n)$$

The conditions for convergence are also well-known:

$$|f'(x)| < 1 \text{ in the vicinity of the solution*}$$

Another iteration procedure is as follows:

Let x_1 be the first guess.

Then x_{n+1} is the intersection of these lines:

$$y = x_{n+1}$$

$$y = \left[f'(x_n)\right] x + \left[f(x_n) - x_n f'(x_n)\right]$$

[The second line is the line through $\left(x_m, f(x_n)\right)$ with slope $f'(x_n)$] .

*Scarborough, J. B., Numerical Mathematical Analysis, third edition, Johns Hopkins Press, Baltimore, 1955.

or,

$$x_{n+1} = x_{n+1} f'(x_n) + f(x_n) - x_n f'(x_n)$$

$$x_{n+1} = \frac{f(x_n) - x_n f'(x_n)}{1 - f'(x_n)}$$

This process will also converge under certain conditions. We will establish convergence under these conditions:

a. $f'(x) < 0$

b. $f'(x)$ monotone

Let x be solution: $\bar{x} = f(\bar{x})$

$$x_{n+1} - \bar{x} = \frac{f(x_n) - \bar{x} - f'(x_n)\left[x_n - \bar{x}\right]}{1 - f'(x_n)}$$

$$\frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} = \frac{\dfrac{f(x_n) - \bar{x}}{x_n - \bar{x}} - f'(x_n)}{1 - f'(x_n)}$$

$$\frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} = \frac{f'(\xi) - f'(x_n)}{1 - f'(x_n)} \quad : \ \xi \text{ is between } x_n \text{ and } \bar{x}$$

$\therefore$,

$$\frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} = \frac{a - t}{a + 1},$$

where $a = -f'(x_n) > 0$

$t = -f'(\xi) > 0$

Note that for $0 \le t \le a$,

$$0 \le \frac{a-t}{a+1} < 1$$

Suppose now that $f'(x)$ is monotonically decreasing: $x_1 < x_2 \Rightarrow f'(x_1) > f'(x_2)$

We have two cases to consider:

a. $x_n > \bar{x}$:

Then $\bar{x} < \xi < x_n$ and $f'(\xi) > f'(x_n)$

or $-f'(x_n) - (-f'(\xi)) > 0$

or

$$a - t > 0$$

$\therefore$,

from above we obtain:

$$0 < \frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} < 1$$

or,

$$\left.\begin{array}{l} x_{n+1} > \bar{x} \\ \text{and} \\ x_{n+1} < x_n \end{array}\right\} \quad \bar{x} < x_{n+1} < x_n$$

Thus, x_{n+1} will indeed converge.

Suppose it does not converge to $\bar{x}$:

Suppose $x_n \to \tilde{x} > \bar{x}$:

$$\frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} \to 1 \Rightarrow + f'(\xi) \Rightarrow + 1,$$

but $f'(\xi) < 0$

b. $x_n < \bar{x}$:

Then $x_n < \xi < \bar{x} \Rightarrow f'(x_n) > f'(\xi)$

$\therefore$,

$$\frac{x_{n+1} - \bar{x}}{x_n - \bar{x}} < 0 \Rightarrow x_{n+1} > \bar{x},$$ or we are back in a.

A similar proof is also possible for the case where $f'(x)$ is monotonically increasing.

We attempt to apply these two methods, and even assume, therefore, that the function satisfies one of these two conditions:

a. $|f'(x)| < 1$ in vicinity of solution

b. $f'(x) < 0$ and monotone in vicinity of solution.

Note that the phrase "vicinity of solution" is actually sufficient if the first guess gets you there. Normally our first guesses are quite good, since the program proceeds in a step-by-step fashion.

A precise application of these methods would require an evaluation of $f'(x)$. This is usually impractical, so the following procedure has been adopted. We hope it will take us to the appropriate method. So far we have had very little difficulty.

Let x_1 be first guess

Let $x_{n+1} = f(x_n)$

1. As long as the $\{x_i\}$ are monotone, we assume the process is converging and we continue.

2. As soon as $x_i < x_{i+1} > x_{i+2}$ or $x_i > x_{i+1} < x_{i+2}$, we have lost monotonicity. We then proceed by halving the interval:

   a. Let $\bar{x}_1 = \min \left[x_i, x_{i+1}, x_{i+2}\right]$

   b. $\bar{x}_2 = \max \left[x_i, x_{i+1}, x_{i+2}\right]$

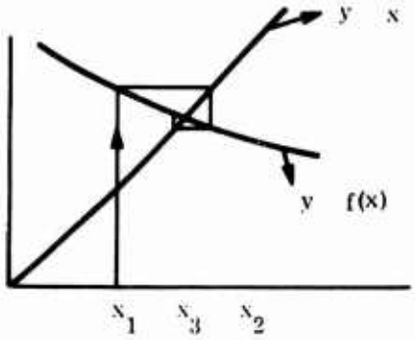
   c. Let $x^* = \dfrac{\bar{x}_1 + \bar{x}_2}{2}$

   d. $x^{**} = f(x^*)$

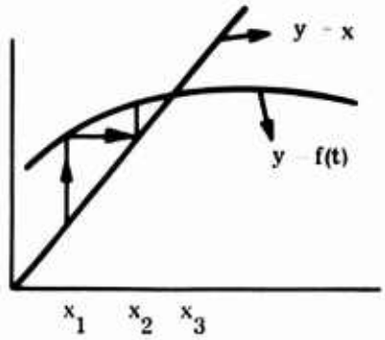
   if $\left\{\begin{matrix} x^* < x^{**} \\ x^* > x^{**} \end{matrix}\right\}$ then $\left\{\begin{matrix} \bar{x}_1 = x^* \\ \bar{x}_2 = x^* \end{matrix}\right\}$ and go back to c

The first step is clearly related to the method of successive approximations. The second step is actually part B of the second procedure. In order to go back to part A we would need the derivative.

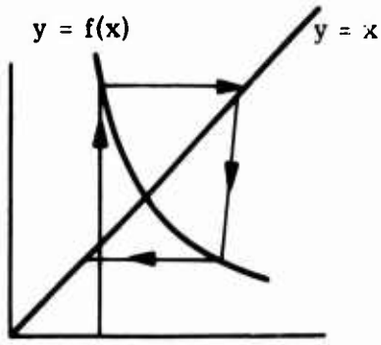
We look at a few examples of the above procedure:



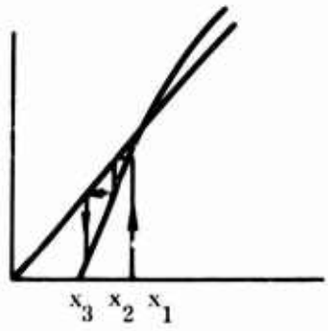
since x_1, x_2, x_3 are not monotone, we would halve the interval



we would proceed by successive approximations



successive approximations will not converge, but halving interval will.



divergence appears imminent!

Because of the possibility that this procedure might not converge under some conditions, the program will stop after a specified number of iterations.

We mention finally that the program is capable of handling simultaneous problems (ten is presently the maximum):

for example,

$$x = f(x, y, z)$$

$$y = g(x, y, z)$$

$$z = h(x, y, z)$$

actually, we could write:

$x = f(x, f_1(x), f_2(x)) = \ell(x)$, which is the correct form. The program proceeds as follows:

choose x_1:

We need to solve:

$$y = g(x_1, y, z)$$

$$z = h(x_1, y, z)$$

choose y_1:

solve $z = h(x_1, y_1, z)$. Let the solution be $\bar{z}$. Then obtain $y_2 = g(x_1, y_1, \bar{z})$, and solve $z = h(x_1, y_2, z)$. Proceed until we obtain

$$\bar{y} = g(x_1, \bar{y}, \bar{z})$$

$$\bar{z} = h(x_1, \bar{y}, \bar{z})$$

Then obtain $x_2 = f(x_1, \bar{y}, \bar{z})$.

Repeat cycle with new guess for x until $x = f(x, \bar{y}, \bar{z})$ is obtained. ($\bar{y}$ and $\bar{z}$ are computed for each x_i.)

APPENDIX D

It is required that the eigenvalues and eigenfunctions of the matrix A, defined in Eq. (I. V. E-12), be found. Therefore it is necessary to consider the system

$$(A - \lambda I)U = 0.$$

Written out explicitly, the equations are

$$-\lambda u_1 - \frac{C_N - 2}{C_N} u_2 - \frac{C_N - 4}{C_N} u_4 - \cdots - \frac{C_0}{C_N} u_N = 0$$

$$u_1 - \lambda u_2 = 0$$

$$u_2 - \lambda u_3 = 0$$

$$\vdots$$

$$u_{N-1} - \lambda u_N = 0$$

With the normalization $u_N = 1$, the last (N - 1) equations give for the eigenfunctions

$$u_{N-j} = \lambda^j$$

or, equivalently,

$$u_j = \lambda^{N-j}.$$

If the last expression is inserted in the first equation of the above system, the result, after rearrangement, can be written

$$\lambda^N \sum_{\substack{j=0 \\ \text{even}}}^{N} C_j \left(\frac{1}{\lambda}\right)^{N-j} = 0$$

or, in terms of $\mu = 1/\lambda$,

$$\frac{1}{\mu^N} \sum_{\substack{j=0 \\ \text{even}}}^{N} C_j \mu^{N-j} = 0.$$

Comparing these equations with Eq. (IV. B-6), it is seen that the eigenvalues of the system satisfy

$$\lambda_i^N P_N\left(\frac{1}{\lambda_i}\right) = 0, \qquad i = 1,2,\ldots,N$$

or

$$P_N(\mu_i) = 0, \qquad i = 1,2,\ldots,N$$

where $\mu_i = 1/\lambda_i$.

APPENDIX E

Presented here are proofs of Eqs. (IV. B-33) and (IV. B-36). Considering first Eq. (IV. B-36), we have

$$\alpha_N = \frac{1}{2} \sum_{i=1}^{N} A_i \mu_i^N .$$

By virtue of the definition and properties of the Gauss quadrature, the right-hand side of this equation is exactly

$$\frac{1}{2} \sum_{i=1}^{N} A_i \mu_i^N = \frac{1}{2} \int_{-1}^{1} \mu^n d\mu = \frac{1 + (-1)^n}{2(n+1)} .$$

Therefore,

$$\alpha_n = \frac{1 + (-1)^n}{2(n+1)}$$

which is identical to Eq. (IV. B-5) and thus completes the proof.

From Eqs. (IV. B-18) and (IV. B-12), it is evident that

$$\gamma_i = \sum_{j=0}^{N-1} \alpha_j \tilde{Q}_{i,j+1} .$$

Substitution of Eq. (IV. B-36), interchanging the order of summation, and a slight rearrangement yields

$$\gamma_i = \frac{1}{2} \sum_{\ell=1}^{N} \mu_\ell^{-1} A_\ell \sum_{j=1}^{N} \mu_\ell^j \tilde{Q}_{i,j} .$$

Because of Eq. (IV. B-23), this reduces to

$$\lambda_i = \frac{1}{2} A_i \mu_i^{N-1}$$

which completes the verification of Eq. (IV. B-33).

APPENDIX F

Although the canonical transformation is not needed in practice, explicit expressions will be derived for the elements of Q^{-1} for the sake of completeness. These can be obtained by inverting the matrix Q by the usual methods. However, a much simpler method is presented here.

First, define a quantity $L_N(\mu;n)$ as

$$L_N(\mu;n) \equiv \sum_{i=1}^{N} \tilde{Q}_{n,i}\mu^i. \tag{F.1}$$

From Eq. (IV. B-23), note that

$$L_N(\mu_j;n) = \mu_j^N \delta_{jn}. \tag{F.2}$$

From the last two equations, it is clear that $L_N(\mu;n)$ is a polynomial of order N in μ whose zeros are identical to those of $P_N(\mu)$ except that the zero μ_n is replaced by zero. Thus

$$L_N(\mu;n) \sim \mu(\mu - \mu_1)(\mu - \mu_2) \cdots (\mu - \mu_{n-1})(\mu - \mu_{n+1}) \cdots (\mu - \mu_N)$$

or

$$L_N(\mu;n) \sim \frac{\mu P_N(\mu)}{\mu - \mu_n}.$$

The constant of proportionality is determined by comparing coefficients of μ^N in the above expression and in the defining equation, Eq. (F.1). This gives

$$L_N(\mu;n) = \frac{\tilde{Q}_{n,N}}{C_0} \frac{\mu P_N(\mu)}{\mu - \mu_n} \tag{F.3}$$

where C_0 is the coefficient of μ^N in $P_N(\mu)$. Using Eq. (F.2) evaluated at $\mu = \mu_n$,

$$L_N(\mu_n;n) = \mu_n^N = \lim_{\mu \to \mu_n} \frac{\tilde{Q}_{n,N}}{C_0} \frac{\mu P_N(\mu)}{\mu - \mu_n} = \frac{\tilde{Q}_{n,N}}{C_0} \mu_n P'_N(\mu_n).$$

Therefore

$$\tilde{Q}_{n,N} = \frac{C_0 \mu_n^{N-1}}{P'_N(\mu_n)}. \tag{F.4}$$

Equation (F.3) becomes

$$L_N(\mu; n) = \left(\frac{\mu_n^{N-1}}{P'_N(\mu_n)} \right) \frac{\mu P_N(\mu)}{\mu - \mu_n}. \tag{F.5}$$

Upon substituting Eq. (F.1) in the last equation, solving for $P_N(\mu)$ and rearranging, it is found that

$$P_N(\mu) = \frac{P'_N(\mu_n)}{\mu_n^{N-1}} \left\{ -\mu_n \tilde{Q}_{n,1} + \tilde{Q}_{n,N} \mu^N + \sum_{i=1}^{N-1} \left[\tilde{Q}_{n,i} - \mu_n \tilde{Q}_{n,i+1} \right] \mu^i \right\}.$$

Recall that $P_N(\mu)$ can be written

$$P_N(\mu) = \sum_{i=0}^{N} C_{N-i} \mu^i.$$

Equating coefficients of like powers of μ in the last two equations yields, in addition to Eq. (F.4),

$$\tilde{Q}_{n,1} = -\frac{\mu_n^{N-2} C_N}{P'_N(\mu_n)} \tag{F.6}$$

$$\tilde{Q}_{n,i} - \mu_n \tilde{Q}_{n,i+1} = \begin{cases} 0 & \text{(i odd)} \\ \dfrac{\mu_n^{N-1} C_{N-i}}{P'_N(\mu_n)} & \text{(i even).} \end{cases} \tag{F.7}$$

By applying Eq. (F.7) recursively in conjunction with Eq. (F.6), it can be shown that

$$\tilde{Q}_{n,i} = \begin{cases} -\dfrac{\mu_n^{N-i-1}}{P'_N(\mu_n)} P_{N,i-1}(\mu_n) & (i \text{ odd}) \\ -\dfrac{\mu_n^{N-i-1}}{P'_N(\mu_n)} P_{N,i-2}(\mu_n) & (i \text{ even}) \end{cases} \tag{F.8}$$

where

$$P_{N,\ell}(\mu_n) \equiv \sum_{k=0}^{\ell} C_{N-k} \mu_n^k = -\sum_{k=0}^{N-\ell-2} C_k \mu_n^{N-k} . \tag{F.9}$$

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13 ABSTRACT This study has been concerned with developing improvements in the physics and in the numerical treatment of the equations governing the dynamics of the plasma produced by a nuclear burst. The studies of the motion of the plasma were based primarily on the Navier-Stokes equations which are applicable at low altitudes where the plasma is a continuum. Considerations were also given to the high altitude rarefied flow regime. Studies were made of the radiative properties of high temperature gases and also of new techniques for the calculation of radiative transfer. We have found that one can apply the complete time-dependent Navier-Stokes equations to the calculation of a spherically symmetric explosion and that no artificial viscosity is present in the solution. In order to maintain desired accuracy, a new mesh size restriction must be imposed, namely that the local spatial mesh utilized in the computations must be of the order of the local mean free path in the gas. In this study, there has also been a successful demonstration of the numerical solution of the time-dependent radiation transfer equation rather than the usual "steady state" formulation.

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