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Derivation of a Numerical Method for Computing 3-D Magnetoplasmadynamic Flows in Thermodynamic Non-equilibrium

Caroline Cecile Marcelle Liron
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Derivation of a Numerical Method for Computing 3-D Magnetoplasmadynamic Flows in Thermodynamic Non-equilibrium

by

Caroline Cécile Marcelle Liron

Thesis

Presented to the Faculty of the Graduate School of Embry-Riddle Aeronautical University in Partial Fulfillment of the Requirements for the Degree of Master of Science in Aerospace Engineering

Embry-Riddle Aeronautical University
Daytona Beach, Florida
May 2005
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Derivation of a Numerical Method for Computing
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Thermodynamic Non-equilibrium

by
Caroline Cécile Marcelle Liron, B.S.
on April 25th, 2005

This thesis was prepared under the direction of the candidate's thesis committee chairman, Dr. Eric Perrell, Department of Aerospace Engineering, and has been approved by the members of his thesis committee. It was submitted to the Aerospace Engineering Department and was accepted in partial fulfillment of the requirements for the degree of Master of Science in Aerospace Engineering.

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Aerospace Engineering Department Chair
For my Brother, my Dad and my Mom

“What we need are more people who specialize in the impossible.”

Theodore Roethke
(American Poet)
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Thank you.
ABSTRACT

Derivation of a Numerical Method for Computing 3-D Magnetoplasmadynamic Flows in Thermodynamic Non-equilibrium

by
Caroline Cécile Marcelle Liron, M.S.A.E.
Embry-Riddle Aeronautical University, 2005
SUPERVISOR: Dr. Eric R. Perrell

Various models exist for the propulsion concept using magnetohydrodynamics (MHD). Various authors, such as Powell, Canupp, Candler, and MacCormack have dealt with issues of solving the magnetic field induction equations simultaneously with Navier-Stokes equations using Computational Fluid Dynamics (CFD). Although most authors deal with species non-equilibrium and thermal non-equilibrium, a new emphasis is set to study the impact of electrons with the electron energy and the electronic excitation energy, as well as a complex energy non-equilibrium.

This thesis presents the derivation of a numerical method for computing 3-D MHD flows for the purpose of modeling steady-state magnetoplasmadynamic thrusters (MPDT). It details the derivations of each equation: both Navier-Stokes and the induction equation when the magnetic term is treated as a body force and the electron pressure as a surface force. The method of flux vector splitting has been chosen to solve the set of $ns + 12$ equations, $ns$ being the number of heavy particles involved in the flow. In addition, it presents the mathematical issues encountered in using this method. The first part of the method has been solved, finding the conserved variables, flux vectors, flux vector Jacobian, and eigenvalues.
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NOMENCLATURE

Note: **Bold characters** indicate vectors, except as noted

**English Symbols (SI unit)**

- $A$: flux-vector Jacobian square matrix
- $A_x$: expanded flux-vector Jacobian square matrix
- $A_p$: Powell’s flux-vector Jacobian square matrix
- $a$: acceleration ($\text{m/s}^2$)
- $\dot{a}$: homogeneity variable
- $B = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}$: magnetic field (T)
- $c_f, c_s$: fast and slow magnetoacoustic wave speeds ($\text{m/s}$)
- $c_v$: specific heat at constant volume ($\text{m}^2 \text{s}^{-2} \text{K}^{-1}$)
- $E$: electric field ($\text{V/m}$)
- $E_{\text{elec}}$: electron energy per unit volume ($\text{J/m}^3$)
- $E_{\text{elec-elec}}$: electron-electronic energy per unit volume ($\text{J/m}^3$)
- $E_r$: rotational energy per unit volume ($\text{J/m}^3$)
- $E_t$: total energy ($\text{J}$)
- $E_i$: vibrational energy per unit volume ($\text{J/m}^3$)
- $e_{\text{elec}}$: electronic energy per unit mass ($\text{J/kg}$)
- $e_r$: rotational energy per unit mass ($\text{J/kg}$)
- $e_i$: vibrational energy per unit mass ($\text{J/kg}$)
\[ \mathbf{F}_{\text{fluxes}} = \begin{pmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{H} \end{pmatrix} \] vector of fluxes

- \( \mathbf{f}_b \) elementary body force – per unit volume (N/m\(^3\))
- \( \mathbf{f}_s \) elementary surface force – per unit surface (N/m\(^2\))
- \( h^0 \) enthalpy of formation (J/kg)
- \( I \) identity matrix
- \( j \) conduction current vector (A/m\(^2\))
- \( J \) electric current vector (A/m\(^2\))
- \( K_0 \) permittivity of vacuum (F/m)
- \( L \) left eigenvectors of flux Jacobian matrix
- \( m \) mass (kg)
- \( M \) molecular weight (kg/mol)
- \( p \) pressure (Pa)
- \( Q \) conserved variables
- \( R \) right eigenvectors of flux Jacobian matrix
- \( R_u \) universal gas constant (J mol\(^{-1}\)K\(^{-1}\))

\[ S = \text{Jacobian matrix} \frac{\partial \mathbf{V}}{\partial \mathbf{Q}} \]

\[ S^{-1} = \text{Jacobian matrix} \frac{\partial \mathbf{Q}}{\partial \mathbf{V}} \]

- \( t \) time (s)
- \( T \) temperature (K)

\[ \mathbf{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} \] velocity vector

- \( \mathbf{V} \) primitive variables
- \( v_\alpha \) General Alfvén velocity (m/s)

\( \mathbf{F}', \mathbf{G}', \mathbf{H}' \) general coordinate flux components
$w$ source vector
$x, y, z$ Cartesian coordinate directions (m)

**Greek Symbols (SI unit)**

$\beta$ phase angle with which the electric field lags the electron speed
$\delta_{ij}$ Kronecker delta
$\Lambda$ diagonal matrix of eigenvalues of flux Jacobian matrix
$\partial S$ boundary surface of the control volume
$\Delta t$ time step (s)
$\eta$ General coordinate direction (m)

viscosity (N s/m$^2$)
$\lambda$ eigenvalue of flux Jacobian matrix
$\mu_0$ magnetic permeability of vacuum (H/m)
$\nabla p$ (vector) – gradient of scalar $p$
$\nabla \cdot \mathbf{u}$ (scalar) – divergence of vector $\mathbf{u}$
$\nabla \times \mathbf{u}$ (vector) – curl of vector $\mathbf{u}$
$\rho$ mass density (kg/m$^3$)
$\sigma$ electrical conductivity ($\Omega^{-1}m^{-1}$)
$\xi$ General coordinate direction (m)
$\zeta$ General coordinate direction (m)
### Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( e, elec )</td>
<td>electron, electronic</td>
</tr>
<tr>
<td>( hp )</td>
<td>heavy particles</td>
</tr>
<tr>
<td>( I )</td>
<td>inviscid</td>
</tr>
<tr>
<td>( s )</td>
<td>denotes species ( s )</td>
</tr>
<tr>
<td>( V )</td>
<td>viscous</td>
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### Superscript

<table>
<thead>
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<th>Superscript</th>
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<tbody>
<tr>
<td>( ( \cdot )' )</td>
<td>denotes General coordinate system</td>
</tr>
<tr>
<td>( ( \cdot )^T )</td>
<td>denotes transpose of vector ( \cdot )</td>
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1 INTRODUCTION

1.1 Background

Magnetoplasmadynamic (MPD) modeling is important for the development of high performance propulsion systems for interplanetary travel. Electromagnetic acceleration of plasmas can be modeled with the MPD equations of motion if the collisional mean free path is small in comparison with the scale length of interest. There are a number of propulsion problems that can be successfully studied with such numerical approach, including fusion, arcjets, magnetohydrodynamic (MHD) nozzles, high Mach number reentry problems, as well as the MPD thruster (MPDT).

The MPDT has a high exhaust velocity (20 to 100 km/s), a high thrust density, and operates at high power levels (~1 MW)\(^1\). These attributes make the MPDT an attractive candidate for manned missions. Examples of such missions are deep-space explorations, rendezvous, and delivery of support payload.

An MPDT is a nozzle shaped structure with two electrodes. The anode is the nozzle-shaped outer structure surrounding a center cylindrical cathode. Current due to the electric field between the two electrodes induces the magnetic field. In some designs, a magnetic field is also applied externally. The interaction of the electric and magnetic fields in a conductive gas results in a Lorentz force, producing thrust. Electrical conductivity arises from arcs between the electrodes producing an ionized plasma from the propellant gas.

High-power MPDT development\(^2\) is currently underway at both the NASA Marshall Space Flight Center (MSFC) and the NASA Glenn Research Center (GRC). While the research at MSFC is presently aimed towards accurate integration of numerical simulations, GRC has achieved experiments of high-power systems using both self-induced magnetic fields and external magnetic fields. This thesis is closely linked to the numerical integration done at MSFC. Together with MSFC, we are
working on developing several numerical codes capable of simulating any propulsion system. Each code would represent one aspect of the propulsion system, e.g. structural behavior or fluid behavior.

This work particularly emphasizes the equations governing electromagnetic propulsion and their numerical solution. Specifically, we will develop our model using the 3-D magnetoplasmadynamic equations of motion. Significantly, Sutton and Biblarz\textsuperscript{1} note the main disadvantage of MPD as “difficult to simulate analytically”.

### 1.2 Previous Research

Current research related to MPD involves software simulations using computational fluid dynamics (CFD) as well as experimental measurements.

To this date, perhaps the most widely applied MPD software is MACH3, which was developed for the US Air Force starting in the mid 1980’s. MACH2, the 2-D version, is a time-marching MHD code solving for two dimensional and axisymmetric single fluid flows\textsuperscript{3}. The governing equations solved by MACH2 are continuity, momentum, electron and ion specific internal energy, and magnetic induction. As a newer version, MACH3, in addition to treating 3-dimensional flows, also includes the radiation energy density and elastic stress equations. The most significant addition to MACH3, however, is its dependence on the varying upstream conditions. Indeed, the operating conditions will influence the time-marching resolution.

To complement and validate software development, some experimental studies have been undertaken. In 1983, Burton \textit{et al}\textsuperscript{4} set up and tested pulsed argon and nitrogen MPD thrusters in order to create a performance database. In 1998, Choueiri and Ziemer\textsuperscript{5} extended this database by including other propellants more likely to find use in practice, such as hydrogen, deuterium and xenon. In 2003, again Choueiri \textit{et al}\textsuperscript{6} compared their experimental measurements with their own computer generated numerical results. They compared current contours, thrust values, velocity, voltage and power input to the plasma. Thrust is over-predicted by 8% then under-predicted by 7% when input current is increased from 12kA to 20kA. Current contours are well
predicted. However, the current contours validations are valid only where the continuum assumption applies. The single continuity equation solved by the code limits the regions where the code is valid. In any case, lack of data restricted comparisons in these regions. The results were satisfactory enough for them to compare other propellants and test the MPDT in other regimes.

The basis of such software development relies on the correct formulation of the governing equations. The governing equations for simple MPD flows have been known for some time. In 1965, Sutton and Sherman\textsuperscript{7} detail the derivations of all governing equations of an electromagnetic flow: mass, momentum, and energy conservation, plus the magnetic induction equation. The last equation is derived starting from Maxwell's equations. However, much latitude exists with regard to the assumptions (hence accuracy) made by individual researchers in formulating the governing equations for MPD studies. Additional equations arise from considerations of multiple species, heavy particles vs. free electrons, the number of dimensions, as well as which energies are considered in non-equilibrium. Each non-equilibrium variable is associated with its own equation. It is easy to see how complex a model can become if energies, most commonly vibrational, rotational, electron, electronic, and total energy are all set in non-equilibrium.

These latter considerations are not adequately addressed by the various mathematical models\textsuperscript{8 9 10 11} that exist for the MPD equations. However, modeling of these effects can be found within a substantial body of literature that addresses hypersonic flows, typically for air-breathing propulsion, and re-entry flow applications. It is again the energy modeling – also referred to as temperature modeling – that distinguishes each work, but also the separation of the electrons from the general flow. Candler\textsuperscript{12}, for example, models multiple species, free electrons, vibrational, and electronic non-equilibrium. However, because flows of interest include electrons, it is necessary to distinguish between the electron and electronic energies. Hatfield\textsuperscript{13} deals with the energy by increasing complexity in its modeling. He studies three, four, and five temperature models considering translational, vibrational, rotational, electron and electronic energies in various equilibrium
schemes. Results are usually similar. However, by consequently increasing the number of temperatures, results are more precise as to which fraction of the energy contributes to the final temperature. As Candler\textsuperscript{12} demonstrates, the setup of non-equilibrium vibrational temperature for individual species is not justified when the chemical species present in the gas have widely the same vibrational relaxation rates. Thus, his later research did not include vibrational non-equilibrium for each species but rather one general vibrational energy.

After choosing which physical phenomenon to study in non-equilibrium, setting up the equations can be straightforward. Nonetheless, solving the MPD equations numerically using modern upwind methods\textsuperscript{14-16} has raised two mathematical issues.

Again, Maxwell's equations are used to derive the magnetic induction equation. One of Maxwell's equations states the invariance of the magnetic divergence, $\nabla \cdot \mathbf{B} = 0$. This property introduces a line of zeroes in the flux Jacobian matrices (derivatives of the fluxes with respect to the conserved variables density, velocity, magnitudes of the magnetic field, and specific energies). This singularity results in an error during the numerical simulation. In order to bypass this matter, Powell, Roe, Myong, Gombosi, and De Zeeuw\textsuperscript{16} introduce a mathematical artifice. By introducing a new term proportional to $\nabla \cdot \mathbf{B}$ and incorporating it into the existing fluxes, the fluxes become non-zero analytically. However, due to the zero value of the divergence, the result remains the same. Thus, Powell \textit{et al} settle the singularity by creating a new non-singular matrix having the same results. This solution has been retained in many works.

The other mathematical problem is unique to a particular type of upwinding. MHD simulations are often solved using the flux vector splitting (FVS) method patterned after Steger and Warming\textsuperscript{17}. This method is favored by hypersonics researchers for its numerical stability and physical accuracy. In order for the method to give valid results, the fluxes need to be homogeneous in the first degree with respect to the conserved variables. Non-homogeneity is introduced by the magnetic induction equation, and can result from certain formulations of the molecular energies. For
example, holding vibrational and translational, or electron and electronic energies in equilibrium, introduces nonlinearities between the conserved variables and the pressures. Both Canupp\cite{Canupp} and MacCormack\cite{MacCormack} have addressed the magnetic induction equation by introducing a homogeneity variable $\alpha$, which when set to unity during resolution does not influence the results.

### 1.3 Approach

This thesis attempts to further derive and solve the governing equations in a manner as physically realistic, and mathematically rigorous, as possible. In particular, ionization and other thermodynamic phenomena, which have been studied for hypersonic flow applications, and which also typify MPD flows, are addressed, in addition to the obvious electromagnetic effects. This case is unique as it specifically treats electrons in non-equilibrium. Indeed, a five-temperature model is chosen, dealing with translational, vibrational, rotational, electron and electronic energies with their own respective temperatures. With the magnetic field components, this formulation yields a number of conserved variables equal to twelve plus the number of molecular and ionic species.

Fluxes of the conserved variables are modeled in an upwind fashion, using flux vector splitting patterned after Steger and Warming\cite{Steger}. First order homogeneity of the fluxes in the conserved variables, as required for flux vector splitting, is strictly enforced in the formulation of the problem. This property rarely is shown and actually verified in other works.

This thesis is split into four parts. In the first part, a general overview of the electric and magnetic field is given. The resulting force between the two interacting fields, known as the Lorentz force, is the acceleration mechanism used by the MPD thruster.

The second part is the main work - modeling of the case and the derivations of all the governing equations. Mass conservation is applied to each chemical species, both heavy particles and electrons. Momentum and magnetic field conservation are written
in three spatial coordinates. Since a five-temperature model is set up, five energy
equations are written. Heavy particle pressure and electron pressure are considered as
surface forces. The Lorentz force is regarded as a body force. As a result, the pressures
and Lorentz forces appear as momentum fluxes, and flow work terms in the electron
energy and total energy equations.

Finally, the third part referring to the resolution method of flux vector splitting is
detailed and applied up to the determination of the eigenvalues, or wave speeds, in a
general coordinate system. The derivation makes use of a simplifying transformation
from conservative to primitive variables, in constructing both the flux Jacobian and the
eigenvalues. Powell’s method of addressing the singularity in the flux Jacobian is
employed, as is MacCormack and Canupp’s method for restoring homogeneity to the
magnetic induction equations.
2 THE INDUCED MAGNETIC FIELD

The law of Biot-Savart relates the magnetic field to the currents that create it. Sketching a wire charged electrically by current \( I \), at any distance \( r \) away from the wire, the current \( I \) traveling through an infinitesimal wire length \( dl \) creates a differential magnetic field \( dB \) of amplitude:

\[
dB = \frac{\mu_0 I \, dl \times r}{4\pi \, r^2}
\]

where \( \mu_0 \) is the magnetic permeability of vacuum.

The direction of the created elementary magnetic \( dB \) field is both perpendicular to the wire and to the direction of the radius. It follows the right-hand rule with \( dl \) and \( r \) as sketched below:

![Diagram showing a wire creating a magnetic field](image)

Figure 2-1 Electrical wire creating a magnetic field

The superposition of all the current elements sum up to create the magnetic field at point A in Figure 2-1. Thus, the amplitude of the magnetic field is given by integrating over the entire wire length:

\[
B = \frac{\mu_0 I}{4\pi} \int \frac{dl \times r}{r^2}
\]
3 THE GOVERNING EQUATIONS

The governing equations reflect the basic principles that govern the evolution of the flow properties. In fluid dynamics, the most common properties are densities (also referred to as mass), velocity, and energies. Since this study focuses on the influence of the magnetic field and its resulting Lorentz force we must also consider Maxwell's equations.

3.1 Continuity

When a fluid is in motion, it must move in such a way that mass is conserved. Assuming no source terms, the equation translating this property is:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \] (3.1)

The charged particles involved in the MPD flow will include both heavy particles and electrons. The density includes both electrons and heavy particles.

\[ \rho = \rho_e + \sum_{s\neq e} \rho_s \] (3.2)

This work will assume non-equilibrium between all species densities, both heavy particles and electrons. Hence a conservation equation is written for each species \( s \), and for free electrons \( e \).

For \( 1 < s < n_s \):

\[ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = 0 \] (3.3)
For electrons,
\[ \frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}) = 0 \]  \hspace{1cm} (3.4)

3.2 Momentum Conservation

The momentum conservation equations for a viscous flow are commonly referred to as the Navier-Stokes equations. With the assumption of inviscid flow taken for this research, the Navier-Stokes equations are reduced to Euler's equations.

The derivation of the momentum equation for a 3-D inviscid-compressible flow including magnetic body forces follows. The starting equation is Newton's second law, which states that the sum of all forces equals the time rate of change of momentum. Let \( m \) refer to the mass and \( \mathbf{a} \) to the acceleration. Assuming the mass is constant, Newton's second law is written as:

\[ \text{Force} = ma \]  \hspace{1cm} (3.5)

In order to evaluate this relation for fluid motion, consider a flow field whose properties such as speed, temperature, and pressure vary in space and time. Consider a fixed finite control volume \( V \) shown below through which the flow field travels. The volume is delimited by a control surface \( S \).

Figure 3-1 Flow field - Control volume
The acceleration is obtained by integrating the rate of change of velocity over the volume:

\[ m \mathbf{a} = \int_V \frac{d (\rho \mathbf{u})}{dt} dV \]  

(3.6)

The force applied to a flow field combines both surface and volume forces, also respectively called pressure and body forces. The surface forces are the ones directly in contact with the control volume. Pressure and viscosity are the most common examples. These forces are localized. Body forces affect the body in its whole while having no direct contact with the control volume; the most common body force is gravity.

Thus the force term can be split into two new terms:

\[ \text{Force} = \text{force}_{\text{surface}} + \text{force}_{\text{volume}} \]  

(3.7)

We introduce the elementary surface and volume forces:

- \( f_s \): elementary surface force
- \( f_b \): elementary body force

In order to obtain the force, we integrate the elementary surface force \( f_s \) over the control surface \( S \) and the elementary body force \( f_b \) over the control volume \( V \):

\[ \text{Force} = \int_S f_s \, dS + \int_V f_b \, dV \]  

(3.8)

The pressure force is the summation over the control surface of the elementary surface force \( p_s \). Expressed in terms of static pressure and viscosity, this force is:

\[ p_s = \left[ p + \frac{2}{3} \eta (\nabla \cdot \mathbf{u}) \right] \delta_{ij} - \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(3.9)
where we introduce the Kronecker delta function:

\[ \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (3.10) \]

and \( p \) and \( \eta \) are the static pressure and viscosity, respectively.

As the flow is considered non-viscous in this research, the elemental pressure force \( p \) simply reduces to the pressure \( p \). Referring to Figure 3-1 on page 9, the pressure is applied inward toward the control surface, thus opposite to the vector \( dS \), and thus giving the negative sign in the integration process. We also introduce the electron pressure \( p_e \) which is treated the same way. The final pressure force \( f_i \) is a combination of both the pressure from heavy particles and the electron pressure. We so define static pressure as:

\[ p = p_e + \sum_{i \neq e} p_i \quad (3.11) \]

We thus write the total surface pressure as:

\[ \text{force}_{\text{surface}} = - \int_S p \, dS \quad (3.12) \]

Using Gauss’ gradient theorem to change each surface integral to volume integrals,

\[ \text{force}_{\text{surface}} = - \int_V \nabla p \, dV \quad (3.13) \]

Thus the equation of motion is rewritten in integral form as:

\[ \int_V \frac{d(\rho u)}{dt} \, dV = - \int_V \nabla p \, dV + \int_V f_s \, dV \quad (3.14) \]
Since the control volume is independent from any variable and all the functions are continuous, all the terms in the above equation can be combined on one side:

\[ \int \left( \frac{d(\rho \mathbf{u})}{dt} + \nabla p - f_b \right) \, dV = 0 \]  

(3.15)

If the integral of a continuous function is zero then the function itself is zero. We then have:

\[ \frac{d(\rho \mathbf{u})}{dt} + \nabla p - f_b = 0 \]  

(3.16)

Expanding the time derivative of the velocity using the general formula:

\[ \frac{d}{dt} (\ ) = \frac{\partial}{\partial t} (\ ) + \mathbf{u} \cdot \nabla (\ ) \]  

(3.17)

We conclude on the formulation of the equation of motion:

\[ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla (\rho \mathbf{u}) = -\nabla p + \mathbf{f}_b \]  

(3.18)

where

\[ \mathbf{uu} = \begin{pmatrix} u^2 & uv & uw \\ uv & v^2 & vw \\ uw & vw & w^2 \end{pmatrix} \]  

(3.19)

Let us now look at the body forces. If the fluid is at least partially ionized, then electric and magnetic fields will act as body forces on the fluid. MHD is the theoretical study of such motion when the Navier-Stokes equations are combined with some form of Maxwell’s equations to model the evolution of the fields.
When a particle with charge $q$ is in an environment where an electric field $E$ is present, the particle is subject to an electric force:

$$F_{\text{electric}} = qE$$ (3.20)

When the same charge $q$ travels through a magnetic field $B$ at a speed $u$, the particle is subject to Laplace's force:

$$F_{\text{Laplace}} = qu \times B$$ (3.21)

Again, when the same charge $q$ travels through an environment where both an electric field and a magnetic field exist, both forces combine to create Lorentz's force:

$$F_{\text{Lorentz}} = q(E + u \times B)$$ (3.22)

The Lorentz force can accelerate or decelerate an ionized particle. If directed in the right direction, this force can contribute to the thrust.

The elementary Lorentz force exerted on an electron is expressed as follows:

$$f_b = \rho_e E + J \times B$$ (3.23)

where:

- $E$ electric field
- $J$ electric current vector
- $B$ magnetic field

Magnetohydrodynamic equations are fairly complex. Two approximations are commonly used to simplify their resolution. These approximations are largely explained by Sutton and Sherman in their book entitled “Engineering Magnetohydrodynamics”. The main steps are retained in the following pages.
The first approximation is to neglect the effect of excess charge \( \rho_e \) on the current flow. By comparing the order of magnitude:

\[
\frac{\rho_e E}{J \times B} \approx \frac{K_0 V}{\sigma L} \approx 10^{-4}
\]  
(3.24)

where in this equation:

- \( K_0 \) permittivity of vacuum
- \( V \) characteristic velocity
- \( \sigma \) electrical conductivity
- \( L \) characteristic length

Thus, we neglect \( \rho_e E \) simplifying the body force to:

\[
f_0 = J \times B
\]
(3.25)

The next steps use Maxwell's equations – magnetic governing equations – to expand further the above equation into pressure and magnetic terms only.

Maxwell's equations can be found in any electromagnetic or MHD literature. They are:

\[
\nabla \cdot E = \frac{\rho_e}{K_0} \tag{3.26} \quad (a)
\]

\[
\nabla \cdot B = 0 \tag{3.27}
\]

\[
\nabla \times E = -\frac{\partial B}{\partial t} \tag{3.28}
\]

\[
\nabla \times B = \mu_0 \left( J + K_0 \frac{\partial E}{\partial t} + \nabla \times M_p \right) \tag{3.29} \quad (a)
\]

with \( \mu_0 \) and \( M_p \) are respectively the magnetic permeability of vacuum and the magnetization.
Neglecting magnetization and displacement current \( \left( \frac{\partial E}{\partial t} = 0 \right) \) (the approximations are again explained by Sutton and Sherman\(^7\)), Maxwell’s equations simplify to:

- **Gauss’ Law:** \( \nabla \cdot E = 0 \) (3.26) (b)
- \( \nabla \cdot B = 0 \) (3.27)
- **Faraday’s Law:** \( \nabla \times E = -\frac{\partial B}{\partial t} \) (3.28)
- **Ampere’s Law:** \( \nabla \times B = \mu_0 J \) (3.29) (b)

Combining Ampere’s Law with the current formulation of the body force:

\[
f_b = J \times B = \left( \frac{\nabla \times B}{\mu_0} \right) \times B
\]  

(3.30)

or:

\[
f_b = \frac{(\nabla \times B) \times B}{\mu_0}
\]  

(3.31)

We conclude on the formulation of the equation of motion for a compressible 3-D inviscid flow in the presence of a magnetic field and a pressure force:

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \frac{(\nabla \times B) \times B}{\mu_0}
\]  

(3.32)

In order to use computational fluid dynamics, we write the equation in the conservation form:

\[
\frac{\partial (\rho)}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = W
\]  

(3.33)

where \( W \) are the source terms.
An additional term is added to the previously written equation of motion,
\[
\frac{B (\nabla \cdot B)}{\mu_0}
\] (3.34)

This term simplifies the writing in conservation form as well as reinforces Equation (3.27) (no magnetic monopoles). Adding the term to the momentum equation will not change the result of the equation since the value of the term is null. On the other hand, it will ensure that the divergence of the magnetic field remains null during calculations. Equation (3.32) becomes:
\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \frac{(\nabla \times B) \times B}{\mu_0} + \frac{B (\nabla \cdot B)}{\mu_0}
\] (3.35)

Also, from non-commutivity of the cross product:
\[
(\nabla \times B) \times B = -B \times (\nabla \times B)
\] (3.36)

Factoring \(\mu_0\) and reorganizing terms, we have:
\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \frac{1}{\mu_0} \left( B (\nabla \cdot B) - B \times (\nabla \times B) \right)
\] (3.37)

Converting the first three terms to conservation form is straightforward. The following steps will cover the conversion of the last two terms into the conservation form, thus a formulation of:
\[
B (\nabla \cdot B) - B \times (\nabla \times B)
\] (3.38)
Using the expansion for the double cross-product:

\[
-B \times (\nabla \times B) = -B_y \times \left( \begin{array}{c} B_x \\ \frac{\partial}{\partial x} B_x \\ \frac{\partial}{\partial y} B_y \\ \frac{\partial}{\partial z} B_z \\ \end{array} \right)
\]

\[
= -B_y \left( \frac{\partial B_x}{\partial y} - \frac{\partial B_y}{\partial x} \right) + B_z \left( \frac{\partial B_y}{\partial z} - \frac{\partial B_z}{\partial y} \right) + B_x \left( \frac{\partial B_z}{\partial x} - \frac{\partial B_x}{\partial z} \right)
\]

\[
= -B_y \left( \frac{\partial B_x}{\partial y} - \frac{\partial B_y}{\partial x} \right) + B_z \left( \frac{\partial B_y}{\partial z} - \frac{\partial B_z}{\partial y} \right) + B_x \left( \frac{\partial B_z}{\partial x} - \frac{\partial B_x}{\partial z} \right)
\]

Treating only the \( x \)-component, Equation (3.38) is equivalent to:

\[
B_x \left( \frac{\partial B_x}{\partial x} + \frac{\partial B_y}{\partial y} + \frac{\partial B_z}{\partial z} \right) - B_y \left( \frac{\partial B_x}{\partial y} - \frac{\partial B_y}{\partial x} \right) + B_z \left( \frac{\partial B_y}{\partial z} - \frac{\partial B_z}{\partial y} \right) + B_y \left( \frac{\partial B_z}{\partial x} - \frac{\partial B_x}{\partial z} \right)
\]

Again, we add a term identically equal to zero by adding and subtracting \( B_x \frac{\partial B_x}{\partial x} \).

Rearranging terms yields:

\[
B_x \left( \frac{\partial B_x}{\partial x} + \frac{\partial B_y}{\partial y} + \frac{\partial B_z}{\partial z} \right) + \left( B_x \frac{\partial B_x}{\partial x} + B_y \frac{\partial B_y}{\partial y} + B_z \frac{\partial B_z}{\partial z} \right)
\]

\[
- \left[ B_x \frac{\partial B_x}{\partial x} + B_y \frac{\partial B_y}{\partial y} + B_z \frac{\partial B_z}{\partial z} \right]
\]
Using index notations, for the \( j \)-component:

\[
\sum_i \left( B_j \frac{\partial B_i}{\partial x_i} + B_i \frac{\partial B_j}{\partial x_i} \right) - \frac{1}{2} \frac{\partial B^2}{\partial x_j} \quad (3.44)
\]

where we define the magnitude of the magnetic field as:

\[
B^2 = B_x^2 + B_y^2 + B_z^2 \quad (3.45)
\]

We note that the first term can be reduced to:

\[
\sum_i \left( \frac{\partial B_j B_i}{\partial x_i} \right) \quad (3.46)
\]

The magnetic field term in the \( j \)-direction is then written as:

\[
\left( \frac{1}{\mu_0} (B \cdot \nabla B) - B \times (\nabla \times B) \right)_j = \frac{1}{\mu_0} \sum_i \left( \frac{\partial B_j B_i}{\partial x_i} \right) - \frac{1}{2 \mu_0} \frac{\partial B^2}{\partial x_j} \quad (3.47)
\]

We introduce a new notation:

\[
\frac{1}{\mu_0} \sum_i \left( \frac{\partial B_j B_i}{\partial x_i} \right) = \left( \nabla \cdot \frac{\mathbf{B B}}{\mu_0} \right)_j \quad (3.48)
\]

where

\[
\mathbf{B B} = \begin{pmatrix}
B_x^2 & B_x B_y & B_x B_z \\
B_y B_x & B_y^2 & B_y B_z \\
B_z B_x & B_z B_y & B_z^2
\end{pmatrix} \quad (3.49)
\]

Finally, recall the original 3-D \((x, y, z)\) momentum equation (3.37) and shift all terms to the left hand side:

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u u}) + \nabla p - \frac{1}{\mu_0} \left( \mathbf{B} \cdot \nabla \mathbf{B} - \mathbf{B} \times (\nabla \times \mathbf{B}) \right) = 0 \quad (3.50)
\]

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This transforms to the final vector notation:

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left( \rho \mathbf{u} \mathbf{u} + I \left( p + \frac{\mathbf{B}^2}{2\mu_0} \right) - \mathbf{B} \mathbf{B} \right) = 0$$  \hspace{1cm} (3.51)

Expanding the momentum equations, where again the components of the velocity vector \( \mathbf{u} \) are \( u, v, \) and \( w \) and the components of the magnetic field vector are \( B_x, B_y, \) and \( B_z \), the expressions are:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u u}{\partial x} + \frac{\partial \rho u v}{\partial y} + \frac{\partial \rho u w}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{\mu_0} \left( \frac{\partial B_x B_x}{\partial x} + \frac{\partial B_x B_y}{\partial y} + \frac{\partial B_x B_z}{\partial z} \right) - \frac{\partial}{\partial x} \left( \frac{\mathbf{B}^2 + \mathbf{B}_y^2 + \mathbf{B}_z^2}{2\mu_0} \right)$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \rho v u}{\partial x} + \frac{\partial \rho v v}{\partial y} + \frac{\partial \rho v w}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{\mu_0} \left( \frac{\partial B_y B_x}{\partial x} + \frac{\partial B_y B_y}{\partial y} + \frac{\partial B_y B_z}{\partial z} \right) - \frac{\partial}{\partial y} \left( \frac{\mathbf{B}^2 + \mathbf{B}_y^2 + \mathbf{B}_z^2}{2\mu_0} \right)$$

$$\frac{\partial \rho w}{\partial t} + \frac{\partial \rho w u}{\partial x} + \frac{\partial \rho w v}{\partial y} + \frac{\partial \rho w w}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{\mu_0} \left( \frac{\partial B_z B_x}{\partial x} + \frac{\partial B_z B_y}{\partial y} + \frac{\partial B_z B_z}{\partial z} \right) - \frac{\partial}{\partial z} \left( \frac{\mathbf{B}^2 + \mathbf{B}_y^2 + \mathbf{B}_z^2}{2\mu_0} \right)$$  \hspace{1cm} (3.52)

We conclude on the momentum equation written in conservation form:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + p + \frac{\mathbf{B}^2}{2\mu_0} \frac{B_x^2}{\mu_0} \right) + \frac{\partial}{\partial y} \left( \rho u v - \frac{\rho B_x B_y}{\mu_0} \right) + \frac{\partial}{\partial z} \left( \rho u w - \frac{\rho B_x B_z}{\mu_0} \right) = 0$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x} \left( \rho v u - \frac{\rho B_x B_y}{\mu_0} \right) + \frac{\partial}{\partial y} \left( \rho v^2 + p + \frac{\mathbf{B}^2}{2\mu_0} \frac{B_y^2}{\mu_0} \right) + \frac{\partial}{\partial z} \left( \rho v w - \frac{\rho B_y B_z}{\mu_0} \right) = 0$$

$$\frac{\partial \rho w}{\partial t} + \frac{\partial}{\partial x} \left( \rho w u - \frac{\rho B_x B_z}{\mu_0} \right) + \frac{\partial}{\partial y} \left( \rho w v - \frac{\rho B_y B_z}{\mu_0} \right) + \frac{\partial}{\partial z} \left( \rho w^2 + p + \frac{\mathbf{B}^2}{2\mu_0} \frac{B_z^2}{\mu_0} \right) = 0$$  \hspace{1cm} (3.53)

Again:

$$\mathbf{B}^2 = B_x^2 + B_y^2 + B_z^2$$  \hspace{1cm} (3.45)
3.3 Magnetic Induction Equation

We use the magnetic induction equation to advance the magnetic field. It relates the change of the magnetic field with respect to time due to the existence of the induced magnetic field. Again, referring to Faraday's Law:

\[
\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (3.28)
\]

In order to express the electric field \( \mathbf{E} \) function of known properties, we use Ohm’s law with ion slip neglected:

\[
\mathbf{j} = \sigma \left[ \mathbf{E} + \mathbf{u} \times \mathbf{B} - \beta (\mathbf{j} \times \mathbf{B}) \right] \quad (3.54)
\]

with:

- \( \sigma \) electrical conductivity
- \( \beta \) phase angle with which the electric field \( \mathbf{E} \) lags \( \mathbf{u} \), (electron speed)

The solution of Ohm’s Law for \( \mathbf{E} \) gives:

\[
\mathbf{E} = \frac{\mathbf{j}}{\sigma} - \mathbf{u} \times \mathbf{B} + \beta (\mathbf{j} \times \mathbf{B}) \quad (3.55)
\]

Using Ampere’s law to substitute for \( \mathbf{j} \):

\[
\mathbf{E} = \frac{\nabla \times \mathbf{B}}{\mu_0 \sigma} - \mathbf{u} \times \mathbf{B} + \beta \left( \frac{\nabla \times \mathbf{B}}{\mu_0} \times \mathbf{B} \right) \quad (3.56)
\]

Taking the curl of both sides of the equation:

\[
\nabla \times \mathbf{E} = \nabla \times \frac{\nabla \times \mathbf{B}}{\mu_0 \sigma} - \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla \times \beta \left( \frac{\nabla \times \mathbf{B}}{\mu_0} \times \mathbf{B} \right) \quad (3.57)
\]
Combining the above equation with Gauss’s Law, we conclude on the general induction equation:

\[
-\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left( \nabla \times \mathbf{B} \right) - \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla \times \beta \left( \frac{\nabla \times \mathbf{B}}{\mu_0} \times \mathbf{B} \right) \quad (3.58)
\]

or

\[
\frac{\partial \mathbf{B}}{\partial t} = -\frac{1}{\mu_0 \sigma} \nabla \times (\nabla \times \mathbf{B}) + \nabla \times (\mathbf{u} \times \mathbf{B}) - \frac{\beta}{\mu_0} \nabla \times ((\nabla \times \mathbf{B}) \times \mathbf{B}) \quad (3.59)
\]

\((1/\mu_0 \sigma) \nabla \times (\nabla \times \mathbf{B})\) and \((\beta/\mu_0) \nabla \times ((\nabla \times \mathbf{B}) \times \mathbf{B})\) are the resistive diffusion and Hall terms, respectively. Physically these terms permit fluid motion transverse to the magnetic field. Mathematically, they behave similarly to viscous diffusion in the momentum equation and thermal conduction in the energy equation. The diffusion term is significant when the conductivity is low, such as in low temperature partially ionized gases. The Hall term is important typically in low density, magnetized flows. While these terms may be important in certain classes of MHD problems including some regions of the flow field of an MPD thruster, the scope of this work is in developing the non-equilibrium flow solver with basic MHD. Thus, we will neglect these terms for the sake of simplicity, and future efforts can use our approach as a starting point for including finite conductivity and the Hall effect. Eliminating these terms leaves:

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) \quad (3.60)
\]
Again, we expand the equation to express it in the conservation form:

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B})
\]

\[
= \nabla \times \left( \begin{bmatrix} u \\ v \\ w \end{bmatrix} \times \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix} \right)
\]

\[
= \frac{\partial(uB_y-vB_x)}{\partial x} - \frac{\partial(wB_x-uB_z)}{\partial y} + \frac{\partial(vB_z-wB_y)}{\partial z} - \frac{\partial(uB_y-vB_x)}{\partial y} + \frac{\partial(wB_x-uB_z)}{\partial z} - \frac{\partial(vB_z-wB_y)}{\partial x}
\]

(3.61)

Using the same technique as in deriving the momentum conservation equation, we add and subtract \( \frac{\partial (\mathbf{u}, \mathbf{B})}{\partial x} \) in the \( j \)-direction, thus:

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left( \mathbf{u} \times \mathbf{B} \right)
\]

\[
= \frac{\partial(uB_y-vB_x)}{\partial x} + \frac{\partial(uB_y-vB_x)}{\partial y} + \frac{\partial(uB_y-vB_x)}{\partial z} + \frac{\partial(vB_z-wB_y)}{\partial x} + \frac{\partial(vB_z-wB_y)}{\partial y} + \frac{\partial(vB_z-wB_y)}{\partial z}
\]

(3.62)

In short notation, the induction equation can be written as:

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \cdot (\mathbf{u} \mathbf{B} - \mathbf{B} \mathbf{u})
\]

(3.63)

Setting all terms on the left hand side of the equal sign yields,

\[
\frac{\partial \mathbf{B}}{\partial t} - \nabla \cdot (\mathbf{u} \mathbf{B} - \mathbf{B} \mathbf{u}) = 0
\]

(3.64)
Inserting the negative sign in the parenthesis yields the final conservation form expression:

\[
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{B}u - u\mathbf{B}) = 0
\]  

(3.65)

where

\[
\mathbf{B}u - u\mathbf{B} = \begin{pmatrix}
u \mathbf{B}_x - B_x u & v \mathbf{B}_y - B_y u & w \mathbf{B}_z - B_z u \\
u \mathbf{B}_x - B_x v & v \mathbf{B}_y - B_y v & w \mathbf{B}_z - B_z v \\
u \mathbf{B}_x - B_x w & v \mathbf{B}_y - B_y w & w \mathbf{B}_z - B_z w 
\end{pmatrix}
\]

(3.66)

3.4 Energy Conservation

For energy conservation, the rule is that energy cannot be created or destroyed. Energy can only be added to, taken away from a system, or transferred between each component in a system.

The internal energy can be broken down into numerous independent kinds of energy. Depending on the accuracy wanted and/or the specific topic studied, various energies are combined. The composition of the species in a gas determines the modes of internal energies present. Here, in addition to translational energy, the nuclei and orbiting electrons – by their non-zero distance from the center of mass – create an energy of rotation, an energy of vibration and finally energies related to the electronic excitation. We will consider in non-equilibrium: molecular translational, rotational, vibrational, free electron translational, and electronic energies.
Referring to the control volume and control surface of Figure 3-1 on page 9, the integral form of the energy equation is:

$$\dot{Q} - \dot{W} = \int_V \int \left( \frac{\partial}{\partial t} (\rho \, e) \right) dV + \int_S \rho \, \mathbf{u} \cdot d\mathbf{S} \quad (3.67)$$

where

- $\dot{Q}$ heat added to the system
- $\dot{W}$ work done by the system

For the study of a flow field initiated by chemical reactions, we assume no heat added to the system and no work done by the system. The changes in energy are due to the actual reactions. Applying Gauss' gradient theorem – Equation (3.13) – we conclude on the energy equation:

$$\frac{\partial}{\partial t} (\rho \, e) + \nabla \cdot (\rho \, e \, \mathbf{u}) = 0 \quad (3.68)$$

### 3.4.1 Total Energy

The total energy $E_T$ regroups all energies previously mentioned – translational, vibrational, rotational, electron and electronic– as well as the kinetic energy of the heavy particles, and the chemical heat of formation. Note also that the magnetic field body forces accelerate the fluid, adding energy to the charged particles, thus the term magnetic energy term is required.

$$E_T = \sum_{i=1}^n \left( \rho_i c_i T_i \right) + E_v + E_r + E_e + E_{elec} + \ldots$$

$$+ \frac{\mathbf{u}^2 + \mathbf{v}^2 + \mathbf{w}^2}{2} \sum_{i=1}^n \rho_i \mathbf{c}_i^2 + \frac{B_i^2 + B_j^2 + B_z^2}{2\mu_0} \sum_{i=1}^n \rho_i \mathbf{h}_i^0 \quad (3.69)$$

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We recast the translational energy in terms of pressure, rather than temperature, using the ideal gas law. This will be useful later, since the pressures appear in expressions for the fluxes. From the original expression of the static pressure, or pressure of the mixture,

\[ p = p_e + \sum_{i \in g} \rho_i \frac{R}{M_i} T \]  \hspace{1cm} (3.70)

then

\[ T = \frac{p - p_e}{\sum_{i \in g} \rho_i \frac{R}{M_i}} \]  \hspace{1cm} (3.71)

The final expression of the total energy expressed as a function of pressure is:

\[ E_T = \sum_{i \in g} \left( \rho_i c_{v_i} \right) \left( p - p_e \right) + E_v + E_r + E_e + E_{elec} + \ldots \]

\[ \begin{align*}
   &+ \frac{u^2 + v^2 + w^2}{2} \sum_{i \in g} \rho_i^2 + \frac{B_x^2 + B_y^2 + B_z^2}{2\mu_0} + \sum_{i \in g} \rho_i h_i^0 
\end{align*} \]  \hspace{1cm} (3.72)

It is interesting to note that the specific heat at constant volume as written in this case only treats the translational energy. Other researchers combine both effects of rotational and translational in this variable. As the rotational energy is treated in non-equilibrium as well, the need to include it again in the specific heat is unnecessary.

Following Powell et al\textsuperscript{16} and Canupp\textsuperscript{18}, the total energy governing equation becomes:

\[ \frac{\partial}{\partial t} (E_T) + \nabla \cdot \left( \left( E_T + p + \frac{B^2}{2\mu_0} \right) u - \frac{B_j}{\mu_0} (u \cdot B) \right) = 0 \]  \hspace{1cm} (3.73)

This formulation illustrates the work done with both magnetic forces and pressure forces.

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3.4.2 Vibrational and Rotational Energies

Vibrational and rotational non-equilibrium are included for completeness. Their importance to the solution of an MPD thruster flow field is not known a priori. It is expected that the propellant molecules will fully dissociate within a short time of entering the chamber, so those energies will be negligible for the most part. Note that Candler treats the vibrational energy as being in non-equilibrium for each species. In other words, each species has a specific vibrational temperature. Nevertheless, Candler concludes that a model using only one vibrational temperature is adequate, as long as the gas consists of chemical species having similar vibrational relaxation rates.

Based on his conclusion, our model will couple the vibrational and rotational energies, $E_v$ and $E_r$, to one vibrational temperature and one rotational temperature, respectively.

Relating them only to their per unit mass equivalent, we have

$$E_v = e \sum_{s \neq e} \rho_s$$

(3.74)

$$E_r = e \sum_{s \neq e} \rho_s$$

(3.75)

Note here that electrons do not have these energy modes, therefore, the density only refers to heavy particles. For further reference to the different variables, note also that

$$\rho = \sum_{s \neq e} \rho_s + \rho_e$$

(3.76)

Using Equation (3.68), both equations written in the conservation form are

$$\frac{\partial}{\partial t} (E_r) + \nabla \left( (\rho - \rho_e) e \mathbf{u} \right) = 0$$

(3.77)

$$\frac{\partial}{\partial t} (E_v) + \nabla \left( (\rho - \rho_e) e \mathbf{u} \right) = 0$$

(3.78)
3.4.3 Electron Energy and Electronic Energy

The electron and electronic energies express the energy of free electrons as well as the energy of the electronic cloud – referring to the energy of the electrons orbiting around each heavy particle.

Again, previous works have dealt very differently with the energies associated with electrons. This energy can be split into specific energies: the translational energy of the free electrons, the kinetic energy of the bulk electron fluid, and finally the energy of the electronic cloud.

\[ E_{e+elec} = E_{\text{trans}} + E_{\text{kin}} + E_{\text{elec}} \]

\[ E_{e+elec} = \frac{P_e}{\gamma} + \frac{E_{\text{kin}}}{2} + \rho_{\text{elec}} \sum \rho_i \]

As for the electron translational energy, it is simply expressed as a function of the electron pressure using the perfect gas relation applied to electrons:

\[ p_e = \rho_e R_e T_e \]

then

\[ \rho_e c_v T_e = \frac{c_v}{R_e} p_e \]
Again, this refers only to the translational energy of the electron. Applying the
principle of equipartition of energy\(^2\) to simplify the ratio of specific heat to gas
constant, with three degrees of freedom:

\[
\rho_e c_v T_e = \frac{3}{2} p_e
\]  

(3.83)
yielding the final version of the electron-electronic energy,

\[
E_{elec} = \frac{3}{2} p_e + \frac{\rho_e}{2} (u^2 + v^2 + w^2) + e_{elec} \sum \rho_i
\]  

(3.84)

The model used to represent the energies linked to the electrons has been the main
issue in deriving fully the governing equations for an MPD thruster.

Candler’s formulation\(^12\) of the model considers non-equilibrium between
translational electron energy \(E_e\) and molecular translational energy. The electronic
energy \(E_{elec}\) is included in the total energy. It is considered to be in equilibrium with
the free electron energy \(E_e\). However, it is not included with the electron energy. The
electronic energy is thus grouped with the heavy particle energy modes, effectively
setting it independent of the electronic excitation. Thus, Candler’s equilibrium
treatment of the electron and electronic energies is something of a numerical artifice.
Strictly speaking, it is not physically correct. We expect this formulation to be
increasingly non-physical in works which follow this idea of constructing source terms
for molecular energy exchange.

However, attempts to model this correctly by grouping \(E_e\) and \(E_{elec}\) in the same
energy pool lead to a mathematical difficulty in the properties of the fluxes (see
Section 4.5.2.1 Homogeneity Criteria page 41). Candler’s formulation, along with his
further assumption (also not strictly correct) that the electron pressure is independent
of the electronic energy, circumvents this difficulty. To make the work mathematically
correct and ensure homogeneity of the fluxes, the electronic excitation state also needs
to be in non-equilibrium.
It was decided for this case that non-equilibrium is assumed between the electron energy and the electronic excitation energy. The electron energy and the electronic energy are not grouped with heavy particles, but are instead evaluated on their own.

Mathematically,
\[ E_{elec} = E_{elec} + E_e \]  \hspace{1cm} (3.85)

with each specific energy written as:
\[ E_{elec} = e_{elec} \sum_{s \neq e} \rho_s \]  \hspace{1cm} (3.86)
\[ E_e = \frac{3}{2} p_e + \frac{\rho_e}{2} (u^2 + v^2 + w^2) \]  \hspace{1cm} (3.87)

Regarding the equations, the electronic conservation energy is written as:
\[ \frac{\partial}{\partial t}(E_{elec}) + \nabla \cdot (E_{elec} \mathbf{u}) = 0 \]  \hspace{1cm} (3.88)

Taking into account both magnetic “pressure” and electron pressure, we conclude on the electron conservation energy governing equation:
\[ \frac{\partial}{\partial t}(E_e) + \nabla \cdot \left( E_e + p_e + \frac{B^2}{2\mu_0} \right) \mathbf{u} - \frac{B^2}{\mu_0} (\mathbf{u} \cdot \mathbf{B}) = 0 \]  \hspace{1cm} (3.89)

### 3.5 Summary of Governing Equations

This section regroups all the differential equations governing the flow studied in this case, each written in vector form.

We assume non-equilibrium for species densities. Thus, there is one continuity equation for each of the \( n_s \) chemical species.
\[ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = 0 \]  \hspace{1cm} (3.1) (a)
This also applies to the electrons.

\[
\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}) = 0 
\]  

(3.1) (b)

The momentum equation will yield one equation in each of the three dimensional directions.

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left( \rho \mathbf{u} \mathbf{u} + I \left( p + \frac{\mathbf{B}^2}{2 \mu_0} \right) - \frac{\mathbf{B} \times \mathbf{B}}{\mu_0} \right) = 0 
\]  

(3.51)

Also for the magnetic field equations, there will be one for each dimensional direction.

\[
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{B} \mathbf{u} - \mathbf{u} \mathbf{B}) = 0 
\]  

(3.65)

There are three simple conservation equations of independent energy for the modes of molecular energy not associated with a pressure, one for rotational, one for vibrational, and one for electronic.

\[
\frac{\partial}{\partial t} \left( (\rho - \rho_e) e_{r\text{rot}} \right) + \nabla \left( (\rho - \rho_e) e_{r\text{rot}} \mathbf{u} \right) = 0 
\]  

(3.68) (b)

The conservation of the electron energy is written as:

\[
\frac{\partial}{\partial t} (E_e) + \nabla \left( E_e + p_e + \frac{\mathbf{B}^2}{2 \mu_0} \right) \mathbf{u} - \frac{\mathbf{B} \times \mathbf{B}}{\mu_0} \mathbf{u} = 0 
\]  

(3.89)

Finally, the conservation of total energy equation is:

\[
\frac{\partial}{\partial t} (E_T) + \nabla \left( E_T + p + \frac{\mathbf{B}^2}{2 \mu_0} \right) \mathbf{u} - \frac{\mathbf{B} \times \mathbf{B}}{\mu_0} \mathbf{u} = 0 
\]  

(3.90)

Considering all the non-equilibrium assumptions, the flow field is represented by \( ns + 12 \) equations. The resolution method is explained in the following chapter.
4 NUMERICAL RESOLUTION

4.1 Formulating the Problem in One Equation

Again, the equations governing the flow motion are the Euler equations. These equations can be written in the conservation form referred to in Section 3.2 Momentum Conservation page 9. We further condense the conservation form using vector notation:

\[
\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = W \tag{4.1}
\]

where \( Q, F, G, H, \) and \( W \) are all vectors: \( Q \) regroups the conserved variables, \( F, G, \) and \( H \) are respectively the \( x, y, \) and \( z \) components of the flux vector \( F_{\text{fluxes}} \), and \( W \) refers to the source terms. The fluxes can be divided into viscous and inviscid components – also referred to as diffusive and convective fluxes – and denoted as \( F_v \) and \( F_i \), \( G_v \) and \( G_i \), and \( H_v \) and \( H_i \). The source terms and viscous fluxes will not be addressed here.

Using the divergence notation, Equation (4.1) can be re-written as:

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F_{\text{fluxes}} = 0 \tag{4.2}
\]

4.2 The General Coordinate System

Until now, the referential system has remained in Cartesian coordinates. In this system, axes are locally and globally orthogonal. The most basic nozzle is axisymmetric and curved; thus there is a need for a body-fitted coordinate system.
(ξ, η, ζ). The normalized metrics (e.g. ξ, η, ζ) are simply direction cosines of the general coordinates with respect to the x, y, and z coordinates. Below is a representation of a general grid cell used in the numerical code.

![Figure 4-1 General grid cells](image)

The Cartesian flux vector components F, G, and H are simply transformed to the general coordinate system (ξ, η, ζ) using basic linear algebra. The flux vectors in the x, y, z directions become respectively the flux vectors in the ξ, η, ζ directions.

The Cartesian coordinate derivatives follow the chain rule:

\[
\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial x} \frac{\partial}{\partial \zeta} \tag{4.3}
\]

\[
\frac{\partial}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial y} \frac{\partial}{\partial \zeta} \tag{4.4}
\]

\[
\frac{\partial}{\partial z} = \frac{\partial \xi}{\partial z} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial z} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial z} \frac{\partial}{\partial \zeta} \tag{4.5}
\]
Equation (4.1) – assuming no source terms – yields:

\[
\frac{\partial Q}{\partial t} + \frac{\partial \xi}{\partial x} \frac{\partial F}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial F}{\partial \eta} + \frac{\partial \zeta}{\partial x} \frac{\partial F}{\partial \zeta} + \frac{\partial \xi}{\partial y} \frac{\partial G}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial G}{\partial \eta} + \frac{\partial \zeta}{\partial y} \frac{\partial G}{\partial \zeta} + \frac{\partial \xi}{\partial z} \frac{\partial H}{\partial \xi} + \frac{\partial \eta}{\partial z} \frac{\partial H}{\partial \eta} + \frac{\partial \zeta}{\partial z} \frac{\partial H}{\partial \zeta} = 0
\]

(4.6)

Regrouping terms:

\[
\frac{\partial Q}{\partial t} + \frac{\partial \xi}{\partial \xi} \left( \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} \right) + \frac{\partial \eta}{\partial \eta} \left( \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} + \frac{\partial H}{\partial z} \right) + \frac{\partial \zeta}{\partial \zeta} \left( \frac{\partial F}{\partial z} + \frac{\partial G}{\partial z} + \frac{\partial H}{\partial z} \right) = 0
\]

(4.7)

The spatial derivative governing equation in general coordinate is:

\[
\frac{\partial Q}{\partial t} + \frac{\partial F'}{\partial \xi} + \frac{\partial G'}{\partial \eta} + \frac{\partial H'}{\partial \zeta} = 0
\]

(4.8)

where the fluxes in general coordinates are

\[
F' = \frac{\partial \xi}{\partial x} F + \frac{\partial \xi}{\partial y} G + \frac{\partial \xi}{\partial z} H
\]

(4.9)

\[
G' = \frac{\partial \eta}{\partial x} F + \frac{\partial \eta}{\partial y} G + \frac{\partial \eta}{\partial z} H
\]

(4.10)

\[
H' = \frac{\partial \zeta}{\partial x} F + \frac{\partial \zeta}{\partial y} G + \frac{\partial \zeta}{\partial z} H
\]

(4.11)

The velocity components are written as:

\[
u' = \xi u + \zeta v + \zeta w
\]

(4.12)

\[
u' = \eta' u + \eta v + \eta w
\]

(4.13)

\[
u' = \xi' u + \zeta v + \zeta w
\]

(4.14)
The magnetic components are:

\[ B_x' = \xi_x B_x + \xi_y B_y + \xi_z B_z \]  
(4.15)

\[ B_y' = \eta_x B_x + \eta_y B_y + \eta_z B_z \]  
(4.16)

\[ B_z' = \zeta_x B_x + \zeta_y B_y + \zeta_z B_z \]  
(4.17)

In this coordinate system, note that:

\[ \xi_x^2 + \xi_y^2 + \xi_z^2 = 1 \]  
(4.18)

\[ \eta_x^2 + \eta_y^2 + \eta_z^2 = 1 \]  
(4.19)

\[ \zeta_x^2 + \zeta_y^2 + \zeta_z^2 = 1 \]  
(4.20)

### 4.3 Temporal Integration and Finite Volume Formulation

The flux-vector splitting method is an upwind method for solving equations of fluid dynamics. The procedure starts using the conservation form equation of the governing fluid equations.

The time derivative is approximated using a forward difference scheme in time:

\[ \frac{\partial Q}{\partial t} = \frac{Q^{n+1} - Q^n}{\Delta t} \]  
(4.21)

The fluxes are evaluated over a finite volume, which is later associated with a difference over two surfaces using Gauss' theorem.

\[ \iiint_V \nabla \cdot F' \text{d}V = \iint_{\partial S} F'_{\text{flux}} \cdot n \text{d}s \]  
(4.22)

where \( n \) is the outward unit normal vector of the control volume \( V \) and \( \partial S \) is the boundary surface of the control volume. Note that this is correct for any coordinate
system. We approximate \( \nabla \cdot F'_{\text{fluxes}} \) to be constant throughout the volume \( V \) thus the divergence of the fluxes can be written as:

\[
\nabla \cdot F'_{\text{fluxes}} = \frac{1}{V} \int_{\partial V} F'_{\text{fluxes}} \cdot n \, ds
\]

(4.23)

This yields the time marching explicit algorithm:

\[
Q^{n+1} = Q^n - \frac{\Delta t}{V} \int_{\partial V} F'_{\text{fluxes}} \cdot n \, ds
\]

(4.24)

Note that the summation of \( F'_{\text{fluxes}} \cdot n \) is simplified because the fluxes are expressed in the general coordinate system. Chronologically, the method can be broken down as follows:

1. **Step 1:** Initialize flow field variables as well as the boundary conditions on the entire grid.
2. **Step 2:** Calculate the integral fluxes using flux vector splitting.
3. **Step 3:** From the flux terms, solve for \( Q^{n+1} \) thus updating the main conserved variables.
4. **Step 4:** Iterate step 2 and 3 until the number of maximum iterations is reached. Note that the number of iterations is directly linked to the integration time since the step used is a time step.
4.4 Flux Vector Splitting

The method employed here follows that of Steger-Warming. Flux vector splitting (FVS) falls in the class of numerical schemes known generally as "upwinding". Numerical stability dictates that the spatial derivatives be finite differenced in the upwind direction. Upwind schemes make use of the wavelike nature of the Euler equations to split (or difference, in other upwind schemes) the fluxes into waves whose directions of travel can be determined. The positive and negative fluxes are then constructed using the wave speeds with positive and negative signs, respectively. The wave speeds are simply the eigenvalues of the flux Jacobian matrices.

The fluxes are each specific to one direction so it is possible to evaluate each independently. This produces three sets of equations, which are nevertheless solved simultaneously. The process is described for the flow in the $i$-advancing direction of the flow (study of $F'$). A similar and simultaneous process could be done for the $j$- and $k$-advancing directions.

Recall the grid cell Figure 4-1 on page 32. In flux vector splitting, the flux at cell face $i + \frac{1}{2}$ is the sum of a positive flux and a negative flux.

$$ F'_{i+\frac{1}{2}} = F'^{+}_{i+\frac{1}{2}} + F'^{-}_{i+\frac{1}{2}} $$

(4.25)

The positive and negative fluxes are functions of $A'^{+}_{i+\frac{1}{2}}$ and $A'^{-}_{i+\frac{1}{2}}$, respectively called positive and negative wave flux Jacobians; the matrix $\frac{\partial F'}{\partial Q}$ being defined as the flux vector Jacobian and denoted as $A'$. The positive and negative fluxes are formed by multiplying the positive and negative flux Jacobians by the conserved variable vector $Q$. 

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This is the direct result of Euler's theorem of homogeneity: let the function $F'(Q)$ be positively homogeneous of degree $n$, then at any point where $F'$ is differentiable, we have:

$$\frac{\partial F'(Q)}{\partial Q} \cdot Q = nF'(Q)$$ \hspace{0.5cm} (4.26)

For a flux vector homogeneity of degree 1 (which is most often the case in computational fluid dynamics), and recalling the variable $A'$ for the flux vector Jacobian, we have:

$$F'(Q) = A' \cdot Q$$ \hspace{0.5cm} (4.27)

The positive flux is calculated using the conserved variables in cell $i$ and the negative flux is calculated using the conserved variables in cell $i+1$. This yields somewhat of an average value, based on the following two expressions:

$$F_{i+\frac{1}{2}}^{+} = A_{i+\frac{1}{2}}^{+} \cdot Q_{i},$$ \hspace{0.5cm} (4.28)

$$F_{i+\frac{1}{2}}^{-} = A_{i+\frac{1}{2}}^{-} \cdot Q_{i+1}.$$ \hspace{0.5cm} (4.29)

Finally, the positive and negative wave flux Jacobians are:

$$A_{i+\frac{1}{2}}^{+} = P_{i+\frac{1}{2}}^{+} \cdot \Lambda^{+}_{i+\frac{1}{2}} \cdot P^{-1}_{i+\frac{1}{2}}$$ \hspace{0.5cm} (4.30)

$$A_{i+\frac{1}{2}}^{-} = P_{i+\frac{1}{2}}^{-} \cdot \Lambda^{-}_{i+\frac{1}{2}} \cdot P^{-1}_{i+\frac{1}{2}}$$ \hspace{0.5cm} (4.31)

Where $P_{i+\frac{1}{2}}$ and $P^{-1}_{i+\frac{1}{2}}$ are respectively the matrices of right and left eigenvectors. Although they can be solved separately, it is easier to invert one to get the other. $\Lambda^{+}_{i+\frac{1}{2}}$ and $\Lambda^{-}_{i+\frac{1}{2}}$ are respectively the diagonal matrices of positive and negative eigenvalues. The eigenvalues and eigenvectors at each cell face are computed with
simple averages of the flow variables at the adjoining cell centers. The signs of the
eigenvalues correspond to the direction of propagation of the different running waves.
They are separated during resolution using the following relations:

\[
\lambda^+_j = \frac{\lambda_j + |\lambda_j|}{2} \quad \text{yields the positive running waves,} \quad (4.32)
\]
\[
\lambda^-_j = \frac{\lambda_j - |\lambda_j|}{2} \quad \text{yields the negative running waves,} \quad (4.33)
\]

Referring to the previous expressions and solving for matrices of positive and
negative eigenvalues, one can note that during resolution the eigenvalues with a
positive value will be equal to themselves in \( \Lambda^+ \) and zero in \( \Lambda^- \). On the contrary,
eigenvalues with a negative value will equal themselves in \( \Lambda^- \) and zero in \( \Lambda^+ \). A
verification process is to check the validity of the following equation:

\[
\Lambda = \Lambda^+ + \Lambda^-
\]

(4.34)

The process of diagonalizing the flux vector Jacobian \( A' \) is complex. We
simplify the problem by introducing a vector of primitive variables \( V \) (explained
later) and writing:

\[
A' = S^{-1} \begin{pmatrix} \frac{\partial V}{\partial Q} & \frac{\partial F'}{\partial V} \end{pmatrix} S
\]

(4.35)

This introduces two new matrices.

\[
S^{-1} = \frac{\partial Q}{\partial V} \quad \text{and} \quad S = \frac{\partial V}{\partial Q}
\]

(4.36)

From algebra relations (refer to the Eigenvalue Problem in any algebra reference)
we know that if the term inside the parentheses in Equation (4.35) can be
diagonalized, then the eigenvalues of \( A \) are the same as the eigenvalues of the term
inside the parentheses. Diagonalizing the inside parentheses term, we have:
\[
\frac{\partial \mathbf{V}}{\partial \mathbf{Q}} \frac{\partial \mathbf{F}'}{\partial \mathbf{V}} = [\mathbf{R}] \cdot \Lambda \cdot [\mathbf{L}] \tag{4.37}
\]

where \([\mathbf{R}]\) and \([\mathbf{L}]\) denote the matrices of right and left eigenvectors, and \(|\Lambda|\) diagonally contains the independent eigenvalues. Note the mathematical relation between the left and right eigenvectors:

\[
[\mathbf{L}] = [\mathbf{R}]^{-1} \tag{4.38}
\]

Regrouping Equations (4.35) and (4.37), it is equivalent to write:

\[
\mathbf{A}' = S^{-1} \cdot [\mathbf{R}] \cdot |\Lambda| \cdot [\mathbf{L}] \cdot S \tag{4.39}
\]

Finally:

\[
\mathbf{P} = S^{-1} [\mathbf{R}] \quad \text{and} \quad \mathbf{P}^{-1} = [\mathbf{L}] S \tag{4.40}
\]

4.5 Resolution

It is now necessary to define the vectors \(\mathbf{Q}\) and \(\mathbf{F}'\) with the studied variables.

4.5.1 The Conserved Variables

The conserved variables chosen to study a reacting flow influenced by the magnetic field where a number \(n_s\) of species are involved are:

- each species density \(\rho_s\)
- electron density \(\rho_e\)
- momentum variables \(\rho u, \rho v, \rho w\)
- magnetic field \(B_x, B_y,\) and \(B_z\)
energies:
- vibrational energy $E_v$
- rotational energy $E_r$
- electronic energy $E_{elec}$
- electron energy $E_e$
- total energy $E_T$

The homogeneity variable is introduced in order for the flux vector to be homogeneous of degree 1 so that Equation (4.27) can be verified. Further details on this variable will be discussed later.

For a number $ns$ of species involved in the flow as well as electrons, we write the conserved variable vector $Q$ as:

$$Q = \begin{pmatrix} 
\rho_1 & \rho_{na} & \rho_e & \rho u & \rho v & \rho w & B_x & B_y & B_z & E_x & E_y & E_z & E_{elec} & E_e & E_r & \dot{a} 
\end{pmatrix}^T$$

(4.41)

Separators facilitate the reading of the vector. We recognize the time variants of: the continuity equation (first and second block), the momentum equations (third block), the induction equation (fourth block) and the energies (fifth block). We will keep the same separators in any one of our matrices for easy referral.

### 4.5.2 The Flux Vector

Setting up the flux vector $F'$ brings forth two analytical concerns. The first concern is to have the flux vector homogeneous in order to apply the method described above. The second concern is how to simplify the calculations in differentiating the homogeneous flux vector.
In order to write the flux vector, we regroup all the fluid mechanics equations derived in Section 3 \textit{THE GOVERNING EQUATIONS} of this report, as well as one additional equation concerning the homogeneity variable \( a \). In this last equation, the flux is set equal to 0.

This yields:

\[
\mathbf{F}_{\text{flux}} = \begin{pmatrix}
\rho u, \\
\rho u^2, \\
\rho u, \\
\rho u + l \left( p + \frac{B^2}{2\mu_0} \right) \frac{B}{\mu_0} \\
\rho u + l \left( p + \frac{B^2}{2\mu_0} \right) \frac{B}{\mu_0} \\
\rho u + l \left( p + \frac{B^2}{2\mu_0} \right) \frac{B}{\mu_0} \\
\mathbf{u} \cdot \mathbf{B} - B u, \\
\mathbf{u} \cdot \mathbf{B} - B v, \\
\mathbf{u} \cdot \mathbf{B} - B w, \\
\mathbf{E} \cdot \mathbf{u}, \\
\mathbf{E} \cdot \mathbf{u}, \\
\mathbf{E} \cdot \mathbf{u}, \\
\left( E_e + p + \frac{B^2}{2\mu_0} \right) \mathbf{u} - \frac{B}{\mu_0} \left( \mathbf{u} \cdot \mathbf{B} \right), \\
\left( E_e + p + \frac{B^2}{2\mu_0} \right) \mathbf{u} - \frac{B}{\mu_0} \left( \mathbf{u} \cdot \mathbf{B} \right), \\
0
\end{pmatrix}
\]  

Recall Equation (3.45) for the magnitude of the magnetic field vector:

\[
B^2 = B_x^2 + B_y^2 + B_z^2
\]

4.5.2.1 Homogeneity Criteria

This simple assembly of equations does not satisfy the homogeneity criterion stated previously, which is required to apply the flux vector splitting method. This is
due to any term where the magnetic field is present at a power of 2: \( \frac{B^2}{\mu_0} \), \( B \cdot \mathbf{B} \), and \( \frac{B_i}{\mu_0} (u \cdot \mathbf{B}) \).

The problem is easily solved by introducing the homogeneity variable \( \hat{a} \) at various locations where the magnetic field is present, as well as in the conserved variables vector and primitive variables vector. MacCormack\(^{21} \) first introduced the homogeneity variable, and his idea is later used by Dietiker and Hoffman\(^{22} \), and Powell\(^{23} \), whenever the magnetic field vector is involved in the equations. Its value being arbitrarily set equal to one will make no changes in any result.

Finally, the homogeneous flux vector can be written:

\[
\begin{pmatrix}
\rho, & u, \\
\rho u, & B_x, \\
\rho v, & B_y, \\
\rho w, & B_z, \\
\rho u u + l \left( p + \frac{B^2}{2 \mu_0 \hat{a}} \right) \frac{B \cdot B}{\mu_0 \hat{a}}, \\
\rho u v + l \left( p + \frac{B^2}{2 \mu_0 \hat{a}} \right) \frac{B \cdot B}{\mu_0 \hat{a}}, \\
\rho u w + l \left( p + \frac{B^2}{2 \mu_0 \hat{a}} \right) \frac{B \cdot B}{\mu_0 \hat{a}}, \\
u_B = -B \cdot u, \\
v_B = -B \cdot v, \\
w_B = -B \cdot w, \\
E, \\
E, \\
\left( E + p + \frac{B^2}{2 \mu_0 \hat{a}} \right) u - \frac{B}{\mu_0 \hat{a}} (u \cdot B), \\
\left( E + p + \frac{B^2}{2 \mu_0 \hat{a}} \right) v - \frac{B}{\mu_0 \hat{a}} (u \cdot B), \\
0
\end{pmatrix}
\] (4.43)
The flux vector is shown more detailed in its $x$, $y$, and $z$ direction in Appendix A, page 68. The proof that it is homogeneous is shown in Appendix B, page 70.

### 4.5.2.2 Fluxes in General Coordinates

The transformation to general coordinates is found in Appendix C, page 76. The result is shown hereafter in the $\xi$-direction only.

$$
F' = \begin{pmatrix}
\rho u' \\
\rho v' \\
\rho w' \\
\rho u' + \frac{B^2}{2\mu_\delta} \left( p + \frac{B B'}{\mu_\delta} \right) \frac{B B'}{\mu_\delta} \\
\rho v' + \frac{B^2}{2\mu_\delta} \left( p + B B' \right) \frac{B B'}{\mu_\delta} \\
\rho w' + \frac{B^2}{2\mu_\delta} \left( p + B B' \right) \frac{B B'}{\mu_\delta} \\
u'B_s - B_{s,\mu} \\
u'B_s - B_{s,\nu} \\
u'B_s - B_{s,w} \\
E_{,u}' \\
E_{,v}' \\
E_{,w}' \\
(E_r + p + \frac{B^2}{2\mu_\delta})u' \frac{B_r}{\mu_\delta} (u B) \\
(E_r + p + \frac{B^2}{2\mu_\delta})u' \frac{B_r}{\mu_\delta} (u B) \\
0 \\
\end{pmatrix}
$$

(4.44)

### 4.5.2.3 Algebra Simplifications

Differentiating the homogeneous flux vector $F'$ directly with respect to the conserved variables $Q$ reveals to be complicated.
The second concern in treating the flux vector appears here. Although it will not be shown, straightforward calculations carried out on this particular flux vector led to eigenvalues for the \(ns+13\) by \(ns+13\) matrix \(\left( \frac{\partial \mathbf{V}}{\partial \mathbf{Q}} \frac{\partial \mathbf{F}'}{\partial \mathbf{V}} \right)\) being equal to zero, thus not having any physical meaning. This is in part due to the divergence of the magnetic field being equal to zero, which is responsible for an entire row of zeros.

In order to bypass this problem, we follow MacCormack's technique detailed by Canupp\(^\text{18}\). We split the general flux vector in two by removing the final terms in each flux component (except for the continuity equations, vibrational, rotational and electron energy flux) and forming two new flux vectors \(\mathbf{F}_j\) and \(\mathbf{P}\):

\[
\mathbf{F}' = \mathbf{F}_j - \mathbf{P} \frac{\mathbf{B}_c}{\mu_0 \hat{\alpha}}
\]

with:

\[
\mathbf{P} = \begin{pmatrix} 0 & \ldots & 0 & B_x & B_y \end{pmatrix}^T
\]

\[
\mathbf{F} = \begin{pmatrix} u \mu_0 \hat{\alpha} & v \mu_0 \hat{\alpha} & w \mu_0 \hat{\alpha} & 0 & 0 & \mathbf{u} \cdot \mathbf{B} \mathbf{u} \cdot \mathbf{B} \end{pmatrix}^T
\]

(4.45)

Then, the altered expanded flux Jacobian matrix is derived using the following expression:

\[
\mathbf{A}'_j = \mathbf{S} \frac{\partial \mathbf{F}_j}{\partial \mathbf{V}} - \mathbf{S} \frac{\partial \mathbf{P} \mathbf{B}_c}{\partial \mathbf{V}} \frac{1}{\mu_0 \hat{\alpha}}
\]

(4.46)

Then:

\[
\mathbf{F}' = \begin{bmatrix} \mathbf{S}_p^{-1} \mathbf{A}_p \mathbf{S}_p & \mathbf{Q}_p \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} \hat{\alpha}
\]

(4.47)

(4.48)

where \(\mathbf{A}'_p\), \(\mathbf{S}_p^{-1}\), and \(\mathbf{S}_p\) are the extracted upper-left \(ns+12\) by \(ns+12\) matrices from \(\mathbf{A}_j\), \(\mathbf{S}^{-1}\), and \(\mathbf{S}\) respectively. Writing the previous fluxes as two new fluxes creates the variable \(\mathbf{b}\), which is simply a mathematical operand related to the
homogeneity variable. In the final resolution of the eigenvalues, $b$ is not looked at, thus $A'_{p}$ is the only matrix for which the eigenvalues are found. A simple description and derivation of $b$ is found in Appendix D page 82. $Q_{p}$ are the original conserved variables elements.

$$Q_{p} = \left( \rho_{1} \ldots \rho_{n} \cdot \rho_{e} \cdot \rho_{n} \cdot \rho_{v} \cdot \rho_{w} \cdot B_{x} \cdot B_{y} \cdot B_{z} \cdot E_{v} \cdot E_{e} \cdot E_{elec} \cdot E_{e} \cdot E_{T} \right)^{T}$$

(4.49)

4.5.3 Differentiating $S$ and $S^{-1}$

The derivation of these matrices is needed in order to ease the calculation of the eigenvectors of the Jacobian matrix. Thus we introduce another vector $V$, somewhat simplified from $Q$. $V$ is called vector of primitive variables and is chosen arbitrarily. The choice of the variables used comes from experience. Usually, it follows the conserved variables using their primitive forms. For example, although we conserve the vibrational and rotational energies themselves, the primitive forms used are their per unit mass equivalent. For the total energy, the most relevant variable to use is the static pressure, since it best translates the energy level. The same is true for the electron energy, for which we choose the electron pressure.

The choice of each primitive variable can be influenced by parallel research efforts currently under way. Although this thesis only deals with the reaction set, parallel studies are underway at NASA for the structure that will host the reaction itself; for structural purposes, pressure (indirectly temperature) is an important factor.

The final version is:

$$V = \left( \rho_{1} \ldots \rho_{n} \cdot \rho_{e} \cdot \rho_{v} \cdot \rho_{w} \cdot B_{x} \cdot B_{y} \cdot B_{z} \cdot e_{v} \cdot e_{e} \cdot e_{elec} \cdot p_{e} \cdot p \cdot \hat{a} \right)^{T}$$

(4.50)

Recall the conserved variables, Equation (4.41):

$$Q = \left( \rho_{1} \ldots \rho_{n} \cdot \rho_{e} \cdot \rho_{v} \cdot \rho_{w} \cdot B_{x} \cdot B_{y} \cdot B_{z} \cdot E_{v} \cdot E_{e} \cdot E_{elec} \cdot E_{e} \cdot E_{T} \cdot \hat{a} \right)^{T}$$
Differentiating $\mathbf{v}$ with respect to $\mathbf{Q}$ is straightforward for species density, electron density, momentum variables, magnetic field components, and finally vibrational, rotational and electronic energies.

Note that it is useful to express each primitive variable as a function of the conserved variables. This is particularly helpful when deriving the momentum variables; remember that $u$ is not a conserved variable but appears in the conserved variable $\rho u$. As an example, when deriving $u$ with respect to $\rho_i$, we introduce $\rho u$ and regard it as a constant later on:

\[
\frac{\partial}{\partial \rho_i}(u) = \frac{\partial}{\partial \rho_i} \left( \frac{\rho u}{\sum_i \rho_i} \right)
= -\frac{\rho u}{\rho^2}
= -\frac{u}{\rho}
\]  

(4.51)
The generally simple terms lead to the following matrix:

\[
S = \frac{\partial V}{\partial Q} =
\begin{pmatrix}
1 & & & & & & & & \\
0 & 1 & & & & & & & \\
0 & 0 & 1 & & & & & & \\
\frac{u}{\rho} & \frac{u}{\rho} & \frac{u}{\rho} & 1 & & & & & \\
\frac{v}{\rho} & \frac{v}{\rho} & \frac{v}{\rho} & 0 & 1 & & & & \\
\frac{w}{\rho} & \frac{w}{\rho} & \frac{w}{\rho} & 0 & 0 & 1 & & & \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \\
\frac{e_e}{\rho - \rho_e} & \frac{e_e}{\rho - \rho_e} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\rho - \rho_e} \\
\frac{e_e}{\rho - \rho_e} & \frac{e_e}{\rho - \rho_e} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\rho - \rho_e} \\
\frac{e_{elec}}{\rho - \rho_e} & \frac{e_{elec}}{\rho - \rho_e} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\rho - \rho_e} \\
\frac{\partial p_t}{\partial \rho_1} & \frac{\partial p_t}{\partial \rho_2} & \frac{\partial p_t}{\partial \rho_3} & \frac{\partial p_t}{\partial \rho_4} & \frac{\partial p_t}{\partial \rho_5} & \frac{\partial p_t}{\partial \rho_6} & \frac{\partial p_t}{\partial \rho_7} & \frac{\partial p_t}{\partial \rho_8} & \frac{\partial p_t}{\partial \rho_9} \\
\frac{\partial p}{\partial \rho_{10}} & \frac{\partial p}{\partial \rho_{11}} & \frac{\partial p}{\partial \rho_{12}} & \frac{\partial p}{\partial \rho_{13}} & \frac{\partial p}{\partial \rho_{14}} & \frac{\partial p}{\partial \rho_{15}} & \frac{\partial p}{\partial \rho_{16}} & \frac{\partial p}{\partial \rho_{17}} & \frac{\partial p}{\partial \rho_{18}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\]

(4.52)

Differentiating the electron pressure as well as the static pressure is done implicitly, using the electron energy equation (3.87) and the total energy equation (3.72), respectively.
4.5.3.1 Differentiating the Electron Pressure

Recall the electron energy equation (3.87). This equation is written as a function of conserved variables only and the electron pressure:

\[ E_e = \frac{3}{2} p_e + \frac{p_e}{2} \left( \left( \rho u \right)^2 + \left( \rho v \right)^2 + \left( \rho w \right)^2 \right) \]  

(4.53)

Solving for the electron pressure gives:

\[ p_e(Q) = \frac{2}{3} \left( E_e - \frac{\rho_e}{2} \left( \left( \rho u \right)^2 + \left( \rho v \right)^2 + \left( \rho w \right)^2 \right) \right) \]  

(4.54)

Differentiating with respect to each primitive variable, the non-zero results are:

\[ \frac{\partial p_e}{\partial \rho_1} = \frac{2}{3} \frac{\rho_e}{\rho} \left( u^2 + v^2 + w^2 \right) \]  

(4.55)

\[ \frac{\partial p_e}{\partial \rho_e} = \frac{2}{3} \left( u^2 + v^2 + w^2 \right) \left( \frac{\rho_e}{\rho} - \frac{1}{2} \right) \]  

(4.56)

\[ \frac{\partial p_e}{\partial \rho u} = \frac{2}{3} \frac{\rho_e}{\rho} u \]  

(4.57)

\[ \frac{\partial p_e}{\partial \rho v} = \frac{2}{3} \frac{\rho_e}{\rho} v \]  

(4.58)

\[ \frac{\partial p_e}{\partial \rho w} = \frac{2}{3} \frac{\rho_e}{\rho} w \]  

(4.59)

\[ \frac{\partial p_e}{\partial E_e} = \frac{2}{3} \]  

(4.60)

All other differentiations are equal to zero. Those are:

\[ \frac{\partial p_e}{\partial B_1} = 0, \quad \frac{\partial p_e}{\partial B_2} = 0, \quad \frac{\partial p_e}{\partial E_c} = 0, \quad \frac{\partial p_e}{\partial E_{dec}} = 0, \quad \frac{\partial p_e}{\partial E_r} = 0, \quad \frac{\partial p_e}{\partial \hat{a}} = 0 \]  

(4.61)
4.5.3.2 Differentiating the Static Pressure

To differentiate the static pressure, it is first expressed as a function of the conserved variables and the electron pressure. Solving for the static pressure from the total energy equation:

$$p(Q) = p_e + \sum_{s \in c} \left( \rho_s \frac{R_s}{M_s} \right) \left( E_T - E_v - E_e - E_{elec} - \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{2(\rho + \ldots + \rho_e)} \sum_{s \in e} \rho_s \ldots \right)$$

$$\ldots - \frac{B_s^2 + B_e^2 + B_{elec}^2}{2 \mu_0 \hat{\alpha}} - \sum_{s \in e} \rho_s h_{e}^s$$

(4.62)

Also, in order to facilitate the writing of the derivatives we introduce:

$$c_v = \sum_{s \in e} \rho_s c_v$$

(4.63)

$$\bar{R} = \sum_{s \in e} \rho_s \frac{R_s}{M_s}$$

(4.64)

The results are expressed as a function of the derivatives of the electron pressure calculated previously:

$$\frac{\partial p}{\partial \rho_{ns}} = \frac{\partial p_e}{\partial \rho_{ns}} + \left( \frac{R_e}{M_e} - c_v \bar{R} \right) T + \frac{\bar{R}}{c_v} \left( u^2 + v^2 + w^2 \right) \left( \frac{1}{2} - \frac{\rho_e}{\rho} \right) - h_{ns}^e$$

(4.65)

$$\frac{\partial p}{\partial \rho_e} = \frac{\partial p_e}{\partial \rho_e} + \frac{\bar{R}}{c_v} \left( u^2 + v^2 + w^2 \right) \left( 1 - \frac{\rho_e}{\rho} \right)$$

(4.66)

$$\frac{\partial p}{\partial \rho u} = \frac{\partial p_e}{\partial \rho u} + \frac{\bar{R}}{c_v} \left( \frac{\rho_e}{\rho} - 1 \right) u$$

(4.67)

$$\frac{\partial p}{\partial \rho v} = \frac{\partial p_e}{\partial \rho v} + \frac{\bar{R}}{c_v} \left( \frac{\rho_e}{\rho} - 1 \right) v$$

(4.68)

$$\frac{\partial p}{\partial \rho w} = \frac{\partial p_e}{\partial \rho w} + \frac{\bar{R}}{c_v} \left( \frac{\rho_e}{\rho} - 1 \right) w$$

(4.69)
\[
\frac{\partial p}{\partial B_x} = -\frac{B_x}{\mu_0 \alpha} \bar{R} \tag{4.70}
\]
\[
\frac{\partial p}{\partial B_y} = -\frac{B_y}{\mu_0 \alpha} \bar{R} \tag{4.71}
\]
\[
\frac{\partial p}{\partial B_z} = -\frac{B_z}{\mu_0 \alpha} \bar{R} \tag{4.72}
\]
\[
\frac{\partial p}{\partial E_r} = -\frac{\bar{R}}{c_v} \tag{4.73}
\]
\[
\frac{\partial p}{\partial E_r} = -\frac{\bar{R}}{c_v} \tag{4.74}
\]
\[
\frac{\partial p}{\partial E_{\text{elec}}} = -\frac{\bar{R}}{c_v} \tag{4.75}
\]
\[
\frac{\partial p}{\partial E_r} = \frac{\partial p_e}{\partial E_r} \frac{\bar{R}}{c_v} \tag{4.76}
\]
\[
\frac{\partial p}{\partial \alpha} = \frac{\partial p_e}{\partial \alpha} + \frac{\bar{R}}{c_v} \frac{B^2}{2 \mu_0 \alpha^2} \tag{4.77}
\]
\[
\frac{\partial p}{\partial \alpha} = \frac{\partial p_e}{\partial \alpha} + \frac{\bar{R}}{c_v} \frac{B^2}{2 \mu_0 \alpha^2} \tag{4.78}
\]

In this work, the specific heats relate only to the translational temperature, thus successively:
\[
c_v \approx = 3 \frac{R_0}{2 M_1 \alpha} \tag{4.79}
\]

which simplifies the ratio \(\bar{R}/c_v\) itself to:
\[
\frac{\bar{R}}{c_v} = 2 \tag{4.80}
\]
Using this, we simplify each equation above to:

\[
\frac{\partial p}{\partial \rho_1} = \frac{u^2 + v^2 + w^2}{3} - \frac{2}{3} \kappa_1 \rho_1 \tag{4.81}
\]

\[
\frac{\partial p}{\partial \rho_e} = \frac{1}{3}(u^2 + v^2 + w^2) \tag{4.82}
\]

\[
\frac{\partial p}{\partial \rho_u} = -\frac{2}{3} u \tag{4.83}
\]

\[
\frac{\partial p}{\partial \rho_v} = -\frac{2}{3} v \tag{4.84}
\]

\[
\frac{\partial p}{\partial \rho_w} = -\frac{2}{3} w \tag{4.85}
\]

\[
\frac{\partial p}{\partial B_r} = -\frac{2}{3} \frac{B_r}{\mu_0 \dot{a}} \tag{4.86}
\]

\[
\frac{\partial p}{\partial B_\theta} = -\frac{2}{3} \frac{B_\theta}{\mu_0 \dot{a}} \tag{4.87}
\]

\[
\frac{\partial p}{\partial B_z} = -\frac{2}{3} \frac{B_z}{\mu_0 \dot{a}} \tag{4.88}
\]

\[
\frac{\partial p}{\partial E_r} = -\frac{2}{3} \tag{4.89}
\]

\[
\frac{\partial p}{\partial E_\theta} = -\frac{2}{3} \tag{4.90}
\]

\[
\frac{\partial p}{\partial E_z} = -\frac{2}{3} \tag{4.91}
\]

\[
\frac{\partial p}{\partial E_{elec}} = 0 \tag{4.92}
\]

\[
\frac{\partial p}{\partial E_r} = \frac{2}{3} \tag{4.93}
\]

\[
\frac{\partial p}{\partial \dot{a}} = \frac{1}{3} \frac{B^2}{\mu_0 \dot{a}^2} \tag{4.94}
\]
The final matrix is:

\[ S = \frac{\partial V}{\partial Q} = \]

\[
\begin{pmatrix}
1 & & & & & & & & & \\
0 & 1 & & & & & & & & \\
0 & 0 & 1 & & & & & & & \\
0 & \frac{\rho}{\rho} & 0 & \frac{1}{\rho} & & & & & & \\
0 & \frac{\rho}{\rho} & 0 & \frac{1}{\rho} & & & & & & \\
0 & \frac{\rho}{\rho} & 0 & \frac{1}{\rho} & & & & & & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\[ (4.95) \]

where again:

\[ \frac{\partial p_e}{\partial \rho_{1 ns}} = \frac{2}{3} \rho_e \left( u^2 + v^2 + w^2 \right) \]

\[ (4.55) \]

\[ \frac{\partial p_e}{\partial \rho_e} = \frac{2}{3} \left( u^2 + v^2 + w^2 \right) \left( \frac{\rho_e}{\rho} - \frac{1}{2} \right) \]

\[ (4.56) \]

\[ \frac{\partial p}{\partial \rho_{1 ns}} = \frac{u^2 + v^2 + w^2}{3} - \frac{2}{3} h_{ns}^e \]

\[ (4.81) \]

\[ \frac{\partial p}{\partial \rho_e} = \frac{1}{3} \left( u^2 + v^2 + w^2 \right) \]

\[ (4.82) \]
\( S^{-1} \) is easily obtained using any analytical software, or by deriving the derivatives by hand.

\[
S^{-1} = \frac{\partial Q}{\partial \mathbf{v}} =
\begin{pmatrix}
1 \\
\vdots \\
0 & 1 \\
0 & 0 & 1 \\
u & u & u & \rho \\
v & v & v & 0 & \rho \\
w & w & w & 0 & 0 & \rho \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 \\
e_r & e_r & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho - \rho_e \\
e_r & e_r & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho - \rho_e \\
e_{\text{elec}} & e_{\text{elec}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho - \rho_e \\
0 & 0 & \frac{u^2 + v^2 + w^2}{2} & \rho u & \rho v & \rho w & \frac{B_1}{\mu_0 \tilde{\alpha}} & \frac{B_2}{\mu_0 \tilde{\alpha}} & \rho - \rho_e & \rho - \rho_e & \rho - \rho_e & 0 & \frac{3}{2} & \frac{1}{2} \frac{B^2}{\mu_0 \tilde{\alpha}^2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\]

(4.96)

The derivatives of the total energy with respect to each species density are:

\[
\frac{\partial E_T}{\partial \rho_{1,nr}} = e_v + e_{\text{elec}} + \frac{u^2 + v^2 + w^2}{2} + h_{\text{ns}}^\sigma
\]

(4.97)

4.5.4 Differentiating the Flux Vector with respect to \( \mathbf{v} \)

Following the method explained in Section 4.5.2.3 Algebra Simplifications starting page 43, the flux vector \( \mathbf{F}_1 \) is written after, followed immediately by its expression using primitive variables only. Again, \( \mathbf{b} \) does not influence the result.
The derivation of all fluxes but the electron energy flux and the total energy flux with respect to \( \mathbf{V} \) is straightforward. \( \mathbf{F}_i \) is a vector of dimension \( ns + 13 \). The differentiation of \( \mathbf{F}_i \) with respect to \( \mathbf{V} \) yields a square matrix of dimension \( ns + 13 \).
\[
\frac{\partial F_e}{\partial V} = \begin{pmatrix}
\begin{bmatrix}
\begin{matrix}
0 & 0 & \xi_1 \rho_1 & \xi_2 \rho_1 & \xi_3 \rho_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{matrix}
\end{bmatrix}
\end{pmatrix}
\]

(4.99)
Again, the derivatives for electron energy flux \( F_{\text{le}} \) and total energy flux \( F_{\text{ls}} \) are evaluated separately.

### 4.5.4.1 Differentiating the Electron Energy Flux

Recall the electron flux expression \( F_{\text{le}} \) from the flux vector above. Reintroducing the electron energy written as a function of the primitive variables only, we have:

\[
F_{\text{le}} = \left( E_e (\mathbf{V}) + p_e + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) \left( \xi_u + \xi_v + \xi_w \right)
\]

\[
= \left( \frac{5}{2} p_e + \frac{\rho_e}{2} (u^2 + v^2 + w^2) + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) \left( \xi_u + \xi_v + \xi_w \right)
\]

so that the non-zero derivatives for each component are:

\[
\frac{\partial F_{\text{le}}}{\partial \rho_e} = \frac{1}{2} (u^2 + v^2 + w^2) u'
\]

\[
\frac{\partial F_{\text{le}}}{\partial u} = \xi_x \left( E_e + p_e + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho_e uu'
\]

\[
\frac{\partial F_{\text{le}}}{\partial v} = \xi_y \left( E_e + p_e + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho_e vu'
\]

\[
\frac{\partial F_{\text{le}}}{\partial w} = \xi_z \left( E_e + p_e + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho_e wu'
\]

\[
\frac{\partial F_{\text{le}}}{\partial B_x} = \frac{B_x}{\hat{\mu}_0} u'
\]

\[
\frac{\partial F_{\text{le}}}{\partial B_y} = \frac{B_y}{\hat{\mu}_0} u'
\]

\[
\frac{\partial F_{\text{le}}}{\partial B_z} = \frac{B_z}{\hat{\mu}_0} u'
\]

\[
\frac{\partial F_{\text{le}}}{\partial p_e} = \frac{5}{2} u'
\]
\[
\frac{\partial F_{1E_T}}{\partial a} = -u, \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{a}^2\mu_0}
\] (4.109)

All other derivatives are zero. Those are:

\[
\frac{\partial F_{1E_T}}{\partial \rho_{1ns}} = 0, \quad \frac{\partial F_{1E_T}}{\partial e_v} = 0, \quad \frac{\partial F_{1E_T}}{\partial e_r} = 0, \quad \frac{\partial F_{1E_T}}{\partial e_{elec}} = 0, \quad \frac{\partial F_{1E_T}}{\partial p} = 0
\] (4.110)

4.5.4.2 Differentiating the Total Energy Flux

Again, the total energy flux expression \( F_{1T} \) is found in the flux vector above. Reintroducing the total energy written as a function of the primitive variables only yields:

\[
F_{1T} = \left( E_T(V) + p + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{a}^2\mu_0} \right) \left( \xi_v u + \xi_r v + \xi_e w \right)
\] (4.111)

with:

\[
E_T(V) = \frac{3}{2} (p - p_e) + e_v \sum_{i \neq e} \rho_s + e_r \sum_{i \neq e} \rho_s + e_{elec} \sum_{i \neq e} \rho_s + p_e + \frac{3}{2} p_e \left( \frac{u^2 + v^2 + w^2}{2} \right) + \ldots
\]

\[
+ e_{elec} \sum_{i \neq e} \rho_s + \frac{u^2 + v^2 + w^2}{2} \sum_{i \neq e} \rho_s + \frac{B_x^2 + B_y^2 + B_z^2}{2\mu_0\hat{a}} \sum_{i \neq e} \rho_s + \sum_{i \neq e} \rho_s h_s^o
\] (4.112)

Each derivative of the total energy has already been shown after obtaining the matrix \( S^{-1} \) at the end of Section 4.5.3 Differentiating \( S \) and \( S^{-1} \), page 53. Thus simple algebra yields the derivatives for the total energy with respect to the primitive variables as:

\[
\frac{\partial F_{1E_T}}{\partial \rho_{1ns}} = \left( e_v + e_r + e_{elec} + \frac{u^2 + v^2 + w^2}{2} + h_{1ns}^o \right) u',
\] (4.113)

\[
\frac{\partial F_{1E_T}}{\partial \rho_e} = \frac{u^2 + v^2 + w^2}{2} u'.
\] (4.114)
\[
\frac{\partial F_{1\xi}}{\partial u} = \xi \left( E_x + p + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho uu' \quad (4.115)
\]

\[
\frac{\partial F_{1\xi}}{\partial v} = \xi_y \left( E_y + p + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho vu' \quad (4.116)
\]

\[
\frac{\partial F_{1\xi}}{\partial w} = \xi_z \left( E_z + p + \frac{B_x^2 + B_y^2 + B_z^2}{2\hat{\mu}_0} \right) + \rho wu' \quad (4.117)
\]

\[
\frac{\partial F_{1\xi}}{\partial B_x} = 2u' \frac{B_x}{\hat{\mu}_0} \quad (4.118)
\]

\[
\frac{\partial F_{1\xi}}{\partial B_y} = 2u' \frac{B_y}{\hat{\mu}_0} \quad (4.119)
\]

\[
\frac{\partial F_{1\xi}}{\partial B_z} = 2u' \frac{B_z}{\hat{\mu}_0} \quad (4.120)
\]

\[
\frac{\partial F_{1\xi}}{\partial e_x} = (\rho - \rho_e) u' \quad (4.121)
\]

\[
\frac{\partial F_{1\xi}}{\partial e_y} = (\rho - \rho_e) u' \quad (4.122)
\]

\[
\frac{\partial F_{1\xi}}{\partial e_z} = (\rho - \rho_e) u' \quad (4.123)
\]

\[
\frac{\partial F_{1\xi}}{\partial p_e} = 0 \quad (4.124)
\]

\[
\frac{\partial F_{1\xi}}{\partial p} = \frac{5}{2} u' \quad (4.125)
\]

\[
\frac{\partial F_{1\xi}}{\partial a} = -u' \frac{B_x^2 + B_y^2 + B_z^2}{\hat{a}^2 \mu_0} \quad (4.126)
\]
4.5.5 Differentiating $\mathbf{P}$

To complete the resolution of the altered flux-vector Jacobian expressed in Equation (4.47), $\mathbf{P}$ is differentiated with respect to the primitive variables. This Jacobian is straightforward.

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

$$
\frac{\partial \mathbf{P}}{\partial \mathbf{V}} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

(4.127)

4.5.6 Finding the Eigenvalues

The matrix $|\Lambda|$ -- needed to solve for the positive and negative wave flux Jacobians -- contains diagonally the independent eigenvalues of $A_p$. Each eigenvalue indicates a wave speed. We obtain the matrices $S \frac{\partial \mathbf{F}}{\partial \mathbf{V}}$ and $S \frac{\partial \mathbf{P}}{\partial \mathbf{V}} B_v$ using the analytic tool of the computer software MatLab®. We further add the resulting matrices to obtain the expanded flux-vector Jacobian $A_v$. Intermediate matrices are shown in Appendix E page 84. We solve for the eigenvalues of only the sub-matrix of dimension $ns+12$ by $ns+12$ of $A_v$. There is no need to include the homogeneity variable equation as it does not relate to any physics.
\[ \frac{S \frac{\partial F}{\partial V} - S \frac{\partial P}{\partial V} \left( \frac{B_z}{\hat{a} \mu_0} \right)}{\hat{a}} = \begin{bmatrix} 0 & 0 & 0 & \xi, \rho_1 & \xi, \rho_2 & \xi, \rho_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \]

Again,

\[ C_1 = \frac{5}{3} \rho + \frac{B^2}{3 \hat{a} \mu_0} \quad (E.2) \]

\[ C_2 = \frac{2}{3 \hat{a} \mu_0} \frac{\rho - \rho_e}{\rho} \quad (E.3) \]

\[ C_3 = -\frac{1}{2} \frac{B^2}{\hat{a}^2 \mu_0 \rho} \quad (E.4) \]
The various wave speeds categorizing an MPDT are well known. They are the convective speeds, two Alfvén wave speeds, and four magnetoacoustic wave speeds, further sub-categorized as fast and slow magnetoacoustic wave speeds. They are usually written in Cartesian coordinates\textsuperscript{16,18}. Since our derivations were done in general coordinates, the eigenvalues found are also written in general coordinates. The $ns+12$ eigenvalues found are:

$$
\frac{u', \ldots, u', 5}{3} u', \ u' \pm v'_{a}, \ u' \pm c'_{f}, \ u' \pm c'_{s}
$$

repeated $ns+5$ times

(4.128)

Two separate convective speeds are found. The convective speed $u'$ is repeated for each species density including the electron, as well as for rotational energy, vibrational energy and electronic energy. A modified convective speed has emerged from treating the translational-rotational non-equilibrium, that is $\frac{5}{3}u'$. Although it has not been fully understood yet, we will likely associate it with the convection of free electrons.

The Alfvén wave appears due to the tension exhibited from the presence of the magnetic field. We define the “general” Alfvén velocity by:

$$
v'_{a} = \frac{B'}{\sqrt{\mu_{0}\rho}}
$$

(4.129)

Thus, the two Alfvén wave speeds found are equal to $u' \pm \frac{B'}{\sqrt{\mu_{0}\rho}}$.

The presence of the magnetic field also engenders another type of waves, referred to as magnetoacoustic waves. (Note that some literatures also refer to magnetosonic waves.)
The fast and slow “general” magnetoacoustic waves \( c'_f \) and \( c'_e \) are respectively:

\[
c'_f^2 = \frac{1}{2} \left[ \left( \frac{5 \rho}{3 \rho} + \frac{B^2}{\mu_0 \rho} \right) + \sqrt{\left( \frac{5 \rho}{3 \rho} + \frac{B^2}{\mu_0 \rho} \right)^2 - 4 \left( \frac{5 \rho}{3 \rho} \right) \left( \frac{B^2}{\mu_0 \rho} \right)} \right]
\]

and

\[
c'_e^2 = \frac{1}{2} \left[ \left( \frac{5 \rho}{3 \rho} + \frac{B^2}{\mu_0 \rho} \right) - \sqrt{\left( \frac{5 \rho}{3 \rho} + \frac{B^2}{\mu_0 \rho} \right)^2 - 4 \left( \frac{5 \rho}{3 \rho} \right) \left( \frac{B^2}{\mu_0 \rho} \right)} \right]
\]

Note the expression of the speed of sound. For both heavy particles and electrons, \( \gamma = 5/3 \), thus the speed of sound is written as:

\[
a^2 = \frac{5 \rho}{3 \rho}
\]
5 CONCLUDING REMARKS - RECOMMENDATIONS

5.1 Summary of Work

The purpose of this thesis was to set up the governing physical equations for the flow of a non-equilibrium ionizing plasma in a magnetic field, and to derive a numerically stable scheme for computing such flows. The flux vector splitting method of upwind biasing the fluxes in a control-volume scheme is selected for its record of stable and accurate performance in hypersonic and thermodynamically complex flows, as evidenced by the literature. The application for such a code is vast and can, with the correct setup, solve the electromagnetic problems mentioned earlier like arcjets, MHD nozzles, and high Mach number reentry. In this work, the intended initial application of such a scheme is the simulation of magnetoplasmadynamic thrusters.

The problem is cast as a total of $n_s + 12$ conservation equations, where the number of species $n_s$ includes heavy particles only. The problem is set up for numerical solution using Steger-Warming flux vector splitting. This technique required some mathematical strategy to address two key issues.

First, the solenoidal nature of the magnetic field ($\nabla \cdot B$ is identically zero) results in a row of zeroes in the flux Jacobian matrix, hence a zero eigenvalue. Powell has engineered a work-around to this problem, which is adopted here. The Jacobian is augmented with additional terms, including the convective speed along the diagonal, the net effect of which is to convect the divergence of the magnetic field. Since the divergence is zero, this has no bearing on the solution.

Secondly, flux vector splitting requires the flux vector's homogeneity of degree one in the conserved variables. Earlier works have addressed homogeneity of the flux vector with varying degrees of rigor. Here it is strictly enforced, and noted inaccuracies are corrected. Non-linearities (with respect to temperature, hence pressure) in the vibrational and electronic energies result in non-homogeneity when
they are held in equilibrium with translational and free electron energies, respectively. Perrell\textsuperscript{25} overlooks the former effect, Hatfield\textsuperscript{13}, and ostensibly Candler\textsuperscript{12}, the latter. Notably however, Candler does not differentiate electronic energy with respect to electron temperature in writing the flux Jacobian. This omission preserves homogeneity of the electron/electronic energy flux, and thus it is a useful artifice to keep in mind, provided numerical results are not degraded. Here, all five of the internal molecular energies are assumed to be in non-equilibrium. As no pressures are associated with the vibrational and electronic energies, homogeneity is preserved.

Fluxes associated with the magnetic field also introduce non-homogeneties. Following MacCormack’s work, a dummy homogeneity variable is introduced in the conserved variables. This leads to \( ns+13 \) equations total, although only the \( ns+12 \) Jacobian matrix is solved for the eigenvalues. Steger-Warming’s flux vector splitting method leads to the expected wave speeds related to MHD flows, including two convective speeds, two Alfvén wave speeds, as well as two slow and two fast magnetoacoustic wave speeds.

The first convective wave speed is associated with each species density as well as energies of rotation, vibration and electronic excitation. In Cartesian coordinates, this speed is respectively \( u, v, \) and \( w \) for each flow direction. In general coordinates, these become \( u', v', \) and \( w' \) where for the \( x \)-direction only again, \( u' = \xi_x u + \xi_y v + \xi_z w \).

The Alfvén waves translate the perturbation generated by the tension exhibited by the magnetic field. This wave travels parallel to \( B \) at the Alfvén speed. In Cartesian coordinates, Powell \textit{et al} formulate this speed as \( B_x / \sqrt{\mu_0 \rho} \). In general coordinates, the expression differs only by the expression of the magnetic term, that is \( v_a' = B_x / \sqrt{\mu_0 \rho} \), where \( B_x' = \xi_x B_x + \xi_y B_y + \xi_z B_z \). Thus the Alfvén wave speeds obtained are \( u' \pm B_x / \sqrt{\mu_0 \rho} \).
Another set of waves results from the presence of the magnetic field. Those are
the fast and slow magnetoacoustic wave speeds, denoted respectively by $c'_f$ and $c'_s$, with:

$$c'_f^2 = \frac{1}{2} \left[ a'^2 + \sqrt{a'^4 - 4 \cdot \frac{5}{3} \rho \cdot v_f^2} \right]$$

$$c'_s^2 = \frac{1}{2} \left[ a'^2 - \sqrt{a'^4 - 4 \cdot \frac{5}{3} \rho \cdot v_s^2} \right]$$

where $a'^2 = \frac{5}{3} \rho + \frac{B^2}{\mu_0 \rho}$ and the Alfvén velocity is mentioned above. Note that since
we have assumed translational energy independent of the other modes, $5/3$ is the ratio
of specific heats for both heavy particles and electrons. Thus, the first term in $a'^2$ is
$a^2$, the square of the sonic velocity. The final four magnetoacoustic wave speeds
obtained from deriving the eigenvalues are $u' \pm c'_f$ and $u' \pm c'_s$.

A second convective speed $\frac{5}{3} u'$ is present. Although it has not been fully
understood yet, we likely associate it with convection of free electrons. This term is
roughly analogous to Candler's "modified convective speed," which he denotes as

$$\overline{u}' = u' \left( 1 - \frac{\rho_e}{\rho} \left( \frac{R_e}{c_{v_e}} - \frac{\overline{R}}{\overline{c_v}} \right) \right)$$

where $\overline{R} = \sum_{s \neq e} \frac{\rho_s R_s}{\rho M_s}$ and $\overline{c_v} = \sum_{s \neq e} \frac{\rho_s c_v}{\rho}$.

Candler maintained translational/rotational equilibrium. In this work, the specific
heats relate only to the translational temperature, thus $\overline{R}/\overline{c_v} = 2/3$, and
$R_e/c_{v_e} = 2/3$. This assumption simplifies the modified convective speed $\overline{u}'$ to our
$u'$.

### 5.2 Recommendations – Future Work

The next step is to find the eigenvectors. This is currently in progress at MSFC. Efforts as of this writing, using the symbolic mathematical capabilities of MatLab,
have failed due to excessive memory requirement. This is thought to result from MatLab's inability to automatically make the correct substitutions for complex expressions during the derivation. In fact, the expressions thus derived for the eigenvalues necessitated considerable simplification by hand. Nevertheless, such computational tools are still deemed essential for completion of the complex linear algebra within a reasonable timeframe.

A worthwhile approach is thought to be to derive the eigenvectors in Cartesian, rather than general coordinates, and then apply a three-dimensional rotation matrix. This has been done in two-dimensional cases by a number of researchers, but no instances of three dimensional rotation matrices have been found in the literature, and it is not known a priori if one can be derived. Also, reconstructing the fluxes still requires the eigenvalues in general coordinates. For future similar efforts, perhaps the eigenvalues should also be derived first in Cartesian coordinates, and those in general coordinates inferred from the observation that speeds with associated directions can simply be replaced with their rotated counterparts.

When the eigenvectors are found, the coding will be straightforward and can be added to the open source CFD code HYP, which is under continuous development at Embry Riddle Aeronautical University. In practice, some revisions may be found to be in order. A first attempt to simplifying the model is due to the fact that temperatures within the MPDT can reach 20,000 K. At these temperatures, complete dissociation occurs, leaving only monatomic gases. For a monatomic gas, rotational and vibrational effects are not present. Consequently, modeling these energies might be unnecessary and thus the size of the numerical model would be reduced. Another reduction in the complexity of the model might be realized by regarding electron/electronic non-equilibrium differently. Electron/electronic non-equilibrium might cause numerical stiffness when source terms are implemented, in which case reproducing Candler's procedure might be a solution. Again, Candler does not differentiate electronic energy with respect to electron temperature, but rather groups it with the heavy-particle energy.
Certain physical processes have not been addressed in this work. As part of this work's assumptions, viscosity, resistive diffusion and Hall terms were nicely, yet justifiably, set aside. The numerical treatment of these diffusive, as opposed to wavelike, processes is much simpler. On the other hand, radiation transport, which is significant at the temperatures typical of an MPDT, is extremely complicated and computationally intensive. Finally, the source terms by which molecular energies are exchanged have not yet been implemented. A body of literature exists on these processes, from which it will be straightforward to construct appropriate models.

Upon completion of the eigensystem, and its inclusion in the CFD code, sample calculations will be performed in association with colleagues at NASA MSFC, Advanced Concepts Office. Subsequently, the revised code's integration into the existing Multiphysics Tool will enable coupled heat transfer and structural analysis calculations. Test cases for the CFD code will be selected from the current literature. Our hope is to apply the code to designs now evolving within the MSFC Propulsion Research Center and elsewhere.
Appendix A

Expansion of the Flux Vector
The flux vector in Cartesian coordinates is split into its three directions as:

\[
\mathbf{F}_{\text{flows}} = \begin{pmatrix}
\rho \mathbf{u} \\
\rho \mathbf{v} \\
\rho \mathbf{w} \\
\rho \mathbf{u}^2 + p + \frac{\mathbf{B}^2}{2 \mu_0 \hat{a}} - \frac{\mathbf{B}^2}{\mu_0 \hat{a}} \\
\rho \mathbf{v}^2 + p + \frac{\mathbf{B}^2}{2 \mu_0 \hat{a}} - \frac{\mathbf{B}^2}{\mu_0 \hat{a}} \\
\rho \mathbf{w}^2 + p + \frac{\mathbf{B}^2}{2 \mu_0 \hat{a}} - \frac{\mathbf{B}^2}{\mu_0 \hat{a}} \\
\rho \mathbf{u} \mathbf{v} - \frac{\mathbf{B} \mathbf{v}}{\mu_0 \hat{a}} \\
\rho \mathbf{u} \mathbf{w} - \frac{\mathbf{B} \mathbf{w}}{\mu_0 \hat{a}} \\
\rho \mathbf{w} \mathbf{v} - \frac{\mathbf{B} \mathbf{v}}{\mu_0 \hat{a}} \\
\mathbf{u} \mathbf{B} - \mathbf{B} \mathbf{u} \\
\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v} \\
\mathbf{w} \mathbf{B} - \mathbf{B} \mathbf{w} \\
\mathbf{e} \mathbf{u} \\
\mathbf{e} \mathbf{v} \\
\mathbf{e} \mathbf{w} \\
\mathbf{e} _{\text{elec}} \mathbf{u} \\
\mathbf{e} _{\text{elec}} \mathbf{v} \\
\mathbf{e} _{\text{elec}} \mathbf{w} \\
\end{pmatrix}
\]

\[
\mathbf{B}^2 = B_x^2 + B_y^2 + B_z^2
\]

\[
\rho = \rho_e \sum_{i \in e} \rho_i \\
p = p_e \sum_{i \in e} p_i
\]

\[
E_e = \frac{\rho_e c_e T_e}{2} + \frac{\rho_e}{2} (u^2 + v^2 + w^2)
\]

\[
E_r = \frac{\sum_{i \in e} (\rho_i c_{r_i})}{\sum_{i \in e} \rho_i} (p - p_e) + E_s + E_v + E_e + E_{\text{elec}} + ...
\]

\[
E_T = \frac{R}{M_s} \sum_{i \in e} \rho_i \mathbf{u}^2 + \mathbf{v}^2 + \mathbf{w}^2 + \frac{\mathbf{B}_x^2 + \mathbf{B}_y^2 + \mathbf{B}_z^2}{2 \mu_0 \hat{a}} + \sum \rho_i h_s
\]

\[
\text{Translational Energy} \\
\text{Vibrational Energy} \\
\text{Rotational Energy} \\
\text{Electronic Energy} \\
\text{Electronic Energy} \\
\text{Kinetic Energy} \\
\text{Magnetic Energy} \\
\text{Chemical Heat of Formation}
\]

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Appendix B

Homogeneity of the Flux Vector
We say that $\mathbf{F}(\mathbf{Q})$ is homogeneous of degree $n$ if the following relation is true:

$$\mathbf{F}(k \cdot \mathbf{Q}) = k^n \cdot \mathbf{F}(\mathbf{Q})$$

(B.1)

Homogeneity of degree one is equivalent to linearity. Again, note that the flux vector in general coordinates is obtained after linear algebra on three separate vectors that are strictly similar. The only difference resides in the place of terms associated with each velocity component: $u$, $v$, and $w$. Those terms shift diagonally. The process below shows homogeneity for the $x$-component only. Linear algebra implies that the process is the same for the two other directions, and that a combination of those processes will make the final flux still homogeneous.

The $x$-flux is:

$$\mathbf{F} = \begin{pmatrix}
\rho \mu \\
\rho u \mu \\
\rho w \mu \\
\rho u^2 + p + \frac{B_x^2}{2\mu_0}\frac{B_x^2}{\mu_0} \\
\rho v u - \frac{B_x B_y}{\mu_0} \\
\rho w u - \frac{B_x B_z}{\mu_0} \\
u B_x - B_x u \\
u B_x - B_x v \\
u B_x - B_x w \\
E_x \mu \\
E_x \mu \\
E_{\text{elec}} \mu \\
\left( E_r + p + \frac{B_r^2}{2\mu_0} \right) u - \frac{B_r}{\mu_0} u \cdot \mathbf{B} \\
\left( E_r + p + \frac{B_r^2}{2\mu_0} \right) u - \frac{B_r}{\mu_0} u \cdot \mathbf{B} \\
0
\end{pmatrix}$$

(B.2)
Again, expressed as a function of the conserved variables:

\[
F = \left( \frac{(\rho u)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho v)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho w)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho u)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho v)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho w)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho u)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho v)}{\rho_1 + \rho_e} \right) + \left( \frac{(\rho w)}{\rho_1 + \rho_e} \right)
\]

The electron pressure as well as the static pressure need to be expressed as a function of the conserved variables only.
Solving for electron pressure from Equation (3.87):

\[
p_e(Q) = \frac{2}{3} \left( E_e - \frac{\rho_e}{2} \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{(\rho_i + .. + \rho_e)^2} \right)
\]  

(4.54)

Checking homogeneity of that term yields:

\[
p_e(k \cdot Q) = \frac{2}{3} \left( k E_e - \frac{k \rho_e}{2} \frac{k^2 (\rho u)^2 + k^2 (\rho v)^2 + k^2 (\rho w)^2}{k^2 (\rho_i + .. + \rho_e)^2} \right) = k \cdot p_e(Q)
\]  

(B.4)

Solving for total pressure from Equation (3.72) (Note that \( \tilde{\alpha} \) was introduced in that equation.):

\[
p(Q) = p_e + \sum_{s \in e} \left( \rho_s \frac{R_s}{M_s} \right) \left( E_r - E_v - E_v - E_{el} - \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{2(\rho_i + .. + \rho_e)^2} \sum_{s \in e} \rho_s \right)
\]

\[
... - \frac{B_s^2 + B_v^2 + B_{el}^2}{2 \mu_0 \tilde{\alpha}} \sum_{s \in e} \rho_s h_s^{e}
\]

(B.5)

Checking for homogeneity:

\[
p(k \cdot Q) = \sum_{s \in e} \left( k \rho_s \frac{R_s}{M_s} \right) \left( k E_r - k E_v - k E_v - k E_{el} - \frac{k^3 (\rho u)^2 + k^3 (\rho v)^2 + k^3 (\rho w)^2}{2k^2 (\rho_i + .. + \rho_e)^2} \sum_{s \in e} k \rho_s \right)
\]

\[
... - \frac{k^3 B_s^2 + k^3 B_v^2 + k^3 B_{el}^2}{2 \mu_0 k \tilde{\alpha}} - \sum_{s \in e} k \rho_s h_s^{e} + p_e(k \cdot Q)
\]

= \( k \cdot p(Q) \)

(B.6)
Overall, replace the conserved variables $Q$ by:

$$k \cdot Q = (k \rho_t, k \rho_m, k \rho_e, k \rho_u, k \rho_v, k \rho_w, k B_y, k B_z, k E_e, k E_\text{elec}, k E_r, k E_e, k E_r, k \hat{\mu})^T$$

(B.7)

$$F(k \cdot Q) =$$

$$
\begin{align*}
&\begin{bmatrix}
\frac{k}{k \rho_t} - \frac{k (\rho_t)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} \\
\end{bmatrix}
\end{align*}
$$

$$
\begin{align*}
&\begin{bmatrix}
\frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} \\
\frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} & \frac{k (\rho_v)}{k \rho_t} - \frac{k (\rho_v)}{k \rho_t + k \rho_r} & \frac{k (\rho_w)}{k \rho_t} - \frac{k (\rho_w)}{k \rho_t + k \rho_r} & \frac{k (\rho_u)}{k \rho_t} - \frac{k (\rho_u)}{k \rho_t + k \rho_r} \\
\end{bmatrix}
\end{align*}
$$

(B.8)
Factoring constant $k$:

$$F(k \cdot Q) =$$

\[
\begin{align*}
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B, \\
&= \frac{(\rho \nu)}{\rho_1 + \rho_e} - B.
\end{align*}
\]

Once constant $k$ is factored out of the vector, the right-hand side is easily seen as equal to $k \cdot F(Q)$. This proves that $F(k \cdot Q) = k \cdot F(Q)$.
Appendix C

Expressing the $\xi$-Component of the Flux Vector in General Coordinates
The initial coordinate system is a Cartesian \((x, y, z)\) system with which the flow relates but not in a smooth manner. The flow does not follow the perfectly orthogonal \(x\), \(y\), and \(z\) axis. The general coordinate system (or normalized metrics) \((\xi, \eta, \zeta)\) follows the geometry, thus is more likely related to the flow field lines. The normalized metrics are just direction cosines of the general coordinates with respect to the \(x\), \(y\), and \(z\) coordinates. The flux vector in the \(x\)-direction becomes the flux vector in the \(\xi\)-direction. The derivations are detailed line by line using the following relations between the two coordinate systems:

\[
\mathbf{F}' = \xi_x \mathbf{F} + \xi_y \mathbf{G} + \xi_z \mathbf{H}
\]

Notations in the final flux vector, the general speed and the general magnetic field expressions are:

\[
u' = \xi_x u + \xi_y v + \xi_z w
\]

\[
B_x' = \xi_x B_x + \xi_y B_y + \xi_z B_z
\]

1. Continuity equations – line 1 to line \(ns+1\)

\[
(F')_1 = \xi_x (F)_1 + \xi_y (G)_1 + \xi_z (H)_1
\]

\[
= \xi_x \rho_1 u + \xi_y \rho_1 v + \xi_z \rho_1 w
\]

\[
= \rho_1 (\xi_x u + \xi_y v + \xi_z w)
\]

\[
= \rho_1 u'
\]

The same procedure is applied for lines 2 to \(ns+1\), lines related to the densities of each species involved in the chemical reaction, both heavy particles and electrons.

\[
(F')_{ns,e} = \rho_{ns,e} u'
\]
2. Momentum equations – line ns+2, ns+3 and ns+4

\[(F')_{n+2} = \xi_x (F)_{n+2} + \xi_y (G)_{n+2} + \xi_z (H)_{n+2}\]
\[= \xi_x \left( \rho u^2 + p + \frac{B^2}{2\mu_0} - \frac{B_z^2}{\mu_0} \right) + \xi_y \left( \rho uv - \frac{B_x B_y}{\mu_0} \right) + \xi_z \left( \rho uw - \frac{B_x B_z}{\mu_0} \right)\]
\[= \rho u \left( \xi_x u + \xi_y v + \xi_z w \right) + \xi_x \left( p + \frac{B^2}{2\mu_0} \right) - \frac{B_z^2}{\mu_0} \left( \xi_x B_x + \xi_y B_y + \xi_z B_z \right)\]
\[= \rho uu'^z \left( \frac{p + B^2}{2\mu_0} \right) - B_z \frac{B_z}{\mu_0} \]  

(C.3)

Line ns+3 and ns+4 are strictly similar to line ns+2. Results are:

\[(F')_{n+3} = \rho uu'^z \left( \frac{p + B^2}{2\mu_0} \right) - B_z \frac{B_z}{\mu_0} \]  

(C.4)

\[(F')_{n+4} = \rho uu'^z \left( \frac{p + B^2}{2\mu_0} \right) - B_z \frac{B_z}{\mu_0} \]  

(C.5)

3. Magnetic equations – line ns+5, ns+6, ns+7

These lines relate to each component of the magnetic field and follow the same derivation process.

\[(F')_{n+5} = \xi_x (F)_{n+5} + \xi_y (G)_{n+5} + \xi_z (H)_{n+5}\]
\[= \xi_x (uB_x - B_x u) + \xi_y (vB_x - B_y u) + \xi_z (wB_x - B_z u)\]
\[= (\xi_x u + \xi_y v + \xi_z w)B_x - u(\xi_x B_x + \xi_y B_y + \xi_z B_z)\]
\[= uu'B_x - uB_x' \]  

(C.6)

\[(F')_{n+6} = uu'B_x - vB_z' \]  

(C.7)

\[(F')_{n+7} = uu'B_z - wB_x \]  

(C.8)
4. Energy equations – Lines ns+8 to ns+12

The next five lines relate to the different energies. They appear in the following order: vibrational, rotational, electronic, electron, and total energy. Vibrational, rotational, and electronic are very similar.

\[
(F')_{ns+8} = \xi_x (F)_{ns+8} + \xi_y (G)_{ns+8} + \xi_z (H)_{ns+8}
= \xi_x E_v u + \xi_y E_v v + \xi_z E_v w
= E_v (\xi_x u + \xi_y v + \xi_z w)
= E_v u'
\] (C.9)

\[
(F')_{ns+9} = E_e u'
\] (C.10)

\[
(F')_{ns+10} = E_{elec} u'
\] (C.11)

For the electron flux, we have

\[
(F')_{ns+10} = \xi_x (F)_{ns+10} + \xi_y (G)_{ns+10} + \xi_z (H)_{ns+10}
= \xi_x \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) u - \frac{B_x}{\mu_a} u \cdot B + \xi_y \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) v - \frac{B_y}{\mu_a} u \cdot B
+ \xi_z \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) w - \frac{B_z}{\mu_a} u \cdot B
+ \xi_x \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) u - \frac{B_x}{\mu_a} u \cdot B
+ \xi_y \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) v - \frac{B_y}{\mu_a} u \cdot B
+ \xi_z \left( E_e + p_e + \frac{B^2}{2\mu_a} \right) w - \frac{B_z}{\mu_a} u \cdot B
\] (C.12)

Similarly, for the total energy flux:

\[
(F')_{ns+11} = \left( E_t + \frac{B^2}{2\mu_a} \right) u - \frac{B_x}{\mu_a} u \cdot B
\] (C.13)
The final ξ homogeneous flux vector is:

\[
\begin{pmatrix}
\rho u' \\
\rho \rho_\Omega u' \\
\rho \rho_\Omega u' \\
\rho \nu u' + \xi_x \left( p + \frac{B^2}{2\mu_\Omega} \right) - \frac{B \cdot B}{\mu_\Omega} \\
\rho \nu u' + \xi_y \left( p + \frac{B^2}{2\mu_\Omega} \right) - \frac{B \cdot B}{\mu_\Omega} \\
\rho \nu u' + \xi_z \left( p + \frac{B^2}{2\mu_\Omega} \right) - \frac{B \cdot B}{\mu_\Omega} \\
\frac{u' B_x - B_y}{\mu_\Omega} \\
\frac{u' B_x - B_y}{\mu_\Omega} \\
\frac{u' B_x - B_y}{\mu_\Omega} \\
\frac{E_x u'}{\mu_\Omega} \\
\frac{E_x u'}{\mu_\Omega} \\
\frac{E_x u'}{\mu_\Omega} \\
\frac{(E_x + p_x + \frac{B^2}{2\mu_\Omega}) u' - \frac{B_x}{\mu_\Omega} (\mathbf{u} \cdot \mathbf{B})}{\mu_\Omega} \\
\frac{(E_y + p_y + \frac{B^2}{2\mu_\Omega}) u' - \frac{B_y}{\mu_\Omega} (\mathbf{u} \cdot \mathbf{B})}{\mu_\Omega} \\
0
\end{pmatrix}
\]  

(4.44)

The derivations of G' and H' follow the same method again using:

\[
v' = \eta_x u + \eta_y v + \eta_z w
\]  

(4.13)

\[
w' = \xi_x u + \xi_y v + \xi_z w
\]  

(4.14)

and

\[
B_y' = \eta_x B_y + \eta_y B_y + \eta_z B_z
\]  

(4.16)

\[
B_z' = \xi_x B_z + \xi_y B_y + \xi_z B_z
\]  

(4.17)
Hence the $\eta$ and the $\zeta$ homogeneous fluxes are respectively:

\[
\begin{align*}
G' &= \begin{pmatrix}
\rho v'

\rho v

\rho \\
\rho v'
\rho w'
\rho w'
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Appendix D

Derivation of Vector $b$
Again, from Section 4.5.2.3 Algebra Simplifications page 43,

\[ F' = \begin{bmatrix} S_p^{-1} A_p S_p Q_p & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} b \\ \hat{a} \end{bmatrix} \]  \hspace{1cm} (4.48)

or,

\[ S^{-1} A_e S = \begin{bmatrix} S_p^{-1} A_p S_p & b \\ 0 & 0 \end{bmatrix} \]  \hspace{1cm} (D.1)

Multiplying each matrix using the software Matlab gives,

\[ \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{6} \xi \frac{B^2}{\hat{a}^2 \mu_0} \\ \frac{1}{6} \xi \frac{B^2}{\hat{a}^2 \mu_0} \\ \frac{1}{6} \xi \frac{B^2}{\hat{a}^2 \mu_0} \\ \frac{1}{6} \xi \frac{B^2}{\hat{a}^2 \mu_0} \\ -u \frac{\hat{a}}{B_x} \\ -v \frac{\hat{a}}{B_x} \\ -w \frac{\hat{a}}{B_x} \\ 0 \\ 0 \\ 0 \\ \frac{1}{2} u \frac{B^2}{\hat{a}^2 \mu_0} \\ \frac{1}{6} u \frac{B^2}{\hat{a}^2 \mu_0} \\ 0 \end{bmatrix} \]

\hspace{1cm} (D.2)
Appendix E
Intermediate Matrices Used
to Find the Eigenvalues
This appendix presents the various matrices involved successively in the flux vector splitting method. These include the various eigensystems of MacCormack and Powell.

\[
S \frac{\partial F}{\partial v} = \begin{bmatrix}
  u' & 0 & 0 & \xi, \rho_1 & \xi, \rho_1 & \xi, \rho_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 & \rho \mu_0 \\
  0 & u' & 0 & \xi, \rho_{wa} & \xi, \rho_{wa} & \xi, \rho_{wa} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & u' & \xi, \rho_e & \xi, \rho_e & \xi, \rho_e & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & u' & 0 & \xi, B_x & \xi, B_x & \xi, B_x & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & u' & \xi, B_x & \xi, B_x & \xi, B_x & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & u' & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

where:

\[
C_1 = \frac{5}{3} \rho e + \frac{B^2}{3 \dot{\rho} \mu_0} \\
C_2 = \frac{2}{3 \dot{\rho} \mu_0} \frac{\rho - \rho_e}{\rho} \\
C_3 = -\frac{1}{2} \frac{B^2}{\dot{\rho}^2 \mu_0 \rho}
\]
with again,

$$C_2 = \frac{2}{3\hat{a}\mu_0} \frac{\rho - \rho_e}{\rho}$$  \hspace{1cm} (E.3)

$A_\varepsilon$ is calculated easily using Equation (4.47):

$$A_\varepsilon = S \frac{\partial F}{\partial V} - S \frac{\partial P}{\partial V} \frac{B_\varepsilon}{\mu_0 \hat{a}}$$
\[
\begin{align*}
S \frac{\partial E}{\partial V} - S \frac{\partial P}{\partial V} \left( \frac{B^i}{\partial \mu_0} \right) = \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
\xi, \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
\xi, \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
\xi, \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
\xi, \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{align*}
\]

Again, \( C_1 = \frac{5}{3} \rho_e + \frac{B^2}{3\partial \mu_0} \) (E.2) \( C_2 = \frac{2}{3\partial \mu_0} \frac{\rho - \rho_e}{\rho} \) (E.3) \( C_3 = -\frac{1}{2} \frac{B^2}{\partial^2 \mu_0 \rho} \) (E.4)
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