MACH REFLECTION INDUCED DETONATION
IN A REACTIVE FLOW

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MACH REFLECTION INDUCED DETONATION
IN A REACTIVE FLOW

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ABSTRACT

MACH REFLECTION INDUCED DETONATION IN A REACTIVE FLOW

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A comparison of a chemically reactive flow versus a non-reactive flow is made in this work to show the possibility of the presence of a detonation wave associated with a Mach stem also known as a Mach reflection wave. A reactive, inviscid, and unsteady flow over a two-dimensional wedge is observed. Then, it is compared to a non-reactive flow over the same geometry and under the same conditions. A range of deflection angles \( \theta \) and incoming flow Mach numbers \( M_i \) is used in this study. The Euler equations are discretized using a finite-volume approach to ensure conservation and to allow proper treatment of discontinuities. A two-step explicit Runge-Kutta integration
scheme is implemented together with a point-implicit treatment of the source terms to obtain a time-accurate solution. In addition, Roe’s flux-difference splitting scheme extended to non-equilibrium flow is used 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. After running several simulations and computations, the results are then compared to theoretical Chapman-Jouguet data. A thorough discussion and analysis is also made for each case included in this work. The variable parameters chosen for this study are the angle of deflection $\theta$, the incoming flow Mach number $M_1$, the initial pressure $P_1$, and the initial temperature $T_1$ as well as the length of the wedge and the height of the domain. It was found that under certain conditions a Mach stem is formed which triggered a detonation in the flow. The detonation and the formation of the mach stem were shown to be dependent on the flow parameters mentioned above and independent on the geometry and the size of the domain.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iv</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>v</td>
</tr>
<tr>
<td>LIST OF ILLUSTRATIONS</td>
<td>ix</td>
</tr>
<tr>
<td>Chapter</td>
<td></td>
</tr>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>2. METHOD</td>
<td>7</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>7</td>
</tr>
<tr>
<td>2.2 Mathematical Formulation</td>
<td>7</td>
</tr>
<tr>
<td>2.2.1. Governing Equations</td>
<td>8</td>
</tr>
<tr>
<td>2.2.2. Thermodynamic Properties</td>
<td>9</td>
</tr>
<tr>
<td>2.2.3. Chemical Kinetics Model</td>
<td>10</td>
</tr>
<tr>
<td>2.2.4. Vibrational Energy Relaxation</td>
<td>11</td>
</tr>
<tr>
<td>2.3 Numerical Formulation</td>
<td>11</td>
</tr>
<tr>
<td>2.4 Geometric Configuration and Grid Study</td>
<td>15</td>
</tr>
<tr>
<td>3. RESULTS</td>
<td>18</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>18</td>
</tr>
<tr>
<td>3.2 Discussion of Selected Cases</td>
<td>19</td>
</tr>
<tr>
<td>3.2.1. Case 1</td>
<td>19</td>
</tr>
</tbody>
</table>
3.2.2. Case 2 ................................................................. 20
3.2.3. Case 3 ................................................................. 21
3.2.4. Case 4 ................................................................. 22
3.2.5. Case 5 ................................................................. 23
3.2.6. Case 6 ................................................................. 25
3.2.7. Case 7 ................................................................. 30
3.2.8. Case 8 ................................................................. 31
3.2.9. Case 9 ................................................................. 32
3.2.10. Case 10 ............................................................ 33
3.2.11. Case 11 ............................................................ 34
3.2.12. Case 12 ............................................................ 36

4. CONCLUSIONS ................................................................. 38

REFERENCES ................................................................. 40

BIOGRAPHICAL INFORMATION ........................................... 402
### LIST OF ILLUSTRATIONS

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Regular reflection wave</td>
<td>2</td>
</tr>
<tr>
<td>1.2</td>
<td>Mach reflection wave</td>
<td>3</td>
</tr>
<tr>
<td>2.1</td>
<td>Geometric configuration</td>
<td>15</td>
</tr>
<tr>
<td>2.2</td>
<td>Change in pressure</td>
<td>16</td>
</tr>
<tr>
<td>2.3</td>
<td>Change in temperature</td>
<td>16</td>
</tr>
<tr>
<td>3.1</td>
<td>Case 1</td>
<td>20</td>
</tr>
<tr>
<td>3.2</td>
<td>Case 2</td>
<td>21</td>
</tr>
<tr>
<td>3.3</td>
<td>Case 3</td>
<td>22</td>
</tr>
<tr>
<td>3.4</td>
<td>Case 4</td>
<td>23</td>
</tr>
<tr>
<td>3.5</td>
<td>Case 5</td>
<td>25</td>
</tr>
<tr>
<td>3.6</td>
<td>Case 6 Isobars</td>
<td>27</td>
</tr>
<tr>
<td>3.7</td>
<td>Case 6 Isotherms</td>
<td>28</td>
</tr>
<tr>
<td>3.8</td>
<td>Case 6 Four different domain regions</td>
<td>29</td>
</tr>
<tr>
<td>3.9</td>
<td>Case 6 water formation</td>
<td>30</td>
</tr>
<tr>
<td>3.10</td>
<td>Case 7</td>
<td>31</td>
</tr>
<tr>
<td>3.11</td>
<td>Case 8</td>
<td>32</td>
</tr>
<tr>
<td>3.12</td>
<td>Case 9</td>
<td>33</td>
</tr>
<tr>
<td>3.13</td>
<td>Case 10</td>
<td>34</td>
</tr>
<tr>
<td>3.14</td>
<td>Case 11</td>
<td>36</td>
</tr>
<tr>
<td>3.15</td>
<td>Case 12</td>
<td>37</td>
</tr>
</tbody>
</table>
CHAPTER I
INTRODUCTION

When opposite families of oblique shock waves generated by sharp wedges intersect, they can create either a regular or a Mach intersection. Consider the symmetrical case where the shocks of opposite family are generated by sharp wedge of the same angle below the shock detachment limit. The symmetry allows half of the domain to be considered. In Figure 1.1, the deflection angle at the corner is \( \theta \), thus generating an oblique shock at point \( A \) with a wave angle \( \beta_1 \). The shock wave generated at \( A \), called the incident shock wave, impinges on the upper wall at point \( B \). Examining Figure 1.1, one can see that the flow in region 2 behind the incident shock is inclined upward at the deflection angle \( \theta \). However, the flow must be tangent everywhere along the upper boundary. Hence, the flow in region 2 must eventually be turned toward the wedge through an angle \( \theta \) in order to maintain a flow tangent to the upper boundary. This downward deflection is via a second shock wave originating at the impingement point \( B \) as shown in Figure 1.1. This second shock is called reflected shock wave.
Another interesting situation can arise as follows. Consider that $M_1$ is only slightly above the minimum Mach number necessary for a straight, attached shock wave at the given deflection angle $\theta$. For this case, the oblique shock is simply a straight, attached incident shock. However, the Mach number decreases across a shock (i.e., $M_2 < M_1$). This decrease may be enough such that $M_2$ is not above the minimum Mach number for the required deflection angle $\theta$ through the reflected shock. In such a case, a solution for a straight reflection shock wave is not possible. The nature of the wave reflection in this case is depicted in Figure 1.2. Here, the originally straight incident shock becomes curved as it nears the upper boundary and becomes a normal shock wave there. This allows the streamline at the wall to continue parallel to the boundary behind the shock intersection. In addition, a curved reflected shock branches from the normal shock and propagates downstream. This wave pattern, shown in Figure 1.2, is called a Mach wave intersection [1].
A detonation wave can occur in a reactive gas flow. It is by far less common than deflagration wave. Since a deflagration flame speed is usually the order of one or more meters per second, a pressure wave which propagates with the speed of sound greatly outdistances the flame front. Thus, the deflagration form of combustion can be modeled as a constant pressure process. Detonation on the other hand, is the more rapid and violent type of combustion. A detonation propagates at a very high velocity, of the order of a few thousand meters per second and, hence, 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 hence, proceed violently. In detonation, all the important energy transfer occurs by mass flow in a strong compression wave, with negligible contribution from other processes such as heat conduction and molecular diffusion which are important in a deflagration flame. Due to the high speed, detonation can be modeled as a constant volume process [2].

Detonation waves are actually complex, oscillatory phenomena with three-dimensional time-dependent cellular structures. However, a rather simple one-dimensional theory was formulated by Chapman (1899) and by Jouguet (1905) after the
phenomenon of detonation was first recognized by Berthelot, Vieille, Mallard and Le Chatelier in 1881. Independently, a fundamental advance was made by Zeldovich (1940) in Russia, Von Neumann (1942) in the United States, and Doering (1943) in Germany. Their contribution is called the ZND model of detonation [3]. The ZND model 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 then proceeds in the reaction zone that follows the shock and is complete in the final state. The shock and the reaction zone then propagate together at the constant detonation velocity $D_{CJ}$ also called the Chapman-Jouguet velocity. Conservation conditions require that the final state lie on both the Hugoniot curve and the Rayleigh line in the pressure-volume plane. At a certain value of $D_{CJ}$, the Rayleigh line is tangent to the Hugoniot curve. This tangent point is called the Chapman-Jouguet point that represents the stable end state for a self-sustaining detonation wave, and the corresponding detonation velocity $D_{CJ}$. Also, it can be shown that at the $CJ$ point, the detonation velocity $D_{CJ}$ relative to the reaction products is equal to the local speed of sound in the reaction products.

In order to capture the discontinuities discussed before, and to study the flow with high accuracy, a numerical algorithm had to be implemented and an accurate scheme had to be chosen. Several computer programs were developed using different algorithms and schemes. Most programs use the upwind or flux-split algorithms that are known to yield accurate solutions of shock-wave dominated flows due to their
superior shock capturing properties. 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 the thermal excitation equations from the flow equations, and solve them separately at each time step. Another approach is to solve the entire equation set governing the fluid dynamics and the non-equilibrium chemistry as well as the thermodynamics simultaneously in a fully coupled fashion. The latter usually introduces extreme stiffness in the system of equations, and results in a very small time step for a stable time-marching solution. Hence, an implicit numerical scheme is often implemented to improve efficiency. This in turn, results in a very complex, large-block structure for the solution algorithm [4].

In this study, a two-dimensional time-accurate numerical simulation model is used for oblique shock waves. The simulation model designed by Kim [4] 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 as well. The simulation code uses a combination of point-implicit scheme introduced by Bussing and Murman [5] that treats the chemical source terms implicitly and all other terms explicitly, and a local ignition averaging is 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. For an accurate capture of the shock wave both in time and space, Roe’s flux-
difference split scheme is combined with the Range-Kutta integration scheme. The chemical reaction for a stoichiometric $N_2 - O_2 - H_2$ flow is described by a simple two-step reaction involving five species, $N_2 - O_2 - H_2 - OH - H_2O$ as follows:

$$H_2 + O_2 \rightarrow 2OH \text{ and } 2OH + H_2 \rightarrow 2H_2O$$

Several different configurations are investigated in this work, with the goal of finding detonation behind the Mach stem of a reactive gas flow. Once detonation is detected, a comparison is made with an inert gas flow to show that the detonation present in the reactive gas flow is solely due to chemical reaction in the flow. The results are then validated against theoretical $CJ$ values. Extensive calculations and simulations are performed with different mesh sizes to select the proper mesh size providing adequate and reasonable CPU time without compromising the resolution of the physical process.

For simplicity, a pair of wedges of opposite family and with equal angles of deflection $\theta$ is chosen and a two-dimensional, inviscid, non-conducting unsteady flow is assumed. In addition to the range of deflection angles $\theta$, a range of incoming flow Mach numbers $M_1$ form a matrix of simulations to cover the most susceptible cases where detonation is even possible. The choice of the angle $\theta$ and the Mach number $M_1$ is made using the $\theta - \beta - M$ curve. Only the angles $\theta$ and Mach numbers $M_1$ that are most likely to generate detonation associated with a Mach stem are considered in this study. The angle $\theta$ is varied between $5^\circ < \theta < 20^\circ$ and the Mach number $M_1$ is varied between $1.16 < M_1 < 3.0$.
CHAPTER II
METHOD

2.1 Introduction

In this chapter, the initial conditions as well as the configuration of the problem are discussed. First, a mathematical formulation is treated, followed by a numerical study, and finally, a geometric configuration of the problem is explored. The mathematical formulation of the problem includes the governing equations, thermodynamic properties, chemical kinetics model, and vibrational energy relaxation. The numerical approach comprises of a brief overview of Kim’s [4] numerical formulation in which the finite-volume formulation, the point implicit time integration, the flux-difference split algorithm, treatment of source terms and the Jacobian, and temperature calculation are treated in depth. Finally, the geometric configuration and test conditions are described.

2.2 Mathematical Formulation

A set of coupled partial differential equations that describe the reactive flow field is derived here, the main application of which will be to calculate initiation and propagation of detonation waves through fuel-air mixture. 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 [4]. The chemical kinetic model is also discussed in this section to ensure accurate prediction of the chemical composition in the mixture as well as a proper description of species and mixture thermodynamics properties including possible excitation of internal energy modes at high temperature, and vibrational energy relaxation process [4].

2.2.1. Governing Equations

Kim [4] formulated the time-dependent conservation equations governing an inviscid, non-heat-conducting, reacting gas flow in which thermal non-equilibrium is modeled with a two-temperature approximation. These equations are summarized here. 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 [6]. In a two-dimensional, Cartesian coordinate system, the conservation equations take the following form:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S$$  \hspace{1cm} (2.1)

where \( U \) is the vector of conserved variables, \( F \) and \( G \) are the convective flux vectors, and \( S \) is the vector of source terms. The vectors are written as
\[ U = \begin{bmatrix} \rho_s \\ \rho u \\ \rho v \\ \rho u e_v \\ \rho E \end{bmatrix}, \quad F = \begin{bmatrix} \rho_s u \\ \rho u^2 + p \\ \rho u v \\ \rho u e_v \\ \rho u E + p u \end{bmatrix}, \quad G = \begin{bmatrix} \rho_s v \\ \rho u v \\ \rho v^2 + p \\ \rho v e_v \\ \rho v E + p v \end{bmatrix}, \quad S = \begin{bmatrix} w_s \\ 0 \\ 0 \\ w_v \end{bmatrix} \] (2.2)

In this equation, the subscript \( s \) ranges from 1 to \( N_s \), where \( N_s \) is the number of species. The first row represents species continuities, followed by the 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 addition, \( u \) and \( v \) are the velocities in the \( x \) and \( y \) directions 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. In addition, \( \rho_s \) 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 [4].

2.2.2. 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 non-equilibrium state. The equilibrium portion of the internal energy is the contribution due to the translational and internal modes that can be assumed to be in equilibrium at the translational temperature \( T \). The remaining non-equilibrium 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 [4].
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 non-equilibrium 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:

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

(2.3)

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. 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. In addition, it is assumed here that each individual species behaves as a thermally perfect gas [7].

2.2.3. 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 estimations of the flow field properties, especially if the flow speed is sufficiently large that the flow timescale is comparable to the chemical reaction timescale. 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 not 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 where a non-equilibrium flow occurs, 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 continuity equations based on the chemical kinetics should be solved together with fluid dynamic equations to account for the possible chemical non-equilibrium [8].

2.2.4. Vibrational Energy Relaxation

The energy exchange between vibrational and translational modes due to inter-molecular collisions can be 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 [9, 10]. The resulting energy exchange rate is given by

\[
Q_{v,s} = \rho_s \frac{e^*_{v,s}(T) - e_{v,s}}{<\tau_s>}
\]

where \(e^*_{v,s}(T)\) is the vibrational energy per unit mass of species \(s\) evaluated at the local translational-rotational temperature, and \(<\tau_s>\) is the averaged Landau-Teller relaxation time of species \(s\) [8].

2.3 Numerical Formulation

The numerical methods used to solve the governing differential equations are derived and discussed in depth in Kim’s dissertation [4]. However, a brief review of the algorithm developed by Kim [4] is given in this section.
The goal is to construct numerical algorithms to obtain a time-accurate solution of the thermo-chemical non-equilibrium flow fields. Discretization is the first step in computer simulation. By discretizing the domain of interest, partial differential equations are reduced to a set of algebraic equations that are easier to solve. The key word in this process is the conservation 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 \([6]\). 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. Implementation of an implicit scheme to solve non-equilibrium 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 \([4]\).
In addition, Roe’s flux-difference splitting scheme extended to non-equilibrium 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 Scheme for Conservation Laws) approach for added spatial accuracy. A MINMOD limiter is applied to limit the scope of the variables used in the extrapolation [4].

2.3.1. Review of Kim’s [4] Numerical 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 [6].

Non-equilibrium 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

\[ \text{Stiffness} = \frac{\tau_{\text{largest}}}{\tau_{\text{smallest}}} \]  \hspace{1cm} (2.5)

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 [5]. 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. Temporal accuracy can be added by using Runge-Kutta integration schemes instead of first-order accurate Euler integration. The flux-difference split algorithm is used 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 [11]. 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 [12], and the flux-difference scheme used here is based on their method. 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 the flow are rewritten here for convenience.

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

(2.6)

Since the term $w_s$ depends explicitly on the species density and temperature, the Jacobian of $w_s$ with respect to $U$ is evaluated as well as the partial derivatives of the vibrational energy production rate $w_v$. The conserved variables at each cell center are updated by a matrix inversion scheme [4]. From these conserved variables, new values of the primitive variables, $\rho_s$, $u$, $v$, $e_v$, and $E$ are easily obtained. However, to close the system of equations and solve 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 [8, 13]:

\[ T^{(k+1)} = T^{(k)} + \frac{\rho e - \sum_s \rho_s e_s (T^{(k)}, T_v^{(k)})}{\rho C_v r_e} \]  

(2.7)

\[ T_v^{(k+1)} = T_v^{(k)} + \frac{\rho e_v - \sum_s \rho_s e_{v,s} (T^{(k)})}{\rho C_{v,v}} \]  

(2.8)

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 [4].

2.4 Geometric Configuration and Grid Study

The geometric configuration used in this study is shown in Figure 2.1 below:

![Figure 2.1 Geometric configuration](image)

The two-dimensional wedge is placed in the supersonic, reactive, inviscid, unsteady flow. The deflection angle \( \theta \) is varied between 5° and 25°. The height of the
domain used for the computational simulation is varied between 0.05 and 0.1 meters.
The length of the wedge is varied between 0.1 and 0.2 meters, depending on the
deflection angle \( \theta \). The domain is varied between 101×51 and 201×101 grid points,
based on a mesh size of 1 mm. The choice of 1 mm for the mesh size is validated by running computational simulations under same conditions with a mesh size of 0.5 mm as well as 1.5 mm as shown in Figure 2.1 and 2.2. The change in pressure vs. change in distance in meters from left to right is shown in Figure 2.1, while the temperature change is shown in Figure 2.2.
A mesh size of 1 mm is chosen because of the best trade-off between accuracy and CPU time. Even though, a mesh size of 0.5 mm should give a better accuracy than 1 mm, it’s shown in Figure 2.1 and Figure 2.2 that due to the computational scheme used for this simulation, the accuracy is compromised. A time-step of $10^{-7}$ seconds does not guarantee a stable solution for a mesh size of 0.5 mm. A time-step of $0.5 \times 10^{-8}$ seconds is needed for the mesh size of 0.5 mm [4], which would have increased the CPU time drastically. However, a time-step of $10^{-7}$ seconds is shown to be adequate for the two other mesh sizes used in this study. On the other hand, a mesh size of 1.5 mm would have saved CPU time, but as one can see in Figure 2.2, the accuracy of the resolution is tremendously compromised. Hence, a mesh size of 1 mm is chosen.

The incoming supersonic flow comprises a premixed stoichiometric hydrogen-air mixture. The initial pressure and temperature of the flow are fixed at $p_i = 2\ atm$ and $T_i = 700\ K$ respectively. The Mach number $M_1$ is varied between 1.16 and 6.0.
CHAPTER III

RESULTS

3.1 Introduction

Of all the different test cases shown in Figure 2.3, only some cases are discussed here for their significance in the objective of this work. The contours of constant pressures forming the oblique shock waves are graphed in this chapter, followed by a graph of constant temperature contours in one case which is thought of as the main objective of this study. Also, a water formation graph is included for the same case to confirm and validate the presence of detonation wave emanated from the Mach stem. Thereafter, a theoretical value of the CJ pressure ratio to the initial pressure is calculated and compared to the data obtained in the simulation of that same case.

Due to the large number of cases studied, this chapter is divided into several cases for simplicity. In addition, an attempt was made to detect parametric trends. For instance, case 1 starts with a low Mach number and a low deflection angle. Case 2, on the other hand, shows a higher Mach number or a higher deflection angle, whichever occurs first. The order of the parameters is as follows: Mach number, angle of deflection, initial pressure, initial temperature, the height of the domain, and finally, the length of the domain. A number of cases are discussed at the end that do not fit the classification scheme and are therefore discussed separately.
3.2 Discussion of Selected Cases

3.2.1. Case 1

This first case is for an incoming flow Mach number of 1.75, and incoming pressures and temperature of 1 atm and 700 K, respectively. The flow domain is 0.075 m high and 0.15 m long. The wedge angle is 15 deg. Figure 3.1 shows the evolution of the flow via isobars.

The incident shock is reflected three times at 0.260 ms and an indication of detonation at the third reflection wave is detected. At 0.265 ms, the third reflection wave initiates a detonation which propagates upstream, passing through the stationary shock system formed previously. A Mach stem is evident at $t = 0.280$ ms and easily noticed at 0.125 m from the left. However, it is not easily shown in this case whether the detonation is Mach stem induced or the Mach stem is a product of the detonation itself. In the final frame of Fig. 3.1, at $t = 0.390$ ms, the detonation wave is almost completely gone from the computational domain.
3.2.2. Case 2

This case is shown below in Figure 3.2 via isobars. The initial and boundary conditions are the same as case 1 but with double the initial pressure. In this case, the third reflection is formed at the same time as in case 1 and detonation initiation also occurs at \( t = 0.265 \text{ ms} \), just as in case 1. However, it is evident in this case that the increase in initial pressure has a minimal, almost negligible effect on the structure and the propagation of the wave system as shown in comparing this case to case 1.
Figure 3.2 Case 2: \( M_1 = 1.75, \theta = 15^\circ, P_1 = 2 \text{ atm}, T_1 = 700 \text{ K}, h = 0.075 \text{ m}, l = 0.15 \text{ m}. \)

### 3.2.3. Case 3

This case is shown below in Figure 3.3 using isobars. It is similar to cases 1 and 2 except that the pressure and temperature of the incoming flow are 2.5 atm and 1000 K respectively. Due to the increase in pressure and temperature compared to the previous cases, this case shows a rather different behavior. As shown in Figure 3.3, at \( t = 0.005 \text{ ms} \) the detonation is formed instantly along the entire ramp. However, the detonation rapidly develops into a normal propagating detonation wave moving upstream to the left and exiting the domain at \( t = 0.245 \text{ ms} \) leaving an oblique detonation wave, which leaves the domain to the left after a very short period of time. In this case, the drastic change in wave behavior is due mostly to the increase in temperature not the pressure.
3.2.4 Case 4

This case is shown below in Figure 3.4 via isobars for the same configuration as cases 1 – 3, except that the incoming flow pressure and temperature are now 3 atm and 1000 K respectively. In this case, a similar behavior like in case 3 is shown. An instant detonation wave is followed by a rapid upstream propagation of the detonation wave. Again, since the pressure in this case is raised from 2.5 to 3.0 atm and the temperature remained the same, the wave structure and behavior is not much different from case 3. Hence, the fact that the temperature change has more effect on the wave structure and behavior than the pressure change is proven.
3.2.5. Case 5

This case for flow past a 15 deg wedge is shown below in Figure 3.5 via isobars. The incoming Mach number is 1.9, while the flow pressure and temperature are 2 atm and 700 K respectively. The height and length of the domain remain the same as the previous cases, 0.075 m and 0.15 m respectively.

This is one of the very few cases that are interesting as far as the objective of this work is concerned. At $t = 0.270$ ms, two regular reflections (RR) waves are seen first. At $t = 0.275$ ms, a detonation kernel appears at the upper right corner of the domain. The detonation kernel is in the form of a third reflection wave. At $t = 0.280$ ms, the detonation becomes a fully developed wave propagating upstream forming a
Mach stem with the second reflection wave. Simultaneously, a normal wave starting at the upper wall, connecting the incident wave with the first reflection wave is appearing, creating a Mach reflection (MR) wave which is clearly shown in the upper magnified picture next to Figure 3.5. At \( t = 0.295 \) ms, the phenomenon sought is making its first appearance as shown in the lower magnified picture next to Figure 3.5; a detonation wave behind the Mach stem, developing instantly to a full detonation wave as seen at \( t = 0.300 \) ms. At this moment, two detonation waves are present. The first detonation wave propagates upstream while the second detonation wave at the Mach stem is getting longer. Finally both waves meet at \( t = 0.305 \) ms. The next frame at \( t = 0.310 \) ms reveals that the first detonation wave is overtaking the Mach stem induced detonation wave as it almost seems to be stationary. Also shown even clearer at \( t = 0.375 \) ms where the first detonation wave is clearing the domain to the left, the MR-induced detonation wave is remaining as it is mixing with the detonation shock formed past the first detonation flame.
3.2.6. Case 6

This case is shown below in Figure 3.6-3.9. In this case, Figure 3.6 shows the isobars where the Mach number is 1.9, the deflection angle is 15 degrees, the initial pressure and temperature are 2 atm and 700 K, respectively. The height of the domain on the hand is 0.1 m and the length is 0.15 m. The change in height allows the (MR) to be captured more clearly and also allows for a more detailed examination of the progress of the detonation wave associated with it. Moreover, for the intriguing
characteristics of this case, an isotherm contour plot is also shown in Figure 3.7 together with a water formation plot in Figure 3.9 to validate the formation of the (MR)-induced detonation wave.

This case is similar to the case 5, yet it shows a slight difference in the behavior of the flow. For instance, in Figure 3.6, the Mach stem in this case appears at \( t = 0.375 \) ms as shown in the upper magnified picture next to Figure 3.6 instead of \( t = 0.295 \) ms in case 5. This delayed appearance of the Mach stem is expected since a longer time is required for the wedge-induced shock to impinge the upper wall and be reflected down due to the increased height. The detonation takes place at \( t = 0.380 \) ms as shown the lower magnified picture next to Figure 3.6. In addition, the first detonation wave in the previous case at the upper right corner is absent in this case due to the raised height which makes it impossible for the wave to reflect a second time within a length of 0.15 m. To show the independency of the geometry and the consistency in these results, case 11 is added at the end of this chapter where it is obvious that after increasing the length to 0.2 m to make it more proportional with a height of 0.1 m, a detonation wave at the upper right corner is formed just like in case 5. When \( t = 0.405 \) ms, the (MR) wave is overtaking the (RR) wave until it finally impinges the lower wall and is reflected back up again to form the detonated reflected wave shown at \( t = 0.445 \) ms. Finally, when \( t = 0.500 \) ms, the Mach stem induced detonation wave propagates out of the domain leaving its trace in a form of slowly decaying detonation wave.
For clarity and a better understanding of this case, Figure 3.7 is added below which shows isotherms under same conditions as in Figure 3.6. Moreover, the same time intervals are used in both figures. It is shown in Figure 3.7 that the isotherms behave in similar manner as the isobars in Figure 3.6 as expected. In other words, similar wave formation is present and a similar Mach stem is impinged at the exact location as in Figure 3.6.
The theoretical $CJ$ values are obtained using a code called CEC and then compared to the pressure ratios of the four different regions of the domain shown in Figure 3.8 obtained from simulation data in Figure 3.7 when $t = 0.405$ ms. Indeed, a detonation is shown above the $CJ$ line at both region 3 and 4 separated by a slip line. The theoretical value of the $CJ$ pressure ratio line is calculated to be 6.75. The pressure ratio of region 3 to the initial pressure in region 1 is equal to the pressure ratio in region 4 to the initial pressure in region 1 and is equal to 7.10 which is slightly higher than the $CJ$ pressure ratio indicating a detonation in both regions 3 and 4. Similarly, the $CJ$
temperature ratio is calculated to be 4.38 and the temperature ratios in region 3 and 4 are 4.5 and 4.7 respectively.

![Figure 3.8 Case 6: Four different domain regions]

In Figure 3.9 below, the water formation is plotted to show the perfect agreement with the detonation location and existence that matches Figures 3.6 and 3.7. By comparing Figure 3.9 below to Figures 3.6 and 3.7, one can see when and where the water formation is initiated and propagated. It is clear that what is seen in Figures 3.6 and 3.7 is indeed a detonation since the reaction in the flow causing the detonation is producing water in the flow.
3.2.7. Case 7

This case is shown below in Figure 3.10. In this case, the isobars are shown where the Mach number is 2.0, the deflection angle is 15 degrees, the initial pressure and temperature are 2 atm and 700 K respectively. The height of the domain is now 0.075 m while the length is 0.15 m.

This case shows similar behavior as case 2. The difference is that the detonation flame starts in the lower right corner whereas in case 2 the detonation flame starts in the upper right corner. Shortly after initiation, the detonation front propagates upstream,
overtaking the stationary shock system. Also, the detonation is initiated at the second reflection wave instead for the third reflection wave as in case 2.

Figure 3.10 Case 7: $M_1 = 2.0$, $\theta = 15^\circ$, $P_1 = 2$ atm, $T_i = 700$ K, $h = 0.075$ m, $l = 0.15$ m

3.2.8. Case 8

This case is shown below in Figure 3.11. In this case, the isobars are shown where the Mach number is 2.4, the deflection angle is 20 degrees, the initial pressure and temperature are now 2 atm and 700 K respectively. The height of the domain is now 0.075 m while the length is 0.15 m.

In this case, no Mach stem is formed. Instead, the reflection wave is detonated instantly upon formation as shown in Figure 3.8 at $t = 0.045$ ms. Thereafter, the detonation is propagating upstream where it clears the ramp at $t=0.225$ ms.
3.2.9. Case 9

This case is shown below in Figure 3.12. In this case, the isobars are shown where the Mach number is now 2.6, the deflection angle is 20 degrees, the initial pressure and temperature are 2 atm and 700 K respectively. The height of the domain is 0.075 m and the length is 0.15 m.

This case is almost identical to case 8. However, it seems like the formation as well as the propagation of the detonation wave in this case is occurring a bit slower than the previous case as can be noticed by comparing $t = 0.110$ ms in this case to $t = 0.105$ ms in the previous case. In addition, it is shown in this case at $t = 0.235$ ms that the detonation is not completely dissipated yet as opposed to in the previous case where the detonation completely left the domain at $t = 0.225$ ms.
This case is shown below in Figure 3.13. In this case, the isobars are shown where the Mach number is 3.0, the deflection angle is now 15 degrees, the initial pressure and temperature are 2 atm and 700 K respectively. The height of the domain is 0.075 m and the length is 0.15 m.

In this case, no Mach stem is shown either. However, a Mach stem that is caused by the detonation wave propagating upstream as shown in Figure 3.10 at $t = 0.150$ ms. Again, the propagation of the detonation upstream in this case is a bit slower than the previous as shown in Figure 3.10 by comparing $t = 0.130$ ms in this case to $t = 110$ in case 9. Also, in this case, the detonation wave is completely dissipated at $t =$
0.375 ms which is 0.140 ms slower than case 9 where the wave was dissipated at $t = 0.235$ ms.

This case is shown below in Figure 3.14. In this case, the isobars are shown where the Mach number is now 1.9, the deflection angle is 15 degrees, the initial pressure and temperature are 2 atm and 700 K respectively. The height of the domain is now 0.10 m and the length is now 0.20 m.

In this case, the domain geometry is changed to show the independency of geometry on the physical aspect of this study. In case 5, a detonation flame started in the upper right corner first and after some time has elapsed another detonation took place at the Mach stem where the height of the domain was 0.075 m and the length was 0.15 m.
0.15 m. In case 6, the height was changed to 0.10 m where only one detonation at the Mach stem was present and no detonation was shown in the corner. The reason of the absence of the detonation in the upper right corner in case 6 is the short length compared to the height which is proven in case 11 where the length is increased to 0.20 m and hence, the detonation wave in the upper right corner is shown leaving the mach stem detonation unaffected as shown in Figure 3.14 at \( t = 0.380 \) ms. However, because of the enlarged domain in case 11, the detonation formation is occurring slower than in case 5 as shown in comparing Figure 3.14 at \( t = 0.380 \) ms and Figure 3.5 at \( t = 0.295 \) ms. The rest of the behavior of case 11 is identical to case 5. In addition, a magnified picture at \( t = 0.375 \) ms is also added here next to Figure 3.14 to show the formation of the mach stem taking place at the same instant as in case 6 where the height of the domain is also 0.1 m as it is in this case.
3.2.12. Case 12

This case is shown below in Figure 3.15. In this case, the isotherms are shown for clarity where the Mach number is 1.9, the deflection angle is 15 degrees, the initial pressure and temperature are 2 atm and 700 K respectively. The height of the domain is 0.10 m and the length is 0.15 m as in case 6. The only difference between case 12 and case 6 is that case 12 represents the non-reactive flow where the hydrogen is given a near-zero or negligible value since an exact value of zero caused the code to blow up.
By simulating an inert flow in this case, it is confirmed that the reaction in the flow caused the detonation behind the Mach stem in case 6 by noticing the absence of the detonation in case 12. Instead, a stagnating shock wave is present throughout the entire computational time period. Moreover, the Mach stem is shown very clearly in the Magnified picture next to Figure 3.15 at $t = 0.375$ ms which is identical to the mach stem in case 6 at the same instant. However, since the isotherms are used for Figure 3.15 in case 12, the slip line is present in the magnified picture, showing the change in flow temperature on both sides of the slip line as expected.

Figure 3.15 Case 12: $M_1 = 1.9$, $\theta = 15^\circ$, $P_1 = 2$ atm, $T_1 = 700$ K, $h = 0.1$ m, $l = 0.15$ m (Inert)
CHAPTER IV

CONCLUSIONS

A Mach reflection induced detonation has been examined in this study. Using previous literature and several simulations, a Mach reflection (MR) induced detonation was captured and analyzed. 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 [4].

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 a personal computer that is 2.4 GHz fast, and an internal memory of 1028 MB. However, in some cases where the domain is large and the mesh size small, the CPU time was a couple of days long. Once the simulations
were performed, the data obtained was compared to the theoretical CJ conditions and a great agreement has been observed.

In Kim’s [4] code, 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 [4]. 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 consideration [4]. The mesh size study has also been performed to show the advantage of a mesh size of 1 mm in CPU time without compromising the accuracy of the model.

Once the Mach reflection (MR) induced detonation was captured, a similar case with the similar initial condition was examined in a non-reactive flow for comparison. Moreover, few changes in domain size have been made to ensure the independency of the geometry or the domain size.

For further studies, it is highly recommended that a major improvement of the code used in this work is made to minimize the limitations encountered in some simulation cases. In addition, a similar study is recommended to be conducted where a Mach stem induced detonation can be captured using a different incoming flow Mach number and initial conditions. Moreover, a double wedged domain is also worth being examined where the deflection angles don’t have to be equal and the domain is not symmetric.
REFERENCES


BIOGRAPHICAL INFORMATION

Walid Cederbond was born 1971 in Lebanon where he received his high school education. At age of 17, Walid moved to Sweden where he received his bachelor degree in double major, computer and electronic engineering in 1992. Right after graduation, He started up his own computer company in Stockholm, Sweden. In 1994, Walid moved to Taiwan where he opened a new branch of his company and stayed for two years. In 1997, Walid came to United States to attend the Tyler International School of Aviation for his flight training. In 1998, He was certified commercial pilot. Thereafter, He became a flight instructor and worked for two years at Meacham airport in Fort Worth, Texas. In the fall of 1999, Walid joined the University of Texas at Arlington where he received his bachelor degree in Aerospace engineering in 2003 and his master degree in Aerospace engineering in 2004. He is planning on doing the PhD program at UTA also starting in the fall of 2005.