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WAZER
A ONE-DIMENSIONAL, TWO-TEMPERATURE HYDRODYNAMIC CODE

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Abstract

The physics and mathematics used in the computer code WAZER is described. This code can perform calculations on plasmas which involve thermal diffusion, heat transfer between ion and electron populations, heat loss from the electrons due to radiation, hydrodynamic effects, absorption of laser light, fusion, and loss of energy across the boundaries in the form of either heat or work. The description includes the mathematical formulation of the physical laws involved and the differencing techniques used to solve the partial differential equations of heat transport and hydrodynamic motion.

I. Introduction

The physical system for which this code (computer program) can be used to perform calculations consists of a one-dimensional volume containing a plasma consisting of two heat-conducting populations, ions and electrons, which may be at different temperatures. This volume may contain several regions in which the properties of the ionic population may be different. The code calculates the effects of various physical processes in this plasma, such as:

- Heat flow due to thermal diffusion in both populations.
- Heat exchange between the two populations.
- Heat loss from the electrons as radiation.
- Hydrodynamic effects of all energy transformations.
- Addition of energy through the absorption of laser light.
- Production of energy by thermonuclear reactions.
- Gain or loss of energy by heat conduction across one boundary or by work done on or by the system at the boundary.

In the hydrodynamic part of the calculations, the gas is treated as a single fluid in each subregion.

II. Hydrodynamic and Heat Transfer Equations

The code performs the calculations in two distinct operations during each time step. First the hydrodynamic motion of the material is calculated; then energy changes produced by heat diffusion and exchange between populations and by creation of new energy through thermonuclear reactions or absorption of laser light is treated. We discuss these two steps in this order.

1. HYDRODYNAMIC EQUATIONS[1]

The conservation of mass in each region may be described in Lagrangian coordinates by

$$\dot{V} = V(\underline{\nabla}\cdot\underline{u}). \tag{1}$$

Here $V = 1/\rho$ is the specific volume of the medium and ρ is the density. In Eq. (1), $\underline{u} = \dot{\underline{r}}$ is the velocity of the medium. Since Lagrangian coordinates are being used, V and $\underline{u}$ are associated with a particle in the medium whose coordinates are $\underline{r}$ rather than with a point in space. The equation of motion of the medium is

$$\dot{\underline{u}} = -V\underline{\nabla}p \tag{2}$$

where

$$p = p_i + p_e. \tag{3}$$

In Eq. (3), p_i and p_e are the pressures exerted by the ions and electrons respectively.

For the purposes of these calculations, it is more convenient to express Eqs. (1) and (2) in terms of partial derivatives with respect to m rather than r, where m is defined in cartesian, cylindrical, and spherical geometries as follows:

$$dm = \rho r^{\delta-1}\,dr = (r^{\delta-1}/V)dr \tag{4}$$

Table I. Dimensions of m.

Geometry	δ	m (units)
Cartesian	1	mass/unit area
Cylindrical	2	mass/unit length-radian
Spherical	3	mass/steradian

In Eq. (4), δ has the values 1, 2, and 3 in each of the three geometries, respectively. Table I shows the dimensions of m for the three cases. Thus Eqs. (1) and (2) take the following forms:

$$\dot{V} = (V/r^{\delta-1})\left[d(r^{\delta-1}u)/dr\right] = d(r^{\delta-1}u)/dm \tag{5}$$

and

$$\dot{u} = -r^{\delta-1}(dp/dm). \tag{6}$$

2. ENERGY CONSERVATION EQUATIONS

The first law of thermodynamics for a system may be expressed by[2]

$$\dot{U} + p\dot{V} = \dot{Q} \tag{7}$$

where $\dot{U}$ is the rate of increase of the internal energy of a system, $p\dot{V}$ is the rate at which work is being done by the system, and $\dot{Q}$ is the rate at which heat is entering the system. U may be expressed as a function of V and θ, the temperature of the system. Therefore in Eq. (7) we let

$$\dot{U} = U_\theta \dot{\theta} + U_V \dot{V} \tag{8}$$

In Eq. (8), $U_\theta = (\partial U/\partial \theta)_V = C$, the heat capacity at constant volume, and $U_V = (\partial U/\partial V)_\theta$. Thus Eq. (7) becomes

$$C\dot{\theta} + (p + U_V)\dot{V} = \dot{Q}. \tag{9}$$

The so-called "energy equation" of thermodynamics is given in Zemansky[2] as

$$U_V = \theta p_\theta - p \tag{10}$$

where $p_\theta = (\partial p/\partial \theta)_V$. Therefore Eq. (9) becomes

$$C\dot{\theta} + \theta p_\theta \dot{V} = \dot{Q}. \tag{11}$$

The ion and electron populations are treated as two subsystems of the whole system, each with its own temperature, and the first law of thermodynamics as expressed by Eq. (11) is applied to each. The flow of heat into (or out of) each small increment of mass, represented by $\dot{Q}$ in Eq. (11), may be caused by four processes:

(1) Exchange of heat between one population and the other through thermal coupling processes.
(2) Loss of heat through radiation.
(3) Diffusion of heat from one point to another in space through each of the two populations.
(4) Various, as yet unspecified, processes which serve as heat sources in the system. Some of these heat sources are described further in Section III.

3. HEAT EXCHANGE BETWEEN POPULATIONS

Heat is transferred between the ion and electron populations because of coulomb interaction. The rate of heat exchange through this mechanism is

$$\dot{Q}_c = 2\omega_c(\theta_i - \theta_e) \tag{12}$$

where θ_i and θ_e are the ion and electron temperatures and ω_c is given by Spitzer[3] as

$$\omega_c = \frac{\sqrt{2\pi/k}\left(N_e Z e^2\right)^2 V L_c}{mM\left[(\theta_e/m) + (\theta_i/M)\right]^{3/2}} . \tag{13}$$

In Eq. (13) N_e is the electron density, Z is the ionic charge, e is the electronic charge, m and M are the electronic and ionic masses respectively, k is Boltzmann's constant, and the quantity $L_c = \ln\left(1 + \Lambda_c^2\right)$ is the so-called "coulombean logarithm."

For partially ionized materials we must use an "effective" value of Z in Eq. (13) above. For most purposes we will use $\overline{Z}$, the average number of electrons stripped off each nucleus, as a sufficiently good approximation for this value recognizing that this may be too small for this and other processes involving Z under some conditions. Thus we will have $N_e = \overline{Z}N_i$ in Eq. (13) where N_i is the ion density. Since it is usually the case that $\theta_i/M \lll \theta_e/m$,

$$\omega_c = (2\pi m/k)^{1/2}\left(N_i\overline{Z}^2 e^2\right)^2 V L_c/M\theta_e^{3/2}. \tag{13'}$$

In Eq. (13'), $N_i = N_o/AV$ where N_o is Avogadro's number and A is the ionic mass in atomic mass units.

The argument Λ_c^2 of the coulombean logarithm is given by Spitzer as

$$\Lambda_c^2 = (9\chi/4\pi N_i)\left(k\theta_e/\overline{Z}e^2\right)^3 \tag{14}$$

where the factor χ, given in Spitzer, is a correction for quantum effects and depends inversely on θ_e.

4. HEAT LOSS THROUGH BREMSSTRAHLUNG

Heat is lost by the electron population through bremsstrahlung. The rate of loss is given by Spitzer[3] as

$$\dot{Q}_r = 2\omega_r\theta_e \tag{15}$$

where ω_r for a Born approximation and a Maxwellian distribution of electron velocity is given as

$$\omega_r = \left(2^5 N_i^2 \overline{Z}^3 e^6 V/3\ hmc^3\right)(2\pi k/m\theta_e)^{\frac{1}{2}} \tag{16}$$

in which c is the speed of light.

It is assumed that any radiation generated by this process passes out of the system without interacting.

5. HEAT DIFFUSION

The rate of flow of heat through each of the populations due to diffusion is

$$\underline{f} = -\lambda\underline{\nabla}\theta = -\lambda(d\theta/dr)\hat{r}. \tag{17}$$

Hence the rate of increase of heat in each population at a point in space is

$$\dot{Q}_D = -V\underline{\nabla}\cdot\underline{f} = -\left[\lambda r^{\delta-1}(d\theta/dr)\right]_m \tag{18}$$

where the subscript m implies differentiation of the quantity in brackets with respect to m. The quantity λ may be calculated by[3]

$$\lambda_i = \frac{40(2/\pi)^{3/2}k(k\theta_i)^{5/2}}{M^{1/2}\,(Ze)^4 L_i} \tag{19a}$$

$$\lambda_e = \frac{40(2/\pi)^{3/2}k(k\theta_e)^{5/2}}{m^{1/2}e^4 L_e(Z + 3.44 + 0.26\ \ln Z)} \tag{19b}$$

for ions and electrons, respectively. The arguments of L_i and L_e, the coulombean logarithms for ions and electrons, respectively, are $\Lambda_i^2 = \Lambda_c^2(\theta_i/Z\theta_e)^2/\chi$ and $\Lambda_e^2 = \Lambda_c^2 Z^2$. As usual Z may be replaced by $\overline{Z}$ for partial ionization.

6. HEAT TRANSFER EQUATIONS

The equations resulting from the application of the first law of thermodynamics to the ion and electron populations are, respectively,

$$C_i\dot{\theta}_i + (p_\theta)_i\dot{V}\theta_i = S_i + \left[\lambda_i r^{\delta-1}(\partial\theta_i/\partial r)\right]_m - 2\omega_c(\theta_i - \theta_e) \tag{20}$$

$$C_e\dot{\theta}_e + (p_\theta)_e \dot{V}\theta_e = S_e + \left[\lambda_e r^{\delta-1}(\partial\theta_e/\partial r)\right]_m - 2\omega_r\theta_e$$

$$+ 2\omega_c(\theta_i - \theta_e) \tag{21}$$

where the subscripts i and e identify the quantities as pertaining to ions or electrons, respectively, and where $(p_\theta)_i = (\partial p_i/\partial\theta_i)_V$ and $(p_\theta)_e = (\partial p_e/\partial\theta_e)_V$. S_i and S_e are the heat source densities for the ion and electron populations. The first law of thermodynamics for the whole system is simply the sum of Eqs. (20) and (21)

$$\dot{U} + p\dot{V} = S + \left[\lambda r^{\delta-1} f\right]_m - 2\omega_r\theta_e \tag{22}$$

where

$$U = U_i + U_e \tag{23}$$

$$p = p_i + p_e \tag{24}$$

$$f = f_i + f_e \tag{25}$$

$$S = S_i + S_e \tag{26}$$

and where U_i, U_e, and U are the internal energy densities of the ions, the electrons, and the whole system, respectively.

7. EQUATIONS OF STATE

An equation of state calculation is necessary to evaluate Eqs. (20) and (21). Such a calculation should provide values of p, U, p_θ, and C for both ions and electrons where their temperatures are distinguished, or common values of these variables where the temperatures are not distinguished. In some problems, this calculation also provides a value of $\overline{Z}$, the average number of electrons stripped off each atom.

For many calculations, the equation of state used for both ions and electrons is that of an ideal gas

$$p = Nk\theta \tag{27}$$

in which k is Boltzmann's constant and N is the number of ions or electrons per unit volume. The internal energy per unit mass is

$$U = (3/2)Nk\theta V. \tag{28}$$

Hence

$$p_\theta = Nk \tag{29}$$

and

$$C = U_\theta = (3/2)NkV. \tag{30}$$

For cases where materials are partially dissociated or ionized, modifications are made in the above equations to incorporate the effect of these phenomena. The numerical coefficient in Eq. (28) must also be increased to account for the internal energy absorbed by molecules or ions with more than three degrees of freedom.

III. Energy Sources

The deposition of energy in plasmas by laser light and thermonuclear reactions is accomplished in the following manner.

1. ABSORPTION OF LASER LIGHT

The mechanism for absorption of laser light by plasmas is assumed to be free-free absorption (the inverse of bremsstrahlung). Bound-free (photoelectric) and bound-bound (spectroscopic line) absorptions are ignored.

Energy is supplied to the electron population by the laser light at a rate S_e where

$$S_e = KV\phi \tag{31}$$

in which K is the absorption coefficient and ϕ is the light intensity (energy/unit time-unit area). Here ϕ is

$$\phi = (\psi^+ + \psi^-)/r^{\delta - 1} \tag{32}$$

where ψ^+ and ψ^- are the outwardly and inwardly directed light fluxes. In this system, the light flux enters at the far boundary where

$$\psi^-(r_{max}) = \Psi(t), \tag{33}$$

$\Psi(t)$ being a sequence of values assigned to the incoming flux at the outer boundary. The light then passes inward through the system being modified by absorption in the following way:

$$d\psi^-/dr = K\psi^-. \tag{34}$$

It is reflected at the inner boundary, i. e.

$$\psi^-(r = 0) = \psi^+ (r = 0) \tag{35}$$

after which it passes out through the system again being modified as follows:

$$d\psi^+/dr = -K\psi^+. \tag{36}$$

At temperatures greater than 10 eV and specific volumes greater than 100 cm^3/g, deuterium gas is almost fully ionized (>90%). Under such conditions, the free-free absorption coefficient for light is given by the following formula derived by means of an unscreened Born approximation with stimulated emission[4] included:

$$K_i = AN_eN_iZ_{eff}^2 (I_o/\hbar\omega)^{7/2}F(\alpha)\epsilon^{-1/2} \tag{37}$$

where

$$A = 64h^2/3cm^5e^8 \text{ and } \alpha = \hbar\omega/k\theta_e. \tag{38}$$

I_o is one Rydberg (13.6 eV), ω is the frequency of the light, Z_{eff} is the effective ionic charge, ϵ is the dielectric constant, and

$$F(\alpha) = 2(\alpha/\pi)^{\frac{1}{2}} \sinh (\alpha/2)K_o(\alpha/2) \tag{39}$$

where $K_o(\alpha/2)$ is a modified Bessel function of the second kind. If damping is neglected, ϵ, the dielectric constant, is given by

$$\epsilon = 1 - (\omega_p/\omega)^2 \tag{40}$$

in which ω_p, the plasma frequency is given by

$$\omega_p^2 = 4\pi e^2N_e/m. \tag{41}$$

At temperatures below 10 eV, the absorption of light by a gas is more complicated. We are mainly interested in the absorption of light by a gas that has already been partially ionized by some other agency and will be rapidly heated to temperatures above 10 eV by absorption of intense laser light. Thus, we may deal with this absorption by approximating the low temperature absorption coefficient by the coefficient for free-free absorption of microwaves in weakly ionized gases,[5] i. e. by

$$K_a = \nu_c(\omega_p/\omega)^2/c \tag{42}$$

in which ν_c, the electron-molecule collision rate, is given by

$$\nu_c = N_a \left\langle \sigma v_e \right\rangle_{ae} \qquad (\nu_c \ll \omega) \tag{43}$$

where N_a is the number of atoms or molecules per unit volume, v_e is the electron velocity, and σ, the electron-molecule cross section for momentum transfer, may be estimated from data in Ref. 4. Hence

$$K_a = 4\pi N_e N_a \sigma(e^2/c\omega^2)\,(3k/m^3)^{\frac{1}{2}} . \tag{44}$$

For the case of hydrogen (or deuterium) where there is one electron per nucleon, the value of K_i and K_a may be calculated by means of the following approximation formulas which are forms of Eqs. (37) and (44):

$$K_i = \frac{2.78 \times 10^9}{V^2(1 + 5.4\sqrt{\theta_e})(1 + 558\theta_e)} \tag{45}$$

$$K_a = (4 \times 10^9)\sqrt{\theta_e}/V^2 \tag{46}$$

where the effect of the dielectric constant ϵ has been left out and where V is in cm^3/g, θ_e is in keV, and K_i and K_a are in cm^{-1}. Values of K for use in Eqs. (31), (34), and (36) are obtained by combining K_i and K_a according to the formula:

$$K = f\left[(1 - f)K_a + fK_i\right] \tag{47}$$

in which f is the degree of ionization. The quantity f may be calculated by means of ionization equilibrium relations, such as those given in Landau and Lifshitz.[6]

As the plasma frequency ω_p given by Eq. (41) approaches the light frequency ω, the coefficient K must be multiplied by $\epsilon^{-\frac{1}{2}}$. Light is totally reflected[7] when $\omega_p \geq \omega$. For laser light from neodymium-doped glass, this occurs at an electron density of approximately $10^{21}/cm^3$ which will therefore be called the critical electron density.

2. ENERGY FROM THERMONUCLEAR REACTIONS

The thermonuclear reactions of interest in the design of this code are

$$D + T \longrightarrow \alpha(3.6\ \text{MeV}) + n(14.1\ \text{MeV})$$

$$D + D \begin{cases} \longrightarrow T(1.0\ \text{MeV}) + p(3.0\ \text{MeV}) \\ \longrightarrow {}^3\text{He}(0.8\ \text{MeV}) + n(2.45\ \text{MeV}) \end{cases}$$

where, as indicated, the D-D reaction goes about 50 percent into each of the two branches. Hence, the rate of change of the densities of the tritium nuclei N_T and the deuterium nuclei N_D are

$$\dot{N}_T = -R_{DT}N_TN_D + (\tfrac{1}{4})R_{DD}N_D^2 \tag{48}$$

$$\dot{N}_D = -R_{DD}N_D^2 - R_{DT}N_TN_D \tag{49}$$

where the rate constants R_{DT} and R_{DD} are given by

$$R_{DT} = \left\langle \sigma_{DT} v \right\rangle = R_{DT}(\theta_i) \tag{50}$$

$$R_{DD} = \left\langle \sigma_{DD} v \right\rangle = R_{DD}(\theta_i). \tag{51}$$

In Eqs. (50) and (51), $\sigma_{DT}(v)$ and $\sigma_{DD}(v)$, the cross-sections for the above two reactions, are averaged over a Maxwellian distribution of velocities in a gas having a temperature θ_i. If the system is small compared to the range of the alpha particles and protons, it may be assumed that these ions and the neutrons carry off their energy, and the only purpose of this calculation is to determine the rate of neutron formation. If the system is large compared to the range of the alphas and protons, it is assumed that the ions deposit their energy immediately and locally in the gas while the neutrons carry off their energy. Thus, the rate of energy production per unit mass by the D-T reaction is

$$S_{DT} = (3.6\ \text{MeV})\ R_{DT}N_DN_TV. \tag{52}$$

The two D-D reactions are lumped and the energies of their product ions are averaged in calculating their energy production per unit mass. Hence

$$S_{DD} = (\tfrac{1}{2})(2.4\ \text{MeV})\ R_{DD}N_D^2\, V. \tag{53}$$

The factor of $\frac{1}{2}$ is included because each deuteron is counted twice in deriving Eq. (53), once as a target and once as a projectile.

It has been estimated[8] that the reaction products apportion their energies between the ion and electron populations in the following amounts:

$$S_i = \frac{\theta_e S_{DT}}{32 + \theta_e} + \frac{\theta_e S_{DD}}{120 + \theta_e} \tag{54}$$

$$S_e = \frac{32\ S_{DT}}{32 + \theta_e} + \frac{120\ S_{DD}}{120 + \theta_e} \tag{55}$$

where θ_e, the electron temperature, is in keV.

IV. Difference Equations

To form difference equation approximations in these calculations, the entire one-dimensional region is divided into J zones. The following conventions will be used here with respect to zones and time steps:

Subscript j indicates the value of a variable at the right boundary (or outer boundary in the case of cylindrical or spherical coordinates) of the jth zone, J indicates the value at the right-hand (or outer) boundary of the whole system. The left-hand boundary (or center) is taken immoveable and non-conducting in these calculations. Subscript j - 1/2 indicates the value of a variable in the middle of the jth zone.

Superscript n indicates the value of a variable at the end of the nth time step; n - 1/2 indicates the value during or at the middle of the nth time step.

1. DIFFERENCING THE HYDRODYNAMIC EQUATIONS

In the difference-equation approximation to Eq. (6), the quantity p (and p_i where it is not part of p) is replaced by p + q (and p_i by p_i + q) where q is the so-called "von Neumann q."[9] The purpose of q is to prevent mathematical instabilities by spreading shock fronts over about three zones. Quantity q is defined by

$$q = \left[b\Delta m(\partial u/\partial m)\right]^2/V \qquad \dot{V} < 0 \text{ (compression)} \tag{56}$$

$$q = 0 \qquad \dot{V} \geq 0 \text{ (expansion)} \tag{57}$$

where usually $b = \sqrt{2}$.

The difference equation approximation to Eq. (6) is

$$u_j^{n+\frac{1}{2}} = u_j^{n-\frac{1}{2}} - \left(r_j^n\right)^{\delta-1}\left[\left(p_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n\right) + \left(q_{j+\frac{1}{2}}^{n-\frac{1}{2}} - q_{j-\frac{1}{2}}^{n-\frac{1}{2}}\right)\right]\left(\Delta t^n/\Delta m_j\right). \tag{58}$$

In Eq. (58), Δt^n and Δm_j are given by

$$\Delta t^n = \tfrac{1}{2}(\Delta t^{n+\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}) \tag{59}$$

$$\Delta m_j = \tfrac{1}{2}(\Delta m_{j+\frac{1}{2}} + \Delta m_{j-\frac{1}{2}}) \tag{60}$$

where $\Delta m_{j+\frac{1}{2}}$ is the mass between the boundaries j + 1 and j, $\Delta t^{n-\frac{1}{2}}$ is the duration of the nth time step, and Eq. (56) is approximated by

$$q_{j-\frac{1}{2}} = \left[b(u_j - u_{j-1})\right]^2 V_{j-\frac{1}{2}}. \tag{61}$$

$\Delta r_{j-\frac{1}{2}}$ is defined as the thickness of the jth zone and is calculated by

$$\Delta r^{n+1}_{j-\frac{1}{2}} = \Delta r^{n}_{j-\frac{1}{2}} + \left(u^{n+\frac{1}{2}}_{j} - u^{n+\frac{1}{2}}_{j-1}\right) \Delta t^{n+\frac{1}{2}} . \qquad (62)$$

Similarly

$$r^{n+1}_{j} = r^{n}_{j} + u^{n+\frac{1}{2}}_{j} \, \Delta t^{n+\frac{1}{2}} . \qquad (63)$$

For the three different geometries, the specific volume is calculated as follows:

Cartesian: $(\delta = 1)$ $$V^{n+1}_{j-\frac{1}{2}} = \Delta r^{n+1}_{j-\frac{1}{2}} \Big/ \Delta m_{j-\frac{1}{2}} \qquad (64)$$

Cylindrical: $(\delta = 2)$ $$V^{n+1}_{j-\frac{1}{2}} = \frac{1}{2}\left(\Delta r^{n+1}_{j-\frac{1}{2}} \Big/ \Delta m_{j-\frac{1}{2}}\right)\left(r^{n+1}_{j} + r^{n+1}_{j-1}\right) \qquad (65)$$

Spherical: $(\delta = 3)$ $$V^{n+1}_{j-\frac{1}{2}} = \left(\Delta r^{n+1}_{j-\frac{1}{2}} \Big/ \Delta m_{j-\frac{1}{2}}\right)\left[r^{n+1}_{j} \, r^{n+1}_{j-1} + \frac{1}{3}\left(\Delta r^{n+1}_{j-\frac{1}{2}}\right)^{2}\right] \qquad (66)$$

and

$$V^{n+\frac{1}{2}}_{j-\frac{1}{2}} = \frac{1}{2}\left(V^{n+1}_{j-\frac{1}{2}} + V^{n}_{j-\frac{1}{2}}\right). \qquad (67)$$

The rate of change of V with time is also needed for the energy equations

$$\dot{V}^{n+\frac{1}{2}}_{j-\frac{1}{2}} = \left(V^{n+1}_{j-\frac{1}{2}} - V^{n}_{j-\frac{1}{2}}\right) \Big/ \Delta t^{n+\frac{1}{2}} \qquad (68)$$

2. DIFFERENCING THE HEAT TRANSFER EQUATIONS

In differencing Eqs. (20) and (21), an implicit backward substitution differencing scheme is used.[10] The difference equation analogue of these equations, written in matrix notation for compactness, are as follows:

$$\begin{aligned} \underline{\underline{\alpha}}_{j-\frac{1}{2}} \cdot \left(\underline{\theta}^{n+1}_{j-\frac{1}{2}} - \underline{\theta}^{n}_{j-\frac{1}{2}}\right) = \underline{\beta}_{j-\frac{1}{2}} &+ \underline{\underline{a}}_{j} \cdot \left[\left(\underline{\theta}^{n+1}_{j+\frac{1}{2}} + \underline{\theta}^{n}_{j+\frac{1}{2}}\right) - \left(\underline{\theta}^{n+1}_{j-\frac{1}{2}} + \underline{\theta}^{n}_{j-\frac{1}{2}}\right)\right] \\ &- \underline{\underline{a}}_{j-1} \cdot \left[\left(\underline{\theta}^{n+1}_{j-\frac{1}{2}} + \underline{\theta}^{n}_{j-\frac{1}{2}}\right) - \left(\underline{\theta}^{n+1}_{j-\frac{3}{2}} + \underline{\theta}^{n}_{j-\frac{3}{2}}\right)\right] - \underline{\underline{\gamma}}_{j-\frac{1}{2}} \left(\underline{\theta}^{n+1}_{j-\frac{1}{2}} + \underline{\theta}^{n}_{j-\frac{1}{2}}\right) \\ &- \underline{\underline{\omega}}_{j-\frac{1}{2}} \cdot \left(\underline{\theta}^{n+1}_{j-\frac{1}{2}} + \underline{\theta}^{n}_{j-\frac{1}{2}}\right) . \end{aligned} \qquad (69)$$

The proper time-step index on all the coefficients in Eq. (69) is $n + \frac{1}{2}$ which is left off for convenience. In Eq. (69), the vector quantities $\underline{\theta}$ and $\underline{\beta}$ are

$$\underline{\theta} = \begin{pmatrix} \theta_i \\ \theta_e \end{pmatrix} \tag{70}$$

and

$$\underline{\beta} = \begin{pmatrix} S_i - q\dot{V} \\ S_e \end{pmatrix} \Delta m. \tag{71}$$

The quantities $\underline{\underline{\alpha}}$, $\underline{\underline{a}}$, and $\underline{\underline{\gamma}}$ are diagonal matrices which are

$$\underline{\underline{\alpha}} = \begin{pmatrix} C_i & 0 \\ 0 & C_e \end{pmatrix} \frac{\Delta m}{\Delta t} , \tag{72}$$

$$\underline{\underline{a}} = \tfrac{1}{2} \begin{pmatrix} \lambda_i & 0 \\ 0 & \lambda_e \end{pmatrix} \frac{r^{\delta - 1}}{\Delta r} , \tag{73}$$

and

$$\underline{\underline{\gamma}} = \tfrac{1}{2} \begin{pmatrix} (p_\theta)_i & 0 \\ 0 & (p_\theta)_e \end{pmatrix} \dot{V} \Delta m \tag{74}$$

The quantity $\underline{\underline{\omega}}$ is a square matrix which is

$$\underline{\underline{\omega}} = \begin{pmatrix} \omega_c & -\omega_c \\ -\omega_c & \omega_c + \omega_r \end{pmatrix} \Delta m \tag{75}$$

Equation (69) may be expanded for use in systems whose state is described by any number of temperatures by merely increasing the dimension of the vector and matrix quantities. The solution of Eq. (69) will be developed with this in mind. Equation (69) may be rearranged in the form

$$\underline{\underline{A}} \cdot \underline{\theta}^{n+1}_{j-\frac{1}{2}} = \underline{\underline{a}}_j \cdot \underline{\theta}^{n+1}_{j+\frac{1}{2}} + \underline{\underline{a}}_{j-1} \underline{\theta}^{n+1}_{j-\frac{3}{2}} + \underline{B}_{j-\frac{1}{2}} \tag{76}$$

where

$$\underline{\underline{A}}_{j-\frac{1}{2}} = \underline{\underline{\alpha}}_{j-\frac{1}{2}} + \underline{\underline{\omega}}_{j-\frac{1}{2}} + \underline{\underline{\gamma}}_{j-\frac{1}{2}} + \underline{\underline{a}}_j + \underline{\underline{a}}_{j-1} \tag{77}$$

and

$$\underline{B}_{j-\frac{1}{2}} = \underline{\beta}_{j-\frac{1}{2}} + \underline{\underline{a}}_{j} \cdot \left(\underline{\theta}^{n}_{j+\frac{1}{2}} - \underline{\theta}^{n}_{j-\frac{1}{2}}\right) - \underline{\underline{a}}_{j-1} \cdot \left(\underline{\theta}^{n}_{j+\frac{1}{2}} - \underline{\theta}^{n}_{j-\frac{1}{2}}\right)$$

$$- \underline{\underline{\gamma}}_{j-\frac{1}{2}} \cdot \underline{\theta}^{n}_{j-\frac{1}{2}} - \underline{\underline{\omega}}_{j-\frac{1}{2}} \cdot \underline{\theta}^{n}_{j-\frac{1}{2}} + \underline{\underline{\alpha}}_{j-\frac{1}{2}} \cdot \underline{\theta}^{n}_{j-\frac{1}{2}} . \qquad (78)$$

Equation (75) may be solved to give

$$\underline{\theta}_{j-\frac{1}{2}} = \underline{\underline{C}}_{j-\frac{1}{2}} \cdot \underline{\theta}_{j+\frac{1}{2}} + \underline{D}_{j-\frac{1}{2}} \qquad (79)$$

where, since Eq. (76) explicitly involves only $\underline{\theta}^{n+1}$, the n + 1 may now be omitted. The matrix $\underline{\underline{C}}$ and the vector $\underline{D}$ may be found as follows. Rewrite Eq. (79) as

$$\underline{\theta}_{j-\frac{3}{2}} = \underline{\underline{C}}_{j-\frac{3}{2}} \cdot \underline{\theta}_{j-\frac{1}{2}} + \underline{D}_{j-\frac{3}{2}} . \qquad (79')$$

Substitute Eq. (79') into Eq. (76) and rearrange to obtain

$$\underline{\underline{K}}_{j-\frac{1}{2}} \cdot \underline{\theta}_{j-\frac{1}{2}} = \underline{\underline{a}}_{j} \cdot \underline{\theta}_{j+\frac{1}{2}} + \underline{E}_{j-\frac{1}{2}} \qquad (80)$$

where

$$\underline{\underline{K}}_{j-\frac{1}{2}} = \underline{\underline{A}}_{j-\frac{1}{2}} - \underline{\underline{a}}_{j-1} \cdot \underline{\underline{C}}_{j-\frac{3}{2}} \qquad (81)$$

and

$$\underline{E}_{j-\frac{1}{2}} = \underline{B}_{j-\frac{1}{2}} + \underline{\underline{a}}_{j-1} \cdot \underline{D}_{j-\frac{3}{2}} . \qquad (82)$$

Hence

$$\underline{\underline{C}}_{j-\frac{1}{2}} = \underline{\underline{K}}^{-1}_{j-\frac{1}{2}} \cdot \underline{\underline{a}}_{j} \qquad (83)$$

and

$$\underline{D}_{j-\frac{1}{2}} = \underline{\underline{K}}^{-1}_{j-\frac{1}{2}} \cdot \underline{E}_{j-\frac{1}{2}} \qquad (84)$$

where $\underline{\underline{K}}^{-1}$ is the inverse of the matrix $\underline{\underline{K}}$.

During each time step, the components of $\underline{\underline{C}}_{j-\frac{1}{2}}$ and $\underline{D}_{j-\frac{1}{2}}$ are evaluated from $\underline{\underline{C}}_{j-\frac{3}{2}}$ and $\underline{D}_{j-\frac{3}{2}}$ by means of Eqs. (81), (82), (83), and (84). To start this evaluation,

$\underline{\underline{a}}_o$ and hence $\underline{\underline{C}}_{-\frac{1}{2}}$ are taken as $\underline{\underline{0}}$, and $\underline{D}_{-\frac{1}{2}}$ is taken as $\underline{\theta}^n_{-\frac{1}{2}}$. The calculation of the components of each $\underline{\theta}_{j-\frac{1}{2}}$ is determined from $\underline{\theta}_{j+\frac{1}{2}}$ by means of Eq. (79) starting with $\underline{\theta}_{J-\frac{1}{2}}$, the temperatures in the outermost zone, which is determined by the boundary conditions at the outermost boundary. These boundary conditions will be described in Section IV.4. The innermost boundary is considered to be a thermally insulated, immoveable wall.

3. EVALUATION OF THE COEFFICIENTS

The evaluation of many of the coefficients in Eq. (69) involves $\theta_i^{n+\frac{1}{2}}$ and $\theta_e^{n+\frac{1}{2}}$. These values of θ are calculated by extrapolation. A quadratic expression for θ in terms of t is fitted to the values of $\frac{1}{2}\ (\theta^{n-m+1} + \theta^{n-m})$ for m equal to 1, 2, and 3 with the corresponding values of t. This expression is then evaluated at $t^{n+\frac{1}{2}}$. There results for each of the θ's in both media

$$\tilde{\theta}^{n+\frac{1}{2}} = \frac{1}{2}\sum_{m=1}^{3} C_m(\theta^{n-m+1} + \theta^{n-m}) \tag{85}$$

where

$$C_3 = 1 - \left[\frac{1}{2}(\Delta t^{n+\frac{1}{2}})^2 - \left(\Delta t^{n+\frac{1}{2}} - \Delta t^{n-\frac{5}{2}}\right)\ (\Delta t^n + \Delta t^{n-2})\right] / D$$

$$D = \Delta t^{n-2}\left[2\Delta t^n - \left(\Delta t^{n+\frac{1}{2}} - \Delta t^{n-\frac{5}{2}}\right)\right]$$

$$C_1 = 1 + (\Delta t^n/\Delta t^{n-1}) + (\Delta t^{n-2}/\Delta t^{n-3})C_3$$

$$C_2 = -(\Delta t^n/\Delta t^{n-1}) - \left[1 + (\Delta t^{n-2}/\Delta t^{n-1})\right] C_3.$$

Other useful values of the θ's and their powers may be computed from those found in Eq. (85) by means of the expressions

$$\bar{\theta}_j^{n+\frac{1}{2}} = \frac{1}{2}\left(\tilde{\theta}^{n+\frac{1}{2}}_{j+\frac{1}{2}} + \tilde{\theta}^{n+\frac{1}{2}}_{j-\frac{1}{2}}\right) \tag{86}$$

and

$$(\overline{\theta^2})^{n+\frac{1}{2}} = \frac{1}{2}\left[\left(\tilde{\theta}^{n+\frac{1}{2}}_{j+\frac{1}{2}}{}^{2} + \tilde{\theta}^{n+\frac{1}{2}}_{j-\frac{1}{2}}\right)^2\right]. \tag{87}$$

Values of the θ's and their powers computed by means of Eqs. (85), (86), and (87) are substituted into the various formulas already given to evaluate the coefficients.

In the evaluation of the a's, it may be noticed that Δr is not evaluated on the boundaries of the zones. The two non-zero components of $\underline{\underline{a}}$ in Eq. (72) are more precisely determined by

$$a_j^{n+\frac{1}{2}} = \left(r_j^{n+\frac{1}{2}}\right)^{\delta-1}\left[\left(\Delta r_{j+\frac{1}{2}}^{n+\frac{1}{2}} \Big/ {}_+\lambda_j^{n+\frac{1}{2}}\right) + \left(\Delta r_{j-\frac{1}{2}}^{n+\frac{1}{2}} \Big/ {}_-\lambda_j^{n+\frac{1}{2}}\right)\right]^{-1}, \tag{88}$$

where

$${}_+\lambda_j^{n+\frac{1}{2}} = \lambda\left(\bar{\theta}_{j+\frac{1}{2}}^{n+\frac{1}{2}},\ V_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right) \quad \text{and} \quad {}_-\lambda_j^{n+\frac{1}{2}} = \lambda\left(\bar{\theta}_{j-\frac{1}{2}}^{n+\frac{1}{2}},\ V_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right).$$

The general method for the evaluation of the λ's is given in Spitzer.[3] The evaluation of the λ's and the other coefficients have differed in detail in various specific applications from the methods given here (even as the equations of state differ from the ideal gas law for ions and electrons in various applications). Since the actual formulas used must be tailored to the specific physical problem, these formulas will not be given in greater detail here.

4. BOUNDARY CONDITIONS

The "inner" boundary ($j = 0$) is taken to be an immoveable, perfectly reflecting, thermally insulated wall. Various combinations of boundary conditions may be used at the outer boundary ($j = J$):

Temperature

- Thermally insulated boundary: $\theta_{J+1/2} = 0$, $\theta_J = 0$, for both ions and electrons.
- Temperature determined: $\theta_{J+1/2} = \theta(t)$ for both ions and electrons.

Here the components of $\underline{\underline{a}}_J$ may be determined from Eq. (73) with the factor of 2 left out of the denominator since the zone center is only a distance $\Delta r/2$ from the boundary.

Velocity and Pressure

- Pressure determined: $p_J = p(t)$.
  Here the velocity u_J of the outer boundary is determined by the code.
- Velocity determined: $u_J = u(t)$.
  Here the pressure on the outer boundary is determined by the code.

5. CALCULATION OF THE ENERGY SOURCES

In difference equation form, Eqs. (34) and (36) may be expressed as follows:

$$\psi_{j-1}^{-} = \psi_j^{-} \exp\left(-K_{j-\frac{1}{2}}\,\Delta r_{j-\frac{1}{2}}/\epsilon_{j-\frac{1}{2}}\right) \tag{89}$$

$$\psi_j^+ = \psi_{j-1}^+ \exp\left(-K_{j-\frac{1}{2}}\Delta r_{j-\frac{1}{2}}/\epsilon_{j-\frac{1}{2}}\right) \tag{90}$$

where ψ_J^- is given by Eq. (33) and ψ_1^+ by Eq. (35). The values of K are calculated by Eq. (47) with Eqs. (45) and (46) or, for more general cases, Eqs. (37) and (44); the energy source density terms are calculated by Eqs. (31) and (32). The divisor $\epsilon_{j-\frac{1}{2}}$ modifies the effective absorption to account for the increase in the dielectric constant as the plasma frequency approaches the frequency of the light. We wish to produce total reflection when the electron density approaches the critical electron density closely (within 98 percent, for instance). Hence we let $y_j = (N_e)_j/N_c$ where N_c is the critical density. Suppose we have

$$y_j < 1 - \xi \quad \text{for } j = J, J-1, J-2, \ldots, k+1$$

$$y_j \geq 1 - \xi \quad \text{for } J = k, k-1, \ldots, 2, 1$$

where $\xi = 0.02$ for the 98 percent case, then

$$\epsilon_{j-\frac{1}{2}} = \left[1 - \tfrac{1}{2}(y_j + y_{j-1})\right]^{\frac{1}{2}} \quad j = J, J-1, \ldots, k+2 \tag{91}$$

$$\epsilon_{k+\frac{1}{2}} = \left[1 - \tfrac{1}{2}(y_{k+1} + 1)\right]^{\frac{1}{2}} \tag{92}$$

$$\psi_k^+ = \psi_k^- \tag{93}$$

and $(S_e)_{j-\frac{1}{2}} = 0$ for $j \leq k$.

In calculations involving fusion, the densities N_T and N_D are expressed in terms of fractions, $f = N_T/N$ and $g = N_D/N$ where $N = N_T^0 + N_D^0$, the superscript 0 on N_T and N_D indicates that these are the initial values of the variables. In terms of the fractions, f and g, the difference equation forms of Eqs. (48) and (49) are

$$f^{n+1} = f^n - C_D\Delta t^{n+\frac{1}{2}}\left[R_{DT}^{n+\frac{1}{2}}\,\tilde{f}^{n+\frac{1}{2}}\,\tilde{g}^{n+\frac{1}{2}} - \tfrac{1}{4}R_{DD}^{n+\frac{1}{2}}\left(\tilde{g}^{n+\frac{1}{2}}\right)^2\right]\Big/V^{n+\frac{1}{2}} \tag{94}$$

$$g^{n+1} = g^n - C_D\Delta t^{n+\frac{1}{2}}\left[R_{DT}^{n+\frac{1}{2}}\,\tilde{f}^{n+\frac{1}{2}}\,\tilde{g}^{n+\frac{1}{2}} + R_{DD}^{n+\frac{1}{2}}\left(\tilde{g}^{n+\frac{1}{2}}\right)^2\right]\Big/V^{n+\frac{1}{2}} \tag{95}$$

where $C_D = N_o/(3f^o + 2g^o)$. The quantities $\tilde{f}^{n+\frac{1}{2}}$ and $\tilde{g}^{n+\frac{1}{2}}$ in Eqs. (94) and (95) are extrapolated values of the variables which may be calculated by means of

$$\tilde{f}^{n+\frac{1}{2}} = f^n + \tfrac{1}{2}\left(\Delta t^{n+\frac{1}{2}}/\Delta t^{n-\frac{1}{2}}\right)\left(f^n - f^{n-1}\right) \tag{96}$$

$$\tilde{g}^{n+\frac{1}{2}} = g^n + \tfrac{1}{2}\left(\Delta t^{n+\frac{1}{2}}/\Delta t^{n-\frac{1}{2}}\right)\left(g^n - g^{n-1}\right). \tag{97}$$

6. Δt CONTROL

During each time step in the calculations, the size of the time step Δt is controlled to satisfy a number of conditions:

- Δt must lie between preselected limits Δt_{max} and Δt_{min}.
- $\Delta x/\Delta t$ should not exceed the rate at which a disturbance would be propagated through the medium hydrodynamically (Courant condition).
- Δt will be increased or decreased in such a way as to hold the percentage change in V and θ below certain selected values.

The Courant condition is given by

$$R_1^{n+1} = \underset{j}{\mathrm{Max}} \left[\left(V_{j-\frac{1}{2}}^{n+1} \, p_{j-\frac{1}{2}}^{n+1} \right)^{\frac{1}{2}} \Big/ \Delta r_{j-\frac{1}{2}}^{n+1} \right] . \qquad (98)$$

The maximum fractional changes in V and θ are given by

$$R_2^{n+1} = \underset{j}{\mathrm{Max}} \left[\left(V_{j-\frac{1}{2}}^{n+1} - V_{j-\frac{1}{2}}^{n} \right) \Big/ V_{j-\frac{1}{2}}^{n+\frac{1}{2}} \right] \qquad (99)$$

$$R_3^{n+1} = \underset{j(i,\, e)}{\mathrm{Max}} \left[\left(\theta_{j-\frac{1}{2}}^{n+1} - \theta_{j-\frac{1}{2}}^{n} \right) \Big/ \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} \right] . \qquad (100)$$

Thus to satisfy all the conditions above we must have

$$\Delta t^{n+\frac{3}{2}} = \mathrm{Max} \left[\Delta t_{min}, \ \mathrm{Min} \left(\Delta t_{max}, K_1 \Big/ R_1^{n+1}, \ K_2 \Delta t^{n+\frac{1}{2}} \Big/ R_2^{n+1}, \ K_3 \Delta t^{n+\frac{1}{2}} \Big/ R_3^{n+1} \right) \right] \qquad (101)$$

where K_1, K_2, and K_3 are parameters which may be selected at the option of the person performing the calculation to modify the effect of these various conditions.

V. Energy Checks

One of the features of computational programs used in these calculations is the incorporation of a system of energy checks. To insure that no machine error in the preparation of the input data has occurred and to assist in troubleshooting the programs when changes or modifications are made, values of the different forms of energy are totalled at the end of each time step to see that the law of conservation of energy is obeyed.

1. INTEGRAL FORMS OF THE FIRST LAW

Equations (20) and (21) may be written in the form:

$$\dot{U}_i + p_i \dot{V} = S_i - \dot{Q}_c + \dot{Q}_{Di} \qquad (102)$$

$$\dot{U}_e + p_e\dot{V} = S_e + \dot{Q}_c - \dot{Q}_r + \dot{Q}_{De} \qquad (103)$$

where

$$\dot{Q}_c = 2\omega_c(\theta_i - \theta_e) \qquad (104)$$

$$\dot{Q}_r = 2\omega_r\theta_e \qquad (105)$$

$$\dot{Q}_D = -V(\underline{\nabla} \cdot \underline{f}) = -(r^{\delta-1}f)_m. \qquad (106)$$

Equation (106) holding for both ions and electrons. Adding Eqs. (102) and (103) gives, in view of Eqs. (23) and (26),

$$\dot{U} + p\dot{V} = S + \dot{Q}_D - \dot{Q}_r \qquad (107)$$

where

$$\dot{Q}_D = \dot{Q}_{Di} + \dot{Q}_{De}. \qquad (108)$$

To find suitable integral forms of Eqs. (102), (103), and (107), we first consider the integration of the $p\dot{V}$ term in each of these equations. From Eq. (5) we have

$$\dot{V}dm = d(ur^{\delta-1}). \qquad (109)$$

From Eq. (6) we have

$$u\dot{u} = -ur^{\delta-1}(dp/dm) = (d/dt)(u^2/2). \qquad (110)$$

Integration of Eq. (110) with respect to m gives

$$\dot{T} = -\int_o^J ur^{\delta-1}(dp/dm)dm \qquad (111)$$

where T is the total kinetic energy. The right-hand side of Eq. (111) may be integrated by parts to give

$$\dot{T} = -\Big[ur^{\delta-1}p\Big]_J + \int_o^J pd(ur^{\delta-1}). \qquad (112)$$

Thus from Eqs. (109) and (112) we have

$$\int_o^J p\dot{V}dm = \dot{T} + \Big[ur^{\delta-1}p\Big]_J. \qquad (113)$$

Equation (102) may be rewritten

$$\dot{U}_i + p\dot{V} = S_i - \dot{Q}_c + \dot{Q}_{Di} + p_e\dot{V}. \tag{114}$$

Equations (114) and (103) may be integrated with respect to m with the help of Eqs. (109) and (113) to give

$$\dot{e}_i + \dot{T} + \left(ur^{\delta-1}p_i\right)_J = s_i - e_c - \left(f_i r^{\delta-1}\right)_J - \int_o^J ur^{\delta-1}\,dp_e \tag{115}$$

$$\dot{e}_e + \left(ur^{\delta-1}p_e\right)_J = s_e + e_c - e_r - \left(f_e r^{\delta-1}\right)_J + \int_o^J ur^{\delta-1}\,dp_e \tag{116}$$

in which

$$e_x = \int_o^J U_x dm, \qquad x = i, e \tag{117}$$

$$s_x = \int_o^J S_x dm, \tag{118}$$

$$\left(f_x r^{\delta-1}\right)_J = -\int_o^J \dot{Q}_{Dx} dm, \tag{119}$$

$$\int_o^J p_x \dot{V} dm = \int_o^J p_x d(ur^{\delta-1}) = \left(p_x ur^{\delta-1}\right)_J - \int_o^J ur^{\delta-1} dp_x, \tag{120}$$

$$e_r = \int_o^J \dot{Q}_r dm, \quad \text{and} \tag{121}$$

$$e_c = \int_o^J \dot{Q}_c dm. \tag{122}$$

Equations (115) and (116) added together give

$$\dot{e} + \dot{T} + (ur^{\delta-1}p)_J = s - (fr^{\delta-1})_J - e_r. \tag{123}$$

The physical significance of the quantities defined by Eqs. (117) through (122) may be described as follows:

e_x - *total internal energy of the ions or electrons.*

s_x - total energy source rate for the ions or electrons.

$\left(f_x r^{\delta-1}\right)_J$ - rate of heat loss by the ions or electrons across the outer boundary.

$\left(p_x u r^{\delta-1}\right)_J$ - rate at which work is done by the ions or electrons on the external environment.

e_r - total rate of heat loss through radiation.

e_c - total rate of heat transfer from the ions to electrons (or from the electrons to the ions).

It may be noted that in these calculations the ions and electrons are somewhat artificially constrained to move together hydrodynamically even though they have their own independent internal energies and exert their own independent pressures. Therefore

$\int_o^J u r^{\delta-1}\, dp_e$ - total rate at which work is done by the ions on the electrons to maintain the above constraint.

2. ENERGY CHECKS

If the computer program is working correctly, Eqs. (115), (116) and (123) must each be satisfied. Hence their integral with respect to time must be satisfied. Therefore let

$$e_x^{n+1} = \sum_j (U_x)_{j-\frac{1}{2}}^{n+1} \Delta m_{j-\frac{1}{2}} \qquad x = i, e \tag{124}$$

$$T^{n+1} = \tfrac{1}{4}\left(u_J^{n+1}\right)^2 \Delta m_{J-\frac{1}{2}} + \tfrac{1}{2}\sum_j \left(u_j^{n+1}\right)^2 \Delta m_j \tag{125}$$

$$H_x^{n+1} = \int_o^{t^{n+1}} s_x dt = H_x^n + \Delta t^{n+\frac{1}{2}} \sum_j (S_x)_{j-\frac{1}{2}}^{n+1} \Delta m_{j-\frac{1}{2}} \tag{126}$$

$$E_c^{n+1} = \int_o^{t^{n+1}} e_c dt = E_c^n + \Delta t^{n+\frac{1}{2}} \sum_j (\dot{Q}_c)_{j-\frac{1}{2}}^{n+\frac{1}{2}} \Delta m_{j-\frac{1}{2}} \tag{127}$$

$$G_e^{n+1} = \int_o^{t^{n+1}} \int_o^J u r^{\delta-1}\, dp_e dt = G_e^n + \Delta t^{n+\frac{1}{2}} \sum_j u_j^{n+\frac{1}{2}} \left(r_j^{n+\frac{1}{2}}\right)^{\delta-1} \left[(p_e)_{j+\frac{1}{2}}^{n+\frac{1}{2}} - (p_e)_{j-\frac{1}{2}}^{n+\frac{1}{2}}\right]$$

$$+ \Delta t^{n+\frac{1}{2}} u_J^{n+\frac{1}{2}} \left(r_J^{n+\frac{1}{2}}\right)^{\delta-1} \left[(p_e)_J^{n+\frac{1}{2}} - (p_e)_{J-1}^{n+\frac{1}{2}}\right] \tag{128}$$

$$E_r^{n+1} = \int_o^{t^{n+1}} e_r dt = E_r^n + \Delta t^{n+\frac{1}{2}} \sum_j (\dot{Q}_r)_{j-\frac{1}{2}}^{n+\frac{1}{2}} \Delta m_{j-\frac{1}{2}}^{n+1} \qquad (129)$$

$$W_x^{n+1} = \int_o^{t^{n+1}} \left(ur^{\delta-1} p_x\right)_J dt = W_x^n + \left[u_J^{n+\frac{1}{2}} \left(r_J^{n+\frac{1}{2}}\right)^{\delta-1} (p_x)_J^{n+\frac{1}{2}}\right] \Delta t^{n+\frac{1}{2}} \qquad (130)$$

$$F_x^{n+1} = \int_o^{t^{n+1}} \left(f_x r^{\delta-1}\right)_J dt = F_x^n - 2(a_x)_J^{n+\frac{1}{2}} \left[(\theta_o)_{J+\frac{1}{2}}^{n+\frac{1}{2}} - (\theta_x)_{J-\frac{1}{2}}^{n+\frac{1}{2}}\right] \Delta t^{n+\frac{1}{2}} \qquad (131)$$

where in Eqs. (124), (126), (127), and (129) the summation is from 1 to J and in Eqs. (125) and (128) it is from 1 to J - 1, and where it must be remembered to use $p_i^{n+\frac{1}{2}} + q^{n+\frac{1}{2}}$ in place of $p_i^{n+\frac{1}{2}}$ in Eq. (130).

Thus, each time the program edits the calculation, a check is made to see how well the following equations are satisfied:

$$e_i^{n+1} + T^{n+1} = e_i^o + T^o + H_i^{n+1} - E_c^{n+1} - F_i^{n+1} - W_i^{n+1} - G_e^{n+1} \qquad (132)$$

$$e_e^{n+1} = e_e^o + H_e^{n+1} + E_c^{n+1} - F_e^{n+1} - W_e^{n+1} + G_e^{n+1} - E_r^{n+1}. \qquad (133)$$

Adding Eqs. (132) and (133) gives

$$e^{n+1} + T^{n+1} = e^o + T^o + H^{n+1} - F^{n+1} - W^{n+1} - E_r^{n+1}. \qquad (134)$$

VI. Sequence of Operations in the Calculations

Figure 1 shows the general order in which the calculations described in this report are performed.

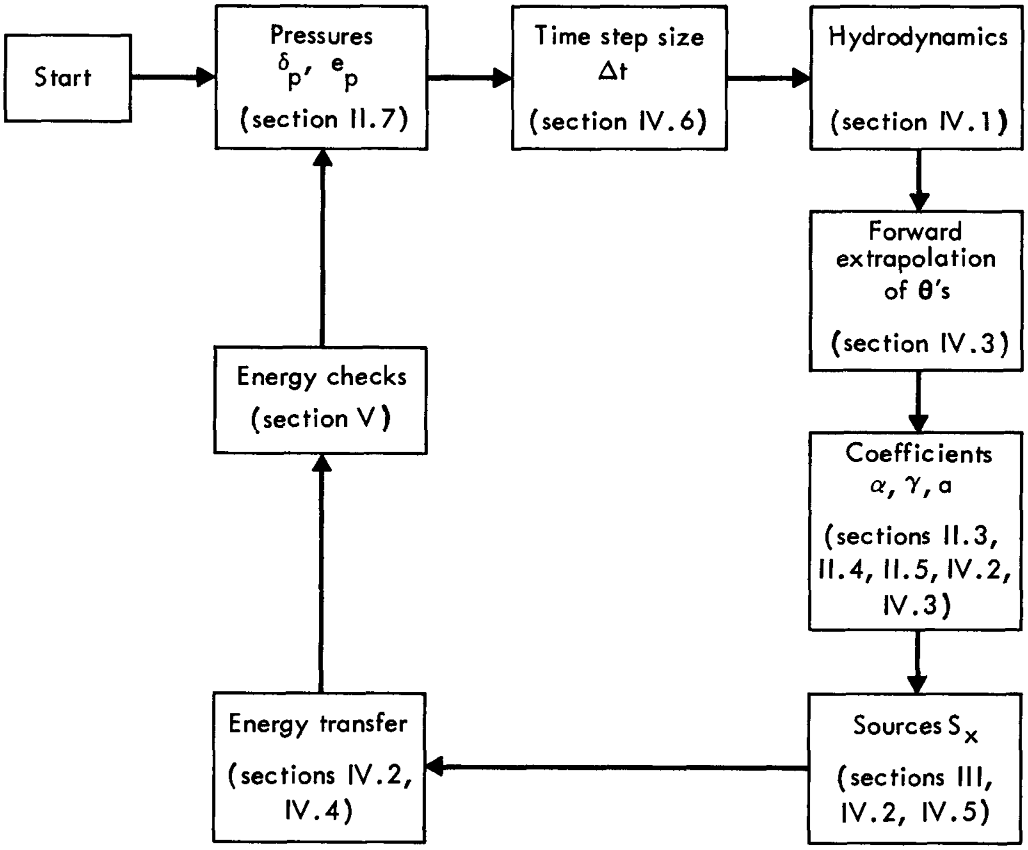

Fig. 1. Flow diagram of calculations.

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