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A COUPLED MHD-MONTE CARLO TRANSPORT MODEL FOR DENSE PLASMAS

MASTER

William Paul Chandler
(Ph. D. Thesis)

June, 1975

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A COUPLED MHD-MONTE CARLO TRANSPORT MODEL FOR DENSE PLASMAS

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ABSTRACT

A two-dimensional, two fluid model of the MHD equations has been coupled to a Monte Carlo transport model of high energy, non-Maxwellian ions. The MHD part of the model assumes complete ionization and includes a perfect gas law for a scalar pressure, a tensor artificial viscosity, electron and ion thermal conduction, electron-ion coupling, and a radiation loss term. A simple Ohm's Law is used with a b_z magnetic field. The MHD equations were solved in Lagrangian coordinates. The conservation equations were differenced explicitly and the diffusion-type equations implicitly using the splitting technique. The Monte Carlo model solves the equation of motion for high energy ions, moving through and suffering small and large angle collisions with the fluid Maxwellian plasma. The source of high energy ions is the thermonuclear reactions of the hydrogen isotopes, or it may be an externally injected beam of neutralized ions. In addition to using the usual Maxwell averaged thermonuclear cross sections for calculating the number of reactions taking place within the Maxwellian plasma, the high energy ions may suffer collisions resulting in a reaction. In the Monte Carlo model all neutrons are assumed to escape, and all energetic ions of $Z \leq 2$ are followed.

This model can be used to calculate the effect of a non-Maxwellian species interacting with a fluid species and is particularly useful in calculating the spatial variations of the energy depositions to a Maxwellian fluid from a high energy non-Maxwellian species. As a demonstration, the model was used to calculate the alpha particle heating of a very dense gas-embedded Z-pinch. Heating from 10 to 45 keV is primarily due to the alpha heating and consequently the pinch expands. The results of this calculation show that the alpha particle energy depositions are in fair agreement with previous calculations, but that energy losses due to drift are lower than expected. The differences can be attributed to the nonlocal energy depositions of the alpha particles.

1. INTRODUCTION

Computer codes and models that have been developed for the study of plasma physics related to the controlled fusion program have primarily been of three types:¹

1. the fluid MHD model;
2. the particle models; and
3. the kinetic equation models.

The fluid MHD model is computationally faster, but is generally limited to dense collision dominated fluids, or when the Larmor orbits of the fluid species is small compared to characteristic sizes of interest in the plasma fluid.

The particle codes give great detail at the expense of computer time and memory capacity, but generally don't consider the macroscopic fluid behavior of the plasma. Particle codes usually do not consider collisions between the plasma components, but do solve the nonlinear Vlasov equation and Maxwell's equations in a self consistent manner.

The kinetic equation codes solve the Vlasov and Fokker-Planck equations directly by differencing of the transport equation or using Fourier transform techniques. In neither case is fluid behavior considered. The Fokker-Planck model is used mainly to calculate the time and velocity variations of a distribution function, but usually not the spatial variations.

The object of this study was to build a model and a code that would not only calculate the behavior of a dense fluid, but also the behavior of a species of high energy non-Maxwellian ions traveling through and interacting with the Maxwellian plasma fluid. The source of these energetic ions within the fluid plasma may be the result of thermonuclear reactions and/or an injected beam of neutralized ions (a neutral cloud of ions and electrons). Computationally, the fluid behavior is modeled with the MHD equations and the high energy non-Maxwellian ions with a Monte Carlo - particle tracking and collision model. These two models are coupled through collisions in the Monte Carlo routines, and source terms in the MHD equations.

In other words, the code does the following physics. The MHD model is a two-dimensional (cylindrical - R, Z) Lagrangian two fluid model. There is a Maxwellian electron fluid at temperature T_e and a Maxwellian ion fluid at temperature T_i . The ion fluid may be composed of all the isotopes of hydrogen and helium, but they are all assumed to be at the temperature T_i . A perfect gas equation of state is used. The fluid equations were explicitly differenced in a manner similar to Schulz,^{2,3} with his scheme for a tensor artificial viscosity. For simplicity, only the $B_\theta(R, Z)$ component of the magnetic field was programmed, although the other components (B_R, B_Z) could be added to the model. A simple Ohm's Law was also assumed. The time derivative of the magnetic field was solved implicitly, since the appropriate Maxwell's equations were easily cast into a diffusion type equation. Electron and ion thermal conduction was also solved implicitly. The transport coefficients; κ_e - electron thermal

conductivity, κ_i - ion thermal conductivity, and σ - electric conductivity were modeled after Braginskii;⁴ i.e., they are functions of B and Z (atomic number) in addition to the usual variables - n_e , n_i , T_e , T_i . Because of the two temperature model, an electron-ion coupling energy loss (gain) term was calculated. A radiation loss term due to bremsstrahlung was included in the electron energy equation.

The source of high energy, non-Maxwellian ions was calculated from the thermonuclear hydrogen isotope reaction rates using the Maxwell averaged cross sections of Greene.⁵ The high energy ion reaction products were then sampled in a Monte Carlo manner, and were transported through the magnetized Maxwellian fluids. The Monte Carlo particles move through the fluid, under the action of the $\vec{v} \times \vec{B}$ Lorentz force, and suffer small and large angle collisions with the fluid electrons and ions. The change in the Monte Carlo bundle's energy and momentum due to small angle collisions is calculated deterministically by integrating an energy loss rate equation (dE/dt). The Monte Carlo bundles may also suffer a large angle scatter or an in-flight thermonuclear reaction. The relatively unimportant large angle scatters and the more important in-flight reactions were done in the usual Monte Carlo manner; i.e., random number selection weighted against collision and reaction probabilities.

In other words, a Monte Carlo high energy ion bundle would be generated and would be moved along its $\vec{v} \times \vec{B}$ orbit for some predetermined time step. At the end of the time step, the energy and momentum changes over that step are calculated due to small angle collisions with electrons and ions. It is assumed that the time to equilibration is less than the

time for a 90° deflection, therefore there would be no deflection of the Monte Carlo bundle due to small angle collisions. Now the probability of having a large angle scatter or in-flight reaction over that path are calculated and compared to a random number. If a collision occurred, then it is assumed to take place at the end of the path and the collision kinematics are calculated. If no collision occurs, the tracking of the particle is continued for another time step. Changes in the fluid's energy and momentum due to the Monte Carlo bundles are then used as source terms in the energy and momentum equations in the MHD section. See Fig. 1 for a very simplified block diagram of the model. In Fig. 1, $\vec{V}$ is the fluid velocity, $\vec{v}$ is the Monte Carlo bundle velocity, ρ the fluid density, $\vec{J}_{MC}$ is the current due to the motion of the high energy Monte Carlo bundles, and T_e and T_i are the electron and ion temperatures.

It should be noted that the model is not self-consistent, in that the Monte Carlo bundles do not see each other, and the electric fields generated between them are ignored. This is valid since the density of the high-energy particles is very small compared to the fluid density.

As a demonstration of this model a code was written on a CDC 7600 computer, and was used to calculate the thermonuclear alpha particle heating of a very dense gas-embedded Z-pinch.⁶ Recent studies have indicated that the Z-pinch may have a lifetime in excess of the shortest growth time for MHD instability;⁷ resulting in a renewed interest in the gas-embedded Z-pinch as a fusion concept. Previous calculations were done on a 1-D MHD code with a crude analytical model to simulate the

energy deposited to the pinched gas from the alpha particles generated from thermonuclear reactions. The results of this calculation show that the alpha particle energy depositions are in fair agreement with the previous calculations, but that energy losses due to drift are lower than expected. These differences can be attributed to the nonlocal energy depositions of the alpha particles. The details of this calculation are described in Appendix 1.

It should be noted that Gaussian c.g.s. units will be used throughout this study.

Figure 1. Block diagram of MHD-Monte Carlo Model: Left hand part of diagram is the MHD, while that on the right is the Monte Carlo Model.

2. MHD MODEL

General

The equations to be solved are:

$$\frac{dm}{dt} = \dot{m}_{MC} \quad (2.0.1)$$

$$\frac{d\vec{V}}{dt} = -\frac{1}{\rho} \nabla (p + q) + \frac{1}{\rho t} \vec{J} \times \vec{B} + \vec{V}_{MC} \quad (2.0.2)$$

$$\rho \frac{dc_i}{dt} = -\rho (p_i + q) \frac{d\tau}{dt} - \omega (KT_i - KT_e) - \nabla \cdot \vec{Q}_i + S_i \quad (2.0.3)$$

$$\begin{aligned} \rho \frac{dc_e}{dt} = & -\rho p_e \frac{d\tau}{dt} + \omega (KT_i - KT_e) - \nabla \cdot \vec{Q}_e \\ & + \eta |\vec{J}|^2 - p_B + S_e \end{aligned} \quad (2.0.4)$$

$$\nabla \times \vec{B} = \frac{4\pi}{c} \vec{J} \quad (2.0.5)$$

$$-\frac{1}{c} \frac{d}{dt} \int_S \vec{B} \cdot \hat{n} da = \int_C \vec{E}' \cdot d\vec{\ell} \quad (2.0.6)$$

with a simple Ohm's law

$$\vec{E}' = \eta \vec{J} \quad (2.0.7)$$

where

- ρ = density of fluid
- $\vec{V}$ = velocity of fluid
- p_e = electron pressure
- p_i = ion pressure
- $p = p_e + p_i$
- q = artificial viscosity
- n_e = density of electrons

- n_i = density of ions
 m = mass of fluid
 η = electric resistivity
 K = Boltzman's constant
 T_e = electron temperature
 T_i = ion temperature
 ω = electron-ion coupling coefficient
 $\vec{Q}_i$ = ion heat flux vector
 $\vec{Q}_e$ = electron heat flux vector
 ϵ_i = internal ion energy
 ϵ_e = internal electron energy
 τ = the specific volume (reciprocal of density)
 $\dot{m}_{MC}$ = Monte Carlo sources to mass
 $\vec{V}_{MC}$ = Monte Carlo sources to momentum
 S_i = Monte Carlo sources to ion energy
 S_e = Monte Carlo sources to electron energy
 P_B = bremsstrahlung energy density loss rate
 $\vec{E}'$ = electric field in the rest frame of $d\vec{l}$

Note that the equations are written in terms of the total derivative which is the form that is differenced in Lagrangian coordinates.

Since only $\vec{B} = B_\theta(R, Z) \hat{\theta}$ is being considered

$$\vec{Q}_i = - \kappa_{i1} \nabla(KT_i) \quad (2.0.8)$$

$$\vec{Q}_e = - \kappa_{1e} \nabla(KT_e) \quad (2.0.9)$$

and from Glasstone and Lovberg⁸

$$P_B = g \frac{32\pi}{3^{3/2}} \cdot \frac{(2\pi KT_e)^{1/2} e^6}{m_e c^3 h} n_e \sum_i (n_i Z_i^2) \quad (2.0.10)$$

or

$$P_B = 5.35 \times 10^{-24} n_e \sum_i (n_i Z_i^2) T_e^{1/2} \text{ ergs/(cm}^3 \text{ sec)}$$

where T_e is given in keV.

From Braginskii (pg. 217 - Eq. 2.17)⁴

$$\omega = \frac{3m_e n_e}{m_i \tau_e} ; \quad \tau_e = \frac{3 \sqrt{m_e} (KT_e)^{3/2}}{4 \sqrt{2\pi} e^4 Z_i^2 n_i \ln \Lambda} \quad (2.0.11)$$

where $\ln \Lambda$ is given by the expression⁹

$$\ln \Lambda = 31.17 + \frac{1}{2} \ln \left[\frac{(KT_e)^2}{n_e} \right]$$

and where (KT_e) is expressed in keV.

The transport coefficients κ_{1e} , κ_{1i} , and σ_1 were modeled after Braginskii, and are described in Appendix 2.

In addition to these above equations, two equations of state are needed. A perfect gas is assumed

$$P_e = n_e KT_e \quad (2.0.12)$$

$$P_i = n_i KT_i$$

Now to solve the above energy equations, a "splitting" technique was used; i.e., the conduction and the joule heating terms were calculated separately and the energy of the zones was adjusted accordingly.

2.1 Conservation Equations

Since the source term $\dot{m}_{MC}$ in Eq. (2.0.1) is to be calculated and added to the problem mass independently, Eq. (2.0.1) becomes

$$\frac{dm}{dt} = 0$$

or the mass in a fluid element remains constant. Therefore this equation need not be considered.

Eliminating the current $\vec{J}$ from Eq. (2.0.2) using Eq. (2.0.5) gives:

$$\rho \frac{d\vec{V}}{dt} = \frac{1}{\rho} \left\{ -\nabla p + q - \frac{B_0}{4\pi R} \nabla(RB_0) \right\} + \vec{V}_{MC} \quad (2.1.1)$$

and splitting off the thermal conduction and joule heating gives for the energy equations

$$\rho \frac{d\epsilon_i}{dt} = -\rho(p_i + q) \frac{d\tau}{dt} - \omega(KT_i - KT_e) + S_i \quad (2.1.2)$$

$$\rho \frac{d\epsilon_e}{dt} = -\rho p_e \frac{d\tau}{dt} + \omega(KT_i - KT_e) - P_B + S_e \quad (2.1.3)$$

Equations (2.1.1)-(2.1.3) are now to be differenced for Lagrangian coordinates, in a manner similar to Schulz.^{2,3}

Letting k and l be defined as Lagrangian coordinates, the Jacobian of the transformation is given by

$$j = -\frac{\partial R}{\partial k} \frac{\partial Z}{\partial l} + \frac{\partial R}{\partial l} \frac{\partial Z}{\partial k} \quad (2.1.4)$$

Figure 2. Lagrangian mesh in Eulerian reference frame.

Note that j is the negative of the usual expression. To convert Eulerian derivatives to Lagrangian, the following expressions can easily be derived.

$$\frac{\partial g}{\partial R} = \frac{1}{j} \left(\frac{\partial Z}{\partial k} \frac{\partial g}{\partial Z} - \frac{\partial Z}{\partial l} \frac{\partial g}{\partial l} \right) \quad (2.1.5)$$

$$\frac{\partial g}{\partial Z} = \frac{1}{j} \left(\frac{\partial R}{\partial l} \frac{\partial g}{\partial R} - \frac{\partial R}{\partial k} \frac{\partial g}{\partial k} \right) \quad (2.1.6)$$

where g is some arbitrary function.

Now consider the two components of the vector Eq. (2.1.1), remembering $\vec{B} = B_\theta(R, Z)\hat{e}$.

$$\frac{d\vec{v}_R}{dt} = \frac{1}{r} \left[-\frac{\partial}{\partial R} (p + q) - \frac{B}{4\pi R} \frac{\partial(RB)}{\partial R} \right] + \left[\vec{v}_R \right]_{MC}$$

and

$$\frac{dV_z}{dt} = \frac{1}{\rho} \left[- \frac{\partial}{\partial Z} (p + q) - \frac{B}{4\pi R} \frac{\partial(RB)}{\partial Z} \right] + \left[\dot{V}_Z \right]_{MC}$$

Transforming to Lagrangian coordinates, using (2.1.5) and (2.1.6) gives

$$\begin{aligned} \frac{dV_R}{dt} = \frac{1}{\rho j} & \left\{ \left[\frac{\partial Z}{\partial \ell} \frac{\partial P}{\partial k} - \frac{\partial Z}{\partial k} \frac{\partial P}{\partial \ell} \right] \right. \\ & \left. + \frac{B}{4\pi R} \left[\frac{\partial Z}{\partial \ell} \frac{\partial(RB)}{\partial k} - \frac{\partial Z}{\partial k} \frac{\partial(RB)}{\partial \ell} \right] \right\} + \left[\dot{V}_R \right]_{MC} \end{aligned} \quad (2.1.7)$$

$$\begin{aligned} \frac{\partial V_Z}{\partial t} = \frac{1}{\rho j} & \left\{ \left[\frac{\partial R}{\partial k} \frac{\partial P}{\partial \ell} - \frac{\partial R}{\partial \ell} \frac{\partial P}{\partial k} \right] \right. \\ & \left. + \frac{B}{4\pi R} \left[\frac{\partial R}{\partial k} \frac{\partial(RB)}{\partial \ell} - \frac{\partial R}{\partial \ell} \frac{\partial(RB)}{\partial k} \right] \right\} + \left[\dot{V}_Z \right]_{MC} \end{aligned} \quad (2.1.8)$$

where

$$P = p + q$$

Since the energy equation has no spatial derivatives, Eqs. (2.1.2) and (2.1.3) are already in proper form. Now Eqs. (2.1.2), (2.1.3), (2.1.7), and (2.1.8) must be differenced.

2.2 Difference Equations: Momentum

To simplify the notation, the following are defined.

$$\frac{\partial}{\partial k} = \Delta \quad ; \quad \frac{\partial}{\partial l} = \delta$$

Equation (2.1.8) becomes

$$\frac{\partial v_z}{\partial t} = \frac{1}{\rho_j} [\Delta R(\delta P + C\delta\psi) - \delta R(\Delta P + C\Delta\psi)] + (\dot{v}_z)_{MC}$$

where $\psi = RB$ and $C = B/4\pi R$

Since the momentum is to be calculated at the (k, l) intersections (see Fig. 2)

$$\left(\frac{\partial v_z}{\partial t}\right)_{k,l} = \left\{ \frac{1}{\rho_j} [\Delta R(\delta P + C\delta\psi) - \delta R(\Delta P + C\Delta\psi)] \right\}_{k,l} + \left\{ (\dot{v}_z)_{MC} \right\}_{k,l}$$

This is differenced as follows

$$\begin{aligned} \left[\frac{v_z^{n+1} - v_z^n}{\Delta t} \right]_{k,l} &= \left[\frac{\Delta R}{2\rho_j} (\delta P + C\delta\psi) \right]_{k+1/2,l}^n \\ &+ \left[\frac{\Delta R}{2\rho_j} (\delta P + C\delta\psi) \right]_{k-1/2,l}^n - \left[\frac{\delta R}{2\rho_j} (\Delta P + C\Delta\psi) \right]_{k,l+1/2}^n \\ &- \left[\frac{\delta R}{2\rho_j} (\Delta P + C\Delta\psi) \right]_{k,l-1/2}^n + \left[(\dot{v}_z)_{MC} \right]_{k,l}^{n+1/2} \end{aligned} \quad (2.2.1)$$

where

$$(\delta P)_{k+1/2,l} = P_{k+1/2,l+1/2} - P_{k+1/2,l-1/2} \quad (2.2.1a)$$

$$(\delta P)_{k-1/2,l} = P_{k-1/2,l+1/2} - P_{k-1/2,l-1/2} \quad (2.2.1b)$$

$$(\Delta P)_{k,l+1/2} = P_{k+1/2,l+1/2} - P_{k-1/2,l+1/2} \quad (2.2.1c)$$

$$(\Delta P)_{k,l-1/2} = P_{k+1/2,l-1/2} - P_{k-1/2,l-1/2} \quad (2.2.1d)$$

$$C\delta\psi_{k+1/2,l} = C_{k+1/2,l} (\psi_{k+1/2,l+1/2} - \psi_{k+1/2,l-1/2}) \quad (2.1.1e)$$

$$C_{k+1/2,l} = \frac{1}{4\pi} (B_{k+1/2,l+1/2} + B_{k+1/2,l-1/2})$$

$$/ (R_{k,l} + R_{k+1,l}) \quad (2.1.1f)$$

The remaining derivatives of ψ are differenced analogously.

It is assumed here that P , B , and ψ is available in the zone centers. The tensor nature of P , because of the tensor definition of q , will be discussed later.

The remaining terms are differenced as follows

$$\left(\frac{\Delta R}{2\rho j}\right)_{k+1/2,l} = \frac{(R_{k+1,l} - R_{k,l})}{[(\rho j)_{k+1/2,l+1/2} + (\rho j)_{k+1/2,l-1/2}]}$$

$$\left(\frac{\Delta R}{2\rho j}\right)_{k-1/2,l} = \frac{(R_{k,l} - R_{k-1,l})}{[(\rho j)_{k-1/2,l+1/2} + (\rho j)_{k-1/2,l-1/2}]}$$

$$\left(\frac{\delta R}{2\rho j}\right)_{k,l+1/2} = \frac{(R_{k,l+1} - R_{k,l})}{[(\rho j)_{k+1/2,l+1/2} + (\rho j)_{k-1/2,l+1/2}]}$$

$$\left(\frac{\delta R}{2\rho j}\right)_{k,l-1/2} = \frac{(R_{k,l} - R_{k,l-1})}{[(\rho j)_{k+1/2,l-1/2} + (\rho j)_{k-1/2,l-1/2}]}$$

Note the (ρj) terms are all zone centered. The density ρ is zone centered by definition, but now the area Jacobian, j , must be calculated in the zone center.

Repeating Eq. (2.1.4) and using new notation

$$j = \frac{\partial R}{\partial \ell} \frac{\partial Z}{\partial k} - \frac{\partial R}{\partial k} \frac{\partial Z}{\partial \ell} = \delta R \Delta Z - \Delta R \delta Z$$

and according to Schulz^{2,3}

$$j_{k-1/2, \ell-1/2} = 1/2 (j_{k, \ell} + j_{k-1, \ell-1}) \quad (2.2.2)$$

where

$$j_{k, \ell} = (R_{k, \ell} - R_{k, \ell-1}) (Z_{k, \ell} - Z_{k-1, \ell}) - (R_{k, \ell} - R_{k-1, \ell}) (Z_{k, \ell} - Z_{k, \ell-1}) \quad (2.2.3)$$

and similarly

$$j_{k-1, \ell-1} = (R_{k-1, \ell} - R_{k-1, \ell-1}) (Z_{k, \ell-1} - Z_{k-1, \ell-1}) - (R_{k, \ell-1} - R_{k-1, \ell-1}) (Z_{k-1, \ell} - Z_{k-1, \ell-1}) \quad (2.2.4)$$

It is interesting to note that $j_{k-1/2, \ell-1/2}$ is the exact area of the quadrilateral (zone) that it is centered in. This can be seen by close inspection of the terms and noting that $j_{k, \ell}$ is the area of a parallelogram defined by its adjacent sides.

The Monte Carlo transport term $\vec{v}_{MC}$ is calculated at time $n + 1/2$, and is zone centered by definition. Therefore $[\vec{v}_Z]_{MC}$ must be averaged.

$$\begin{aligned} [\vec{v}_Z]_{MC, \ell} &= \left[(m\vec{v}_Z)_{k+1/2, \ell+1/2}^{MC} + (m\vec{v}_Z)_{k+1/2, \ell-1/2}^{MC} \right. \\ &\quad \left. + (m\vec{v}_Z)_{k-1/2, \ell+1/2}^{MC} + (m\vec{v}_Z)_{k-1/2, \ell-1/2}^{MC} \right] / [m_{k+1/2, \ell+1/2} \\ &\quad + m_{k+1/2, \ell-1/2} + m_{k-1/2, \ell+1/2} + m_{k-1/2, \ell-1/2}] \end{aligned} \quad (2.2.5)$$

This concludes the differencing of the axial momentum equation.

The radial momentum equation should be differenced in a similar manner

$$\begin{aligned} \left[\frac{v_R^{n+1} - v_R^n}{\Delta t} \right]_{k,l} &= \left[\frac{\delta Z}{2\rho_j} (\Delta P + C\Delta\psi) \right]_{k,l-1/2}^n \\ &+ \left[\frac{\delta Z}{2\rho_j} (\Delta P + C\Delta\psi) \right]_{k,l+1/2}^n - \left[\frac{\delta Z}{2\rho_j} (\delta P + C\delta\psi) \right]_{k+1,l}^n \\ &- \left[\frac{\delta Z}{2\rho_j} (\delta P + C\delta\psi) \right]_{k-1/2,l}^n + \left[(\dot{v}_R)_{MC} \right]_{k,l}^{n+1/2} \end{aligned} \quad (2.2.6)$$

Note that (ρ_j) , δP , ΔP , $C\delta\psi$, $C\Delta\psi$ have all previously been defined in Eqs. (2.2.1a-f) for this set of k and l , therefore the remaining terms are defined as:

$$(\delta Z)_{k,l-1/2} = Z_{k,l} - Z_{k,l-1}$$

$$(\delta Z)_{k,l+1/2} = Z_{k,l+1} - Z_{k,l}$$

$$(\Delta Z)_{k+1/2,l} = Z_{k+1,l} - Z_{k,l}$$

$$(\Delta Z)_{k-1/2,l} = Z_{k,l} - Z_{k-1,l}$$

The Monte Carlo transport term, $\dot{v}_R$, is averaged in a manner identical to Eq. (2.2.5).

The above Eqs. (2.2.1) and (2.2.6) are the Lagrangian difference equations for momentum conservation in cylindrical coordinates. The only remaining loose end is the calculation of the P terms

$$P \equiv p + q$$

$$P_{k-1/2, l-1/2} = p_{k-1/2, l-1/2} + q_{k-1/2, l-1/2}^i$$

where

$$P_{k-1/2, l-1/2} = \{n_e^{KT_e} + n_i^{KT_i}\}_{k-1/2, l-1/2}$$

and q^i symbolizes the tensor nature of q . Four q terms will be defined; each a measure of the compression along the four sides of the quadrilateral $(k-1/2, l-1/2)$. Let q^1 be associated with side $(k-1/2, l)$, and q^2, q^3, q^4 for the remaining sides going clockwise around the zone. (See Fig. 3.)

Figure 3. Quadrilateral zones with tensor artificial viscosities.

The actual definition of q is discussed in Appendix 3. The four q^i terms can now be inserted into Eqs. (2.2.1a)-(2.2.1d). For example:

$$\begin{aligned}(\delta P)_{k+1/2, l} &= [\delta(p + q^4)]_{k+1/2, l} \\&= p_{k+1/2, l+1/2} + q_{k+1/2, l+1/2}^4 - p_{k+1/2, l-1/2} \\&\quad - q_{k+1/2, l-1/2}^4\end{aligned}\quad (2.2.7)$$

Note that $(\delta P)_{k+1/2, l}$ is the pressure gradient with respect to l , $\delta \equiv \frac{\partial}{\partial l}$, and to the right of the point k, l . Therefore the correct q^i to use is q^4 , similarly for the others

$$(\delta P)_{k-1/2, l} = [\delta(p + q^2)]_{k-1/2, l} \quad (2.2.8)$$

$$(\Delta P)_{k, l+1/2} = [\Delta(p + q^3)]_{k, l+1/2} \quad (2.2.9)$$

$$(\Delta P)_{k, l-1/2} = [\Delta(p + q^3)]_{k, l-1/2} \quad (2.2.10)$$

Equations (2.2.1) and (2.2.6) are now easily solved for v_Z^{n+1} and v_R^{n+1} for a given Δt . After solving for v_Z^{n+1} and v_R^{n+1} , integrating again gives

$$R^{n+1} = R^n + v_R^{n+1} \Delta t \quad (2.2.11)$$

$$Z^{n+1} = Z^n + v_Z^{n+1} \Delta t \quad (2.2.12)$$

This concludes the discussion of the momentum equations and now the energy equations will be discussed.

2.3 Difference Equations: Energy

The energy equations to be differenced are Eqs. (2.1.2) and (2.1.3). Remember that the thermal conduction and joule heating have been split from the equation and their contributions to the energy transport will be calculated separately. The electron and ion equations are differenced in time as follows:

$$\begin{aligned} \epsilon_i^{n+1} - \epsilon_i^n + \left(\frac{p_i^{n+1}}{2} + \frac{p_i^n}{2} + q^{n+1/2} \right) d\tau^{n+1/2} \\ + (\omega\tau)^{n+1} \left(KT_i^{n+1} - KT_e^{n+1} \right) \Delta t - (S_i\tau)^{n+1/2} \Delta t = 0 \end{aligned} \quad (2.3.1)$$

$$\begin{aligned} \epsilon_e^{n+1} - \epsilon_e^n + \left(\frac{p_e^{n+1}}{2} + \frac{p_e^n}{2} \right) d\tau^{n+1/2} - (\omega\tau)^{n+1} \left(KT_i^{n+1} - KT_e^{n+1} \right) \Delta t \\ + (p_B\tau)^{n+1/2} \Delta t - (S_e\tau)^{n+1/2} \Delta t = 0 \end{aligned} \quad (2.3.2)$$

Now let

$$p_i = n_i KT_i$$

$$p_e = n_e KT_e$$

$$\epsilon_i = \frac{3}{2} n_i \tau KT_i$$

$$\epsilon_e = \frac{3}{2} n_e \tau KT_e$$

and substitute these into the above equations and solve for KT_i^{n+1} and KT_e^{n+1} . After a little algebra, Eqs. (2.3.1) and (2.3.2) become

$$KT_i^{n+1} = \frac{B}{A} + \frac{C}{A} KT_e^{n+1} \quad (2.3.3)$$

where A, B, and C are defined as follows

$$A = \frac{3}{2} (n_i \tau)^{n+1} + \frac{1}{2} n_i^{n+1} d\tau^{n+1/2} + (\omega \tau)^{n+1} \Delta t \quad (2.3.3a)$$

$$B = \frac{3}{2} (n_i \tau)^n K T_i^n - \left(\frac{1}{2} n_i^n K T_i^n + q^{n+1/2} \right) d\tau^{n+1/2} + (S_i \tau)^{n+1/2} \Delta t \quad (2.3.3b)$$

$$C = (\omega \tau)^{n+1} \Delta t \quad (2.3.3c)$$

similarly for the electron equation

$$K T_e^{n+1} = \frac{E}{D} + \frac{F}{D} K T_i^{n+1} \quad (2.3.4)$$

where

$$D = \frac{3}{2} (n_e \tau)^{n+1} + \frac{1}{2} n_e^{n+1} d\tau^{n+1/2} + (\omega \tau)^{n+1} \quad (2.3.4a)$$

$$E = \frac{3}{2} (n_e \tau)^n K T_e^n - \frac{1}{2} n_e^n K T_e^n d\tau^{n+1/2} - (P_B \tau)^{n+1/2} \Delta t + (S_e \tau)^{n+1/2} \Delta t \quad (2.3.4b)$$

$$F = (\omega \tau)^{n+1} \Delta t \quad (2.3.4c)$$

Now use Eq. (2.3.4) to solve (2.3.3)

$$K T_i^{n+1} = \frac{DB + CF}{AD - CF} \quad (2.3.5)$$

Now $K T_i^{n+1}$ can be used to calculate $K T_e^{n+1}$ from Eq. (2.3.4). This completes the time differencing and now the spatial averaging will be discussed.

We want the energy to be a zone centered quantity, and all the variables, except q , are zone centered, so the rest is simple. For a scalar, zone centered q , which is needed in Eq. (2.3.3b), use

$$q_{k-1/2, \ell-1/2}^{n+1/2} = \frac{1}{2} (q^{n+1} + q^n)_{k-1/2, \ell-1/2}$$

and let

$$q_{k-1/2, \ell-1/2}^{n+1/2} = \frac{1}{2} (q^1 + q^2 + q^3 + q^4)_{k-1/2, \ell-1/2}$$

Note that q^{n+1} is calculated after the momentum, when the coordinates and velocities are known at time $n + 1$. Likewise

$$\begin{aligned} d\tau^{n+1/2} &= \tau^{n+1} - \tau^n \\ \tau^{n+1/2} &= \frac{1}{2} (\tau^{n+1} + \tau^n) \end{aligned}$$

where τ^{n+1} can be calculated after the momentum

$$\begin{aligned} \tau_{k-1/2, \ell-1/2}^{n+1} &= \frac{1}{m_{k-1/2, \ell-1/2}} \left\{ \frac{\pi}{3} \left[j_{k, \ell}^{n+1} (R_{k-1, \ell}^{n+1} + R_{k, \ell-1}^{n+1} \right. \right. \\ &\quad \left. \left. + R_{k, \ell}^{n+1} \right) + j_{k-1, \ell-1}^{n+1} (R_{k-1, \ell}^{n+1} + R_{k, \ell-1}^{n+1} + R_{k-1, \ell-1}^{n+1}) \right] \right\} \quad (2.3.6) \end{aligned}$$

The term in the curled brackets $\{ \dots \}$ is the volume of the zone, and the j terms are as defined in the previous section on momentum - Eqs. (2.2.3) and (2.2.4).

Except for joule heating and thermal conduction, this completes the section on differencing the energy equation. Since the joule heating and thermal conduction depend on solving the magnetic and thermal diffusion equations, it is more convenient to describe the solutions to these equations first and then update the energy equations.

2.4 Magnetic Field Diffusion

The time and space variations of the magnetic field were solved by casting the field equations into the form of a diffusion equation. This diffusion equation was then solved implicitly by the splitting method.

Using Eq. (2.0.7) in Eq. (2.0.6) gives

$$-\frac{1}{c} \frac{d}{dt} \int_S \vec{B} \cdot \hat{n} \, da = \int \eta \vec{J} \cdot d\vec{\ell}$$

Use Stokes theorem:

$$-\frac{1}{c} \frac{d}{dt} \int_S \vec{B} \cdot \hat{n} \, da = \int_S \nabla \times (\eta \vec{J}) \cdot \hat{n} \, da$$

and now use Eq. (2.0.5) to eliminate $\vec{J}$

$$-\frac{1}{c} \frac{d}{dt} \int_S \vec{B} \cdot \hat{n} \, da = \int_S \nabla \times \left[\eta \frac{c}{4\pi} \nabla \times \vec{B} \right] \cdot \hat{n} \, da$$

or

$$\frac{1}{A} \frac{d\Phi}{dt} = -\frac{c^2}{4\pi} \nabla \times (\eta \nabla \times \vec{B}) \cdot \hat{n}$$

where A = area (A will equal the zonal area, and $\vec{B}$ is parallel to the normal of A) and $\Phi = BA$ is the magnetic flux

Letting $\vec{B} = \frac{\psi}{R} \hat{\theta}$ and expanding the cross products gives

$$\frac{1}{A} \frac{d\Phi}{dt} = \frac{c^2 R}{4\pi} \nabla \cdot \left(\frac{\eta}{R^2} \nabla \psi \right)$$

This is a diffusion equation, that can now be differenced implicitly.

Transform this equation to Lagrangian form, using the transform Eqs.

(2.1.5) and (2.1.6)

$$\frac{1}{A} \frac{d\Phi}{dt} = \frac{c^2 R}{4\pi} \nabla \cdot \left\{ \hat{r} \frac{\eta}{R^2 j} \left(-\frac{\partial Z}{\partial \ell} \frac{\partial \psi}{\partial k} + \frac{\partial Z}{\partial k} \frac{\partial \psi}{\partial \ell} \right) + \hat{k} \frac{\eta}{R^2 j} \left(\frac{\partial R}{\partial \ell} \frac{\partial \psi}{\partial k} - \frac{\partial R}{\partial k} \frac{\partial \psi}{\partial \ell} \right) \right\}$$

Expanding the divergence for cylindrical coordinates gives

$$\begin{aligned} \frac{1}{A} \frac{d\Phi}{dt} = \frac{c^2 R}{4\pi} & \left\{ \frac{1}{Rj} \left[-\frac{\partial Z}{\partial \ell} \frac{\partial}{\partial k} + \frac{\partial Z}{\partial k} \frac{\partial}{\partial \ell} \right] \frac{\eta}{Rj} \left[-\frac{\partial Z}{\partial \ell} \frac{\partial \psi}{\partial k} + \frac{\partial Z}{\partial k} \frac{\partial \psi}{\partial \ell} \right] \right. \\ & \left. + \frac{1}{j} \left[\frac{\partial R}{\partial \ell} \frac{\partial}{\partial k} - \frac{\partial R}{\partial k} \frac{\partial}{\partial \ell} \right] \frac{\eta}{R^2 j} \left[\frac{\partial R}{\partial \ell} \frac{\partial \psi}{\partial k} - \frac{\partial R}{\partial k} \frac{\partial \psi}{\partial \ell} \right] \right\} \end{aligned}$$

After some algebra this reduces to

$$\begin{aligned} \frac{1}{A} \frac{\partial \Phi}{\partial t} = \frac{c^2}{4\pi j} & \left\{ \frac{\partial}{\partial k} \left[\frac{\eta \left(\frac{\partial Z}{\partial \ell} \right)^2}{Rj} \frac{\partial \psi}{\partial k} \right] - \frac{\partial}{\partial k} \left[\frac{\eta \left(\frac{\partial Z}{\partial \ell} \right) \left(\frac{\partial Z}{\partial k} \right)}{Rj} \frac{\partial \psi}{\partial \ell} \right] \right. \\ & - \frac{\partial}{\partial \ell} \left[\frac{\eta \left(\frac{\partial Z}{\partial k} \right) \left(\frac{\partial Z}{\partial \ell} \right)}{Rj} \frac{\partial \psi}{\partial k} \right] + \frac{\partial}{\partial \ell} \left[\frac{\eta \left(\frac{\partial Z}{\partial k} \right)^2}{Rj} \frac{\partial \psi}{\partial \ell} \right] \\ & + \frac{\partial}{\partial k} \left[\frac{\eta \left(\frac{\partial R}{\partial \ell} \right)^2}{Rj} \frac{\partial \psi}{\partial k} \right] - \frac{\partial}{\partial k} \left[\frac{\eta \left(\frac{\partial R}{\partial \ell} \right) \left(\frac{\partial R}{\partial k} \right)}{Rj} \frac{\partial \psi}{\partial \ell} \right] \\ & \left. - \frac{\partial}{\partial \ell} \left[\frac{\eta \left(\frac{\partial R}{\partial k} \right) \left(\frac{\partial R}{\partial \ell} \right)}{Rj} \frac{\partial \psi}{\partial k} \right] + \frac{\partial}{\partial \ell} \left[\frac{\eta \left(\frac{\partial R}{\partial k} \right)^2}{Rj} \frac{\partial \psi}{\partial \ell} \right] \right\} \end{aligned}$$

Let $\frac{\partial R}{\partial \ell} = R_\ell$, $\frac{\partial R}{\partial k} = R_k$, etc.

Making the approximation that the cross terms are small^{10,11} compared to the others the above becomes

$$\frac{1}{A} \frac{\partial \Phi}{\partial t} = \frac{c^2}{4\pi j} \left\{ \frac{\partial}{\partial k} \frac{\eta(R_\ell^2 + Z_\ell^2)}{Rj} \frac{\partial \psi}{\partial k} + \frac{\partial}{\partial \ell} \frac{\eta(R_k^2 + Z_k^2)}{Rj} \frac{\partial \psi}{\partial \ell} \right\} \quad (2.4.1)$$

It is this equation which will be differenced. Since the magnetic field is to be defined at the zone center, Eq. (2.4.1) should be calculated at $(k - 1/2, \ell - 1/2)$. Consider the terms separately.

The term $\left(\frac{c^2}{4\pi j}\right)_{k-1/2, l-1/2}$ is easily obtained using Eq. (2.2.3), (2.2.4), (2.2.2).

The terms in the brackets become

$$\begin{aligned} & \left[\frac{\partial}{\partial k} \frac{\eta(R_l^2 + Z_l^2)}{R_j} \frac{\partial \psi}{\partial k} \right]_{k-1/2, l-1/2} - \left[\frac{\eta(R_l^2 + Z_l^2)}{R_j} \frac{\partial \psi}{\partial k} \right]_{k, l-1/2} \\ & - \left[\frac{\eta(R_l^2 + Z_l^2)}{R_j} \frac{\partial \psi}{\partial k} \right]_{k-1, l-1/2} \\ & \left[\frac{\partial}{\partial l} \frac{\eta(R_k^2 + Z_k^2)}{R_j} \frac{\partial \psi}{\partial l} \right]_{k-1/2, l-1/2} - \left[\frac{\eta(R_k^2 + Z_k^2)}{R_j} \frac{\partial \psi}{\partial l} \right]_{k-1/2, l} \\ & - \left[\frac{\eta(R_k^2 + Z_k^2)}{R_j} \frac{\partial \psi}{\partial l} \right]_{k-1/2, l-1} \end{aligned}$$

Now difference the remaining derivatives of ψ and rearrange terms

$$\begin{aligned} & \left[\frac{1}{\partial A} \frac{\partial \psi}{\partial t} \right]_{k-1/2, l-1/2} = \epsilon_1 (\psi_{k+1/2, l-1/2} - \psi_{k-1/2, l-1/2}) \\ & - \epsilon_2 (\psi_{k-1/2, l-1/2} - \psi_{k-3/2, l-1/2}) \\ & + \epsilon_3 (\psi_{k-1/2, l+1/2} - \psi_{k-1/2, l-1/2}) \\ & - \epsilon_4 (\psi_{k-1/2, l-1/2} - \psi_{k-1/2, l-3/2}) \end{aligned} \quad (2.4.2)$$

where

$$\begin{aligned} \epsilon_1 &= \left[\frac{\eta(R_l^2 + Z_l^2)}{R_j} \right]_{k, l-1/2} \\ \epsilon_2 &= \left[\frac{\eta(R_l^2 + Z_l^2)}{R_j} \right]_{k-1, l-1/2} \end{aligned} \quad (2.4.2a)$$

$$\xi_3 = \left[\frac{n(R_k^2 + Z_k^2)}{R_j} \right]_{k-1/2, 2}$$

$$\xi_4 = \left[\frac{n(R_k^2 + Z_k^2)}{R_j} \right]_{k-1/2, l-1}$$

where

$$\xi = \left(\frac{c}{4\pi} \right)_{k-1/2, l-1/2}$$

Note that $\xi_1 - \xi_4$ are defined at the zone boundaries, therefore they were averaged in the following way

$$\xi_1 = \frac{4\pi [\alpha_{k+1/2, l-1/2} + \alpha_{k-1/2, l-1/2}]}{\left(\frac{V}{n} \right)_{k+1/2, l-1/2} + \left(\frac{V}{n} \right)_{k-1/2, l-1/2}} \quad (2.4.2b)$$

$$\xi_2 = \frac{4\pi [\alpha_{k-1/2, l-1/2} + \alpha_{k-3/2, l-1/2}]}{\left(\frac{V}{n} \right)_{k-1/2, l-1/2} + \left(\frac{V}{n} \right)_{k-3/2, l-1/2}}$$

$$\xi_3 = \frac{4\pi [\gamma_{k-1/2, l+1/2} + \gamma_{k-1/2, l-1/2}]}{\left(\frac{V}{n} \right)_{k-1/2, l+1/2} + \left(\frac{V}{n} \right)_{k-1/2, l-1/2}}$$

$$\xi_4 = \frac{4\pi [\gamma_{k-1/2, l-1/2} + \gamma_{k-1/2, l-3/2}]}{\left(\frac{V}{n} \right)_{k-1/2, l-1/2} + \left(\frac{V}{n} \right)_{k-1/2, l-3/2}}$$

where

$$\alpha = (R_z^2 + Z_z^2)$$

$$\gamma = (R_k^2 + Z_k^2)$$

$$V = \text{volume of zone} \approx 2\pi R_j \tilde{z}$$

and

$$R_l = \frac{1}{2} [(R_{k,l} - R_{k,l-1}) + (R_{k-1,l} - R_{k-1,l-1})]$$

$$Z_l = \frac{1}{2} [(Z_{k,l} - Z_{k,l-1}) + (Z_{k-1,l} - Z_{k-1,l-1})]$$

$$R_k = \frac{1}{2} [(R_{k,l} - R_{k-1,l}) + (R_{k,l-1} - R_{k-1,l-1})]$$

$$Z_k = \frac{1}{2} [(Z_{k,l} - Z_{k-1,l}) + (Z_{k,l-1} - Z_{k-1,l-1})]$$

The volume V is calculated as described in Eq. (2.3.6). Also note that η , the electric resistivity is defined in the zone center. Thus using the above definitions, Eq. (2.4.2) has been spatially differenced. The magnetic diffusion must now be differenced with respect to time.

Noting that ξ_1 and ξ_2 are differences in k and ξ_3 and ξ_4 are differences in l , an implicit splitting scheme may be tried.

$$\begin{aligned} \phi^{n'} = & AB (\Delta t) [\xi_3 \psi_{k-1/2, l+1/2}^{n'} - \xi_3 \psi_{k-1/2, l-1/2}^{n'} \\ & - \xi_4 \psi_{k-1/2, l-1/2}^{n'} + \xi_4 \psi_{k-1/2, l-3/2}^{n'}] + \phi^n \end{aligned}$$

$$\begin{aligned} \phi^{n+1} = & AB (\Delta t) [\xi_1 \psi_{k+1/2, l-1/2}^{n+1} - \xi_1 \psi_{k-1/2, l-1/2}^{n+1} \\ & - \xi_2 \psi_{k-1/2, l-1/2}^{n+1} + \xi_2 \psi_{k-3/2, l-1/2}^{n+1}] + \phi^{n'} \end{aligned}$$

noting that $j = A$, $\beta = \frac{c^2}{4\pi j}$ and $\phi = \frac{A}{R} \psi$ and after a little algebra the above two equations can be written in the tridiagonal form

$$-a \psi_{k-1/2, l+1/2}^{n'} + b \psi_{k-1/2, l-1/2}^{n'} - c \psi_{k-1/2, l-3/2}^{n'} = d \quad (2.4.3)$$

$$-e \psi_{k+1/2, l-1/2}^{n+1} + f \psi_{k-1/2, l-1/2}^{n+1} - g \psi_{k-3/2, l-1/2}^{n+1} = h \quad (2.4.4)$$

where

$$a = \frac{c^2 \Delta t}{4\pi} \xi_3$$

$$b = \left[\left(\frac{\Delta}{R} \right)^{n+1} + \frac{c^2 \Delta t}{4\pi} (\xi_3 + \xi_4) \right]$$

$$c = \frac{c^2 \Delta t}{4\pi} \xi_4$$

$$d = \left(\frac{\Delta}{R} \right)^n \psi_{k-1/2, l-1/2}$$

$$e = \frac{c^2 \Delta t}{4\pi} \xi_1$$

$$f = \left[\left(\frac{\Delta}{R} \right)^{n+1} + \frac{c^2 \Delta t}{4\pi} (\xi_1 + \xi_2) \right]$$

$$g = \frac{c^2 \Delta t}{4\pi} \xi_2$$

$$h = \left(\frac{\Delta}{R} \right)^{n'} \psi_{k-1/2, l-1/2}^{n'}$$

It is assumed that the coefficients a-h are centered at $(k-1/2, l-1/2)$. This is slightly in error since $\xi_1 - \xi_4$ are in the centers of a zone boundary. It is to be noted that time n' is equal to time $n+1$. Equations (2.4.3) and (2.4.4) are now easily solved using the standard tridiagonal technique.

$$\psi_{k-1/2, l-1/2}^{n'} = E_{k-1/2, l-1/2}^{n'} \psi_{k-1/2, l+1/2}^{n'} + F_{k-1/2, l-1/2}^{n'}$$

$$E_{k-1/2, l+1/2}^{n'} = \frac{a_{k-1/2, l+1/2}}{b_{k-1/2, l+1/2} - c_{k-1/2, l+1/2} E_{k-1/2, l-1/2}^{n'}}$$

$$F_{k-1/2, l+1/2}^{n+1} = \frac{c_{k-1/2, l+1/2} F_{k-1/2, l-1/2}^{n+1} + d_{k-1/2, l+1/2}}{b_{k-1/2, l+1/2} - c_{k-1/2, l+1/2} L_{k-1/2, l-1/2}^{n+1}}$$

$$\psi_{k-1/2, l-1/2}^{n+1} = G_{k-1/2, l-1/2}^{n+1} \psi_{k+1/2, l-1/2}^{n+1} + H_{k-1/2, l-1/2}^{n+1}$$

$$G_{k+1/2, l-1/2}^{n+1} = \frac{e_{k+1/2, l-1/2}}{f_{k+1/2, l-1/2} - g_{k+1/2, l-1/2} G_{k-1/2, l-1/2}^{n+1}}$$

$$H_{k+1/2, l-1/2}^{n+1} = \frac{g_{k+1/2, l-1/2} H_{k-1/2, l-1/2}^{n+1} + h_{k+1/2, l-1/2}}{f_{k+1/2, l-1/2} - g_{k+1/2, l-1/2} G_{k-1/2, l-1/2}^{n+1}}$$

Computationally, dummy zones are carried along the boundaries, where boundary values of ψ can be stored.

Using the above methods, the values of ψ at time $n+1$ are calculated, and since $\psi = BR$, B at $n+1$ is known.

2.5 Joule Heating

Having described the magnetic diffusion, it is convenient now to derive the joule heating term. Since the energy equation has already been differenced without joule heating, it is only necessary to calculate the incremental change to the zone's energy due to the joule heating. The heating will be added to the electrons. Let E_e^J denote the energy deposited due to joule heating. For a simple Ohm's law,

$$E_e^J = \iiint dv dt \, \eta |\vec{J}|^2$$

and for a particular zone of volume V

$$\Delta E_e^J = V(\Delta t) \, \eta |\vec{J}|^2 \quad (2.5.1)$$

Now let $\vec{J} = \frac{c}{4\pi} \nabla \times \vec{B}$, $\vec{B} = B_0(R, Z) \hat{\theta}$, and $\psi = B_0 R$.

Equation (2.5.1) becomes

$$\Delta E_e^J = V(\Delta t) \, \eta \left(\frac{c}{4\pi R} \right)^2 \left[\left(\frac{\partial \psi}{\partial Z} \right)^2 + \left(\frac{\partial \psi}{\partial R} \right)^2 \right] \quad (2.5.2)$$

This equation now has to be transformed to Lagrangian coordinates. Using Eqs. (2.1.5) and (2.1.6), expanding, and dropping the cross terms with the assumption they are small compared to the others, gives the following

$$\begin{aligned} \Delta E_e^J = V(\Delta t) \left(\frac{c}{4\pi} \right)^2 & \left[\frac{\eta}{R^2 j^2} \left\{ (R_k^2 + Z_k^2) \left(\frac{\partial \psi}{\partial \ell} \right)^2 \right. \right. \\ & \left. \left. + (R_\ell^2 + Z_\ell^2) \left(\frac{\partial \psi}{\partial k} \right)^2 \right\} \right] \end{aligned} \quad (2.5.3)$$

The volume of a Lagrangian zone can be approximated by

$$V = 2\pi j \langle R \rangle$$

where $\langle R \rangle$ is the average R of the zone, i.e.,

$$\langle R \rangle = R_{k-1/2, l-1/2}$$

Therefore

$$\Delta E_e^J = \frac{c^2(\Delta t)}{8\pi} \left(\frac{\eta}{R_j} \right) \left[(R_k^2 + Z_k^2) \left(\frac{\partial \psi}{\partial t} \right)^2 + (R_l^2 + Z_l^2) \left(\frac{\partial \psi}{\partial k} \right)^2 \right] \quad (2.5.4)$$

Equation (2.5.4) will now be differenced

$$\begin{aligned} [\Delta E_e^J]_{k-1/2, l-1/2} &= \frac{c^2(\Delta t)}{8\pi} \left\{ \frac{\eta (R_k^2 + Z_k^2)}{R_j} \left(\frac{\partial \psi}{\partial t} \right)^2 \right. \\ &\quad \left. + \frac{\eta (R_l^2 + Z_l^2)}{R_j} \left(\frac{\partial \psi}{\partial k} \right)^2 \right\}_{k-1/2, l-1/2} \end{aligned} \quad (2.5.5)$$

For conservation of energy, the joule heating should be consistent with the magnetic diffusion model, therefore the terms in the brackets $\left\{ \right\}$ were cast in the form

$$\left\{ \frac{2\pi(R_k^2 + Z_k^2)}{\frac{V}{\eta}} \right\}.$$

But this bracket was calculated on the zone boundary for the diffusion, therefore one must calculate the energy deposited at the boundary centers and then share the energy with the zones common to the boundary. The sharing was based on a volume weighting of the resistivity. In a manner analogous to the magnetic diffusion,

Eq. (2.5.5) becomes

$$\begin{aligned} [\Delta E_e^J]_{k-1/2, l-1/2} = \beta \left\{ \xi_3 W_3 (\psi_{k-1/2, l+1/2} - \psi_{k-1/2, l-1/2})^2 \right. \\ + \xi_4 W_4 (\psi_{k-1/2, l-1/2} - \psi_{k-1/2, l-3/2})^2 \\ + \xi_1 W_1 (\psi_{k+1/2, l-1/2} - \psi_{k-1/2, l-1/2})^2 \\ \left. + \xi_2 W_2 (\psi_{k-1/2, l-1/2} - \psi_{k-3/2, l-1/2})^2 \right\} \quad (2.5.6) \end{aligned}$$

where ξ_1 , ξ_2 , ξ_3 and ξ_4 were defined by Eqs. (2.4.2a) and (2.4.2b);
and

$$\begin{aligned} W_1 &= \frac{(\eta V)_{k-1/2, l-1/2}}{(\eta V)_{k-1/2, l-1/2} + (\eta V)_{k+1/2, l-1/2}} \\ W_2 &= \frac{(\eta V)_{k-1/2, l-1/2}}{(\eta V)_{k-1/2, l-1/2} + (\eta V)_{k-3/2, l-1/2}} \\ W_3 &= \frac{(\eta V)_{k-1/2, l-1/2}}{(\eta V)_{k-1/2, l+1/2} + (\eta V)_{k-1/2, l-1/2}} \\ W_4 &= \frac{(\eta V)_{k-1/2, l-1/2}}{(\eta V)_{k-1/2, l-1/2} + (\eta V)_{k-1/2, l-3/2}} \\ \beta &= \frac{c^2 \Delta t}{8\pi} \end{aligned}$$

The resistivity is already zone centered, and V is calculated using Eq. (2.3.6).

Now the timing of the term ΔE_e^J should be considered. It is computationally easier to calculate the magnetic diffusion (ψ^{n+1}) after the energy equation is solved. Also R, Z, and V are available at time n+1,

but since $\eta = \eta(T_e)$, it is not fully advanced in time. This is because T_e cannot be advanced to time $n+1$ until the thermal conduction and joule heating have been considered. Overall it seems advantageous to calculate ΔE_e^J after the energy equation, and after the magnetic diffusion using J at t^{n+1} and η at almost t^{n+1} .

The joule heating is calculated as outlined above and is added to the electron internal energy.

2.6 Thermal Conduction

The changes to the electron and ion internal energy due to thermal conduction, from Eqs. (2.0,3) and (2.0,4) are

$$\frac{dE_e}{dt} = -\nabla \cdot \vec{Q}_e \quad \text{and} \quad \frac{dE_i}{dt} = -\nabla \cdot \vec{Q}_i \quad (2.6.1)$$

where E_e and E_i are energy densities, and $\vec{Q}_i$ and $\vec{Q}_e$ are the heat flux vectors. Since the electron and ion conduction equations are identical in form, the subscript will be dropped and a general equation of that form will be discussed. The heat flux is defined

$$\vec{Q} = -\kappa_{\perp} \nabla T \quad (2.6.2)$$

where only $\kappa_{\perp}$ is considered (since $\vec{B} = B_0(R, Z) \hat{\theta}$) and T is the temperature. Using $E = \frac{3}{2} nKT$, Eq. (2.6.1), and dropping the $\perp$ subscript

$$\frac{\partial T}{\partial t} = G \nabla \cdot (\kappa \nabla T) \quad (2.6.3)$$

where $G = \frac{2}{3nK}$, and Eq. (2.6.3) is the standard diffusion equation.

The Lagrangian difference scheme used to solve this type of equation was discussed in detail in the section on magnetic diffusion. Therefore, the differencing of Eq. (2.6.3) will be covered with a minimum of details.

Transforming to Lagrangian space, and dropping the cross terms gives

$$\frac{\partial T}{\partial t} = \frac{G}{Rj} \left[\frac{\partial}{\partial k} \left\{ \frac{(R_{\ell}^2 + Z_{\ell}^2) R \kappa}{j} \frac{\partial T}{\partial k} \right\} + \frac{\partial}{\partial \ell} \left\{ \frac{(R_k^2 + Z_k^2) R \kappa}{j} \frac{\partial T}{\partial \ell} \right\} \right] \quad (2.6.4)$$

Differencing as before

$$\begin{aligned}
 \frac{\partial T}{\partial t} = & Y_1 (T_{k+1/2, l-1/2} - T_{k-1/2, l-1/2}) \\
 & - Y_2 (T_{k-1/2, l-1/2} - T_{k-3/2, l-1/2}) \\
 & + Y_3 (T_{k-1/2, l+1/2} - T_{k-1/2, l-1/2}) \\
 & - Y_4 (T_{k-1/2, l-1/2} - T_{k-1/2, l-3/2})
 \end{aligned} \tag{2.6.5}$$

where $Y_1 - Y_4$ are defined as

$$\begin{aligned}
 Y_1 &= \lambda \left[\frac{(R_l^2 + Z_l^2) R \kappa}{j} \right]_{k, l-1/2} \\
 Y_2 &= \lambda \left[\frac{(R_l^2 + Z_l^2) R \kappa}{j} \right]_{k-1, l-1/2} \\
 Y_3 &= \lambda \left[\frac{(R_k^2 + Z_k^2) R \kappa}{j} \right]_{k-1/2, l} \\
 Y_4 &= \lambda \left[\frac{(R_k^2 + R_k^2) R \kappa}{j} \right]_{k-1/2, l-1}
 \end{aligned}$$

$$\lambda = \frac{G}{Rj} \quad k-1/2, l-1/2$$

and

$$\begin{aligned}
 \left[\frac{(R_l^2 + Z_l^2) R \kappa}{j} \right]_{k, l-1/2} &= \frac{1}{8} \left[\left\{ \frac{(R_l^2 + Z_l^2)}{j} \right\}_{k+1/2, l-1/2} \right. \\
 &+ \left. \left\{ \frac{(R_l^2 + Z_l^2)}{j} \right\}_{k-1/2, l-1/2} \right] \\
 &\cdot (R_{k, l} + R_{k, l-1}) (\kappa_{k+1/2, l-1/2} + \kappa_{k-1/2, l-1/2})
 \end{aligned}$$

with similar expressions for the factors in Y_2 , Y_3 and Y_4 . Using splitting, and differencing implicitly in time, Eq. (2.6.5) becomes

$$\begin{aligned} & - Y_3 T_{k-1/2, \ell+1/2}^{n'} + (1 + Y_3 + Y_4) T_{k-1/2, \ell-1/2}^{n'} \\ & - Y_4 T_{k-1/2, \ell-3/2}^{n'} = T_{k-1/2, \ell-1/2}^n \end{aligned} \quad (2.6.6)$$

$$\begin{aligned} & - Y_1 T_{k+1/2, \ell-1/2}^{n+1} + (1 + Y_1 + Y_2) T_{k-1/2, \ell-1/2}^{n+1} \\ & - Y_2 T_{k-3/2, \ell-1/2}^{n+1} = T_{k-1/2, \ell-1/2}^{n'} \end{aligned} \quad (2.6.7)$$

Once again, the above equations are in a form easily solved by the tridiagonal method, which was discussed earlier. Solving Eqs. (2.6.6) and (2.6.7) gives the change in the zone temperature due to conduction.

This equation is solved twice, once for electrons, and once for ions, where the transport coefficients κ_{le} , and κ_{li} are modeled after Braginskii⁴ and are discussed in Appendix 2.

3. QUALITATIVE DESCRIPTION OF MONTE CARLO MODEL

The basic idea of any Monte Carlo model is that the cumulative effect of many independent events can be calculated by summing over a finite number of events chosen at random but in accord with the appropriate probability distribution. Specifically, the effect of high energy charged particles on a Maxwellian fluid plasma can be calculated if the probabilities for all the individual events are known. For Monte Carlo transport, one must calculate the equation of motion for a finite but representative sample of the charged particles. Since the equation of motion is very complicated, it is not solved in an analytic fashion, but is calculated by moving the Monte Carlo test bundle through the medium over many small time steps, according to the forces acting on the bundle. During the travel of a bundle, the probability of collision is calculated, and using a random number, weighted against the probability of collision, one can force the bundle to collide with the fluid at various points along its orbit. These collisions will alter the bundle's energy and momentum, and could also result in a thermonuclear reaction.

The equation of motion for a high energy particle in a Maxwellian fluid plasma might be written

$$\frac{d\vec{v}}{dt} = \frac{q}{mc} \vec{v} \times \vec{B} + \left\{ \text{small angle collision drag term} \right\} + \left\{ \text{large angle scattering term} \right\} \quad (3.0.1)$$

where the force term $q\vec{E}$ has been assumed to be small compared to the Lorentz force. This equation was solved in three steps. For a selected

time step (Δt), a $\Delta \vec{v}$ and a $\Delta \vec{x}$ were calculated from the Lorentz force. The Monte Carlo bundle was then advanced in configurational and velocity space accordingly. The change in energy due to small angle collisions for this Δt was now calculated by integrating the equation for the energy loss rate of the energetic ions to the electron and ion Maxwellians¹²⁻¹⁵.

$$\left. \frac{dE_1}{dt} \right)_{\text{elec}} = \beta_e E_1 \quad (3.0.2)$$

$$\left. \frac{dE_1}{dt} \right)_{\text{ions}} = \beta_i E_1^{-1/2} \quad (3.0.3)$$

where E_1 is the energetic ion's energy, and

$$\beta_i = 2\sqrt{2m_1} \pi e^4 Z_1^2 \ln \Lambda_i \sum_{i=1}^N \frac{n_i Z_i^2}{m_i}$$

$$\beta_e = \frac{8\sqrt{2\pi m_e} Z_1^2 e^4 n_e \ln \Lambda_e}{3m_1 (KT_e)^{3/2}}$$

The derivation of these equations is discussed in Appendix 4, and their integration is developed in a following section. Thus for a given Δt , Eqs. (3.0.2) and (3.0.3) are integrated, giving a ΔE_1 , the change in the ions energy due to small angle collisions. This ΔE_1 yields a new Δv (speed) and it is assumed that the direction does not change, i.e., the ion's relaxation time is less than the deflection time.

It should be noted that this solution of the small angle drag term is done deterministically and not with Monte Carlo techniques. To calculate this term in a pure Monte Carlo fashion would be prohibitive considering the very large number of electron-ion collisions, and probably would not be any more accurate.

The last term, the large angle collision term is calculated in a Monte Carlo manner. Having moved the particle a $\Delta\vec{x}$ in a Δt one can calculate the probability that the particle suffered a large angle nuclear collision or an in-flight thermonuclear reaction. This probability is compared to a random number, and if a collision occurs the approximation is made that it occurred at the end of the increment $\Delta\vec{x}$ at time $t + \Delta t$. It is possible to randomly allow the collision anywhere along its incremental path, but then the small angle term and the Lorentz term would have to be reversed in time to the collision point, which is computationally very tedious.

Admittedly, the large angle collision term is small compared to the small angle term and could be dropped without significant effect, but the collisions which result in in-flight reactions may represent a very significant part of the energy generated for some types of problems¹⁵. The reason for doing the large angle scattering with the in-flight reactions was more a matter of convenience than a physics necessity. The cross section data used¹⁶⁻²², contained both pieces of physics and it was simple to do both.

The orbit of the high energy particle is thus calculated over many time steps until one of the following happens: it thermalizes (reaches $3/2 kT_1$ and becomes part of the Maxwellian), it escapes beyond the boundary of the problem, or the problem reaches its conclusion. Of course the ion may have an in-flight reaction resulting in two different particles. For example: ${}^3\text{H}({}^2\text{H},n)\alpha$ -- an energetic triton may collide with a Maxwellian deuteron resulting in a neutron and alpha particle. The neutron is assumed

to escape with all its energy, and the alpha is scattered isotropically and followed in lieu of the incoming triton. The tracking of these ions is further complicated by the Lagrangian definition of the zones. The variables that affect the orbit change from zone to zone, so that the $\Delta \vec{x}$ an ion bundle moves can never be greater than the distance to a zone boundary crossing. When a bundle reaches a new zone, the appropriate cross sections, and variables are updated and the bundle tracking is resumed. The method used to track bundles in a Lagrangian mesh is covered in Appendix 5.

At the end of each Δt in a particle's orbit, the change in the momentum and energy to the Maxwellian fluids are calculated and saved as source terms for the MHD conservation equations. When a bundle is born from the fluid, or thermalizes, the mass of the zone is adjusted.

This section has been a qualitative description of the Monte Carlo transport model that was used, and the following sections and the appendices will cover more of the specifics. In doing a Monte Carlo calculation the techniques used by one person on one type of computer may not be useful for another problem on a different computer. Therefore the nonphysics Monte Carlo techniques that were used (sample size determination, etc.) will be discussed only briefly in Appendix 6.

3.1 Integration of the Lorentz Force

As stated in an earlier section, the first step in solving the equation of motion, Eq. (3.0.1), was to integrate the Lorentz force, i.e., solve the equation

$$\frac{d\vec{v}}{dt} = \frac{q}{mc} \vec{v} \times \vec{B} \quad (3.1.1)$$

This equation has been solved for particle codes by a large number of people^{1,23}, and in most of these cases the plasma is considered collisionless. Kruer's paper²³ reviews particle codes and their use in plasma simulation and gives a fairly extensive list of further references on the subject. Since this model considers collisions and the high energy charged particles have a fairly good chance of thermalizing, one does not need the high degree of accuracy that one would want in a collisionless plasma simulation.

For a given time step (more will be said about this time step control in another paragraph in this section), Eq. (3.1.1) is differenced approximately as follows

$$\vec{v}_i^{n+1} = \vec{v}_i^n + \frac{\Delta t}{c} \left(\frac{q}{m} \right)_i [\vec{v}_i^n \times \vec{B}]^{n+1/2} \quad (3.1.2)$$

where i denotes the i th Monte Carlo ion sample. The word approximately was used because the Lorentz force was not readily available at time $n + 1/2$, therefore a 2 pass iterative scheme was used to calculate it (a predictor-corrector if you prefer). Equation (3.1.2) was solved in cartesian (x , y , z) space for a full 3 component magnetic field:

$\vec{B} = B_\theta \hat{\theta} + B_r \hat{r} + B_z \hat{k}$. This is inconsistent with the MHD section which only had a B_θ component, but was programmed this way in anticipation of

future changes to the code. For this project, B_r and B_z were set equal to zero. To do the tracking in cartesian space the magnetic field (in cylindrical coordinates) was decomposed to its cartesian components. The details of the cartesian tracking in a 2-D Lagrangian mesh are covered in Appendix 5. The particle tracking could probably be done in cylindrical coordinates, but it appeared to be simpler in cartesian, particularly when calculating the distance to zonal boundary crossing.

Therefore given a Δt , $\vec{v} \times \vec{B}$ was predicted at time $n + 1/2$ and using this time centered Lorentz force, the velocity at time $n + 1$ is calculated. The velocity is then simply integrated to get a new position coordinate

$$\vec{x}^{n+1} = \vec{x}^n + \Delta t \vec{v}^n \quad (3.1.3)$$

It seemed logical that the time step for the Lorentz force integration should be controlled by the magnetic field strength. For a strong $\vec{B}$ field and tight orbits, a small Δt would be needed and for very weak fields a large Δt could be tolerated. Therefore the Δt used in solving Eq. (3.1.1) was arbitrarily set such that

$$f_c F \Delta t_{\text{mag}} \frac{|\vec{v}_\perp|}{|\vec{v}|} \leq 1 \quad (3.1.4)$$

where $f_c = \frac{qB}{2\pi mc}$ = the cyclotron frequency, and F was an arbitrary multiplier, usually set to 20. In other words, with $F = 20$, one is allowing the ion to only move along 1/20 of its local Larmor orbit. For a uniform $\vec{B}$ field and a circular orbit, the ion's track would be a 20 sided polygon (icosogon). Experimentation with F seemed to indicate a value of

20 was adequate provided a time centered second order accurate scheme (Eq. (3.1.2)) was used.

It should be noted that in the actual programming of Eq. (3.1.2) other considerations may require the Δt to be even smaller. For example one does not want the particle's orbit to carry it into another zone, but only to its boundary, therefore the time to boundary must be calculated (Δt_{BNDRY}).

$$\Delta t_{\text{BNDRY}} = (\vec{X}_{\text{BNDRY}} - \vec{X}^n) / \vec{v}^n \quad (3.1.5)$$

And in addition one must calculate the time to thermalization (Δt_{TH}) - the time it takes for the energetic ion to reach $3/2 K T_i$, when it no longer is a Monte Carlo bundle, but becomes part of the Maxwellian ion fluid. (See Section 3.2) for the Δt_{TH} calculation). It is the minimum of $\{\Delta t_{\text{MAG}}, \Delta t_{\text{BNDRY}}, \Delta t_{\text{TH}}\}$ that is used for the tracking of the ion.

Now that the Monte Carlo ion bundle has been advanced in velocity and configurational space due to the Lorentz force, the energy and momentum losses to the bundle (gains to the fluid plasma) are calculated for that time step.

3.2 Integration of Small Angle Collision Term

The object of this section is to develop the equations used to calculate the energy loss to an energetic ion as it travels through a Maxwellian fluid of electrons and ions. Only small angle collisions are considered in this section and the approximation is made that the equilibration time of the energetic ion is less than the 90° deflection time. Therefore a straight line path is assumed. The energy loss of the energetic ions is given to the Maxwellian fluids. The fractional amounts given to each are also calculated.

From Appendix 4 the energy loss rate equations were derived as (Note: minus sign dropped)

$$\left(\frac{dE_1}{dt}\right)_e = \frac{32 n_e z_1^2 e^4}{3m_1 \langle v_e \rangle} \left(\frac{E_1}{KT_e}\right) \ln \Lambda_e \quad (3.2.1)$$

$$\left(\frac{dE_1}{dt}\right)_i = \frac{4\pi e^4 z_1^2 \ln \Lambda_i}{v_1} \sum_{i=1}^N \frac{n_i z_i^2}{m_i} \quad (3.2.2)$$

where the i subscript refers to the energetic ion, the e subscript to the electron fluid, and the i subscript to the ion fluid. Letting

$$\langle v_e \rangle = \sqrt{\frac{8 KT_e}{\pi m_e}} ; \quad v_i = \sqrt{\frac{2E_1}{m_i}}$$

Eqs. (3.2.1), (3.2.2) become

$$\left(\frac{dE_1}{dt}\right)_e = \beta_e E_1 \quad (3.2.3)$$

$$\left(\frac{dE_1}{dt}\right)_1 = \beta_i E_1^{-1/2} \quad (3.2.4)$$

$$\beta_e = \frac{8 \sqrt{2\pi} m_e Z_1^2 e^4 n_e \ln \Lambda_e}{3m_1 (KT_e)^{3/2}}$$

$$\beta_i = 2\sqrt{2\pi} \pi e^4 Z_1^2 \ln \Lambda_i \sum_{i=1}^N \frac{n_i Z_i^2}{m_i}$$

Equation (3.2.3) is the energy loss rate of an energetic ion in a Maxwellian of electrons where $v_1 \ll \langle v_e \rangle$. Equation (3.2.4) is the energy loss rate of an energetic ion in a Maxwellian of ions where $v_1 \gg v_i$.

The total energy loss rate is just the sum of (3.2.3) and (3.2.4)

$$\frac{dE_1}{dt} = \beta_e E_1 + \beta_i E_1^{-1/2} \quad (3.2.5)$$

With a little algebra, Eq. (3.2.5) becomes

$$dt = \frac{E_1^{1/2} dE_1}{\beta_i (1 + \beta_T E_1^{3/2})} \quad (3.2.6)$$

where $\beta_T = \beta_e/\beta_i$. Integrating

$$\Delta t = \int_{E_f}^{E_s} \frac{E_1^{1/2} dE_1}{\beta_i (1 + \beta_T E_1^{3/2})} \quad (3.2.7)$$

where E_s is the energy of the energetic ion at the start of the time step and E_f is the energy at the end of Δt . Since β_i and β_e are not functions

of E_1 , Eq. (3.2.7) is easily integrated

$$\Delta t = \frac{2}{3\beta_e} \ln \frac{(1 + \beta_T E_s^{3/2})}{(1 + \beta_T E_f^{3/2})} \quad (3.2.8)$$

This is a very useful equation. We know E_s , β_T , and β_e , and if E_f is known we can calculate the Δt needed to reach E_f . Or if Δt is known, then E_f can be calculated. Equation (3.2.8) is easily rearranged to give the equation for E_f

$$E_f = \left\{ \frac{1}{\beta_T} \left[(1 + \beta_T E_s^{3/2}) e^{-\frac{3\beta_e \Delta t}{2}} - 1 \right] \right\}^{2/3} \quad (3.2.9)$$

As was stated earlier, the Δt to be used in the Monte Carlo tracking must be less than the time it takes for the ion to reach thermalization. Therefore Eq. (3.2.8) is used to calculate this Δt_{TH}

$$\Delta t_{TH} = \frac{2}{3\beta_e} \ln \frac{(1 + \beta_T E_s^{3/2})}{(1 + \beta_T E_{TH}^{3/2})} \quad (3.2.10)$$

where $E_{TH} = 3/2 kT_i$; a known quantity. Having calculated Δt_{MAC} (Eq. 3.1.4) and Δt_{BNDRY} (Eq. 3.1.5), and Δt_{TH} (Eq. 3.2.10), the minimum of these three is selected and used to advance the Monte Carlo bundle. This Δt is substituted into Eqs. (3.1.2) and (3.1.3) to advance the bundle and into Eq. (3.2.9) to calculate its final energy. The total energy change is simply

$$\Delta E_1 = E_s - E_f \quad (3.2.11)$$

Now we must calculate that fraction of ΔE_1 which goes to the fluid ions and that which goes to the electrons. The energy given to the Maxwellian fluid ions is given by

$$(\Delta E_1)_i = \int_{E_f}^{E_s} \left(\frac{dE_1}{dt} \right)_i dt$$

Using Eqs. (3.2.4) and (3.2.6), the above becomes

$$(\Delta E_1)_i = \int_{E_f}^{E_s} \frac{dE_1}{(1 + \beta_T E_1^{3/2})}$$

This can be integrated and gives

$$(\Delta E_1)_i = \frac{2}{3\beta_T E} \left[\frac{1}{2} \ln \frac{g^2 - gx + x^2}{(g+x)^2} + \sqrt{3} \tan^{-1} \left(\frac{2x-g}{g\sqrt{3}} \right) \right] \Bigg|_{E_f}^{E_s}$$

where $g = (1/\beta_T)^{1/3}$ and $x = E_1^{1/2}$. This is computationally tedious and it is simpler to use the approximation¹⁷

$$(\Delta E_1)_i = \left(\frac{1}{\beta_T} \right)^{2/3} F(u) \quad (3.2.12)$$

$$F(u) = \int_{u_f}^{u_s} \frac{du}{u^{3/2} + 1}$$

where $u^{3/2} = \beta_T E^{3/2}$ and $F(u)$ can be approximated by

$$F(u) = \begin{cases} u - .25u^2 & , \quad u \leq 1 \\ 2.4 - 2u^{-1/2} + .35u^{-1} & , \quad u > 1 \end{cases}$$

This set of equations is used to calculate the fraction of energy that goes to the ions. From conservation of energy the remaining energy goes to the electrons

$$(\Delta E_1)_e = \Delta E_1 - (\Delta E_1)_i \quad (3.2.13)$$

Now the speed of the energetic ion is decreased to be consistent with its new energy. Note that the direction is not altered.

$$v_x^{n''} = v_x^{n'} \frac{|\vec{v}|^{n''}}{|\vec{v}|^{n'}} \quad (3.2.14)$$

$$|\vec{v}|^{n''} = \sqrt{\frac{2E_f}{m_1}}$$

etc. for y and z components; where n'' refers to the time after the small angle collisions (but before any large angle collision) and n' refers to time at the end of the Lorentz motion (but before large and small angle collisions).

The completes the integration of the small angle collision term, but a summary might clarify the procedure. The following is a word description of the flow of the Monte Carlo calculation up to this point.

1. Δt_{MAG} is calculated from Eq. (3.1.4).
2. Δt_{TH} is calculated from Eq. (3.2.10).
3. Δt_{BNDY} is calculated from Eq. (3.1.5).
4. Select minimum of $\{\Delta t_{MAG}, \Delta t_{TH}, \Delta t_{BNDY}\}$.
5. Calculate $\Delta \vec{v}$ from Eq. (3.1.2).
6. Calculate $\Delta \vec{X}$ from Eq. (3.1.3).
7. Calculate ΔE_1 from Eq. (3.2.11).
8. Calculate $(\Delta E_1)_i$ from Eq. (3.2.12).

9. Calculate $(\Delta E_1)_e$ from Eq. (3.2.13).
10. Calculate $|\vec{v}|$ from Eq. (3.2.14).

The large angle collisions can now be calculated.

3.3 Integration of the Large Angle Collision Term

In the last two sections the Monte Carlo bundle was advanced in velocity and configuration space due to the Lorentz force, and the speed and energy were updated from small angle coulomb collisions. Now the probability of the Monte Carlo bundle to have a large angle nuclear scattering, or an in-flight nuclear reaction over the specified time step (Δt) can be calculated. The cross sections and data used were adapted from papers written by Corman and others.¹⁶⁻²² Only the following scatterings and reactions were considered:

1. Deuterons: an energetic deuteron was able to undergo the following in-flight reactions

and could scatter elastically from other Maxwellian deuterium ions. Elastic scattering of deuterons on tritium was not modeled.

2. Tritons: energetic tritons were allowed to have an in-flight reaction with Maxwellian deuterium; Eq. (3.3.3).

3. Alphas: energetic alpha particles could undergo nuclear elastic scatterings with Maxwellian deuterium ions. Scattering of alphas on tritium was not calculated.

The only reason for not considering elastic collisions on tritium was that the cross section data was not readily available, and the relative unimportance of large angle scattering to the overall problem didn't justify spending the time needed to compile it.

In all cases above, the probability for an event happening over the given Δt is given by the following general type of equation.

$$P_i = 1 - \exp \left[- \Delta t \sum_{j=1}^N n_j (\sigma V)_{i-j} \right] \quad (3.3.4)$$

where i denotes the energetic particle and j the Maxwellian species it is colliding and reacting with. The term (σV) is replaced by $\langle \sigma V \rangle$, the Maxwell averaged cross section, for the in-flight reactions. The cross sections are tabulated in the code as a function of the test ion energy and plasma ion temperature. As an example of Eq. (3.3.4), the probability of an energetic deuteron event (case 1 above) is

$$P_d = 1 - \exp \left[- \Delta t (n_d \langle \sigma V \rangle_{d-d}^{(1)} + n_d \langle \sigma V \rangle_{d-d}^{(2)} + n_t \langle \sigma V \rangle_{d-t} + n_d (\sigma V)_{d-d}^{(s)}) \right] \quad (3.3.5)$$

where the superscripts (1) and (2) refer to the different branches of the d-d reaction, and the (s) refers to the elastic scattering cross section. The data and equations needed to determine $\langle \sigma V \rangle$ and (σV) are given in the references mentioned earlier.

Having calculated the total probability for an event using Eq. (3.3.4), one now compares this with a random number. If the random number is less

than P_i , then an event is assumed and a second random number is selected and compared to the individual probabilities to decide which event occurred. For simplicity it is assumed the event takes place at the end of the Δt . The event could have taken place anywhere along its elemental path, but this would require "backing up" the Lorentz force and the small angle collision terms to the collision point; which would be very tedious.

When the event is an in-flight reaction, then the reaction products are created and scattered isotropically with their appropriate energies. When the event is an elastic scatter, the scattering angle must be randomly determined from a table. This table of angles was generated in the usual fashion, by integrating the differential cross section (which is a function of the test ions energy) over a given set of angles and equating the results to a set of random numbers. Thus given a random number and the energy of the test ion, a scattering angle is easily determined. Using conservation of energy and momentum, the energy and remaining angles of the scatter for the test and target particles are easily calculated using the usual center of mass equations for elastic scattering.

It is interesting to note that after an event, one may be left with two high energy bundles to track. All high energy neutrons generated from the reactions are assumed to escape immediately with their energy. But any resultant charged particles from a reaction or, the scattered test particle and its scattered target particle must be tracked as Monte Carlo particles until they reach thermalization energy. Thus particles

may be scattered out of the Maxwellian model into the Monte Carlo model, and vice versa.

This completes the Monte Carlo time step. The particle tracking continues for another Δt until the sum of the Monte Carlo Δt 's equals an MHD Δt , at which time the Monte Carlo bundles are stored on disc (census) until after the MHD has been advanced a time step.

3.4 Momentum Conservation

The last three sections have described how the equation of motion for a Monte Carlo bundle of energetic ions was solved. It involved three computational steps: 1. the integration of the Lorentz force, 2. integration of the small angle coulomb collision term, and 3. integration of the large angle scattering and in-flight reaction term. In addition to calculating the energetics of these processes, one must also calculate the momentum changes between the fluid and the Monte Carlo system of particles. Changes in the fluid's momentum from the Monte Carlo processes are saved as a source term and added to the MHD momentum equation (Eq. (2.0.2)). This source term is of the form

$$(\vec{v})_{MC} = \left(\frac{\Delta \vec{v}}{\Delta t} \right)_{MC} = \left(\frac{\vec{v}^{n+1} - \vec{v}^n}{\Delta t} \right)_{MC} \quad (3.4.1)$$

where $\vec{v}$ is the fluid velocity. Thus one needs to know what the fluids final velocity would be as a result of the Monte Carlo processes. The term $(\vec{v})_{MC}$ is the resultant of the sum of all processes for all Monte Carlo bundles. Note that the fluid velocity is not changed after each Monte Carlo event, but is changed only through the Monte Carlo momentum term in the MHD momentum equation.

A. Lorentz Force

When integrating the Lorentz force, the particle's velocity vector was rotated, but the speed and energy remained constant. Since the vector velocity has changed, the momentum of the bundle has changed at the expense of the momentum of the magnetic field. One might assume that the fluid and field are strongly coupled, therefore the momentum change ought

to be given to the fluid. But this creates a problem. If the fluid is to receive the momentum, then by conservation, one can't hold the particle energy constant over the Lorentz rotation unless the energy is to come from the magnetic field. The physics of this three component process was not understood, so the assumption was made that

$$(\vec{v})_{\text{MC-LORENTZ}} = 0$$

i.e., the Lorentz rotation of the Monte Carlo bundle contributed no momentum changes to the fluid.

B. Small Angle Coulomb Collisions

The calculation of momentum exchange from small angle coulomb collisions was modeled by considering the collision between a zone of mass M and velocity $\vec{V}$ with a particle of mass m and velocity $\vec{v}$. The collision kinematics are conveniently described in the center of mass (momentum) coordinates. Letting the subscript CM denote a variable in the center of mass coordinates, the following can easily be derived

$$\vec{v}_{\text{CM}} = \left(\frac{M}{m + M} \right) (\vec{v} - \vec{V}) \quad (3.4.2)$$

$$\vec{V}_{\text{CM}} = \left(\frac{m}{m + M} \right) (\vec{V} - \vec{v}) \quad (3.4.3)$$

and $\vec{U}_L$, the CM velocity in the laboratory is

$$\vec{U}_L = \left(\frac{M}{m + M} \right) \vec{V} + \left(\frac{m}{m + M} \right) \vec{v} \quad (3.4.4)$$

The kinetic energy of the system in the CM is given by the equation

$$(\text{KE})_{\text{CM}} = \frac{1}{2} m v_{\text{CM}}^2 + \frac{1}{2} M V_{\text{CM}}^2$$

and using Eqs. (3.4.2) - (3.4.4) it becomes

$$\langle KE \rangle_{CM} = \frac{1}{2} \left(\frac{m M}{m + M} \right) |\vec{v}_{CM} - \vec{v}_{CM}|^2 \quad (3.4.5)$$

Letting the superscripts n and $n + 1$ refer to the time at the start and end of the Monte Carlo time step; assuming straight line slowing down (scattering angle of the energetic ion is zero) and invoking conservation of energy and momentum gives

$$\vec{v}^{n+1} = \mu \vec{v}^n + (1 - \mu) \vec{v}_L^n \quad (3.4.6)$$

where

$$\mu = \left[\frac{\langle KE \rangle_{CM}^{n+1}}{\langle KE \rangle_{CM}^n} \right]^{1/2} \quad (3.4.7)$$

The object is to now determine the cylindrical components of Eq. (3.4.6) by taking the dot product of $\vec{v}^{n+1}$ with the unit vectors, $\hat{r}$, $\hat{\theta}$, $\hat{z}$. Note that $v_{\theta}^n = 0$, but v_{θ}^n is not, therefore a v_{θ}^{n+1} is generated. From symmetry there should be cancellation of the various v_{θ}^{n+1} components for each particle. Thus there will be no $\hat{\theta}$ component of momentum, but there will be an energy deposited to the fluid from this v_{θ}^n component. Thus the final lab components of the fluid velocity are

$$v_R^{n+1} = \left[\mu + (1 - \mu) \frac{M}{m + M} \right] v_R^n + (1 - \mu) \left(\frac{m}{m + M} \right) v_R^n \quad (3.4.8a)$$

$$v_z^{n+1} = \left[\mu + (1 - \mu) \frac{M}{m + M} \right] v_z^n + (1 - \mu) \left(\frac{M}{m + M} \right) v_z^n \quad (3.4.8b)$$

$$v_{\theta}^{n+1} = (1 - \mu) \left(\frac{m}{m + M} \right) v_{\theta}^n \quad (3.4.8c)$$

Now the Monte Carlo momentum depositions for small angle coulomb collisions can be calculated using Eqs. (3.4.1) and (3.4.8)

$$\begin{aligned}
 \vec{v}_{MC-SMALL\ ANGLE} = \hat{r} \left\{ \left[\mu + (1 - \mu) \frac{M}{m + M} \right] v_R^n \right. \\
 \left. + (1 - \mu) \frac{m}{m + M} v_R^n - v_R^n \right\} + \hat{z} \left\{ \left[\mu + \right. \right. \\
 \left. \left. (1 - \mu) \frac{M}{m + M} \right] v_z^n + (1 - \mu) \left(\frac{m}{m + M} \right) v_z^n - v_z^n \right\} \quad (3.4.9)
 \end{aligned}$$

Note that v_R , v_z , and v_θ are to be calculated from the cartesian components v_x , v_y , and v_z and their direction cosines which are used in the tracking (see Appendix 5). The components of Eq. (3.4.9) thus represent axial and radial momentum depositions to the fluid from small angle coulomb collisions.

Since both energy and momentum must be conserved, a few words are in order concerning the energy depositions calculated in Section 3.2. The terms $(\Delta E_1)_e$ and $(\Delta E_1)_i$ calculated from Eqs. (3.2.12) and (3.2.13) must be slightly modified. The equations to calculate the energy loss rate assumed the Maxwellian fluid was at rest, but since it is not the terms $(\Delta E_1)_i$ and $(\Delta E_1)_e$ should be calculated in the fluid rest frame before using the equations of Section 3.2. This is simply done by subtracting $\vec{v}$ from $\vec{v}$ and calculating E_1 using the rest frame speed.

Thus the energy deposited to the fluid internal energy is the difference between the $(KE)_{CM}$ over the time step, plus the energy

deposited due to the v_{θ}^n component of velocity (see Eq. 3.4.8c).

$$\Delta \epsilon = (KE)_{CM}^n - (KE)_{CM}^{n+1} + \frac{1}{2} M \left[(1 - \nu) \frac{m}{m + M} v_{\theta}^n \right]^2 \quad (3.4.10)$$

The term $(KE)_{CM}$ is related to the kinetic energy of the Monte Carlo bundle in the fluid rest frame by the relation

$$(KE)_{CM} = \frac{M}{m + M} (E_1)_{\text{fluid rest frame}} \quad (3.4.11)$$

Thus knowing E_1 in the above equation, we calculate $(KE)_{CM}$ for time n and $n + 1$ and then calculate ν in Eq. (3.4.7). Now the amount of energy given to the internal energy of the electron and ion fluids is

$$(\Delta \epsilon)_i = \frac{M}{m + M} (\Delta E_1)_i + f_i E_{\theta} \quad (3.4.12)$$

$$(\Delta \epsilon)_e = \frac{M}{m + M} (\Delta E_1) - (\Delta \epsilon)_i + (1 - f_i) E_{\theta} \quad (3.4.13)$$

$$f_i = \frac{(\Delta E_1)_i}{(\Delta E_1)} \quad (3.4.14)$$

$$E_{\theta} = \frac{1}{2} M (1 - \nu) \frac{m}{m + M} v_{\theta}^n{}^2 \quad (3.4.15)$$

where $(\Delta E_1)_i$ is from Eq. (3.2.12), (ΔE_1) from Eq. (3.2.11), remembering that E_1 is in the fluid rest frame.

C. Large Angle Scattering and In-Flight Reactions

When an elastic nuclear scattering event takes place the CM scattering angle is randomly selected from the appropriate distribution. Thus the collision kinematics between the Maxwellian ion (which is assumed to be at rest) and the Monte Carlo bundle are easily done using the usual collision equations for an elastic scatter in the CM coordinates.²⁴ Thus the target particle is kicked out of the Maxwellian and becomes a

Monte Carlo particle. Momentum is conserved between the test and target particles, therefore the zone fluid does not receive any momentum from the collision. For an in-flight reaction the reaction products are created at their appropriate energies and no momentum is given to the fluid. Therefore no momentum from large angle scattering and in-flight reactions is given to the fluid; i.e.,

$$(\vec{V})_{MC-LARGE\ ANGLE}^+ = 0$$

D. Summary

Thus in summary the only contribution to the fluid momentum is from the small angle coulomb collisions, as given by Eq. (3.4.9). And the energy terms of Section 3.2 must be modified as in Eq. (3.4.12) - (3.4.15) to be consistent with this momentum deposition.

3.5 Monte Carlo Current

As indicated in the introduction and in Figure 1, a Monte Carlo current ($\vec{J}_{MC}$) term should be calculated and used in calculating the magnetic field. This current could be added to the current in Ampere's Law. However, in this study, $\vec{J}_{MC}$ was assumed to be zero. The values of $\vec{J}_{MC}$ could be calculated by tallying the fluxes of electrons and ions as they move through the mesh.

$$\vec{J}_{MC} = (\vec{J}_{MC})_i + (\vec{J}_{MC})_e$$

or

$$\vec{J}_{MC} = n_i Z_i e \vec{v}_i - n_e e \vec{v}_e \quad (3.5.1)$$

The determination of $(\vec{J}_{MC})_i$ is very simple. One simply counts the Monte Carlo ion bundles that traverse the zone. However calculating $(\vec{J}_{MC})_e$ is not so obvious as there are no Monte Carlo electrons. Because of the coulomb forces generated, the ion will tend to drag electrons along with it. If the electrons were not dragged along, then one would not have local charge neutrality.

In the absence of a $\vec{B}$ field the assumption $\vec{J}_{MC} = 0$ seems quite reasonable for hydrodynamic time scales. However when there is a strong $\vec{B}$ field, the gradient and curvature drift complicate the picture as they tend to separate the ion and its companion electrons. The picture is further complicated by the fact the companion electrons will be of much lower energy than the ion and will have a much shorter mean free path, thus suffering many collisions while moving with the ion. Despite these complications, one would think that the coulomb attractive force would

dominate and that the Monte Carlo ions would move as neutrals; i.e., they would have companion electrons with them. Thus $\vec{J}_{MC}$ was assumed to be zero in this study.

Assuming one did know how to calculate a $\vec{J}_{MC}$, then the question arises as to what to do with it. One simple suggestion would be to calculate the change in $\vec{B}$ due to $\vec{J}_{MC}$, by solving Ampere's Law, $\nabla \times \vec{B} = \frac{4\pi}{c} \vec{J}_{MC}$, explicitly. This may (without care) cause instabilities, but it would be a simple way to account for a Monte Carlo current in the MHD equations. A self-consistent scheme is described by T. Johnson in his Ph.D. thesis.²⁵

4. CONCLUSION

In the preceding pages a model for simulating the transport of non-Maxwellian ions in a Maxwellian fluid plasma has been developed. The non-Maxwellian ions were modeled using a Monte Carlo model and the Maxwellian fluid with a MHD model. The non-Maxwellian ions suffered small angle coulomb collisions, large angle scatterings, and in-flight reactions while orbiting in the plasma under the influence of a magnetic field. Energy and momentum depositions to the Maxwellian fluids from Monte Carlo collisions were added to the electron and ion conservation equations as source terms. The model was developed in a two-dimensional (R, Z) coordinate system, with a Lagrangian representation for the MHD equations. A B_0 magnetic field with a simple Ohm's law was assumed. A two temperature model was used, with a perfect gas equation of state, a scalar pressure and a tensor artificial viscosity. Electron and ion thermal conduction was also calculated. All physics and transport coefficients are calculated assuming a fully ionized gas, and a bremsstrahlung radiation loss term is included to simulate the free-free transitions. The MHD conservation equations were differenced explicitly and the diffusion type equations (magnetic and thermal conduction) were differenced implicitly.

The model was developed primarily to study the effect of thermonuclear reaction products upon a dense hot plasma. The Monte Carlo model is particularly useful when the Larmor radii of the non-Maxwellian ions are comparable in size to the problem size. A diffusion transport model is not valid in this regime. Of course, when the magnetic field is strong and the orbits are small, the Monte Carlo model becomes too

expensive and impractical to use. The assumption of a perfect gas and full ionization are valid for hot plasmas that are burning, but must be used with caution. One would not want to simulate the magnetohydrodynamics of a cold, partially ionized gas with this model. The Lagrangian fluid equations are useful for problems that may have multiple fluid species or a plasma that is interacting with a wall or liner. On the other hand the hydro motion must not be so turbulent that the mesh distorts and bowties to the point where one can't run. In other words, the model should be used for hot systems that are close to hydrodynamic equilibrium, but where the non-Maxwellian energy and momentum depositions from the thermonuclear reactions will affect the motion of the fluid.

The Monte Carlo model might also be useful for beam-injection and/or Fokker-Planck type studies.

The model was used to calculate the thermonuclear alpha particle heating of a gas-embedded Z-pinch. The problem description and results are described in detail in Appendix 1. In summary, the results of this test calculation show that the nonlocal energy depositions of the alphas to the pinched gas result in nonuniform spatial heating and significantly lower drift losses. Despite these differences, the overall heating and resulting expansion are in fair agreement with other computer studies. With respect to the computer model, the conclusion can be drawn that Monte Carlo is a valid calculational tool for certain plasma physics studies.

Three problems were run; all were initially identical except that each had different currents (different circuit parameters). Two of the

problems (the smaller of the currents) ran without any difficulties, but the problem with the largest current created large B fields and very small time steps in the Monte Carlo. Problem 3 (MC-3) would probably be better run on a diffusion model. Each problem used about 6 hours of 7600 computer time, and each problem generated and followed approximately 10,000 alpha particles for 1,000 cycles (approximately .4 μ sec).

The usefulness of the model could be significantly improved with the addition of the K and Z components of the magnetic field. This was essentially done in the Monte Carlo section, but were set to zero to be consistent with the MHD. Other possible improvements would be the inclusion of partially ionized gas physics, a non-perfect equation of state, and a better Ohm's law. Any of these additions could be made to the model within the current configuration of the code. Another desirable change would be to add the θ dependence to the model, but this would require redoing the Monte Carlo tracking scheme -- a difficult task. The assumed θ symmetry greatly simplified the tracking by allowing one to perform a coordinate transformation to track in a plane. Without θ symmetry a new tracking model must be developed.

Although there is room for improvement in this model, the concept of a Monte Carlo-MHD hybrid code has been shown to be useful. The model will aid in the understanding of plasma behavior and the transport properties within a hot dense magnetized gas.

APPENDIX 1: TEST PROBLEM - ALPHA PARTICLE HEATING OF A Z-PINCH

To test the model developed in this report, a study was made of the alpha particle heating of a Z-pinch. Hartman and others have reported on their investigation and their modeling of the alpha particle heating of a gas-embedded Z-pinch^{26,27} using a 1-D MHD code.²⁸ It was decided to repeat the calculation using this MHD/Monte Carlo model.

The problem reported by Hartman was essentially as follows. A one-dimensional D-T plasma (50%-50%) of radius 10 centimeters with $T = 1$ eV for $r \leq .047$ cm; and $T =$ room temperature for $.047 < R \leq 10$ cm, and $\rho = .1$ gm/cm³ for all r was subdivided (zoned) in 40 zones. The inner region of the problem was heated up to $T = 390$ eV in $2.25 \mu s$ by a resistive pinch preheat. At $t = 2.25 \mu s$ a capacitor ($c = .1 \mu fd$) with internal inductance $L = 50$ nhenry, charged to $V = 50$ MV was switched on and crowbarred at peak current $I = 30$ MA. The plot of the current as a function of time is given by curve #1 in Fig. 5.1.1. The D-T reaction rates were calculated as a function of the material temperature, T . The alpha particle heating was calculated assuming that the alpha particles lose energy to the plasma by classical collisions with time constant τ_c and are lost out the end of the pinch by VB drift with time constant τ_D . The alpha particle lifetime for each zone was given by $1/\tau_\alpha = 1/\tau_c + 1/\tau_D$. In the loss due to drift calculation, the axial dimension of the plasma was assumed to be 10 cm. The alpha particle energy heated the plasma from 10 to 50 keV and in consequence the pinch expanded radially.

Now to describe the problem as it was run on this MHD/Monte Carlo model. Although the code written to simulate this model is as yet

unnamed, it will be referred to as the MC code. The code used by Hartman is called MAGPIE.

Since the MC model assumed a perfect gas and full ionization it was decided to not try and run the entire problem as was done on MAGPIE, but to pick up (link) the problem from MAGPIE at $t = 2.3 \mu s$. This was after preheat, but before the final pinch and thermonuclear burn. Only the hot plasma (inner 19 zones) was linked to MC and the remaining 21 zones were hydrodynamically simulated using a time varying pressure profile on the outer boundary of the mesh. Since MC is two-dimensional, it was possible to specify the axial dimension of 10 cm. To compare with MAGPIE and to keep the MC Lagrangian zones from sausaging (and becoming bowtied), the radial accelerations were forced to be constant along a line of constant Z . Thus the problem was essentially one dimensional in the MHD but the Monte Carlo was still two-dimensional.

Three problems were run on MC. They all had identical initial conditions, but the current profile as a function of time was different. Problem MC-1 was run with the current given by curve #1, Fig. 5.1.1; MC-2 with current #2 and MC-3 with current #3. At currents much higher than #3, the MC code became too expensive to run since the Larmor orbits became very small and hence the Monte Carlo magnetic time step (Δt_{MC} - Eq.(3.1.4)) became prohibitively small.

Before describing the results a few words about the physics differences between the MC and MAGPIE codes should be made. The key difference is the model describing the transport of the alpha particles,

which has already been described. Another possibly significant difference is that MC is a two temperature code (T_e and T_i) while MAGPIE has only a single temperature T . Both codes calculated thermal conduction, and for times greater than $2.3 \mu s$ and $r < .2$ cm (first 19 zones of MAGPIE) the full ionization and perfect gas assumptions of MC are probably valid. Both codes had a radiation loss term and ignored the neutron energy from the D-T reactions.

It is important to note that the problems labeled MC-1 and MAGPIE had identical currents, therefore should be comparable. MC-2 had a smaller current and MC-3 a larger current.

When comparing MC-1 and MAGPIE in Figs. 5.1.2-5.1.9, one sees that the results are reasonably similar in most respects (within a factor of 2). The biggest discrepancy seems to be the energy lost to the problem from drift. MAGPIE's drift energy was approximately 8 times larger than MC-1. In MC-1 the energy is not drifting out of the problem as fast as it did in MAGPIE. The lower drift can partly be attributed to a smaller gradient in the magnetic field (off axis) in MC-1 and also due to the higher densities and lower temperatures (on axis) one sees in MC-1. The temperature and density differences can significantly reduce the time it takes a particle to thermalize (and hence reduces the chance to escape). For example a 3.5 MeV alpha particle in D-T at density $.01 \text{ gm/cm}^3$ and $T_e = 40 \text{ keV}$ (MAGPIE conditions) will thermalize in approximately $.1 \mu s$, whereas at $T_e = 20 \text{ keV}$ and $\rho = .02 \text{ gm/cm}^3$ (MC-1 conditions) the time to thermalization is approximately $.03 \mu s$. These ∇B , ρ , and T_e differences can easily justify the factor of 8 difference in the drift energy loss.

The scenario in MC-1 as compared to MAGPIE seems to be the following. The pinch in MC-1 is more effective, resulting in higher initial densities and higher radiation loss; thermonuclear burn starts similarly, but in MC-1 it tends to be off axis (about $r = .05$ cm), *whereas in MAGPIE it is fairly uniform. This is probably caused by* the lower B field on axis, which doesn't trap the alpha particles as effectively as the stronger B field off axis. Both problems overall have similar energy deposition from the alphas, but MC-1 initially loses more energy from bremsstrahlung. Later in time the MC-1 seems to expand faster causing a large drop-off in density at $r = .1$. The large difference in loss due to drift is probably explained by higher initial densities, lower temperatures, and a significantly smaller gradient in the B field. See Figs. 5.1.7-5.1.9 for MC-1 and MAGPIE comparisons of B, T_e , T_i , T, and ρ at 2.6 μ s.

It should be noted that MC-3 was not run to completion (2.7 μ s) because it was becoming too expensive in terms of computer time (for a student running a test problem). The increased current caused better pinching and better burn, but the large B field ($\sim 10^8$ gauss) created very small Monte Carlo time steps.

Figure 5.1.1. Current vs time profile for the three MC problems and the one MAGPIE problem. Note current #1 is for MC-1 and MAGPIE.

Figure 5.1.2. Alpha energy created from thermonuclear reactions versus time.

Figure 5.1.3. Rate alpha energy created from thermonuclear reactions versus time.

Figure 5.1.4. Alpha energy deposited versus time.

Figure 5.1.5. Rate alpha energy deposited versus time.

Figure 5.1.6. Energy lost to plasma from drift versus time.

Figure 5.1.7. Magnetic field versus radius at 2.6 μ s.

Figure 5.1.8. Temperature versus radius at 2.6 μ s. Note that MAGPIE has only one temperature.

Figure 5.1.9. Density versus radius at 2.6 μ s.

APPENDIX 2: TRANSPORT COEFFICIENTS

Electric Conductivity

From Braginskii,⁴ the electric conductivity was calculated from the following formulas

$$\sigma_{\perp} = \frac{e^2 n_e^2}{a_{\perp}} \quad \{\text{sec}^{-1}\} \quad (5.2.1)$$

where

$$a_{\perp} = \frac{m_e n_e}{\tau_e} \left(1 - \frac{a'_1 X^2 + a'_0}{\Delta_e} \right)$$

and

$$X = \omega_e \tau_e, \quad \Delta_e = X^4 + \delta_1 X^2 + \delta_0. \quad (5.2.2)$$

The electron collision time is given as

$$\tau_e = \frac{3 \sqrt{m_e} (KT_e)^{3/2}}{4 \sqrt{2\pi} e^4 Z^2 n_i \ln \Lambda_e} \quad \{\text{sec}\}$$

For τ_e in sec where KT_e is given in keV

$$\tau_e = \frac{1.088 \times 10^{10} [KT_e \{\text{keV}\}]^{3/2}}{n_i Z^2 \ln \Lambda_e} \quad \{\text{sec}\} \quad (5.2.3)$$

also

$$\omega_e = \frac{eB}{m_e c} = 1.7588 \times 10^7 B \{\text{gauss}\} \quad \{\text{sec}^{-1}\} \quad (5.2.4)$$

The coefficients a'_1 , a'_0 , δ_1 , δ_0 are given in Braginskii in tabular form.

They were fitted to polynomials as a functions of Z , the atomic number.

$$a'_1 = 4.63 + 1.786Z^{-1} \quad (5.2.5)$$

$$a'_0 = .0678 + .49242^{-1} + .9762^{-2} + .3008^{-3}$$

$$\delta_1 = 7.482 + 5.9582^{-1} + 1.352^{-2}$$

$$\delta_0 = .0961 + .77782^{-1} + 1.59562^{-2} + 1.30082^{-3}$$

The $\ln \Lambda_e$ term in Eq. (5.2.2) was given by Shkarofsky²⁹ and Garelis³⁰ to be the smaller of the classical expression and the quantum mechanical expression

$$(\ln \Lambda_e)_{\text{classical}} = 33.825 + \frac{1}{2} \ln \left[\frac{(KT_e)^3}{Z^2 n_e} \right] \quad (5.2.6)$$

$$(\ln \Lambda_e)_{\text{Q.M.}} = 32.167 + \frac{1}{2} \ln \left[\frac{(KT_e)^2}{n_e} \right]$$

where (KT_e) is expressed in keV, and n_e = density of electrons.

Thus by using the above definition, Eq. (5.2.1) was used to calculate the electric conductivity.

Electron Thermal Conductivity

Also from Braginskii, the electron thermal conductivity was modeled with the following

$$\kappa_1 = \frac{n_e (KT_e) \tau_e}{n_e} = \frac{(\gamma'_1 X^2 + \gamma'_0)}{\Delta_e} \left\{ \frac{1}{\text{cm-sec}} \right\}$$

where (KT_e) is given in ergs. For (KT_e) to be expressed in keV

$$\kappa_1 = 1.7588 \times 10^{18} n_e (KT_e) \tau_e \frac{(\gamma'_1 X^2 + \gamma'_0)}{\Delta_e} \left\{ \frac{1}{\text{cm-sec}} \right\} \quad (5.2.7)$$

where τ_e is given by Eq. (5.2.3), and X and Δ_e by Eq. (5.2.2). The coefficients γ'_1 and γ'_0 were approximated by

$$\gamma'_1 = 2.5 \quad (5.2.8)$$

$$\gamma'_0 = 10.23 \div 9.13Z^{-1} + 2.31Z^{-2}$$

Ion Thermal Conductivity

Again from Braginskii, the ion thermal conductivity

$$\kappa_i = \frac{n_i (KT_i) \tau_i}{m_i} \frac{(2X^2 + 2.645)}{\Delta_i} \quad \frac{1}{\text{cm-sec}} \quad (5.2.9)$$

If (KT_i) is to be expressed in keV

$$\kappa_i = 9.59 \times 10^{14} \frac{n_i (KT_i) \tau_i}{A} \frac{(2X^2 + 2.645)}{\Delta_i} \quad \frac{1}{\text{cm-sec}} \quad (5.2.10)$$

where $\Delta_i = X^4 + 2.7 X^2 + .667$, A is the average atomic mass of the plasma, and τ_i , the ion collision time is given by

$$\tau_i = \frac{6.59 \times 10^{11} A^{1/2} [KT_i]^{3/2}}{n_i Z^4 \ln \Lambda_i} \quad \{\text{sec}\} \quad (5.2.11)$$

In Eq. (5.2.11), KT_i is also in keV. The variable X for ions is $\omega_i \tau_i$ where $\omega_i = 9.59 \times 10^3 \text{ ZB/A } \{\text{sec}^{-1}\}$. The $\ln \Lambda_i$ term, similarly to the $\ln \Lambda_e$, is given by the minimum of the following two expressions^{29,30}

$$(\ln \Lambda_i)_{\text{classical}} = 33.825 + \frac{1}{2} \ln \left[\frac{(KT_e)(KT_i)^2}{n_e Z^4} \right] \quad (5.2.12)$$

$$(\ln \Lambda_i)_{\text{Q.M.}} = 35.924 + \frac{1}{2} \ln \left[\frac{A(KT_e)(KT_i)}{n_e} \right]$$

where (KT_e) and (KT_i) are in keV.

APPENDIX 3: ARTIFICIAL VISCOSITY

When solving MHD differential equations one needs a mechanism to smooth out shock discontinuities. Von Neumann and Richtmyer³¹ developed such a mechanism, an artificial viscosity, denoted by the symbol q . Unfortunately, their model doesn't work well in a 2D system, especially a 2D Lagrangian system. Schulz proposed a tensor viscosity,² or a set of four q^1 per zone where each q is a measure of the compression along each side of the zone. (See Fig. 5.3.1.) Schulz's equations for q are

$$q^k = -c_0^2 \rho \left[\frac{\partial V}{\partial \ell} \right]^{1/2} \left[\frac{\partial}{\partial \ell} \left(\frac{\partial V}{\partial \ell} \right) \right]^{3/2} \quad (5.3.1)$$

$$q^\ell = -c_0^2 \rho \left[\frac{\partial V}{\partial k} \right]^{1/2} \left[\frac{\partial}{\partial k} \left(\frac{\partial V}{\partial k} \right) \right]^{3/2}$$

where q^ℓ is the q along a k line, but differenced with respect to ℓ ; i.e., q^2 and q^4 . Also q^k is along an ℓ line; q^1 and q^3 . The quantity V is the speed

$$V = |\vec{V}| = |V_R \hat{r} + V_Z \hat{k}|$$

The partial derivatives are defined as follows

$$\frac{\partial V}{\partial \ell} \equiv \frac{\vec{x}_k \cdot \vec{v}_\ell}{|\vec{x}_k|} \quad \frac{\partial V}{\partial k} \equiv \frac{\vec{x}_\ell \cdot \vec{v}_k}{|\vec{x}_\ell|} \quad (5.3.2)$$

where $\vec{x} \equiv Z\hat{r} - R\hat{k}$, and the subscript refers to differentiation with respect to that variable.

Since the differencing of Eq. (5.3.1), using Eq. (5.3.2) is fairly messy, and also given in detail in Schulz's papers, it will not be repeated here.

Figure 5.3.1. Lagrangian zones in R, Z space, showing the position of the tensor artificial viscosity terms.

APPENDIX 4: ENERGY LOSS RATE EQUATION

The usual starting point for calculating the energy loss (or gain) of an energetic ion to a Maxwellian plasma of density n_p is with the equation.^{13,29,32,33}

$$-\frac{dE_1}{dt} = \frac{4\pi n_p z_1^2 z_p^2 e^4 \ln \Lambda}{m_p v_1} \left[\phi - \frac{m_p}{\nu} y \phi' \right] \quad (5.4.1)$$

where

$$\phi = \text{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} dx$$

$$y = \frac{m_p}{m_1} \frac{E_1}{K T_p} = \frac{3}{2} \frac{v_1^2}{\langle v_p^2 \rangle}$$

$$\frac{1}{\nu} = \frac{1}{m_1} + \frac{1}{m_p}$$

and where the subscript 1 refers to the energetic ion and the subscript p refers to the Maxwellian plasma. These equations will now be analyzed for the specific cases where $v_1 \gg v_p$ and $v_1 \ll v_p$.

A velocity dependent coulomb logarithm by Cooper³⁴ was used for $\ln \Lambda$ in the equations described here.

Case 1 ($v_1 \ll v_p$)

If we consider a high energy ion slowing down in a Maxwellian of electrons, then $v_1 \ll v_p$ for cases where the ion is in the low MeV range and the electron temperature is greater than 1 keV. When this is

the case then $y^2 \ll 1$ and ϕ and ϕ' from Eq. (5.4.1) can be simplified.

$$\phi = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} dx \approx \frac{2}{\sqrt{\pi}} \left(y - \frac{1}{3} y^3 \right)$$

and

$$y \phi' = \frac{2}{\sqrt{\pi}} (y - y^3)$$

Substituting the above into Eq. (5.4.1) gives

$$\left(\frac{dE_1}{dt} \right)_e = \frac{8 \sqrt{\pi} n_e Z_1^2 e^4 \ln \Lambda_e}{\sqrt{2} m_1} \sqrt{\frac{m_e}{KT_e}} \left(1 - \frac{2}{3} \frac{E_1}{KT_e} \right)$$

We note that

$$\langle v_e \rangle = \sqrt{\frac{8KT_e}{\pi m_e}}$$

therefore

$$\left(\frac{dE_1}{dt} \right)_e = \frac{16 n_e Z_1^2 e^4 \ln \Lambda_e}{m_1 \langle v_e \rangle} \left(1 - \frac{2E_1}{3KT_e} \right) \quad (5.4.2)$$

We visually note that for most of the energetic ion's lifetime Eq. (5.4.2) is negative since $E_1 > \frac{3}{2} KT_e$. When $E_1 < \frac{3}{2} KT_e$ the equation becomes positive, but the range of the ion once it reaches the electron thermal energy is very small compared to the total range. Therefore since $E_1 > \frac{3}{2} KT_e$ for most of the ion's range, the factor of 1 in Eq. (5.4.2) is usually dropped. This results in the form

$$\left(\frac{dE_1}{dt} \right)_e = - \frac{32 n_e Z_1^2 e^4}{3 m_1 \langle v_e \rangle} \left(\frac{E_1}{KT_e} \right) \ln \Lambda_e \quad (5.4.3)$$

Case 2 ($v_1 \gg v_p$)

If we consider a high energy ion slowing down in a Maxwellian of ions then $v_1 \gg v_p$ for most of the range. In this case $y^2 \gg 1$, therefore the bracketed part of Eq. (5.4.1) becomes

$$\phi - \frac{m_i}{\mu} y \phi' = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} dx - \left(1 + \frac{m_i}{m_1}\right) y e^{-y^2}$$

In the limit as $y \rightarrow \infty$, the above goes to 1. Therefore

$$\left(\frac{dE_1}{dt}\right)_i = - \frac{4\pi n_i Z_1^2 Z_i^2 e^4 \ln \Lambda_i}{m_i v_1} \quad (5.4.4)$$

This is the desired form of the equation for a single ion fluid Maxwellian.

For a multi ion fluid

$$\left(\frac{dE_1}{dt}\right)_i = - \frac{4\pi e^4 Z_1^2}{v_1} \ln \Lambda_i \sum_{i=1}^N \frac{n_i Z_i^2}{m_i} \quad (5.4.5)$$

where N is the total number of Maxwellian ion species.

The total energy loss to the energetic ion is just the sum of Eqs. (5.4.3) and (5.4.5).

$$\frac{dE_1}{dt} = \left(\frac{dE_1}{dt}\right)_e + \sum_{i=1}^N \left(\frac{dE_1}{dt}\right)_i \quad (5.4.6)$$

Equation (5.4.6) can now be integrated to obtain the energy losses to the Monte Carlo ion bundles due to the small angle coulomb collisions (Section 3.2).

APPENDIX 5: TRACKING IN A 2D LAGRANGIAN CYLINDRICAL MESH

In doing particle simulations one needs to push a particle through a coordinate mesh. As explained in Section 3.1, given a Δt one can calculate a new velocity $\vec{v}$ and a new position $\vec{X}$ for a particle provided one knows the equation of motion. The tracking of a particle in a 2D Lagrangian (quadrilateral) mesh was programmed in cartesian coordinates, hence the elemental distance ($\Delta\vec{X}$) a particle moves in some given Δt is a straight line, i.e., the curved orbital path of the ion is composed of many short straight line segments. Also since variables change from zone to zone it is necessary to guarantee that a chosen Δt does not carry a particle beyond the boundaries of the zone it was in. Instead a particle is advanced just to the boundary and the zonal parameters in the equation of motion are changed accordingly. Then the particle is allowed to enter the new zone and continue on its way. The scheme used and about to be described was modeled from one proposed by the late Calvin Gardner³⁵.

Two important calculations must be made to do the tracking (particle pushing): first a coordinate transformation is made on the velocity vector to simplify the tracking and second, the distance to the zone boundary is calculated. Doing the coordinate transformation also greatly simplifies the distance to boundary calculation.

The Monte Carlo bundle has a cartesian 3D velocity and position.

$$\begin{aligned}\vec{X} &= x_0\hat{i} + y_0\hat{j} + z_0\hat{k} \\ \vec{v} &= v_x\hat{i} + v_y\hat{j} + v_z\hat{k}\end{aligned}\tag{5.5.1}$$

but because of cylindrical symmetry a coordinate transformation can be performed which essentially reduces the velocity to two dimensions. Figure 5.5.1a shows the projection of $\vec{v}$ in the R-Z plane and Fig. 5.5.1b shows the projection of $\vec{v}$ in a constant z plane (x, y plane). Since there is no θ dependence in the variables, the cylinder can be rotated such that v_x goes to zero and v_y is positive; Fig 5.5.1c. The motion is now confined to a y-z plane provided the track is linear, which it is for each elemental $\Delta\vec{x}$. At the end of each $\Delta\vec{x}$ a particle will deflect out of the y-z plane due to a rotation from the Lorentz force or a collision. Therefore a coordinate rotation is done after each time step while tracking each particle. After rotation the particle has a new position and velocity

$$\begin{aligned}\vec{x}' &= x_0' \hat{i} + y_0' \hat{j} + z_0' \hat{k} \\ \vec{v}' &= v_y' \hat{j} + v_z' \hat{k}\end{aligned}\tag{5.5.2}$$

The rotation is done using the following procedure.

$$\begin{aligned}\alpha &= \frac{v_x}{v} \quad ; \quad \beta = \frac{v_y}{v} \quad , \quad \gamma = \frac{v_z}{v} \\ \alpha' &= 0 \quad ; \quad \gamma' = \gamma \quad ; \quad \beta' = \sqrt{1 - \gamma^2} \\ x_0' &= (\beta x_0 - \alpha y_0) / \beta' \\ y_0' &= (\alpha x_0 + \beta y_0) / \beta' \\ z_0' &= z_0 \quad ; \quad v_x' = 0 \\ v_y' &= \beta' v \quad ; \quad v_z' = v_z\end{aligned}\tag{5.5.3}$$

where α , β , and γ are the usual direction cosines and the prime superscript refers to the new coordinate frame. Note that v , the speed, remains constant in the rotation.

The problem now is to calculate the distance to boundary along the straight line trajectory of the velocity vector in this y - z plane.

The straight line segments in the R - Z plane that define a Lagrangian zone are really conic sections in the cylinder -- see Fig. 5.5.2a. From Fig. 5.5.2a, b, c, it can be seen that the intersection of the surface generated by the line 1-2 and a y - z plane is a curved line -- a hyperbola. Hence the distance to boundary calculation is the intersection of the velocity vector projection with a hyperbola. Since there are four sides to a zone and the particle doesn't know which one it will hit, one must look at the intersection of the velocity vector with the 4 hyperbolas generated by the 4 zone sides.

Without going into the algebra, the distance to boundary for one of the four sides is given by

$$L = \frac{SK + \frac{\beta'}{\gamma'} y'_0 \pm \sqrt{\left[S^2 - \left(\frac{\beta'}{\gamma'}\right)^2\right] x_0'^2 + \left[\frac{\beta'}{\gamma'} K + S y'_0\right]^2}}{\gamma' \left[S^2 - \left(\frac{\beta'}{\gamma'}\right)^2\right]} \quad (5.5.4)$$

where

$$S = \frac{R_1 - R_2}{Z_1 - Z_2} \quad \text{and} \quad K = S(Z_2 - Z_0') - R_2$$

and where (R_1, Z_1) , (R_2, Z_2) are the cylindrical coordinates of a Lagrangian line element. This equation is a quadratic and yields two solutions, and

since this calculation must be done for all four sides of the zone, eight solutions for λ are obtained. The smallest, positive, real solution is the valid one.

Having calculated the distance to boundary, the ion bundle can be advanced in the y - z plane the appropriate $\Delta \vec{x}$ -- the distance to boundary or the distance calculated from the Lorentz force for the specified Δt , whichever is smaller.

5.5.1a

5.5.1b

5.5.1c

Figure 5.5.1a,b,c. A particle velocity vector in cylindrical coordinates (Fig. a,b); and after a coordinate transformation (Fig. c).

5.5.2a

5.5.2b

5.5.2c

Figure 5.5.2a,b,c. A Lagrangian line element (Fig. a) represents a conic surface of revolution (Fig. b). The intersection of a y - z plane with the conic surface is a hyperbola (Fig. b).

APPENDIX 6: MONTE CARLO TECHNIQUES

A rough outline of the Monte Carlo process might be summarized as follows:

1. A source of non-Maxwellian energetic ions must exist in the physical system being simulated.
2. This source of ions is subdivided into N bundles, where N is called the sample size. The determination of N will be discussed below.
3. The bundles are given an initial position, velocity vector, etc., that completely describe the bundle.
4. Bundles are now tracked and suffer collisions for a series of minor Δt 's until a major Δt is reached. At the end of the major Δt , the particle is stored away on disc (census). Another bundle is now tracked. When all bundles have been tracked for the major Δt , the code advances the other pieces of physics (MHD) for the major Δt . When this is completed a new major Δt is started; new source particles may be generated, and the census particles are retrieved for further tracking.

A critically important parameter in running any Monte Carlo calculation is the determination of N. It must be large enough such that the cumulative history of the bundles is representative of the problem, but small enough to be practical to run. In this model N was determined automatically within the code and was constantly varying depending on the source strength.

$$N = \text{Integer part of } \left\{ \frac{E_s}{E_0} \right\} \quad (5.6.1)$$

where E_s is the source energy and E_0 is an input parameter. In other words E_0 is approximately the energy of the Monte Carlo bundles to be tracked. The weight is the actual number of ions within the bundle. A simple example may help.

Suppose in an actual source we had 10^{20} alpha particles, each of 2 MeV energy. The total energy of the source is thus 2×10^{20} MeV. Now suppose the user decides that he doesn't want Monte Carlo bundles roaming around his problem with energies greater than 10^{17} MeV. Then he would set $E_0 = 10^{17}$ and N would be calculated to be 2000; i.e., the code would track 2000 bundles, each of 10^{17} MeV. Since the weight is the actual number of alphas in the bundle

$$WT = \frac{\text{bundle energy}}{\text{ion energy}} = \frac{10^{17} \text{ MeV}}{2 \text{ MeV}} = 5 \times 10^{16}$$

The sample size was determined in this way to avoid having very energetic bundles traveling through the mesh with the potential to wreak havoc with a small zone. Also N is a function of the source; you don't want to generate a large N when the source is negligible or off. If the source is substantial and if N is small, then it is quite possible to have bundles (generated in a large zone) that are larger in mass and energy than another zone. And if this bundle should interact with this small zone, then the entire energy and mass of the small zone could be depleted -- causing disaster. Normally one would set E_0 to be equal to some fraction of the internal energy of the smallest zone. Thus all bundles would be assured of being small enough to not create too much trouble.

There is one problem with this approach. If E_0 is based upon the smallest zone, and if there are also many large zones, then one ends up with a very large number of small bundles. This problem is easily overcome by splitting bundles when they pass into small zones, or randomly throwing out bundles when they pass into large zones (Russian Roulette). When playing Russian Roulette, one must multiply the surviving bundles weight and energy by an appropriate factor to conserve energy, mass and momentum. It is only conserved on the average.

Because the calculation of N was a function of E_s , the sample size can grow without bound as the source grows. But machine limitations force an upper maximum of N to be approximately 5×10^5 for a time step. Practically though, a "reasonable" value of N (for an entire mesh -- over a single Δt) would be approximately 5×10^4 bundles. A CDC 7600 computer was able to process this many bundles for a single major time step in one to two minutes of CPU time. Monte Carlo can be expensive!

There are obviously lots of ways one may determine a sample size criteria for a Monte Carlo calculation, but this method seemed to be fairly simple and trouble free. Of course what it boils down to is that one wants a sample size that is somewhere between the regions of nonsense (N too small) and non-affordability (N too large).

APPENDIX 7: ENERGETIC ION SOURCES FOR MONTE CARLO MODEL

The energetic ions of the Monte Carlo model may come from one or from several programmed sources, depending on the problem. One may generate the problem with the ions already in the problem. In other words, the particles may exist within the problem when the problem is started. Another source may be an externally injected beam of neutralized ions. By neutralized, it is meant that the ion beam being injected into the plasma has free companion electrons traveling along with it. The ion beam description is supplied by the user, where any ion of $Z \leq 2$ may be specified. It is not necessary to go into details, but in a Monte Carlo model it is quite easy to build very complicated ion beams; such as an anisotropic, mixed isotope, time and energy dependent source. A third source of Monte Carlo particles is one that has already been mentioned; the scattered target particles from a Monte Carlo event (see Section 3.3). This is a secondary source, in that it takes other Monte Carlo particles to create them.

The principal source of the Monte Carlo, non-Maxwellian energetic ions modeled was the thermonuclear reaction products of a burning Maxwellian plasma. Accommodations were made to simulate the following reactions

Knowing the Maxwellian averaged cross sections, the ion temperature (T_i) and the ion densities, the reaction rates (R) are simply calculated between the i^{th} and j^{th} species

$$R_{ij} = n_i n_j \langle \sigma v \rangle_{i-j} \quad (5.7.5)$$

and when $i = j$

$$R_{ii} = \frac{1}{2} n_i^2 \langle \sigma v \rangle_{i-i}$$

The Maxwell averaged cross sections were tabulated from Greene⁵, as a function of T_i . Multiplying Eq. (5.7.5) by a zone's volume and a time step gives the actual number of reactions that took place, and the actual number of the reaction products in that zone. These reaction products are then grouped into representative bundles, given an appropriate energy, a weight, isotropic scattering angles, and a random initial position within the zone. Now they are Monte Carlo bundles of energetic ions and the tracking can proceed.

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