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NUMERICAL SIMULATION OF TRANSIENT COMBUSTION PROCESS IN PULSE DETONATION WAVE ENGINE

The members of the Committee approve the doctoral dissertation of Hyungwon Kim

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[Signatures]
NUMERICAL SIMULATION OF TRANSIENT
COMBUSTION PROCESS IN PULSE
DETONATION WAVE ENGINE

by

HYUNGWON KIM

Presented to the Faculty of the Graduate School of
The University of Texas at Arlington in Partial Fulfillment
of the Requirements
for the Degree of

DOCTOR OF PHILOSOPHY

THE UNIVERSITY OF TEXAS AT ARLINGTON
August 1999
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wife HaeRan. I would like to share the joy of this accomplishment with my proud son SangYup and lovely daughter SooYeon.

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June 29, 1999
ABSTRACT

NUMERICAL SIMULATION OF TRANSIENT COMBUSTION PROCESS IN PULSE DETONATION WAVE ENGINE

Publication No. ________

Hyungwon Kim, Ph.D.

The University of Texas at Arlington, 1999

Supervising Professor: Dale A. Anderson

A two-dimensional time-accurate numerical model to simulate the transient combustion process in a pulse detonation engine is presented in this dissertation. Inviscid, non-heat conducting flow equations are fully coupled with a finite-rate chemistry model for a general description of chemical non-equilibrium, and the vibrational energy equation based on a two-temperature model is used to account for possible thermal non-equilibrium. The governing equations are discretized using the finite-volume formulation to ensure conservation and to allow a correct treatment of discontinuities. A time-accurate solution is obtained from the Runge–Kutta integration scheme, with a point-implicit treatment of the source terms. Roe's flux-difference splitting scheme extended to non-equilibrium flow is implemented for the cell face fluxes, and the MUSCL approach is used for higher-order spatial accuracy. For the purpose of constructing an efficient numerical tool, while maintaining a reasonable accuracy, a two-step global model has been selected and validated for a hydrogen–air mixture. The inherent stiffness in the chemical reaction model is properly taken care of by the point-implicit
treatment of source terms, together with the application of a Local Ignition Averaging Model to each mesh where ignition starts. The calculated results from the present model are compared with the theoretical Chapman–Jouguet and experimental data. Excellent agreement in the detonation wave velocities as well as detonation pressure, density, and temperature are observed. A series of calculations is also performed using different orders of numerical schemes in spatial and temporal accuracy and different mesh sizes to select a proper scheme and a mesh size to provide adequate resolution of the physical process. Detonation initiation is extensively studied in this dissertation. Criteria for direct initiation are presented from the observation of the effect of initial hot spot conditions on the development of a detonation wave. A simulation of a shock-induced detonation experiment is also performed to provide a validation of the present model in the unsteady propagation of a detonation wave and its interactions with the boundaries as well as other waves.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>iii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>v</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>ix</td>
</tr>
<tr>
<td>LIST OF ABBREVIATIONS</td>
<td>xiii</td>
</tr>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Review of Detonation Physics</td>
<td>2</td>
</tr>
<tr>
<td>1.2 Review of Computational Studies</td>
<td>4</td>
</tr>
<tr>
<td>1.3 The Scope of Current Work</td>
<td>6</td>
</tr>
<tr>
<td>2. MATHEMATICAL FORMULATION</td>
<td>8</td>
</tr>
<tr>
<td>2.1 Governing Equations</td>
<td>10</td>
</tr>
<tr>
<td>2.2 Thermodynamic Properties</td>
<td>13</td>
</tr>
<tr>
<td>2.3 Chemical Kinetics Model</td>
<td>18</td>
</tr>
<tr>
<td>2.4 Vibrational Energy Relaxation</td>
<td>20</td>
</tr>
<tr>
<td>3. NUMERICAL FORMULATION</td>
<td>22</td>
</tr>
<tr>
<td>3.1 Finite-Volume Formulation</td>
<td>23</td>
</tr>
<tr>
<td>3.2 Point Implicit Time Integration</td>
<td>25</td>
</tr>
<tr>
<td>3.3 Flux-Difference Split Algorithm</td>
<td>27</td>
</tr>
</tbody>
</table>
**LIST OF FIGURES**

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Vibrational energy near reference temperature</td>
<td>17</td>
</tr>
<tr>
<td>4.1</td>
<td>Species mass fraction history from chemical kinetics</td>
<td>38</td>
</tr>
<tr>
<td>4.2</td>
<td>Species mole fraction history from the flow solver</td>
<td>40</td>
</tr>
<tr>
<td>4.3</td>
<td>Time evolution of detonation pressure profiles</td>
<td>42</td>
</tr>
<tr>
<td>4.4</td>
<td>Time evolution of detonation density profiles</td>
<td>42</td>
</tr>
<tr>
<td>4.5</td>
<td>Time evolution of detonation temperature profiles</td>
<td>43</td>
</tr>
<tr>
<td>4.6</td>
<td>Time evolution of particle velocity profiles</td>
<td>43</td>
</tr>
<tr>
<td>4.7</td>
<td>Profile of typical detonation wave</td>
<td>45</td>
</tr>
<tr>
<td>4.8</td>
<td>Profile of typical detonation wave front</td>
<td>45</td>
</tr>
<tr>
<td>4.9</td>
<td>Downstream Mach number and convergence to CJ state</td>
<td>46</td>
</tr>
<tr>
<td>4.10</td>
<td>Wave profiles from different order of accuracy</td>
<td>47</td>
</tr>
<tr>
<td>4.11</td>
<td>Detonation velocities from different order of accuracy</td>
<td>48</td>
</tr>
<tr>
<td>4.12</td>
<td>Detonation pressures from different order of accuracy</td>
<td>48</td>
</tr>
<tr>
<td>4.13</td>
<td>Detonation densities from different order of accuracy</td>
<td>49</td>
</tr>
<tr>
<td>4.14</td>
<td>Detonation temperatures from different order of accuracy</td>
<td>49</td>
</tr>
<tr>
<td>4.15</td>
<td>Wave profiles from different mesh sizes</td>
<td>51</td>
</tr>
<tr>
<td>4.16</td>
<td>Detonation velocities from different mesh sizes</td>
<td>51</td>
</tr>
<tr>
<td>4.17</td>
<td>Detonation pressures from different mesh sizes</td>
<td>52</td>
</tr>
<tr>
<td>4.18</td>
<td>Detonation densities from different mesh sizes</td>
<td>52</td>
</tr>
<tr>
<td>4.19</td>
<td>Detonation temperatures from different mesh sizes</td>
<td>53</td>
</tr>
</tbody>
</table>
5.10 Wave profiles of EHS of $T=3000\text{K}, p=100\text{atm}$ ........................................ 75
5.11 Detonation velocities with varying hot spot states ................................................. 76
5.12 Detonation pressures with varying hot spot states ............................................... 76
5.13 Detonation densities with varying hot spot states ................................................. 77
5.14 Detonation temperatures with varying hot spot states .......................................... 77
5.15 Downstream Mach No. with varying hot spot states ............................................. 78
5.16 Pressure build-up for EHS of $T=2000\text{K}, p=10\text{atm}$ ....................................... 79
5.17 Temperature build-up for EHS of $T=2000\text{K}, p=10\text{atm}$ .............................. 80
5.18 Pressure build-up for EHS of $T=1500\text{K}, p=10\text{atm}$ ....................................... 81
5.19 Temperature build-up for EHS of $T=1500\text{K}, p=10\text{atm}$ .............................. 81
5.20 Successful initiation for RHS of $T=1500\text{K}, p=10\text{atm}$ ............................... 83
5.21 Unsuccessful initiation for RHS of $T=1500\text{K}, p=5\text{atm}$ .............................. 84
5.22 Critical volume of hot spot ................................................................. 85
5.23 Critical level of energy deposition ............................................................... 86
5.24 Pressure profiles when $p_1 = 1 \text{ atm}$ .......................................................... 87
5.25 Temperature profiles when $p_1 = 1 \text{ atm}$ ....................................................... 87
5.26 Pressure profiles when $p_1 = 2 \text{ atm}$ .......................................................... 88
5.27 Temperature profiles when $p_1 = 2 \text{ atm}$ ....................................................... 89
5.28 Initiation by reflection for energy deposition of 1.75 J ................................... 91
5.29 Early pressure build-up by reflecting waves ....................................................... 92
5.30 Pressure development in critical initiation of 1.75 J ...................................... 92
5.31 Initiation by reflection for energy deposition of 1.24 J ................................... 94
5.32 Pressure development in critical initiation of 1.24 J ...................................... 95
5.33 Temperature development in critical initiation of 1.24 J ................................... 95

xi
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>The schematic of the UT Arlington experiment</td>
<td>97</td>
</tr>
<tr>
<td>6.2</td>
<td>Pressure measurements at station 4 and 5 for test No.14</td>
<td>98</td>
</tr>
<tr>
<td>6.3</td>
<td>Pressure measurements at station 4 and 5 for test No.23</td>
<td>98</td>
</tr>
<tr>
<td>6.4</td>
<td>Calculated pressure histories at station 4 and 5</td>
<td>100</td>
</tr>
<tr>
<td>6.5</td>
<td>Wave interactions in shock-induced detonation tube</td>
<td>101</td>
</tr>
</tbody>
</table>
LIST OF ABBREVIATIONS

$A_k^s$ curve fit constant for evaluating $C_p^s$
$A_{f,r}$ pre-exponential term for evaluating $K_{f,r}$
$A_{c,r}$ pre-exponential term for evaluating $K_{c,r}$
$A_{s,j}$ constant for determining $\tau_{s,j}$
a frozen speed of sound
$C_p^s$ specific heat at constant pressure for species $s$
$C_{p,q}$ specific heat at constant pressure for mixture for energy mode $q$
$C_{p,r}^s$ specific heat at constant pressure for species $s$ for rotational energy
$C_{p,t}^s$ specific heat at constant pressure for species $s$ for translational energy
$C_{p,v}^s$ specific heat at constant pressure for species $s$ for vibrational energy
$C_v^s$ specific heat at constant volume for species $s$
$C_{v,q}$ specific heat at constant volume for mixture for energy mode $q$
$C_{v,r}^s$ specific heat at constant volume for species $s$ for rotational energy
$C_{v,t}^s$ specific heat at constant volume for species $s$ for translational energy
$C_{v,v}^s$ specific heat at constant volume for species $s$ for vibrational energy
$D_s$ dissociation energy per unit mass of molecule $s$
$E$ total energy per unit mass of mixture
$E_i$ eigenvectors
$E_s$ total energy per unit mass of species $s$
$E_{f,r}$ activation energy for forward reaction $r$
\( e \quad \text{internal energy per unit mass of mixture} \\
\( e_{eq,s} \quad \text{equilibrium portion of internal energy per unit mass of species } s \\
\( e_s \quad \text{internal energy per unit mass of species } s \\
\( e_{s,o} \quad \text{energy of formation of species } s \\
\( e_v \quad \text{vibrational energy per unit mass of mixture} \\
\( e_{v,s} \quad \text{vibrational energy per unit mass of species } s \\
\( e_{v,s}^* \quad \text{vibrational energy per unit mass of species } s \text{ evaluated at temperature } T \\
\( F \quad \text{convective flux vector in } x\text{-direction} \\
\( G \quad \text{convective flux vector in } y\text{-direction} \\
\( H \quad \text{total enthalpy per unit mass of mixture} \\
\( h_s \quad \text{enthalpy per unit mass of species } s \\
\( h_{v,s} \quad \text{vibrational enthalpy per unit mass of species } s \\
\( I \quad \text{identity matrix} \\
\( K_{b,r} \quad \text{backward reaction rate coefficient for reaction } r \\
\( K_{c,r} \quad \text{equilibrium constant for reaction } r \\
\( K_{f,r} \quad \text{forward reaction rate coefficient for reaction } r \\
\( M_s \quad \text{molecular weight of species } s \\
\( N_r \quad \text{number of reactions in chemical kinetic model} \\
\( N_s \quad \text{number of species in the chemical kinetic model} \\
\( n_j \quad \text{number density of species } s \\
\( P_{si} \quad \text{momentum transfer rate of species } s \text{ in the } i \text{ direction} \\
\( p \quad \text{static pressure} \\
\( p_s \quad \text{partial pressure due to species } s \\
\( Q_s \quad \text{energy transfer rate of species } s \)
$Q_{v,s}$  vibrational energy exchange rate of species $s$
$q$  any primitive variable
$\tilde{R}$  universal gas constant, 8314.3 J/kg-mole-K
$R_{b,r}$  backward reaction rate for reaction $r$
$R_{f,r}$  forward reaction rate for reaction $r$
$R_i$  gas constant of species $i$
$\bar{R}$  mixture gas constant
$S$  vector of source terms
$T$  translational-rotational temperature
$T_{ref}$  reference temperature for thermodynamic relation
$T_v$  vibrational temperature
$t$  time
$U$  vector of conserved variables
$u$  velocity component in $x$-direction
$u_{Dsi}$  diffusion velocity of species $s$ in the $i$ direction
$u_{si}$  velocity of species $s$ in the $i$ direction
$v$  velocity in $y$-direction
$w_s$  mass rate of production of species $s$ per unit volume
$w_v$  vibrational energy production rate
$\alpha_i$  wave strengths
$\alpha_{s,r}$  Stoichiometric coefficient in forward reaction
$\beta_{s,r}$  Stoichiometric coefficient in backward reaction
$\tilde{\gamma}$  ratio of specific heats of equilibrium portion of energy
$\mu_{sj}$  reduced molecular weights of species $s$ and $j$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>mixture density</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>density of species $s$</td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>eigenvalues</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>cell face length</td>
</tr>
<tr>
<td>$&lt; \tau_s &gt;$</td>
<td>averaged Landau-Teller relaxation time of species $s$</td>
</tr>
<tr>
<td>$\tau_{sj}$</td>
<td>vibrational relaxation time of species $s$ caused by species $s$</td>
</tr>
<tr>
<td>$\tau_v$</td>
<td>number weighted average vibrational relaxation time for mixture</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>cell area</td>
</tr>
</tbody>
</table>
CHAPTER 1

INTRODUCTION

The Pulse detonation engine (PDE) has received considerable interest in recent years due to its potential advantages in performance and inherent simplicity over current propulsion concepts. The PDE uses detonation waves that are initiated repeatedly at either end of a detonation chamber and propagate through a fuel—oxidizer mixture with supersonic speed to produce high pressure which is the main thrusting mechanism. This rapid detonation process permits the PDE to achieve nearly constant volume combustion resulting in better efficiencies compared with the usual constant pressure Brayton cycle. In addition, the PDE does not necessarily need a compressor or a turbine, and this makes the engine mechanically simple and cost effective. Furthermore, PDE’s can be operated in a wide range of flight speeds, from low subsonic to high supersonic, regardless of the engine size and shape [1]—[4].

Conceptually there seems to be no doubt that the PDE will be a good alternative to conventional engines, as well as a revolutionary propulsion system for future space transportation. However, there are still many problems to be solved and many complex phenomena to be understood for the PDE to be operable in a real world. Detonation initiation, the PDE cycle analysis and optimization are included among the problems [5, 6].

The PDE can be classified as an unsteady propulsion engine which operates in an intermittent manner governed by a cycle frequency. The cycle frequency of the PDE is defined as the inverse of the time required to complete a full detonation cycle. One
full cycle is comprised of several distinct processes: (a) filling the chamber with a fresh fuel/oxidizer mixture, (b) initiating detonation, (c) propagation of detonation waves, and (d) expansion of burned gases to reduce the chamber pressure to the refill level. All of these processes are interdependent, and the interaction and timing are crucial to multi-cycle engine efficiency. The wide range of time scales in the PDE cycle as well as the requirement to capture the time-accurate motion of detonation waves pose important challenges for any computational approach [5]. Time-accurate computational fluid dynamics (CFD) methods can be used to perform cycle analysis and performance optimization of the PDE from the simulations of the corresponding flow fields with variations in design parameters.

This dissertation presents an unsteady numerical simulation model for these purposes. The key words here are accuracy and efficiency. The object of this study includes the construction of a basic CFD module that is efficient to be used for design parametric studies, while maintaining sufficient accuracy to simulate details like detonation initiation.

In this chapter, the relevant physics of detonation is reviewed shortly. The previous computational research is briefly summarized, followed by a presentation of the scope of the current work.

1.1 Review of Detonation Physics

In an explosive gas mixture, waves can be propagated in the form of a chemical reaction [7]. There are two essentially different conditions under which propagation of the reaction is possible. One is deflagration that is the most common type of combustion. Since a deflagration flame speed is the order of one or more meters per second for most
cases, a pressure wave which propagates with the speed of sound greatly outdistances the flame front. Laminar or turbulent molecular diffusion plays an important role in the propagation of a deflagration flame. This form of combustion can be modeled as a constant pressure process.

Another form of combustion that is rapid and violent is called detonation. In detonation, all the important energy transfer occurs by mass flow in a strong compression wave, with negligible contribution from other processes like heat conduction and molecular diffusion which are important in a deflagration flame [8]. A detonation propagates at a very large velocity (a few thousand meters per second relative to an unburned gas mixture), and produces very high pressures. The leading part of a detonation front is a strong shock wave propagating into the unburned gas mixture. This shock heats the gas mixture to a very high temperature by compressing it. Chemical reactions are triggered by the shock heating, and proceed violently. The energy from the chemical reactions support the travelling shock wave in turn, and a balance is attained to form a self-sustaining detonation wave. Due to the high speed, detonation closely approximates a constant volume process [1].

Detonation waves are actually complex, oscillatory phenomena with three dimensional time-dependent cellular structures. However, it is worth while to review the relatively simple description of detonation to understand its basic features. The elements of the simplest one-dimensional theory were formulated by Chapman (1899) and by Jouguet (1905) after the phenomenon of detonation had been first recognized by Berthelot and Vieille, and by Mallard and Le Chatelier in 1881 during studies of flame propagation. A fundamental advance was made independently by Zeldovich (1940) in Russia, von Neumann (1942) in the United States, and Doering (1943) in Germany, and
their treatment has come to be called the ZND model of detonation [8]. The ZND description neglects transport processes, and assumes one-dimensional flow. The shock at the head of the wave is a jump discontinuity. It heats the gas mixture, and triggers the chemical reaction. The reaction proceeds in the reaction zone that follows the shock, and is complete in the final state. The shock and the reaction zone propagate together at the constant detonation velocity, $D$. The conservation conditions require that the final state lie on both the Hugoniot curve and the Rayleigh line in the pressure–volume plane. There will be a particular value of $D$ that makes the Rayleigh line tangent to the Hugoniot curve. This tangent point is called the Chapman–Jouguet(CJ) point that represents the stable end state for a self-sustaining detonation wave, and the corresponding detonation velocity $D$ is called the CJ velocity. It can be shown from the tangency condition that at the CJ point, the detonation velocity relative to the reaction products is equal to the local speed of sound in the reaction products.

1.2 Review of Computational Studies

During the 1960s, the computation of real gas flows was an active research area for application in hypersonic flows. Much effort was devoted in obtaining numerical and quasi-analytical solutions to high temperature non-equilibrium flows [9]–[15]. However, it subsequently languished. In the 1980s, numerical simulations of high temperature gas flow resurged on a national scale due to the renewed interest in the field of hypersonics including the proposed development of a National Aerospace Plane(NASP) that would travel in the atmosphere at a very high Mach number. The availability of accurate, robust and efficient simulation tools for the complex physical phenomena in the hypersonic regime became an essential priority for the scientists and designers [16]. Several computer programs for chemical and thermal non-equilibrium flows were developed to
this end [17]–[24]. Most of them used upwind or flux-split algorithms that are known to yield accurate solutions of shock-wave dominated flows due to their superior shock capturing properties. Grossman and Cinnella [24] presented extensions of the flux-vector split schemes and flux-difference split scheme of the Roe type to non-equilibrium flows. Liu and Vinokur [22] also presented flux-split formulations for nonequilibrium flows, with provisions for a more general gas model.

There have been two standard approaches to solve the equation set for non-equilibrium flows. One approach has been to uncouple the chemical reaction and thermal excitation equations from the flow equations, and solve them separately at each time step [25]–[27]. Another approach has been to solve the entire equation set governing the fluid dynamics and non-equilibrium chemistry and thermodynamics simultaneously in a fully coupled fashion. This usually introduces extreme stiffness in the system of equations, and results in a very small time step for a stable time-marching solution. To improve efficiency, the numerical scheme has been made implicit [18]. This results in a very complex, large-block structure for the solution algorithm which, however, fully accounts for the non-equilibrium effects. Bussing and Murman [28] introduced a point-implicit scheme treating the chemical source terms implicitly and all other terms explicitly.

Computational work on a detonation wave and its application to the PDE has progressed following the development of numerical methods on a high-temperature non-equilibrium flow. Cambier and Adelman [29] performed quasi one-dimensional computations with a shock-capturing total variation diminishing (TVD) algorithm for multiple species that is second-order accurate in space and is monotone. Lynch and Edelman [5, 30] used a spatially-third-order TVD discretization scheme with a special
treatment on source terms, while Eidelman et al. [31]—[34] performed computational studies using a second-order Godunov solver on unstructured grids.

1.3 The Scope of the Current Work

The objective of this work is to construct a two-dimensional time-accurate numerical simulation model to be used for PDE’s, efficient enough to be used for design parametric studies while maintaining a reasonable accuracy. The simulation model is constructed to formulate the corresponding physical phenomena as precisely as possible including chemical and thermal non-equilibrium, and to numerically solve the resulting mathematical formulation as accurately as possible. The novel aspect of this work includes a combination of point-implicit treatment and Local Ignition Averaging applied to the global two-step reaction model for efficient time-accurate solution of a propagating detonation wave. The partition of internal energy is based on the two-temperature model, and the vibrational energy of each species is obtained by subtracting out fully-excited translational and rotational energy from total internal energy. Roe’s flux-difference split scheme is combined with the Runge–Kutta integration scheme for an accurate capture of the shock wave both in space and in time.

The present model is validated by comparing the calculated results with the theoretical CJ and experimental data. Extensive calculations are performed with numerical schemes of different orders in space and time, and with different mesh sizes to select the proper scheme and mesh size providing adequate resolution of the physical process.

One of the common simplifications made in the computational work on PDE’s consists in modeling the detonation initiation by having a sufficiently large energy deposition [35]. Detonation initiation is extensively studied in this dissertation to derive
the criteria for direct initiation, as well as to provide a proper initiation model from the observation of the effect of initial hot spot conditions on the development of a detonation wave. Shock-induced detonation experiments are also simulated to provide a validation of the numerical simulation model, and as an aid in understanding the experimental results.
CHAPTER 2

MATHEMATICAL FORMULATION

A set of coupled partial differential equations that describe gas phase reactive flow fields is derived here, the main application of which will be to calculate initiation and propagation of detonation waves through quiescent fuel–air mixture in a pulse detonation engine. Inviscid, non-heat-conducting flow equations are used, since the major physical processes involved are inviscid phenomena such as shock compression of the gas mixture, chemical reactions in the shock compressed region, generation of pressure waves due to energy release from chemical reactions, wave interactions, formation and propagation of detonation waves, and expansion of burned gases.

The flow fields are assumed to be accurately described by a continuum formulation, even though the processes simulated result from the interactions of molecules and atoms in a reactive medium. The continuum formulation requires that the Knudsen number be much less than one to ensure a large number of particles within a computational volume. This implies little statistical variation at any point in the domain. This continuum approximation incorporates statistical averaging processes performed over the small-scale particle phenomena. This natural process in which the small-scale phenomena are averaged to produce a global quantity is called “chunking” by Hofs-tadter [36], and has been used as a basis of many scientific studies. We use a macroscopically chunked fluid or continuum picture of the particles, which give us distinct chemical species.
At high temperature, portions of the internal energy may be out of equilibrium. The internal energy of each species will generally depend upon the various internal energy modes such as translational and rotational, vibrational, electronic excitation, and free electron energy mode. An adequate description of the energy distribution is rather subjective, and depends upon the problem to be solved. The primary application in this work is to hydrogen—air reactive flows, and since the temperature range for this application is expected to be around 3000 K, it is assumed that the translational and rotational energy modes are fully excited, while the electronic excitation and the effect of ionization can be ignored.

The energy in the translational modes of all the species is assumed to be characterized by a single temperature $T$, and the rotational state of the diatomic molecules is assumed to be in equilibrium with this translational temperature. Thus, a single temperature $T$ is used to characterize the translational and rotational state of the gas mixture, which is assumed to be fully excited in the temperature range of interest.

A two-temperature model is selected to describe the remaining energy modes. The energy in the vibrational modes of all the molecules is assumed to be described by a single vibrational temperature $T_v$. This model has been assessed by Chul Park [37] in high temperature flow fields and observed to yield accurate results while requiring much less computing time. More detailed thermal models can be constructed in which the vibrational energy of each molecular species is modeled by its own vibrational temperature. This requires additional conservation equations of vibrational energy for each species, and thus much more computing time. The application of a multi-vibrational temperature model is also limited by the availability and accuracy of the relaxation time data required to describe the energy exchanges due to collisions among species.
The other main ingredients of the formulation include a chemical kinetic model to ensure accurate prediction of the chemical composition in the mixture, proper description of species and mixture thermodynamic properties including possible excitation of internal energy modes at high temperature, and vibrational energy relaxation process.

2.1 Governing Equations

The time-dependent conservation equations governing inviscid, non-heat-conducting, reacting gas flow in which thermal nonequilibrium is modeled with a two-temperature approximation are derived in this section. The conservation equations for the individual species are derived first, and then these are combined to yield the complete set of equations. This more general approach will make clear the underlying assumptions embodied in the governing equations.

The mass conservation equation for species $s$ of the gas mixture is given by [38]

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_{sj}) = w_s$$  \hspace{1cm} (2.1)

The species momentum, total energy, and vibrational energy conservation equations are written as

$$\frac{\partial}{\partial t} (\rho_s u_{si}) + \frac{\partial}{\partial x_j} (\rho_s u_{si} u_{sj}) = -\frac{\partial p_s}{\partial x_i} + P_{si}$$  \hspace{1cm} (2.2)

$$\frac{\partial}{\partial t} (\rho_s E_s) + \frac{\partial}{\partial x_j} [\rho_s (E_s + p_s) u_{sj}] = Q_s$$  \hspace{1cm} (2.3)

$$\frac{\partial}{\partial t} (\rho_s e_{v,s}) + \frac{\partial}{\partial x_j} (\rho_s e_{v,s} u_{sj}) = Q_{v,s} + w_s e_{d,s}$$  \hspace{1cm} (2.4)

where $u_{si}$ is the velocity of species $s$ in the $i$ direction, and $w_s$, $P_{si}$, $Q_s$ represent the mass, momentum, and energy transfer rates, respectively, of species $s$ from the interaction with other species in the mixture. The first term in the right hand side of the
vibrational conservation equation, \( Q_{us} \) represents the vibrational energy exchange rate of species \( s \) due to the relaxation process with translational energy, and the second term, \( w_s e_{ds} \) represents the amount of vibrational energy gained or lost due to production or depletion of species \( s \) from chemical reactions.

For a gas mixture of \( N_s \) species, this approach would entail \( 5N_s \) equations to solve simultaneously for two-dimensional problem, and the evaluation of the momentum transfer term \( P_{si} \). This may not be feasible for a multi-dimensional flow field with some species. The problem can be simplified by using the mass-averaged velocity \( u_i \), and the diffusion velocity \( u_{Dsi} \) defined by

\[
 u_i = \sum_s \frac{\rho_s}{\rho} u_{si}, \quad u_{Dsi} = u_{si} - u_i \quad (2.5)
\]

Using these new variables, the species mass conservation equation 2.1 becomes

\[
 \frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_j) = -\frac{\partial}{\partial x_j} (\rho_s u_{Dsj}) + w_s \quad (2.6)
\]

The species momentum, total energy, and vibrational energy equations can be summed over all the species to yield the following mass-averaged equations:

\[
 \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} \quad (2.7)
\]

\[
 \frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} [\rho (E + p) u_j] = -\frac{\partial}{\partial x_j} \sum_s h_s u_{Dsi} \quad (2.8)
\]

\[
 \frac{\partial}{\partial t} (\rho e_v) + \frac{\partial}{\partial x_j} (\rho e_v u_j) = \sum_s Q_{us} + \sum_s w_s e_{ds} - \frac{\partial}{\partial x_j} \sum_s h_{us} u_{Dsi} \quad (2.9)
\]

where the total pressure and density are defined as the sum of the species quantities. In the momentum equation, the momentum transfer rates between species, \( P_{si} \), as well as the diffusion flux terms identically sum to zero. This produces a significant simplification.
Another simplification comes from the assumption that molecular diffusion is not significant and can be safely neglected when the chemical reactions and the corresponding energy release occur rapidly as in a detonation process [39]. When we assume zero diffusion velocity, the following simplified set of equations is obtained.

\[
\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_j) = w_s \tag{2.10}
\]

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} \tag{2.11}
\]

\[
\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} [\rho (E + p) u_j] = 0 \tag{2.12}
\]

\[
\frac{\partial}{\partial t} (\rho e_v) + \frac{\partial}{\partial x_j} (\rho e_v u_j) = \sum_i Q_{v,i} + \sum_i w_s e_{d,i} \tag{2.13}
\]

The governing equations are written in the conservation law form which has the property that the coefficients of the derivative terms are either constant or, if variable, their derivatives appear nowhere in the equation. Normally this means that the divergence of a physical quantity can be identified in the equation. This form is advantageous in numerical simulations to correctly capture shock waves [40]. In two dimensional Cartesian coordinate system, this takes the following form:

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S \tag{2.14}
\]

where \( U \) is the vector of conserved variables, \( F \) and \( G \) are the convective flux vectors, and \( S \) is the vector of source terms. Each vector is written as

\[
U = \begin{bmatrix} \rho_s \\ \rho v \\ \rho E \end{bmatrix}, \quad F = \begin{bmatrix} \rho_s u \\ \rho u^2 + p \\ \rho u E + pu \end{bmatrix}, \quad G = \begin{bmatrix} \rho_s v \\ \rho u v \\ \rho v e_v \\ \rho v E + pv \end{bmatrix}, \quad S = \begin{bmatrix} w_s \\ 0 \\ w_v \end{bmatrix} \tag{2.15}
\]
In this equation, subscript $s$ ranges 1 to $N_s$, where $N_s$ is the number of species. The first $N_s$ rows represent species continuities, followed by two momentum conservation equations for the mixture. The next row describes the rate of change in the vibrational energy, and the final row is the total energy conservation equation. In the above equation, $u$ and $v$ are the velocities in the $x$ and $y$ direction respectively, $\rho$ is the mixture density, $p$ is the pressure, $e_v$ is the vibrational energy, and $E$ is the total energy per unit mass of mixture. $\rho_s$ is the $s$-th species density, $w_s$ is the mass production rate of species $s$ per unit volume, and $w_v$ is the vibrational energy source term which is defined as

$$w_v = \sum_s Q_{vs} + \sum_s w_se_{d,s}$$ \hspace{1cm} (2.16)

For an axisymmetric flow, the conservation equation take the form as

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{1}{y} \frac{\partial (yG)}{\partial y} = S$$ \hspace{1cm} (2.17)

where $U, F$ and $G$ are the same as in equation 2.15, but $S$ is given by

$$S = \begin{bmatrix} w_i \\ 0 \\ p/y \\ w_v \\ 0 \end{bmatrix}$$ \hspace{1cm} (2.18)

### 2.2 Thermodynamic Properties

A general representation of species internal energy includes a portion of the internal energy in thermodynamic equilibrium and the remaining portion in a nonequilibrium state. The equilibrium portion of the internal energy is the contribution due to translation and internal modes that can be assumed to be in equilibrium at the translational
temperature $T$. The remaining nonequilibrium portion is the contribution due to internal modes that are not in equilibrium at the translational temperature $T$, but may be assumed to satisfy a Boltzmann distribution at a different temperature.

For the temperature range of interest as stated earlier in this chapter, the rotational mode is assumed to be fully excited and in equilibrium with translational temperature $T$, while the electronic excitation and free electron modes can be safely ignored. Thus, the only remaining energy mode that could be in nonequilibrium with translational temperature $T$ is the vibrational energy mode. Therefore, the species internal energy based on the two-temperature model can be written as follows:

$$ e_s = e_{eq,s}(T) + e_{v,s}(T_v) \quad (2.19) $$

where $e_{eq,s}$ is the equilibrium portion of the internal energy and $e_{v,s}$ is the vibrational energy which is not in thermodynamic equilibrium. The equilibrium portion of the energy can be further defined as

$$ e_{eq,s} = \int_{T_{ref}}^{T} (C_{v,t}^s + C_{v,r}^s) \, d\tau + e_{s,o} \quad (2.20) $$

where $T_{ref}$ is the reference temperature, $e_{s,o}$ is the energy of formation, and $C_{v,t}^s$ and $C_{v,r}^s$ are the translational and rotational portion of specific heat at constant volume, respectively. Since the translational and rotational modes are assumed to be fully excited, $C_{v,t}^s$ and $C_{v,r}^s$ can be written as

$$ C_{v,t}^s = 1.5\tilde{R}/M_s \quad (2.21) $$

$$ C_{v,r}^s = \begin{cases} \tilde{R}/M_s, & \text{diatomic molecule} \\ 1.5\tilde{R}/M_s, & \text{polyatomic molecule} \end{cases} \quad (2.22) $$
where \( R \) is the universal gas constant and \( M_s \) is the molecular weight of species \( s \). The energy of formation \( e_{s,o} \) can be obtained from readily available heat of formation data as

\[
e_{s,o} = h_{s,o} - \frac{R}{M_s} T_{ref}
\]  

(2.23)

Therefore, the equilibrium portion of energy can be written as follows:

\[
e_{eq,s}(T) = K_s \frac{R}{M_s} (T - T_{ref}) - \frac{R}{M_s} T_{ref} + h_{s,o}
\]  

(2.24)

where \( K_s \) is 1.5, 2.5, 3.0 for monatomic, diatomic or linear polyatomic, and nonlinear polyatomic species respectively.

The heat capacity of the vibrational energy mode can now be obtained from the fact that the translational and rotational heat capacities are independent of temperature. This can be evaluated by utilizing the readily available curve fit for total heat capacity evaluated at temperature \( T_v \) and subtracting out the constant contributions from the translation and rotational heat capacities as follows:

\[
C^s_{u,v}(T_v) = C^s_u(T_v) - C^s_{u,t} - C^s_{u,r}
\]  

(2.25)

where

\[
C^s_u(T_v) = C^s_p(T_v) - \frac{R}{M_s}
\]

\( C^s_u \) and \( C^s_p \) are specific heats at constant volume and constant pressure respectively, and curve fit data for \( C^s_p(T) \) can be found in the following form [41, 42):

\[
C^s_p(T) = \frac{R}{M_s} \sum_{k=1}^{5} A_k^s T^{k-1}
\]  

(2.26)
Therefore we can obtain $C_{v,u}^s$ as follows:

$$C_{v,u}^s(T_v) = \begin{cases} \frac{\bar{R}}{M_s} \left( \sum_{k=1}^{5} A_k^s T_v^{k-1} - \frac{7}{2} \right), & \text{diatomic molecule} \\ \frac{\bar{R}}{M_s} \left( \sum_{k=1}^{5} A_k^s T_v^{k-1} - 4 \right), & \text{polyatomic molecule} \end{cases} \quad (2.27)$$

The species vibrational energy $e_{v,s}$ can be obtained by integrating $C_{v,u}^s$ such that

$$e_{v,s}(T_v) = \int_{T_{ref}}^{T_v} C_{v,u}^s(\tau) \, d\tau \quad (2.28)$$

An alternative formulation using the enthalpy relation may be used as follows [43]:

$$h_{v,s}(T_v) = h_s(T_v) - (C_{p,t}^s + C_{p,r}^s)(T_v - T_{ref}) - h_{s,0} \quad (2.29)$$

$$h_s(T, T_v) = h_{v,s}(T_v) + (C_{p,t}^s + C_{p,r}^s)(T - T_{ref}) + h_{s,0}$$

where

$$C_{p,t}^s = C_{v,t}^s + \frac{\bar{R}}{M_s}, \quad C_{p,r}^s = C_{v,r}^s$$

Here, $h_{v,s}(T_v)$ and $h_s(T, T_v)$ are vibrational enthalpy and enthalpy per unit mass of species $s$, and $h_s(T_v)$ which includes the heat of formation is readily available as the following form:

$$h_s(T_v) = \frac{\bar{R}}{M_s} \left( \sum_{k=1}^{5} A_k^s T_v^{k} + A_6^s \right) \quad (2.30)$$

Therefore, $e_{v,s}$ and $e_s$ can be directly obtained from $h_{v,s}$ and $h_s$ as follows:

$$e_{v,s}(T_v) = h_{v,s}(T_v)$$

$$e_s(T, T_v) = h_s(T, T_v) - \frac{\bar{R}}{M_s} T$$ \quad (2.31)

Thus, vibrational energy is obtained basically from the difference between total internal energy in equilibrium and the fully excited translational/rotational mode of internal energy. At the reference temperature where $T_v = T_{ref} = 298.15$ K, $h_s(T_v)$ in
equation 2.30 is made equal to the heat of formation $h_{s,0}$. Therefore, $e_{v,s} = h_{v,s} = 0$

at and below this reference temperature, and vibrational energy will increase gradually as temperature increases. However, in the temperature range slightly higher than the reference temperature, equation 2.30 yields small negative values of vibrational energy, as shown in figure 2.1. This negative vibrational energy is caused by using fully excited translational/rotational mode of heat capacity from the assumption that translational/rotational energy mode is fully excited, which is apparently not true for this temperature range. This can cause problems in determining vibrational temperature using a Newton–Raphson iteration method near the reference temperature. To avoid this problem, a limiter on the vibrational energy needs to be introduced, which makes the vibrational energy zero if it has a negative value in the lower temperature range. This limiter will not have any actual effects on the calculations of the thermodynamic properties.

Figure 2.1. Vibrational energy near reference temperature.
The mixture relations are expressed in the following way:

\[ C_{p,q} = \frac{1}{\rho} \sum_s \rho_s C_{p,q}^s \]

\[ C_{v,q} = \frac{1}{\rho} \sum_s \rho_s C_{v,q}^s \]

\[ e_u = \frac{1}{\rho} \sum_s \rho_s e_{u,s} \]

\[ e = \frac{1}{\rho} \sum_s \rho_s e_s \]

where

\[ \rho = \sum_{s=1}^{N_s} \rho_s \]

Total energy and total enthalpy are obtained from

\[ E = \frac{u^2 + v^2}{2} + e \]

\[ H = E + \frac{p}{\rho} \]

(2.33)

It is assumed here that each individual species behaves as a thermally perfect gas. With this assumption, the pressure can be given as

\[ p = \sum_s p_s = \sum_s \frac{\rho_s \tilde{R}T}{M_s} = \rho \tilde{R}T \]

(2.34)

where

\[ \tilde{R} = \frac{1}{\rho} \sum_s \rho_s \frac{\tilde{R}}{M_s} \]

2.3 Chemical Kinetics Model

High temperature flows typically involve some chemical reactions, and the time scale in which the chemical reactions take place is important in the estimation of the flowfield properties. When a characteristic flow time is compared to a typical chemical
reaction time, three cases can occur. The first case is when a reaction time is much
greater than the flow time, in which the reaction has no enough time to occur. In
this case, a frozen flow can be assumed with respect to that specific reaction. The
second case is for a reaction time much shorter than a fluid dynamic time, in which
the reaction has virtually infinite time to evolve, and consequently an equilibrium state
will be reached during a fluid dynamic time scale. The third case is the general case of
finite-rate chemistry, when both times are of the same order. In this case, the actual
kinetics of the reaction must be considered together with fluid dynamic equations.

For accurate modeling of a detonation wave, especially in the detonation front
where rapid chemical reactions take place in the shock compressed region, species con-
tinuity equations based on the chemical kinetics should be solved together with fluid
dynamic equations to account for the possible chemical nonequilibrium. The mass
production rate of species $s$ from the chemical reactions can be written as [43]

$$w_s = M_s \sum_{r=1}^{N_r} (\beta_{s,r} - \alpha_{s,r})(R_{f,r} - R_{b,r})$$  \hspace{1cm} (2.35)

where $M_s$ is the molecular weight of species $s$, $N_r$ is the number of reactions, $\alpha_{s,r}$ and $\beta_{s,r}$ are the stoichiometric coefficients for reactants and productants, respectively, in
the $r$ reaction. $R_{f,r}$ and $R_{b,r}$ are the forward and backward reaction rate of $r$ reaction,
respectively, defined by

$$R_{f,r} = 1000 \left[ K_{f,r} \prod_{s=1}^{N_s} (0.001\rho_s/M_s)^{\alpha_{s,r}} \right]$$

$$R_{b,r} = 1000 \left[ K_{b,r} \prod_{s=1}^{N_s} (0.001\rho_s/M_s)^{\beta_{s,r}} \right]$$  \hspace{1cm} (2.36)

The factors 1,000 and 0.001 are required to convert from CGS units to MKS units, since
most reaction rate data in the literature are found in CGS units.
The forward reaction rate coefficient can be expressed by

\[ K_{f,r} = A_{f,r} T^{N_{f,r}} \exp(-E_{f,r}/R_T) \]  \hspace{1cm} (2.37)

where \( E_{f,r} \) is the activation energy of the \( r \)-th forward reaction. The values of parameters \( A_{f,r}, N_{f,r}, E_{f,r} \) are usually found in table format according to the reactions involved. The backward reaction rate coefficient is evaluated using the equilibrium constant for the reaction such that

\[ K_{b,r} = \frac{K_{f,r}}{K_{e,r}} \]  \hspace{1cm} (2.38)

2.4 Vibrational Energy Relaxation

The energy exchange between vibrational and translational modes due to intermolecular collisions has been well described by the Landau–Teller formulation where it is assumed that the vibrational level of a molecule can change by only one quantum level at a time [44, 45]. The resulting energy exchange rate is given by

\[ Q_{v,s} = \rho_s \frac{e^*_{v,s}(T) - e_{v,s}}{\langle \tau_s \rangle} \]  \hspace{1cm} (2.39)

where \( e^*_{v,s}(T) \) is the vibrational energy per unit mass of species \( s \) evaluated at the local translational–rotational temperature, and \( \langle \tau_s \rangle \) is the averaged Landau–Teller relaxation time of species \( s \) given by [43]

\[ \langle \tau_s \rangle = \frac{\sum_{j=1}^{N_s} n_j \tau_{sj}}{\sum_{j=1}^{N_s} n_j} \]  \hspace{1cm} (2.40)

where \( \tau_{sj} \) is the vibrational–translational relaxation time of species \( s \) caused by intermolecular collision with species \( j \), and \( n_j \) is number density of species \( j \).
The Landau–Teller inter-species relaxation time $\tau_{sj}$ can be obtained in seconds using semi-empirical expression developed by Millikan and White [46] such that

$$\tau_{sj} = \frac{1}{p} \exp \left[ A_{sj} \left( T^{-1/3} - 0.015 \mu_{sj}^{1/4} \right) - 18.42 \right]$$  (2.41)

where

- $p$ ; pressure in atm
- $A_{sj} = 1.16 \times 10^{-3} \mu_{sj} \theta_{sj}$
- $\mu_{sj} = M_s M_j / (M_s + M_j)$; reduced mass
- $\theta_{sj}$; Characteristic vibrational temperature of harmonic oscillator

The vibrational energy relaxation rate can be simplified using the following approximation [43]:

$$\sum_s \rho_s \frac{e_{v^*} - e_{v}}{\langle \tau_s \rangle} \approx \sum_s \rho_s C_{v,v}^s \frac{T - T_v}{\tau_v} \approx \frac{\rho C_{v,v}}{\tau_v} (T - T_v)$$  (2.42)

where

$$\frac{1}{\tau_v} = \frac{\sum_s \rho_s / (M_s \langle \tau_s \rangle)}{\sum_s \rho_s / M_s}$$

This approximation not only reduces the number of species dependent parameters but also simplifies the evaluation of the vibrational relaxation as a single relaxation term multiplied by the difference in the translational and vibrational temperature. When a point implicit formulation is used on the source terms in the numerical algorithm, the above approximation greatly simplifies an implicit treatment of the temperature difference which drives the relaxation process.
CHAPTER 3

NUMERICAL FORMULATION

The numerical methods used to solve the governing differential equations are derived and discussed in this chapter. The goal is to construct numerical algorithms to obtain a time-accurate solution of the thermo-chemical nonequilibrium flow fields.

The first step to a computer simulation must be a discretization, which reduces partial differential equations to a set of algebraic equations to be solved. The key word in this process is the conservative property. The discrete algorithm that maintains the conservation statement “exactly” for any mesh size over an arbitrary finite region containing any number of grid points is said to have the conservative property [40]. Finite-volume methods which have the conservative property are used in this study.

The next step is to decide how to advance the numerical solution in time. In this regard, one major difficulty often encountered in the numerical simulations of thermo-chemical nonequilibrium flow is the stiffness problem caused by the order differences in the various characteristic time scales. An implicit time integration scheme is one choice to overcome this problem. However, the implicit scheme may not be a good choice for the unsteady flow fields where a time-accurate solution is needed. The implicit scheme loses overall efficiency it used to have from its unconditional stability and the consequent increase in time step, when a smaller time step is needed anyhow. It means that a huge linear problem needs to be solved at every time step small enough to ensure a time-accurate solution. Implementation of an implicit scheme to solve nonequilibrium flows creates another problem in the derivation of the Jacobian. When flux-difference
splitting schemes of the Roe type are used for cell face fluxes, the flux Jacobian becomes too complicated to derive. An explicit time integration scheme, on the other hand, may result in extreme inefficiencies in obtaining a time-accurate solution. For stability and accuracy, the integration time step should be much smaller than the characteristic times associated with chemical reactions and thermal relaxation. This may be impractical in many cases. The point implicit scheme whereby the source terms are treated implicitly and the fluxes remain explicit is chosen here together with two-step Runge–Kutta method as a time integration procedure. The advantages from both implicit and explicit schemes can be expected, such as rescale of the various characteristic times, simple and efficient nature of the explicit scheme, no need to derive complicated flux Jacobian for flux difference splitting scheme.

Roe’s flux-difference splitting scheme extended to nonequilibrium flow is implemented for the cell interface fluxes. The implemented scheme itself is first-order accurate, and a higher-order approximation is obtained by the MUSCL (Monotone Upstream-centered Schemes for Conservation Laws) approach for added spatial accuracy. A MINMOD limiter is applied to limit the slope of the variables used in the extrapolation.

3.1 Finite-Volume Formulation

A discretized set of equations is derived in this section from the governing partial differential equations using the finite-volume method. The advantage of this method is its use of the integral form of the equations, which ensures conservation, and allows the correct treatment of discontinuities [40]. In the following derivation, the cell-centered approach will be described.
For an arbitrary volume $\omega$, enclosed by a boundary $\sigma$, the governing equations in integral form can be written

$$
\frac{\partial}{\partial t} \iiint U \, d\Omega + \oint_{\sigma} \vec{H} \cdot \vec{n} \, d\sigma = \iiint S \, d\Omega
$$

(3.1)

where

$$
\vec{H} = (F, G)
$$

where $U$ is the vector of conserved variables, $S$ is the vector of source terms, and $H$ is the flux vector, respectively. The unit vector $n$ is normal to the infinitesimal area $d\sigma$ and points outwards. The first step to discretize the above equation is to introduce volume averaged values of the conserved variables and the source term as follows:

$$
< U > = \frac{1}{\Omega} \iiint U \, d\Omega, \quad < S > = \frac{1}{\Omega} \iiint S \, d\Omega
$$

(3.2)

These volume averaged variables are substituted into the integral form of the governing equations to yield

$$
\frac{\partial}{\partial t}(< U > + \Omega) + \oint_{\sigma} (F, G) \cdot \vec{n} \, d\sigma = < S > + \Omega
$$

(3.3)

For two-dimensional Cartesian coordinate system where the computational cell is defined by two constant lines of both $x$ and $y$ directions, the surface integral can be split into four contributions, one from each bounding surface. When the index of the cell centered variables is $(i, j)$, the above surface integral can be written as

$$
\oint_{\sigma} (F, G) \cdot \vec{n} \, d\sigma = \int_{\sigma_{i+1/2}} F \, d\sigma + \int_{\sigma_{i-1/2}} F \, d\sigma + \int_{\sigma_{j+1/2}} G \, d\sigma + \int_{\sigma_{j-1/2}} G \, d\sigma
$$

(3.4)

Then, area-averaged values of fluxes can be defined such that

$$
< F >_{i+1/2} = \frac{1}{\sigma_{i+1/2}} \int_{\sigma_{i+1/2}} F \, d\sigma, \quad < G >_{i+1/2} = \frac{1}{\sigma_{i+1/2}} \int_{\sigma_{i+1/2}} G \, d\sigma
$$

(3.5)

where the bounding surface area $\sigma_{i+1/2}, \sigma_{j+1/2}$ actually represent cell face lengths in two-dimensional Cartesian coordinate system. After substituting these definitions of
averaging into the equation 3.3, the following discrete form of conservation equations written in two-dimensional Cartesian coordinate system can be obtained.

\[
\frac{\partial}{\partial t} (<U>_{i,j} \Omega) + <F>_{i+1/2} \sigma_{i+1/2} - <F>_{i-1/2} \sigma_{i-1/2} \\
+ <G>_{j+1/2} \sigma_{j+1/2} - <G>_{j-1/2} \sigma_{j-1/2} = <S>_{i,j} \Omega
\]  
(3.6)

After dropping brackets, it can be rearranged to give the final form of the discrete equations as follows:

\[
\frac{\partial U_{i,j}}{\partial t} = - \left( F_{i+1/2} \frac{\sigma_{i+1/2}}{\Omega_{i,j}} - F_{i-1/2} \frac{\sigma_{i-1/2}}{\Omega_{i,j}} \right) \\
- \left( G_{j+1/2} \frac{\sigma_{j+1/2}}{\Omega_{i,j}} - G_{j-1/2} \frac{\sigma_{j-1/2}}{\Omega_{i,j}} \right) + S_{i,j}
\]  
(3.7)

A discrete form of conservation equations for axisymmetric geometry can be obtained similarly as follows:

\[
\frac{\partial U_{i,j}}{\partial t} = - \left( F_{i+1/2} \frac{\sigma_{i+1/2}}{\Omega_{i,j}} - F_{i-1/2} \frac{\sigma_{i-1/2}}{\Omega_{i,j}} \right) \\
- \frac{1}{y_j} \left( y_{j+1/2} G_{j+1/2} \frac{\sigma_{j+1/2}}{\Omega_{i,j}} - y_{j-1/2} G_{j-1/2} \frac{\sigma_{j-1/2}}{\Omega_{i,j}} \right) + S_{i,j}
\]  
(3.8)

3.2 Point Implicit Time Integration

Nonequilibrium flows involving finite-rate chemistry and thermal energy relaxation often can be very difficult to solve numerically because of the stiffness. The stiffness in terms of time scale can be defined as the ratio of the largest to the smallest time scale such that

\[
\text{Stiffness} = \tau_{\text{largest}} / \tau_{\text{smallest}}
\]

where \(\tau\) can be any characteristic time in the flow field. For reactive flow problems, there can be several chemical time scales and relaxation time scales in addition to the
fluid dynamic time scale associated with convection. The stiffness parameter can be as high as order $10^6$. The point implicit formulation evaluating the source terms at time level $n+1$ has been an effective method used to numerically integrate stiff systems [28]. The point implicit treatment is known to reduce the stiffness of the system by effectively rescaling all the characteristic times in the flow fields into the same order of magnitude.

Equation 3.8 is rewritten here with source terms evaluated at the time level $n+1$ as follows:

$$\frac{\partial U_{i,j}}{\partial t} = - \left( F^n_{i+1/2} \frac{\sigma_{i+1/2}}{\Omega_{i,j}} - F^n_{i-1/2} \frac{\sigma_{i-1/2}}{\Omega_{i,j}} \right)$$

$$- \left( G^n_{j+1/2} \frac{\sigma_{j+1/2}}{\Omega_{i,j}} - G^n_{j-1/2} \frac{\sigma_{j-1/2}}{\Omega_{i,j}} \right) + S_{i,j}^{n+1}$$

(3.9)

The source vector is then linearized about the present time level such that

$$S^{n+1} = S^n + \left( \frac{\partial S}{\partial U} \right)^n \Delta U$$

(3.10)

When simple Euler time integration is used, substituting this linearization into the above equation and rearranging yields

$$\left[ \frac{I}{\Delta t} - \left( \frac{\partial S}{\partial U} \right)^n \right] \Delta U = - \left( F^n_{i+1/2} \frac{\sigma_{i+1/2}}{\Omega_{i,j}} - F^n_{i-1/2} \frac{\sigma_{i-1/2}}{\Omega_{i,j}} \right)$$

$$- \left( G^n_{j+1/2} \frac{\sigma_{j+1/2}}{\Omega_{i,j}} - G^n_{j-1/2} \frac{\sigma_{j-1/2}}{\Omega_{i,j}} \right) + S_{i,j}^{n}$$

(3.11)

Similarly the axisymmetric version of the equation can be written as follows:

$$\left[ \frac{I}{\Delta t} - \left( \frac{\partial S}{\partial U} \right)^n \right] \Delta U = - \left( F^n_{i+1/2} \frac{\sigma_{i+1/2}}{\Omega_{i,j}} - F^n_{i-1/2} \frac{\sigma_{i-1/2}}{\Omega_{i,j}} \right)$$

$$\frac{1}{y_i} \left( y_{j+1/2} G^n_{j+1/2} \frac{\sigma_{j+1/2}}{\Omega_{i,j}} - y_{j-1/2} G^n_{j-1/2} \frac{\sigma_{j-1/2}}{\Omega_{i,j}} \right) + S_{i,j}^{n}$$

(3.12)

These equations can be evaluated to get $\Delta U$ entirely at the current time level at the expense of matrix inversion containing source term Jacobian.
Temporal accuracy can be added by using Runge–Kutta integration schemes instead of first-order accurate Euler integration. The two-step explicit Runge–Kutta time integration schemes can be written as follows:

\[
U^{n+\frac{1}{2}} = U^n + \gamma_1 \Delta U^n
\]

\[
U^{n+1} = U^{n+\frac{1}{2}} + \gamma_2 \Delta U^{n+\frac{1}{2}} + \zeta_2 \Delta U^n
\]  \hspace{1cm} (3.13)

where \( \gamma_1 = 1.0, \gamma_2 = 0.5, \text{ and } \zeta_2 = -0.5 \), and the three step scheme is given by

\[
U^{n+\frac{1}{2}} = U^n + \gamma_1 \Delta U^n
\]

\[
U^{n+\frac{3}{2}} = U^{n+\frac{1}{2}} + \gamma_2 \Delta U^{n+\frac{1}{2}} + \zeta_2 \Delta U^n
\]

\[
U^{n+1} = U^{n+\frac{3}{2}} + \gamma_3 \Delta U^{n+\frac{3}{2}} + \zeta_3 \Delta U^{n+\frac{1}{2}}
\]  \hspace{1cm} (3.14)

where \( \gamma_1 = 8/15, \gamma_2 = 5/12, \gamma_3 = 3/4, \text{ and } \zeta_2 = -17/60, \zeta_3 = -5/12 \).

3.3 Flux-Difference Split Algorithm

The basic feature of the flux-difference split algorithm is to solve a local Riemann problem at the cell interface in order to determine the cell-face flux. Roe’s scheme was originally developed for a perfect gas [47]. An approximate Riemann problem is used with Roe’s scheme, and this approach has been used very successfully. An extension of this method to a thermo-chemical non-equilibrium gas was made by Grossman and Cinnella [24], and the flux-difference scheme used here is based on their method.

The approximate Riemann solver is implemented by computing the cell face flux as a summation of the contributions from each wave component.

\[
F_{i+1/2} = \frac{1}{2} (F_R + F_L) - \frac{1}{2} \sum_{i=1}^{N_{x+4}} \hat{\alpha}_i \lambda_i \hat{E}_i
\]

\[
= \frac{1}{2} (F_R + F_L) - \frac{1}{2} ([F]_A + [F]_B + [F]_C)
\]  \hspace{1cm} (3.15)
where subscript $R$ and $L$ represent right and left state respectively, $\lambda_i$ are eigenvalues, $E_i$ are eigenvectors, $\alpha_i$ are corresponding wave strengths, and $^\wedge$ indicates Roe averaged quantity. The $[F]_A$ term corresponding to the repeated eigenvalues $\lambda_i = u$ can be written as

$$[F]_A = (\rho - \frac{[p]}{\hat{a}^2}) |\hat{u}| \begin{bmatrix} \hat{\rho}_i \\ \hat{u} \\ \hat{v} \\ \hat{e}_v \\ \hat{H} - \hat{a}^2/(\hat{\gamma} - 1) \end{bmatrix} + \hat{\rho} |\hat{u}| \begin{bmatrix} \rho_i/\rho \\ 0 \\ [v] \\ [e_v] \\ \theta \end{bmatrix}$$

(3.16)

where

$$[(\cdot)] = (\cdot)_R - (\cdot)_L$$

$$\theta = [e_v] - \sum_{i=1}^{N_s} \hat{\Psi}_i [\rho_i/\rho] + \hat{v} [v]$$

$$\Psi_i \equiv \frac{1}{\hat{\gamma} - 1} \frac{\partial p}{\partial \rho_i} = \frac{R_i T}{\hat{\gamma} - 1} - e_{eq,i} + \frac{u^2 + v^2}{2}$$

$$\hat{\gamma} = \frac{\hat{C}_p}{\hat{C}_v} = \frac{C_{p,t} + C_{p,r}}{C_{v,t} + C_{v,r}}$$

$$R = \hat{R}/M_a$$

The $[F]_B$ and $[F]_C$ terms which are contributions from the eigenvalues $\lambda_i = u \pm a$, are found to be

$$[F]_{B,C} = \frac{1}{2 \hat{a}^2} (|p| \pm \hat{\rho} \hat{a}|u|) (\hat{u} \pm \hat{a})$$

(3.17)

When equations 3.16, 3.17 are inserted into equation 3.16 to get the cell-face flux, the absolute values of the wave speeds should be substituted in equations 3.16 and 3.17.

Similarly, the cell-face flux in $y$-direction can be written as

$$G_{j+1/2} = \frac{1}{2} (G_U + G_L) - \frac{1}{2} ([G]_A + [G]_B + [G]_C)$$

(3.18)
and $[G]_A$, $[G]_B$ and $[G]_C$ terms can be found similarly as in the $x$ direction.

Following the derivation of Grossman and Cinnella, the Roe-averaged quantities are determined to be

$$ r \equiv \sqrt{\rho_R / \rho_L} $$

$$ \hat{\rho} = \sqrt{\rho_R \rho_L} $$

$$ \hat{u} = \frac{u_L + ru_R}{1 + r} $$

$$ \hat{v} = \frac{v_L + rv_R}{1 + r} $$

$$ \hat{\rho}_i = \frac{(\rho_i)_R + r(\rho_i)_L}{\hat{\rho}_i(1 + r)} \quad i = 1, \cdots, N_s $$

$$ \hat{e}_v = \frac{(e_v)_L + (e_v)_R}{1 + r} $$

$$ \hat{H} = \frac{H_L + rH_R}{1 + r} $$

$$ \hat{\psi} = \frac{R_i \hat{T}}{\hat{\gamma} - 1} - \hat{e}_i + \frac{\hat{u}^2 + \hat{v}^2}{2}, \quad i = 1, \cdots, N_s \quad (3.19) $$

$$ \hat{a}^2 = (\hat{\gamma} - 1) \left( \hat{H} - \frac{\hat{u}^2 + \hat{v}^2}{2} + \hat{C}_v^* \hat{T} - \sum_{i=1}^{N_s} \hat{\rho}_i \hat{e}_i - \hat{e}_v \right) $$

$$ \hat{T} = \frac{T_L + rT_R}{1 + r} $$

$$ \hat{C}_v^* = \sum_{i=1}^{N_s} \hat{\rho}_i C_{v,i}^* \quad \text{where} \quad C_{v,i}^* = \frac{1}{[T]} \int_{T_L}^{T_R} \tilde{C}_v^i dT = C_{v,i}^i + C_{v,r}^i $$

$$ \hat{\gamma} = 1 + \frac{\hat{R}}{\hat{C}_v^*} $$

$$ \hat{R} = \frac{(\hat{R})_L + (\hat{R})_R}{1 + r}, \quad \text{where} \quad \hat{R} = \sum_{i=1}^{N_s} \frac{\rho_i}{\rho} R_i $$

For added spatial accuracy, higher-order approximation using the MUSCL approach can be applied. When the MUSCL approach is employed, the primitive variables of right and left states at the cell interface are evaluated using the following
extrapolation formulas [40]:

\[ q^L_{i+1/2} = q_i + \frac{1-\kappa}{4} \delta^+ q_{j-1/2} + \frac{1+\kappa}{4} \delta^- q_{j+1/2} \]
\[ q^R_{i+1/2} = q_{i+1} - \frac{1+\kappa}{4} \delta^+ q_{j+1/2} - \frac{1-\kappa}{4} \delta^- q_{j+3/2} \]  

(3.20)

where \( q \) is any primitive variable, superscript \( L \) and \( R \) represent left and right extrapolation respectively, and the value of \( \kappa \) determines the type of extrapolation method such that

\[
\kappa = \begin{cases} 
-1 & \text{2nd order upwind scheme} \\
1/3 & \text{3rd order upwind scheme} \\
1 & \text{2nd order classic centered scheme}
\end{cases}
\]  

(3.21)

In the above equations, the slopes of the variables are limited to prevent nonphysical oscillations and to preserve the TVD (Total Variation Diminishing) property. The limited slopes can be written using minmod limiter as follows:

\[
\delta^- q_{i+1/2} = \min \mod(\delta q_{i+1/2}, \omega \delta q_{i-1/2})
\]
\[
\delta^+ q_{i+1/2} = \min \mod(\delta q_{i+1/2}, \omega \delta q_{i+3/2})
\]  

(3.22)

The minmod limiter is a function that selects the smallest number from a set when all have the same sign but is zero if they have different signs such that

\[
\min \mod(x, y) = \begin{cases} 
x & \text{if } |x| < |y| \text{ and } xy > 0 \\
y & \text{if } |x| > |y| \text{ and } xy > 0 \\
0 & \text{if } xy < 0
\end{cases}
\]  

(3.23)

with the limits on \( \omega \) given as

\[ 1 \leq \omega \leq \frac{3 - \kappa}{1 - \kappa} \]  

(3.24)
3.4 Source Terms and Jacobian

The Jacobian of the source terms needs to be developed. This arises from the point implicit treatment of source terms. The vector of conserved variables $U$ and the vector of source terms $S$ for axisymmetric flow are rewritten here for convenience.

$$
U = \begin{bmatrix}
\rho_s \\
\rho u \\
\rho v \\
\rho e_v \\
\rho E
\end{bmatrix}, \quad S = \begin{bmatrix}
w_s \\
0 \\
p/y \\
w_v \\
0
\end{bmatrix}
$$

where

$$
w_s = M_s \sum_{r=1}^{N_a} (\beta_{s,r} - \alpha_{s,r})(R_{f,r} - R_{b,r})
$$

$$
w_v = \frac{\rho C_{v,v}}{\tau_v} (T - T_v) + \sum_s w_s e_{d,s}
$$

The second term in $w_v$ is the average vibrational energy created or destroyed according to the mass production rate. If preferential reaction of molecules is assumed (i.e., a molecule in a higher vibrational state is more likely to react and be depleted, and molecules produced are more likely to be in a higher vibrational state), then $e_{d,s}$ should be larger than the average vibrational energy $e_{v,s}$ of the system. At the same time it should be smaller than the dissociation energy of the molecule [43]. One of Chul Park’s models [48] for preferential reaction is used here such that

$$
e_{d,s} = 0.3 \tilde{D}_s, \quad \text{where} \quad \tilde{D}_s; \text{ dissociation energy of molecules}
$$

Since the term $w_s$ depends explicitly on the species density and temperature, the Jacobian of $w_s$ with respect to $U$ is evaluated using the chain rule such that

$$
\frac{\partial w_s}{\partial U_j} = \frac{\partial w_s}{\partial U_j} \bigg|_{T} + \frac{\partial w_s}{\partial T} \bigg|_{U} \frac{\partial T}{\partial U_j}
$$
Partial derivatives of $w_s$ can be obtained directly from the partial derivatives of the reaction rates.

$$
\frac{\partial R_{f,r}}{\partial \rho_s} \bigg|_T = \frac{\alpha_{s,r}}{\rho_s} R_{f,r}, \\
\frac{\partial R_{b,r}}{\partial \rho_s} \bigg|_T = \frac{\beta_{s,r}}{\rho_s} R_{b,r}, \\
\frac{\partial R_{f,r}}{\partial T} \bigg|_U = \left(N_{f,r} + \frac{E_{f,r}}{RT}\right) \frac{R_{f,r}}{T}, \\
\frac{\partial R_{b,r}}{\partial T} \bigg|_U = \left[(N_{f,r} - N_{c,r}) + \frac{(E_{f,r} - E_{c,r})}{RT}\right] \frac{R_{b,r}}{T}
$$

(3.28)

Equation 3.27 is made complete by defining the partial derivatives of temperature which are found to be

$$
\rho C_{v,\text{tr}} \frac{\partial T}{\partial U_j} = \begin{cases} 
\frac{u^2 + v^2}{2} - e_{eq,j} , & j = 1, \cdots, N_s \\
-u , & j = N_s + 1 \\
-v , & j = N_s + 2 \\
-1 , & j = N_s + 3 \\
1 , & j = N_s + 4
\end{cases} 
$$

(3.29)

where

$$
C_{v,\text{tr}} = C_{c,t} + C_{v,r}
$$

The partial derivatives of the vibrational energy production rate can be written as

$$
\frac{\partial w_v}{\partial U_j} = \frac{\rho C_{v,v}}{\tau_v} \left( \frac{\partial T}{\partial U_j} - \frac{\partial T_v}{\partial U_j} \right) + \sum_s \frac{\partial w_s}{\partial U_j} e_{d,s}
$$

(3.30)

All of the terms in this equation are described if the partial derivatives of the vibrational temperature is additionally defined to be [49]

$$
\rho C_{v,\text{tr}} \frac{\partial T}{\partial U_j} = \begin{cases} 
-e_{v,j} , & j = 1, \cdots, N_s \\
0 , & j = N_s + 1 \\
0 , & j = N_s + 2 \\
1 , & j = N_s + 3 \\
0 , & j = N_s + 4
\end{cases} 
$$

(3.31)
The last term to be considered is due to the axisymmetric formulation of the equation set, and is written as
\[
\frac{\partial (p/y)}{\partial U_j} = \frac{1}{y} \frac{\partial p}{\partial U_j}
\]  
(3.32)
where the pressure derivatives are found to be
\[
\frac{1}{\bar{\gamma} - 1} \frac{\partial p}{\partial U_j} = \begin{bmatrix}
\xi_j & , & j = 1, \ldots, N_s \\
u & , & j = N_s + 1 \\
v & , & j = N_s + 2 \\
-1 & , & j = N_s + 3 \\
1 & , & j = N_s + 4 
\end{bmatrix}
\]  
(3.33)
and
\[
\xi_j = \frac{R_j T}{\bar{\gamma} - 1} - e_{eq,j} + \frac{u^2 + v^2}{2}
\]

3.5 Temperature Calculation

The conserved variables at each cell center are updated using the equation 3.12 or 3.13 by a matrix inversion scheme. From these conserved variables, new values of the primitive variables, \(\rho, u, v, e_v, E\) are easily obtained. However, to close the problem, the temperature and vibrational temperature are determined at each iteration cycle. In order to obtain the temperatures, a Newton–Raphson method is used in the following manner [43, 49]:
\[
T^{(k+1)} = T^{(k)} + \frac{\rho e - \sum_s \rho_s e_s (T^{(k)}, T^{(k)}_v)}{\rho C_{v,ir}}
\]
(3.34)
\[
T^{(k+1)}_v = T^{(k)}_v + \frac{\rho e_v - \sum_s \rho_s e_{v,s} (T^{(k)})}{\rho C_{v,v}}
\]
While total internal energy \(e\) and vibrational energy \(e_v\) are directly obtained from the updated conservative variables, species internal energies \(e_s\) and vibrational energies \(e_{v,s}\)
are calculated from the gas model using the current values of both temperatures. The iteration is carried out until converged values of both temperatures are obtained.
CHAPTER 4
VALIDATION STUDIES

4.1 H₂—Air Reaction Model

The major application of this study includes initiation and propagation of detonation waves for a mixture of hydrogen and air that can be used in a pulse detonation engine. The proper chemical reaction model needs to be selected from several different models available for this gas mixture, from the complex to the simplest. The scope of this research includes the construction of a numerical simulation model for PDE’s and the actual application of this tool to various calculations, which should be efficient enough to be used in the parametric studies, as well as accurate enough to be used in the analysis and design. The introduction of detailed chemical reaction mechanisms can often cause excessive computing time and storage requirement, since the number of equations solved is directly dependent upon the number of species involved in the reactions. A simple chemistry mechanism, while still modeling the overall nature of the reactions with reasonable accuracy, can be a desirable choice.

The two-step reaction model proposed by Rogers and Chinitz [50] is used in this study. This model was developed to represent H₂—Air chemical kinetics with as few reaction steps as possible while still giving reasonably accurate global results. This model consists of the following two steps:

\[
\begin{align*}
H_2 + O_2 & \leftrightarrow 2OH \\
2OH + H_2 & \leftrightarrow 2H_2O
\end{align*}
\]
where the forward reaction rate constants are given by

\[
K_{f,r} = A_{f,r}(\phi) T^{N_{f,r}} \exp(-E_{f,r}/\bar{R}T)
\]  \hspace{1cm} (4.2)

and the pre-exponential \( A_{f,r}(\phi) \) is a function of the equivalence ratio \( \phi \), the fuel-to-air ratio divided by the stoichiometric fuel-to-air ratio. Values of the parameters used in this model are

\[
\begin{align*}
A_{f,1}(\phi) &= [8.917\phi + (31.433/\phi) - 28.950] \times 10^{47} \text{ cm}^3/\text{mole-s} \\
N_{f,1} &= -10 \\
E_{f,1} &= 4,865 \text{ cal/mole}
\end{align*}
\]  \hspace{1cm} (4.3)

\[
\begin{align*}
A_{f,2}(\phi) &= [2.000 + (1.333/\phi) - 0.833\phi] \times 10^{54} \text{ cm}^6/\text{mole}^2\text{-s} \\
N_{f,2} &= -13 \\
E_{f,2} &= 42,500 \text{ cal/mole}
\end{align*}
\]  \hspace{1cm} (4.4)

The backward reaction rate can be obtained from

\[
K_{b,r} = K_{f,r}/K_{c,r}
\]  \hspace{1cm} (4.5)

where the equilibrium constant \( K_{c,r} \) is given by

\[
K_{c,r} = A_{c,r} T^{N_{c,r}} \exp(-E_{c,r}/\bar{R}T)
\]  \hspace{1cm} (4.6)

where

\[
\begin{align*}
A_{c,1} &= 26.164 \times 10^3 \text{ cm}^3/\text{mole-s} \\
N_{c,1} &= 0 \\
E_{c,1} &= 17,867 \text{ cal/mole}
\end{align*}
\]  \hspace{1cm} (4.7)

\[
\begin{align*}
A_{c,2} &= 2.682 \times 10^{-3} \text{ cm}^6/\text{mole}^2\text{-s} \\
N_{c,2} &= 1 \\
E_{c,2} &= -137,930 \text{ cal/mole}
\end{align*}
\]  \hspace{1cm} (4.8)

This model is valid for initial temperatures of 1,000–2,000 K and equivalence ratios of 0.2–2.0. Since the chemistry model is not valid below temperature of 1,000 K, an ignition temperature must be specified.
Nitrogen is also counted as a collisional partner in the thermodynamic model and the relaxation process, but not included in the chemical reaction model since the maximum temperature in hydrogen-air reaction does not reach the dissociation temperature of Nitrogen.

4.1.1 Local Ignition Averaging Model

Before an actual calculation using the flow solver is made, the chemical kinetic model needs to be examined to see how each species concentration is changing, and on what time scale. This may provide some insight on the stiffness of the system and some clues to establish a flow solver time step that permits species concentrations to follow the correct kinetics.

The mass production rate equation 2.35 can be independently integrated using the reaction data in equations 4.2–4.8 to yield the species mass fraction history. The typical result obtained using a Runge–Kutta integration method is in figure 4.1. The mass fraction of OH is shown to rise very rapidly as soon as the ignition starts. The OH production reaction is instantaneous at its initial stage and goes to equilibrium very quickly in less than $10^{-11}$ seconds. After that, the reactions seem to remain in equilibrium until H$_2$O production reaction begins around $10^{-9}$ seconds. It is interesting to note that all these major changes in the species concentrations take place within the first $10^{-7}$ seconds, a time interval that is a typical fluid dynamic time step. Moreover, the integration time step should remain at or below $10^{-12}$ seconds to ensure stable integration using the Runge–Kutta scheme, and to properly follow the chemical kinetics. This shows the stiffness of the chemical reaction model.

From the above observation, it could be deduced that the integration time step for the flow solver should be the order of $10^{-12}$ seconds or less to properly include the
Figure 4.1. Species mass fraction history from chemical kinetics.

chemical kinetics. Moreover, it should be much less than this order in regions of OH production. However, it is practically impossible to use this small time step in the flow solver. When using $10^{-12}$ seconds as a flow solver time step, the order of $10^9$ integration steps might be needed to solve a typical detonation wave propagation problem which has a time scale of interest of the order of $10^{-3}$ seconds. This would result in $10^4$ days of CPU time when 1 second of CPU time per computation cycle, which is a proper estimate for this code on a typical front-end workstation, is assumed. Fortunately, however, most of this stiffness problem can be taken care of by the point implicit treatment of source terms, as explained in section 3.2, through effectively rescaling all the characteristic time scales involved. Thus, a typical fluid dynamic time step of the order of $10^{-7}$ seconds can be safely used throughout the calculation, since the species production rates during this time interval can be properly treated by the effective rescaling of the chemical reaction time scale.
However, the very first time step where all the drastic changes take place within that short period of time cannot be properly described by rescaling time alone. Another special treatment for the igniting cell is needed to be able to use a typical flow solver time step. For this purpose, a Local Ignition Averaging Model (LIAM) is proposed here. The basic idea of this model comes from the fact that the species mass fractions are changing drastically in a very short period of time as soon as ignition starts, and goes to equilibrium soon afterwards. LIAM separates the cell in which the ignition condition is met, and then integrates the chemical kinetics equations alone for that cell. A time step less than $10^{-12}$ seconds is used in the integration within the interval of the flow solver time step. The average production rate of each species during this time interval is then estimated using

$$w_s = \frac{\Delta \rho_s}{\Delta t_f}$$

(4.9)

where $\Delta \rho_s$ is the density change of species $s$ obtained from a separate integration of chemical kinetic equations during this time interval, and $\Delta t_f$ is the flow solver time step. The average value of the forward reaction rate for each reaction during this time interval can be estimated from the following relations.

$$R_{f,1} = -\frac{W_{O_2}}{M_{O_2}}, \quad R_{f,2} = \frac{W_{OH}}{2M_{OH}}$$

(4.10)

These terms need to be obtained for the calculation of the source term Jacobian. Here, backward reaction rates during this first reaction time step are assumed to be zero.

LIAM turns out to work well together with the point implicit scheme to accurately describe chemical kinetics in the flow solver using a typical flow solver time step of $10^{-7}$ seconds. Figure 4.2 shows calculated results of the species mole fraction history at a fixed location inside the detonation chamber initially filled with hydrogen–air mixture. Excellent agreement can be seen with the equilibrium concentration data from the CEA.
code [51]. This assures that the chemical kinetics are properly modeled and coupled to the flow solver.

![Graph showing species mole fraction history from the flow solver.](image)

Figure 4.2. Species mole fraction history from the flow solver.

### 4.1.2 Species Density Limiter

For a stoichiometric mixture, it is natural that mass fractions of both oxygen and hydrogen species become nearly zero when the reactions reach equilibrium. For some cases, however, the densities of one or more species may have very small negative densities during the reaction process as a result of truncation errors in the integration. This may cause a failure of computation. To prevent this negative density, the following density limiter is introduced.

\[
\begin{align*}
\rho^n_s + \Delta \rho^n_s & \leq 0 \quad ; \quad \rho^{n+1}_s = \rho^n_s \\
\text{otherwise} & \quad ; \quad \rho^{n+1}_s = \rho^n_s + \Delta \rho^n_s
\end{align*}
\]  

(4.11)
\[
\rho_s^{n+1} = \frac{\sum_{i=2}^{N_s} (\rho_i^n + \Delta \rho_i^n)}{\sum_{i=2}^{N_s} \rho_i^{n+1}}
\]

4.2 Various Tests and Verification

Various tests are performed in this section to evaluate efficiency, accuracy, and robustness of the present numerical model for calculations of unsteady detonation wave propagation.

4.2.1 Qualitative Overlook

A typical calculated result showing the formation and the propagation of a detonation wave is presented in this section to assure that qualitatively correct behavior of the detonation wave is predicted. Dimensional variables and physical lengths are used to simplify later validation with available raw experimental data. Figures 4.3—4.6 show a detonation wave travelling into a quiescent hydrogen—air mixture initially at 1 atmosphere pressure and 298.15 K temperature. Ignition has been initiated near the left-end wall. These figures show the time evolution of pressure, density, temperature, and particle velocity profiles, respectively, as a function of distance from the initiation point.

The first thing that can be observed from this result is the self-sustaining nature of the propagating detonation wave, with limiting values of the variables which may correspond to the CJ state. The shape of the wave can be seen to adequately follow the usual description of a detonation wave. A strong shock wave that is the leading part of a detonation front compresses the gas mixture, and the chemical reactions are triggered by a temperature rise from this strong shock compression. A balance is maintained such
Figure 4.3. Time evolution of detonation pressure profiles.

Figure 4.4. Time evolution of detonation density profiles.
Figure 4.5. Time evolution of detonation temperature profiles.

Figure 4.6. Time evolution of particle velocity profiles.
that the leading shock is supported in turn by the energy released from the chemical reactions. The expansion of burned gas immediately follows thereafter to match the boundary condition, and the values in the constant region are determined to meet the left wall boundary condition of zero velocity.

A closer examination of the detonation wave front shows the interesting features of the CJ state. Figure 4.7 shows the time histories of pressure and temperature for a typical detonation wave at a fixed location. Figure 4.8 shows the enlarged portion of the detonation front that corresponds to the dotted circle of figure 4.7. It is interesting to note the discrepancy in the peaks of pressure and temperature, and this can be explained from the simple picture of detonation theory of the Zeldovich–von Neumann–Doering (ZND) model as a time lag between the ZND spike and the CJ state. The CJ point is defined as the final state of the reaction zone which corresponds here to the peak point in the temperature history, whereas the peak value in the pressure history corresponds to the ZND spike. Practically, the residence time of the ZND spike is so short that its contribution to the total impulse seems to be negligible. Therefore, interest in further calculations for the validation and the application is in the CJ state, with a qualitatively correct description of the detonation front.

Another interesting feature often used as a confirmation of the CJ state is that the downstream speed at the CJ plane is locally sonic with respect to the moving shock front, as reviewed in section 1.1. Figure 4.9 depicts the downstream Mach number relative to the shock front together with the pressure, where both values are taken at the final state of the reaction zone. The data are taken from the same calculation as shown in figure 4.3. The downstream Mach number is observed to converge to unity at some distance from the initiation point, and it is interesting to note that the pressure also converges to a limiting value at the same distance. Therefore, it can be said that
Figure 4.7. Profile of typical detonation wave.

Figure 4.8. Profile of typical detonation wave front.
this propagating detonation wave reaches the CJ state at the corresponding distance of convergence, and that the limiting value reached at this distance corresponds to the CJ value of this simulation. This confirms in another way that the wave front and the corresponding CJ properties of a detonation wave are properly described.

![Graph showing Detonation Pressure and Downstream Mach Number](image)

Figure 4.9. Downstream Mach number and convergence to CJ state.

4.2.2 Spatial and Temporal Accuracy

Generally speaking, a higher-order scheme may yield more accurate results, in turn requiring more computing time. As explained in chapter 3, the present computer model accommodates the options to choose numerical schemes of both space and time integration up to third-order accuracy. For temporal accuracy, Euler integration for first-order, two-step Runge–Kutta(RK) integration for second-order, and three-step RK for third-order are contained in the computer. And for the spatial accuracy, the MUSCL approach is prepared for the higher-order approximations. The purpose of this
section is to study the effect of the order of the numerical schemes on the predicted detonation wave. The results of this study can then be used to select the order of the scheme necessary to provide adequate resolution of the physical process.

Figure 4.10 shows a comparison of detonation wave pressure profiles along a detonation chamber when numerical schemes of different order of accuracy are implemented. This figure compares detonation wave profiles, propagating into the quiescent hydrogen–air mixture initially at 1 atmosphere pressure. The higher-order calculation captures the higher peak pressure as expected. However, it is interesting to note that the second-order calculation is close to the third-order calculation, and that the overall shapes of the two waves are almost the same.

![](image)

Figure 4.10. Wave profiles from different order of accuracy.

This convergence trend can be seen more clearly in figures 4.11–4.14. Figure 4.11 shows detonation wave velocities, and figures 4.12–4.14 depict pressure, density, and
Figure 4.11. Detonation velocities from different order of accuracy.

Figure 4.12. Detonation pressures from different order of accuracy.
Figure 4.13. Detonation densities from different order of accuracy.

Figure 4.14. Detonation temperatures from different order of accuracy.
temperature at the CJ plane of the detonation waves, respectively, as a function of
distance from the initiation point for each scheme. From this observation, a second-
order calculation is a reasonable choice when efficiency and accuracy are considered
together. Thus, a second-order accurate scheme in both space and time is employed to
be used for further calculations, unless otherwise noted.

4.2.3 Mesh Convergence

A mesh convergence test is performed to determine the proper mesh size to insure
accurate resolution of the physical process. The same configuration and parameters are
used as before but with different mesh sizes. A second-order accurate scheme in both
space and time is used throughout the calculation.

Figure 4.15 shows detonation wave profiles resulting from three different mesh
sizes. Actual dimensional sizes of 5.0, 2.5, and 0.5 mm are used, respectively, in mod-
eling a two-meter long tube with planar initiation model. For calculations of both 5.0
and 2.5 mm mesh size, a time step of $10^{-7}$ seconds has been used successfully to yield
stable solutions. However, for the smallest mesh size of 0.5 mm, a smaller time step of
$5 \times 10^{-8}$ seconds has been used, since a time step of $10^{-7}$ seconds does not yield a stable
solution for this mesh size. The calculated results are summarized in figures 4.16–4.19.

The convergence trend can be seen clearly from these figures which depict deto-
nation wave velocities, and the CJ plane values of pressure, density, and temperature of
the detonation waves, respectively, along the distance from an initiation point for each
mesh size used. The results of 2.5 mm mesh shows almost converged values to the 0.5
mm mesh, in detonation velocity as well as in overall wave shape. The non-monotonic
convergence trends observed in the pressure and density profiles seem to be due to the
inconsistent time step used. If we assume the computing time of 2.5 mm mesh case to
Figure 4.15. Wave profiles from different mesh sizes.

Figure 4.16. Detonation velocities from different mesh sizes.
Figure 4.17. Detonation pressures from different mesh sizes.

Figure 4.18. Detonation densities from different mesh sizes.
Figure 4.19. Detonation temperatures from different mesh sizes.

be 1 CPU, then the corresponding computing times of 5.0 mm and 0.5 mm case will be about 1/4 CPU and 50 CPU, respectively, for two-dimensional calculation. When we take into account accuracy as well as efficiency in choosing mesh size, mesh size of 2.5 mm can be a reasonable choice. This mesh size will be used throughout on further calculations, if no additional comment is given.

4.2.4 Independence on the Geometry

The properties of fully developed detonation waves should be the same regardless of the geometry involved whenever the initial condition and composition of the fuel–air mixture are the same. Four different calculations are performed here to confirm the results to follow this known postulate. We take four cases with two kinds of geometry and two initiation methods, which are two-dimensional calculations with planar initiation and with point initiation, and repeat for axi-symmetric flow with the
same initiation methods. The calculation domain is 68.5 cm × 3.75 cm for both and filled with stoichiometric hydrogen—air mixture. Initiation occurs near the left-end wall.

Figures 4.20–4.23 show pressure contour plots at specified times for the above four combinations of geometry. The resulting shapes of the propagating detonation wave can be observed from these figures. It is interesting to note that the formation of a planar detonation wave is clearly captured. In figure 4.21 and 4.23, a planar wave can be observed to evolve from a spherical wave originated from a point initiation through the interactions of the reflecting waves. The interaction of the waves and the formation of the resulting detonation wave can be seen more easily in figures 4.24 and 4.25 that depict the time evolution of the pressure profiles along the center line. The large jump in the pressure behind the wave front emerging after 50 μsec is due to the reflection of waves from the circumferential wall. It is interesting to note that this reflecting wave finally catches up the wave front to form a fully developed detonation wave.

The calculated results are summarized in figures 4.26 and 4.27. These figures show detonation wave velocities and the CJ plane pressures, respectively, along two different lines which are lower boundary (actually, center line) and upper wall. For point initiation cases, detonation velocities and the pressures on the axis are observed to remain lower than those of planar initiation cases and keep increasing, while the detonation velocities and the pressures on the wall are much higher than those of planar initiation cases and keep decreasing until the formation of the planar wave. The higher pressure and velocity on the wall are due to the reflection of the detonation wave. It is interesting to note that the detonation velocities and the pressures for all four cases converge to the same value at a certain distance from the initiation point where fully developed planar waves are formed. And this result confirms the known postulate previously stated.
Figure 4.20. Planar initiation in 2D geometry.
Figure 4.21. Point initiation in 2D geometry.
Figure 4.22. Planar initiation in axi-symmetric geometry.
Figure 4.23. Point initiation in axi-symmetric geometry.
Figure 4.24. Early profiles of pressure propagation.

Figure 4.25. Developing profiles of pressure propagation.
Figure 4.26. Detonation velocities from different geometries in use.

Figure 4.27. Detonation pressures from different geometries in use.
4.3 Comparison with Theoretical CJ and Test Data

The calculated detonation wave properties are finally compared with the theoretical CJ data to validate the present numerical model for unsteady detonation wave propagation. Since the property of the fully developed detonation wave is converging to the same value regardless of the geometry involved as seen in the previous section, and since we are interested in the final converged state of the CJ condition, calculations can be properly performed on the one-dimensional planar geometry for the sake of efficiency.

The computational domain is, thus, composed of a detonation tube of semi-infinite length filled with a mixture of hydrogen and air initially at 1 atmosphere and 298.15 K. The detonation is initiated just adjacent to the left-end wall, and the planar wave propagates to the right through the quiescent gas mixture. Figures 4.28–4.30 show the resulting detonation wave properties when the equivalence ratios of the gas mixture are 0.75, 1.0, and 1.5, respectively. The detonation wave velocity, pressure, density, and temperature as a function of distance from an initiation point are recorded and compared with the theoretical CJ data. The theoretical CJ data are obtained from the CEA code [51]. The converging trend of all the variables of the detonation wave is confirmed in each calculation of different equivalence ratios. These converged values can be compared to the theoretical CJ data. The results are summarized in figure 4.31, which depicts the converged values of each detonation variable with varying equivalence ratios, and compares these values with the theoretical CJ data. Excellent agreement between them is observed.

An additional calculation has been done to simulate the test performed by Hinkey, et al [52]. The thrust wall pressure history was measured in this test, when the detonation is initiated near the left-end thrust wall and is propagating into the two inch
Figure 4.28. Comparison with theoretical CJ data when $\phi=0.75$. 
Figure 4.29. Comparison with theoretical CJ data when $\phi=1.0$. 
Figure 4.30. Comparison with theoretical CJ data when $\phi=1.50$. 
Figure 4.31. Comparison with theoretical CJ data.
diameter detonation tube filled with stoichiometric mixture of hydrogen and air initially at 1 atmosphere and 298 K. Figure 4.32 shows the measured thrust wall pressure history, and figure 4.33 shows the computed thrust wall pressure history of a simulated experiment utilizing the Mozart code originally developed at NASA Ames. The result from the present simulation model for the same configuration is found in figure 4.34, and a good agreement with the test result is observed in an overall shape of the pressure history. In the test result, the wall pressure is observed to reach the post-detonation pressure by the retonation wave. In the calculation, however, the wall pressure does not reach the CJ level since a direct initiation is forced on the cells adjacent to the thrust wall. Although a similar pressure level might be reached if a different initiation model is implemented to properly simulate the retonation wave, the pressure peak does not contribute much to the total impulse due to the short period of time. Excellent agreement is seen, instead, in the pressure level and the duration of the steady region before the rarefaction wave from the open end of the tube quickly reduces the pressure. The pressure in this region is the main contribution to the total impulse.

![Figure 4.32. Thrust wall pressure measurement by Hinkey, et al.](image-url)
Figure 4.33. Thrust wall pressure prediction using Mozart code.

Figure 4.34. Thrust wall pressure prediction using the present model.
CHAPTER 5

STUDIES ON THE DETONATION INITIATION

Initiation of detonation may be achieved either by transition from deflagration or by deposition of energy to directly initiate the detonation. Deflagration-to-detonation transition (DDT) can be said to be a sudden evolution of a turbulent flame into a self-sustaining detonation [53]. DDT has been observed in experiments as a complex process involving deflagration, shocks and shock reflections, boundary layers, and all of their mutual interactions, but exactly how DDT occurs remains unclear. Although there has been recent progress towards a full understanding of DDT [53, 54], accurate and predictive modeling of the process is a very difficult task [35]. The simulation of this process constitutes another research topic, and it is outside scope of the current project. This may require that some other physical phenomena not considered in the present simulation model such as thermal conduction, molecular diffusion, etc., be included in the model for a gas-phase flame simulation, as well as the implementation of a more detailed chemical reaction model.

On the other hand, the direct initiation of detonation can be achieved from the deposition of energy into the gas either by an electrical discharge or by a laser. The process in which the hot spot created from the energy deposition develops into a shock wave of sufficient strength and finally a self-sustaining detonation wave can be simulated using the present model. Therefore, throughout the calculations, it is assumed that some method of directly initiating the detonation is implemented, or that the length for transition from deflagration to detonation is sufficiently short to avoid modeling the
DDT process. The purpose of this chapter is to derive the criteria for direct initiation, as well as a proper initiation model to yield self-sustaining CJ detonation, from the observations of the effect of hot spot conditions such as pressure, temperature, size, and their combinations on detonation.

5.1 Independence on the Initiation Models

There are different ways to create a hot spot for the simulation of energy deposition. The sequence of events occurring in the hot spot when depositing energy consists of the exposure of a portion of gas mixture to a high temperature for a certain period of time, triggering of chemical reactions, energy release from the reactions, and formation of a high pressure and high temperature spot. One way of modeling a hot spot is just to raise the temperature of the corresponding cells and let it start from the chemical reactions. This will be called the "reacting hot spot (RHS)". Another way is to assign a certain condition of pressure, temperature, and species concentration as a modeling of after-burn condition to the corresponding cells. This is called the "equilibrium hot spot (EHS)" approach.

The first series of calculations is performed on a one-dimensional planar initiation. A detonation tube of infinite length is filled with a stoichiometric mixture of hydrogen and air at 1 atm and 298.15 K, and a hot spot is modeled by two cells just adjacent to the left-end wall. A series of calculations is performed for the RHS with varying initial temperature and pressure at the hot spot. Figures 5.1 and 5.2 show the history of the build-up of temperature and pressure at the hot spots for different initial conditions. The reason for choosing these temperatures is that the validation range of initial temperature for the current chemical reaction model is 1,000–2,000 K. The resulting profiles of the propagating detonation wave is shown in figures 5.3–5.7.
Figure 5.1. Histories of temperature build-up in the hot spot.

Figure 5.2. Histories of pressure build-up in the hot spot.
Figure 5.3. Wave profiles for RHS of $T=1100K$, $p=3.7$ atm.

Figure 5.4. Wave profiles of RHS of $T=1500K$, $p=5.0$ atm.
Figure 5.5. Wave profiles of RHS of $T=2000\text{K}$, $p=6.7\text{atm}$.

Figure 5.6. Wave profiles of RHS of $T=1500\text{K}$, $p=15.0\text{atm}$.
Figure 5.7. Wave profiles of RHS of $T=1500K, p=50.0$atm.

An interesting result shown in these figures is that the properties of the propagating detonation waves finally converge to the same values, regardless of the different initial conditions and the resulting differences in the early stage build-up of temperature and pressure in the hot spot.

Another series of calculations has been performed for EHS for the same configuration. A wide variety of hot spot conditions has been tested including some extreme cases. Figures 5.8–5.10 show the typical results. Pressure profiles of propagating detonation waves are shown for different hot spot conditions. The same trend as in the RHS approach can be observed in these figures. This can be seen more clearly in figures 5.11–5.14, which summarize the EHS results together with those of the RHS. These figures depict detonation velocities, pressures, densities, and temperatures as a function of distance from the initiation point. It is very interesting to note that no matter what the hot spot conditions are, the properties of the propagating detonation
wave always converge to the same limiting values. In some over-driven cases, the detonation velocities and peak pressures are observed to decrease to the limiting values, and in under-driven cases to increase to the same values. The limiting values can be shown to be CJ state for the given condition. This can be further confirmed from figure 5.15 that shows the downstream Mach number relative to the detonation wave front. The downstream Mach numbers of all the cases are observed to converge to unity at some distance from the initiation point, even though the converging paths are all different. This converged state of the sonic condition of downstream speed is, as reviewed in section 1.1, consistent with the CJ state.

![Image](image_url)

Figure 5.8. Wave profiles of EHS of $T=3000K$, $p=10atm$.

Therefore, virtually any initiation model can be chosen, that is appropriate for the intent of each calculation, as long as it ensures the formation of a self-sustaining detonation wave. If the final CJ state is of interest, then either $T = 1500 K$, $p = 50$
Figure 5.9. Wave profiles of EHS of $T=3000\text{K}$, $p=50\text{atm}$.

Figure 5.10. Wave profiles of EHS of $T=3000\text{K}$, $p=100\text{atm}$.
Figure 5.11. Detonation velocities with varying hot spot states.

Figure 5.12. Detonation pressures with varying hot spot states.
Figure 5.13. Detonation densities with varying hot spot states.

Figure 5.14. Detonation temperatures with varying hot spot states.
atm of RHS or $T = 3000$ K, $p = 100$ atm of EHS may be a proper choice of the hot spot state for an advantage of a fast convergence to the CJ state. On the other hand, if a more realistic simulation of the transient process in the formation of a detonation wave is of interest, then $T = 1500$ K, $p = 5$ atm of RHS may be an appropriate choice of the initiation model.

5.2 Critical Level of Energy Deposition

Another interesting result can be observed in figures 5.16—5.19 where the early stage profiles of pressure and temperature from two different hot spot conditions are shown. The initial hot spot condition of figures 5.16 and 5.17 is an equilibrium state of $T = 2000$ K, $p = 10$ atm, whereas the condition of figures 5.18 and 5.19 is an equilibrium state of $T = 1500$ K, $p=10$ atm, both of which are planar initiation cases. It is interesting to note that the entirely different results are obtained from the small
difference in the initial conditions. Figures 5.16 and 5.17 show a gradual increase in the pressure and the temperature that finally ends up with a successful formation and a propagation of a self-sustaining detonation wave. On the other hand, figures 5.18 and 5.19 show a gradual decrease in the pressure and the temperature that finally leads to the decay of the wave without forming a self-sustaining detonation wave. This result suggests that a certain critical level of energy exists with an initial temperature, pressure, and hot spot size, below which a successful initiation and propagation of a detonation wave does not take place. It is the object of this section to closely examine this critical hot spot condition.

![Graph showing pressure build-up for EHS of T=2000K, p=10 atm.](image)

Figure 5.16. Pressure build-up for EHS of $T=2000K$, $p=10\text{ atm}$.

An axi-symmetric configuration is chosen here for more realistic calculations. The calculation is performed on the 21 inch long, 3 inch inner diameter detonation tube filled with a stoichiometric mixture of hydrogen and air. The initiation occurs at the lower
Figure 5.17. Temperature build-up for EHS of $T=2000\text{K}$, $p=10\text{atm}$. 

The deposition of energy into a hot spot for direct initiation of detonation is simulated by increasing the temperature and the pressure of a certain portion of the gas mixture. The calculation starts from the chemical reactions initiated by the increased temperature in the hot spot. The deposited energy can be estimated from the resulting increase in the internal energy of the hot spot together with its size. For instance, when the temperature and the pressure of the hot spot increase to 1,500 K and 5 atm from the initial fuel–air mixture state of 298.15 K and 1 atm, the increase in the internal energy for the corresponding cells is $1.348 \times 10^6$ J/Kg, or $1.149 \times 10^6$ J/m$^3$ using a density of 0.8523 Kg/m$^3$. When the size of the hot spot is assumed to be 3×3 cells in the axial and radial directions with the mesh size of 2.5 mm, the total internal energy increase in the hot spot is 1.523 Joule. Although this value that reflects the resulting
Figure 5.18. Pressure build-up for EHS of $T=1500$K, $p=10$atm.

Figure 5.19. Temperature build-up for EHS of $T=1500$K, $p=10$atm.
increased level of internal energy may not be directly comparable to the energy level of a spark igniter or a laser, this can be used as a good estimation of the energy deposition in the hot spot.

Figures 5.20 and 5.21 show the typical results of successful and unsuccessful formation of a detonation wave, respectively. Figure 5.20 is the resulting pressure contour plot for a hot spot state of $T = 1500 \text{ K}$, $p = 10 \text{ atm}$, and a size of $3 \times 3$ meshes, the energy deposition of which is calculated to be 3.046 Joules. Figure 5.21 shows the results from the same initial set-up as figure 5.20 except for $p = 5 \text{ atm}$. The internal energy increase in the hot spot for this case turns out to be 1.523 Joules.

An extensive series of calculations has been performed with varying states and size of the hot spot. The results are summarized in figures 5.22 and 5.23. Figure 5.22 depicts the critical levels of the hot spot volume that lead to successful and unsuccessful formation of a detonation wave. The initial pressure in the hot spot is varied while the temperature of the hot spot is increased to 1,500 K. Here the energy density can be defined as the increased energy per unit volume, and can be obtained from the corresponding initial conditions of the hot spot, which turns out to be proportional to the initial pressure. An interesting result can be observed that there exists a certain critical condition of the hot spot for successful initiation. The expected trend can be also observed from this figure that the higher the energy density is, the smaller the size of the hot spot required to successfully initiate the detonation and vice versa. Figure 5.23 depicts the critical level of the energy deposition in the hot spot for both a successful and an unsuccessful formation of a detonation wave as a function of hot spot volume. It clearly shows the minimum level of the energy deposition in a hot spot for successful initiation. An interesting trend can be also observed that the critical energy level is not constant but increases as the volume of the hot spot increases, which means
Figure 5.20. Successful initiation for RHS of $T=1500\text{K}$, $p=10\text{atm}$. 
Figure 5.21. Unsuccessful initiation for RHS of $T=1500$K, $p=5$atm.
the minimum energy deposition required for a successful initiation is decreasing as the energy density of the hot spot is increasing.

![Graph showing critical volume of hot spot vs. pressure in hot spot.](image)

*Figure 5.22. Critical volume of hot spot.*

### 5.3 Reproduction of an Experimental Observation

A typical result of unsuccessful initiation presented in the previous section as figure 5.21 will be reviewed here and qualitatively compared with the experimental result. The initiation model for this case is just to increase the temperature of 3×3 hot spot to 1,500 K from the initial state of hydrogen—air stoichiometric mixture at 298.15 K and 1 atm. Figures 5.24 and 5.25 show the time evolution of the pressure and the temperature profiles, respectively, along the center line in the axial direction. Very slow (almost stationary) propagation of the flame front compared to the pressure
wave is observed especially after 40 $\mu$sec, and this results in the loss in synchronization between the compression by pressure wave and the reactions. In turn, the pressure wave is not supported by the energy release from the reactions, and finally ends up with the decaying wave.

A similar result was reported from the experiments performed on the same configuration as used in the above calculation [55]. In this experiment, the reactants were a stoichiometric mixture of hydrogen and oxygen, and an arc device located next to the left-end plate was used as an initiation mechanism. It was reported from the experiments that the initial pressure of the reactants strongly influenced the detonation wave development. When the initial pressure of the reactants was 1 atm, the detonation wave was not fully developed, and instead a wave propagation speed of about 800 m/s was observed which is far less than CJ detonation velocity of 2850 m/s. However, when
Figure 5.24. Pressure profiles when $p_1 = 1$ atm.

Figure 5.25. Temperature profiles when $p_1 = 1$ atm.
the initial pressure of the reactants was increased to 2 atm, a successful transition to CJ detonation was observed at a distance of about 23 cm from the ignition source.

A calculation has been performed on the same configuration with the initial reactant pressure of 2 atm to evaluate the influence of the initial pressure on the development of the detonation wave. The same initiation model increasing the temperature of $3 \times 3$ hot spot zone to 1,500 K has been also used in this calculation. Figures 5.26 and 5.27 show the resulting time evolution of pressure and temperature profiles, respectively, along the center line in axial direction. As expected, a successful evolution to a CJ detonation wave is observed in this case.

![Pressure profile graph](image)

Figure 5.26. Pressure profiles when $p_1 = 2$ atm.

From these observations, the calculation with the specific initiation model turns out to yield the same result as the experimentally observed one concerning the influence of the initial pressure on the detonation wave development. Even though the reactant
used in the calculation is different from the one in the experiment, it is worth while to note the same qualitative trend in both the calculation and the experiment.

5.4 Initiation by Reflecting Wave

It has been observed and discussed in sections 4.2.4 and 5.2 that a spherical detonation wave originating from a hot spot finally develops into a planar detonation wave corresponding to the CJ state through the interactions of the reflecting waves. The typical shape of the detonation wave development can be seen in figure 5.20. This pattern of detonation wave formation, however, takes place when the energy deposition in the hot spot is high enough to directly initiate the spherical detonation wave. Different patterns of detonation wave development have been observed during extensive calculations to find the critical level of energy deposition in a hot spot.
An interesting shape of wave formation can be observed in figure 5.28 that shows the evolution of the pressure contour when the energy deposition in the hot spot is slightly higher than the critical value. This is the result when the $3 \times 3$ hot spot (corresponding to 1.325 cm$^3$) is given the energy deposition of 1.75 Joule. The spherical wave originating from the hot spot is observed not to fully develop into the self-sustaining detonation wave until the wave reaches the circumferential wall, which appears to be caused by insufficient initial energy deposition. The wave shape until then looks very similar to the unsuccessful initiation that is shown in figure 5.21. However, when the wave reaches the circumferential wall, a reinforcement of the detonation by the high pressure and temperature from the reflecting wave occurs, and the self-sustaining detonation wave is observed to develop from the circumference of the axi-symmetric configuration. Through the complex wave interactions among this re-initiated detonation wave, the original wave from the hot spot, and the reflection waves from the circumferential wall and again from the center, the fully developed planar wave of a CJ detonation is finally obtained. The interaction of the waves and the developing process of the CJ detonation wave formation can be seen more easily in figures 5.29 and 5.30 that show the time evolution of the pressure profiles along the center line in the axial direction.

Another typical example of the initiation by the reflecting waves is seen in figure 5.31 that plots the evolution of the pressure contours when a $3 \times 2$ hot spot (corresponding to 0.884 cm$^3$) at the lower left corner is modeled with an energy deposition of 1.24 Joule. The detonation wave development from the circumferential wall by the reflecting wave, and the propagation of the corresponding self-sustaining wave back into the direction of the axial axis can be seen more clearly in this figure. Figures 5.32 and 5.33 show the time evolution of the corresponding pressure and temperature profiles along the center line in the axial direction. The process of detonation wave formation
Figure 5.28. Initiation by reflection for energy deposition of 1.75 J.
Figure 5.29. Early pressure build-up by reflecting waves.

Figure 5.30. Pressure development in critical initiation of 1.75 J.
resulting from the complicated interactions of the waves can be seen more easily in these figures.

Comparison of the results shown in figure 5.30 and 5.32 with those shown in figure 4.25 shows that the fully developed states of the detonation waves, even though initiated by reflecting waves, also converge to the same values of the CJ state that have been already observed in figures 5.11—5.14, independent of the entirely different shapes of the wave developing process.
Figure 5.31. Initiation by reflection for energy deposition of 1.24 J.
Figure 5.32. Pressure development in critical initiation of 1.24 J.

Figure 5.33. Temperature development in critical initiation of 1.24 J.
CHAPTER 6
SIMULATION OF
SHOCK-INDUCED DETONATION

A series of shock-induced detonation experiments has been performed at The University of Texas at Arlington (UTA), to study a hypersonic propulsion test facility concept based on magnetohydrodynamic (MHD) augmentation of high-pressure arc heaters [56]. A detonation driver, 15.24 cm in diameter and 2.74 m in length, was added to an existing shock tube to enhance its performance so that measurements of the electrical conductivity of high-pressure, seeded air plasmas could be obtained. A schematic of the experimental facility is shown in figure 6.1. The driver tube was highly pressurized with either air or helium, and the detonation tube was filled with a stoichiometric mixture of fuel and oxygen/air. These two tubes were separated by a double-diaphragm section as shown. The pressure histories were recorded at several stations on the wall of the detonation tube during this experiment. In this chapter, the results of a numerical simulation of this experiment are compared with experimental data. This provides validation for the numerical simulation and an aid in understanding the experimental results as well.

Figure 6.2 shows the pressure histories from an experiment, recorded at stations 4 and 5 corresponding to 166.4 cm and 224.8 cm, respectively, from the location of the diaphragm [57]. In this experiment, the initial pressure of the stoichiometric hydrogen-air mixture inside the detonation tube was 3 atm and the driver tube was pressurized initially to 200 atm with helium. Another experimental result from a different shot, but
Figure 6.1. The schematic of the UT Arlington experiment.

with the exactly same initial set-up is seen in figure 6.3. These two figures are observed to show almost identical results, and this suggests a reliability of the experimental data. Both the incident detonation wave and the reflected wave were clearly captured at each station. The reflected wave is travelling toward the left after reflecting from the diaphragm separating the driven tube and detonation tube. It is interesting to note that the pressure history after arrival of the reflected wave is observed to increase with additional step-like shapes.

The modeling of the experiment with a numerical simulation requires that some assumptions and simplifications be made. In this experiment, the double diaphragm section between driver tube and detonation tube measures 11.43 cm long, and is pressurized initially to 100 atm, about a half of the pressure in the driver tube. Therefore, complex wave interactions may exist inside the double diaphragm section and driver tube until the second diaphragm ruptures and shock-induced detonation is initiated in the detonation tube adjacent to the diaphragm. The details caused by the double diaphragm section are not modeled in the simulation, and instead are replaced by an effective pressure inside the driver tube. This effective pressure is assumed to act directly on the hydrogen-air mixture in the detonation tube as if the diaphragm is effectively removed at $t = 0$. The effective pressure should be lower than the actual initial pressure
Figure 6.2. Pressure measurements at station 4 and 5 for test No.14.

Figure 6.3. Pressure measurements at station 4 and 5 for test No.23.
in the driver tube that was 200 atm in this experiment, and higher than the pressure inside the double diaphragm section that was 100 atm. Therefore, we take 150 atm as a reasonable first guess for the effective pressure in the driver tube.

In the experimental set-up, another diaphragm separated the right-end of the detonation tube and the driven tube. The inner diameter of the driven tube was 4.11 cm, much smaller than the 15.24 cm diameter detonation tube. The right-end of the detonation tube is modeled by a reflective boundary based on the fact that the area opening to the driven tube, even after a rupture of the diaphragm, corresponds to only 7 percent of the cross-sectional area of the detonation tube.

Figure 6.4 shows the resulting pressure histories at the station 4 and 5 from the simulation using the previously described modeling. It is quite amazing that the simulation result nearly reproduces the experimental data, in spite of the assumptions and simplifications used. The arrival time lag in the incident detonation wave between station 4 and 5 is observed to be almost the same as the experimental measurement, which suggests excellent agreement in the detonation wave velocities. The same agreement is observed in the reflected waves. The pressure levels of both incident and reflected waves are also seen to be in good agreement. It is interesting that the calculated pressure history also shows an increase at each station after the arrival of the reflected wave. The increasing pattern and the level of pressure from the calculation almost exactly reproduce the experimental result.

This step-like increasing pattern of the pressure history is closely examined from the simulation results. Figure 6.5 shows time evolution of the pressure and the density profiles inside the detonation tube. The incident detonation wave is clearly seen to propagate to the right, and the driver material interface is also clearly observed from the density profile to follow the incident wave. The reflection of the incident wave
Figure 6.4. Calculated pressure histories at station 4 and 5.

from the right boundary can be seen in the graph at 1.5 msec, and the reflected wave propagates to the left until it meets the right-running material interface around 2.4 msec. The left-running reflected wave reflects again from the material interface, and as a result, a higher pressure and density are generated from this reflection and propagates back to the right. The material interface travels back toward the left as can be seen in the graphs after 2.4 msec. The right-running wave reflected from the material interface is observed to reflect once again from the right boundary around 3.1 msec and the resulting shock-increased pressure and density are seen to propagate back to the left. From these observations, the step-like increasing pattern of the pressure history turns out to be a result of these multiple wave reflections.

The simulation result using the current numerical model is in excellent agreement with the experimental data. From this observation, the assumptions and the simplifi-
Figure 6.5. Wave interactions in shock-induced detonation tube.
cations made to model the experiment are also justified. Especially the effective driver pressure appears to be a reasonable simplification to model the double diaphragm section. This simulation validates the current numerical model to be used with confidence to calculate the unsteady propagation of a detonation wave and its interactions with the boundaries as well as other waves.
CHAPTER 7
CONCLUSION

A numerical model to simulate the transient combustion process in a pulse detonation engine has been presented in this dissertation. Inviscid, non-heat-conducting flow equations are fully coupled with the chemical kinetics of the reactions for a general description of the chemical non-equilibrium. Vibrational energy conservation based on the two-temperature model is used to account for the possible thermal excitation and the relaxation of the vibrational energy mode. The governing equations are discretized using the finite-volume formulation, and a time-accurate solution is obtained from the Runge–Kutta integration scheme with a point-implicit treatment of the source terms. Roe's flux-difference splitting scheme extended to non-equilibrium flow is implemented for the cell face fluxes, and the MUSCL approach is used for higher-order spatial accuracy.

For the purpose of constructing an efficient numerical tool to be used in parametric studies, while maintaining a reasonable accuracy to be used for analysis, a two-step global model has been selected and validated for the chemical reactions of a hydrogen–air mixture. The inherent stiffness in the chemical reaction model has been properly taken care of by point-implicit treatment of source terms, together with the application of a Local Ignition Averaging Model to each mesh where ignition starts. The simulation model for a hydrogen–air mixture has resulted in an algorithm to perform the calculation of typical detonation wave initiation and propagation problems within several hours of CPU time on Sun Sparkstation for most configurations.
The calculated results from the present model have been compared with the theoretical Chapman-Jouguet data and experimental data. Excellent agreement has been observed. These observations validate the efficiency and the accuracy of the present model.

Numerical schemes of different order have been tested both in temporal and spatial accuracy up to the third-order. The higher-order calculation has been observed to capture the higher peak pressure in the propagating detonation wave, as expected. However, from the observation of the convergence trends, the second-order accurate scheme in both space and time seems to be a reasonable choice when the efficiency and the accuracy are taken into account. Mesh convergence tests have also been performed for three different mesh sizes of 5.0 mm, 2.5 mm, and 0.5 mm. Convergence has been clearly observed in the detonation wave velocity as well as in the pressure, density and temperature of the detonation wave. The calculated result using the 2.5 mm mesh shows nearly converged values that are almost the same as those computed with the 0.5 mm mesh, whereas the CPU time for 0.5 mm mesh is about 50 times more than the CPU time for 2.5 mm mesh. As a conclusion of these observations, the second-order accurate scheme in both space and time integration applied to 2.5 mm mesh size seems to be an appropriate choice from the trade-offs of accuracy and efficiency.

Geometry independence of detonation wave properties has been confirmed. The propagation of a detonation wave through a stoichiometric mixture of hydrogen and air has been calculated on four different combinations of the configuration taken from two kinds of geometry (two-dimensional and axi-symmetric) and two types of initiation (planar and point initiation). The detonation wave velocities and pressures from four different calculations are observed to converge finally to the same values through the complex process of the reflections and interactions of the waves.
The fully developed detonation wave property has been found to be independent on the initiation model implemented, as long as it ensures self-sustaining formation of the detonation wave. Extensive calculations have been performed both on the "reacting hot spot" and the "equilibrium hot spot." The properties of propagating detonation waves have been observed to converge finally to the same values, regardless of the different initial states of the hot spots and the resulting differences in the early stage building-up profiles.

The critical condition of a hot spot has been observed to exist for a successful initiation. A small decrease in the initial pressure and/or temperature of a hot spot has resulted in an unsuccessful initiation when the energy deposition in the hot spot is in the vicinity of the critical condition. The hot spot criteria for a successful initiation of the self-sustaining detonation wave has been found as a function of initial temperature, pressure, and size of the hot spot from an extensive series of calculations. These conditions have been converted to the equivalent minimum level of energy deposition in the hot spot.

An experimental observation that the initial pressure of the reactants strongly influenced the detonation wave development has been simulated with the specific initiation model. In the experiment, the reactant at 1 atm pressure was observed to be unsuccessful in developing into a CJ detonation, whereas the reactant at 2 atm was successful. The same result has been obtained from the calculation with the initiation mechanism modeled as a reacting hot spot on 3×3 meshes.

When the energy deposition in the hot spot is insufficient to directly initiate the detonation but just above the minimum critical level of the energy, an interesting pattern of detonation wave development that suggests an example of the deflagration-to-detonation transition process has been observed to take place. The spherical wave
originating from a hot spot is too weak to develop into a self-sustaining detonation wave until reflected from the circumferential wall. The re-initiation by the reflecting wave takes place near the wall, and the self-sustaining detonation wave is developing from the circumference to the direction of the axis. The fully developed planar wave of CJ detonation is finally obtained through the complex wave interactions.

The shock-induced detonation experiment has been simulated. In the experiment, a stoichiometric mixture of hydrogen and air in the detonation tube was detonated by a highly pressurized helium gas in the driver tube. The pressure histories recorded at the specific stations on the wall of the detonation tube have been compared with the time-accurate calculation results, and an excellent agreement has been observed. The calculated result has almost exactly reproduced the experimental data. The step-like increasing pattern of the pressure history after arrival of the reflected wave has been found to be due to multiple wave reflections between the material interface and the right boundary.

A basic unit of the simulation model for a pulse detonation wave engine has been developed and validated in this dissertation. There seems to be two main directions for future work. One direction is to emphasize the analysis capability of the present model. This could include the provision for a gas-phase flame simulation that may require some other physical phenomena such as thermal conduction, molecular diffusion, etc. to be included in the simulation model, as well as a more detailed chemical reaction model to be implemented. This may provide a tool for more detailed studies on the initiation mechanism including the deflagration-to-detonation transition. Another direction is to extend the design capability with the confidence of efficiency and accuracy of the present model. Coupling of the flow inside an engine with the outer flow field could be
included for this purpose. This may provide a tool for performance studies including the complete cycle analysis of a pulse detonation engine.
BIBLIOGRAPHY


BIOGRAPHICAL STATEMENT

Hyungwon Kim was born in Busan, Korea in 1955. He received his elementary education in the Joongang Elementary School and completed secondary education in the Busan Middle School and the Busan High School. He entered the Seoul National University in 1974, and graduated in 1978 with a Bachelor of Science degree in Aerospace Engineering. He joined the Agency for Defense Development (ADD) in 1978, and had worked until 1995 as a senior research engineer in the various fields of research and development of weapon systems and related technologies. He entered the Chungnam National University in 1988 as a part-time graduate student, and completed his Master of Science degree in Physics in 1990. He came to the United States to pursue graduate studies in Aerospace Engineering at The University of Texas at Arlington in 1995. His areas of research included computational studies of high temperature nonequilibrium gas flows and transient combustion process in pulse detonation engine, which was the subject of his dissertation.