

Abstract

AMAR, ADAM JOSEPH. Modeling of One-Dimensional Ablation with Porous Flow Using Finite Control Volume Procedure. (Under the direction of Dr. Jack R. Edwards.)

The development and verification of a one-dimensional (planar) material thermal response code with ablation is presented. The mixture energy, gas phase continuity, and solid phase continuity equations are solved with Fourier's law to model heat conduction, Darcy's law to model porous flow, and the ideal gas law to model the state of the pyrolysis gases. Consequently, the temperature, gas density, and solid density profiles are predicted for a decomposing ablator and the resulting gas flux, porosity, and pore pressure can be determined.

The control volume finite element spatial discretization method (CVFEM), the Euler implicit time integrator, and a contracting grid scheme are used for the solution of the mixture energy and gas phase continuity equations. The solid continuity equation is solved through direct integration of decomposition kinetics under the assumption of a constant temperature rise rate within a given time step. The mixture energy and gas phase continuity equations are solved using segregated Newton solvers, which allow for nonlinear iteration on the entire system of nodal equations that are discretized according to a residual formulation. The block Gauss-Seidel segregated solution procedure has been implemented to globally iterate on the system of governing equations resulting in a fully coupled solution.

Formal verification studies were performed that show the implemented model exhibits second order spatial accuracy and first order temporal accuracy. In addition, the second order nonlinear convergence of the Newton solvers was verified for

temperature dependent material properties, the thermochemical ablation model, the heat of ablation model, decomposing materials, and several nonlinear boundary conditions. While not considered a part of the formal verification process, code-to-code comparisons are also presented.

Timing studies were performed, and when comparable accuracy is considered, the method developed in this study exhibits significant time savings over the property lagging approach typically used in legacy codes. In addition, maximizing the Newton solver's convergence rate by including sensitivities to the surface recession rate for the mixture energy equation reduces the overall computational time when compared to lagging the grid convection terms in the iteration process.

Modeling of One-Dimensional Ablation with Porous Flow Using Finite Control Volume Procedure

by

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Biography

Adam Joseph Amar was born in Green Bay, Wisconsin on March 9, 1982 to Jack and Diane Amar and is the younger brother of Jason Amar, Rebecca Dees, and Sarah Amar. He attended St. Patrick's Catholic Elementary School, Holy Trinity Catholic Middle School, and Charlotte Catholic High School all in Charlotte, North Carolina. He began his college career at North Carolina State University in the fall of 2000 and completed his Bachelor of Science degree in Aerospace Engineering in May of 2004. At that time, he enrolled in graduate school at North Carolina State University in pursuit of a Master of Science degree in Aerospace Engineering. Upon completion of his thesis requirements in August of 2006, he will begin employment in the Applied Aerosciences and CFD Branch at the National Aeronautics and Space Administration Lyndon B. Johnson Space Center in Houston, Texas.

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List of Symbols

Roman symbols:

A	Area
$\mathbf{A}$	Area vector
a, b	Constants
B'_c	Dimensionless char ablation rate
Bi	Biot number
C_h	Corrected heat transfer Stanton number
C_{ho}	Uncorrected heat transfer Stanton number
C_m	Mass transfer Stanton number
C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
D_p	Pore hydraulic diameter
DE	Discretization error
E	Activation energy in Arrhenius relationship
$\dot{E}$	Energy transfer rate due to control volume convection
$\tilde{E}$	Energy content
e	Specific internal energy
(e)	Element
$\dot{G}$	Energy transfer rate from gas flux
H	Convective heat transfer coefficient
h	Specific enthalpy
h_f°	Heat of formation
k	Thermal conductivity or pre-exponential factor in Arrhenius relationship
L	Time dependent domain length

$\hat{M}$	Molecular weight
$\tilde{M}$	Gas mass flux with grid convection contribution
$\tilde{M}$	Gas mass content
$\dot{m}''$	Mass flux
$\dot{m}'''$	Volumetric mass source term
N	Shape function
Pr	Prandtl number
$\mathbf{Q}$	Volumetric flow rate vector
Q^*	Heat of ablation
$\dot{Q}$	Heat conduction rate
$\dot{q}''$	Heat flux
$\dot{\mathbf{q}}''$	Heat flux vector
R	Residual
$\mathbf{R}$	Residual vector
$\hat{R}$	Universal gas constant
r	Recovery factor or ratio of characteristic mesh lengths
Re	Reynolds number
s	Surface recession
$\dot{s}$	Surface recession rate
T	Temperature
t	Time
u	Velocity
u'	Superficial velocity
V	Volume
$\mathbf{v}$	Velocity vector
$\mathbf{v}'$	Superficial velocity vector

w	Dimensionless relative density
$\overline{X}$	Average of adjacent nodal values of any quantity X
x	Coordinate with respect to instantaneous ablation front
y	Mass fraction
z	Coordinate with respect to initial ablation front
$\dot{z}$	Nodal velocity

Greek symbols:

α	Thermal diffusivity
β	Extent of reaction (degree of char)
Γ	Initial resin volume fraction
δ	Perturbation
ϵ	Emissivity
η	Landau coordinate
Θ	Time rate of change of temperature
θ	Transformed temperature
κ	Permeability
λ	Blowing reduction parameter
μ	Dynamic viscosity
ν_n	Eigenvalue
ξ	Local coordinate
ρ	Density
σ	Stefan-Boltzman constant
ϕ	Porosity
ψ	Reaction order in Arrhenius relationship
Ω	Stanton number correction factor

Subscripts:

A, B, C	Solid composite components
abl	Ablation
ah	Aerodynamic heating
$back$	Back boundary
blw	Blowing
bnd	Boundary
c	Char
$conv$	Convection
cs	Control surface
cv	Control volume
cw	Cold wall
e	Boundary layer edge condition
$elem$	Elements
f	Front boundary
$full$	Full sensitivity matrix
g	Gas
h, j	Nodal or element indices
hw	Hot wall
i	Composite component index
$iter$	Iterative solution procedure
lag	Property lagging solution procedure
N	Total number of elements or nodes
$nodes$	Nodes
o	Initial value
r	Value at recovery conditions

<i>rad</i>	Radiation
<i>ref</i>	Reference value
<i>res</i>	Reservoir property
<i>s</i>	Solid
<i>spec</i>	Specified quantity such as an input parameter
<i>surf</i>	Surface
<i>tri</i>	Tridiagonal sensitivity matrix
<i>v</i>	Virgin plastic
<i>w</i>	Property of the gases adjacent to the wall (surface)

Superscripts:

<i>converged</i>	Converged value
<i>g.c.</i>	Globally converged value
<i>n</i>	Time level
ν	Iteration level
*	Reference value

1 Introduction

For nearly half of a century, numerical heat transfer and ablation modeling have been important tools in the design and analysis of thermal protection systems. Researchers designing ballistic reentry vehicles for weapons applications in the 1950's introduced the idea of using ablative materials as heat shields. The National Aeronautics and Space Administration (NASA) helped pioneer the use of ablative materials for thermal protection systems during the development of Mercury, Gemini, and Apollo reentry capsules. Over the years, ablative materials have been used on reentry vehicle heat shields and drag flaps for weapons applications, rocket nozzle linings, and leading edges of hypersonic vehicles. Recently, NASA has introduced a new initiative for human exploration of the moon, and ablative heat shields have been chosen as the thermal protection system on the blunt body reentry capsule[1]. Due to the importance and cost of these aerospace systems, it is necessary to verify and validate predictions of material thermal response to ensure payload safety and maximize the performance of ablative thermal protection systems in extreme heating conditions.

1.1 Background

During atmospheric entry or reentry, a hypersonic vehicle will induce a shock wave that will greatly increase the pressure and temperature of the gases adjacent to the vehicle's surface. This can also prompt chemical reactions that dissociate and even ionize the gaseous species. The increase in pressure coupled with viscous effects creates drag and causes the vehicle to rapidly decelerate while heat is transferred to the body through the boundary layer. Heat transfer at the vehicle's surface is dominated by convection while heat can also be absorbed or rejected from the body through radiation. It is the function of the thermal protection system to minimize the heat conducted into the body so the vehicle's substructure will not fail under the

intense thermal loads.

The most well-known thermal protection system to the general public is the ceramic tile array that covers the underbody of NASA's space shuttle orbiters. Upon reentry into the Earth's atmosphere, these tiles provided the vehicle and payload with insulation against extreme heating conditions during the rapid deceleration process. In general, if the integrity of a given tile has not been compromised, then it can be reused on subsequent flights since it has the same structure and protective capabilities as it did pre-flight. On the other hand, ballistic reentry vehicles are subject to more intense heating conditions than NASA's orbiters, and it is necessary to provide these vehicles with another type of thermal protection system that can protect the vehicle during atmospheric reentry. Ablative materials have been a common and proven choice for this application for nearly half of a century.

Ablation is the process by which a system rejects energy through mass loss from the system. In general, this mass loss can be instigated by phase change, chemical erosion, oxidation, and mechanical removal. Most commonly, materials that lose mass due to phase change and/or chemical reactions are of interest for heat shield applications. Since mass loss occurs at the surface, energy incident on the body is used to remove mass (through any means mentioned above), and consequently a portion of the heat is prevented from transferring into the body. As a result, ablative thermal protective systems are considered non-reusable since the materials can change shape and composition throughout flight.

In general, there are two types of ablative materials: surface ablaters and decomposing ablaters. Surface ablaters are non-decomposing ablaters that only chemically erode, oxidize, or change phase at the exposed surface. Some common surface ablaters are metals, Teflon, graphite, and carbon-carbon. Carbon-carbon is a material that is commonly used to protect reentry vehicle sections that are subject to the high-

est mechanical stresses such as stagnation point regions, nose cones, and drag flaps, and it is used on the leading edges of NASA's shuttle orbiters[2]. Although surface ablators can generally withstand higher shear stresses than decomposing ablators, they are also generally heavier. Therefore if their use is necessary, they are limited to vehicle sections that are exposed to the highest structural loads when vehicle weight is a concern. In addition, carbon-carbon has a higher thermal conductivity than many decomposing ablators which makes it less effective at keeping heat from transferring to the substructure.

Decomposing or charring ablators, which are typically used for rocket nozzle linings and heat shield regions that are not subject to large shear stresses, undergo both surface erosion and in-depth decomposition. These materials are typically resin/binder composites that are less dense than surface ablators and are structurally weaker. Phenolic resins are commonly injected into binder materials such as carbon, silica, asbestos, and quartz. When in-depth temperatures are sufficiently high, the resin (and sometimes the binder material) pyrolyzes creating porous charred solid and gas that is free to move within the material and out to the surface depending on in-depth pressure gradients. Figure 1.1 shows the regions of interest in a decomposing ablator problem. The virgin and char layers have a constant solid density while the decomposition (or pyrolysis) zone is characterized by a steep solid density gradient. Each of the ablator's three layers is porous so gases are also free to move toward the impermeable substructure although the bulk motion is out of the ablating surface since the char layer has the least flow resistance.

1.2 Research Motivation and Previous Work

The goal of this study is to develop a one-dimensional material thermal response code with ablation that can predict the transient heat conduction and pyrolysis ef-

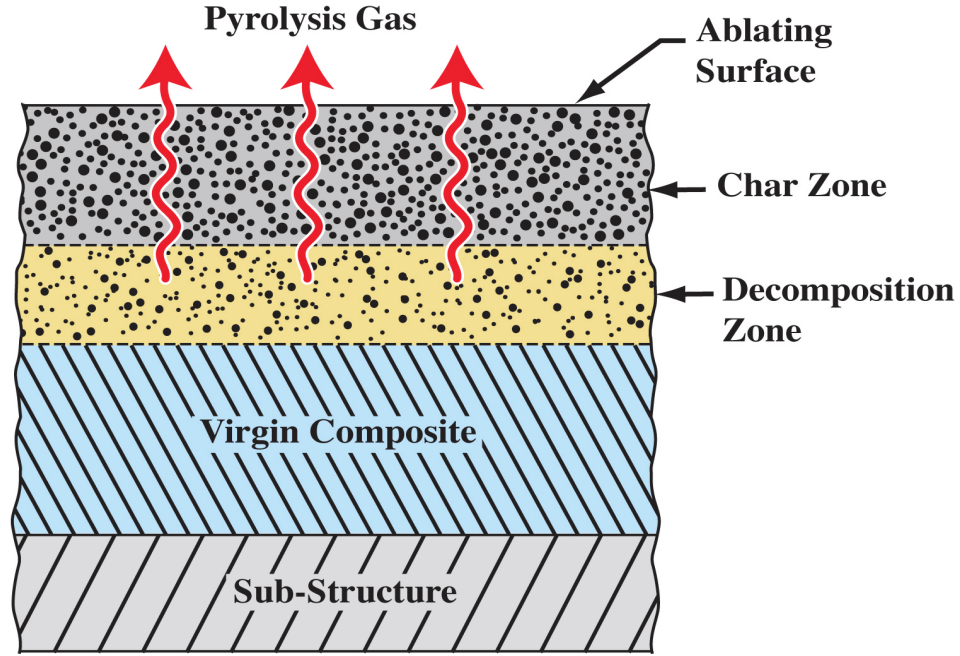


Figure 1.1: Schematic of a decomposing ablator.

fects within a porous charring ablator including in-depth gas flux, porosity, and pore pressure. Not only does this work provide a one-dimensional thermal response tool, but it also serves as a test-bed for algorithm development and verification methodology that is expected to be applied to multidimensional tools.

Due to the overwhelming amount of studies that have been performed over the past fifty years concerning ablation phenomenon, polymer decomposition, reentry heating, and their associated numerical methods, this literature review is in no way an attempt to examine all of the published work in this field. Rather, it is summary of the significant contributions that have been made to the field that were relevant throughout the course of this study and provide a historical perspective of the evolution of ablation modeling.

During the 1950s and 1960s, it is evident that NASA and defense contractors recognized the importance of accurate material thermal response predictions of reen-

try heat shields, and one means of providing this analysis was through the use of numerical methods and computational tools. Aerotherm Corporation, one of NASA's contractors during that time, developed Charring Materials Ablation[3] (CMA), and it has served as the industry standard for several decades. CMA is a one-dimensional material thermal response code with in-depth decomposition that solves the energy equation with pyrolysis gas effects. One of the primary physical assumptions that the developers, Moyer and Rindal, made was that for a given time step, the pyrolysis gas generated further in-depth than a given node was assumed to flow pass that node during the time step. Consequently, all of the gas generated during a time step was assumed to leave the material and the associated computational domain without any residence time in the porous ablator. As a result, gas phase continuity and momentum equations were not solved to predict the local state (density, pressure, and velocity) of the gas. Although this may be a valid assumption for most cases, it is of interest to know if the pore pressure is ever high enough to cause mechanical removal or in-depth damage to the solid. Consequently, it is important to include the gas phase continuity equation. In addition, CMA accounts for a loose-coupling between the solid phase continuity and energy equations where the updated solid density field is used in the energy equation solution, but the temperature profile is lagged one time step for the solid phase continuity equation solution. These assumptions are highly effective at keeping computational loads to a minimum, which was an issue during that era.

In terms of numerics, CMA has a finite difference spatial discretization of the governing differential equations and the Euler implicit time integrator. Moyer and Rindal implemented a translating grid scheme in which the grid is attached to the receding surface and the overall number of nodes in the domain is reduced as mass is removed at the ablating surface. With this method, each node, except the back

boundary node, translates with the same velocity as the surface node, and the size of grid cells remains fixed except for the back boundary cell which reduces in size until the cell reaches a critical thickness. Once the critical thickness has been reached, the last node is removed from the domain. An implementation of this method requires the developer to account for the energy in the dropped cell whether it be by assuming it is negligible or by including it in the updated domain.

Since the energy equation is nonlinear in both surface recession rate and temperature, a linearization method is necessary to find a solution. Moyer and Rindal accomplished this by lagging the thermophysical properties and surface recession rate one time step for the interior node equations while they iteratively solve the surface energy balance to find the updated recession rate. On a per time level basis, this method obviously saves time over iterating on the entire system of nodal equations, but it compromises accuracy at the same time. Aerotherm Corporation eventually became a division of Acurex Corporation and went on to develop a two-dimensional axisymmetric material thermal response code, ABRES Shape Change Code (ASCC)[4, 5], that included a fully coupled solid-fluid interaction but did not account for in-depth decomposition.

Although CMA was the most well-known and widely used tool developed during that time, another notable study is that of Valle, Pike, and April[6, 7]. This group not only solved the energy equation for a charring ablator, but they also modeled frozen, equilibrium, and nonequilibrium reacting gas flow to determine the gas composition, in-depth pressure, and the corresponding effects on the energy equation assuming thermal equilibrium between the solid and gaseous species.

Clark[8] went a step further and predicted the transient thermal response of a charring ablator with chemical and thermal nonequilibrium. In addition to allowing the pyrolysis gases to react among themselves, he also modeled the pyrolysis gas re-

actions with the decomposed solid in the char layer and the oxidation reaction at the ablator's surface. Although Clark's analysis of the gas phase was more sophisticated, he assumed that the pyrolysis zone was infinitely thin resulting in two constant density sections (charred and virgin) and the inability to predict a solid density profile through decomposition kinetics. It is also of interest to note that Clark did present comparisons between numerical and analytical results as a crude form of verification but did not present a formal verification study.

More recently Blackwell[9] presented the control volume finite element method (CVFEM) for solving ablation problems on translating/node-dropping grids with a fully implicit time integrator with which he implemented the Moyer and Rindal approach to iterating only on the nonlinear surface energy balance. The CVFEM requires a discretization of the integral form of the governing equations where information is known at element boundaries (nodes) and control volume boundaries are located at element centers. Consequently, the element assembly approach to generating the linearized system of energy balance equations, common in many finite element codes, can be used with the CVFEM. Blackwell also implemented exponential differencing which improves accuracy by allowing the discretization method to take advantage of the "exponential-like" temperature profile characteristic of many ablation problems.

Later, a contracting grid scheme for one-dimensional ablation was presented by Blackwell and Hogan[10] in which the relative size of grid cells and the total number of cells is fixed throughout the problem, and each node translates at a fraction of the surface recession rate. This eliminates the node-dropping complexity, but adds a change in energy content due to cell volume reduction. This method also has a more logical extension to multidimensions in which the mesh deformation is determined by treating the domain as a linear elastic solid as presented by Hogan et al.[11].

Blackwell's and Hogan's work also implemented the CVFEM with a fully implicit time integrator that again lagged material properties and iterated only on the surface energy balance.

Keyhani, Krishnan, and Polehn[12, 13, 14, 15] had a series of publications, concurrent with Blackwell's and Hogan's works, in which they developed finite difference models to predict the thermal response of one-dimensional, axisymmetric, and two-dimensional decomposing ablators with thermal nonequilibrium and in-depth pyrolysis gas flow analysis. They investigated the effects of loosely and fully coupling the energy and gas continuity equations and found that the two methods give significantly different predictions for pore pressure, but the temperature solution is relatively unaffected.

More recent one and two-dimensional studies with application work have been performed by several researchers at the Japan Aerospace Exploration Agency and Tohoku University[16, 17, 18]. Their one-dimensional work includes attempts at implicit integration of the loosely coupled, finite differenced governing equations to predict in-depth decomposition and gas effects. In their two-dimensional work, they implement a finite volume spatial discretization, implicit integration of the gas continuity and momentum equations, and explicit integration of the solid continuity and mixture energy equations. All of their work is presented with validation data from ground, flight, and wind tunnel tests.

Chen and Milos[19, 20, 21] have also done one, two, and three-dimensional ablation studies with applications. The one-dimensional work presents a finite difference method that includes in-depth gas effects and a fluids solver interface but only iterates on the nonlinear surface energy balance. Their two-dimensional work includes fully coupled fluid and material thermal response solutions using a finite difference method for the thermal response solution while the three-dimensional study couples their ab-

lation program (TITAN) with a finite-element thermal and structural analysis code used to determine the solution for the non-ablating, non-decomposing substructure.

Although there have been significant advances in ablation modeling techniques over the past fifty years, one aspect that all of the research is collectively lacking is published formal verification studies. Advances in the understanding of numerical methods can now give code developers insight into model behavior. As a result, it is necessary that modern code development practices include formal verification studies to ensure that developers have implemented what they intended to implement especially when the model is being developed for engineering/production applications. Detailed discussions on verification theory and practices can be found in Roache[22] and Knupp and Salari[23].

This study presents the development and verification of a one-dimensional planar material thermal response code that includes:

1. Implicit integration of the mixture (gas and solid) energy equation assuming thermal equilibrium between the solid and gas phases
2. Implicit integration of the gas phase continuity equation assuming the following:
 - Darcy's law is the momentum equation for the pyrolysis gases, and it can be used to determine the gas velocity in the pore space
 - The pyrolysis gases are a single entity that has a temperature dependent molecular weight, which accounts for a change in composition over a range of temperatures
3. Direct integration of the solid phase decomposition kinetics for the solution of the solid phase continuity equation

4. Fully coupled governing equations through the block Gauss-Seidel segregated solution procedure
5. Residual formulation of nodal energy and gas mass balance equations
6. Nonlinear iteration on the entire system of nodal residual equations for the mixture energy and gas phase continuity equations
7. The CVFEM spatial discretization on a contracting grid for the mixture energy and gas phase continuity equations
8. Energy equation time dependent boundary conditions including:
 - Specified temperature
 - Specified heat flux
 - Standard convection
 - Far-field radiation
 - Aerodynamic heating with corrections for hot wall and blowing effects on the convective heat transfer coefficient
9. Ablation models including:
 - Heat of ablation (Q^*)
 - Thermochemical ablation
10. Gas phase continuity equation time dependent boundary conditions including:
 - Specified pressure
 - Impermeable wall

It is also a goal of this study to publish detailed documentation of equation derivations and algorithm development. Many of the previous works only present outlines of the implemented equations, perhaps due to length limitations, without regard to future use by an outside party. Therefore this document is intended to be both a theory manual for the analysts using this code and a thorough reference for future code developers.

2 Governing Equations and Material Model

2.1 Governing Equations

The equations that govern the solid/gas system of the porous charring ablator include solid energy and continuity equations as well as the Navier-Stokes equations as applied to all of the gaseous species considered. In the general case, it is possible that the pyrolysis gases react among themselves, erode the remaining solid, or deposit residue (coke) on the solid, but these phenomena are neglected. Under the assumptions that the pyrolysis gas is a single nonreactive entity, the solid and gas are in thermal equilibrium, and there is no in-depth energy source, then the solid and gas energy equations for a moving grid reduce to a mixture energy equation given by¹

$$\underbrace{\int_{cs} \dot{\mathbf{q}}'' \cdot d\mathbf{A}}_{\text{conduction}} + \underbrace{\int_{cs} \phi \rho_g h_g \mathbf{v}_g \cdot d\mathbf{A}}_{\text{gas flux}} - \underbrace{\int_{cs} \rho h \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} + \frac{d}{dt} \underbrace{\int_{cv} \rho e dV}_{\text{energy content}} = 0 \quad (2.1)$$

and the mixture continuity equation is

$$\underbrace{\int_{cs} \phi \rho_g \mathbf{v}_g \cdot d\mathbf{A}}_{\text{gas flux}} - \underbrace{\int_{cs} \rho \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} + \frac{d}{dt} \underbrace{\int_{cv} \rho dV}_{\text{mass content}} = 0 \quad (2.2)$$

which is the sum of the solid and gas phase continuity equations given by

$$\text{solid: } \frac{d}{dt} \underbrace{\int_{cv} \rho_s dV}_{\text{solid mass content}} - \underbrace{\int_{cs} \rho_s \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} = \underbrace{\int_{cv} \dot{m}_s''' dV}_{\text{solid mass source}} \quad (2.3)$$

and

$$\text{gas: } \frac{d}{dt} \underbrace{\int_{cv} \phi \rho_g dV}_{\text{gas mass content}} + \underbrace{\int_{cs} \phi \rho_g \mathbf{v}_g \cdot d\mathbf{A}}_{\text{gas flux}} - \underbrace{\int_{cs} \phi \rho_g \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} = \underbrace{\int_{cv} \dot{m}_g''' dV}_{\text{gas mass source}} \quad (2.4)$$

¹Due to the nature of the CVPFEM, it is more convenient to deal with the integral form of the governing equations as opposed to the differential governing equations that can be found in the majority of the literature.

where

$$\int_{cv} \dot{m}_g''' dV + \int_{cv} \dot{m}_s''' dV = 0 \quad (2.5)$$

Applying the Navier-Stokes momentum equations to flow through the char layer would require detailed knowledge of the pore structure, and that information is not known. In 1856, Darcy[24] published results from a series of experiments in which he determined how the volumetric flow rate of a laminar flowing fluid relates to the local pressure gradient within a fully saturated porous medium.

$$\mathbf{Q} = -A \frac{\kappa}{\mu} \nabla P \quad (2.6)$$

The superficial or filtration velocity is the volumetric flow rate averaged over the cross-sectional area of the medium and is given by

$$\mathbf{v}' = \frac{\mathbf{Q}}{A} = -\frac{\kappa}{\mu} \nabla P \quad (2.7)$$

The average or seepage velocity of the fluid is the volumetric flow rate averaged over the cross-sectional area through which the fluid can flow (porous area) and is given by

$$\mathbf{v} = \frac{\mathbf{Q}}{\phi A} = -\frac{\kappa}{\phi \mu} \nabla P \quad (2.8)$$

which assumes that the surface porosity is equal to the volumetric porosity. Darcy's law is valid for laminar flows with "sufficiently" low Reynolds numbers based on pore hydraulic diameter and superficial velocity.

$$\text{Re} = \frac{|\mathbf{v}'| \rho D_p}{\mu} \quad (2.9)$$

The word "sufficiently" is ambiguous because several studies present different results as to what Reynolds number must be exceeded so that flow is no longer described by Darcy's law. This is mostly due to the indeterminacy of the hydraulic length scale of a given porous medium through hydraulic radius theory[25]. According

to Darcy's law, the fluid velocity is inversely proportional to the flow resistance and directly proportional to the pressure gradient. At higher velocities these relationships become nonlinear and Darcy's law is no longer valid. Since the flow of pyrolysis gas in the char layer is expected to be at low velocities, it is assumed that the flow can be described by Darcy's law. If the velocities were expected to be high enough for nonlinear effects to manifest themselves, then Darcy's law can be modified with a quadratic term to give the Darcy-Forchheimer relationship[15, 25].

Since the momentum equation for the pyrolysis gases is assumed to be Darcy's law, which provides a simple relationship between fluid velocity and the pressure gradient, Darcy's law in conjunction with the perfect gas law is treated as a closure relationship for the energy-continuity system of equations with surface recession rate, temperature, solid density, and gas density being the dependent variables. As a result, there is no independent solution of a momentum equation since this is inherent in the gas phase continuity equation solution.

Newton's method for a system of nonlinear equations is used to solve the mixture energy and gas phase continuity equations. Consequently, a residual formulation, or Δ -formulation, of the control volume energy and gas mass balance equations is solved resulting in the linear system's Jacobian matrix, $[A]$ in Eq. 2.10, being comprised of the residuals' sensitivities to the dependent variables.

$$[A] \Delta \mathbf{x} = \mathbf{R} \quad (2.10)$$

As a result, convergence can be monitored as the correction vector, $\Delta \mathbf{x}$, or the residual vector, $\mathbf{R}$, approaches zero. The solid continuity equation is not solved in this manner and is instead solved through direct integration of the decomposition kinetics as described in Section 6.

The solution procedure for the entire system of governing equations can be outlined as follows:

1. Iteratively solve the mixture energy equation with nodal temperatures and surface recession rate as the dependent variables
 - Adjust grid throughout iteration procedure
 - Hold nodal density and gas velocity values constant
2. Integrate kinetic relationships to solve solid phase continuity equation
 - Use updated grid and temperature field
3. Iteratively solve the gas phase continuity equation with nodal gas densities as the dependent variables
 - Use Darcy's law to determine pyrolysis gas velocity in the pore space
 - Use updated grid, temperature field, and gas source field
 - Hold solid density, temperature, and recession rate constant

This segregated solution procedure in which updated information is being used as soon as it is available is commonly referred to as the block Gauss-Seidel method which converges linearly if implemented correctly[26]. Steps 1-3 are repeated until global convergence of the Gauss-Seidel method is reached, and the system is considered globally converged when no local nonlinear iteration is necessary to converge the mixture energy equation.

2.2 Boundary Conditions

The mixture energy and gas mass conservation equations allow for heat and mass transfer respectively out of the domain, while the solid phase continuity equation is constrained to no solid mass flux at the boundaries. Since direct integration of the kinetic equations is used to solve the solid phase continuity equation resulting in

nodal solid density changes being independent of solid density changes at all other nodes, the application formal boundary conditions is not necessary.

An array of boundary conditions for the mixture energy equation has been implemented and the most commonly used for engineering applications are convective aerodynamic heating and radiation. Assuming equal species diffusion coefficients and equal mass and heat transfer Stanton numbers, the aerodynamic heating/radiation boundary condition with ablative and pyrolysis gas flux energy terms is given by

$$\dot{q}'' = \underbrace{\rho_e u_e C_{h_o} \left(\frac{C_h}{C_{h_o}} \right) (h_w - h_r)}_{\text{aerodynamic heating}} + \underbrace{\epsilon \sigma (T_{bnd}^4 - T_{res}^4)}_{\text{radiation}} + \underbrace{\dot{m}_s'' h_w}_{\text{ablation}} + \underbrace{\dot{m}_g'' h_w}_{\text{pyrolysis gas}} \quad (2.11)$$

where C_h/C_{h_o} is an empirical Stanton number correction for mass blowing and hot wall effects discussed in Section 5.5.5. The wall gas enthalpy (h_w) is defined as the enthalpy resulting from equilibrated reactions between ablation products, pyrolysis gases being injected into the boundary layer, and boundary layer gases from the surrounding environment. A detailed discussion of the general aerodynamic heating boundary condition with unequal species diffusion coefficients and unequal heat and mass transfer Stanton numbers is provided by Moyer and Rindal[3] and Kendall et al.[27].

Other implemented boundary conditions include specified heat flux, standard convection, and specified surface temperature, and the discretization of these terms is also discussed. These boundary conditions can be applied to engineering problems, but they also proved to be valuable tools throughout the debugging and verification processes. In addition, two ablation models, heat of ablation and thermochemical ablation, have been implemented to predict surface recession and energy loss due to mass rejection.

The boundary conditions for the gas phase continuity equation are limited to a specified pressure on the exposed surface and an impermeable back face. Both the

gas phase continuity and mixture energy equations' boundary conditions are time dependent.

2.3 Material Model

In order to complete the explanation of the governing equations and boundary conditions, it is important to understand the material model used to characterize the state of the solid/gas mixture. It is assumed that all the pores are interconnected, and therefore pyrolysis gases occupy all of the pore space and are free to flow through it. Consequently, the density of the solid/gas mixture is described by

$$\rho = \phi \rho_g + \rho_s \quad (2.12)$$

where the solid density is a bulk density, the gas density is a true density, and the porosity is equal to the gas volume fraction. In terms of units, Eq. 2.12 can be expressed as

$$\frac{\overbrace{[\text{mixture mass}]}^{\rho}}{\overbrace{[\text{mixture vol}]}^{\phi}} = \frac{\overbrace{[\text{pore vol}]}^{\phi}}{\overbrace{[\text{mixture vol}]}^{\phi}} \frac{\overbrace{[\text{gas mass}]}^{\rho_g}}{\overbrace{[\text{pore vol}]}^{\phi}} + \frac{\overbrace{[\text{solid mass}]}^{\rho_s}}{\overbrace{[\text{mixture vol}]}^{\phi}} \quad (2.13)$$

It is assumed that the thermodynamic state of the pyrolysis gases can be described by the perfect gas law, and that the solid and gas phases are in thermal equilibrium resulting in

$$P = \rho_g \frac{\hat{R}}{\hat{M}_g(T_g)} T_g \quad (2.14)$$

where

$$T_g = T_s = T \quad (2.15)$$

The solid material model adopted in this study is similar to the model used in CMA and is consistent with many of the studies mentioned in Section 1.2. The solid bulk density is given by

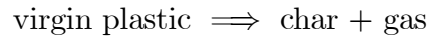
$$\rho_s = \underbrace{\Gamma(\rho_A + \rho_B)}_{\text{resin}} + \underbrace{(1 - \Gamma)\rho_C}_{\text{binder}} \quad (2.16)$$

where Γ is the resin volume fraction in the virgin composite. The component density terms are not truly densities, but they can be more appropriately considered component concentrations. Although using the symbol ρ to represent the concentrations is misleading, this nomenclature along with the "density" verbiage will continue to be used to be consistent with the precedent established by fifty years of published studies. The units associated with the solid bulk density model in Eq. 2.16 are

$$\begin{aligned} \frac{\overbrace{[\text{solid mass}]}^{\rho_s}}{[\text{mixture vol}]} &= \frac{\overbrace{[\text{initial resin vol}]}^{\Gamma}}{[\text{mixture vol}]} \left(\frac{\overbrace{[\text{comp. } A \text{ mass}]}^{\rho_A}}{[\text{initial resin vol}]} + \frac{\overbrace{[\text{comp. } B \text{ mass}]}^{\rho_B}}{[\text{initial resin vol}]} \right) \\ &\quad + \underbrace{\frac{[\text{initial binder vol}]}{[\text{mixture vol}]}}_{1-\Gamma} \underbrace{\frac{[\text{binder mass}]}{[\text{initial binder vol}]}}_{\rho_C} \end{aligned} \quad (2.17)$$

It is assumed that the solid does not change volume due to thermal expansion, and therefore the mixture volume is constant. It is important to note that the solid description in Eq. 2.16 is only a modeling assumption, and the solid is not truly comprised of three components or species. In other words, there are no distinctly distinguishable materials A , B , and C in a general decomposable resin/binder composite. This modeling assumption comes as a result of decomposition data obtained from thermogravimetric analyses (TGA). It has been observed that phenolic resins undergo a two-stage decomposition process that can be appropriately captured by the two resin component model[28]. The decomposition of the binder material, which occurs in asbestos and nylon phenolics, is accounted for in this model, but materials such as silica and carbon phenolics undergo no binder decomposition.

It is assumed that all decomposed solid mass results in gas mass generation, and the general model of the decomposition process is described by



This is a generalized description of the initial and final states of the system between which there are transitional states at which the solid can exist. The reaction is irreversible, and the pyrolysis gases are assumed to not react among themselves or with the remaining solid in the pore space.

Taking the temporal derivative of Eq. 2.16 gives the solid decomposition rate in terms of component decomposition rates.

$$\frac{\partial \rho_s}{\partial t} = \Gamma \left(\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_B}{\partial t} \right) + (1 - \Gamma) \frac{\partial \rho_C}{\partial t} \quad (2.18)$$

It is assumed that the decomposition of each component can be described by an Arrhenius relationship of the form

$$\frac{\partial \rho_i}{\partial t} = -k_i \rho_{v_i} \left(\frac{\rho_i - \rho_{c_i}}{\rho_{v_i}} \right)^{\psi_i} e^{-E_i/RT} \text{ for } i = A, B, \text{ and } C \quad (2.19)$$

which applies at a constant spatial location.

Since most thermophysical properties of the solid are only known for the virgin plastic and fully charred states, the intermediate solid is modeled as some interpolated state between virgin and char. This interpolated state is characterized by the extent of reaction (β), or degree of char, given by

$$\beta = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \quad (2.20)$$

where the virgin and char bulk densities are known constants. It is evident that as the solid decomposes from virgin to char, the extent of reaction ranges from 0 to 1. The definition in Eq. 2.20 can be rearranged to more clearly describe the interpolated state.

$$\rho_s = (1 - \beta) \rho_v + \beta \rho_c \quad (2.21)$$

Although the virgin and char materials are not distinguishable entities within the intermediate solid, Eq. 2.21 reveals that the degree of char represents an "imaginary"

char volume fraction within the solid (not in the solid/gas mixture). In a similar light, CMA defines an "imaginary" virgin mass fraction given by

$$y_v = \frac{\rho_v}{\rho_v - \rho_c} \left(1 - \frac{\rho_c}{\rho_s} \right) \quad (2.22)$$

which can be related to the extent of reaction through

$$y_v = \frac{\rho_v}{\rho_s} (1 - \beta) \quad (2.23)$$

Similarly the char mass fraction is given by

$$y_c = 1 - y_v = \frac{\rho_c}{\rho_s} \beta \quad (2.24)$$

These "imaginary" parameters are used to determine several solid and mixture properties.

3 Property Models

A summary of the thermophysical and thermodynamic properties that are input parameters is given in Table 3.1, while a discussion of the properties required for the solution of the governing equations follows. The listed functions in Table 3.1 are all tabulated.

Table 3.1: Thermophysical and thermodynamic property input parameters.

Input Parameter	Description
$C_{v_v}(T)$	Specific heat of the virgin material vs. temperature
$C_{v_c}(T)$	Specific heat of the char material vs. temperature
T_{ref}	Reference temperature for heats of formation
$(h_f^o)_v$	Virgin plastic heat of formation
$(h_f^o)_c$	Char heat of formation
$(h_f^o)_g$	Pyrolysis gas heat of formation
$k_v(T)$	Thermal conductivity of the virgin material vs. temperature
$k_c(T)$	Thermal conductivity of the char material vs. temperature
$\epsilon_v(T)$	Emissivity of the virgin material vs. temperature
$\epsilon_c(T)$	Emissivity of the char material vs. temperature
$h_g(T)$	Pyrolysis gas enthalpy vs. temperature
$\hat{M}_g(T)$	Pyrolysis gas molecular weight vs. temperature
$\phi(\beta)$	Porosity vs. extent of reaction
$\kappa(\beta)$	Permeability vs. extent of reaction
$\mu(T)$	Pyrolysis gas dynamic viscosity vs. temperature

3.1 Specific Internal Energy and Gas Enthalpy Models

The specific internal energy of the mixture will take into account both the solid and gas phases. The solid specific internal energy and enthalpy can be found from

$$e_s(T) = h_s(T) = y_v e_v(T) + (1 - y_v) e_c(T) \quad (3.1)$$

where $e_v(T)$ and $e_c(T)$ are determined through parabolic interpolation in the virgin and char specific internal energy tables developed in Appendix A, which also provides

details regarding the parabolic interpolation routine. The gas specific internal energy can be found from

$$e_g(T) = h_g(T) - \frac{P}{\rho_g} \quad (3.2)$$

and substituting in the ideal gas law gives

$$e_g(T) = h_g(T) - \frac{\hat{R}}{\hat{M}_g(T)}T \quad (3.3)$$

The mixture specific internal energy and enthalpy can then be determined from

$$e(T) = y_g e_g(T) + (1 - y_g) e_s(T) \quad (3.4)$$

and

$$h(T) = y_g h_g(T) + (1 - y_g) h_s(T) \quad (3.5)$$

where the gas mass fraction is defined as

$$y_g = \frac{\phi \rho_g}{\rho} \quad (3.6)$$

These definitions can be expanded in terms of extent of reaction to give

$$\rho e(T) = \phi \rho_g e_g(T) + \rho_v (1 - \beta) e_v(T) + \rho_c \beta e_c(T) \quad (3.7)$$

and

$$\rho h(T) = \phi \rho_g h_g(T) + \rho_v (1 - \beta) h_v(T) + \rho_c \beta h_c(T) \quad (3.8)$$

3.2 Specific Heats

Since internal energy and enthalpy are the same for solids, then

$$\frac{\partial e_s}{\partial T} = \frac{\partial h_s}{\partial T} \quad (3.9)$$

or

$$C_{v_s} = C_{p_s} \quad (3.10)$$

and the solid specific heat can be determined from

$$C_{v_s}(T) = C_{p_s}(T) = y_v C_{v_v}(T) + (1 - y_v) C_{v_c}(T) \quad (3.11)$$

Since the nodal density values are fixed while iteratively solving the mixture energy equation, the mass fraction terms have no temperature sensitivity.

The gas specific heat at constant volume is given by

$$C_{v_g}(T) = \frac{\partial e_g}{\partial T} \quad (3.12)$$

where $e_g(T)$ is defined in Eq. 3.3. Performing the differentiation gives

$$C_{v_g}(T) = C_{p_g}(T) - \frac{\hat{R}}{\hat{M}_g(T)} \left[1 - \frac{T}{\hat{M}_g(T)} \frac{\partial \hat{M}_g}{\partial T} \right] \quad (3.13)$$

where

$$C_{p_g}(T) = \frac{\partial h_g}{\partial T} \quad (3.14)$$

which can be determined from a finite difference of the pyrolysis gas enthalpy table.

The mixture specific heats can now be calculated from

$$C_p(T) = y_g C_{p_g}(T) + (1 - y_g) C_{p_s}(T) \quad (3.15)$$

and

$$C_v(T) = y_g C_{v_g}(T) + (1 - y_g) C_{v_s}(T) \quad (3.16)$$

3.3 Thermal Conductivity and Emissivity

It is assumed that the virgin and char thermal conductivities and emissivities are bulk properties of the porous solid, which is a feasible assumption since realistic experiments to determine these properties would be performed on a porous sample. In addition, it is assumed that the conductivity of the gas can be neglected, and therefore the mixture property is equal to the solid property. Unlike internal energy and specific heat, the definitions of thermal conductivity and emissivity do not inherently suggest

a natural weighting parameter (volume or mass fraction). Using either extent of reaction[29] or mass fraction[3] have both been utilized in previous studies, and a mass fraction weighting is used in this model. The resulting thermal conductivity and emissivity expressions are

$$k(T) = y_v k_v(T) + (1 - y_v) k_c(T) \quad (3.17)$$

and

$$\epsilon(T) = y_v \epsilon_v(T) + (1 - y_v) \epsilon_c(T) \quad (3.18)$$

and their sensitivities to temperature are

$$\frac{\partial k(T)}{\partial T} = y_v \frac{\partial k_v(T)}{\partial T} + (1 - y_v) \frac{\partial k_c(T)}{\partial T} \quad (3.19)$$

and

$$\frac{\partial \epsilon(T)}{\partial T} = y_v \frac{\partial \epsilon_v(T)}{\partial T} + (1 - y_v) \frac{\partial \epsilon_c(T)}{\partial T} \quad (3.20)$$

It is necessary to note that determining thermal conductivity and emissivity using mass weighted averages of the virgin and char states is strictly a modelling assumption in order to apply a physically meaningful property to the intermediate solid. There is not experimental data to ensure that these assumptions are correct, but available data is limited to virgin and char properties so an appropriate assumption must be made.

3.4 Porosity, Permeability, Viscosity, and Molecular Weight

The solution to the governing equations also accounts for variable porosity, permeability, pyrolysis gas viscosity, and pyrolysis gas molecular weight, and these properties are determined through linear interpolation in the tabulated functions described in Table 3.1. Since porosity and permeability data is known for the intermediate solid and both quantities are assumed to have no dependence on temperature, they are

tabulated as functions of extent of reaction, and beyond interpolation no further calculations are necessary to determine these properties.

4 Domain Description and Discretization Method

Before discussing the discretization of the governing equations and their respective solution procedures, it is necessary to provide a description of the coordinate systems, grid motion scheme, and spatial discretization method. The code developed during the current study has several grid generation options including:

1. Two manual node generation options
 - Specified nodal depths and initial temperatures
 - Specified element thicknesses and initial nodal temperatures
2. Automatic uniform grid generation based on domain length and number of elements specified
3. Automatic nonuniform grid generation with a geometric progression based on domain length, number of elements specified, and either first or last element thickness where

$$\frac{\Delta z_{j+1}}{\Delta z_j} = \text{constant} \quad (4.1)$$

and $\Delta z_j = z_{j+1} - z_j$

4.1 Spatial Discretization

The control volume finite element method, which has been previously used for ablation problems[9, 10], associates a control volume with each node in the discretized domain. For each internal node j , the nodal control volume has a left sub-control volume contained in element $(e)_{j-1}$ and a right sub-control volume in element $(e)_j$ as shown in Figure 4.1. As a result, control volume boundaries are always located at element centers, but element boundaries (or nodes) are only located at control volume centers when $\Delta z_{j-1} = \Delta z_j$.

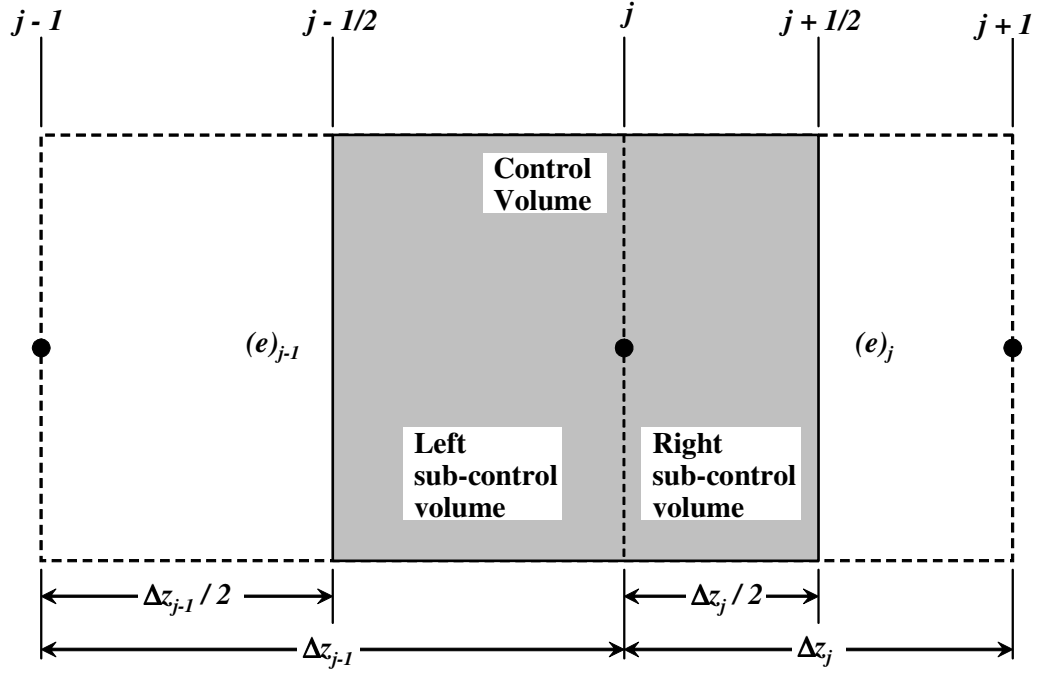


Figure 4.1: Schematic of control volume surrounding node j with elements $(e)_{j-1}$ and $(e)_j$.

Boundary nodes on the other hand can be conceptualized as having half-control volumes or control volumes containing only one sub-control volume. The first nodal control volume only has a right sub-control volume that is in the first element, and the last nodal control volume only has a left sub-control volume that is in the last element.

Data is stored at nodes and properties are assumed to vary linearly within each element for this study although assuming an exponential temperature variation has been shown to work for ablation problems[9, 10]. Throughout the development process, the CVFEM has provided several advantages over finite difference, and traditional finite volume methods including:

1. ease of handling thermophysical properties at material interfaces since different

profiles can be associated with each sub-control volume as opposed to determining effective control volume properties using averaging techniques

2. naturally occurring zero flux boundary conditions which is explained further in Sections 5.5.2 and 7.4.2

4.2 Coordinate Systems and Contracting Grid Scheme

Since ablation problems involve moving grids it is convenient to describe the domain with different coordinate systems for different applications. A few examples are:

1. a moving grid problem could be steady-state in one coordinate system while it is transient in another
2. one coordinate system is more convenient for domain discretization
3. one coordinate system is more intuitive to the analyst for post-processing such as plot generation
4. one coordinate system simplifies the grid motion scheme

Figure 4.2 shows the three coordinate systems that describe the evolving domain for ablation problems. The z -coordinate system is stationary with its origin at the original ablator surface, and as a result, the surface recession is measured from $z = 0$. This coordinate system is convenient for domain discretization and post-processing since its frame of reference is consistent with an observer watching a body ablate in a wind tunnel setting. The x -coordinate system has a translating origin that is attached to the receding surface and it is often useful in describing steady-state ablation problems. The x -coordinate system is also used in conjunction with the translating/node-dropping grid scheme since the x -coordinate of a given node is constant throughout the problem with the exception of the ablator back face node.

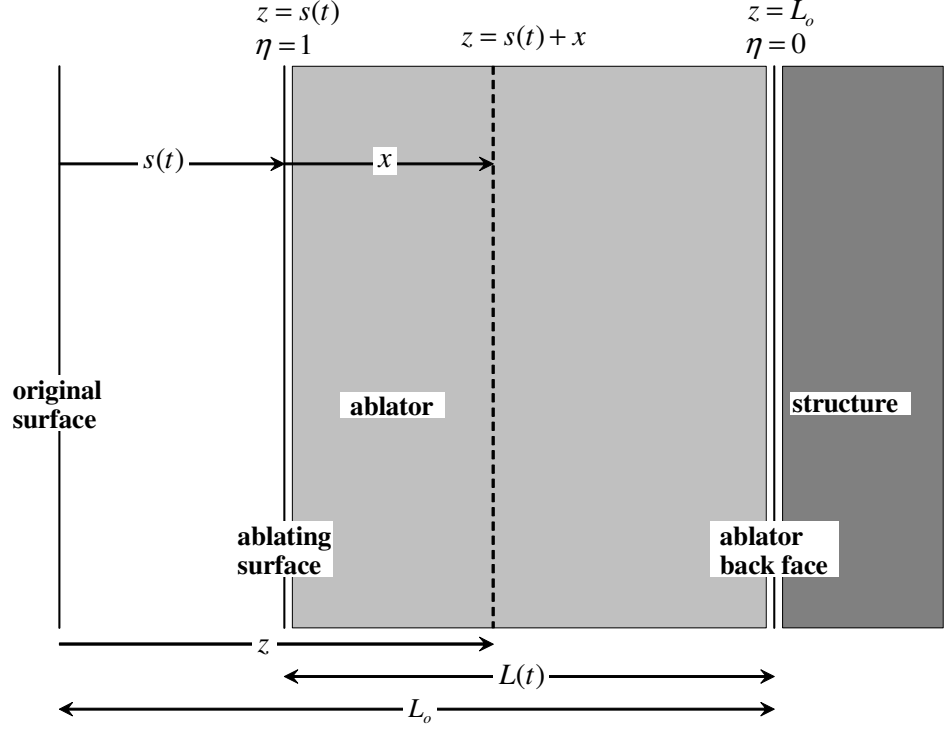


Figure 4.2: Schematic of coordinate systems for one-dimensional planar geometry.

However, this is not the case with the contracting grid scheme in which the x and z coordinates of each node is changing with the exceptions of the surface node in the x -coordinate system and the ablator back face node in the z -coordinate system. The contracting grid scheme implements a Landau[30] coordinate transformation as presented by Blackwell and Hogan[10], which transforms the spatial coordinate such that the non-dimensional thickness of the remaining domain in Landau-space is always unity and that the Landau coordinate of a given node is constant. The Landau coordinate at any location is given as

$$\eta = \frac{L(t) - x}{L(t)} = \frac{L_o - z}{L_o - s} \quad (4.2)$$

It is evident that at the ablation front, $x = 0$, $z = s(t)$, and $\eta = 1$, while at the back face, $x = L(t)$, $z = L_o$, and $\eta = 0$. As a result, the velocity of any node can be

related to the surface recession rate by

$$\dot{z}_j^{n+1} = \eta_j \dot{s}^{n+1} \quad (4.3)$$

Consequently, the translation of any node in a given time step is related to the nodal recession rate through

$$z_j^{n+1} - z_j^n = \dot{z}_j^{n+1} \Delta t^{n+1} \quad (4.4)$$

Since control volume boundaries are at element centers, which is explained in the previous section, the velocity of the control volume boundary is given by

$$(u_{cs})_{j+1/2}^{n+1} = \dot{s}^{n+1} \frac{1}{2} (\eta_j + \eta_{j+1}) \quad (4.5)$$

Figure 4.3 shows an initial to final mesh comparison for a one-dimensional uniform mesh problem. Although the nodal displacement relationship is simpler for the translating grid scheme, it creates a large discontinuity in adjacent cell sizes at the back face which could have negative numerical implications. Also, the contracting grid scheme avoids the node dropping complexity and ensures that the accuracy of the scheme is maintained throughout the problem since the number of nodes and the dimensionless element thickness $(\Delta z_j(t) / L(t))$ is constant.

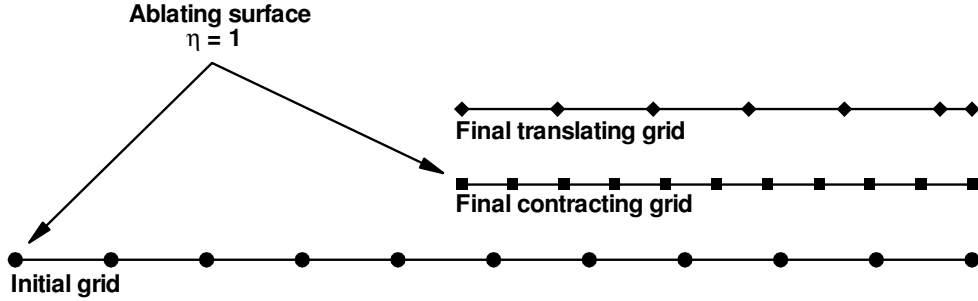


Figure 4.3: Initial to final mesh comparison for contracting grid scheme on a uniform mesh.

It is also necessary for moving mesh problems to satisfy the geometric conservation law, introduced by Thomas and Lombard[31], which is essentially a conservation

of volume statement given by

$$\int_{cs} \mathbf{v}_{cs} \cdot d\mathbf{A} = \frac{d}{dt} \int_{cv} dV \quad (4.6)$$

Consistent with the CVFEM, the geometric conservation equation in semi-discrete form for a one-dimensional planar geometry becomes

$$(Au_{cs})_{j+1/2} - (Au_{cs})_{j-1/2} = \frac{d}{dt} \int_{\bar{z}_{j-1}}^{z_j} dV + \frac{d}{dt} \int_{z_j}^{\bar{z}_j} dV \quad (4.7)$$

where $\bar{z}_{j-1} = z_{j-1/2}$ and $\bar{z}_j = z_{j+1/2}$. Evaluating the terms gives

$$A\dot{s}^{n+1}(\eta_{j+1/2} - \eta_{j-1/2}) = A\left(\dot{z}_{j+1/2}^{n+1} - \dot{z}_{j-1/2}^{n+1}\right) \quad (4.8)$$

and using the relationship in Eq. 4.3 shows that the geometric conservation law is identically satisfied. Similar analyses can show that quasi-one-dimensional spherical and cylindrical geometries also satisfy the geometric conservation law for the contracting grid scheme.

5 Mixture Energy Equation

The mixture energy conservation equation given in Eq. 2.1 is

$$\underbrace{\int_{cs} \dot{\mathbf{q}}'' \cdot d\mathbf{A}}_{\text{conduction}} + \underbrace{\int_{cs} \phi \rho_g h_g \mathbf{v}_g \cdot d\mathbf{A}}_{\text{gas flux}} - \underbrace{\int_{cs} \rho h \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} + \frac{d}{dt} \underbrace{\int_{cv} \rho e dV}_{\text{energy content}} = 0$$

where the discretization of each term is discussed in the subsequent sections. For both the mixture energy and gas mass conservation equations, a consistent sign convention is adopted such that

$$[\text{outflow terms}] - [\text{inflow terms}] + [\text{rate of change of content}] = [\text{source terms}]$$

For one-dimension, Eq. 2.1 in semi-discrete form for a nodal control volume becomes

$$\begin{aligned} 0 = & (\dot{q}'' A)_{j+1/2} - (\dot{q}'' A)_{j-1/2} - (\phi \rho_g h_g u_g A)_{j-1/2} + (\phi \rho_g h_g u_g A)_{j+1/2} \\ & + (\rho h u_{cs} A)_{j-1/2} - (\rho h u_{cs} A)_{j+1/2} \\ & + \frac{d}{dt} \int_{\bar{z}_{j-1}}^{z_j} \rho e A dz + \frac{d}{dt} \int_{z_j}^{\bar{z}_j} \rho e A dz \end{aligned} \quad (5.1)$$

and the energy balance terms can be seen in Figure 5.1. Section 3 presented the model for determining thermophysical and thermodynamic properties of the gas, solid, and mixture that are necessary for the solution of the mixture energy equation.

While solving the mixture energy equation, nodal temperatures and the surface recession rate are treated as the dependent variables while nodal values of solid density, gas density, and gas velocity are constant. The gas velocity is held constant since the flow work associated with the moving gas is small compared to the internal energy of the solid. Therefore, recalculating the gas velocity and its associated sensitivities during every energy equation iteration would not be expected to accelerate global convergence or reduce computational time.

For non-ablating intervals (when the surface recession rate is zero), the linear system in Eq. 2.10 is tridiagonal since the only unknowns in the residual equations

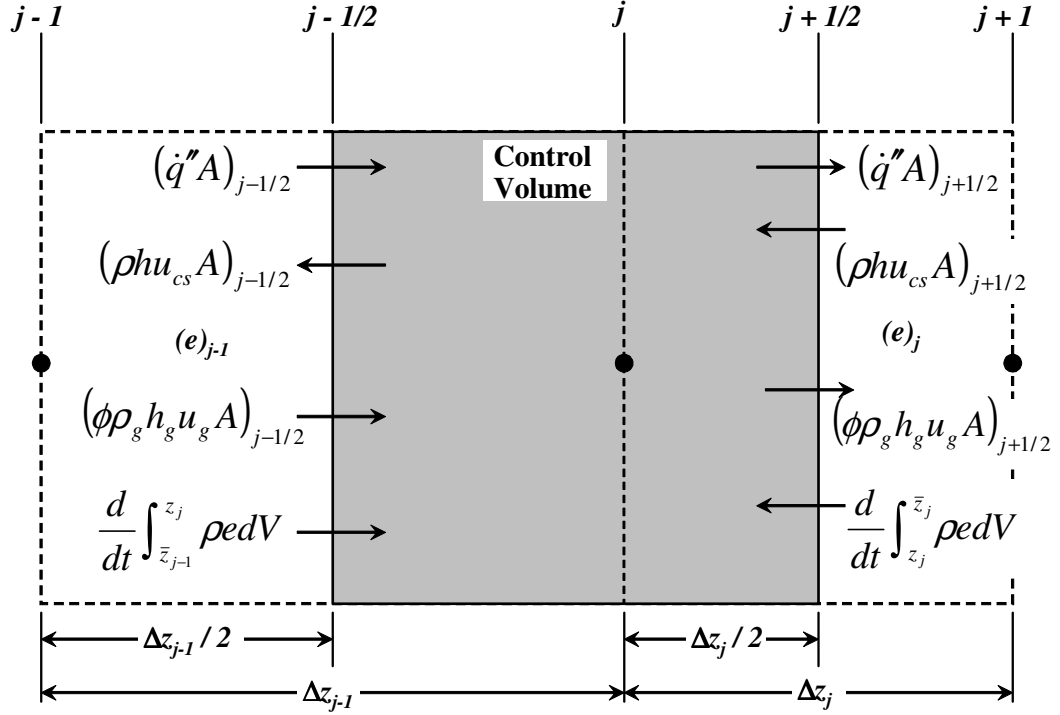


Figure 5.1: Energy balance terms for the control volume surrounding node j .

are nodal temperatures. The linear system for a five node domain is given by

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 \\ 0 & 0 & a_4 & b_4 & c_4 \\ 0 & 0 & 0 & a_5 & b_5 \end{bmatrix}^{\nu} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}^{\nu} \quad (5.2)$$

On the other hand when the material is ablating, the residual equations have a non-linear dependence on the surface recession rate. The resulting linear system, for the same five node domain, is of the form

$$\begin{bmatrix} e_0 & c_0 & 0 & 0 & 0 & 0 \\ e_1 & b_1 & c_1 & 0 & 0 & 0 \\ e_2 & a_2 & b_2 & c_2 & 0 & 0 \\ e_3 & 0 & a_3 & b_3 & c_3 & 0 \\ e_4 & 0 & 0 & a_4 & b_4 & c_4 \\ e_5 & 0 & 0 & 0 & a_5 & b_5 \end{bmatrix}^{\nu} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}^{\nu} \quad (5.3)$$

where the vector $\mathbf{e}$ in the first column of the sensitivity matrix contains residuals' sen-

sivities to the surface recession rate. It is evident that an additional relationship to provide the "zeroth" residual equation is necessary for the solution of this system, and this relationship is provided by the ablation models discussed in Section 5.6. An algorithm, described in detail in Appendix B, was developed to solve this system by eliminating the superdiagonal using Gaussian elimination followed by back substitution to determine the correction vector. For simulations that have both ablating and non-ablating intervals, the code switches between a tridiagonal solver and the new linear system solver in order to minimize computational time. Timing study results are presented in Section 9 to show that given the same convergence criteria, solving a problem with the entire recession rate sensitivity vector is more computationally efficient than solving the problem with the traditional tridiagonal formulation used in legacy codes.

An element assembly approach to generating the global sensitivity matrix entries is used for the mixture energy and gas phase continuity equations. As a result, each term in the governing equations is discretized on an element-by-element basis and the appropriate sub-control volume contributions are made to the nodal control volume residual equations. Consequently, each element $(e)_j$ has contributions to the residual equations associated with nodes j and $j + 1$ as seen in Figure 5.1. In order to provide element assembly routine implementation details for each term, a summary of the global sensitivity matrix and residual vector contributions is given for each term and boundary condition. These contributions are presented in a mixed mathematical and programming language syntax such that

$$\mathbf{b}(j) = \mathbf{b}(j) + X \quad (5.4)$$

means that the j th entry in vector $\mathbf{b}$, which is the variable in the computer program corresponding to b_j in Eq. 5.2 or Eq. 5.3, has some quantity X added to it.

5.1 Conduction

Fourier's law is used to model the heat conducted at a control volume boundary and the heat conduction rate is given by

$$\dot{Q}_{j+1/2} = \left[-k(T)A \frac{dT}{dz} \right]_{j+1/2} = \frac{-\bar{k}(T)A}{\Delta z_j} (T_{j+1} - T_j) \quad (5.5)$$

where $\bar{X} = (X_{j+1} + X_j) / 2$, and X is any quantity. The elemental representation of the heat conduction rate is

$$\begin{bmatrix} \dot{Q}_j \\ \dot{Q}_{j+1} \end{bmatrix} = \frac{\bar{k}(T)A}{\Delta z_j} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} T_j \\ T_{j+1} \end{bmatrix} \quad (5.6)$$

In general, the heat conduction vector is a nonlinear function of temperature and recession rate since the thermal conductivity depends on temperature and Δz_j depends on the surface recession rate. Therefore an iterative solution procedure is necessary to solve for the time accurate nonlinearities. To aid in the iterative process, it is convenient to linearize the element conduction vector with a Taylor series expansion in iteration space treating the nodal temperatures and surface recession rate as the independent variables

$$\begin{bmatrix} \dot{Q}_j \\ \dot{Q}_{j+1} \end{bmatrix}^{\nu+1} = \begin{bmatrix} \dot{Q}_j \\ \dot{Q}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \dot{Q}_j}{\partial \dot{s}} & \frac{\partial \dot{Q}_j}{\partial T_j} & \frac{\partial \dot{Q}_j}{\partial T_{j+1}} \\ \frac{\partial \dot{Q}_{j+1}}{\partial \dot{s}} & \frac{\partial \dot{Q}_{j+1}}{\partial T_j} & \frac{\partial \dot{Q}_{j+1}}{\partial T_{j+1}} \end{bmatrix} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_j \\ \Delta T_{j+1} \end{bmatrix}^{\nu+1} + \dots \quad (5.7)$$

Performing the required differentiation for planar geometry ($A(z) = 1$) gives

$$\left. \begin{aligned}
\frac{\partial \dot{Q}_j}{\partial \dot{s}} &= -\frac{\bar{k}A}{\Delta z_j^2} (T_j - T_{j+1}) \frac{\partial \Delta z_j}{\partial \dot{s}} \\
\frac{\partial \dot{Q}_{j+1}}{\partial \dot{s}} &= \frac{\bar{k}A}{\Delta z_j^2} (T_j - T_{j+1}) \frac{\partial \Delta z_j}{\partial \dot{s}} \\
\frac{\partial \dot{Q}_j}{\partial T_j} &= \frac{\bar{k}A}{\Delta z_j^2} \left[1 + \frac{(T_j - T_{j+1})}{2\bar{k}} \left(\frac{\partial k}{\partial T} \right)_j \right] \\
\frac{\partial \dot{Q}_j}{\partial T_{j+1}} &= \frac{\bar{k}A}{\Delta z_j^2} \left[-1 + \frac{(T_j - T_{j+1})}{2\bar{k}} \left(\frac{\partial k}{\partial T} \right)_{j+1} \right] \\
\frac{\partial \dot{Q}_{j+1}}{\partial T_j} &= \frac{\bar{k}A}{\Delta z_j^2} \left[-1 - \frac{(T_j - T_{j+1})}{2\bar{k}} \left(\frac{\partial k}{\partial T} \right)_j \right] \\
\frac{\partial \dot{Q}_{j+1}}{\partial T_{j+1}} &= \frac{\bar{k}A}{\Delta z_j^2} \left[1 - \frac{(T_j - T_{j+1})}{2\bar{k}} \left(\frac{\partial k}{\partial T} \right)_{j+1} \right]
\end{aligned} \right\} \quad (5.8)$$

where

$$\frac{\partial \Delta z_j}{\partial \dot{s}} = \Delta t^{n+1} (\eta_{j+1} - \eta_j) = \Delta t^{n+1} \Delta \eta_j \quad (5.9)$$

Note that for cylindrical and spherical one-dimensional geometries, the area variation is a function of position ($A = A(z)$) resulting in additional terms in the surface recession rate sensitivities for all of the terms discussed. The resulting linear system

contributions for each j th element are

$$\left. \begin{aligned} \mathbf{e}(j) &= \mathbf{e}(j) + \frac{\partial \dot{Q}_j}{\partial \dot{s}} \\ \mathbf{e}(j+1) &= \mathbf{e}(j+1) + \frac{\partial \dot{Q}_{j+1}}{\partial \dot{s}} \\ \mathbf{b}(j) &= \mathbf{b}(j) + \frac{\partial \dot{Q}_j}{\partial T_j} \\ \mathbf{c}(j) &= \mathbf{c}(j) + \frac{\partial \dot{Q}_j}{\partial T_{j+1}} \\ \mathbf{d}(j) &= \mathbf{d}(j) - \dot{Q}_j^\nu \\ \mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{\partial \dot{Q}_{j+1}}{\partial T_j} \\ \mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{\partial \dot{Q}_{j+1}}{\partial T_{j+1}} \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) - \dot{Q}_{j+1}^\nu \end{aligned} \right\} \quad (5.10)$$

5.2 Grid Convection

The energy transfer rate due to convection of a control volume boundary is given by

$$\dot{E} = (\rho h u_{cs} A)_{j+1/2} \quad (5.11)$$

and the corresponding element convection vector, consistent with the established sign convention, is

$$\begin{bmatrix} \dot{E}_j \\ \dot{E}_{j+1} \end{bmatrix} = [\rho h u_{cs} A]_{j+1/2} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad (5.12)$$

Substituting in the mixture enthalpy definition in Eq. 3.5 gives

$$\begin{bmatrix} \dot{E}_j \\ \dot{E}_{j+1} \end{bmatrix} = \left[(\phi \rho_g h_g)_{j+1/2} + (\rho_s h_s)_{j+1/2} \right] (u_{cs})_{j+1/2} A \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad (5.13)$$

Since properties are assumed to vary linearly within elements, the enthalpy per unit volume at the control volume boundary is given by

$$(\rho_s h_s)_{j+1/2} = \overline{\rho_s h_s} = \frac{1}{2} [(\rho_s h_s)_{j+1} + (\rho_s h_s)_j] \quad (5.14)$$

and

$$(\phi \rho_g h_g)_{j+1/2} = \overline{\phi \rho_g h_g} = \frac{1}{2} [(\phi \rho_g h_g)_{j+1} + (\phi \rho_g h_g)_j] \quad (5.15)$$

The control surface velocity according to the contracting grid scheme in Section 4.2 is given by Eq. 4.5

$$(u_{cs})_{j+1/2} = \dot{s} \bar{\eta}_j$$

Linearizing the convection vector in iteration space according to a Taylor series expansion gives

$$\begin{bmatrix} \dot{E}_j \\ \dot{E}_{j+1} \end{bmatrix}^{\nu+1} = \begin{bmatrix} \dot{E}_j \\ \dot{E}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \dot{E}_j}{\partial \dot{s}} & \frac{\partial \dot{E}_j}{\partial T_j} & \frac{\partial \dot{E}_j}{\partial T_{j+1}} \\ \frac{\partial \dot{E}_{j+1}}{\partial \dot{s}} & \frac{\partial \dot{E}_{j+1}}{\partial T_j} & \frac{\partial \dot{E}_{j+1}}{\partial T_{j+1}} \end{bmatrix} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_j \\ \Delta T_{j+1} \end{bmatrix}^{\nu+1} + \dots \quad (5.16)$$

where the sensitivity matrix entries are

$$\left. \begin{aligned} \frac{\partial \dot{E}_j}{\partial \dot{s}} &= -\overline{\rho h} \bar{\eta}_j A \\ \frac{\partial \dot{E}_{j+1}}{\partial \dot{s}} &= \overline{\rho h} \bar{\eta}_j A \\ \frac{\partial \dot{E}_j}{\partial T_j} &= -\frac{A}{2} (u_{cs})_{j+1/2} (\rho C_p)_j \\ \frac{\partial \dot{E}_j}{\partial T_{j+1}} &= -\frac{A}{2} (u_{cs})_{j+1/2} (\rho C_p)_{j+1} \\ \frac{\partial \dot{E}_{j+1}}{\partial T_j} &= \frac{A}{2} (u_{cs})_{j+1/2} (\rho C_p)_j \\ \frac{\partial \dot{E}_{j+1}}{\partial T_{j+1}} &= \frac{A}{2} (u_{cs})_{j+1/2} (\rho C_p)_{j+1} \end{aligned} \right\} \quad (5.17)$$

and the expression for the specific heat is given in Eq. 3.15. The resulting linear system contributions for each j th element are

$$\left. \begin{aligned} \mathbf{e}(j) &= \mathbf{e}(j) + \frac{\partial \dot{E}_j}{\partial \dot{s}} \\ \mathbf{e}(j+1) &= \mathbf{e}(j+1) + \frac{\partial \dot{E}_{j+1}}{\partial \dot{s}} \\ \mathbf{b}(j) &= \mathbf{b}(j) + \frac{\partial \dot{E}_j}{\partial T_j} \\ \mathbf{c}(j) &= \mathbf{c}(j) + \frac{\partial \dot{E}_j}{\partial T_{j+1}} \\ \mathbf{d}(j) &= \mathbf{d}(j) - \dot{E}_j^\nu \\ \mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{\partial \dot{E}_{j+1}}{\partial T_j} \\ \mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{\partial \dot{E}_{j+1}}{\partial T_{j+1}} \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) - \dot{E}_{j+1}^\nu \end{aligned} \right\} \quad (5.18)$$

5.3 Gas Flux

For both moving and stationary grid problems, in-depth decomposition of the material may be occurring which results in gas generation and convection within the porous material. The superficial gas velocity at control volume boundaries is determined from Darcy's law (described in Section 2.1), which is given in one-dimensional discrete form at the control volume boundary as

$$u'_g = \frac{\bar{\kappa}}{\bar{\mu}} \frac{P_j - P_{j+1}}{\Delta z_j} \quad (5.19)$$

where the average permeability and viscosity are determined by averaging adjacent nodal values

$$\bar{\kappa} = \frac{1}{2} (\kappa_j + \kappa_{j+1}) \quad (5.20)$$

and

$$\bar{\mu} = \frac{1}{2} (\mu_j + \mu_{j+1}) \quad (5.21)$$

Since the permeability can vary several orders of magnitude between adjacent nodes, the averaging technique proposed in this study may not be the ideal approach for all situations. Other averaging techniques such as harmonic mean approaches have been used for ablation problems[15].

The element energy convection vector from gas flux is given by

$$\begin{bmatrix} \dot{G}_j \\ \dot{G}_{j+1} \end{bmatrix} = u'_g (\rho_g h_g A)_{j+1/2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (5.22)$$

and a Taylor series expansion of the energy convection vector from gas flux is

$$\begin{bmatrix} \dot{G}_j \\ \dot{G}_{j+1} \end{bmatrix}^{\nu+1} = \begin{bmatrix} \dot{G}_j \\ \dot{G}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \dot{G}_j}{\partial \dot{s}} & \frac{\partial \dot{G}_j}{\partial T_j} & \frac{\partial \dot{G}_j}{\partial T_{j+1}} \\ \frac{\partial \dot{G}_{j+1}}{\partial \dot{s}} & \frac{\partial \dot{G}_{j+1}}{\partial T_j} & \frac{\partial \dot{G}_{j+1}}{\partial T_{j+1}} \end{bmatrix}^{\nu} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_j \\ \Delta T_{j+1} \end{bmatrix}^{\nu+1} + \dots \quad (5.23)$$

Since the gas enthalpy per unit volume at the control volume boundary is expressed as

$$(\rho_g h_g)_{j+1/2} = \overline{\rho_g h_g} = \frac{1}{2} [(\rho_g h_g)_j + (\rho_g h_g)_{j+1}] \quad (5.24)$$

and the gas velocity is assumed to be constant while solving the energy equation, performing the required differentiation gives

$$\left. \begin{aligned}
\frac{\partial \dot{G}_j}{\partial \dot{s}} &= 0 \\
\frac{\partial \dot{G}_{j+1}}{\partial \dot{s}} &= 0 \\
\frac{\partial \dot{G}_j}{\partial T_j} &= \frac{1}{2} u'_g A (\rho_g C_{p_g})_j \\
\frac{\partial \dot{G}_j}{\partial T_{j+1}} &= \frac{1}{2} u'_g A (\rho_g C_{p_g})_{j+1} \\
\frac{\partial \dot{G}_{j+1}}{\partial T_j} &= -\frac{1}{2} u'_g A (\rho_g C_{p_g})_j \\
\frac{\partial \dot{G}_{j+1}}{\partial T_{j+1}} &= -\frac{1}{2} u'_g A (\rho_g C_{p_g})_{j+1}
\end{aligned} \right\} \quad (5.25)$$

The resulting linear system contributions for each j th element are

$$\left. \begin{aligned}
\mathbf{b}(j) &= \mathbf{b}(j) + \frac{\partial \dot{G}_j}{\partial T_j} \\
\mathbf{c}(j) &= \mathbf{c}(j) + \frac{\partial \dot{G}_j}{\partial T_{j+1}} \\
\mathbf{d}(j) &= \mathbf{d}(j) - \dot{G}_j^\nu \\
\mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{\partial \dot{G}_{j+1}}{\partial T_j} \\
\mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{\partial \dot{G}_{j+1}}{\partial T_{j+1}} \\
\mathbf{d}(j+1) &= \mathbf{d}(j+1) - \dot{G}_{j+1}^\nu
\end{aligned} \right\} \quad (5.26)$$

5.4 Energy Content and Time Integration

The energy content for an element can be divided into terms corresponding to each of the two sub-control volumes within an element.

$$\begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix} = \begin{bmatrix} \int_{z_j}^{\bar{z}_j} \rho e(T) Adz \\ \int_{\bar{z}_j}^{z_{j+1}} \rho e(T) Adz \end{bmatrix} \quad (5.27)$$

The internal energy per unit volume in Eq. 5.27 can be expressed by a Taylor series expansion in position about the element center

$$(\rho e)_z = (\rho e)_{\bar{z}_j} + \left. \frac{\partial(\rho e)}{\partial z} \right|_{\bar{z}_j} (z - \bar{z}_j) + \dots \quad (5.28)$$

The elemental energy content vector can now be expressed as

$$\begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix} = \begin{bmatrix} \int_{z_j}^{\bar{z}_j} \left(\overline{\rho e} + \left. \frac{\partial(\rho e)}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) \right) Adz \\ \int_{\bar{z}_j}^{z_{j+1}} \left(\overline{\rho e} + \left. \frac{\partial(\rho e)}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) \right) Adz \end{bmatrix} \quad (5.29)$$

where

$$(\rho e)_{\bar{z}_j} = \overline{\rho e} = \frac{1}{2} \left[(\rho e)_j + (\rho e)_{j+1} \right] \quad (5.30)$$

To aid in the integration process it is convenient to employ a local coordinate system in which the shape functions within an element are written as

$$\left. \begin{aligned} N_1(\xi) &= \frac{1}{2}(1 - \xi) \\ \text{and} \\ N_2(\xi) &= \frac{1}{2}(1 + \xi) = 1 - N_1(\xi) \end{aligned} \right\} \text{for } -1 \leq \xi \leq 1 \quad (5.31)$$

The global coordinate, z , and local coordinate, ξ , are related through

$$z = N_1(\xi) z_j + N_2(\xi) z_{j+1} = \bar{z}_j + \frac{\xi}{2} \Delta z_j \quad (5.32)$$

and consequently the differential length is

$$dz = \frac{\Delta z_j}{2} d\xi \quad (5.33)$$

If a finite central difference is used to approximate $\partial(\rho e)/\partial z$, the energy capacitance terms can be rewritten in terms of local coordinates as

$$\begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix} = \begin{bmatrix} \overline{\rho e} \frac{\Delta z_j}{2} \int_{-1}^0 A(\xi) d\xi + [(\rho e)_{j+1} - (\rho e)_j] \frac{\Delta z_j}{4} \int_{-1}^0 \xi A(\xi) d\xi \\ \overline{\rho e} \frac{\Delta z_j}{2} \int_0^1 A(\xi) d\xi + [(\rho e)_{j+1} - (\rho e)_j] \frac{\Delta z_j}{4} \int_0^1 \xi A(\xi) d\xi \end{bmatrix} \quad (5.34)$$

Performing the integration for planar geometry ($A(\xi) = 1$) gives

$$\begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix} = \frac{A\Delta z_j}{2} \begin{bmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{bmatrix} \begin{bmatrix} (\rho e)_j \\ (\rho e)_{j+1} \end{bmatrix} \quad (5.35)$$

The result is simply a weighted average of nodal values where the weighting factor matrix is geometry dependent. The time rate of change of energy content according to an implicit time integrator can be expressed as

$$\frac{d}{dt} \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^{n+1} = \left\{ \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^{n+1} - \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^n \right\} \frac{1}{\Delta t^{n+1}} \quad (5.36)$$

and linearizing in iteration space according to a Taylor series expansion gives

$$\begin{aligned} \frac{d}{dt} \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^{\nu+1} &= \left\{ \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^\nu + \begin{bmatrix} \frac{\partial \tilde{E}_j}{\partial \dot{s}} & \frac{\partial \tilde{E}_j}{\partial T_j} & \frac{\partial \tilde{E}_j}{\partial T_{j+1}} \\ \frac{\partial \tilde{E}_{j+1}}{\partial \dot{s}} & \frac{\partial \tilde{E}_{j+1}}{\partial T_j} & \frac{\partial \tilde{E}_{j+1}}{\partial T_{j+1}} \end{bmatrix}^\nu \begin{bmatrix} \Delta \dot{s} \\ \Delta T_j \\ \Delta T_{j+1} \end{bmatrix} \right. \\ &\quad \left. - \begin{bmatrix} \tilde{E}_j \\ \tilde{E}_{j+1} \end{bmatrix}^n \right\} \frac{1}{\Delta t^{n+1}} \end{aligned} \quad (5.37)$$

where the sensitivity matrix entries are

$$\left. \begin{aligned} \frac{\partial \tilde{E}_j}{\partial \dot{s}} &= A \frac{\partial \Delta z_j}{\partial \dot{s}} \left[\frac{3}{8} (\rho e)_j + \frac{1}{8} (\rho e)_{j+1} \right] \\ \frac{\partial \tilde{E}_{j+1}}{\partial \dot{s}} &= A \frac{\partial \Delta z_j}{\partial \dot{s}} \left[\frac{1}{8} (\rho e)_j + \frac{3}{8} (\rho e)_{j+1} \right] \\ \frac{\partial \tilde{E}_j}{\partial T_j} &= \frac{3A\Delta z_j}{8} (\rho C_v)_j \\ \frac{\partial \tilde{E}_j}{\partial T_{j+1}} &= \frac{A\Delta z_j}{8} (\rho C_v)_{j+1} \\ \frac{\partial \tilde{E}_{j+1}}{\partial T_j} &= \frac{A\Delta z_j}{8} (\rho C_v)_j \\ \frac{\partial \tilde{E}_{j+1}}{\partial T_{j+1}} &= \frac{3A\Delta z_j}{8} (\rho C_v)_{j+1} \end{aligned} \right\} \quad (5.38)$$

The resulting linear system contributions for each j th element are

$$\left. \begin{aligned} \mathbf{e}(j) &= \mathbf{e}(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_j}{\partial \dot{s}} \\ \mathbf{e}(j+1) &= \mathbf{e}(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_{j+1}}{\partial \dot{s}} \\ \mathbf{b}(j) &= \mathbf{b}(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_j}{\partial T_j} \\ \mathbf{c}(j) &= \mathbf{c}(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_j}{\partial T_{j+1}} \\ \mathbf{d}(j) &= \mathbf{d}(j) - \frac{1}{\Delta t^{n+1}} \left(\tilde{E}_j^\nu - \tilde{E}_j^n \right) \\ \mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_{j+1}}{\partial T_j} \\ \mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{E}_{j+1}}{\partial T_{j+1}} \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) - \frac{1}{\Delta t^{n+1}} \left(\tilde{E}_{j+1}^\nu - \tilde{E}_{j+1}^n \right) \end{aligned} \right\} \quad (5.39)$$

5.5 Boundary Conditions

For generality, the boundary conditions are presented in a form in which they can be applied to either the exposed surface or the back face consistent with the established sign convention in which an inflow term is a negative quantity. In addition, since the analysis in this study is restricted to planar geometry, several of the boundary conditions have no sensitivity to the surface recession rate, but for quasi-one-dimensional geometries the surface area has a recession rate dependence. Therefore for nonplanar geometries, a given boundary condition has a recession rate sensitivity if the surface area is a factor in the residual contribution.

5.5.1 Specified Temperature

A time dependent specified temperature boundary condition can be applied if the surface temperature history is known (perhaps through experimental data). If desired, the converged temperature solution can be post-processed to compute the surface heat flux consistent with the specified temperature boundary condition. This condition can only be applied to non-ablating problems when the linear system is in the tridiagonal form given in Eq. 5.2. The residual equation for either boundary (*bnd*) node is

$$R_{bnd} = T_{bnd}^{n+1} - T_{bnd}^\nu \quad (5.40)$$

Expanding the boundary residual according to a Taylor series expansion gives

$$R_{bnd}^{\nu+1} = R_{bnd}^\nu + \left. \frac{\partial R}{\partial T} \right|_{T=T_{bnd}} \Delta T_{bnd}^{\nu+1} + \dots \quad (5.41)$$

and the final form of the boundary residual is

$$\Delta T_{bnd}^{\nu+1} = T_{bnd}^{n+1} - T_{bnd}^\nu \quad (5.42)$$

The resulting linear system contributions are

$$\left. \begin{aligned} \mathbf{a}(\mathbf{bnd}) &= 0 \\ \mathbf{b}(\mathbf{bnd}) &= 1 \\ \mathbf{c}(\mathbf{bnd}) &= 0 \\ \mathbf{d}(\mathbf{bnd}) &= R_{bnd}^\nu \end{aligned} \right\} \quad (5.43)$$

5.5.2 Specified Heat Flux

Any heat flux incident on the body's surface can be expanded in iteration space according to

$$(\dot{q}_{spec}'')^{\nu+1} \approx (\dot{q}_{spec}'')^\nu + \left. \frac{\partial \dot{q}_{spec}''}{\partial T} \right|_{T=T_{bnd}}^\nu (\Delta T_{bnd}^{\nu+1}) + \left. \frac{\partial \dot{q}_{spec}''}{\partial \dot{s}} \right|^\nu (\Delta \dot{s}^{\nu+1}) \quad (5.44)$$

Since a specified input heat flux is neither temperature nor recession rate dependent, then

$$\left. \frac{\partial \dot{q}_{spec}''}{\partial T} \right|_{T=T_{bnd}} = 0 \quad (5.45)$$

and

$$\frac{\partial \dot{q}_{spec}''}{\partial \dot{s}} = 0 \quad (5.46)$$

giving

$$(\dot{q}_{spec}'')^{\nu+1} = (\dot{q}_{spec}'')^{\nu} \quad (5.47)$$

This results in the boundary residual being updated according to

$$\mathbf{d}(\mathbf{bnd}) = \mathbf{d}(\mathbf{bnd}) - A_{bnd} (\dot{q}_{spec}'')^{\nu} \quad (5.48)$$

It is evident that an adiabatic boundary condition requires no modification to the linear system; thus, the adiabatic condition is said to occur naturally with this scheme.

5.5.3 Standard Convection

The standard convective heat flux is given by

$$\dot{q}_{conv}'' = H (T_{bnd} - T_r) \quad (5.49)$$

where the driving potential is a temperature difference. This phenomenon is labeled "standard" since the aerodynamic heating flux is also convective but an enthalpy difference is the driving potential. The temperature and recession rate sensitivities are

$$\left. \frac{\partial \dot{q}_{conv}''}{\partial T} \right|_{T=T_{bnd}} = H \quad (5.50)$$

and

$$\frac{\partial \dot{q}_{conv}''}{\partial \dot{s}} = 0 \quad (5.51)$$

where the heat transfer coefficient is a time dependent input parameter that is independent of temperature. This results in the linear system coefficients being updated

according to

$$\left. \begin{aligned} \mathbf{b}(\mathbf{bnd}) &= \mathbf{b}(\mathbf{bnd}) + A_{bnd} \left. \frac{\partial \dot{q}_{conv}''}{\partial T} \right|_{T=T_{bnd}} \\ \mathbf{d}(\mathbf{bnd}) &= \mathbf{d}(\mathbf{bnd}) - A_{bnd} (\dot{q}_{conv}'')^\nu \end{aligned} \right\} \quad (5.52)$$

However if the heat transfer coefficient was a function of temperature, then a simple modification would be necessary.

5.5.4 Radiation

The radiation flux in Eq. 2.11 is written as

$$\dot{q}_{rad}'' = \epsilon \sigma (T_{bnd}^4 - T_{res}^4) \quad (5.53)$$

and the sensitivities are given by

$$\frac{\partial \dot{q}_{rad}''}{\partial \dot{s}} = 0 \quad (5.54)$$

and

$$\left. \frac{\partial \dot{q}_{rad}''}{\partial T} \right|_{T=T_{bnd}} = 4\epsilon \sigma T_{bnd}^3 + \left. \frac{\partial \epsilon}{\partial T} \right|_{T=T_{bnd}} (T_{bnd}^4 - T_{res}^4) \quad (5.55)$$

This results in the linear system coefficients being updated according to

$$\left. \begin{aligned} \mathbf{b}(\mathbf{bnd}) &= \mathbf{b}(\mathbf{bnd}) + A_{bnd} \left. \frac{\partial \dot{q}_{rad}''}{\partial T} \right|_{T=T_{bnd}} \\ \mathbf{d}(\mathbf{bnd}) &= \mathbf{d}(\mathbf{bnd}) - A_{bnd} (\dot{q}_{rad}'')^\nu \end{aligned} \right\} \quad (5.56)$$

5.5.5 Aerodynamic Heating

The aerodynamic heat flux in Eq. 2.11 is given by

$$\dot{q}_{ah}'' = \rho_e u_e C_h (h_w - h_r) \quad (5.57)$$

where h_w is the specific enthalpy of the gases adjacent to the wall which is tabulated as a function of pressure, pyrolysis gas blowing rate, and wall temperature in

the surface thermochemistry data that is generated by ACE[32] or some other equilibrium chemistry code. The equilibrium chemistry solution at the body's surface accounts for the species in the free-stream gas (air for Earth reentry), gaseous ablation products, and pyrolysis gases from in-depth decomposition. Therefore for a non-ablating and non-decomposing materials, thermochemistry data accounting for the ionization and dissociation of the free-stream gas is required if the aerodynamic heating boundary condition is applied. The thermochemistry table organization and the three-dimensional interpolation routine used to extract data from it is discussed in detail in Appendix C. The required time dependent input parameters for the aerodynamic heating boundary condition include: heat transfer coefficient ($\rho_e u_e C_h$), recovery enthalpy (h_r), boundary layer edge velocity (u_e), boundary pressure (P), and a parameter indicating either laminar or turbulent flow.

The code includes corrections to the Stanton number for both hot wall and blowing effects since the legacy codes used to generate the aerodynamic heating input assume a cold wall and no mass injection into the boundary layer. The resulting aerodynamic heat flux is

$$\dot{q}_{ah}'' = \underbrace{\rho_e u_e C_{h_o}}_{\text{input value}} \underbrace{\left(\frac{C_h}{C_{h_o}} \right)}_{\text{correction}} (h_w - h_r) \quad (5.58)$$

where

$$\frac{C_h}{C_{h_o}} = \Omega_{hw} \Omega_{blw} \quad (5.59)$$

Note that the overall Stanton number correction model assumes that the hot wall and blowing corrections are independent of each other and they can therefore be applied either separately or in the multiplicative fashion in Eq. 5.59.

Blowing Correction When ablation and/or in-depth decomposition is occurring, the mass injection into the boundary layer is known to thicken the boundary layer

and cause a corresponding decrease in the convective heat transfer coefficient. As a result, corrections should be applied to the Stanton number to more accurately model the physics at the ablator surface. The empirical blowing correction used in this study, which is presented by Kays et al.[33], is given by

$$\Omega_{blw} = \frac{\Phi}{e^{\Phi} - 1} \quad (5.60)$$

where

$$\Phi = 2\lambda \frac{\dot{m}''}{\rho_e u_e C_{h_o}} \quad (5.61)$$

The gas blowing flux into the boundary layer, which is relative to the moving surface, includes the mass loss rate from ablation and the pyrolysis gas flux at the surface and is given by

$$\dot{m}'' = \dot{m}_{abl}'' + \dot{m}_g'' \quad (5.62)$$

where the mass flux from ablation products is

$$\dot{m}_{abl}'' = \rho_s \dot{s} \quad (5.63)$$

and the pyrolysis gas blowing rate from in-depth is

$$\dot{m}_g'' = \rho_g (\phi \dot{s} - u_g') \quad (5.64)$$

Thus the overall blowing rate can be rewritten as

$$\dot{m}'' = \rho \dot{s} - \rho_g u_g' \quad (5.65)$$

The blowing reduction parameter (λ) in Eq. 5.61 is 0.5 for laminar flow and 0.4 for turbulent flow. In order to avoid numerical precision issues, four different blowing

corrections have been implemented over a range of Φ values given by

$$\Omega_{blw} = \begin{cases} 1 - \frac{\Phi}{2} + \frac{\Phi^2}{12} & \text{for } \Phi < 10^{-7} \\ \frac{\Phi}{e^\Phi - 1} & \text{for } 10^{-7} \leq \Phi \leq 20 \\ \Phi e^{-\Phi} & \text{for } 20 < \Phi \leq 100 \\ 10^{-8} & \text{for } \Phi > 100 \end{cases} \quad (5.66)$$

The blowing corrections have no temperature dependence, and the surface recession rate sensitivities are given by

$$\frac{\partial \Omega_{blw}}{\partial \dot{s}} = \begin{cases} \frac{1}{2} \frac{\partial \Phi}{\partial \dot{s}} \left(\frac{\Phi}{3} - 1 \right) & \text{for } \Phi < 10^{-7} \\ \frac{\partial \Phi}{\partial \dot{s}} \frac{[e^\Phi (1 - \Phi) - 1]}{(e^\Phi - 1)^2} & \text{for } 10^{-7} \leq \Phi \leq 20 \\ \frac{\partial \Phi}{\partial \dot{s}} e^{-\Phi} [1 - \Phi] & \text{for } 20 < \Phi \leq 100 \\ 0 & \text{for } \Phi > 100 \end{cases} \quad (5.67)$$

where

$$\frac{\partial \Phi}{\partial \dot{s}} = \frac{2\lambda\rho}{\rho_\epsilon u_\epsilon C_{h_o}} \quad (5.68)$$

Hot Wall Correction For the hot wall correction, one of two methods is used depending on whether the flow is laminar or turbulent. For laminar and stagnation point flows, the method presented by Cohen and Reshotko[34] is used and is given by

$$\Omega_{hw} = \left(\frac{\rho_{hw}\mu_{hw}}{\rho_{cw}\mu_{cw}} \right)^{0.1} \quad (5.69)$$

For this method, the gas density and viscosity at both the hot and cold wall conditions must be obtained. The code contains tabulated functions of pressure, temperature, enthalpy, molecular weight, viscosity, and Prandtl number where pressure and any

one of the other properties can be chosen as the independent variables. As a result, the tabulated data in conjunction with the perfect gas law can be used to determine the laminar hot wall correction in Eq. 5.69.

For turbulent flows, a correction based on Eckert's reference enthalpy method[35, 36] is used.

$$\Omega_{hw} = \left(\frac{\mu_{hw}^*}{\mu_{cw}^*} \right)^{0.2} \left(\frac{\rho_{hw}^*}{\rho_{cw}^*} \right)^{0.8} \quad (5.70)$$

The reference properties in Eq. 5.70 are calculated from the tabulated data mentioned above given the pressure and reference enthalpies²

$$h_{hw}^* = \frac{1}{2} (h_e + h_{hw}) + 0.11ru_e^2 \quad (5.71)$$

and

$$h_{cw}^* = \frac{1}{2} (h_e + h_{cw}) + 0.11ru_e^2 \quad (5.72)$$

where the boundary layer edge enthalpy is given by

$$h_e = h_r - r \frac{u_e^2}{2} \quad (5.73)$$

and the recovery factor can be found from

$$r = \text{Pr}_{hw}^{1/3} \quad (5.74)$$

Due to the complexity of the hot wall correction, its sensitivity to temperature is determined from a central finite difference by means of perturbation of the boundary temperature. Thus, the hot wall correction sensitivities are given by

$$\left. \frac{\partial \Omega_{hw}}{\partial T} \right|_{T=T_{bnd}} = \frac{\Omega_{hw}(T_{bnd} + \delta) - \Omega_{hw}(T_{bnd} - \delta)}{2\delta} \quad (5.75)$$

and

$$\frac{\partial \Omega_{hw}}{\partial \dot{s}} = 0 \quad (5.76)$$

where

$$\delta = T_{bnd} \times 10^{-8} \quad (5.77)$$

²The 0.11 factor in the reference enthalpies' definitions is a unitless quantity.

Aerodynamic Heating Sensitivities The aerodynamic heat flux's sensitivity to temperature is given by

$$\left. \frac{\partial \dot{q}_{ah}''}{\partial T} \right|_{T=T_{bnd}} = \rho_e u_e C_{h_o} \left\{ \left[\frac{C_h}{C_{h_o}} \right] \left. \frac{\partial h_w}{\partial T} \right|_{T=T_{bnd}} + (h_w - h_r) \left. \frac{\partial}{\partial T} \left[\frac{C_h}{C_{h_o}} \right] \right|_{T=T_{bnd}} \right\} \quad (5.78)$$

where

$$\left. \frac{\partial}{\partial T} \left[\frac{C_h}{C_{h_o}} \right] \right|_{T=T_{bnd}} = \Omega_{blw} \left. \frac{\partial \Omega_{hw}}{\partial T} \right|_{T=T_{bnd}} \quad (5.79)$$

The wall gas enthalpy is found from interpolation within the thermochemistry tables, and its functional dependencies are

$$h_w = h_w(P, T_{bnd}, B'_g(\dot{s}, T_{bnd}))$$

where the dimensionless pyrolysis gas blowing rate is defined as

$$B'_g = \frac{\dot{m}_g''}{\rho_e u_e C_m} \quad (5.80)$$

The mass transfer coefficient is related to the heat transfer coefficient according to

$$\rho_e u_e C_m = \rho_e u_e C_{h_o} \frac{C_h}{C_{h_o}} \frac{C_m}{C_h} \quad (5.81)$$

where C_m/C_h is an input parameter that is assumed to be constant. For the analyses presented in this study, $C_m/C_h = 1$. When the recession rate is held constant, the differential wall gas enthalpy is given by

$$dh_w = \left. \frac{\partial h_w}{\partial T} \right|_{B'_g} dT + \left. \frac{\partial h_w}{\partial B'_g} \right|_T dB'_g \quad (5.82)$$

and differentiating with respect to temperature gives

$$\frac{\partial h_w}{\partial T} = \left. \frac{\partial h_w}{\partial T} \right|_{B'_g} + \frac{\partial B'_g}{\partial T} \left. \frac{\partial h_w}{\partial B'_g} \right|_T \quad (5.83)$$

where $(\partial h_w / \partial T)|_{B'_g}$ and $(\partial h_w / \partial B'_g)|_T$ are calculated with finite differences from the tabulated thermochemistry data. The dimensionless pyrolysis gas blowing rate's sensitivity to temperature is

$$\frac{\partial B'_g}{\partial T} = - \frac{B'_g}{C_h / C_{h_o}} \frac{\partial}{\partial T} \left[\frac{C_h}{C_{h_o}} \right] \quad (5.84)$$

The aerodynamic heating flux's surface recession rate sensitivity is given by

$$\frac{\partial \dot{q}_{ah}''}{\partial \dot{s}} = \rho_e u_e C_{h_o} \left\{ \left[\frac{C_h}{C_{h_o}} \right] \frac{\partial h_w}{\partial \dot{s}} + (h_w - h_r) \frac{\partial}{\partial \dot{s}} \left[\frac{C_h}{C_{h_o}} \right] \right\} \quad (5.85)$$

where

$$\frac{\partial}{\partial \dot{s}} \left[\frac{C_h}{C_{h_o}} \right] = \Omega_{hw} \frac{\partial \Omega_{blw}}{\partial \dot{s}} \quad (5.86)$$

The wall gas enthalpy's sensitivity to surface recession rate can now be expressed as

$$\frac{\partial h_w}{\partial \dot{s}} = \frac{\partial h_w}{\partial B'_g} \frac{\partial B'_g}{\partial \dot{s}} \quad (5.87)$$

where

$$\frac{\partial B'_g}{\partial \dot{s}} = \frac{\rho_g}{\rho_e u_e C_m} \left(\phi - \frac{(\phi \dot{s} - u'_g)}{C_h/C_{h_o}} \frac{\partial}{\partial \dot{s}} \left[\frac{C_h}{C_{h_o}} \right] \right) \quad (5.88)$$

The final implication of the application of the aerodynamic heating flux boundary condition is an update of the linear system coefficients according to

$$\left. \begin{aligned} \mathbf{e}(\mathbf{bnd}) &= \mathbf{e}(\mathbf{bnd}) + A_{bnd} \frac{\partial q_{ah}}{\partial \dot{s}} \\ \mathbf{b}(\mathbf{bnd}) &= \mathbf{b}(\mathbf{bnd}) + A_{bnd} \frac{\partial \dot{q}_{ah}''}{\partial T} \Big|_{T=T_{bnd}} \\ \mathbf{d}(\mathbf{bnd}) &= \mathbf{d}(\mathbf{bnd}) - A_{bnd} (\dot{q}_{ah}'')^\nu \end{aligned} \right\} \quad (5.89)$$

5.5.6 Pyrolysis Gas Injection Into the Boundary Layer

At the surface boundary there are pyrolysis gases being injected into the boundary layer due to both gas flow and surface recession, and each phenomenon will be treated separately. The energy transfer rate due to surface recession is

$$\dot{E}_{surf} = \dot{s} (\phi \rho_g h_w A)_1 \quad (5.90)$$

where the wall gas enthalpy (h_w) is not the pyrolysis gas enthalpy at the surface temperature, but it is the enthalpy of the gases adjacent to the wall after the reactions with ablation products and boundary layer gases occur. It is evident that pyrolysis

gases are injected into the boundary layer when ablation is occurring even if the gases themselves are not moving. Linearizing the energy transfer rate according to a Taylor series expansion in iteration space gives

$$\dot{E}_{surf}^{\nu+1} = \dot{E}_{surf}^{\nu} + \left. \frac{\partial \dot{E}_{surf}}{\partial T} \right|_{T=T_1} \Delta T_1^{\nu+1} + \frac{\partial \dot{E}_{surf}}{\partial \dot{s}} \Delta \dot{s}^{\nu+1} + \dots \quad (5.91)$$

and its sensitivity to temperature is given by

$$\left. \frac{\partial \dot{E}_{surf}}{\partial T} \right|_{T=T_1} = \dot{s} \left(\phi \rho_g A \frac{\partial h_w}{\partial T} \right)_1 \quad (5.92)$$

where $\partial h_w / \partial T$ is given in Eq. 5.83. The recession rate sensitivity is given by

$$\frac{\partial \dot{E}_{surf}}{\partial \dot{s}} = (\phi \rho_g A)_1 \left(\dot{s} \frac{\partial h_w}{\partial \dot{s}} + h_w \right)_1 \quad (5.93)$$

where $\partial h_w / \partial \dot{s}$ is given in Eq. 5.87. The resulting linear system contributions are

$$\left. \begin{aligned} \mathbf{e}(1) &= \mathbf{e}(1) + \frac{\partial \dot{E}_{surf}}{\partial \dot{s}} \\ \mathbf{b}(1) &= \mathbf{b}(1) + \left. \frac{\partial \dot{E}_{surf}}{\partial T} \right|_{T=T_1} \\ \mathbf{d}(1) &= \mathbf{d}(1) - \dot{E}_{surf}^{\nu} \end{aligned} \right\} \quad (5.94)$$

The energy transfer rate due to gas flow is

$$\dot{G}_{surf} = - (u'_g \rho_g h_w A)_1 \quad (5.95)$$

and linearizing in iteration space gives

$$\dot{G}_{surf}^{\nu+1} = \dot{G}_{surf}^{\nu} + \left. \frac{\partial \dot{G}_{surf}}{\partial T} \right|_{T=T_1} \Delta T_1^{\nu+1} + \frac{\partial \dot{G}_{surf}}{\partial \dot{s}} \Delta \dot{s}^{\nu+1} + \dots \quad (5.96)$$

where

$$\left. \frac{\partial \dot{G}_{surf}}{\partial T} \right|_{T=T_1} = - \left(u'_g \rho_g A \frac{\partial h_w}{\partial T} \right)_1 \quad (5.97)$$

and

$$\frac{\partial \dot{G}_{surf}}{\partial \dot{s}} = - (u'_g \rho_g A)_1 \frac{\partial h_w}{\partial \dot{s}} \quad (5.98)$$

The resulting linear system contributions are

$$\left. \begin{aligned} \mathbf{e}(1) &= \mathbf{e}(1) + \frac{\partial \dot{G}_{surf}}{\partial \dot{s}} \\ \mathbf{b}(1) &= \mathbf{b}(1) + \frac{\partial \dot{G}_{surf}}{\partial T} \Big|_{T=T_1} \\ \mathbf{d}(1) &= \mathbf{d}(1) - \dot{G}_{surf}^{\nu} \end{aligned} \right\} \quad (5.99)$$

Since the back node is stationary and impermeable, there are no energy fluxes due to grid convection and gas flow across the boundary, and these conditions occur naturally without any modification to the linear system.

5.6 Ablation Models

Since the code only allows ablation to occur at the front face, the development of the ablation models and the linear system contributions will only apply to the zeroth and first residual equations in the linear system.

5.6.1 Heat of Ablation (Q^*) Model

The heat of ablation model assumes that ablation occurs at a fixed temperature and that there is a fixed amount of energy consumed per unit mass of material ablated. This fixed amount of energy, Q^* , is the difference between the wall gas enthalpy and the charred solid enthalpy and is given by

$$Q^* = h_w - h_s \quad (5.100)$$

As a result, the enthalpy associated with the material being convected out of the surface control volume is the gas enthalpy adjacent to the wall.

$$h_w = h_s + Q^* \quad (5.101)$$

The resulting energy flux resulting from the ablation process is

$$q''_{abl} = \rho_s \dot{s} h_w = \rho_s \dot{s} (h_s + Q^*) \quad (5.102)$$

Since the surface temperature is known and is fixed while ablation is occurring for this model, the zeroth residual equation needed to complete the linear system in Eq. 5.3 is

$$\Delta T_1^{\nu+1} = 0 \quad (5.103)$$

and the resulting linear system contributions are

$$\left. \begin{aligned} \mathbf{e}(0) &= 0 \\ \mathbf{c}(0) &= 1 \\ \mathbf{d}(0) &= 0 \end{aligned} \right\} \quad (5.104)$$

The sensitivity of the ablative flux to the surface recession rate is

$$\frac{\partial q''_{abl}}{\partial \dot{s}} = \rho_s h_w \quad (5.105)$$

and the temperature sensitivity is

$$\left. \frac{\partial q''_{abl}}{\partial T} \right|_{T=T_1} = \rho_s \dot{s} \left. \frac{\partial h_s}{\partial T} \right|_{T=T_1} = \rho_s \dot{s} C_{ps} (T_1) \quad (5.106)$$

As a result, the linear system coefficients are updated according to

$$\left. \begin{aligned} \mathbf{e}(1) &= \mathbf{e}(0) + A_1 \frac{\partial q''_{abl}}{\partial \dot{s}} \\ \mathbf{b}(1) &= \mathbf{b}(0) + A_1 \left. \frac{\partial q''_{abl}}{\partial T} \right|_{T=T_1} \\ \mathbf{d}(1) &= \mathbf{d}(0) - A_1 (q''_{abl})^\nu \end{aligned} \right\} \quad (5.107)$$

Simple modifications could be added if the surface temperature was allowed to vary and the heat of ablation was a function of temperature.

$$Q^* = Q^* (T)$$

Note that a weakness of the heat of ablation model is that the wall gas enthalpy in the ablative flux is different from the wall gas enthalpy in the aerodynamic heating flux which is determined from non-ablating thermochemistry data. Unlike the thermochemical ablation model discussed in Section 5.6.2, the heat of ablation model does not have to be used in conjunction with the aerodynamic heating boundary condition.

Specified Recession Rate Option Instead of specifying the ablation temperature and heating rate, it is also feasible to have a problem in which the surface temperature and surface recession rate are known functions of time possibly from experiments. For this situation the zeroth and first equations in the linear system are

$$\Delta \dot{s}^{\nu+1} = \dot{s}^{n+1} - \dot{s}^{\nu} \quad (5.108)$$

and

$$\Delta T_1^{\nu+1} = T_1^{n+1} - T_1^{\nu} \quad (5.109)$$

respectively. Consequently, the linear system coefficient contributions are

$$\left. \begin{aligned} \mathbf{e}(0) &= 1 \\ \mathbf{c}(0) &= 0 \\ \mathbf{d}(0) &= \Delta \dot{s}^{\nu+1} \end{aligned} \right\} \quad (5.110)$$

and

$$\left. \begin{aligned} \mathbf{e}(1) &= 0 \\ \mathbf{b}(1) &= 1 \\ \mathbf{c}(1) &= 0 \\ \mathbf{d}(1) &= \Delta T_1^{\nu+1} \end{aligned} \right\} \quad (5.111)$$

5.6.2 Thermochemical Ablation Model

Like the Q^* ablation model, the ablative flux in the thermochemical ablation model is given by

$$\dot{q}_{abl}'' = \rho_s \dot{s} h_w \quad (5.112)$$

but now the surface temperature is not constant. The minimum ablation temperature is the temperature below which surface thermochemical processes are not significant enough to cause feasible surface recession, and therefore it is assumed that ablation is not occurring below this temperature. The minimum ablation temperature is a function of pressure and pyrolysis gas blowing rate

$$T_{abl_{\min}} = T_{abl_{\min}}(P, B'_g(\dot{s}, T_{bnd}))$$

where this two-dimensional function can be extracted from the thermochemistry data as described in Appendix C. The wall gas enthalpy is a function of surface temperature, pressure, and dimensionless pyrolysis gas blowing rate which can also be determined from the thermochemistry data.

$$h_w = h_w(P, T_{bnd}, B'_g(\dot{s}, T_{bnd}))$$

The ablative flux's sensitivities to surface temperature and recession rate are

$$\left. \frac{\partial \dot{q}_{abl}''}{\partial T} \right|_{T=T_1} = \rho_s \dot{s} \left. \frac{\partial h_w}{\partial T} \right|_{T=T_1} \quad (5.113)$$

and

$$\frac{\partial \dot{q}_{abl}''}{\partial \dot{s}} = \rho_s \left(h_w + \dot{s} \frac{\partial h_w}{\partial \dot{s}} \right) \quad (5.114)$$

where $(\partial h_w / \partial T)|_{T=T_1}$ is determined from Eq. 5.83 and $\partial h_w / \partial \dot{s}$ is given in Eq. 5.87.

The thermochemical ablation model results in linear system contributions given by

$$\left. \begin{aligned} \mathbf{e}(1) &= \mathbf{e}(1) + A_1 \frac{\partial \dot{q}_{abl}''}{\partial \dot{s}} \\ \mathbf{b}(1) &= \mathbf{b}(1) + A_1 \left. \frac{\partial \dot{q}_{abl}''}{\partial T} \right|_{T=T_1} \\ \mathbf{d}(1) &= \mathbf{d}(1) - A_1 (\dot{q}_{abl}'')^\nu \end{aligned} \right\} \quad (5.115)$$

The auxiliary relationship for thermochemical ablation provides the zeroth residual equation in the linear system and relates the surface recession rate and dimensionless char ablation rate through

$$\dot{m}_{abl}'' = \rho_s \dot{s} = \rho_e u_e C_m B'_c \quad (5.116)$$

where the dimensionless char ablation rate is tabulated as a function of pressure, temperature, and dimensionless pyrolysis gas blowing rate in the thermochemistry data.

$$B'_c = B'_c(P, T_1, B'_g(\dot{s}, T_{bnd}))$$

The relationship in Eq. 5.116 can be rewritten to give the definition of the dimensionless char ablation rate

$$B'_c = \frac{\rho_s \dot{s}}{\rho_e u_e C_{h_o} \frac{C_h}{C_{h_o}} \frac{C_m}{C_h}} \quad (5.117)$$

Now the zeroth residual equation can be written as

$$R_0 = \frac{\rho_s \dot{s}}{\rho_e u_e C_{h_o} \frac{C_h}{C_{h_o}} \frac{C_m}{C_h}} - B'_c \quad (5.118)$$

Performing the required differentiation to find the sensitivities gives

$$\frac{\partial R_0}{\partial \dot{s}} = \frac{\rho_s}{\rho_e u_e C_m} \left[1 - \frac{\dot{s}}{C_h / C_{h_o}} \frac{\partial (C_h / C_{h_o})}{\partial \dot{s}} \right] - \frac{\partial B'_c}{\partial \dot{s}} \quad (5.119)$$

and

$$\left. \frac{\partial R_0}{\partial T} \right|_{T=T_1} = - \left[\left. \frac{\rho_s \dot{s}}{\rho_e u_e C_m \frac{C_h}{C_{h_o}}} \frac{\partial (C_h / C_{h_o})}{\partial T} \right|_{T=T_1} + \left. \frac{\partial B'_c}{\partial T} \right|_{T=T_1} \right] \quad (5.120)$$

where

$$\frac{\partial B'_c}{\partial \dot{s}} = \frac{\partial B'_c}{\partial B'_g} \bigg|_T \frac{\partial B'_g}{\partial \dot{s}} \quad (5.121)$$

$\partial B'_g/\partial \dot{s}$ is given in Eq. 5.88 while $(\partial B'_c/\partial B'_g)|_T$ is calculated using a finite difference from the thermochemistry data. When the recession rate is held constant, the differential dimensionless ablation rate is given as

$$dB'_c = \frac{\partial B'_c}{\partial T} \bigg|_{B'_g} dT + \frac{\partial B'_c}{\partial B'_g} \bigg|_T dB'_g \quad (5.122)$$

and differentiating with respect to temperature gives

$$\frac{\partial B'_c}{\partial T} = \frac{\partial B'_c}{\partial T} \bigg|_{B'_g} + \frac{\partial B'_g}{\partial T} \frac{\partial B'_c}{\partial B'_g} \bigg|_T \quad (5.123)$$

where $(\partial B'_c/\partial T)|_{B'_g}$ is calculated using a finite difference from the thermochemistry data and $\partial B'_g/\partial T$ is given in Eq. 5.84. For the zeroth equation, the linear system contributions are

$$\begin{aligned} \mathbf{e}(0) &= \frac{\partial R_0}{\partial \dot{s}} \\ \mathbf{c}(0) &= \frac{\partial R_0}{\partial T} \bigg|_{T=T_1} \\ \mathbf{d}(0) &= -R'_0 \end{aligned} \quad (5.124)$$

5.7 Net Surface Heat Flux

Once a converged solution has been reached, the net heat flux at the surface of the body can be determined through examination of the surface control volume's energy balance. If the in-depth contributions to the first residual, $\mathbf{d}(1)$, are recalculated or saved while the boundary condition terms are not included, then the residual represents the heating rate at the surface necessary to satisfy the energy balance.

The surface control volume's energy balance is given by

$$\begin{aligned} (\dot{q}'' A)_1 = -\mathbf{d}(1) &= (\dot{q}'' A)_{1+1/2} - (\rho h u_{cs} A)_{1+1/2} - (\phi \rho_g h_g (u_g - u_{cs}) A)_1 \\ &+ (\phi \rho_g h_g u_g A)_{1+1/2} + \frac{d}{dt} \int_{z_1}^{\bar{z}_1} \rho e A dz \end{aligned} \quad (5.125)$$

which is evident from the internal contributions in the element assembly routines.

As a result,

$$\dot{q}'' = -\mathbf{d}(1)\frac{1}{A_1} \quad (5.126)$$

and a similar analysis can be performed for the back face.

6 Solid Phase Continuity Equation

The solid mass conservation equation for a moving grid given by Eq. 2.3 is

$$\frac{d}{dt} \underbrace{\int_{cv} \rho_s dV}_{\text{solid mass content}} - \underbrace{\int_{cs} \rho_s \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} = \underbrace{\int_{cv} \dot{m}_s''' dV}_{\text{solid mass source}}$$

Since the solid density gradient in the decomposition region is known to be much larger than the temperature gradients in the domain, a finer mesh is necessary for the solution of the solid phase continuity equation than was needed to solve the energy equation. CMA and several other studies employ a sub-mesh scheme in which there are a given number of nodelets (or sub-nodes) within each element on which the solid phase continuity equation is solved. Integral effects of the nodelet solutions are applied at nodes during the solution of the mixture energy equation. This method saves a significant amount of computational time since it avoids excessive grid points during the mixture energy equation solution. The nodelet scheme has not been implemented in the current model, therefore each governing equation is solved on the same mesh.

Implicit integration of the solid mass conservation equation through the CVFEM and nodal mass balance equations is not performed. Instead, direct integration of the kinetic relationships accounting for the moving grid, which has been used in previous studies[3], was chosen to determine the solution. The development of the fixed grid solid continuity equation solution procedure is presented, and the moving grid effects are considered afterwards.

6.1 Solution Procedure

The solid phase continuity equation on a fixed grid is given by

$$\frac{d}{dt} \underbrace{\int_{cv} \rho_s dV}_{\text{solid mass content}} = \underbrace{\int_{cv} \dot{m}_s''' dV}_{\text{solid mass source}} \quad (6.1)$$

Substituting Eq. 2.16 into Eq. 6.1 and knowing that the component source terms can be volumetrically weighted like the component densities in Eq. 2.16 gives

$$\frac{d}{dt} \int_{cv} [\Gamma(\rho_A + \rho_B) + (1 - \Gamma)\rho_C] dV = \int_{cv} [\Gamma(\dot{m}_A''' + \dot{m}_B''') + (1 - \Gamma)\dot{m}_C'''] dV \quad (6.2)$$

Since the decomposition of each component is independent of the other components when coupling effects from the other governing equations are ignored, the solid phase continuity equation can be further reduced to component continuity equations given by

$$\frac{d}{dt} \int_{cv} \Gamma \rho_A dV = \int_{cv} \Gamma \dot{m}_A''' dV \quad (6.3)$$

$$\frac{d}{dt} \int_{cv} \Gamma \rho_B dV = \int_{cv} \Gamma \dot{m}_B''' dV \quad (6.4)$$

$$\frac{d}{dt} \int_{cv} (1 - \Gamma) \rho_C dV = \int_{cv} (1 - \Gamma) \dot{m}_C''' dV \quad (6.5)$$

Removing the constant volume fractions gives

$$\frac{d}{dt} \int_{cv} \rho_i dV = \int_{cv} \dot{m}_i''' dV \text{ for } i = A, B, \text{ and } C \quad (6.6)$$

Now there are four equations (Eqs. 6.2 and 6.6) with three unknowns (ρ_A , ρ_B , ρ_C , and ρ_s), and the procedure is to solve the component continuity equations and then determine the solid density as a post-processing step via Eq. 2.16. The analogous finite difference relationship to Eq. 6.6 is

$$\left. \frac{\partial \rho_i}{\partial t} \right|_z = \dot{m}_i''' = -k_i \rho_{v_i} \left(\frac{\rho_i - \rho_{c_i}}{\rho_{v_i}} \right)^{\psi_i} e^{-E_i/RT} \text{ for } i = A, B, \text{ and } C \quad (6.7)$$

Since the density history at a given location only depends on the temperature history at that location, Eq. 6.7 can be integrated on a location-by-location basis (accounting for the moving grid) and the updated solid density can be determined.

6.2 Integration of Kinetic Equations

Since ρ_{v_i} and ρ_{c_i} are constants, the kinetic equation in Eq. 6.7 can be rearranged to give

$$\left. \frac{d}{dt} \left(\frac{\rho_i - \rho_{c_i}}{\rho_{v_i}} \right) \right|_z = -k_i \left(\frac{\rho_i - \rho_{c_i}}{\rho_{v_i}} \right)^{\psi_i} e^{-E_i/RT} \text{ for } i = A, B, \text{ and } C \quad (6.8)$$

or

$$\left. \frac{dw_i}{dt} \right|_z = -k_i w_i^{\psi_i} e^{-E_i/RT} \text{ for } i = A, B, \text{ and } C \quad (6.9)$$

where the dimensionless relative density is given by

$$w_i = \frac{\rho_i - \rho_{c_i}}{\rho_{v_i}} \quad (6.10)$$

Direct integration of Eq. 6.9 over one time step while treating temperature explicitly in time, gives

$$w_i(z_j^{n+1}, t^{n+1}) = \left\{ [w_i(z_j^{n+1}, t^n)]^{(1-\psi_i)} - \Delta t^{n+1} (1 - \psi_i) k_i e^{-E_i/RT(z_j^{n+1}, t^n)} \right\}^{\frac{1}{1-\psi_i}} \quad (6.11)$$

for $\psi_i \neq 1$

and

$$w_i(z_j^{n+1}, t^{n+1}) = [w_i(z_j^{n+1}, t^n)] e^{-k_i \Delta t^{n+1} e^{-E_i/RT(z_j^{n+1}, t^n)}} \quad (6.12)$$

for $\psi_i = 1$

Eqs. 6.11 and 6.12 were implemented in CMA to integrate the kinetic equations regardless of the temperature change over the time interval. They are applied in the current model only if the temperature remains constant over the time interval $[T(z_j^{n+1}, t^{n+1}) = T(z_j^{n+1}, t^n)]$. Also note that $w_i(z_j^{n+1}, t^{n+1})$, $w_i(z_j^{n+1}, t^n)$, $T(z_j^{n+1}, t^{n+1})$, and $T(z_j^{n+1}, t^n)$ are evaluated at the same spatial location (z -coordinate) and not at the same node (η -coordinate).

An alternative approach to determining the dimensionless relative densities at time level $n + 1$ is to assume that the temperature rise rate over the time interval

Δt^{n+1} is a constant, Θ .

$$\left. \frac{dT}{dt} \right|_z = \Theta = \frac{T(z_j^{n+1}, t^{n+1}) - T(z_j^{n+1}, t^n)}{\Delta t} \quad (6.13)$$

This is consistent with the implicit time integrator's ability to at best capture a linear temperature rise rate since the method is first order. Using Eq. 6.9 and the chain rule gives

$$\left. \frac{dw_i}{dT} \right|_z \Theta = -k_i w_i^{\psi_i} e^{-E_i/RT} \text{ for } i = A, B, \text{ and } C \quad (6.14)$$

Integrating and solving for $w_i(z_j^{n+1}, t^{n+1})$ gives

$$w_i(z_j^{n+1}, t^{n+1}) = \left\{ [w_i(z_j^{n+1}, t^n)]^{1-\psi_i} + \frac{k_i(\psi_i - 1)}{\Theta} \int_{T(z_j^{n+1}, t^n)}^{T(z_j^{n+1}, t^{n+1})} e^{-E_i/RT} dT \right\}^{\frac{-1}{\psi_i - 1}} \quad (6.15)$$

for $\psi_i \neq 1$

and

$$w_i(z_j^{n+1}, t^{n+1}) = \exp \left(\ln [w_i(z_j^{n+1}, t^n)] - \frac{k_i}{\Theta} \int_{T(z_j^{n+1}, t^n)}^{T(z_j^{n+1}, t^{n+1})} e^{-E_i/RT} dT \right) \quad (6.16)$$

for $\psi_i = 1$

$\int_{T(z_j^{n+1}, t^n)}^{T(z_j^{n+1}, t^{n+1})} e^{-E_i/RT} dT$ can be determined through the use of exponential integrals or numerical integration techniques such as trapezoidal or Simpson's rules, and Simpson's rule was chosen for this study. Since the new dimensionless relative densities are known, the component densities can be determined via Eq. 6.10, and the solid bulk density can now be determined from

$$\rho_s^{n+1} = \Gamma (\rho_A^{n+1} + \rho_B^{n+1}) + (1 - \Gamma) \rho_C^{n+1} \quad (6.17)$$

or in terms of dimensionless relative densities

$$\rho_s^{n+1} = \rho_{c_s} + \Gamma (\rho_{v_A} w_A^{n+1} + \rho_{v_B} w_B^{n+1}) + (1 - \Gamma) \rho_{v_C} w_C^{n+1} \quad (6.18)$$

Since problems are solved on contracting grids for which the spatial coordinate of each node changes while the Landau coordinate of each node is fixed, it is necessary to determine temperature and dimensionless relative density profiles at the previous time level and current nodal locations $(T(z_j^{n+1}, t^n)$ and $w_i(z_j^{n+1}, t^n)$). Since properties are assumed to vary linearly within elements, linear interpolation in the old (time level n) profiles is used to calculate these properties. Say that node j now lies between the old locations of nodes h and $h + 1$. Then

$$X(z_j^{n+1}, t^n) = fX(z_{h+1}^n, t^n) + (1 - f)X(z_h^n, t^n) \quad (6.19)$$

where $X = T$ or w_i and

$$f = \frac{z_j^{n+1} - z_h^n}{z_{h+1}^n - z_h^n} \quad (6.20)$$

The above procedure for determining the solution to the solid phase continuity equation requires that the component density and temperature profiles and the nodal locations at the previous time level (time level n) are known. Also the most recently updated temperature profile and nodal locations at the current time level and global iteration (time level $n + 1$ and global iteration $\nu + 1$) must be provided.

7 Gas Phase Continuity Equation and Darcy's Law

The gas mass conservation equation given by Eq. 2.4 is

$$\underbrace{\frac{d}{dt} \int_{cv} \phi \rho_g dV}_{\text{gas mass content}} + \underbrace{\int_{cs} \phi \rho_g \mathbf{v}_g \cdot d\mathbf{A}}_{\text{gas flux}} - \underbrace{\int_{cs} \phi \rho_g \mathbf{v}_{cs} \cdot d\mathbf{A}}_{\text{grid convection}} - \underbrace{\int_{cv} \dot{m}_g''' dV}_{\text{gas mass source}} = 0$$

For one-dimension, Eq. 2.4 in semi-discrete form for a nodal control volume is

$$\begin{aligned} 0 = & \frac{d}{dt} \int_{\bar{z}_{j-1}}^{z_j} \phi \rho_g A dz + \frac{d}{dt} \int_{z_j}^{\bar{z}_j} \phi \rho_g A dz - (\phi \rho_g u_g A)_{j-1/2} + (\phi \rho_g u_g A)_{j+1/2} \\ & + (\phi \rho_g u_{cs} A)_{j-1/2} - (\phi \rho_g u_{cs} A)_{j+1/2} - \int_{\bar{z}_{j-1}}^{z_j} \dot{m}_g''' A dz - \int_{z_j}^{\bar{z}_j} \dot{m}_g''' A dz \end{aligned} \quad (7.1)$$

and the gas mass balance terms can be seen in Figure 7.1. During the local iteration

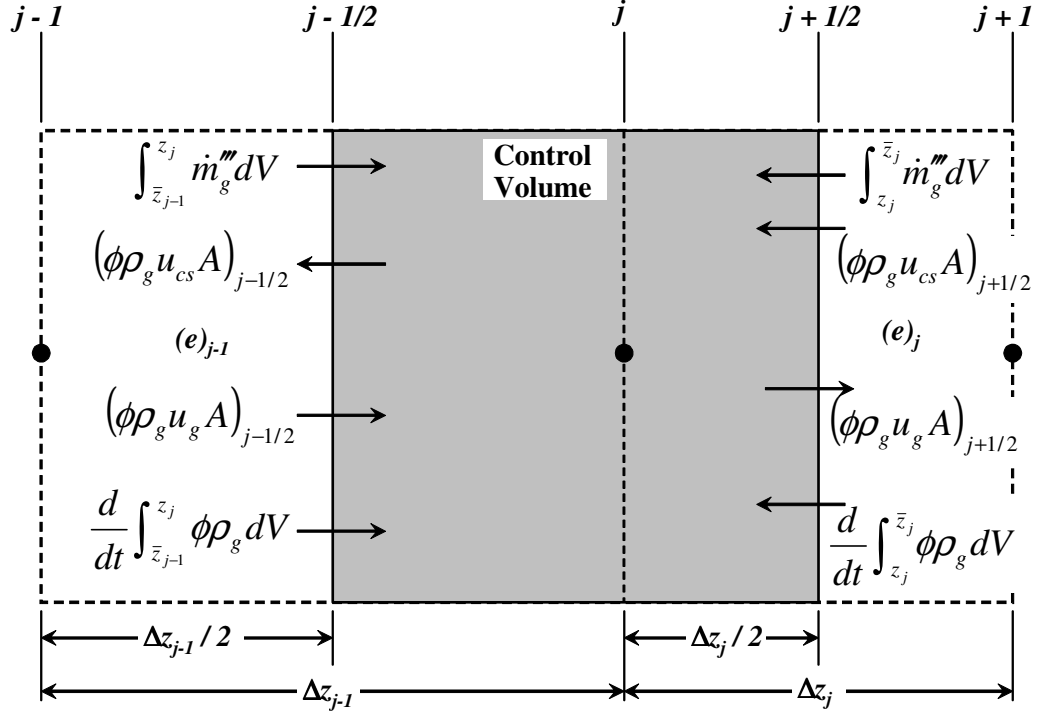


Figure 7.1: Gas mass balance terms for the control volume surrounding node j .

process, temperature and surface recession rate are held constant. Consequently, gas density is the only dependent variable changing during the iterative solution of the gas

phase continuity equation. The resulting linear system of nodal residual equations is always tridiagonal since the grid position is constant throughout the solution process.

The linear system for a five node domain is given by

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 \\ 0 & 0 & a_4 & b_4 & c_4 \\ 0 & 0 & 0 & a_5 & b_5 \end{bmatrix}^\nu \begin{bmatrix} \Delta(\rho_g)_1 \\ \Delta(\rho_g)_2 \\ \Delta(\rho_g)_3 \\ \Delta(\rho_g)_4 \\ \Delta(\rho_g)_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}^\nu \quad (7.2)$$

It is unknown what the true initial conditions for the solution of the gas phase continuity equation should be. For a ballistic reentry vehicle, atmospheric gases (air) fill the pore space before flight and are free to exit the pore space to adjust to the surface pressure as the vehicle leaves the atmosphere. Upon reentry but before in-depth decomposition begins to occur, air can reenter the pore space, but it is unknown how quickly this may occur. Once in-depth decomposition begins, both air and pyrolysis gases occupy the pore space and this cohabitation may occur throughout the remainder of the flight.

For the current study, it is assumed that the atmospheric gases never occupy any of the pore space, which is initially assumed to be filled with pyrolysis gases at the initial temperature and pressure. Although it is assumed that pyrolysis gases initially reside in the pore space, the solution of the gas phase continuity equation is not determined until in-depth decomposition begins to occur. Consequently, the mixture energy equation is solved with trace amounts of stagnant pyrolysis gas which is not expected to significantly change the solution since the gas's heat capacity is much lower than the solid's heat capacity. Initializing the pore space as a vacuum was also attempted, but this resulted in numerical predictions with negative pressures in the beginning of simulations. In addition, a discontinuous pressure front translates from the pyrolysis front to the ablator back face when decomposition first begins. Although initializing the pore space as a vacuum results in the prediction

of nonphysical transient behavior at the beginning of simulations, once an adequate amount of gas occupies the pore space these issues do not arise. With the exception of the results at early problem times, the solutions do not have a significant sensitivity to the gas density initialization.

7.1 Gas Mass Flux and Grid Convection

The gas flux and grid convection terms are treated simultaneously for the gas phase continuity equation since there is not the complexity of two phases in the grid convection terms that there was in the mixture energy equation. The combined gas flux and convection terms in Eq. 7.1 for the $j + 1/2$ boundary in element vector form are given by

$$\begin{bmatrix} \check{M}_j \\ \check{M}_{j+1} \end{bmatrix} = [\phi \rho_g A (u_g - u_{cs})]_{j+1/2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (7.3)$$

Introducing the superficial velocity found from Darcy's law in Eq. 5.19 gives

$$\begin{bmatrix} \check{M}_j \\ \check{M}_{j+1} \end{bmatrix} = \bar{\rho}_g A [u'_g - \bar{\phi}(u_{cs})_{j+1/2}] \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (7.4)$$

where

$$\phi u_g = u'_g \quad (7.5)$$

Linearizing the gas mass flux vector in iteration space according to a Taylor series expansion treating the nodal gas densities as the independent variables gives

$$\begin{bmatrix} \check{M}_j \\ \check{M}_{j+1} \end{bmatrix}^{\nu+1} = \begin{bmatrix} \check{M}_j \\ \check{M}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \check{M}_j}{\partial (\rho_g)_j} & \frac{\partial \check{M}_j}{\partial (\rho_g)_{j+1}} \\ \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_j} & \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_{j+1}} \end{bmatrix}^{\nu} \begin{bmatrix} \Delta (\rho_g)_j \\ \Delta (\rho_g)_{j+1} \end{bmatrix}^{\nu+1} + \dots \quad (7.6)$$

where the sensitivity matrix entries are

$$\left. \begin{aligned} \frac{\partial \check{M}_j}{\partial (\rho_g)_j} &= A \left\{ \frac{1}{2} [u'_g - \bar{\phi}(u_{cs})_{j+1/2}] + \bar{\rho}_g \frac{\partial u'_g}{\partial (\rho_g)_j} \right\} \\ \frac{\partial \check{M}_j}{\partial (\rho_g)_{j+1}} &= A \left\{ \frac{1}{2} [u'_g - \bar{\phi}(u_{cs})_{j+1/2}] + \bar{\rho}_g \frac{\partial u'_g}{\partial (\rho_g)_{j+1}} \right\} \\ \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_j} &= -A \left\{ \frac{1}{2} [u'_g - \bar{\phi}(u_{cs})_{j+1/2}] + \bar{\rho}_g \frac{\partial u'_g}{\partial (\rho_g)_j} \right\} \\ \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_{j+1}} &= -A \left\{ \frac{1}{2} [u'_g - \bar{\phi}(u_{cs})_{j+1/2}] + \bar{\rho}_g \frac{\partial u'_g}{\partial (\rho_g)_{j+1}} \right\} \end{aligned} \right\} \quad (7.7)$$

Substituting the equation of state into Darcy's law gives

$$\begin{bmatrix} \frac{\partial u'_g}{\partial (\rho_g)_j} \\ \frac{\partial u'_g}{\partial (\rho_g)_{j+1}} \end{bmatrix} = \frac{\bar{\kappa} \hat{R}}{\bar{\mu} \Delta z_j} \begin{bmatrix} \left(\frac{T}{\hat{M}_g} \right)_j \\ - \left(\frac{T}{\hat{M}_g} \right)_{j+1} \end{bmatrix} \quad (7.8)$$

The resulting linear system contributions for each j th element are

$$\left. \begin{aligned} \mathbf{b}(j) &= \mathbf{b}(j) + \frac{\partial \check{M}_j}{\partial (\rho_g)_j} \\ \mathbf{c}(j) &= \mathbf{c}(j) + \frac{\partial \check{M}_j}{\partial (\rho_g)_{j+1}} \\ \mathbf{d}(j) &= \mathbf{d}(j) - \check{M}_j^\nu \\ \mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_j} \\ \mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{\partial \check{M}_{j+1}}{\partial (\rho_g)_{j+1}} \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) - \check{M}_{j+1}^\nu \end{aligned} \right\} \quad (7.9)$$

7.2 Gas Source

The element mass source vector is given by

$$-\begin{bmatrix} \dot{M}_j \\ \dot{M}_{j+1} \end{bmatrix} = \begin{bmatrix} -\int_{\bar{z}_j}^{z_j} \dot{m}_g''' Adz \\ -\int_{\bar{z}_j}^{z_{j+1}} \dot{m}_g''' Adz \end{bmatrix} \quad (7.10)$$

where the negative sign is for consistency with Eq. 7.1. The source term at any location can be determined by a Taylor series expansion in position about the element center given by

$$(\dot{m}_g''')_z = (\dot{m}_g''')_{\bar{z}_j} + \left. \frac{\partial \dot{m}_g'''}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) + \dots \quad (7.11)$$

Substituting Eq. 7.11 into 7.10 gives

$$-\begin{bmatrix} \dot{M}_j \\ \dot{M}_{j+1} \end{bmatrix} = -\begin{bmatrix} \int_{\bar{z}_j}^{z_j} \left[\bar{\dot{m}}_g''' + \left. \frac{\partial \dot{m}_g'''}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) \right] Adz \\ \int_{\bar{z}_j}^{z_{j+1}} \left[\bar{\dot{m}}_g''' + \left. \frac{\partial \dot{m}_g'''}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) \right] Adz \end{bmatrix} \quad (7.12)$$

where

$$(\dot{m}_g''')_{\bar{z}_j} = \bar{\dot{m}}_g''' \quad (7.13)$$

Since it is assumed that all solid decomposition results in gas generation, the nodal gas mass source terms can be determined from

$$(\dot{m}_g''')_j^{n+1} = -(\dot{m}_s''')_j^{n+1} = -[\Gamma (\dot{m}_A''' + \dot{m}_B''') + (1 - \Gamma) \dot{m}_C''']^{n+1} \quad (7.14)$$

where

$$(\dot{m}_i''')^{n+1} = -k_i \rho_{v_i} [w_i (z_j^{n+1}, t^{n+1})]^{\psi_i} e^{-E_i/RT(z_j^{n+1}, t^{n+1})} \text{ for } i = A, B, \text{ and } C \quad (7.15)$$

Consequently, the mass source term and its spatial derivative at the element center are determined from

$$\bar{\dot{m}}_g''' = \frac{1}{2} [(\dot{m}_g''')_j + (\dot{m}_g''')_{j+1}] \quad (7.16)$$

and

$$\left. \frac{\partial \dot{m}_g'''}{\partial z} \right|_{z=\bar{z}_j} = \frac{(\dot{m}_g''')_{j+1} - (\dot{m}_g''')_j}{\Delta z_j} \quad (7.17)$$

respectively. To aid in the integration process it is convenient to again employ the local coordinate system described in Eqs. 5.31-5.33. Thus the mass source vector in terms of local coordinates becomes

$$-\begin{bmatrix} \dot{M}_j \\ \dot{M}_{j+1} \end{bmatrix} = -\begin{bmatrix} \frac{\Delta z_j}{2} \bar{m}_g''' \int_0^0 A(\xi) d\xi + [(\dot{m}_g''')_{j+1} - (\dot{m}_g''')_j] \frac{\Delta z_j}{4} \int_0^0 \xi A d\xi \\ \frac{\Delta z_j}{2} \bar{m}_g''' \int_0^1 A(\xi) d\xi + [(\dot{m}_g''')_{j+1} - (\dot{m}_g''')_j] \frac{\Delta z_j}{4} \int_0^1 \xi A d\xi \end{bmatrix} \quad (7.18)$$

For planar geometry, the gas mass source vector simplifies to

$$-\begin{bmatrix} \dot{M}_j \\ \dot{M}_{j+1} \end{bmatrix} = -\frac{\Delta z_j}{2} \begin{bmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{bmatrix} \begin{bmatrix} (\dot{m}_g''')_j \\ (\dot{m}_g''')_{j+1} \end{bmatrix} \quad (7.19)$$

It is evident that the mass source vector has no dependence on nodal gas density, and as a result, the mass source term has a residual vector contribution but no sensitivity matrix contributions.

$$\left. \begin{aligned} \mathbf{d}(j) &= \mathbf{d}(j) + \dot{M}_j^\nu \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) + \dot{M}_{j+1}^\nu \end{aligned} \right\} \quad (7.20)$$

7.3 Gas Mass Content and Time Integration

The element gas mass content vector is given by

$$\begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix} = \begin{bmatrix} \int_{\bar{z}_j}^{\bar{z}_j} \phi \rho_g A dz \\ \int_{\bar{z}_j}^{z_{j+1}} \phi \rho_g A dz \end{bmatrix} \quad (7.21)$$

where the gas bulk density at any point can be determined through a Taylor series expansion about the element center.

$$(\phi \rho_g)_z = (\phi \rho_g)_{\bar{z}_j} + \left. \frac{\partial (\phi \rho_g)}{\partial z} \right|_{z=\bar{z}_j} (z - \bar{z}_j) + \dots \quad (7.22)$$

Substituting Eq. 7.22 into Eq. 7.21 gives

$$\begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix} = \begin{bmatrix} \int_{z_j}^{\bar{z}_j} \left(\overline{\phi \rho_g} + \frac{\partial(\phi \rho_g)}{\partial z} \Big|_{z=\bar{z}_j} (z - \bar{z}_j) \right) Adz \\ \int_{\bar{z}_j}^{z_{j+1}} \left(\overline{\phi \rho_g} + \frac{\partial(\phi \rho_g)}{\partial z} \Big|_{z=\bar{z}_j} (z - \bar{z}_j) \right) Adz \end{bmatrix} \quad (7.23)$$

where

$$(\phi \rho_g)_{\bar{z}_j} = \overline{\phi \rho_g} \quad (7.24)$$

Using a finite central difference for $\partial(\phi \rho_g)/\partial z$ and invoking the local coordinate system reduces the gas mass content vector to

$$\begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix} = \begin{bmatrix} \overline{\phi \rho_g} \frac{\Delta z_j}{2} \int_{-1}^0 A(\xi) d\xi + [(\phi \rho_g)_{j+1} - (\phi \rho_g)_j] \frac{\Delta z_j}{4} \int_{-1}^0 \xi A d\xi \\ \overline{\phi \rho_g} \frac{\Delta z_j}{2} \int_{-1}^0 A(\xi) d\xi + [(\phi \rho_g)_{j+1} - (\phi \rho_g)_j] \frac{\Delta z_j}{4} \int_0^1 \xi A d\xi \end{bmatrix} \quad (7.25)$$

Performing the integration for planar geometry gives

$$\begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix} = \frac{\Delta z_j}{2} \begin{bmatrix} \frac{3}{4} \phi_j & \frac{1}{4} \phi_{j+1} \\ \frac{1}{4} \phi_j & \frac{3}{4} \phi_{j+1} \end{bmatrix} \begin{bmatrix} (\rho_g)_j \\ (\rho_g)_{j+1} \end{bmatrix} \quad (7.26)$$

The time rate of change of gas mass content according to an implicit time integrator can be expressed as

$$\frac{d}{dt} \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^{n+1} = \left\{ \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^{n+1} - \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^n \right\} \frac{1}{\Delta t^{n+1}} \quad (7.27)$$

Expanding the time rate of change of the gas mass content vector in iteration space according to a Taylor series expansion gives

$$\begin{aligned} \frac{d}{dt} \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^{\nu+1} &= \left\{ \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^{\nu} + \begin{bmatrix} \frac{\partial \tilde{M}_j}{\partial (\rho_g)_j} & \frac{\partial \tilde{M}_j}{\partial (\rho_g)_{j+1}} \\ \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_j} & \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_{j+1}} \end{bmatrix}^{\nu} \begin{bmatrix} \Delta (\rho_g)_j \\ \Delta (\rho_g)_{j+1} \end{bmatrix}^{\nu+1} \right. \\ &\quad \left. - \begin{bmatrix} \tilde{M}_j \\ \tilde{M}_{j+1} \end{bmatrix}^n \right\} \frac{1}{\Delta t^{n+1}} \end{aligned} \quad (7.28)$$

where the sensitivity matrix entries are

$$\left. \begin{aligned} \frac{\partial \tilde{M}_j}{\partial (\rho_g)_j} &= \frac{3\Delta z_j}{8} \phi_j \\ \frac{\partial \tilde{M}_j}{\partial (\rho_g)_{j+1}} &= \frac{\Delta z_j}{8} \phi_{j+1} \\ \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_j} &= \frac{\Delta z_j}{8} \phi_j \\ \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_{j+1}} &= \frac{3\Delta z_j}{8} \phi_{j+1} \end{aligned} \right\} \quad (7.29)$$

The resulting linear system contributions for each j th element are

$$\left. \begin{aligned} \mathbf{b}(j) &= \mathbf{b}(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{M}_j}{\partial (\rho_g)_j} \\ \mathbf{c}(j) &= \mathbf{c}(j) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{M}_j}{\partial (\rho_g)_{j+1}} \\ \mathbf{d}(j) &= \mathbf{d}(j) - \frac{1}{\Delta t^{n+1}} \left(\tilde{M}_j^\nu - \tilde{M}_j^n \right) \\ \mathbf{a}(j+1) &= \mathbf{a}(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_j} \\ \mathbf{b}(j+1) &= \mathbf{b}(j+1) + \frac{1}{\Delta t^{n+1}} \frac{\partial \tilde{M}_{j+1}}{\partial (\rho_g)_{j+1}} \\ \mathbf{d}(j+1) &= \mathbf{d}(j+1) - \frac{1}{\Delta t^{n+1}} \left(\tilde{M}_{j+1}^\nu - \tilde{M}_{j+1}^n \right) \end{aligned} \right\} \quad (7.30)$$

7.4 Boundary Conditions

7.4.1 Specified Pressure

On the front face, a time dependent specified boundary pressure is applied, and it is either provided by the aerodynamic heating input data or a separate specified

pressure table if an aerodynamic heating boundary condition is not applied. The residual equation for the first node is

$$R_1 = P_1^{n+1} - P_1^\nu = 0 \quad (7.31)$$

where

$$P_1^\nu = \left[\rho_g \frac{\hat{R}}{\hat{M}_g} T \right]_1^\nu \quad (7.32)$$

Expanding the residual in iteration space gives

$$R_1^{\nu+1} = R_1^\nu + \left[\frac{\partial R_1}{\partial (\rho_g)_1} \right]_1^\nu [\Delta (\rho_g)_1]^{\nu+1} + \dots \quad (7.33)$$

where

$$\frac{\partial R_1}{\partial (\rho_g)_1} = - \left[\frac{\hat{R}T}{\hat{M}_g} \right]_1^\nu \quad (7.34)$$

The residual equation can now be expressed as

$$[\Delta (\rho_g)_1]^{\nu+1} = \left[\frac{\hat{M}_g P^{n+1}}{\hat{R}T} \right]_1 - (\rho_g)_1^\nu \quad (7.35)$$

and the resulting linear system contributions are

$$\left. \begin{aligned} \mathbf{b}(1) &= 1 \\ \mathbf{c}(1) &= 0 \\ \mathbf{d}(1) &= [\Delta (\rho_g)_1]^{\nu+1} \end{aligned} \right\} \quad (7.36)$$

7.4.2 Impermeable Wall Condition

The back face is treated as an impermeable boundary which results in no gas flux and no pressure gradient. Since no gas flux terms are applied at the back boundary in the gas mass flux routine described in Section 7.1, this boundary condition occurs naturally without any additional calculation in the same manner that the adiabatic condition occurred naturally for the energy equation as described in Section 5.5.2.

7.4.3 Surface Pyrolysis Gas Flux

Once a converged solution has been reached, the net pyrolysis gas mass flux and velocity at the surface of the body can be determined through examination of the surface control volume's mass balance. If the in-depth contributions to the first residual, $d(1)$, are recalculated or saved while the boundary condition terms are not included, then the residual represents the pyrolysis gas mass flow rate at the surface necessary to satisfy the mass balance. The surface control volume's mass balance is given by

$$\begin{aligned} (\rho_g A (u'_g - \phi \dot{s}))_1 = -d(1) = (\phi \rho_g A (u'_g - \phi u_{cs}))_{1+1/2} \\ + \frac{d}{dt} \int_{z_1}^{\bar{z}_1} \phi \rho_g A dz - \int_{z_1}^{\bar{z}_1} \dot{m}_g''' A dz \end{aligned} \quad (7.37)$$

Therefore

$$(u'_g)_1 = -d(1) \frac{1}{(\rho_g A)_1} + \phi_1 \dot{s} \quad (7.38)$$

and the pyrolysis gas injection rate into the boundary layer (positive into boundary layer) is

$$\dot{m}_g'' = d(1) \frac{1}{A_1} \quad (7.39)$$

8 Model Verification

Before using the code for engineering applications, model verification is a necessary step in the code development process in order to ensure that the chosen model equations have been implemented correctly. The verification process allows the developers to identify derivation and coding errors (bugs) when the results deviate from theoretical expectations. However, code verification does not ensure that the correct equations have been implemented to describe the physical phenomenon being modeled. In order to accomplish this, code validation through comparison with experimental observations is necessary.

The spatial discretization method for both the mixture energy and gas phase continuity equations is expected to be second order, $O(\Delta z^2)$, while the implicit time integrator is expected to be first order, $O(\Delta t)$. As a result, the discretization error is expected to be of the form

$$DE = a\Delta t + b\Delta z^2 + (\text{higher order terms}) \quad (8.1)$$

Factoring out a $b\Delta z^2$ and ignoring the higher order terms gives

$$DE = b\Delta z^2 \left(1 + \frac{a\Delta t}{b\Delta z^2} \right) \quad (8.2)$$

It is evident that if the spatial and temporal grids are simultaneously refined while keeping $\Delta t/\Delta z^2$ constant, then the spatial and temporal orders of accuracy can be confirmed if the grid convergence rate is second order. This method is valid only when $a\Delta t/b\Delta z^2$ is greater than or on the order of 1. If $a\Delta t/b\Delta z^2 \ll 1$, then only the spatial order of accuracy can be confirmed.

Independent refinements of Δz while keeping Δt sufficiently small and Δt while keeping Δz sufficiently small can yield the spatial and temporal orders of accuracy respectively without making any assumption about the form of the discretization error.

However the proposed method only requires one refinement study for each verification problem and neither the time step nor the spatial step is required to be extremely small which would result in long computations. Also, the independent refinement method is an iterative process in order to ensure that Δz or Δt is sufficiently small. If the order of accuracy of the implicit time integrator is independently verified, which is also presented, then the application of the simultaneous refinement can be used to confirm the spatial order of accuracy of various terms.

Two methods are presented to verify the grid convergence rates of the implemented model. The first is the comparison of numerical solutions to analytical solutions where the numerical solutions are found on successively refined space time grids to reveal if the analytical solution is being approached at the theoretical rate. This method can isolate terms in a governing equation or boundary condition for select problems that have analytical solutions, and if the convergence rate does not agree with expectations, then the term in which the error resides is easy to identify.

The other method is the use of the Grid Convergence Index and Richardson extrapolation as described by Roache[22], which is used to verify the grid convergence rate when solving a real-world problem in which the material properties and time dependence are too complicated to determine an analytical solution. Richardson extrapolation can be used to approximate the exact solution, f_{exact} , according to

$$f_{exact} \approx f_1 + \frac{f_1 - f_2}{r^2 - 1} \quad (8.3)$$

where r is the ratio of initial characteristic mesh lengths given by

$$r = \left. \frac{\Delta z_2}{\Delta z_1} \right|_o \quad (8.4)$$

For $r = 2$, the expression for the approximate exact solution reduces to

$$f_{exact} \approx \frac{4}{3}f_1 - \frac{1}{3}f_2 \quad (8.5)$$

where the subscript 1 denotes the finer mesh. This method was developed based on finite difference theory, but it has also been applied to finite element and finite volume methods. The approximation of the exact solution is fourth order accurate if the two numerical solutions used in the extrapolation are second order accurate through the use of second order central differences. In addition, Richardson extrapolation must be applied at a consistent spatial location. Therefore, for moving grid problems there is an added complexity since nodal locations at the end of a simulation are not the same for each of the grids with the exception of the ablator back face node. The presented analyses assume that the error associated with inconsistent nodal locations is small, therefore it is sometimes necessary to integrate over small time intervals so these errors do not accumulate.

In addition to verifying the temporal and spatial orders of accuracy, it is necessary to verify the order of nonlinear convergence of the Newton solvers. Theoretically, a correct implementation of a full Newton's method for a system of nonlinear equations should exhibit second order convergence. If the method converges at a rate other than second order, then it is likely that a mistake exists in the derivation or implementation. The theoretical error relationship for successive iterations is given by

$$(error)^{\nu+1} = a [(error)^\nu]^2 \quad (8.6)$$

Therefore a plot of $\log |(error)^{\nu+1}|$ versus $\log |(error)^\nu|$ should result in a line with a slope of 2 if the method is correctly implemented[37]. Since the Newton solvers will converge to the exact solution plus discretization error, the difference in some quantity, X , between the current iteration and the converged solution is used as the error metric.

$$(error)^\nu = (X)^\nu - (X)^{converged} \quad (8.7)$$

As a result, nonlinear convergence plots have no data points for the final two iterations

of a time step since this will result in coordinates with zero values which compromises the value of the logarithmic plot.

It is important to note that the presence of second order nonlinear convergence does not imply that the method is converging to the correct answer nor does the absence of second order convergence imply that the converged solution is incorrect. Second order nonlinear convergence reveals that the implemented sensitivity matrix contains the correct sensitivities for the implemented residual equations and that the efficiency of the solution procedure is maximized. Therefore incorrect residual equations can be implemented but second order nonlinear convergence can still exist if their associated sensitivities were correctly derived and implemented.

8.1 Transient Conduction

8.1.1 Problem Statement

The transient conduction verification problem is intended to isolate the constant property and constant density terms in the energy content, conduction, and specified heat flux boundary condition routines. Consider a constant property, non-ablating, non-decomposing, one-dimensional, uniform density, planar slab with a specified constant heat flux on the front face and an adiabatic back face. The governing equation, boundary conditions, and initial conditions associated with this problem are

$$\left. \begin{aligned} \rho C_v \frac{\partial T}{\partial t} &= k \frac{\partial^2 T}{\partial z^2} \text{ for } 0 \leq z \leq L \\ -k \frac{\partial T}{\partial z} \Big|_{z=0} &= \dot{q}'' \\ -k \frac{\partial T}{\partial z} \Big|_{z=L} &= 0 \\ T(z, t=0) &= T_o \end{aligned} \right\} \quad (8.8)$$

and the parameters for the problem are given in Table 8.1. Since this is a linear problem, convergence is reached in one iteration per time step and a nonlinear convergence rate study is unnecessary. Consequently, if more than one iteration is required, then it is likely that a mistake exists.

Table 8.1: Transient conduction verification problem parameters.

$T_o = 300 \text{ K}$
$\dot{q}'' = 7.5 \times 10^5 \text{ W/m}^2$
$L = 0.01 \text{ m}$
$\rho = 8000 \text{ kg/m}^3$
$C_v = 500 \text{ J/kg-K}$
$k = 10 \text{ W/m-K}$
$\alpha = k/(\rho C_v) = 2.5 \times 10^{-6} \text{ m}^2/\text{s}$

8.1.2 Analytical Solution

The analytical solution to this problem can be found in Arpaci[38] or Beck et al.[39] and is given by

$$\frac{T(z, t) - T_o}{\dot{q}'' L/k} = \frac{\alpha t}{L^2} + \frac{1}{3} - \frac{z}{L} + \frac{1}{2} \left(\frac{z}{L} \right)^2 - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp \left(-n^2 \pi^2 \frac{\alpha t}{L^2} \right) \cos \left(n \pi \frac{z}{L} \right) \quad (8.9)$$

where the analytical solution for $t = 4 \text{ s}$ and $t = 40 \text{ s}$ is shown in Figure 8.1.

8.1.3 Grid Refinement Study

In order to independently verify the order of accuracy of the implicit time integrator, the domain was discretized with a 2000 element uniform grid so that the error associated with the time integration in Eq. 8.1 is dominant over the error associated with the spatial discretization.

$$a\Delta t \gg b\Delta z^2$$

The coarsest temporal grid has a time step of 0.5 s while the time step is refined by a factor of 4 for each of the subsequent temporal grids, and the grid parameters can

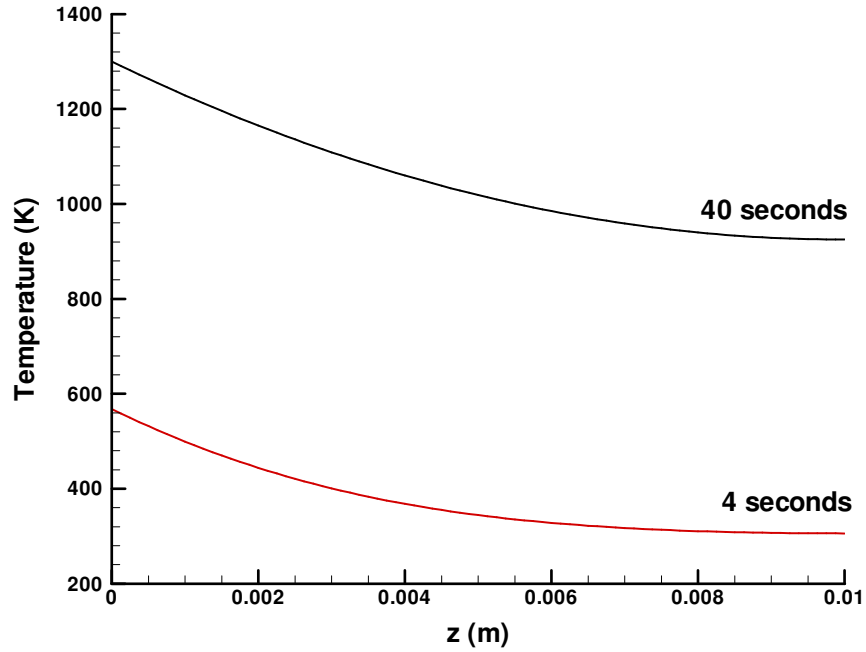


Figure 8.1: Transient conduction verification problem analytical solution for $t = 4$ s and $t = 40$ s.

be seen in Table 8.2. Figure 8.2 shows that the implicit time integrator does exhibit first order convergence at both problem times.

Since the temporal order of accuracy has been independently verified to be first order, the simultaneous refinement can be performed to confirm the spatial order of accuracy. The grid parameters for the four grids used in this study with $\alpha\Delta t/\Delta z^2 = 1.25$ can be seen in Table 8.3. The study results, which show second order grid convergence for the simultaneous refinement, can be seen in Figure 8.3.

Table 8.2: Grid parameters for temporal order of accuracy study.

Grid	# elem	Δz , m	Δt , s
coarse	2000	5×10^{-6}	0.5
medium	2000	5×10^{-6}	0.125
fine	2000	5×10^{-6}	0.03125

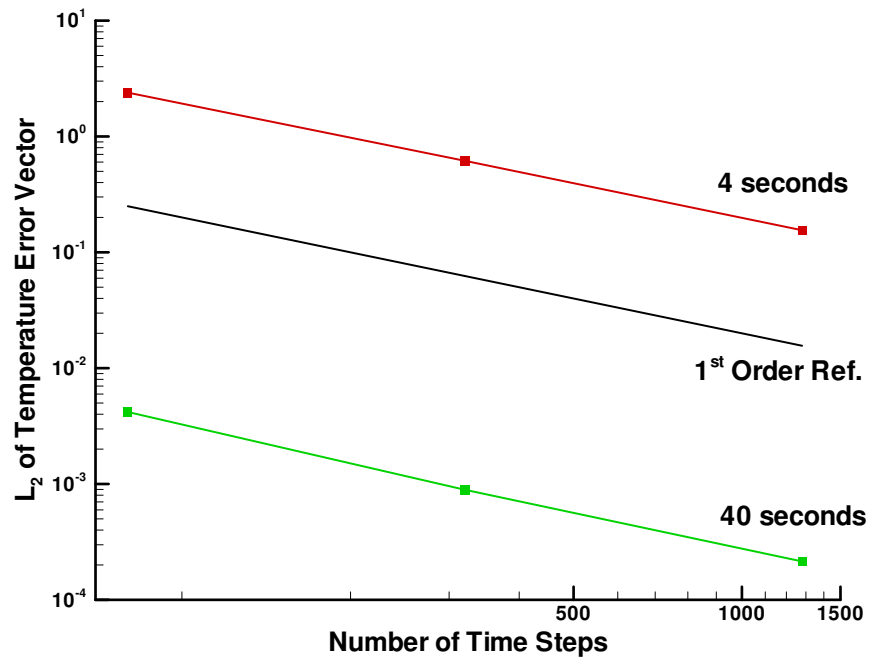


Figure 8.2: Temporal grid refinement study for transient conduction verification problem.

Table 8.3: Grid parameters for simultaneous space/time grid refinement study.

Grid	# elem	Δz , m	Δt , s
coarse	10	0.001	0.5
medium	20	0.0005	0.125
fine	40	0.00025	0.03125
extra-fine	80	0.000125	0.0078125

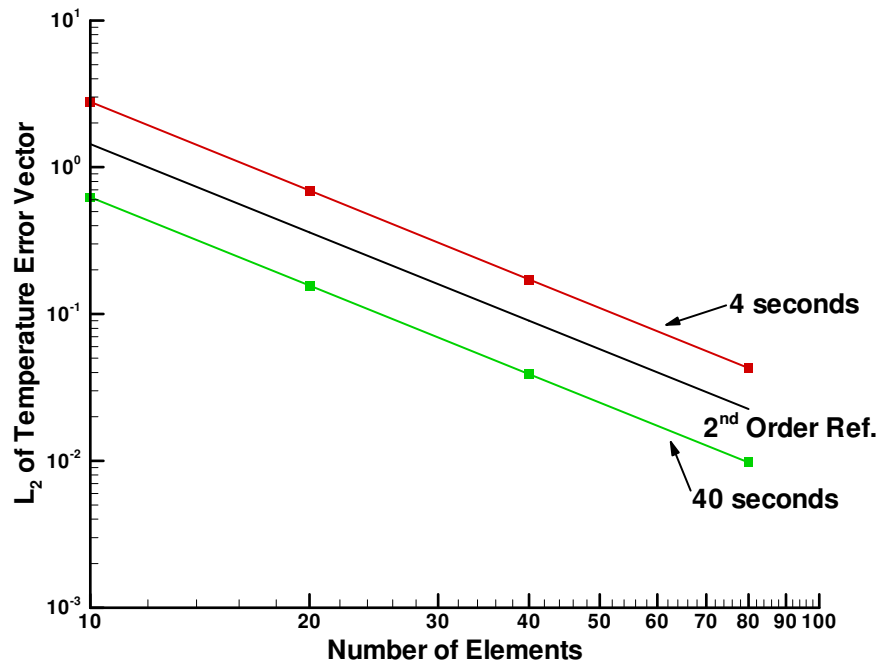


Figure 8.3: Grid refinement study for transient conduction verification problem.

8.2 Transient Conduction with Standard Convection

8.2.1 Problem Description

Since the constant property energy content and conduction terms have already been verified, this problem is intended to verify the standard convection boundary condition described in Section 5.5.3 while reconfirming the order of accuracy of the energy content and conduction terms. Consider a constant property, non-ablating,

non-decomposing, one-dimensional, uniform density, planar slab that is subject to a convective heating environment on the back face and an adiabatic front face. The governing equation, boundary conditions, and initial conditions associated with this problem are

$$\left. \begin{aligned} \rho C_v \frac{\partial T}{\partial t} &= k \frac{\partial^2 T}{\partial z^2} \text{ for } 0 \leq z \leq L \\ -k \frac{\partial T}{\partial z} \Big|_{z=0} &= 0 \\ -k \frac{\partial T}{\partial z} \Big|_{z=L} &= H (T(t) - T_r) \\ T(z, t = 0) &= T_o \end{aligned} \right\} \quad (8.10)$$

and the parameters for this problem are given in Table 8.4.

Table 8.4: Standard convection verification problem parameters.

$T_o = 300 \text{ K}$
$H = 1000 \text{ W/m}^2\text{-K}$
$T_r = 1300 \text{ K}$
$L = 0.01 \text{ m}$
$\rho = 8000 \text{ kg/m}^3$
$C_v = 500 \text{ J/kg-K}$
$k = 10 \text{ W/m-K}$
$\alpha = k/(\rho C_v) = 2.5 \times 10^{-6} \text{ m}^2/\text{s}$

8.2.2 Analytical Solution

The analytical solution to this problem can be found in Arpaci[38] and is given by

$$\frac{T(z, t) - T_r}{T_o - T_r} = 2 \sum_{n=1}^{\infty} \left(\frac{\sin \nu_n}{\nu_n + \sin \nu_n \cos \nu_n} \right) \exp(-\nu_n^2 \alpha t / L^2) \cos(\nu_n z / L) \quad (8.11)$$

for all $\nu_n > 0$ where the eigenvalues can be found by solving the implicit relationship

$$\nu_n \sin \nu_n = \text{Bi} \cos \nu_n \quad (8.12)$$

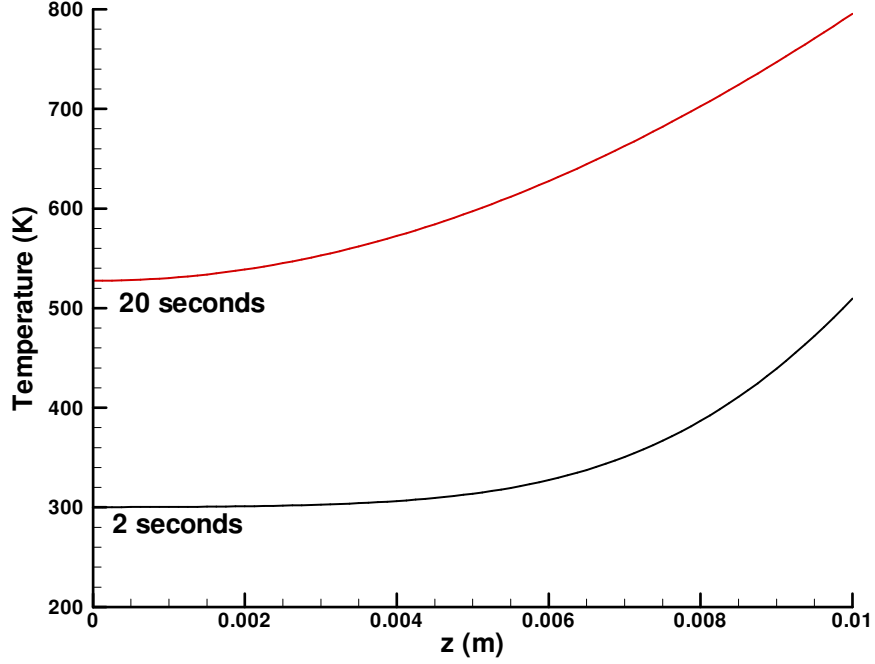


Figure 8.4: Standard convection verification problem analytical solution for $t = 2$ s and $t = 20$ s.

and the Biot number is given by

$$\text{Bi} = \frac{HL}{k} \quad (8.13)$$

The analytical solution for $t = 2$ s and $t = 20$ s is shown in Figure 8.4.

8.2.3 Grid Refinement Study

The domain was discretized with three different uniform grids denoted by coarse, medium, and fine. The coarse grid had ten uniform elements while each subsequent grid doubled the number of elements thereby halving the mesh spacing. The grid parameters for the three grids with $\alpha\Delta t/\Delta z^2 = 1.25$ can be seen in Table 8.5. Figure 8.5 shows that the solutions at both $t = 2$ s and $t = 20$ s exhibit second order grid convergence. Since the convective boundary condition does not introduce any nonlinearities into the problem, it is again not necessary to investigate the Newton solver's convergence rate since the problem converges in one iteration.

Table 8.5: Parameters for standard convection problem grid refinement study.

Grid	# elem	Δz , m	Δt , s
coarse	10	0.001	0.5
medium	20	0.0005	0.125
fine	40	0.00025	0.03125

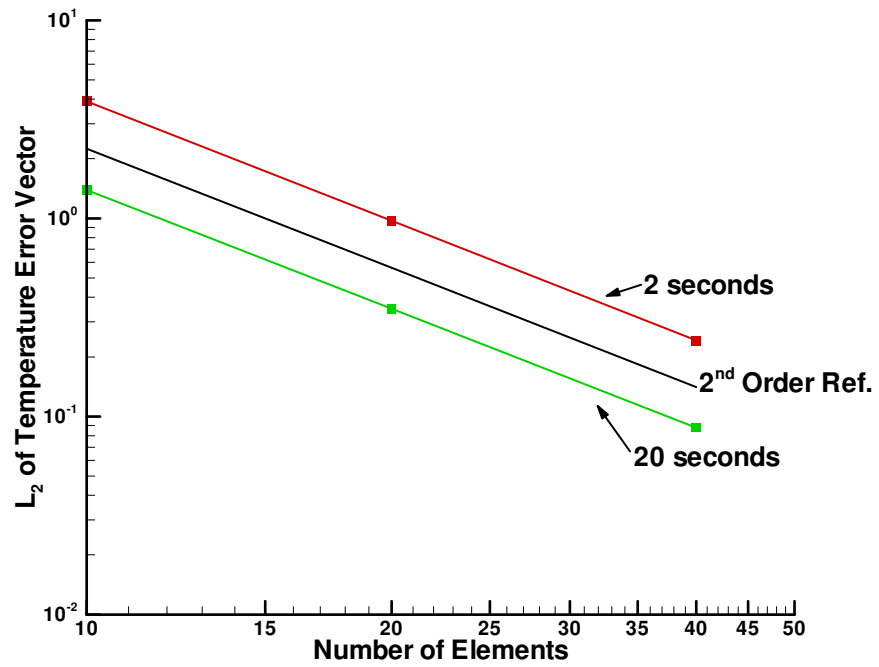


Figure 8.5: Grid refinement study for standard convection verification problem.

8.3 Steady-State Radiation

8.3.1 Problem Statement

The steady state radiation problem is intended to verify the implementation of the radiation boundary condition described in Section 5.5.4 where the radiation boundary flux is given in Eq. 5.53 as

$$\dot{q}_{rad}'' = \epsilon \sigma (T_{bnd}^4 - T_{res}^4)$$

Consider a constant property, non-ablating, non-decomposing, one-dimensional, uniform density, planar slab with a far-field radiation boundary condition on the front face and specified temperature on the back face. The differential equation and boundary conditions are

$$\left. \begin{aligned} \frac{d^2 T}{dz^2} &= 0 \\ -k \frac{dT}{dz} \Big|_{z=0} &= \epsilon \sigma (T_{res}^4 - T_f^4) \\ T(z=L) &= T_{back} \end{aligned} \right\} \quad (8.14)$$

and the problem parameters are given in Table 8.6.

Table 8.6: Steady-state radiation verification problem parameters.

$k = 10 \text{ W/m-K}$
$\epsilon = 0.9$
$\sigma = 5.6704 \times 10^{-8} \text{ W/m}^2 \text{ K}^4$
$T_{res} = 1300 \text{ K}$
$T_{back} = 300 \text{ K}$
$L = 0.01 \text{ m}$

8.3.2 Analytical Solution and Computational Result

Instead of formally solving the differential equation, the steady-state solution can be determined by knowing that the applied radiative heat flux must be balanced by the

heat conducted through the slab, and consequently the temperature profile is linear. As a result, the front face temperature can be determined from the energy balance relationship

$$\epsilon\sigma (T_{res}^4 - T_f^4) = \frac{k}{L} (T_f - T_{back}) \quad (8.15)$$

where T_f is the unknown front face temperature. Newton's method can be used to solve this fourth order polynomial, and the numerical result to machine precision is

$$T_f = 443.7777348036277 \text{ K} \quad (8.16)$$

Since the temperature profile for this problem is linear in position, a second order spatial discretization method should reproduce the temperature profile to within machine precision, and the absence of agreement to machine precision would indicate an error. Therefore it is not necessary to perform a formal grid refinement study, which would be a weakness of this verification problem had the conduction routine not been previously verified. The calculations performed did reproduce the result given in Eq. 8.16 to within machine precision.

If the initial guess is chosen to be sufficiently different from the steady-state solution, then the solution process can require enough iterations to reveal the nonlinear convergence rate. If the error metric is chosen to be

$$(error)^\nu = (T_f)^\nu - (T_f)^{converged} \quad (8.17)$$

then the second order nonlinear convergence rate can be seen in Figure 8.6.

8.4 Transient Conduction with Temperature Dependent Properties

8.4.1 Problem Statement

The temperature dependent property problem is intended to isolate the variable material property and constant density terms in the energy content and conduction

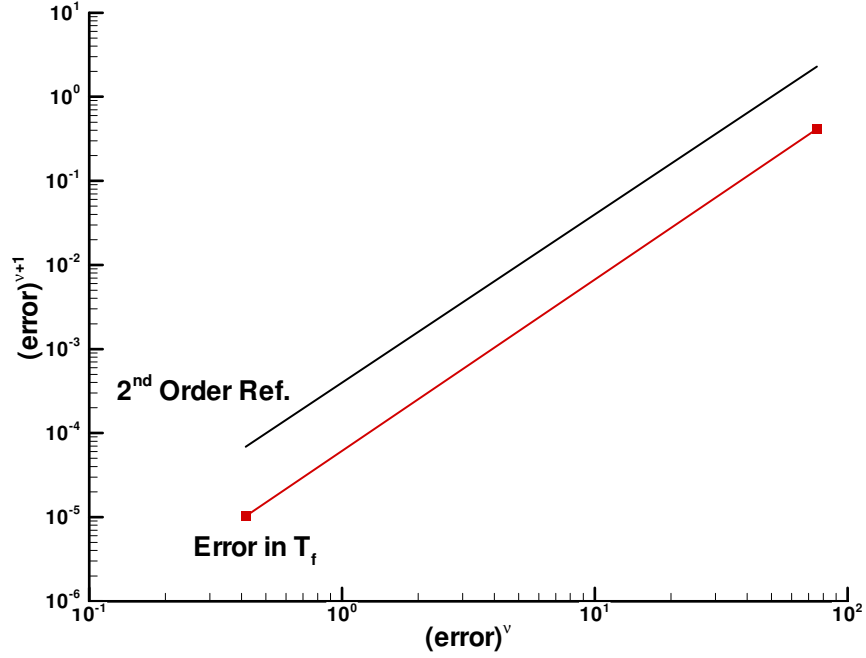


Figure 8.6: Nonlinear convergence rate for steady-state radiation verification problem.

routines, and this verification study can be found in Amar et al.[40]. Consider a non-ablating, non-decomposing, one-dimensional, uniform density, planar slab subject to a constant specified heat flux on the front face and an adiabatic back face. The governing equation, boundary conditions, and initial conditions that characterize the problem are

$$\left. \begin{aligned} \rho C_v \frac{\partial T}{\partial t} &= \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \text{ for } 0 \leq z \leq L \\ -k \frac{\partial T}{\partial z} \Big|_{z=0} &= \dot{q}'' \\ -k \frac{\partial T}{\partial z} \Big|_{z=L} &= 0 \\ T(z, t=0) &= T_o \end{aligned} \right\} \quad (8.18)$$

and the parameters for this problem are given in Table 8.7. The thermal conductivity and specific heat are given in Table 8.8 and are assumed to vary linearly with

temperature while the thermal diffusivity is constant giving

$$k(T) = k_1 + \frac{k_2 - k_1}{T_2 - T_1} (T - T_1) \quad (8.19)$$

$$C_v(T) = C_{v,1} + \frac{C_{v,2} - C_{v,1}}{T_2 - T_1} (T - T_1) \quad (8.20)$$

$$\alpha = \frac{k_1}{\rho C_{v,1}} = \frac{k_2}{\rho C_{v,2}} = \frac{k(T)}{\rho C_v(T)} \quad (8.21)$$

Table 8.7: Temperature dependent properties verification problem parameters.

$T_o = 300 \text{ K}$
$\dot{q}'' = 7.5 \times 10^5 \text{ W/m}^2$
$L = 0.01 \text{ m}$
$\rho = 8000 \text{ kg/m}^3$
$\alpha = k/(\rho C_v) = 2.5 \times 10^{-6} \text{ m}^2/\text{s}$

Table 8.8: Material properties for temperature dependent properties verification problem.

$T, \text{ K}$	$k, \text{ W/m-K}$	$C_v, \text{ J/kg-K}$
$T_1 = 300$	10	500
$T_2 = 1300$	100	5000

8.4.2 Analytical Solution

The analytical solution to this problem can be found by first applying Kirchoff's transformation

$$\theta = \frac{1}{k_{ref}} \int_{T_{ref}}^T k(\hat{T}) d\hat{T} \quad (8.22)$$

as described by Arpaci[38] and then using the related constant property solution shown in the Section 8.1.2 or in Beck et al.[39]. Performing the integration with $T_{ref} = T_1$ and $k_{ref} = k_1$ gives

$$\theta = (T - T_1) + \frac{k_2 - k_1}{T_2 - T_1} \frac{1}{2k_1} (T - T_1)^2 \quad (8.23)$$

The above equation is quadratic in $(T - T_1)$, and can be solved to yield

$$T - T_1 = (T_2 - T_1) \left(\frac{k_1}{k_2 - k_1} \right) \left[-1 \pm \sqrt{1 + \frac{2\theta}{T_2 - T_1} \left(\frac{k_2 - k_1}{k_1} \right)} \right] \quad (8.24)$$

where the physically meaningful root is denoted by the plus sign since

$$T > T_1 \text{ when } \frac{k_2 - k_1}{T_2 - T_1} > 0$$

The transformed energy equation, boundary conditions, and initial conditions become

$$\left. \begin{aligned} \frac{\partial \theta}{\partial t} &= \alpha \frac{\partial^2 \theta}{\partial z^2} \text{ for } 0 \leq z \leq L \\ -k_1 \frac{\partial \theta}{\partial z} \Big|_{z=0} &= \dot{q}'' \\ -k_1 \frac{\partial \theta}{\partial z} \Big|_{z=L} &= 0 \\ \theta(z, t=0) &= \theta_o = \theta(T = T_o) \end{aligned} \right\} \quad (8.25)$$

The transformed energy equation now has the same form as the related constant property case presented in Section 8.1, and the analytical solution is

$$\frac{\theta(z, t) - \theta_o}{\dot{q}'' L / k_1} = \frac{\alpha t}{L^2} + \frac{1}{3} - \frac{z}{L} + \frac{1}{2} \left(\frac{z}{L} \right)^2 - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp \left(-n^2 \pi^2 \frac{\alpha t}{L^2} \right) \cos \left(n \pi \frac{z}{L} \right) \quad (8.26)$$

The analytical solution for $t = 4$ s and $t = 40$ s is shown in Figure 8.7.

8.4.3 Grid Refinement and Nonlinear Convergence Studies

The domain was discretized with four different uniform grids denoted by coarse, medium, fine, and extra-fine. The coarse grid has ten uniform elements while each subsequent grid doubles the number of elements thereby halving the mesh spacing. The grid parameters for the four grids with $\alpha \Delta t / \Delta z^2 = 1.25$ can be seen in Table 8.9. Figure 8.8 shows that the solutions at both $t = 4$ s and $t = 40$ s exhibit second order grid convergence.

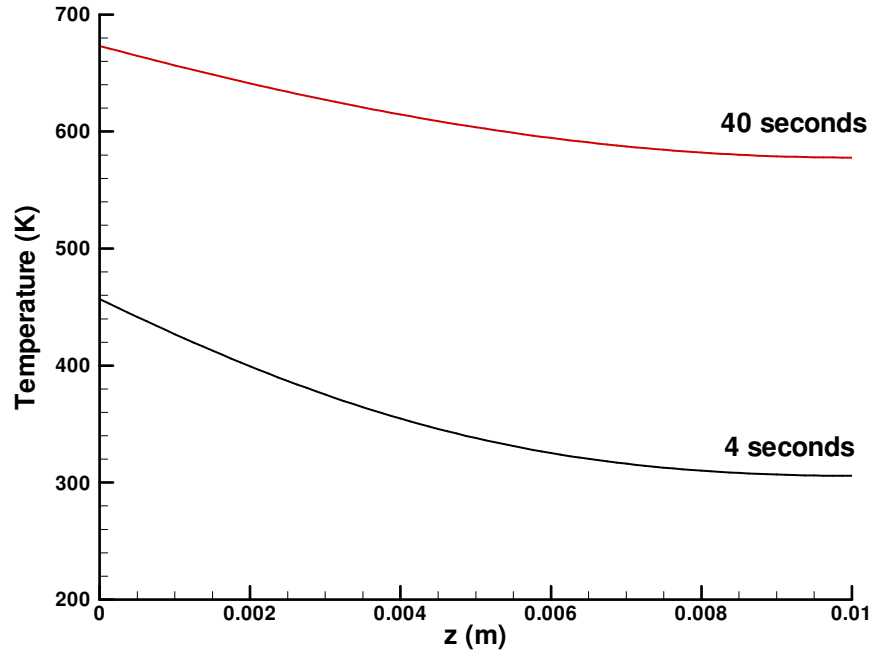


Figure 8.7: Variable property verification problem analytical solution for $t = 4$ s and $t = 40$ s.

Table 8.9: Parameters for variable property problem grid refinement study.

Grid	# elem	Δz , m	Δt , s
coarse	10	0.001	0.5
medium	20	0.0005	0.125
fine	40	0.00025	0.03125
extra-fine	80	0.000125	0.0078125

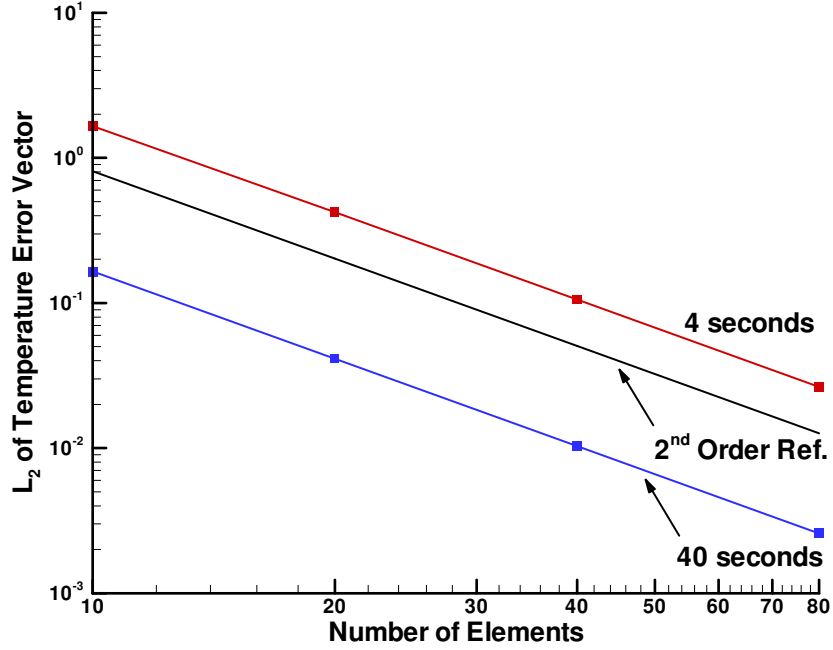


Figure 8.8: Grid refinement study for variable property verification problem.

Since the analytical solution is known for this problem, the error metric for determining the nonlinear convergence rate is chosen to be the L_2 of the temperature error vector.

$$(error)^\nu = (L_2)^\nu - (L_2)^{converged} \quad (8.27)$$

Figure 8.9 shows the second order nonlinear convergence rate for a single time step that had a total of four iterations.

8.5 Steady-State Heat of Ablation with Blowing Correction

8.5.1 Problem Statement

The steady-state ablation problem is intended to verify the implementation of the solid grid convection, Q^* ablation, aerodynamic heating, and blowing correction routines, and this verification study can be found in Amar et al.[40]. Consider a non-decomposing, one-dimensional, uniform density, ablative, semi-infinite, planar slab

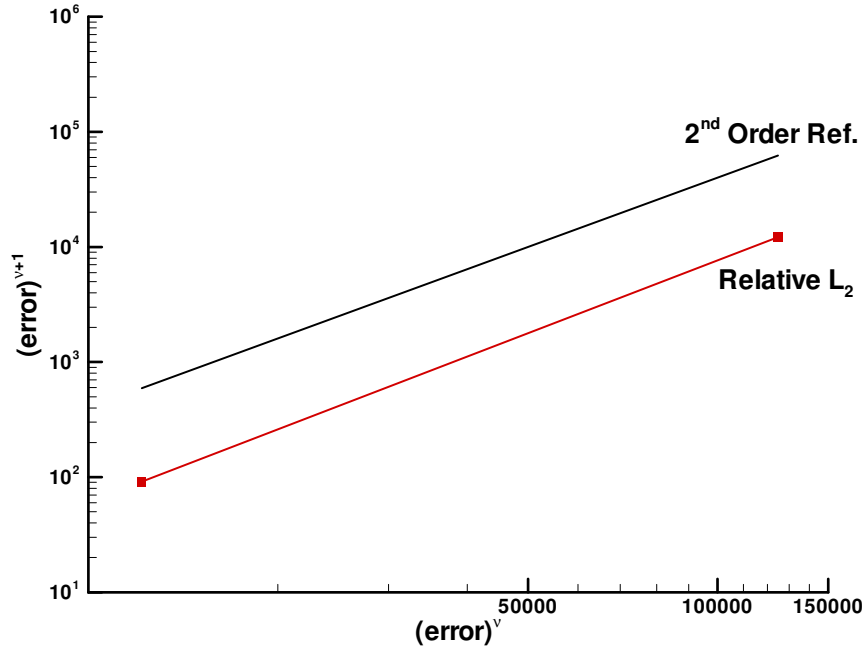


Figure 8.9: Nonlinear convergence rate for variable property verification problem.

with constant material properties and isothermal boundaries. The governing equation and boundary conditions that characterize the problem are

$$\left. \begin{aligned} k \frac{d^2 T}{dx^2} + \rho \dot{s} C_v \frac{dT}{dx} &= 0 \\ T(x=0) &= T_{abl} \\ T(x=\infty) &= T_o \end{aligned} \right\} \quad (8.28)$$

and the material properties and problem parameters are given in Table 8.10. While the differential equation assumes there is a boundary at $x = \infty$, the corresponding numerical simulation must be for a finite computational domain. For consistency between the numerical and analytical solutions, the computational domain must be chosen sufficiently large for the semi-infinite assumption to be valid.

Table 8.10: Q^* ablation verification problem parameters.

$k = 0.2 \text{ W/m-K}$
$\rho = 2000 \text{ kg/m}^3$
$C_v = 1000 \text{ J/kg-K}$
$L_o = 3.0 \times 10^{-2} \text{ m}$
$Q^* = 2 \times 10^6 \text{ J/kg}$
$\dot{q}'' = 2 \times 10^6 \text{ W/m}^2$
$\dot{s} = 4.0 \times 10^{-4} \text{ m/s}$
$T_{abl} = 800 \text{ K}$
$T_o = T_{ref} = 300 \text{ K}$

8.5.2 Analytical Solution

The analytical solution is

$$\frac{T(x) - T_o}{T_{abl} - T_o} = \exp(-\dot{s}x/\alpha) \quad (8.29)$$

where the steady-state temperature profile with respect to the x -coordinate system translates through the remaining material as the ablation front moves. It is important to note that although the problem is steady-state in the x -coordinate system, the numerical solution takes place in the z -coordinate system in which the problem is transient and therefore the contracting control volume contribution to the energy content term is exercised.

The surface energy balance can be written as

$$-k \left. \frac{dT}{dx} \right|_{x=0} = \dot{q}'' - \rho \dot{s} Q^* \quad (8.30)$$

and substituting the analytical temperature profile into the surface energy balance gives the necessary heat flux found in Table 8.10.

$$\dot{q}'' = \rho \dot{s} [C_v (T_{abl} - T_o) + Q^*] \quad (8.31)$$

In order to use this as a verification problem, the procedure is to numerically solve a problem with a specified heat flux on the front face and a nonuniform initial

temperature profile given by Eq. 8.29 and see how well the computed surface recession rate compares to the known recession rate given in Table 8.10.

The aerodynamic heating boundary flux with blowing correction is given by

$$\dot{q}'' = \rho_e u_e C_{h_o} \frac{C_h}{C_{h_o}} (h_w - h_r) \quad (8.32)$$

where

$$\frac{C_h}{C_{h_o}} = \Omega_{blw} \quad (8.33)$$

The gas enthalpy model adopted for this verification problem is a constant specific heat (corresponding to air) and is given as

$$h_w(T) = C_{p_w} (T - T_{ref}) \quad (8.34)$$

where

$$C_{p_w} = 1.00416 \times 10^3 \text{ J/kg-K}$$

It is assumed that the recovery temperature of the boundary layer edge gases is 1800 K, and the corresponding recovery enthalpy is

$$h_r(T_r = 1800 \text{ K}) = 1.506240 \times 10^6 \text{ J/kg}$$

While ablation is taking place, $T_w = T_{abl} = 800 \text{ K}$ with a corresponding wall gas enthalpy of

$$h_w(T_w = 800 \text{ K}) = 5.02080 \times 10^5 \text{ J/kg}$$

The corrected heat transfer coefficient can now be determined from Eq. 8.32 and is found to be

$$\rho_e u_e C_h = 1.9917145 \text{ kg/m}^2\text{-s}$$

If the laminar blowing correction described in Section 5.5.5 is used, the uncorrected heat transfer coefficient is

$$\rho_e u_e C_{h_o} = 2.3692465 \text{ kg/m}^2\text{-s}$$

An aerodynamic heating flux and thermochemistry data with the above values for $\rho_e u_e C_{h_o}$, h_r , C_{p_w} , and h_w is imposed on the ablating surface while the other boundary condition for the numerical model is adiabatic.

8.5.3 Grid Refinement and Nonlinear Convergence Studies

The problem was solved using three different grids designated as coarse, medium, and fine. Each grid is nonuniform and is based on an exponential grid with a geometric progression modification. The motivation behind the piecewise nonuniform grid technique is as follows:

1. Realistic uniform grids for which the method is known to be second order spatially were inadequate to ensure the results were in the asymptotic regime. Several uniform grids were tried, and while they could capture the steep gradients, the location of the largest error typically was at the back face where no activity is supposed to be happening.
2. A nonuniform grid, which would be expected to do a better job of capturing the steep gradients, is not necessarily second order spatially. Since the profile is exponential, several exponentially stretched grids were tried in which the initial temperature drop between nodes was constant. Again, the largest temperature error tended to be at the back face, and the errors were never in the asymptotic regime.
3. Next, a modified exponential grid was devised. For a ten element exponential grid, the tenth element was replaced by ten more elements in an expanding sequence based on a geometric progression with $\Delta z_{j+1}/\Delta z_j = 1.5$. The resulting grid and initial conditions are shown in Figure 8.10. The sequence of grid refinements was accomplished by taking the 19-element baseline grid given in

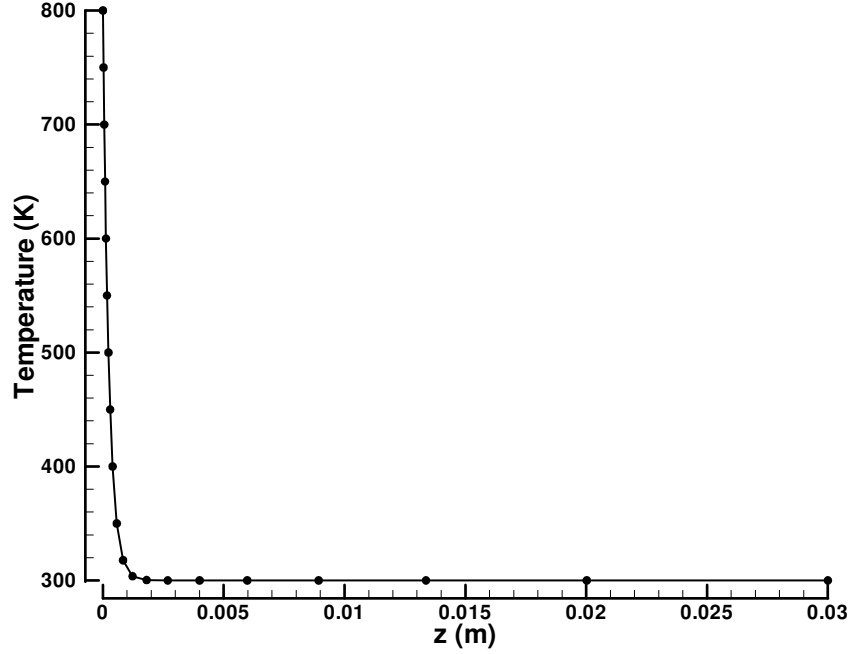


Figure 8.10: Initial temperature profile on the 19-element grid for the Q^* ablation verification problem.

Figure 8.10 and successively dividing each element in half. This process was repeated so that a total of three grids was produced. Similar grid refinement studies for nonuniform grids have been performed by Blottner[41, 42].

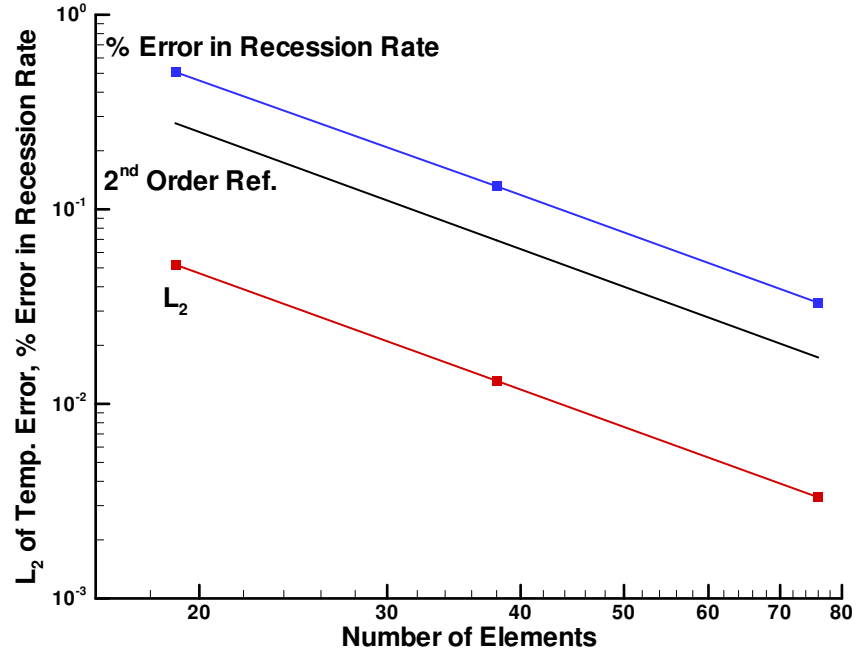
The time step was determined by keeping the grid scale Fourier number based on the initial first element thickness $(\alpha \Delta t / (\Delta z_1)_o^2)$ constant at approximately 1.44133. The grid parameters are given in Table 8.11, and the grid refinement study, which shows second order convergence for both the predicted temperature profile and recession rate at $t = 2$ s, can be seen in Figure 8.11.

The nonlinear convergence rate for the Q^* model was determined by using the difference in surface recession rate between the current iteration and the converged solution as the error metric

$$(error)^\nu = \dot{s}^\nu - \dot{s}^{converged} \quad (8.35)$$

Table 8.11: Parameters for Q^* ablation verification problem grid refinement study.

Grid	# elem	$(\Delta z_1)_o$, m	Δt , s
coarse	19	2.6340×10^{-5}	0.5
medium	38	1.3170×10^{-5}	0.0025
fine	76	6.5850×10^{-6}	0.000625

Figure 8.11: Grid refinement study for the Q^* ablation verification problem.

and the second order results are shown in Figure 8.12, which confirms a correct implementation of the Jacobian terms.

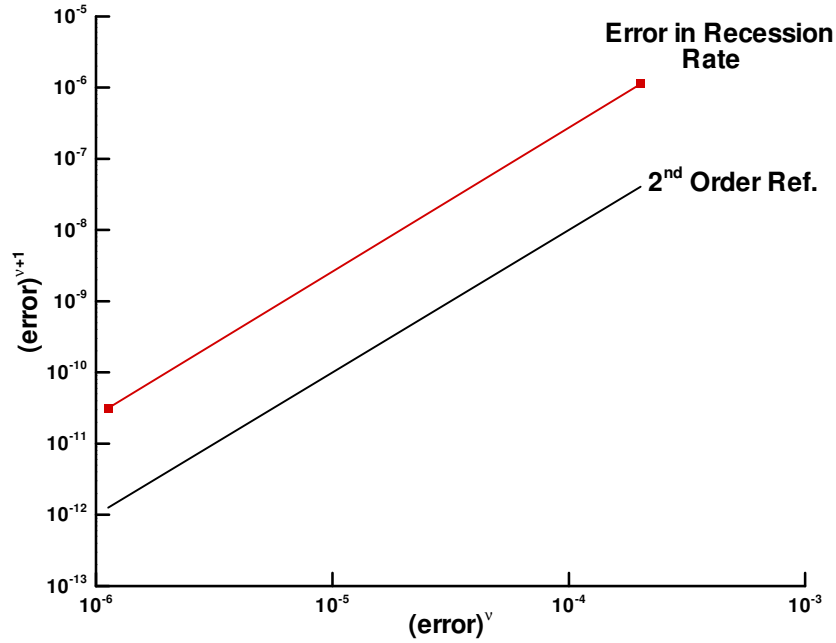


Figure 8.12: Nonlinear convergence of surface recession rate for the Q^* ablation verification problem.

8.6 Steady-State Ablation with Specified Recession Rate

The steady-state Q^* ablation problem described in the previous section can be modified to verify the implementation of the specified recession rate and surface temperature option which is described in Section 5.6.1. If the surface temperature and recession rate are specified as given in Table 8.10, then the solution error can either be measured by the temperature field or the calculated incident heat flux. The grid parameters used in this study are given in Table 8.11. Since specifying the surface temperature and recession rate makes the problem linear, a nonlinear convergence rate study is not necessary. Figure 8.13 shows that the method exhibits second order grid convergence for both error metrics at $t = 2$ s.

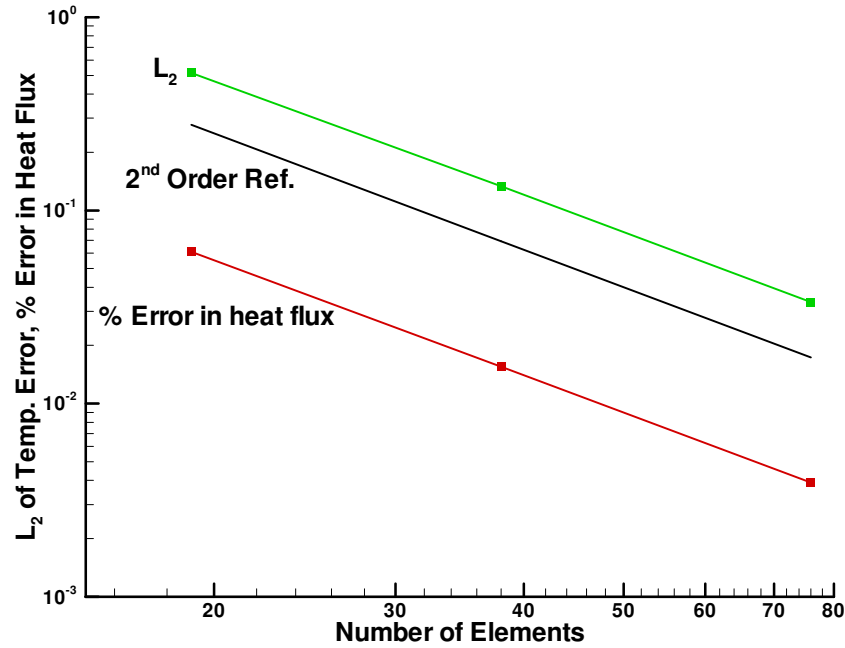


Figure 8.13: Grid refinement study for the specified recession rate Q^* ablation verification problem.

8.7 Thermochemical Ablation of a Non-Decomposing Material

8.7.1 Problem Statement

The carbon-carbon thermochemical ablation problem is intended to simultaneously verify all of the constant density terms in the mixture energy equation in addition to the thermochemical ablation routine and aerodynamic heating boundary condition with hot wall and blowing corrections, and this verification study can also be found in Amar et al.[40]. Carbon-carbon is a non-decomposing ablator with specific heat and thermal conductivity functions given in Table 8.12, and the emissivity is 0.8 and is assumed to be independent of temperature.³ The carbon-in-air surface thermochemistry data was generated by ACE and is excluded from this document due to

³The carbon-carbon material properties come from personal communication with Don Potter and David Kuntz of Sandia National Laboratories.

length, but it is discussed in detail in Appendix C.

Table 8.12: Thermophysical properties of carbon-carbon.

Temperature (°R)	Specific Heat (Btu/lb _m -°R)	Conductivity (Btu/ ft- s-°R)
460.0	0.130	0.0103
960.0	0.220	0.0104
1460.0	0.315	0.0086
1960.0	0.388	0.0074
2460.0	0.424	0.0063
2960.0	0.460	0.0056
3460.0	0.480	0.0051
3960.0	0.497	0.0049
4460.0	0.507	0.0048
4960.0	0.512	0.0048
5460.0	0.520	0.0047
10000.0	0.520	0.0047

The problem is characterized by a typical ballistic reentry trajectory where the time dependent aerodynamic heating parameters are given in Figures 8.14 and 8.15, and the numerical solutions for surface temperature and recession rate histories are shown in Figure 8.16. The discontinuities in recovery enthalpy and boundary layer edge velocity result from the numerical scheme used in 2IT/SANDIAC/HIBLARG[43, 44, 45, 46], which is the series of programs that generated this aerodynamic heating information. Simply put, the model in HIBLARG predicts a discontinuity in boundary layer edge location when switching from laminar to turbulent calculations, and consequently the calculated properties have discontinuities also.

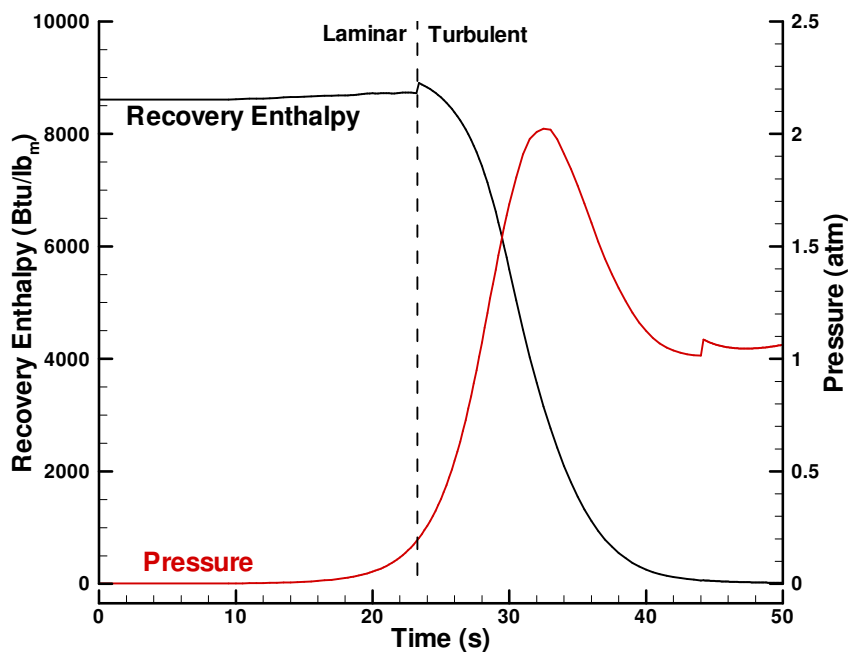


Figure 8.14: Time dependent recovery enthalpy and pressure in aerodynamic heating boundary condition.

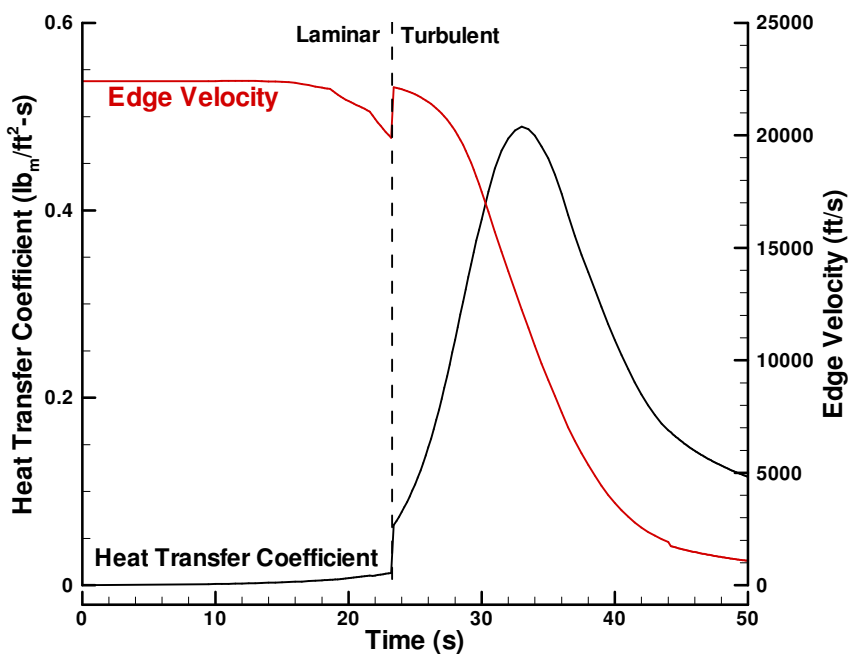


Figure 8.15: Time dependent heat transfer coefficient and edge velocity in aerodynamic heating boundary condition.

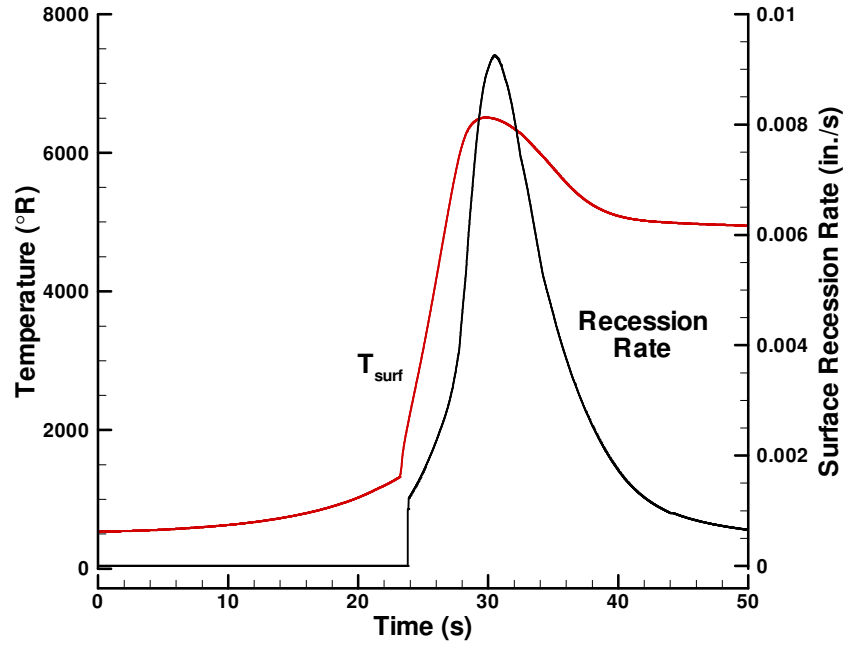


Figure 8.16: Surface temperature and recession rate histories for carbon-carbon thermochemical ablation verification problem.

8.7.2 Grid Refinement and Nonlinear Convergence Studies

Due to the complexity of determining an analytical solution to a thermochemical ablation problem with Stanton number corrections, the Grid Convergence Index based on Richardson extrapolation, as described in Section 8, is used to confirm the order of accuracy of the constant density thermochemical ablation solution procedure. For this process, a 0.5 inch domain was discretized with a series of four uniform grids which are denoted by coarse, medium, fine, and extra-fine. The grid parameters can be seen in Table 8.13 where $\Delta t / \Delta z_o^2 = \text{constant}$.

Richardson extrapolation was performed on the surface temperature and recession rate at $t = 25$ s and 50 s according to Eq. 8.5 using the extra-fine and fine grids giving

$$T_{exact} \approx \frac{4}{3}T_{extra-fine} - \frac{1}{3}T_{fine} \quad (8.36)$$

Table 8.13: Parameters for carbon-carbon thermochemical ablation problem grid refinement study.

Grid	# elem	Δz_o , in	Δt , s
coarse	50	0.01	0.1
medium	100	0.005	0.025
fine	200	0.0025	0.00625
extra-fine	400	0.00125	0.0015625

and

$$\dot{s}_{exact} \approx \frac{4}{3}\dot{s}_{extra-fine} - \frac{1}{3}\dot{s}_{fine} \quad (8.37)$$

If the error reduction for the coarse and medium grids is colinear with the error reduction for the fine and extra-fine grids, then the second order accuracy of the scheme can be confirmed. Figure 8.17 shows that the scheme in fact exhibits second order grid convergence for both error metrics.

The nonlinear convergence rate was determined for this problem using the same error metric described in Eq. 8.35, and the second order results can be seen in Figure 8.18.

8.7.3 Code-to-Code Comparison

Although it is not a part of the formal verification process, it is sometimes beneficial to perform code-to-code comparisons throughout the development process. The thermochemical ablation verification problem was solved on the medium grid in Table 8.13 using SODDIT[9, 10, 47], CMA, and the code developed during the current study for a consistency check with established codes. It is important to note that the major differences between the codes are as follows:

1. SODDIT and CMA iterate only on the surface energy balance and lag temperature dependent properties and surface recession rate for the interior node solution

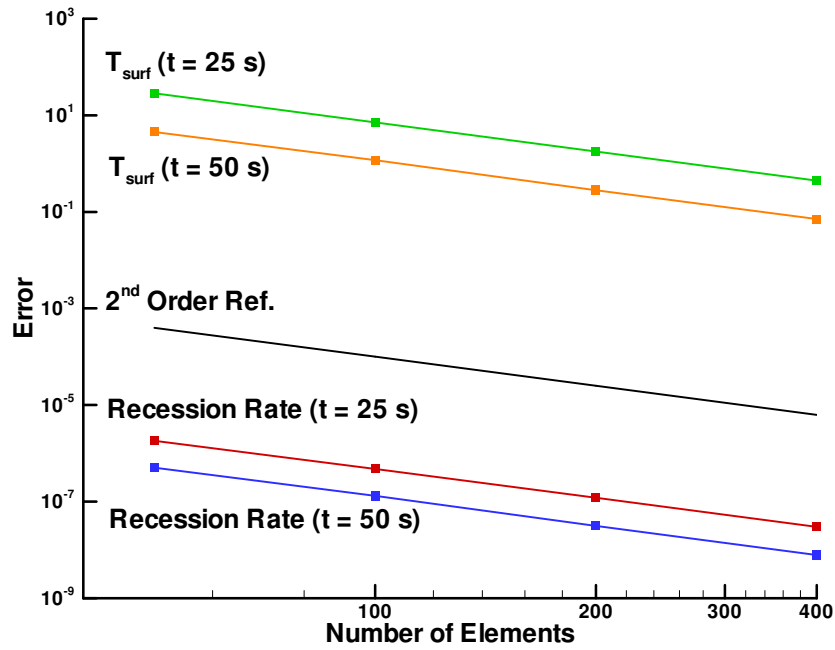


Figure 8.17: Richardson extrapolation grid convergence results for carbon-carbon thermochemical ablation verification problem.

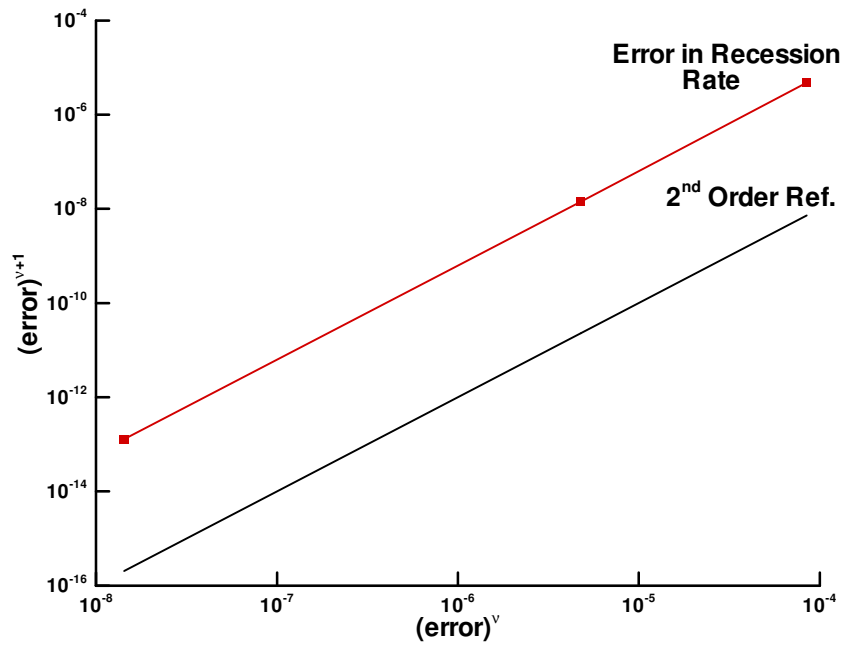


Figure 8.18: Nonlinear convergence of surface recession rate for carbon-carbon thermochemical ablation verification problem.

2. SODDIT uses the contracting grid scheme and CMA use a translating/node-dropping grid scheme
3. SODDIT and CMA use a lumped capacitance method while the research code uses a distributed capacitance method⁴
4. SODDIT and CMA linearly interpolate on $\ln(B'_c)$ while the research code linearly interpolates on B'_c

Figures 8.19, 8.20, and 8.21 compare the predictions from the three codes for surface temperature, back boundary temperature, and recession rate respectively, and Table 8.14 shows the relative difference between the three predictions at the peak values. The CMA results are difficult to decipher since the SODDIT and CMA solutions are nearly coincident on the scale shown in the figures.

It is evident that the three programs have good agreement which gives additional indication that the method has been implemented correctly. The largest discrepancy is at the time of the peak surface recession rate where the research code predicts a higher recession rate than CMA and SODDIT. However, the results do not suggest which difference in the models is causing this discrepancy or if this is a combined effect of several of the differences.

Table 8.14: Peak value comparison for the research code, CMA, and SODDIT.

Peak value in research code	CMA % difference	SODDIT % difference
$T_{surf} = 6508 \text{ }^{\circ}\text{R}$ at 29.8 s	1.29 at 30.1 s	1.26 at 30.1 s
$T_{back} = 5094 \text{ }^{\circ}\text{R}$ at 41.5 s	0.93 at 41.5 s	0.91 at 41.5 s
$\dot{s} = 9.251 \times 10^{-3} \text{ in/s}$ at 30.5 s	-3.85 at 30.5 s	-4.35 at 30.5 s

⁴SODDIT also has the control volume and Galerkin finite element methods, but the lumped capacitance option was excersized in order to behave more like CMA.

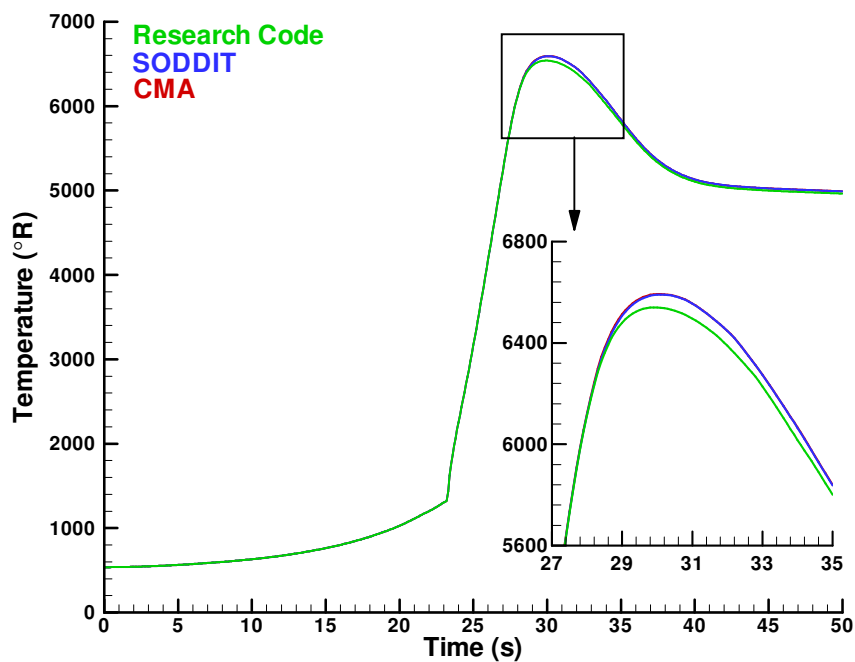


Figure 8.19: Three code comparison of surface temperature predictions for the carbon-carbon thermochemical ablation verification problem.

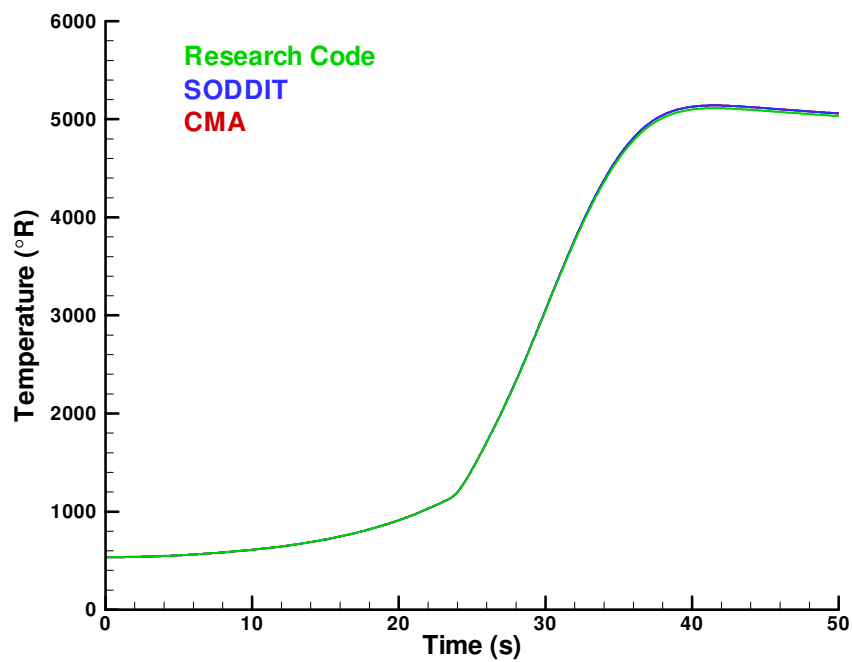


Figure 8.20: Three code comparison of back boundary temperature predictions for the carbon-carbon thermochemical ablation verification problem.

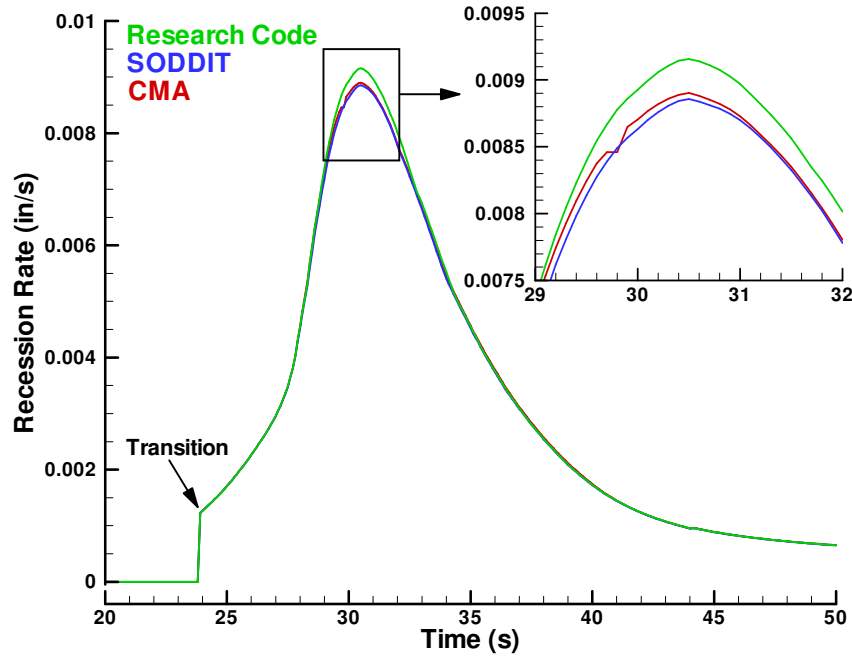


Figure 8.21: Three code comparison of recession rate predictions for the carbon-carbon thermochemical ablation verification problem.

8.8 Thermochemical Ablation of a Decomposing Material

8.8.1 Problem Statement

The decomposing material thermochemical ablation problem is intended to verify the implementation of the gas phase continuity equation in addition to the pyrolysis gas effects in the mixture energy equation. Due to the difficulty in determining an analytical solution, Richardson extrapolation is used to approximate the exact solution, and the global convergence rate and nonlinear convergence rates of the mixture energy and gas phase continuity equations are determined.

Consider a 0.5 inch thick planar slab of carbon-phenolic with material properties given in Appendix D that is subject to the same aerodynamic heating condition used in the carbon-carbon verification problem in Section 8.7. The Stanton number is corrected for both hot wall and blowing effects and the surface is subject to a far-field

Table 8.15: Parameters for carbon-phenolic thermochemical ablation problem grid refinement study.

Grid	# elem	Δz_o , in	Δt , s
coarse	50	0.01	0.1
medium	100	0.005	0.025
fine	200	0.0025	0.00625
extra-fine	400	0.00125	0.0015625

radiation condition where the source temperature is 414.0 °R. The back boundary is adiabatic and impermeable, and the time dependent specified surface pressure is provided by the aerodynamic heating boundary condition input displayed in Figure 8.14.

8.8.2 Grid Refinement Studies

The domain was discretized with a series of four grids with $\Delta t / \Delta z_o^2 = \text{constant}$, and the grid parameters can be seen in Table 8.15. Since the solid continuity equation is solved through direct integration of the decomposition kinetics, it is unclear how its solution and consequently its coupling with the other governing equations will behave as the mesh is refined. As a result, an alternative procedure to the previous verification problems was used in order to isolate the mixture energy and gas phase continuity equations from the solid phase continuity equation solution. The procedure is as follows:

1. Solve the problem on the extra-fine mesh until a problem time of $t = 25\text{ s}$ is reached
2. The conditions found at $t = 25\text{ s}$ can then be used to re-initialize the problem on the entire series of grids resulting in
 - Nonuniform initial profiles for:

- a. Temperature
- b. Solid density
- c. Porosity
- d. Permeability
- e. Gas density
- f. Gas generation rate
- g. Gas velocity
- Contracted grid
- Re-initialization during an ablating interval

3. Verify the mixture energy equation

- Integrate over 0.1 s (restarting at $t = 25$ s) for the entire series of grids only advancing the mixture energy equation in time while holding all other terms constant
 - a. Integration over a small time interval reduces errors associated with inconsistent nodal locations
 - b. Result is as revealing as integrating over a long time interval if all of the relevant terms are being employed which is ensured by the nonuniform initialization
- Perform Richardson extrapolation at $t = 25.1$ s on the surface temperature, recession rate, and back face temperature. The results showing the second order grid convergence can be seen in Figure 8.22.

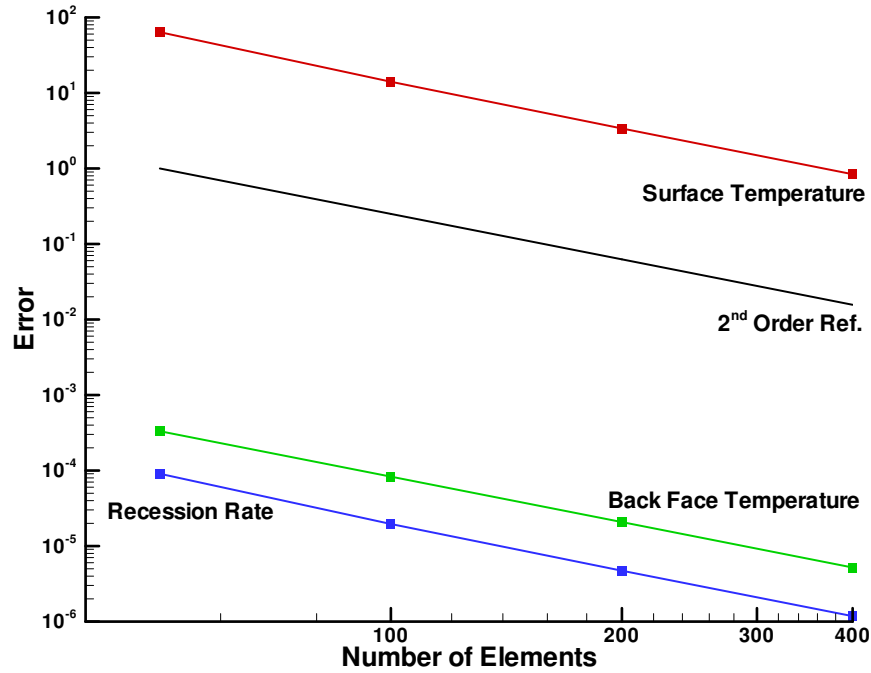


Figure 8.22: Mixture energy equation grid convergence results for carbon-phenolic thermochemical ablation verification problem.

4. Verify the gas phase continuity equation

- Integrate over 1.0 s (restarting at $t = 25$ s) for the entire series of grids only advancing the gas phase continuity equation in time while holding all other terms constant
- Perform Richardson extrapolation at $t = 26.0$ s on the surface gas flux, an interior gas density value at a consistent spatial location, and back face gas density. The results showing the second order grid convergence can be seen in Figure 8.23.
 - a. An interior location is chosen for Richardson extrapolation on the gas density because the surface gas density is specified through the boundary conditions. $z = 1.07 \times 10^{-2}$ in is the position of the first interior

node on the coarsest mesh which has a collocated node on each of the finer meshes.

- b. Integration over a longer time interval was performed since the mesh does not contract during the solution of the gas phase continuity equation

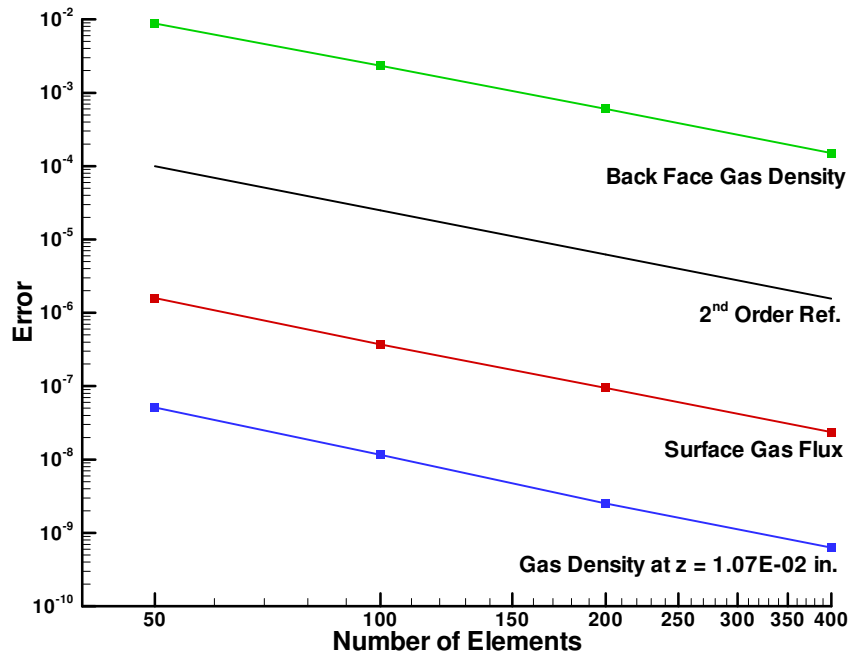


Figure 8.23: Gas continuity equation grid convergence results for carbon-phenolic thermochemical ablation verification problem.

8.8.3 Nonlinear Convergence Studies

For the mixture energy equation, the error metric used to determine the nonlinear convergence rate is the recession rate as given by Eq. 8.35, and the error metric for the gas phase continuity equation is the relative L_2 of the density correction vector.

$$(error)^\nu = (L_2)^\nu - (L_2)^{converged} \quad (8.38)$$

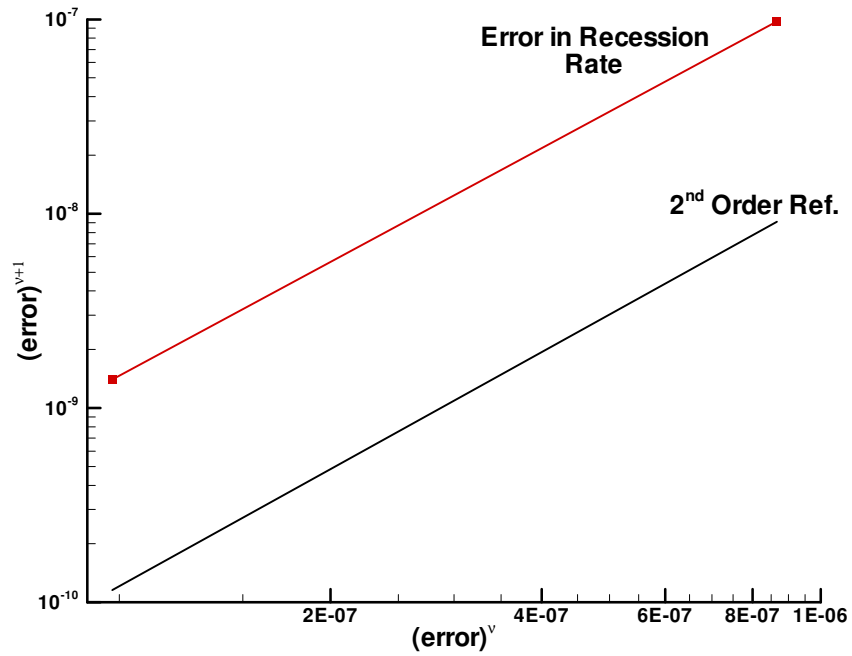


Figure 8.24: Nonlinear convergence of surface recession rate for carbon-phenolic thermochemical ablation verification problem.

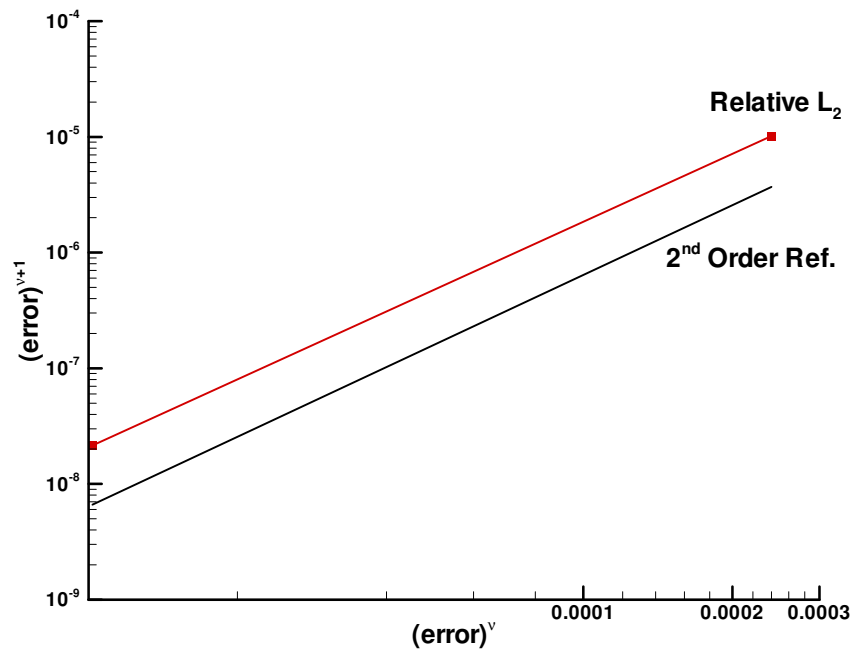


Figure 8.25: Nonlinear convergence of gas continuity equation for carbon-phenolic thermochemical ablation verification problem.

The convergence rates are shown in Figures 8.24 and 8.25, and the results follow the second order line.

The block Gauss-Seidel method used to solve the entire system of governing equations is expected to exhibit linear convergence. Since the solution procedure achieves coupling through iteration, information can only be used as soon as it is updated and a smooth convergence curve should not be expected. To examine the global convergence, it is necessary to view the problem in global iteration space as opposed to local (Newton) iteration space. Let the iteration index (ν) now represent the global iteration. Since the solution globally converges to the exact solution plus some discretization error, the difference between the locally converged solution at a given global iteration (X^ν) and the globally converged solution ($X^{g.c.}$) is used as the error metric.

$$(error)^\nu = X^\nu - X^{g.c.} \quad (8.39)$$

The global convergence rates of the surface recession rate and gas density are shown in Figure 8.26 while the global convergence rates for the surface temperature and solid density are shown in Figure 8.27. It is important to note that the surface gas density only changes with surface temperature since the boundary pressure is known from the boundary conditions. As a result, the surface gas density and temperature will always converge to machine precision in the same number of global iterations. On the other hand, the surface solid density reaches global convergence in fewer iterations and experience has shown that this is generally the case.

8.8.4 Code-to-Code Comparison

The carbon-phenolic thermochemical ablation problem was solved on the medium grid in Table 8.15 using both CMA and the code developed during this study. Although CMA has the capability to integrate the decomposition kinetics on a finer mesh than

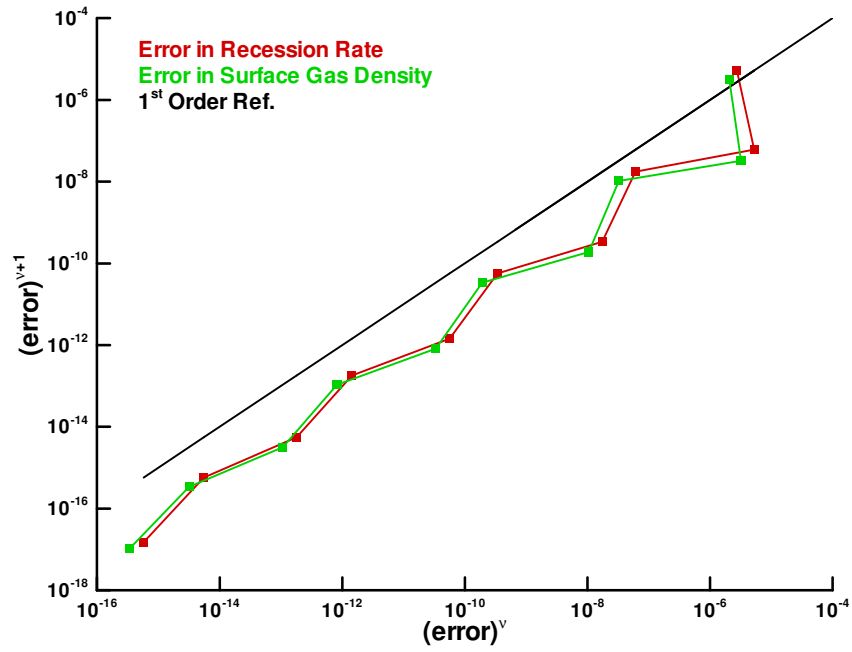


Figure 8.26: Global convergence rate for surface recession rate and gas density where ν is the global iteration index.

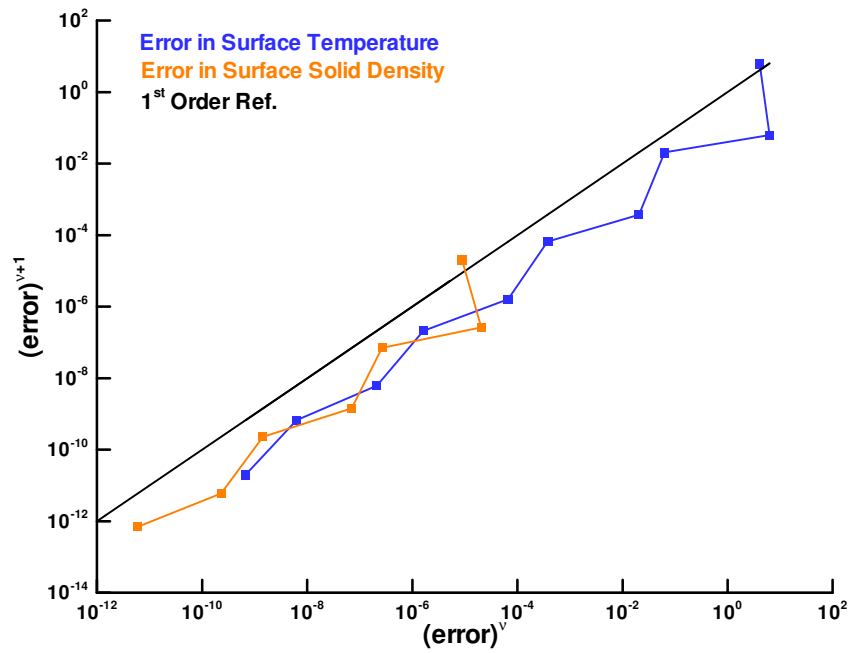


Figure 8.27: Global convergence rate for surface temperature and solid density where ν is the global iteration index.

is used to solve the mixture energy equation as discussed in Section 6, this option was not exercised in order to make a more direct comparison. It is also important to note that the primary differences between the two codes for this simulation are as follows:

1. CMA iterates only on the surface energy balance and lags temperature dependent properties and surface recession rate for the interior node solution while the research code iterates on the entire system of residual equations to determine time accurate nonlinearities
2. CMA uses a translating/node-dropping grid scheme, and the research code uses a contracting grid scheme
3. CMA uses a lumped capacitance method, and the research code uses a distributed capacitance method
4. CMA linearly interpolates on $\ln(B'_c)$, and the research code linearly interpolates on B'_c
5. CMA assumes that all gas generated further in-depth than a given node passes that node in the time interval in which the gas was generated and the flow work is accounted for, and the research code allows internal pressure gradients to drive the flow of pyrolysis gases through the pore space
6. CMA does not account for the gas phase internal energy in the energy capacitance term, and the research code does account for the gas phase internal energy

The comparisons for the predicted surface temperature, back face temperature, recession, and recession rate histories can be seen in Figures 8.28, 8.29, 8.30, and

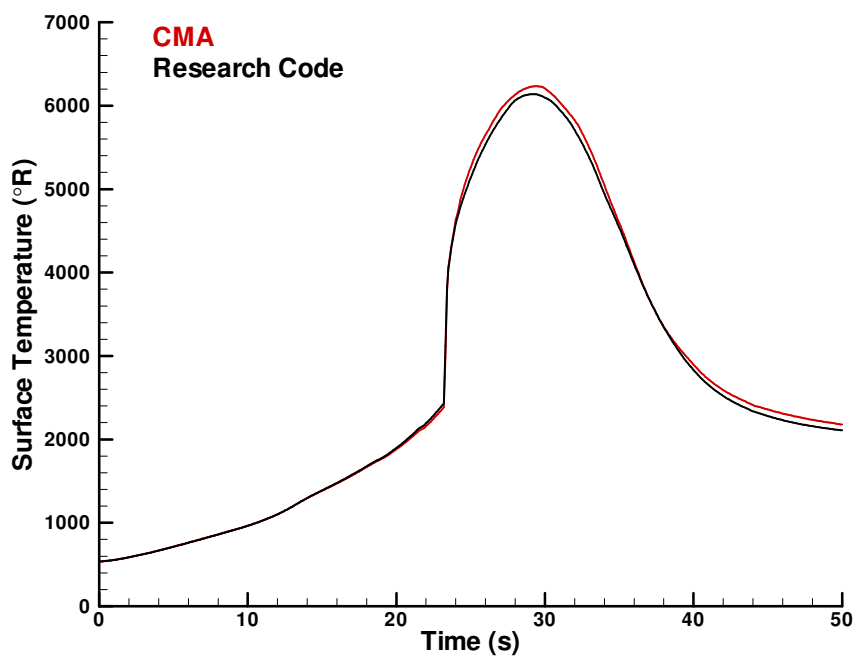


Figure 8.28: Comparison of surface temperature predictions for the carbon-phenolic thermochemical ablation verification problem.

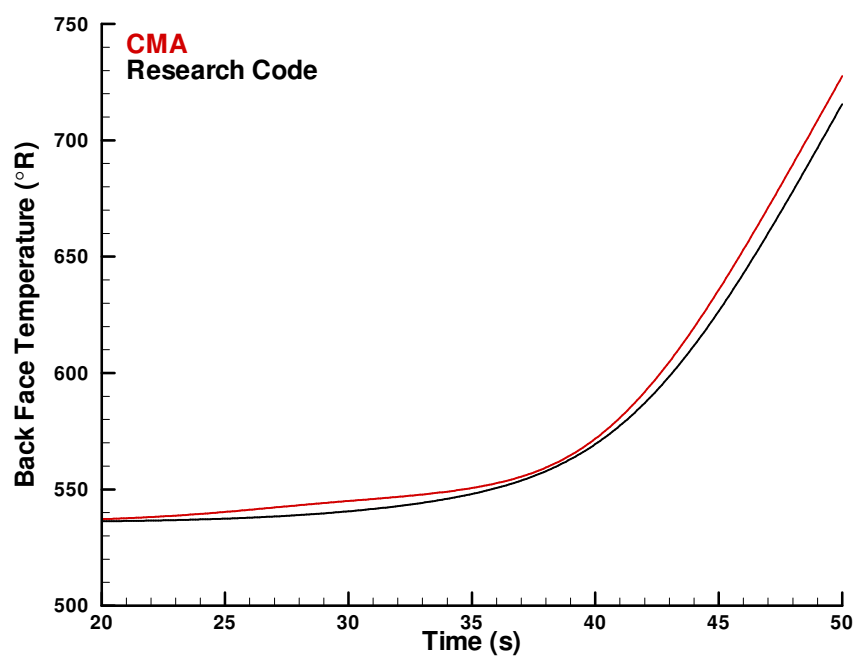


Figure 8.29: Comparison of back face temperature predictions for the carbon-phenolic thermochemical ablation verification problem.

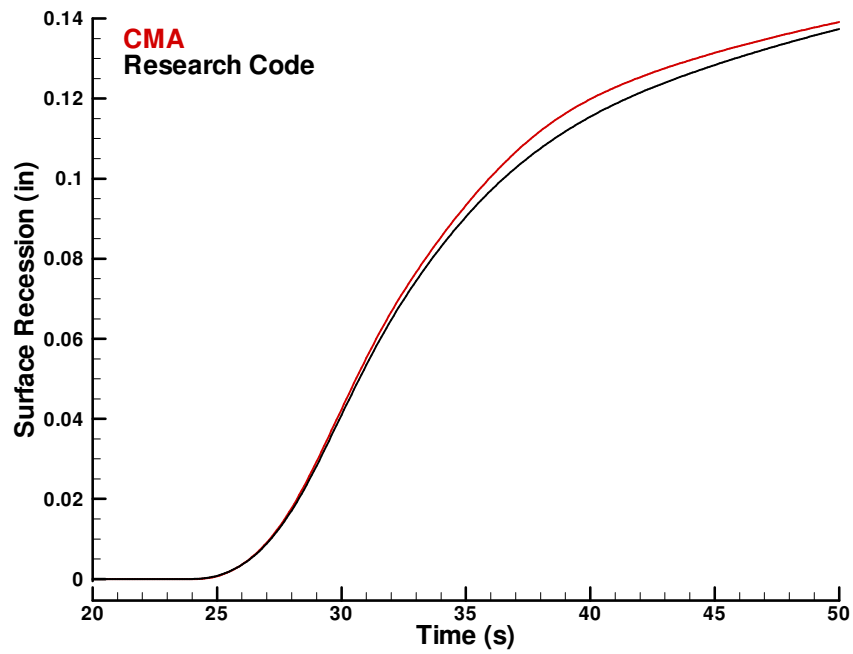


Figure 8.30: Comparison of surface recession predictions for the carbon-phenolic thermochemical ablation verification problem.

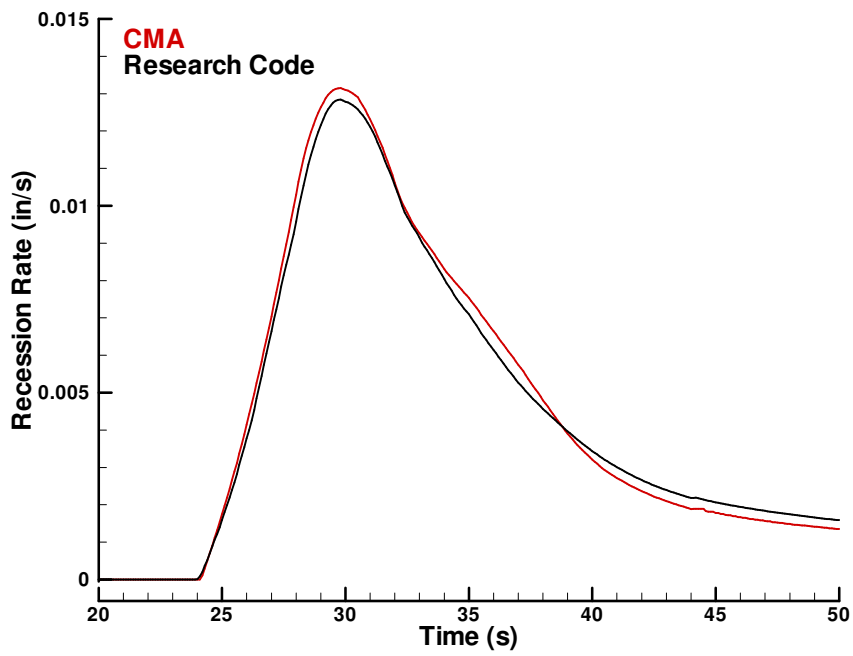


Figure 8.31: Comparison of surface recession rate predictions for the carbon-phenolic thermochemical ablation verification problem.

8.31 respectively. Due to the number of numerical differences between the codes and the number of physical phenomenon that are being modeled throughout the solution procedure, it is difficult to discern what modeling differences between the two codes is causing the discrepancy in the solutions. From these results it is evident that CMA's pyrolysis gas assumptions, described in items 5 and 6 in the above list, are valid since the exclusion of these assumptions (as is done in the research code) does not significantly change the mixture energy equation solution. This suggests a dominantly one-way coupling between the mixture energy equation and the gas phase continuity equation, which is expected since gas velocities are low and the heat capacity and thermal conductivity for gases are generally much lower than they are for a solid.

8.8.5 Porous Flow Results

One of the primary goals of this study is the implementation and verification of the gas phase continuity equation with porous flow assumptions in order to predict in-depth pressure in a charring ablator. Figures 8.32-8.40 show profile histories for several properties in the charring carbon-phenolic ablator including gas density, pressure, and gas superficial velocity, which are predicted through solving the gas phase continuity equation with porous flow assumptions. It is evident that the gas density, pressure, and solid decomposition (or gas generation) rate profiles have steep gradients when compared to the temperature profile. This suggests that if a sub-mesh scheme is implemented (as described in Section 6), then both the solid and gas phase continuity equations should be solved on the nodelet mesh.

Figure 8.36 shows that ablation begins to occur before the surface solid becomes fully charred meaning that there is still non-decomposed resin in the solid. This creates a discrepancy since the surface thermochemical solution assumes that the solid participating in the reactions is fully charred. According to the decomposition

kinetics, it takes an infinite amount of time for the composite to decompose to its char state. As a result, to ensure that the thermochemistry data is accurately describing the surface ablation phenomenon, a tolerance in the vicinity of the char density could be implemented with which the solid density is automatically adjusted to the char value once this tolerance has been reached. This method is implemented in CMA, but it adds the additional complication of accounting for this mass when solving the gas phase continuity equation.

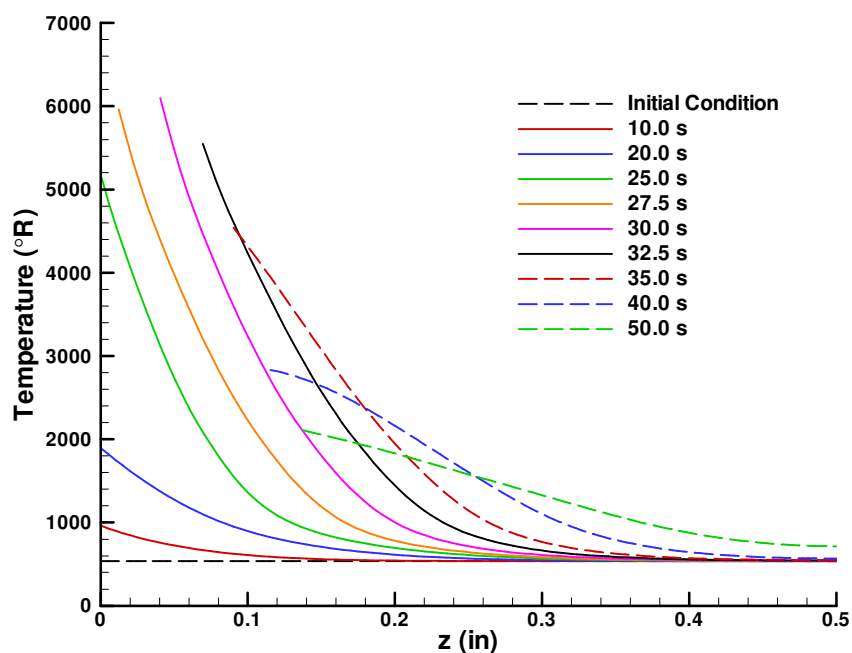


Figure 8.32: Temperature profile history for the carbon-phenolic thermochemical ablation verification problem.

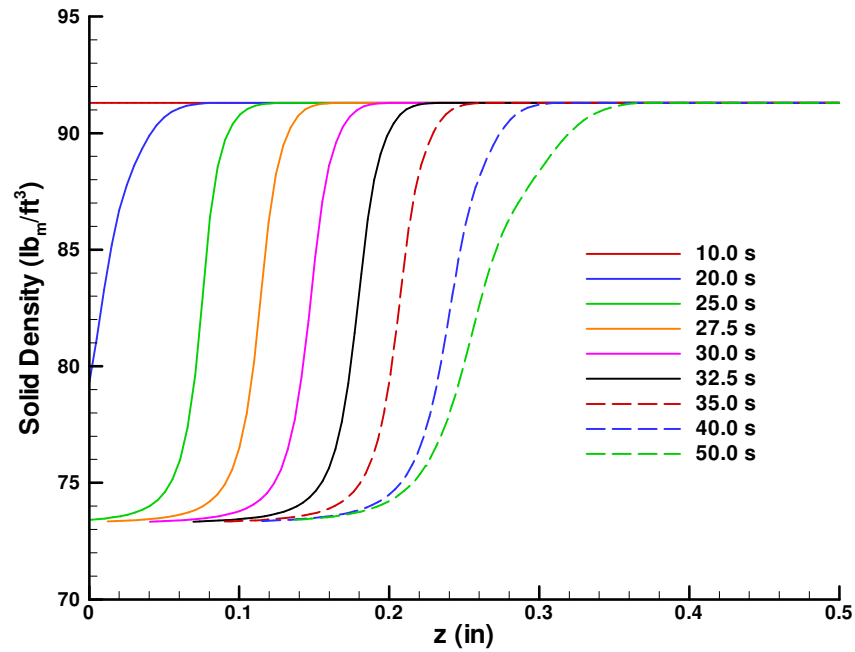


Figure 8.33: Solid density profile history for the carbon-phenolic thermochemical ablation verification problem.

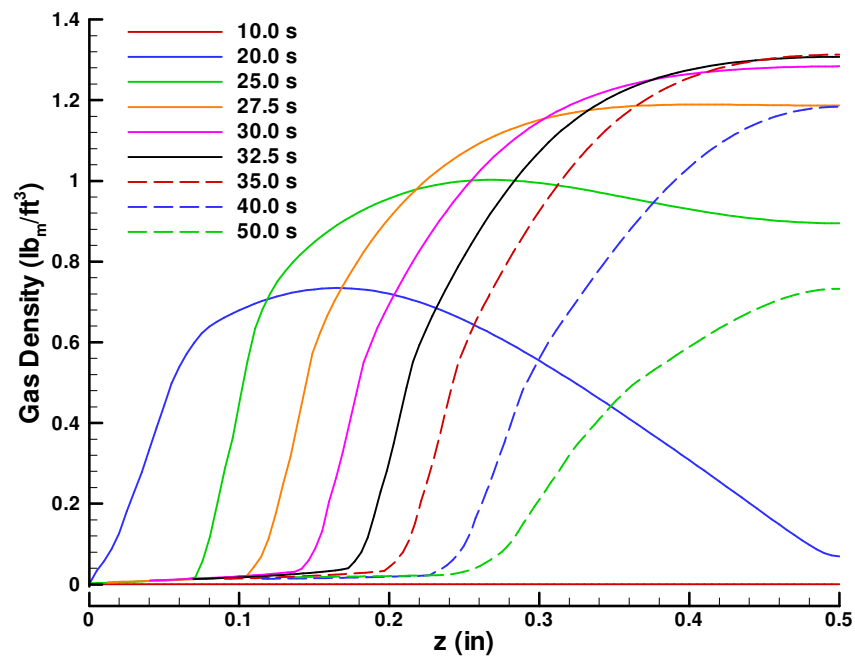


Figure 8.34: Gas density profile history for the carbon-phenolic thermochemical ablation verification problem.

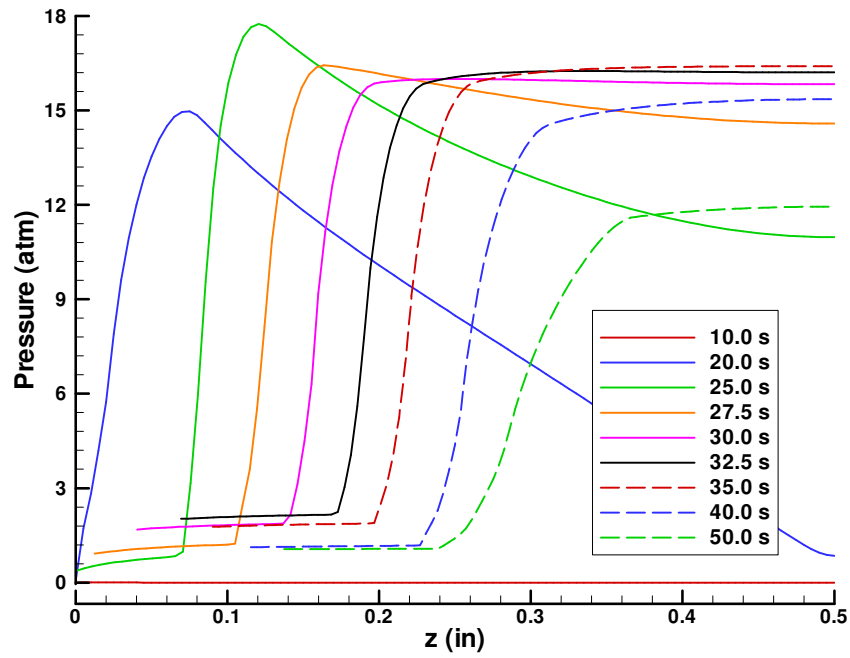


Figure 8.35: Pressure profile history for the carbon-phenolic thermochemical ablation verification problem.

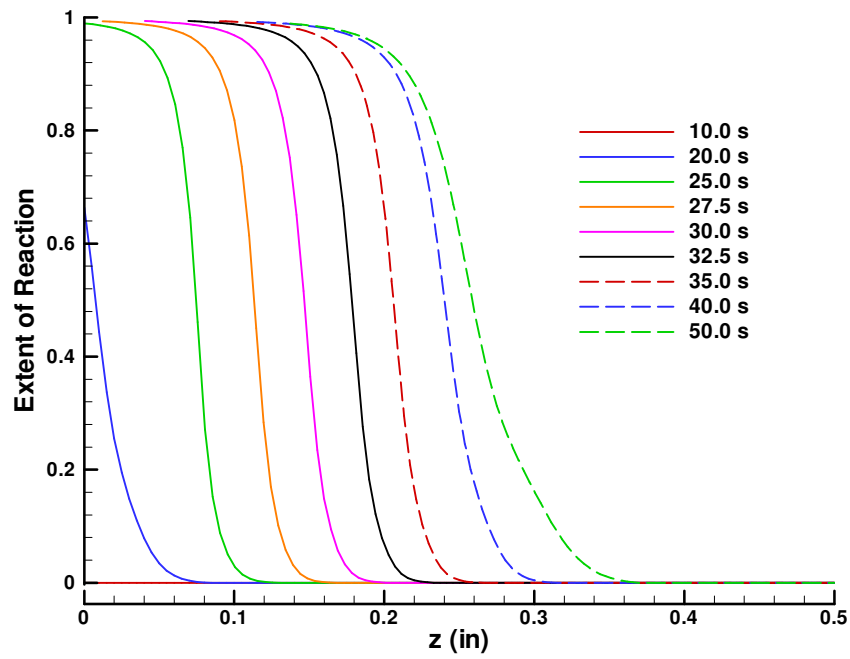


Figure 8.36: Extent of reaction (β) profile history for the carbon-phenolic thermochemical ablation verification problem.

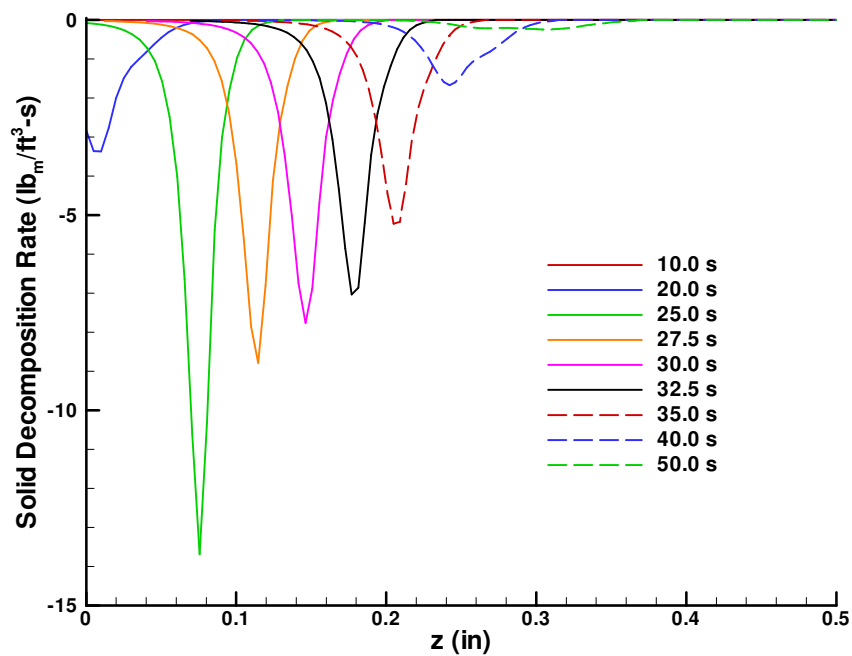


Figure 8.37: Solid decomposition rate profile history for the carbon-phenolic thermochemical ablation verification problem.

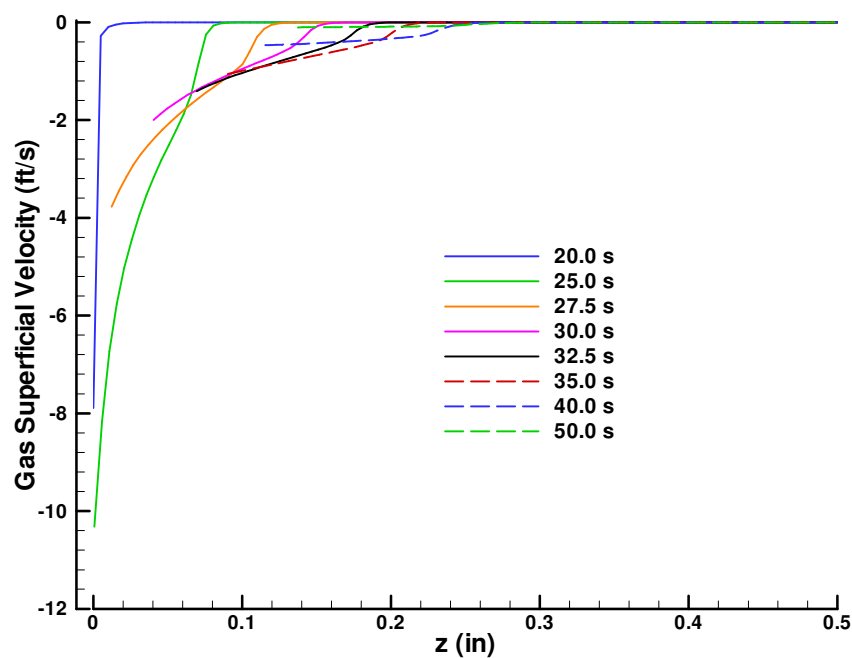


Figure 8.38: Gas superficial velocity profile history for the carbon-phenolic thermochemical ablation problem where a negative velocity is toward the ablating surface.

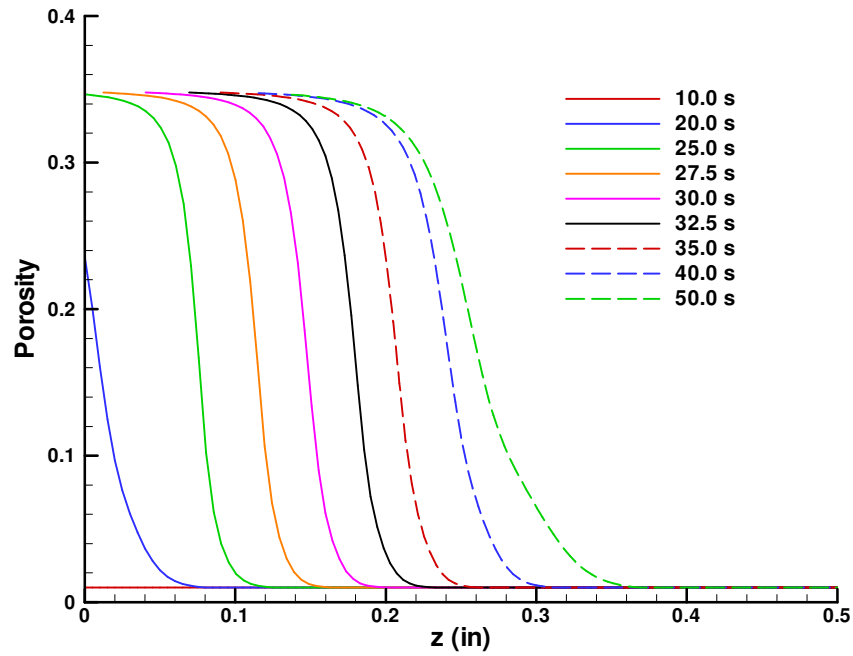


Figure 8.39: Porosity profile history for the carbon-phenolic thermochemical ablation verification problem.

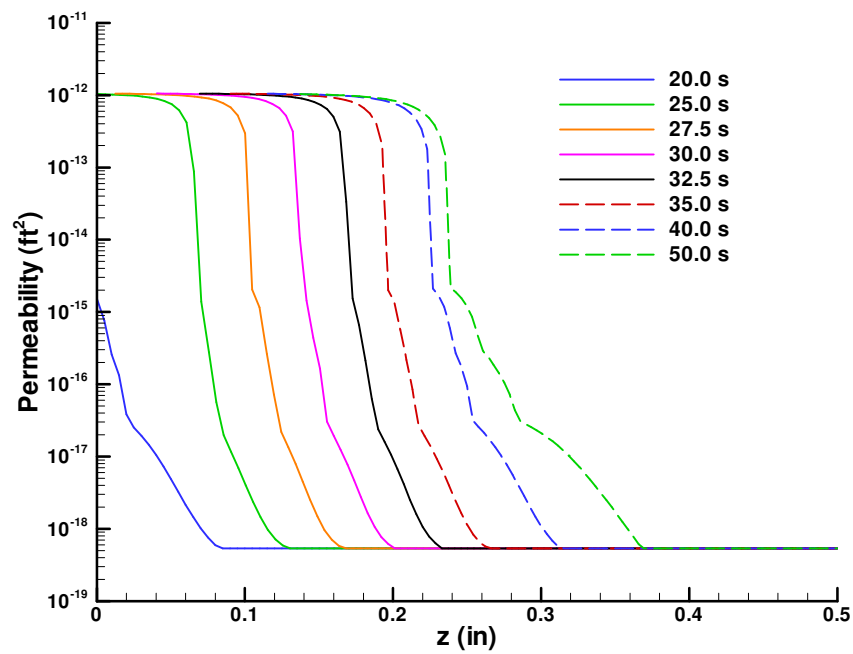


Figure 8.40: Permeability profile history for the carbon-phenolic thermochemical ablation verification problem.

9 Timing Studies

Timing studies, which are also presented in Amar et al.[40], were performed to determine if the model developed in this study provides advantages or disadvantages when compared to other models.

9.1 Complete Sensitivity Matrix vs. Tridiagonal Formulation

The first timing study was performed to determine the advantage of including the entire sensitivity matrix versus only including the tridiagonal terms when identical convergence criteria are imposed.

$$\begin{array}{c}
 \text{full sensitivity matrix:} \\
 \left[\begin{array}{cccccc} e_0 & c_0 & 0 & 0 & 0 & 0 \\ e_1 & b_1 & c_1 & 0 & 0 & 0 \\ e_2 & a_2 & b_2 & c_2 & 0 & 0 \\ e_3 & 0 & a_3 & b_3 & c_3 & 0 \\ e_4 & 0 & 0 & a_4 & b_4 & c_4 \\ e_5 & 0 & 0 & 0 & a_5 & b_5 \end{array} \right]^\nu \left[\begin{array}{c} \Delta \dot{s} \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{array} \right]^{\nu+1} = \left[\begin{array}{c} d_0 \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{array} \right]^\nu
 \end{array}$$

versus

$$\begin{array}{c}
 \text{tridiagonal matrix:} \\
 \left[\begin{array}{cccccc} e_0 & c_0 & 0 & 0 & 0 & 0 \\ e_1 & b_1 & c_1 & 0 & 0 & 0 \\ 0 & a_2 & b_2 & c_2 & 0 & 0 \\ 0 & 0 & a_3 & b_3 & c_3 & 0 \\ 0 & 0 & 0 & a_4 & b_4 & c_4 \\ 0 & 0 & 0 & 0 & a_5 & b_5 \end{array} \right]^\nu \left[\begin{array}{c} \Delta \dot{s} \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{array} \right]^{\nu+1} = \left[\begin{array}{c} d_0 \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{array} \right]^\nu
 \end{array}$$

Experience has shown that both methods converge to the same solution, but the tridiagonal system exhibits first order nonlinear convergence. Consequently, it is of interest to determine if the extra development, verification, and computational time necessary to calculate the entire recession rate sensitivity vector benefits the analyst.

For the Q^* ablation verification problem described in Section 8.5, the spatial and temporal grids were refined separately to isolate the effects of each refinement. The parameters for the uniform grids used in the spatial refinement study are given in

Table 9.1, and the results can be seen in Figure 9.1. It is evident that including the full sensitivity matrix requires approximately 60% of the computational time and 45 – 50% of the total iterations necessary to solve the problem when compared to the tridiagonal approach. This reduction has the potential to save the analyst significant amounts of time especially if the model is extended to multidimensions.

The parameters and results for the temporal grid refinement timing study are given in Table 9.2 and Figure 9.2 respectively. Consistent with the spatial refinement results, the temporal refinement suggests that the full sensitivity matrix approach takes 60% of the computational time and 50% of the total iterations necessary to solve the problem. It is evident that although including the entire sensitivity matrix is about 19% to 30% slower (increases as the spatial grid is refined) per iteration than the tridiagonal formulation, it provides a significant reduction in overall computational time which will benefit the analyst.

Table 9.1: Grid parameters for spatial refinement.

# elem	Δz_o , m	Δt , s
20	1.5×10^{-3}	0.01
40	7.5×10^{-4}	0.01
80	3.75×10^{-4}	0.01
160	1.875×10^{-4}	0.01
320	9.375×10^{-5}	0.01
640	4.6875×10^{-5}	0.01

Table 9.2: Grid parameters for temporal refinement.

Δt , s	# elem	Δz_o , m
0.01	20	1.5×10^{-3}
0.005	20	1.5×10^{-3}
0.0025	20	1.5×10^{-3}
0.00125	20	1.5×10^{-3}

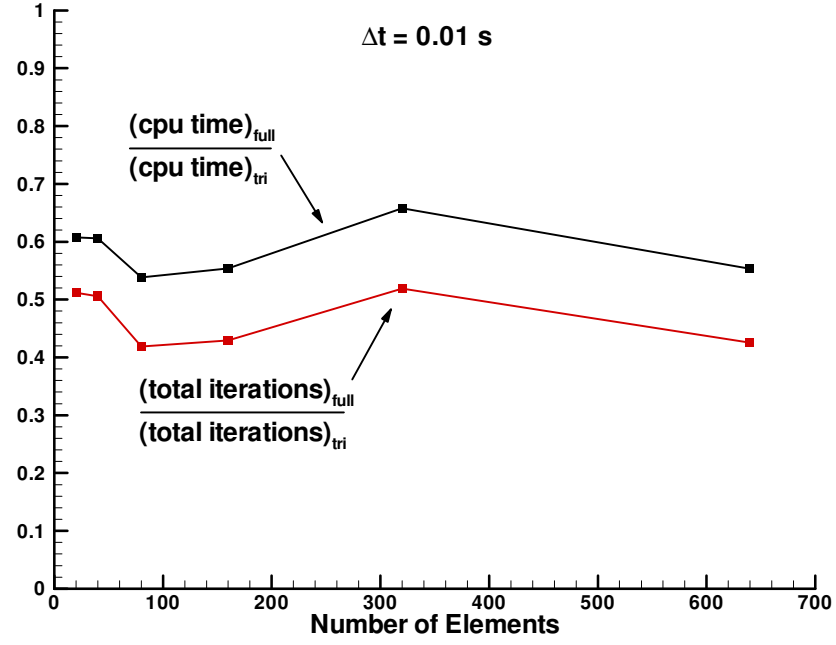


Figure 9.1: Timing study results for the spatial grid refinement on the Q^* ablation verification problem where both methods have the same convergence criteria.

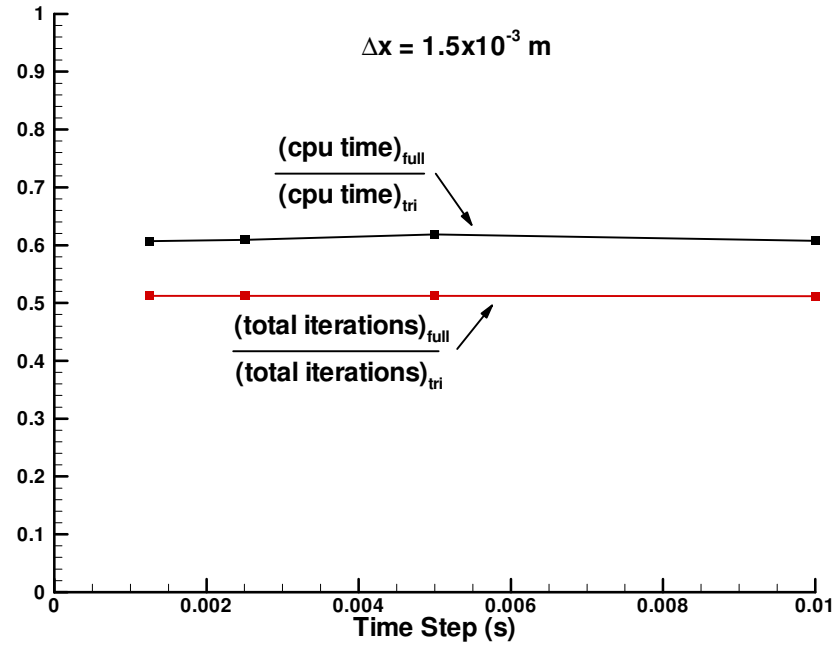


Figure 9.2: Timing study results for temporal grid refinement on the Q^* ablation verification problem where both methods have the same convergence criteria.

9.2 Nonlinear Iteration vs. Material Property Lagging

It is also of interest to determine if iteratively solving the entire system of equations saves computational time when compared to the material property lagging approach used in legacy codes. The variable property verification problem was solved on all four spatial grids in Table 8.9 using both approaches in order to compare the computational time necessary to give **equally** accurate solutions. The time step for the iterative method solutions was chosen to be 0.5 s for each grid, and the L_2 of the temperature error vector was calculated at the final time ($t = 40$ s). The time step for the lagging method solutions was varied until the desired accuracy at the final computational time was achieved on each grid, and the results can be seen in Figure 9.3.

It is evident that there is a second order relationship between computational time savings and grid refinement in order to achieve the same accuracy for the variable property problem. As a result, using the iterative solution procedure as opposed to the lagging method can significantly decrease the computational time necessary to find solutions on relatively fine grids since considerably larger time steps can be used. For example, to achieve the required accuracy on the finest spatial grid, the full iterative approach developed in this study requires less than 1% of the computational time when compared to lagging the thermal properties. This is another improvement that will benefit the analyst especially if the model is extended to multidimensions.

Since the allowable modes of operation in the research code do not include solving ablation problems by lagging the grid convection terms one time step at the interior nodes while only iterating on the surface energy balance, an associated timing study was unable to be performed. Results similar to the nonlinear iteration versus thermal property lagging timing study are expected since both cases are comparing lagging a nonlinearity versus nonlinear iteration on the entire system of residual equations.

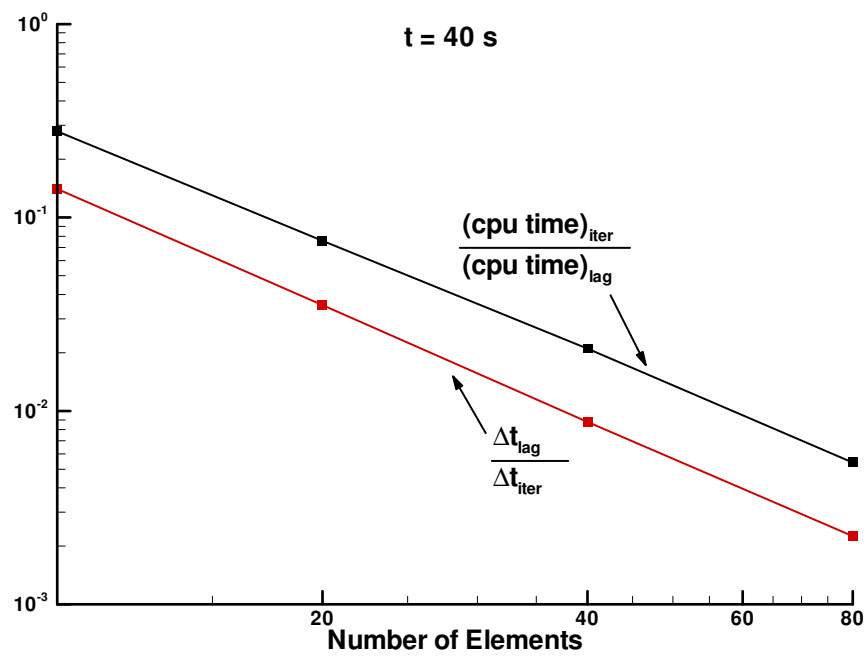


Figure 9.3: Timing study results comparing iterative and lagging methods for variable property verification problem.

10 Conclusion

10.1 Summary

The development of a one-dimensional material thermal response code with ablation has been presented. The model has been implemented and verified to be first order temporally and second order spatially for all terms in the governing equations, boundary conditions, and ablation models considered. Newton's method for nonlinear iteration on the entire system of nodal residual equations has been implemented for the mixture energy and gas phase continuity equations' solution procedures, and they both exhibit second order nonlinear convergence for the entire verification suite. In addition, the block Gauss-Seidel segregated solution procedure has been verified to exhibit first order nonlinear convergence for the entire system of equations.

The model presented in this study includes several improvements over methods in legacy codes. The contracting grid scheme avoids the node-dropping complexity inherent in the translating grid scheme, and it maintains solution accuracy when the domain is significantly thinner than the initial domain. The control volume finite element method not only provides a conservative discretization of the governing equations, but it also simplifies the model's derivation and implementation when compared to finite difference discretizations of the governing differential equations. Nonlinear iteration on the mixture energy and gas phase continuity equations provides time accurate nonlinearities which has been shown to allow for significantly larger time steps than are required for the property lagging approach for the same accuracy. Including the recession rate sensitivities in the mixture energy equation's Jacobian matrix has been shown to accelerate convergence and reduce the overall computation time necessary to solve moving grid problems when compared to lagging the grid convection terms throughout the iteration process. The block Gauss-Seidel method provides a full coupling of the governing equations and allows for larger time steps

than the loose-coupling approach implemented in CMA when accuracy is considered. Integration of the kinetic relationships assuming a constant temperature rise rate has been implemented which is more expensive than treating temperature explicitly in time but it provides a more accurate solution.

The gas density and pore pressure are able to be predicted through the solution of the gas phase continuity equation with porous flow assumptions. This provides a more accurate prediction of the gas generation and gas flux effects on the energy equation solution and it better predicts the pyrolysis gas injection rate into the boundary layer. In addition, knowing the pore pressure allows the analyst to determine if stress limits are exceeded which could lead to in-depth structural damage and eventual failure of the thermal protection system.

10.2 Future Work

The model developed in this study does not include all of the relevant physics involved in the ablation of a decomposable material, but it provides a model development and verification methodology that can be applied when more of the physics is added. Some of the phenomena that should be considered for a more complete model of a charring ablator includes:

1. Multiple pyrolysis gas species and the reactions among them in the pore space
2. Reactions between the pyrolysis gases and the solid in the pore space
3. Deposition of residue (coking) from the pyrolysis gases to the solid
4. Thermal and chemical nonequilibrium
5. The solid not being fully charred at the ablating surface for decomposing materials as discussed in Section 8.8.5

6. Nonlinear effects on the relationship between gas velocity and flow resistance in the porous medium
7. Inclusion of surface thermochemistry solution within the code to avoid thermochemistry table generation and interpolation and associated convergence issues due to lack of smoothness and resolution of the table
8. Ability to handle unequal species mass diffusion coefficients in the thermochemical ablation model and the aerodynamic heating boundary condition

In addition to the improvements to the physical model, the numerics can also be improved by adding a sub-mesh scheme for the solution of the continuity equations which could significantly reduce computational time without significantly compromising accuracy.

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Appendices

Appendix A: Specific Internal Energy Table Generation and Interpolation Routine

A.1 Specific Internal Energy and Gas Enthalpy Table Generation

Through integration of the tabulated specific heat functions, specific internal energy tables can be generated for the virgin and char. The code requires an input reference temperature, T_{ref} , that will serve as the "zero" datum for both the specific internal energy functions and the pyrolysis gas specific enthalpy table. It is important to note that although the pyrolysis gas specific enthalpy is a function of pressure and temperature, it is assumed that there is a weak pressure dependence, and therefore the gas enthalpy is a function of temperature only. The gas specific enthalpy table, which is generated by ACE or some other equilibrium chemistry code, is modified for every entry according to

$$h_g(T_k) = [h_g(T_k)]_{\text{input}} + (h_f^o)_g \quad (\text{A.1})$$

so that the enthalpy at the reference temperature is consistent with the solid internal energy tables.

For n virgin or char specific heat entries tabulated versus temperature, the input table is of the form:

$T(T)$	$C_v(T)$
T_1	$C_v(T_1)$
.	.
.	.
T_i	$C_v(T_i)$
T_{i+1}	$C_v(T_{i+1})$
.	.
.	.
T_n	$C_v(T_n)$

and the virgin and char specific heat tables are not required to have the same number of entries. The generated specific internal energy tables have identical temperature

entries resulting in tables of the form:

T	$C_v(T)$	$e(T)$
T_1	$C_v(T_1)$	$e(T_1)$
$\cdot$	$\cdot$	$\cdot$
$\cdot$	$\cdot$	$\cdot$
T_i	$C_v(T_i)$	$e(T_i)$
T_{i+1}	$C_v(T_{i+1})$	$e(T_{i+1})$
$\cdot$	$\cdot$	$\cdot$
$\cdot$	$\cdot$	$\cdot$
T_n	$C_v(T_n)$	$e(T_n)$

Direct integration of the specific heat tables starting from the lowest temperature entry will result in

$$e(T_{ref}) \neq h_f^o \quad (\text{A.2})$$

Therefore to ensure that $e(T_{ref}) = h_f^o$, the specific internal energy at each temperature entry is determined from

$$e(T_k) = h_f^o + \int_{T_{ref}}^{T_k} C_v(T) dT = h_f^o - \int_{T_1}^{T_{ref}} C_v(T) dT + \int_{T_1}^{T_k} C_v(T) dT \quad (\text{A.3})$$

where

$$\begin{aligned} \int_{T_1}^{T_{ref}} C_v(T) dT &= \left[\sum_{j=1}^{i-1} \frac{1}{2} [C_v(T_j) + C_v(T_{j+1})] (T_{j+1} - T_j) \right] \\ &\quad + \frac{1}{2} (C_v(T_{ref}) + C_v(T_i)) (T_{ref} - T_i) \end{aligned} \quad (\text{A.4})$$

if $T_i < T_{ref} < T_{i+1}$. The specific internal energy at the k th temperature entry can then be found from

$$e(T_k) = \begin{cases} h_f^o - \int_{T_1}^{T_{ref}} C_v(T) dT & \text{for } k = 1 \\ e(T_1) + \sum_{j=2}^k \frac{1}{2} (C_v(T_j) + C_v(T_{j-1})) (T_j - T_{j-1}) & \text{for } k = 2 \dots n \end{cases} \quad (\text{A.5})$$

A.2 Parabolic Interpolation

Since it is assumed that the specific heat functions are linear in temperature between tabulated entries, it would be inconsistent to also assume a linear variation in internal

energy. As a result, treating internal energy parabolic in temperature properly accounts for the integration of the specific heat functions up to the temperature of interest.

The specific internal energy at any temperature, T , is given by

$$e(T) = h_f^o + \int_{T_{ref}}^T C_v(\hat{T}) d\hat{T} \quad (\text{A.6})$$

If the temperature of interest, T , is between two tabulated temperature entries, namely T_k and T_{k+1} , then Eq. A.6 can be expressed as

$$e(T) = h_f^o + \int_{T_{ref}}^{T_k} C_v(\hat{T}) d\hat{T} + \int_{T_k}^T C_v(\hat{T}) d\hat{T} = e(T_k) + \int_{T_k}^T C_v(\hat{T}) d\hat{T} \quad (\text{A.7})$$

where $e(T_k)$ is a tabulated specific internal energy entry determined by Eq. A.5, and the tabulated specific heat curve can be integrated to obtain $\int_{T_k}^T C_v(\hat{T}) d\hat{T}$. This gives

$$e(T) = e(T_k) + (T - T_k) \frac{1}{2} [C_v(T_k) + C_v(T)] \quad (\text{A.8})$$

where

$$C_v(T) = f C_v(T_{k+1}) + (1 - f) C_v(T_k) \quad (\text{A.9})$$

and the interpolation parameter is defined to be

$$f = \left[\frac{T - T_k}{T_{k+1} - T_k} \right] \quad (\text{A.10})$$

The final expression for the specific internal energy interpolation is given by

$$e(T) = e(T_k) + (T - T_k) \frac{1}{2} [(2 - f) C_v(T_k) + f C_v(T_{k+1})] \quad (\text{A.11})$$

As a result, the routine must be provided with tabulated specific internal energy and specific heat tables with the same temperature entries as described in the previous section.

If one segment of the specific heat and specific internal energy functions is given by

T K	$C_v(T)$ J/(kg-K)	$e(T)$ J/kg
$T_k = 300$	$C_v(T_k) = 500$	$e(T_k) = 0$
$T_{k+1} = 1300$	$C_v(T_{k+1}) = 5000$	$e(T_{k+1}) = 2.75 \times 10^6$

then the linear and parabolic interpolation curves can be seen in Figure A.1. It is evident that the two interpolation methods agree at the tabulated temperatures but are different when $T_k < T < T_{k+1}$.

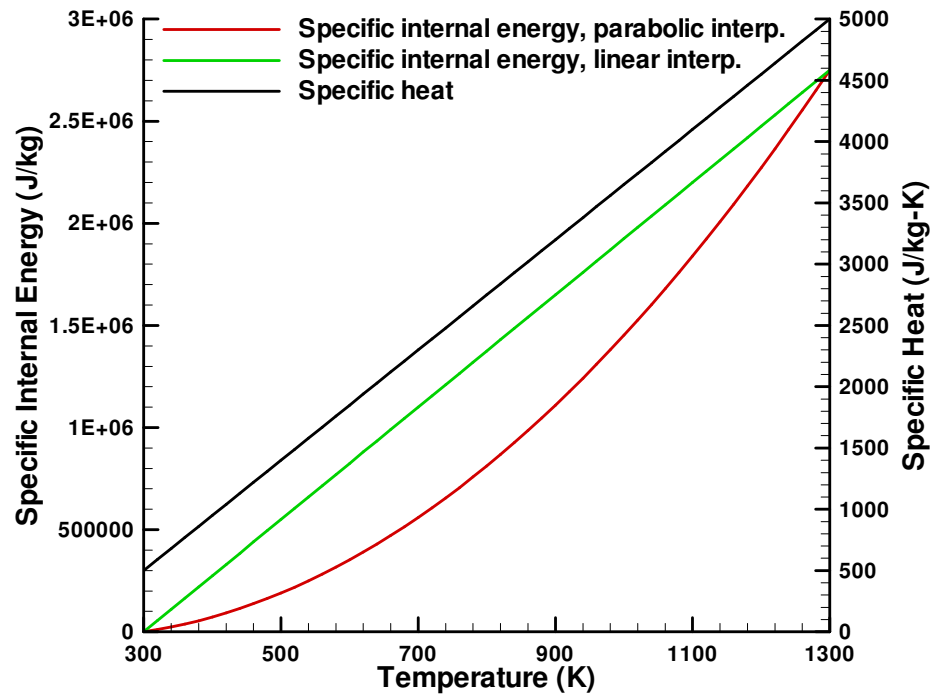


Figure A.1: Specific heat and specific internal energy interpolation curves.

Appendix B: Linear System Solver

For non-ablating problems and ablation problems when ablation is not occurring, the linear system of energy residual equations resulting from boundary conditions and the element assembly routines is tridiagonal with temperature correction $\Delta T_1^{\nu+1}$ as the first unknown. For example, a five node domain would have the matrix structure given by Eq. 5.2

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 \\ 0 & 0 & a_4 & b_4 & c_4 \\ 0 & 0 & 0 & a_5 & b_5 \end{bmatrix} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}$$

An efficient way to solve for the unknown vector would be to implement a forward elimination/back substitution routine or some other Gaussian elimination algorithm that is tailored for solving tridiagonal systems.

For ablation problems when ablation is occurring, a zeroth equation is added to the linear system and is given by

$$Q^* \text{ ablation: } \Delta T_1^{\nu+1} = 0 \quad (\text{B.1})$$

or

$$\text{Thermochemical ablation: } B'_c = \frac{\rho_s \dot{s}}{\rho_e u_e C_m} \quad (\text{B.2})$$

Since ablation problems on moving grids are nonlinear in surface recession rate in addition to temperature, the resulting linear system from boundary conditions and element assembly routines is given by Eq. 5.3

$$\begin{bmatrix} e_0 & c_0 & 0 & 0 & 0 & 0 \\ e_1 & b_1 & c_1 & 0 & 0 & 0 \\ e_2 & a_2 & b_2 & c_2 & 0 & 0 \\ e_3 & 0 & a_3 & b_3 & c_3 & 0 \\ e_4 & 0 & 0 & a_4 & b_4 & c_4 \\ e_5 & 0 & 0 & 0 & a_5 & b_5 \end{bmatrix} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}$$

The following algorithm description is written in mixed FORTRAN90/math syntax, therefore there may be more convenient ways of expressing the routine when being applied in other programming languages. Upon inspection of the linear system in Eq. 5.3, it is evident that the coefficient matrix is a lower triangular matrix with the exception of the superdiagonal represented by c_0 , c_1 , c_2 , c_3 , and c_4 . Given an arbitrary size $(J_{\max} + 1 \times J_{\max} + 1)$ square matrix with the same structure as Eq. 5.3, where $J_{\max}$ is the number of nodes, eliminating the superdiagonal results in a lower triangular matrix, and back substitution is used to solve for the unknown vector. In order to eliminate any entry in the superdiagonal array, $c(j)$, equation $j + 1$ can be multiplied by the appropriate elimination factor, f , and added to equation j . The elimination factor is

$$f = -c(j)/b(j + 1) \quad (\text{B.3})$$

As a result

$$c(j) = f * b(j + 1) + c(j) = 0 \quad (\text{B.4})$$

Consequently the other coefficients in equation j need to be adjusted appropriately.

$$b(j) = f * a(j + 1) + b(j) \quad (\text{B.5})$$

$$e(j) = f * e(j + 1) + e(j) \quad (\text{B.6})$$

$$d(j) = f * d(j + 1) + d(j) \quad (\text{B.7})$$

Note that $a(j)$ is not affected by the row operation because its corresponding term in equation $j + 1$ is zero. These operations apply to equations 1 through $J_{\max} - 1$ as equation $J_{\max}$ already falls into the lower triangular form and equation 0 needs special considerations. Equation 0 requires fewer operations than the internal node equations, and the elimination factor is of the same form

$$f = -c(0)/b(1) \quad (\text{B.9})$$

Since there is no $\mathbf{b}(0)$, only $\mathbf{e}(0)$ and $\mathbf{d}(0)$ need to be dealt with.

$$\mathbf{c}(0) = \mathbf{f} * \mathbf{b}(1) + \mathbf{c}(0) = 0 \quad (\text{B.10})$$

$$\mathbf{e}(0) = \mathbf{f} * \mathbf{e}(1) + \mathbf{e}(0) \quad (\text{B.11})$$

$$\mathbf{d}(0) = \mathbf{f} * \mathbf{d}(1) + \mathbf{d}(0) \quad (\text{B.12})$$

The modified linear system, after the Gaussian elimination process, has the following lower triangular structure

$$\begin{bmatrix} e_0 & 0 & 0 & 0 & 0 & 0 \\ e_1 & b_1 & 0 & 0 & 0 & 0 \\ e_2 & a_2 & b_2 & 0 & 0 & 0 \\ e_3 & 0 & a_3 & b_3 & 0 & 0 \\ e_4 & 0 & 0 & a_4 & b_4 & 0 \\ e_5 & 0 & 0 & 0 & a_5 & b_5 \end{bmatrix} \begin{bmatrix} \Delta \dot{s} \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \\ \Delta T_4 \\ \Delta T_5 \end{bmatrix}^{\nu+1} = \begin{bmatrix} d_o \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix} \quad (\text{B.13})$$

and back substitution can now be applied.

In the back substitution routine, equations 0 and 1 need special consideration since they have fewer coefficients than the rest of the nodes. For equation 0

$$\Delta \dot{s} = \mathbf{d}(0)/\mathbf{e}(0) \quad (\text{B.14})$$

and for equation 1

$$\Delta T(1) = (\mathbf{d}(1) - \mathbf{e}(1)\Delta \dot{s})/\mathbf{b}(1) \quad (\text{B.15})$$

For the rest of the nodes the unknown is given by

$$\Delta T(j) = (\mathbf{d}(j) - \mathbf{e}(j)\Delta \dot{s} - \mathbf{a}(j)\Delta T(j-1))/\mathbf{b}(j) \quad (\text{B.16})$$

In summary:

```

DO  j = Jmax-1, 1, -1
      f = -c(j)/b(j+1)
      b(j) = f * a(j+1) + b(j)
      e(j) = f * e(j+1) + e(j)
      d(j) = f * d(j+1) + d(j)
END DO

      f = -c(0)/b(1)
      e(0) = f * e(1) + e(0)
      d(0) = f * d(1) + d(0)

!NOW WE HAVE A LOWER TRIANGULAR MATRIX
!BEGIN BACK SUBSTITUTION

      Δṡ = d(0)/e(0)

      ΔT(1) = (d(1) - e(1) * Δṡ)/b(1)

DO  j = 2, Jmax
      ΔT(j) = (d(j) - e(j) * Δṡ - a(j) * ΔT(j-1))/b(j)
END DO

```

Appendix C: Thermochemistry Data Organization and 3-D Interpolation Routine

Thermochemistry Data Organization

The thermochemistry tables are arranged in a series of pressure (P) tables each associated with one pressure value. For each pressure value, there are a series of dimensionless pyrolysis gas blowing rate (B'_g) sub-tables each associated with one dimensionless pyrolysis gas blowing rate value. For each dimensionless pyrolysis gas blowing rate sub-table, there are a series of entries for dimensionless char ablation rate (B'_c), wall temperature (T), and equilibrium gas specific enthalpy (h_w). The dimensionless rates are defined as

$$B'_g = \frac{\dot{m}''_g}{\rho_e u_e C_m} \quad (\text{C.1})$$

and

$$B'_c = \frac{\dot{m}''_{abl}}{\rho_e u_e C_m} \quad (\text{C.2})$$

where

$$\rho_e u_e C_m = \rho_e u_e C_{h_o} \frac{C_h}{C_{h_o}} \frac{C_m}{C_h} \quad (\text{C.3})$$

It is also necessary that the reference temperature associated with the equilibrium gas enthalpy function is consistent with the reference temperature for the internal energy and pyrolysis gas enthalpy functions discussed in Appendix A. Each pressure table is organized as follows:

(atm)	—	—	(°R)	(Btu/lb _m)
$P_1 = 1$	$(B'_g)_{3,1} = 5$	$(B'_c)_{5,3,1} = 4$	$T_{5,3,1} = 1300$	$(h_w)_{5,3,1} = 600$
$P_1 = 1$	$(B'_g)_{3,1} = 5$	$(B'_c)_{4,3,1} = 3$	$T_{4,3,1} = 1000$	$(h_w)_{4,3,1} = 400$
$P_1 = 1$	$(B'_g)_{3,1} = 5$	$(B'_c)_{3,3,1} = 2$	$T_{3,3,1} = 800$	$(h_w)_{3,3,1} = 200$
$P_1 = 1$	$(B'_g)_{3,1} = 5$	$(B'_c)_{2,3,1} = 0$	$T_{2,3,1} = 800$	$(h_w)_{2,3,1} = 250$
$P_1 = 1$	$(B'_g)_{3,1} = 5$	$(B'_c)_{1,3,1} = 0$	$T_{1,3,1} = 500$	$(h_w)_{1,3,1} = 50$
$P_1 = 1$	$(B'_g)_{2,1} = 2$	$(B'_c)_{5,2,1} = 6$	$T_{5,2,1} = 1200$	$(h_w)_{5,2,1} = 550$
$P_1 = 1$	$(B'_g)_{2,1} = 2$	$(B'_c)_{4,2,1} = 4$	$T_{4,2,1} = 900$	$(h_w)_{4,2,1} = 300$
$P_1 = 1$	$(B'_g)_{2,1} = 2$	$(B'_c)_{3,2,1} = 2$	$T_{3,2,1} = 700$	$(h_w)_{3,2,1} = 50$
$P_1 = 1$	$(B'_g)_{2,1} = 2$	$(B'_c)_{2,2,1} = 0$	$T_{2,2,1} = 700$	$(h_w)_{2,2,1} = 200$
$P_1 = 1$	$(B'_g)_{2,1} = 2$	$(B'_c)_{1,2,1} = 0$	$T_{1,2,1} = 500$	$(h_w)_{1,2,1} = -50$
$P_1 = 1$	$(B'_g)_{1,1} = 0$	$(B'_c)_{5,1,1} = 7$	$T_{5,1,1} = 1300$	$(h_w)_{5,1,1} = 500$
$P_1 = 1$	$(B'_g)_{1,1} = 0$	$(B'_c)_{4,1,1} = 5$	$T_{4,1,1} = 900$	$(h_w)_{4,1,1} = 200$
$P_1 = 1$	$(B'_g)_{1,1} = 0$	$(B'_c)_{3,1,1} = 2$	$T_{3,1,1} = 600$	$(h_w)_{3,1,1} = -50$
$P_1 = 1$	$(B'_g)_{1,1} = 0$	$(B'_c)_{2,1,1} = 0$	$T_{2,1,1} = 600$	$(h_w)_{2,1,1} = 100$
$P_1 = 1$	$(B'_g)_{1,1} = 0$	$(B'_c)_{1,1,1} = 0$	$T_{1,1,1} = 500$	$(h_w)_{1,1,1} = -200$

where from right to left the subscripts denote an entry's association with a given pressure, dimensionless pyrolysis gas blowing rate, and wall temperature. Therefore $(B'_c)_{k,j,i}$ is the dimensionless char ablation rate entry associated with the k th temperature entry in the j th dimensionless gas ablation rate sub-table in the i th pressure table. This particular pressure table, which is only an example and does not describe any certain ablator/gas interaction, has 3 gas blowing rate sub-tables and 5 temperature entries within each of those sub-tables. In general, each pressure table includes a $(B'_g)_{j,i} = 0$ (no pyrolysis gas rejection) sub-table, and each gas blowing rate sub-table includes a series of $(B'_c)_{k,j,i} = 0$ (non-ablating) entries.

Typically there is a pair of consecutive entries within a given gas blowing rate sub-table that contains one ablating entry ($B'_c > 0$) and one non-ablating entry ($B'_c = 0$) that have an identical temperature value which represents the minimum ablation temperature at the given pressure and gas blowing rate. From the thermochemistry data, the code generates an auxiliary table containing the minimum ablation temperature

as a function of pressure and dimensionless gas blowing rate.

$$T_{abl_{\min}} = T_{abl_{\min}}(P, B'_g(T, \dot{s}))$$

In order to extract information from a thermochemistry table, the pressure and dimensionless gas ablation rate must be known in addition to one of the other three quantities. CMA and SODDIT use the dimensionless char ablation rate as the third independent variable for ablation problems and the wall temperature as the third independent variable for non-ablating problems and non-ablating intervals of ablation problems when the dimensionless char ablation rate is zero. The code developed during this study uses the wall temperature as the third independent variable for all intervals of all problems.

Sample Thermochemistry Data

In order to clarify the thermochemistry data organization described in the previous section, thermochemical data for carbon in an air environment is presented in more detail. The wall gas enthalpy is given as a function of temperature with pressure as a parameter in Figure C.1.

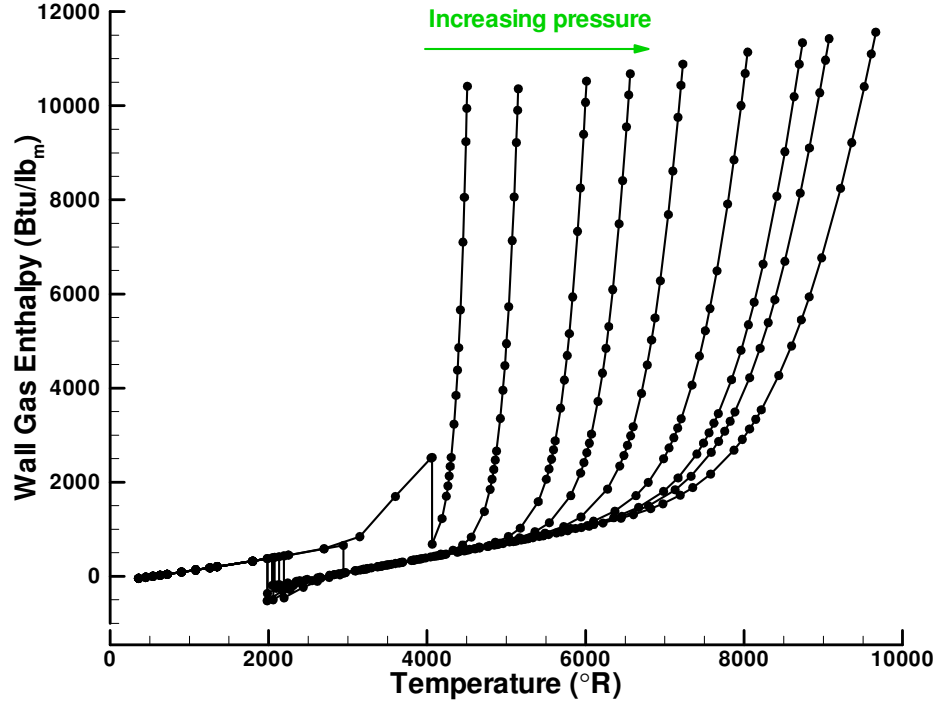


Figure C.1: Carbon-in-air wall gas enthalpy functions with pressure as a parameter.

Since carbon-carbon is a non-decomposing ablator, there is no pyrolysis gas blowing rate dependence, which gives

$$B'_c = B'_c(P, T)$$

$$h_w = h_w(P, T)$$

and

$$T_{abl_{\min}} = T_{abl_{\min}}(P)$$

Consequently, the family of curves in Figure C.1 shows all of the gas enthalpy data (one curve per pressure value) for carbon-carbon, but a decomposing ablator has multiple gas enthalpy curves for each pressure value (one for each pyrolysis gas blowing rate). The same is true for the dimensionless ablation rate which is shown in Figure C.2.

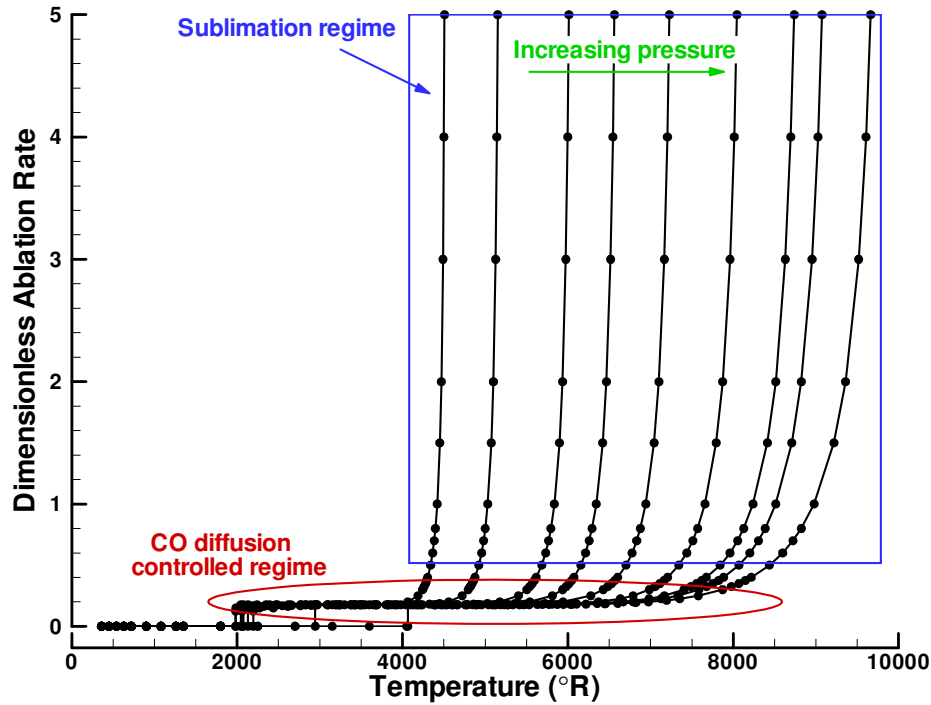
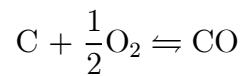
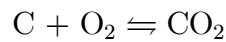


Figure C.2: Carbon-in-air ablation rate functions with pressure as a parameter.

The thermochemical ablation of carbonaceous solids is characterized by two distinct regimes. The ablation rate in the diffusion controlled regime is limited by the availability of oxygen at the surface to participate in the oxidation reactions

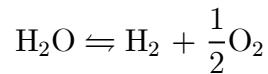
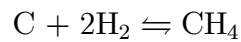
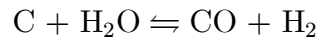
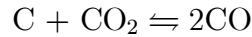


and



where the creation of carbon-monoxide (CO) is dominant at high temperatures. If just the carbon monoxide reaction is considered, then a thermochemical analysis reveals that the dimensionless ablation rate is approximately 0.174, and this is the value at which the family of curves is coincident in the CO diffusion controlled regime in Figure C.2. If more data points were considered at the lower ablation rate values,

then the data would reveal another plateau of coincident curves in the CO_2 diffusion controlled regime. As the temperature increases, other chemical reactions become more common and deviation from the diffusion controlled limit is evident. The other possible reactions include



and a more detailed discussion of the carbon thermochemical ablation processes is explained by Kays et al.[33] and Welsh and Chung[48]. At extremely high temperatures, mass loss due to sublimation effects becomes dominant over chemical reactions, and for a given pressure, the maximum allowable temperature is limited to the sublimation temperature.

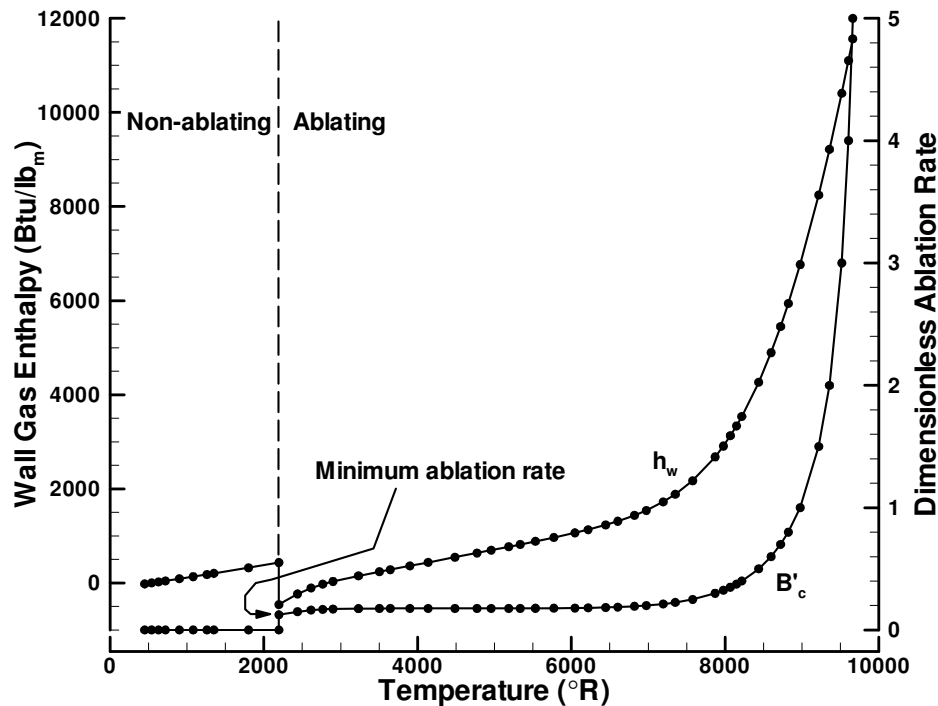


Figure C.3: Carbon-in-air ablation rate and wall gas enthalpy for a single pressure.

Figure C.3 shows both the gas enthalpy and ablation rate functions for a given pressure. The ablating/non-ablating boundary is pointed out to show that the data contains two entries at the minimum ablation temperature. In addition, all of the dimensionless ablation rate curves in Figure C.2 coincide in the CO diffusion controlled regime and the assumed minimum ablation rate is pointed out in Figure C.3. Note that the discontinuities in the enthalpy functions are results of the solution procedure in the program used to generate the thermochemical data. The discontinuities are nonphysical and a better approach to generating this information is needed. However, using erroneous data does not effect the code's ability to demonstrate the model.

Three-Dimensional Interpolation

When dealing with tabulated functions, it is necessary to use interpolation to determine dependent variable values and their derivatives with respect to the independent variables. Since, in general, the thermochemistry tables provide

$$B'_c = B'_c(P, T, B'_g)$$

and

$$h_w = h_w(P, T, B'_g)$$

a three-dimensional interpolation is necessary to calculate the desired information.

The following outline provides step-by-step instructions for performing a three-dimensional interpolation to find wall enthalpy, dimensionless ablation rate, and their derivatives with respect to wall temperature and dimensionless gas ablation rate.

Known going into routine: P , B'_g , and T

Calculated in routine: B'_c , h_w , $\left. \frac{\partial B'_c}{\partial T} \right|_{B'_g}$, $\left. \frac{\partial B'_c}{\partial B'_g} \right|_T$, $\left. \frac{\partial h_w}{\partial T} \right|_{B'_g}$, and $\left. \frac{\partial h_w}{\partial B'_g} \right|_T$

Finding B'_c and h_w

Since the pressure difference between consecutive tables can be as large as an order of magnitude, it is often more desirable to perform linear interpolation on $\ln(P)$ rather than P , and the code allows for both options. Linear interpolation on $\ln(P)$ is presented in the example, but the procedure is the same if the independent variable is chosen to be P .

1. Find $\ln(P_i)$ and $\ln(P_{i+1})$ such that $\ln(P_i) \leq \ln(P) \leq \ln(P_{i+1})$
2. For $\ln(P_i)$
 - a. Find $(B'_g)_{j,i}$ and $(B'_g)_{j+1,i}$ such that $(B'_g)_{j,i} \leq B'_g \leq (B'_g)_{j+1,i}$
 - b. For $(B'_g)_{j,i}$
 - Find $T_{k,j,i}$ and $T_{k+1,j,i}$ such that $T_{k,j,i} \leq T \leq T_{k+1,j,i}$
 - Calculate the interpolation factor $(f_{j,i})$ according to

$$f_{j,i} = \frac{T - T_{k,j,i}}{T_{k+1,j,i} - T_{k,j,i}} \quad (\text{C.4})$$

- $(B'_c)_{j,i}$ and $(h_w)_{j,i}$ can now be determined from

$$(B'_c)_{j,i} = f_{j,i} (B'_c)_{k+1,j,i} + (1 - f_{j,i}) (B'_c)_{k,j,i} \quad (\text{C.5})$$

and

$$(h_w)_{j,i} = f_{j,i} (h_w)_{k+1,j,i} + (1 - f_{j,i}) (h_w)_{k,j,i} \quad (\text{C.6})$$

- c. Similarly for $(B'_g)_{j+1,i}$
 - Find $T_{k,j+1,i}$ and $T_{k+1,j+1,i}$ such that $T_{k,j+1,i} \leq T \leq T_{k+1,j+1,i}$
 - Calculate the interpolation factor $(f_{j+1,i})$ according to

$$f_{j+1,i} = \frac{T - T_{k,j+1,i}}{T_{k+1,j+1,i} - T_{k,j+1,i}} \quad (\text{C.7})$$

- $(B'_c)_{j+1,i}$ and $(h_w)_{j+1,i}$ can now be determined from

$$(B'_c)_{j+1,i} = f_{j+1,i} (B'_c)_{k+1,j+1,i} + (1 - f_{j+1,i}) (B'_c)_{k,j+1,i} \quad (\text{C.8})$$

and

$$(h_w)_{j+1,i} = f_{j+1,i} (h_w)_{k+1,j+1,i} + (1 - f_{j+1,i}) (h_w)_{k,j+1,i} \quad (\text{C.9})$$

- d.** Calculate the interpolation factor (f_i) according to

$$f_i = \frac{B'_g - (B'_g)_{j,i}}{(B'_g)_{j+1,i} - (B'_g)_{j,i}} \quad (\text{C.10})$$

- e.** $(B'_c)_i$ and $(h_w)_i$ can now be determined from

$$(B'_c)_i = f_i (B'_c)_{j+1,i} + (1 - f_i) (B'_c)_{j,i} \quad (\text{C.11})$$

and

$$(h_w)_i = f_i (h_w)_{j+1,i} + (1 - f_i) (h_w)_{j,i} \quad (\text{C.12})$$

3. Similarly for $\ln(P_{i+1})$

- a.** Find $(B'_g)_{j,i+1}$ and $(B'_g)_{j+1,i+1}$ such that $(B'_g)_{j,i+1} \leq B'_g \leq (B'_g)_{j+1,i+1}$

- b.** For $(B'_g)_{j,i+1}$

- Find $T_{k,j,i+1}$ and $T_{k+1,j,i+1}$ such that $T_{k,j,i+1} \leq T \leq T_{k+1,j,i+1}$
- Calculate the interpolation factor $(f_{j,i+1})$ according to

$$f_{j,i+1} = \frac{T - T_{k,j,i+1}}{T_{k+1,j,i+1} - T_{k,j,i+1}} \quad (\text{C.13})$$

- $(B'_c)_{j,i+1}$ and $(h_w)_{j,i+1}$ can now be determined from

$$(B'_c)_{j,i+1} = f_{j,i+1} (B'_c)_{k+1,j,i+1} + (1 - f_{j,i+1}) (B'_c)_{k,j,i+1} \quad (\text{C.14})$$

and

$$(h_w)_{j,i+1} = f_{j,i+1} (h_w)_{k+1,j,i+1} + (1 - f_{j,i+1}) (h_w)_{k,j,i+1} \quad (\text{C.15})$$

c. Similarly for $(B'_g)_{j+1,i+1}$

- Find $T_{k,j+1,i+1}$ and $T_{k+1,j+1,i+1}$ such that $T_{k,j+1,i+1} \leq T \leq T_{k+1,j+1,i+1}$
- Calculate the interpolation factor $(f_{j+1,i+1})$ according to

$$f_{j+1,i+1} = \frac{T - T_{k,j+1,i+1}}{T_{k+1,j+1,i+1} - T_{k,j+1,i+1}} \quad (\text{C.16})$$

- $(B'_c)_{j+1,i+1}$ and $(h_w)_{j+1,i+1}$ can now be determined from

$$(B'_c)_{j+1,i+1} = f_{j+1,i+1} (B'_c)_{k+1,j+1,i+1} + (1 - f_{j+1,i+1}) (B'_c)_{k,j+1,i+1} \quad (\text{C.17})$$

and

$$(h_w)_{j+1,i+1} = f_{j+1,i+1} (h_w)_{k+1,j+1,i+1} + (1 - f_{j+1,i+1}) (h_w)_{k,j+1,i+1} \quad (\text{C.18})$$

d. Calculate the interpolation factor (f_{i+1}) according to

$$f_{i+1} = \frac{B'_g - (B'_g)_{j,i+1}}{(B'_g)_{j+1,i+1} - (B'_g)_{j,i+1}} \quad (\text{C.19})$$

e. $(B'_c)_{i+1}$ and $(h_w)_{i+1}$ can now be determined from

$$(B'_c)_{i+1} = f_i (B'_c)_{j+1,i+1} + (1 - f_{i+1}) (B'_c)_{j,i+1} \quad (\text{C.20})$$

and

$$(h_w)_{i+1} = f_{i+1} (h_w)_{j+1,i+1} + (1 - f_{i+1}) (h_w)_{j,i+1} \quad (\text{C.21})$$

4. Calculate the interpolation factor (f) according to

$$f = \frac{\ln(P) - \ln(P_i)}{\ln(P_{i+1}) - \ln(P_i)} \quad (\text{C.22})$$

5. Finally, B'_c and h_w can now be determined from

$$B'_c = f (B'_c)_{i+1} + (1 - f) (B'_c)_i \quad (\text{C.23})$$

and

$$h_w = f (h_w)_{i+1} + (1 - f) (h_w)_i \quad (\text{C.24})$$

Finding $\left. \frac{\partial B'_c}{\partial T} \right|_{B'_g}, \left. \frac{\partial B'_c}{\partial B'_g} \right|_T, \left. \frac{\partial h_w}{\partial T} \right|_{B'_g},$ and $\left. \frac{\partial h_w}{\partial B'_g} \right|_T$

$\left. \frac{\partial}{\partial T} \right|_{B'_g}$ of either quantity is determined by weighting finite-difference derivatives according to

$$\left. \frac{\partial}{\partial T} \right|_{B'_g} = f \left. \frac{\partial}{\partial T} \right|_{i+1} + (1-f) \left. \frac{\partial}{\partial T} \right|_i \quad (\text{C.25})$$

where

$$\left. \frac{\partial}{\partial T} \right|_i = f_i \left. \frac{\partial}{\partial T} \right|_{j+1,i} + (1-f_i) \left. \frac{\partial}{\partial T} \right|_{j,i} \quad (\text{C.26})$$

and

$$\left. \frac{\partial}{\partial T} \right|_{i+1} = f_{i+1} \left. \frac{\partial}{\partial T} \right|_{j+1,i+1} + (1-f_{i+1}) \left. \frac{\partial}{\partial T} \right|_{j,i+1} \quad (\text{C.27})$$

The remaining derivatives are finite differences given by

$$\left. \frac{\partial ()}{\partial T} \right|_{j+1,i} = \frac{()_{k+1,j+1,i} - ()_{k,j+1,i}}{T_{k+1,j+1,i} - T_{k,j+1,i}} \quad (\text{C.28})$$

$$\left. \frac{\partial ()}{\partial T} \right|_{j,i} = \frac{()_{k+1,j,i} - ()_{k,j,i}}{T_{k+1,j,i} - T_{k,j,i}} \quad (\text{C.29})$$

$$\left. \frac{\partial ()}{\partial T} \right|_{j+1,i+1} = \frac{()_{k+1,j+1,i+1} - ()_{k,j+1,i+1}}{T_{k+1,j+1,i+1} - T_{k,j+1,i+1}} \quad (\text{C.30})$$

and

$$\left. \frac{\partial ()}{\partial T} \right|_{j,i+1} = \frac{()_{k+1,j,i+1} - ()_{k,j,i+1}}{T_{k+1,j,i+1} - T_{k,j,i+1}} \quad (\text{C.31})$$

f , f_i , and f_{i+1} can be found from Eqs. C.22, C.10, and C.19 respectively.

$\left. \frac{\partial}{\partial B'_g} \right|_T$ for either quantity is determined according to

$$\left. \frac{\partial}{\partial B'_g} \right|_T = f \left. \frac{\partial}{\partial B'_g} \right|_{i+1} + (1-f) \left. \frac{\partial}{\partial B'_g} \right|_i \quad (\text{C.32})$$

where

$$\left. \frac{\partial ()}{\partial B'_g} \right|_i = \frac{()_{j+1,i} - ()_{j,i}}{(B'_g)_{j+1,i} - (B'_g)_{j,i}} \quad (\text{C.33})$$

and

$$\left. \frac{\partial ()}{\partial B'_g} \right|_{i+1} = \frac{()_{j+1,i+1} - ()_{j,i+1}}{(B'_g)_{j+1,i+1} - (B'_g)_{j,i+1}} \quad (\text{C.34})$$

Appendix D: Carbon-Phenolic Material Properties

The following tables present the material properties associated with carbon-phenolic and its pyrolysis gases that was used for the calculations in Section 8.8. It is important to note that the properties used in the calculations were gathered from various sources, and therefore they may not all apply to the same carbon-phenolic composite. Since the purpose of the calculations is to demonstrate and verify the computational model and not to make predictive calculations for the design of a system, it is acceptable to use slightly inconsistent data. In addition, the carbon-phenolic-in-air surface thermochemistry data was generated by ACE and is excluded from this document due to length.

Table D.1: Decomposition kinetics for carbon-phenolic[49].

	A	B	C
Virgin density (lb_m/ft^3)	60.75	20.25	97.4
Char density (lb_m/ft^3)	32.4	0.0	97.4
Pre-exponential factor ($1/\text{s}$)	4.48×10^9	1.40×10^4	—
Reaction order	3.0	3.0	—
Scaled activation energy, E/R ($^\circ\text{R}$)	3.68×10^4	1.54×10^4	—
Minimum reaction temperature ($^\circ\text{R}$)	600.0	1000.0	—

Table D.2: Heats of formation and initial resin mass fraction for carbon-phenolic.⁵

Virgin heat of formation (Btu/lb_m)	−363.0
Char heat of formation (Btu/lb_m)	0.0
Pyrolysis gas heat of formation (Btu/lb_m)	0.0
Resin volume fraction in virgin composite, Γ in Eq. 2.16	0.372

⁵These carbon-phenolic material properties come from personal communication with Don Potter and David Kuntz of Sandia National Laboratories.

Table D.3: Thermophysical properties of virgin carbon-phenolic.⁶

Temperature (°R)	Specific Heat (Btu/lb _m -°R)	Conductivity (Btu/ft ² -s)	Emissivity
460.0	0.24	9.5×10^{-5}	0.85
760.0	0.36	1.30×10^{-4}	0.85
960.0	0.48	1.42×10^{-4}	0.85
1460.0	0.50	1.78×10^{-4}	0.85
1960.0	0.50	2.16×10^{-4}	0.85
2460.0	0.50	2.60×10^{-4}	0.85
2960.0	0.50	2.91×10^{-4}	0.85
3460.0	0.50	3.66×10^{-4}	0.85
5000.0	0.50	4.55×10^{-4}	0.85
7000.0	0.50	4.55×10^{-4}	0.85

Table D.4: Thermophysical properties of char carbon-phenolic.⁶

Temperature (°R)	Specific Heat (Btu/lb _m -°R)	Conductivity (Btu/ft ² -s)	Emissivity
500.0	0.05	1.0×10^{-4}	0.85
860.0	0.0602	1.01×10^{-4}	0.85
1060.0	0.0794	1.05×10^{-4}	0.85
2000.0	0.274	1.625×10^{-4}	0.85
3000.0	0.341	2.18×10^{-4}	0.85
4000.0	0.3715	2.75×10^{-4}	0.85
5000.0	0.384	3.33×10^{-4}	0.85
6000.0	0.400	3.89×10^{-4}	0.85

⁶These carbon-phenolic material properties come from personal communication with Don Potter and David Kuntz of Sandia National Laboratories.

Table D.5: Porosity and permeability of a carbon composite[15].⁷

Extent of Reaction	Porosity	Permeability (ft ²)
0.0	0.01	5.38×10^{-19}
0.25	0.095	3.23×10^{-17}
0.5	0.18	3.23×10^{-16}
0.75	0.265	2.15×10^{-15}
1.0	0.35	1.08×10^{-12}

Table D.6: Carbon-phenolic pyrolysis gas enthalpy at $P = 1$ atm generated by ACE.

Temperature (°R)	Enthalpy (Btu/lb _m)
900.0	−2941.0
1800.0	−1891.0
2700.0	−540.0
3600.0	450.0
4500.0	1350.0
5400.0	2250.0
6300.0	5771.0
7200.0	9151.0
8100.0	14241.0
9000.0	24926.0

Table D.7: Carbon-phenolic pyrolysis gas molecular weight[13].⁸

Temperature (°R)	Molecular Weight (lb _m /lb _{mole})
1210.0	32.0
1460.0	26.0

⁷The porosity and permeability data is representative of a general reinforced carbon composite, and does not specifically apply to any certain carbon-phenolic composite.

⁸It is assumed that the composition of the pyrolysis gases is only changing between the temperatures given in the table. Therefore the pyrolysis gas molecular weight is constant outside the boundaries of the table.

Table D.8: Carbon-phenolic pyrolysis gas viscosity[13].

Temperature (°R)	Viscosity (lb _m /ft-s)
500.0	3.366×10^{-7}
720.0	4.127×10^{-7}
2880.0	9.988×10^{-7}
3600.0	1.151×10^{-6}