

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE
ENGINEERING AND TECHNOLOGY

**COMPUTATIONAL INVESTIGATIONS
FOR SHOCK WAVE – BOUNDARY LAYER INTERACTIONS OF
A THERMALLY NON-EQUILIBRIUM HYPERSONIC FLOW**



M.Sc. THESIS

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Department of Aeronautical and Astronautical Engineering

Aeronautical and Astronautical Engineering Programme

JULY 2020

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

**ISIL DENGEDEN OLMAYAN HİPERSONİK BİR AKIŞTAKİ
ŞOK DALGASI – SINIR TABAKA ETKİLEŞİMLERİNİN HESAPLAMALI
YÖNTEMLERLE İNCELENMESİ**

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To my family,



FOREWORD

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ABBREVIATIONS

OPENFOAM	: Open-source Field Operation And Manipulation
JANAF	: Joint Army-Navy-NASA-Air Force
2-D	: Two-Dimensional
3-D	: Three-Dimensional
NASA	: National Aeronautics and Space Administration
DSMC	: Direct Simulation Monte Carlo
V-T	: Vibrational-Transrotational
V-V	: Vibrational-Vibrational
C-V	: Chemistry-Vibrational
CFL	: Courant–Friedrichs–Lewy



SYMBOLS

R	: Gas constant
ρ	: Density
c_v	: Specific heat at constant volume
c_p	: Specific heat at constant pressure
C_p	: Pressure coefficient
Cf	: Friction coefficient
Y	: Mass fraction
X	: Molar fraction
e	: Internal energy per unit mass
M	: Molecular weight
$n_{m,s}$	: Number density of the colliding pair
c_m	: Average molecular speed
$\sigma_{v,m}$	: Limited collision cross-section
u, v, w	: Velocity components in x, y and z directions
δ	: Kronecker delta



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COMPUTATIONAL INVESTIGATIONS FOR SHOCK WAVE – BOUNDARY LAYER INTERACTIONS OF A THERMALLY NON- EQUILIBRIUM HYPERSONIC FLOW

SUMMARY

A hypersonic solver has been developed and validated in order to investigate high enthalpy behavior of shock wave - boundary layer interactions for thermally equilibrium and non-equilibrium conditions. The newly developed code is based on two standard OpenFOAM solvers, which are *rhoCentralFoam* and *reactingFoam*. *rhoCentralFoam* is a density based Navier-Stokes solver that is able to capture shock waves in high speed regimes. *reactingFoam*, on the other hand, is capable of solving chemistry physics of low speed flows. The developed solver has been blended from these two open-source codes for modeling hypersonic reacting flows in thermally/chemically equilibrium and non-equilibrium conditions.

Additional models and equations have also been implemented into the blended solver for a true representation of flow physics. Thermally non-equilibrium solution requires the addition of Two-Temperature model into the hypersonic solver. Two temperature model decomposes equilibrium temperature into trans-rotational and vibrational temperatures at molecular level. While trans-rotational temperature is computed from standard Navier-Stokes energy equation with a small modification, vibrational temperature for each molecule in the mixture is obtained from an additional energy equation, which has been externally implemented into the solver. This additional vibrational energy equation, just as in standard energy equation, is solved in two steps, which are composed of predictor and corrector parts. Finite volume discretization of Navier-Stokes' equations in the solver is performed by using Kurganov - Tadmor flux scheme.

Standard JANAF package in OpenFOAM libraries for calculation of thermodynamic properties in relatively low temperatures has been extended to include a higher temperature range in order to represent high enthalpy reacting flow physics more accurately. As opposed to Sutherland model available in existing libraries, thermophysical property of each specie is adapted to high temperatures by a different formulation. Furthermore, the mixture value of thermophysical properties is updated with a mixing rule which takes into account molar fractions and molecular weight of each specie.

Chemical model for air has been selected according to the high enthalpy equilibrium flow conditions of an experimental study in which mass fractions of various species are reported. In computational results, air is modeled with 5 species including 19 irreversible chemical reactions whose reaction rates are calculated from Arrhenius equation. In validation processes, however, several other chemical models have also been used in accordance with other solvers available in the literature.

The solver has been tested against both non-reactive and reactive flow conditions in thermally equilibrium and non-equilibrium conditions. The validation tests were conducted on benchmark cases such as adiabatic heat bath, double cone and blunted cone models. The results obtained from hypersonic solver were compared against to

some other high-speed non-equilibrium reactive solvers as well as experimental studies performed on these benchmark models.

Both 2-D and 3-D shock wave – boundary layer interactions were investigated for a double wedge geometry which has a fixed fore and various aft angles. The differences in shock structures were analyzed by systematically increasing the second angle by 5° . The results obtained from 2-D and 3-D solutions were compared between themselves and against to an experimental study conducted on a same aft angle. For comparison purposes, numerical Schlieren images and surface heat flux distribution were examined. In addition, distinctions between equilibrium and non-equilibrium solutions were reported.



ISIL DENGEDEN OLMAYAN HİPERSONİK BİR AKIŞTAKİ ŞOK DALGASI – SINIR TABAKA ETKİLEŞİMLERİNİN HESAPLAMALI YÖNTEMLERLE İNCELENMESİ

ÖZET

Dünya ve diğer gezegenlerin atmosferine giriş yapan uzay araçlarının tasarlanması aşamasında aracın etrafında aerodinamik ısınmadan, şok-şok ve şok sınır tabaka etkileşimlerinden kaynaklanan problemlerin çözümü hayati bir önem arz etmektedir. Gezegenin çekim etkisine giren uzay aracı hipersonik hızlara ulaştığından şok etkileşimlerinden kaynaklı ani sıcaklık ve basınç yükselmeleri uzay aracı etrafında bölgesel ısınmalara ve kalıcı deformasyonlara neden olarak hasar yaratmaktadır. Belirtilen bu zorluğun üstesinden gelebilmek ve güvenli uçuşlar yapabilmek adına yüksek hız ve entalpi koşullarında deneyler ve sayısal çalışmalar sürdürülmektedir. 1960’lardan beri yapılagelen çalışmalar var olsa da, akışın uzay hava aracı üzerindeki aerotermodinamik ve kimyasal etkileri hala tam olarak anlaşılabilmiş değildir.

Yüksek hızlarda çalışan rüzgar tünellerinde düşük ve yüksek entalpide deneysel koşullar oluşturularak bu etkiler incelenmektedir. Ancak hipersonik hız rejimindeki atmosfer koşullarını deneysel olarak modellemek oldukça maliyetli olmakla birlikte yüksek kapasiteli deney merkezleri de oldukça sınırlıdır. Analitik ve ampirik olarak elde edilen çözümler ise sadece çok basit geometrilerle sınırlı kalmakta ve karmaşık geometrilerdeki parçalara sahip olan uzay araçları için yetersiz kalmaktadır. Bu yüzden Hesaplamalı Akışkanlar Dinamiği yöntemi ile hem daha hızlı ve ucuza çözümler elde edilebilmekte hem de deneysel bulgulardan çok daha detaylı bir şekilde veri sunulabilmektedir. Hesaplamalı Akışkanlar Dinamiği yöntemi ile akışı yöneten denklemler olarak bilinen Navier-Stokes denklemleri cebirsel ifadelerle dönüştürülüp yüksek performanslı bilgisayar ve sunucularda paralel işlemcilerde çözdürülebilmektedir. Geçmişte Hesaplamalı Akışkanlar Dinamiği yöntemi, Huygens-Cassini, Mars Pathfinder ve Mars Science Lab gibi birçok uzay aracının tasarımında kullanılmıştır.

Bu tez çalışmasında, Hesaplamalı Akışkanlar Dinamiği yöntemi temel alınarak yüksek entalpi koşullarında çözüm yapabilen hipersonik bir sonlu hacimler çözücüsü geliştirilmiştir. Geliştirilen çözücü ısı denge ve ısı dengesinden uzak koşullar için sınır tabaka-şok dalgası etkileşimlerini ve bu etkileşimlerden kaynaklı kimyasal tepkimeleri çözümleyebilmektedir. Çözücü nesne temelli modüler bir programlama yapısına sahip olan OpenFOAM yazılımı bünyesindeki açık kaynak kodlu iki temel çözücü yardımıyla oluşturulmuştur. rhoCentralFoam ve reactingFoam isimli bu iki çözücü sırasıyla yüksek hızda meydana gelen şok yapılarını ve kimyasal tepkimeleri analiz etme kabiliyetine sahiptir. rhoCentralFoam çözücüsü yoğunluk temelli hücre merkezli bir sonlu hacimler çözücüsüdür. Zamanda birinci derecenen uzayda ise ikinci dereceden doğrulukta çözüm yapabilmekte fakat kimyasal tepkimeli akış koşullarını modelleyememektedir. reactingFoam çözücüsü ise sıkıştırılamaz akış rejiminde

kimyasal tepkimeleri çözümleyebilmesine rağmen şok yapılarını elde etme kabiliyetine sahip değildir.

Bu yüzden, geliştirilen hipersonik çözücünde, akışın iki temel fiziksel mekanizması olan şok yapıları ve kimyasal reaksiyonlar bu iki çözücü vasıtasıyla birbirine bağlanmıştır. Yani, hipersonik çözücü ısı dengede ve ısıl dengeden uzak koşullarda şok dalgası - sınır tabaka etkileşimlerinden kaynaklanan yüksek sıcaklık ve basınç artışları sebebiyle tetiklenen kimyasal reaksiyonları modelleyebilmektedir.

Yüksek hızlarda ve sıcaklıklardaki akışın fiziğini doğru temsil edebilmek adına hipersonik çözücüye bu iki çözücünde halihazırda bulunmayan bazı modeller ve denklemler de ilave edilmiştir. Isıl dengeden uzak akış çözümleri için literatürde İki-Sıcaklık Modeli olarak bilinen bir model çözücüye entegre edilmiştir. Makro düzeyde tanımlanan gazların denge sıcaklığı, mikro düzeydeki atom ve moleküllerin serbestlik derecesinden kaynaklı farklı enerji modlarındaki sıcaklıkların Maxwell dağılımını sağladığı durumu ifade etmektedir. Fakat yüksek hız ve sıcaklık koşullarında termal dengeden uzaklaşıldığı için denge sıcaklığı Maxwell dağılımından uzaklaşmaktadır. Bu yüzden İki-Sıcaklık Modeli vasıtasıyla, denge sıcaklığı öteleme-dönme ve titreşimsel sıcaklık olarak ikiye ayrılmaktadır. Öteleme-dönme sıcaklığı bir molekül veya atomun öteleme ve dönme hareketlerinden kaynaklı sıcaklıklarının dengede olduğu kabulünü içerir. Bu modelde titreşimsel sıcaklıklar moleküllere has olarak tanımlanmakta ve atomlar için sadece öteleme-dönme sıcaklığı geçerli olmaktadır. Bu tür etkilerin hesaplanabilmesi için eş zamanlı olarak çözülen süreklilik, momentum ve enerji denklemlerinin yanı sıra akış alanındaki her bir molekül ve atom için çeşit kütle korunum denklemleri ve moleküller için titreşimsel sıcaklıkların hesaplanabildiği ek bir enerji denkleminin de çözülmesi gerekmektedir. Öteleme-dönme sıcaklığı, rhoCentralFoam çözücüsü içerisinde halihazırda bulunan standart enerji denkleminde yapılan küçük bir değişiklik ile hesaplanabilmekte iken moleküllerin titreşimsel sıcaklıklarının bulunabilmesi için çözücüye ayrıca ek bir titreşimsel enerji denklemi entegre edilmiştir. Eklenen bu titreşimsel enerji denklemi, tıpkı standart formdaki enerji denklemi gibi iki parçada çözümlenebilmektedir. Çözücünde yer alan bu ek enerji denkleminin ayrıklaştırması diğer kütle, momentum ve enerji denklemlerinde olduğu gibi Kurganov-Tadmor şemasına dayanmaktadır.

OpenFOAM bünyesi altındaki termodinamik kütüphanelerinde entropi, entalpi ve sabit basınçta özgül ısı gibi her bir çeşide ait termodinamiksel özellikler JANAF paketi yardımıyla hesaplanmaktadır. Halihazırda kütüphanelerde mevcut olan JANAF paketi ile termofiziksel özellikler sıcaklığın 200K ve 6000K arasında kaldığı değerler için hesaplanabilmektedir. Fakat, yüksek ses üstü hız koşullarında bu sıcaklık aralığı aşılabildiğinden standart JANAF hesaplamaları yeterli olmamaktadır. Bu yüzden NASA tarafından geliştirilmiş olan daha geniş bir sıcaklık aralığını kapsayan termodinamik bağıntıları kütüphanelere entegre edilmiştir. Hipersonik çözücü eklenmiş yeni JANAF bağıntıları sayesinde termodinamik özellikleri 200K – 20000K sıcaklık aralığı için hesaplayabilmektedir. Ayrıca, hipersonik çözücünün diğer geliştirilmiş çözücülerle karşılaştırma sırasında uyumlu olabilmesi adına viskozite ve iletim katsayısı gibi termofiziksel özellikler kütüphanelerde tanımlı olan Sutherland bağıntısının yerine Blottner tarafından önerilen bir ifade ile hesaplanmıştır. Karışımın termofiziksel özelliklerini hesaplayabilmek için çözücüye bir bağıntı eklenmiştir. Wilke tarafından önerilen bu karışım bağıntısında karışımın toplam termofiziksel katsayısının büyüklüğü her bir çeşidin kütle oranı ve molekül ağırlığının hesaba katılmasıyla elde edilebilmektedir.

Hipersonik çözücü ile gerçekleştirilen analizlerde kimyasal olarak aktif bir hava modeli kullanılmıştır. Bu hava modeli referans olarak alınan bir deneysel çalışmanın akış koşullarında bulguların çeşitlerinin kütle oranına ve cinsine göre belirlenmiştir. Sayısal hesaplamalarda kullanılan hava modeli toplam 5 farklı tipte çeşit içermekte ve bu çeşitler farklı kombinasyonlarda olmak üzere 19 adet tersinmez tepkimeye uğramaktadırlar. Her bir kimyasal tepkimenin reaksiyon hızları Arrhenius bağıntısı yardımıyla hesaplanabilmektedir. Çözücünün doğrulama çalışmalarında ise diğer çözücülerin kullandığı hava modelleri ile uyumlu olabilmesi açısından belirtilen hava modelinden farklı seçimler de yapılmıştır.

Geliştirilen hipersonik çözücü hem ısı dengede hem de ısı dengeden uzak koşullarda olmak üzere kimyasal tepkimelerin aktif olduğu ve olmadığı durumlar için test edilmiştir. Doğrulama çalışmaları hipersonik çalışmalarda yaygın olarak kullanılan adyabatik ısı banyosu, sivri burunlu koni ve küt burunlu koni gibi modeller üzerinde gerçekleştirilmiştir. Doğrulama testleri, akış fiziğinin görece basit olduğu durumlardan daha karmaşık olduğu durumlara kadar aşama aşama yapılmıştır. Belirtilen modeller üzerinde yapılan hesaplamalardan elde edilen çözümler, aynı sınır ve başlangıç koşulları altında hesaplamaları gerçekleştirilen diğer hipersonik çözücülerden elde edilen sonuçlarla ve deneysel bulgularla karşılaştırılmıştır.

Hipersonik çözücü ile şok-şok ve şok-sınır tabaka etkileşim mekanizmalarının incelenmesinde sıklıkla kullanılan iki açılı rampa geometrisi üzerinde ısı dengede ve ısı dengeden uzak kimyasal akış analizleri gerçekleştirilmiştir. İki açılı rampa geometrisinin ilk açısı 30° 'de sabit tutulurken ikinci açısı 45° 'den başlamak üzere sistematik olarak 60° 'ye kadar arttırılmıştır. Hem iki boyutlu hem de üç boyutlu ısı dengede ve ısı dengeden uzak analizler bu dört farklı rampa geometrisi için tekrarlanmıştır. Şok dalgası – sınır tabaka etkileşimlerinin ve akışın kimyasal davranışının ikinci açı değişimi ile etkisi incelenmiştir. Rampa modeli üzerinde hesaplanan ısı akısı dağılımı ikinci açının 55° olduğu model üzerinde yapılmış olan deneysel çalışmadan ve diğer hipersonik çözücülerden elde edilen ısı akısı dağılımları ile karşılaştırılmıştır. Akışın üç boyutluluk etkisi ve zamana bağlı davranışı incelenmiştir. İki boyutlu ve üç boyutlu çözümlerden elde edilen şok yapıları için sayısal Schlieren görüntüleri oluşturulup farklı durumlar için karşılaştırmalar yapılmıştır.



1. INTRODUCTION

The study of aerodynamics of high speed re-entering vehicles still remains one of the most challenging tasks for engineers and scientists. Flight speeds of vehicles during re-entry might go up to 10 km/s and gas temperature can increase to about 10000 K. Material selection and design processes of these vehicles are very much dependent upon the complex physical behavior of shock wave interactions in hypersonic regime. In 2006, after completing its mission, the maximum velocity and temperature of gas around Stardust probe during re-entry were measured as 12.8 km/s and 25000 K, respectively [1]. Another hypersonic test vehicle X-51 flew for 210 seconds in a speed more than Mach 5 in 2013 [2]. In addition to these successful flights, there have also been some catastrophic accidents in the history of aviation. For instance, the body of X-15 designed by NASA was damaged severely by local aerodynamic heating resulting from unpredicted shock interaction mechanisms [3]. In 2003, disaster of Columbia Space Shuttle was due to problems in thermal protection system triggered by high temperatures during re-entry [3].

As it is understood, predicting the physical behavior of hypersonic flow around such vehicles becomes crucial for ensuring safety and preventing tragic accidents. There have been some experimental studies regarding high enthalpy, low pressure flows in order to overcome these difficulties. Nevertheless, because such experiment facilities are limited and cost too much to produce required hypersonic conditions, researchers have also tried different techniques to cope with such problems. Some of them are predicting the physics of flow by means of analytical, empirical and semi-empirical methods. Even though these methods are fundamentally quite accurate, they are only valid for simple geometries and boundary conditions. In the case of complex geometries, solution to high-speed flows becomes impossible. Therefore, Computational Fluid Dynamics (CFD) gained popularity for the design of aerial vehicles thanks to advancing computer technology. CFD plays crucial role to reduce costs that cannot be achieved by wind tunnel experiments. However, CFD solutions still require wind tunnel experiment validations, which mean that an optimization

process for choosing the best solution among hundreds of cases is mandatory. In the past, CFD was used in the design process of Mars Pathfinder, Stardust, Mars Science Lab and Huygens-Cassini [4-5].

In the present study, a Finite Volume Navier-Stokes hypersonic solver was developed within the framework of OpenFOAM. This study aims to investigate the complex shock – shock, shock wave – boundary layer interactions in high enthalpy, low-pressure conditions. Newly developed hypersonic solver provides an alternative to the present codes available in the literature. The results of this hypersonic solver compare prediction capabilities of different solvers run at similar flow conditions.

The novelty of this study is to systematically investigate interaction mechanisms around the same model with different aft-angles. Besides, the present work also provides a comparison between 2D and 3D shock interactions in thermally equilibrium and non-equilibrium reacting flow conditions.

1.1 Literature Review

There exist some numerical solvers capable of simulating hypersonic flows in the literature. *DPLR* and *LAURA* codes [6] developed by NASA were two of hypersonic solvers that can successfully calculate hypersonic flow properties around flying objects. *DPLR* code is a three-dimensional structured finite volume Navier-Stokes solver with reaction kinetics, thermal and chemical non-equilibrium flow physics implemented. The implicit time integration method Data-Parallel Line Relaxation implemented into the solver gives the name for *DPLR* code. In *DPLR*, Steger-Warming flux splitting scheme [7] for calculating inviscid fluxes was used with MUSCL extrapolation technique. The code achieves a third order spatial accuracy with a minmod limiter coupled to MUSCL extrapolation [8]. In *LAURA*, thermal non-equilibrium effects for reactive flows can also be simulated. Differently from *DPLR*, *LAURA* uses either point or line implicit time integration scheme in order to achieve steady state. Inviscid fluxes are calculated with the help of Roe's average [9] and Harten's fixed entropy [10] schemes with Yee's symmetric TVD limiter [11].

Researchers from University of Minnesota developed another hypersonic code by the name of *US3D*. *US3D* code [6] acquired much of its capability from the development stages of *DPLR* solver. While the codes generated by NASA are suitable for

structured mesh only, *US3D* is able to perform unstructured mesh solutions as well. All of these three codes employ Two-Temperature Model of Park [12] in order to represent thermally non-equilibrium flows by separating distinct energy modes. In the case of reacting computation, ionization processes as well as dissociation reactions are also taken into account in these codes. Another hypersonic non-equilibrium finite volume code called *LEMANS* [13] was developed by the University of Michigan. Similar to DPLR, numerical fluxes between adjacent cells are handled by Stegger-Warming flux splitting scheme. Two temperature model accounts for thermal non-equilibrium conditions. Time marching is achieved by a point implicit technique. *hy2Foam* [14] is an open-source CFD solver which is able to compute non-equilibrium hypersonic flows. With the help of two temperature model, *hy2Foam* has the capability to represent the energy transfers between different energy modes in reacting mixtures. Flux interpolations between neighbor cells are handled using central-upwind scheme proposed by Kurganov and Tadmor [15].

dsmcFoam [16] and *MONACO* [17] codes include the implementation of DSMC method for rarefied re-entry problems in which molecular effects becomes crucial in thermally and chemically non-equilibrium flow. Contrary to continuum approach, DSMC directly computes particle collisions rather than dealing with macroscopic averages of collisional effects. DSMC approach is currently the most popular technique in the simulation of rarefied gas flows.

In addition to numerical studies, there have also been experimental tests conducted in high speed regimes. For example, in 2001 and 2002, Holden et al. performed low Reynolds number hypersonic test experiments [18] on a double cone model for Mach numbers ranging from 9 to 11. These experiments took place in CUBRC LENS I facilities provided Schlieren images of shock waves as well as surface heat flux and pressure distributions on cone model. Similar to that, in 2006, Schrijer et al. used PIV and Schlieren measurement techniques to obtain details about flow field around a double wedge model on Mach 7 [19]. Swantek et.al., who studied on the same double wedge model, also contributed a great deal of experimental data conducted on high enthalpy flow conditions for Mach numbers between 4-7 [20-21]. Their experiments were performed for nitrogen and air flow both in low and high enthalpy conditions at different Mach speeds.

In 2011, AVT-136, which is a subgroup of The North Atlantic Treaty Organization (NATO), also realized other supersonic experimental studies on the double cone model [22-23]. Apart from the double cone, this group carried out high speed flow experiments on a cylinder model as well. In the following years, six different researchers from Europe and USA made studies on AVT-136 group's experiments in order to compare and validate their own numerical solvers. All the numerical studies on double cone model from various researchers proved that the flow around double cone showed time-dependent behavior [23], which is not observable in the experiment. For this reason, another group AVT-205 was established so that more detailed hypersonic experimental studies could be conducted to observe shock-wave boundary layer interactions. AVT-205 chose three different test cases in order to investigate heat transfer rates originating from separation and reattachment shocks in the boundary layer. One of these benchmark cases was selected from the double wedge experiments of Swantek [24], on which many numerical solutions, including the results of this thesis, compared with each other.

1.2 Shock Wave – Boundary Layer Interactions

1.2.1 Shock induced separation on a surface

A typical shock wave – boundary layer interaction mechanism can be understood from a supersonic viscous flow over a flat plate on which an incident shock wave impinges upon a growing boundary layer [25]. The pressure jump across the impinging shock wave, with the effect of adverse pressure gradient, separates the boundary layer from the surface. The high pressure information behind the shock wave is transmitted through the subsonic flow region of the boundary layer, thus allows the location of separation point to move upstream of impinging shock wave. As a result of separated boundary layer, a second shock wave, which is called as “induced separation shock”, is formed ahead of incident shock wave. Nevertheless, the separated boundary layer reattaches to the surface at some specific downstream location, where nature forms another shock wave called the “reattachment shock”. Along the profile of boundary layer, Prandtl-Meyer expansion waves are also generated where the flow turns back to the surface. A relatively thin boundary layer forms at the reattachment location due to high pressure within this region. In addition to high pressure, immense local heat transfers are encountered behind the

reattachment shock. Besides, at a certain distance, induced separation and reattachment shocks interact and the interaction causes a formation of another shock wave called “reflected shock”.

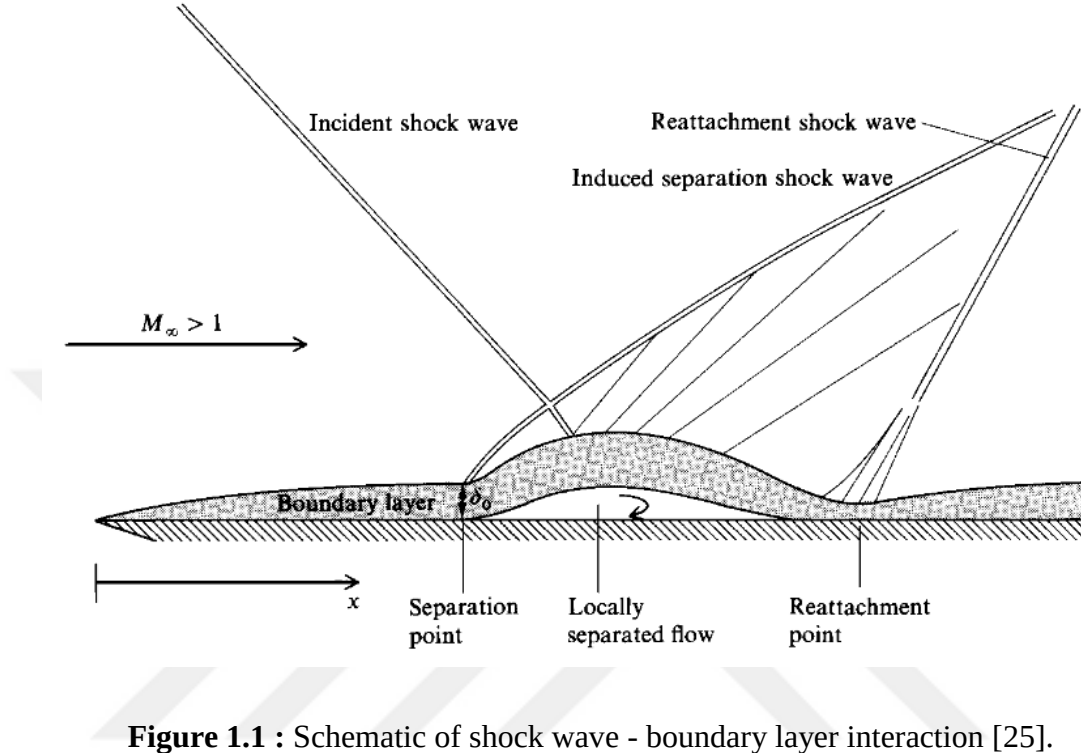


Figure 1.1 : Schematic of shock wave - boundary layer interaction [25].

1.2.2 Edney type-V interaction mechanism

In the case of hypersonic viscous flows on double cone and double wedge surfaces, more complicated forms of shock-shock, shock-boundary layer interactions might develop and excessive heat fluxes might be observed on the surfaces. Various experimental and numerical studies [20-21, 26-28] showed that a unique type of interaction called Edney type-V is present if the aft angle exceeds a threshold value depending on free-stream Mach number. In addition to shock waves created at the leading edge and the compression corner (CC), extra shock waves, depending on the aft angle and free-stream velocity, might occur due to the separation of boundary layer as explained in the previous section. Also, a detached bow shock forms due to the high aft angle of the double wedge model. Deformation of the boundary layer causes formation of reattachment shocks (RS) upstream and downstream of the CC. From the interaction point of leading edge shock (LS) and bow shock (BS), another shock called transmitted shock (TS) emerges and impinges upon the second surface

of the double wedge. This impingement creates a separation bubble in addition to the one near the CC. When LS, TS and BS interact at the triple point a contact discontinuity (CD) also occurs from this location. It should also be noted that additional triple points TP_1 and TP_2 might be present if RS and TS do not directly interact at the TP. In this case, new triple points of TP_1 and TP_2 are connected through a Mach stem (MS).

Nevertheless, the interaction mechanism is not limited to the one illustrated in the Figure 1.2. Depending on the Mach number and the geometrical dimensions of double wedge, formations of more complex and unsteady interaction mechanisms are also possible on these types of flows [29].

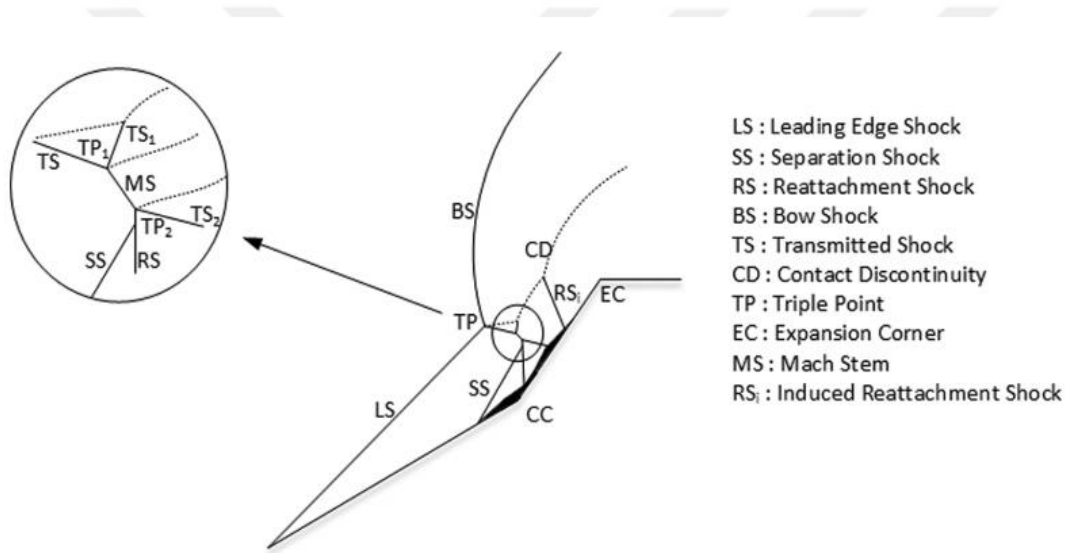


Figure 1.2 : Edney type-V interaction mechanism.

1.3 Thermally and Chemically Non-Equilibrium Hypersonic Flows

Trajectories of a re-entry craft travelling through an atmosphere contain a number of several degrees of rarefied regions ranging from the continuum to the free-molecular. Usually, the rarefaction spectrum in the upper layers of atmosphere is classified in three categories: continuum regime, continuum-transition regime and free molecular regime [30]. In the continuum-transition flow regime, collisional impacts on the surface of the space vehicle become important in order to truly represent non-equilibrium nature of the flow. In addition to atmospheric rarefaction, shock wave –

boundary layer interactions around the re-entry vehicle also contribute to thermal and chemical non-equilibrium effects.

Non-equilibrium effects in a flow becomes observable if the required time of a process to accommodate itself to local conditions within a certain region is of the same order as the transit time across the entire region. Equilibrium conditions are satisfied as long as the accommodation time is very short compared to transit time. On the other hand, the process is called “frozen” if the accommodation time is very long in comparison to transit time. The determination of length scale of the region is a problem-specific issue. For example, the parameters such as boundary layer thickness, shock standoff distance, chord length and shock-transition zone thickness might be useful to decide on length scale of the region for re-entry problems. Possible processes can be chemical reactions, energy relaxations among distinct modes and ionizations. The accommodation time is a direct function of frequency of effective collisions among molecules, atoms, electrons and ions in the gas mixture. The effect of non-equilibrium conditions takes more importance in the low-density atmosphere for hypersonic flows. The collisional frequency is lower when the vehicle travelling in the rarefied regions of upper layers of atmosphere. The lack of effective collisions among the molecules increases the accommodation time of any process in the flow. The transit time, however, is lowered due to high speed during re-entry missions. Therefore, the combination of low transit time and high accommodation time makes non-equilibrium effects a non-negligible phenomenon in these types of flows [31].

1.4 Two-Temperature Model

Normally Navier-Stokes equations are only applicable for continuum regions. In order to extend the applicability of equations for continuum-transition regime, Park’s Two-Temperature formulation [12] was used in this study. In hypersonic speeds, the two-temperature formulation models thermally non-equilibrium flow. Due to the flow conditions explained in the previous subsection, thermal non-equilibrium effects become important for re-entry and the internal energy of gas needs to be characterized by various energy modes, which are representation of distinct motions in molecular level. These energy modes correspond to translational, rotational, vibrational and electronic internal energies. Unlike single temperature formulation,

the two-temperature model assumes that there are only two different temperatures associated with these energy modes. The first temperature, T_{tr} , represents equilibrium state of translational and rotational energies, whereas the second one, T_{ve} , is assumed to be equilibrium temperature of vibrational and electronic modes [32]. An additional equation called vibrational energy equation is needed to determine T_{ve} in the two-temperature model.



2. GOVERNING EQUATIONS

2.1 Flow Equations for Thermal Non-Equilibrium

Adopting the continuum approach, transient solution of hypersonic flows for thermal non-equilibrium conditions can be obtained by utilizing Navier-Stokes-Fourier equations [33]. In these set of equations, mixture and specie partial densities are calculated from total continuity and specie continuity equations, respectively. Together with three momentum equations and a total energy equation, vibrational energy equations for each molecule in the mixture must also be taken into account so that thermal non-equilibrium can be represented. Since ionization effects are neglected in this study, all the terms related to the electronic mode are dropped from the original governing equations. Therefore, in vector form the governing equations can be written as below:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial (\mathbf{F}_{i,inv} - \mathbf{F}_{i,vis})}{\partial x_i} = \mathbf{W} \quad (2.1)$$

where the primitive vector is expressed as:

$$\mathbf{U} = [\rho, \rho_s, \rho u, \rho v, \rho w, E_{v,m}, E]^T, \quad s \in N_s, \quad m \in N_m \quad (2.2)$$

N_s and N_m represent the total number of species and molecules in the gas mixture, respectively. The inviscid and viscid flux vectors can be stated as:

$$\mathbf{F}_{i,inv} = \begin{bmatrix} \rho u_i \\ \rho_s u_i \\ \rho u_i u + \delta_{i1} p \\ \rho u_i v + \delta_{i2} p \\ \rho u_i w + \delta_{i3} p \\ E_{v,m} u_i \\ (E + p) u_i \end{bmatrix}, \quad \mathbf{F}_{i,vis} = \begin{bmatrix} 0 \\ J_{s,i} \\ \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ -q_{v,i,m} - e_{v,m} J_{m,i} \\ \tau_{ij} u_j - q_{tr,i} - q_{v,i} - \sum_s h_s J_{r,i} \end{bmatrix} \quad (2.3)$$

In equation (2.3), both i and j denotes one of three dimensions in Euclidean space. The second row in $\mathbf{F}_{i,inv}$ shows s^{th} specie's inviscid mass flux through the cell faces whereas the sixth row indicates the inviscid vibrational energy flux through the cell faces. In the vector $\mathbf{F}_{i,vib}$, the second row illustrates s^{th} specie's mass diffusion flux. In the sixth row, the first term represents vibrational conductivity due to vibrational energy gradient in the flow domain while the second term indicates vibrational energy transfer due to species' mass diffusion. In the last row, $q_{tr,i}$ and $q_{v,i}$ are heat conduction terms due to the gradient of trans-rotational and vibrational temperatures in the flow domain. The last term in this row includes diffusion of species' enthalpies, which contains chemical related information.

Total pressure, p , can be obtained by adding the partial pressure of each specie using Dalton's Law:

$$p = \sum_s p_s = \sum_s \rho_s R_s T_{tr} \quad (2.4)$$

Shear stress tensor, τ_{ij} , is calculated according to the following formula:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + (\lambda + \mu_b) \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (2.5)$$

where Stokes' hypothesis holds such that second and shear viscosities are dependent variables with the relation $\lambda = -\frac{2}{3}\mu$, whereas bulk viscosity is assumed as $\mu_b = 0$. The calculation of trans-rotational and vibrational heat conduction terms follows Fourier's law:

$$q_{tr,i} = \sum_s q_{tr,i,s} = \sum_s -\kappa_{tr,s} \frac{\partial T_{tr}}{\partial x_i}, \quad (2.6)$$

$$q_{v,i} = \sum_s q_{v,i,s} = \sum_s -\kappa_{v,s} \frac{\partial T_{v,s}}{\partial x_i} \quad (2.7)$$

Eucken relation [34] provides approximate calculations for trans-rotational and vibrational thermal conductivities terms:

$$\kappa_{tr,s} = \mu_s \left(\frac{5}{2} c_{vts} + c_{vrs} \right), \quad \kappa_{v,s} = \eta_v \mu_s \quad (2.8)$$

where the coefficient $\eta_v = 1.2$ is predicted from kinetic theory [35]. Eucken relation gives reasonable results only up to temperatures around 6000 K. For better accuracy for higher temperatures, other valid methods should be used instead. The terms related to translational and rotational heat capacities at constant volume, c_{vts} and c_{vrs} , can be found out from the internal energy relations given in equations (2.27 and 2.28). The pure specie viscosity is obtained by a viscosity model offered by Blottner et al. [36]:

$$\mu_s = 0.1 e^{[(A_s \ln T + B_s) \ln T + C_s]} \quad (2.9)$$

where A_s , B_s , and C_s coefficients for each species are determined from the thermo-chemistry model used. Mixture thermo-physical quantities are calculated from specie properties by incorporating Wilke's mixing rule [37]:

$$\mu = \sum_s \frac{X_s \mu_s}{\phi_s} \quad (2.10)$$

$$\kappa = \sum_s \frac{X_s \kappa_s}{\phi_s} \quad (2.11)$$

where X_s is the molar fraction of specie "s". The expansion of ϕ_s can be expressed as:

$$\phi_s = \sum_r X_r \left[1 + \sqrt{\frac{\mu_s}{\mu_r} \left(\frac{M_r}{M_s} \right)^{\frac{1}{4}}} \right]^2 \left[\sqrt{8 \left(1 + \frac{M_s}{M_r} \right)} \right]^{-1} \quad (2.12)$$

where M_s denotes the molecular weight of s^{th} specie. It is assumed that diffusion flux of each specie is calculated through the gradient of the mass fraction, $Y_{s,i}$. Fick's Law [33] can find out diffusion flux among mixtures of similar particles:

$$J_{s,i} = \rho D_s \frac{\partial Y_{s,i}}{\partial x_i} \quad (2.13)$$

For low Knudsen numbers, reasonable accuracy in the determination of the diffusion coefficient, D_s , can be obtained from constant Lewis number, Le , approximation:

$$Le = \frac{\rho D c_p}{\kappa} \quad (2.14)$$

where constant Le number of 1.4 assumed. However, constant Lewis approximation for the calculation of diffusion coefficient cannot produce good results for high Kn numbers that is encountered during atmospheric entries. The right hand side of equation (2.1) includes source term vector:

$$\dot{W} = [0, \dot{w}_s, 0, 0, 0, \dot{w}_{v,m}, 0]^T \quad (2.15)$$

where $\dot{w}_s$ is the net rate of mass production term of s^{th} specie in the mixture whereas the term $\dot{w}_{v,m}$ contains the rate of energy transfers among the available energy modes. Expansion of vibrational source term is written as:

$$\dot{w}_{v,m} = Q_{m,V-T} + Q_{m,V-V} + Q_{m,C-V} \quad (2.16)$$

The energy transfer between vibrational-transrotational, vibrational-vibrational and chemistry-vibrational modes are represented by the indices V-T, V-V and C-V, respectively. Landau-Teller equation [38] expresses the exchange of energy between vibrational and trans-rotational modes as follows:

$$Q_{m,V-T} = \rho_m \frac{e_{v,m}(T_{tr}) - e_{v,m}(T_{v,m})}{\tau_{m,V-T}} \quad (2.17)$$

where $\tau_{m,V-T}$ symbolizes the molar averaged relaxation time between vibrational and trans-rotational modes. The calculation of this term is done by utilizing Millikan and White semi-empirical correlation [39] with Park's correction factor [40]:

$$\tau_{m,V-T} = \frac{\sum_s X_s}{\sum_s X_s / \tau_{m-s,V-T}} \quad (2.18)$$

where Landau-Teller inter-species relaxation time [33], $\tau_{m-s,V-T}$, is governed by the relation:

$$\tau_{m-s,V-T} = \frac{1}{p} \exp \left[A_{m,s} \left(T_{tr}^{-1/3} - B_{m,s} - 18.42 \right) + \frac{1}{c_m \sigma_{v,m} n_{m,s}} \right] \quad (2.19)$$

where the unit of the pressure term, p , is in “atm”. The calculation of the coefficients $A_{m,s}$ and $B_{m,s}$ can be obtained from the equations provided in reference [14]. The second term in the square bracket shows the collision-limited relaxation time term offered by Park [40]. The formula proposed by Knab et al [41-42] is used to calculate the vibrational-vibrational energy relaxation term, $Q_{m,V-V}$:

$$Q_{m,V-V} = \sum_{l \neq m} N_A \sigma_{m,l} P_{m,l} \sqrt{\frac{8RT_{tr}}{\pi M_{m,l}}} \frac{\rho_l}{M_l} \rho_m \left(e_{v,m}(T_{tr}) \frac{e_{v,l}(T_{v,l})}{e_{v,l}(T_{tr})} - e_{v,m}(T_{v,m}) \right), \quad m, l \in N_m \quad (2.20)$$

where N_A is the Avogadro number, R is the universal gas constant and the value of the assessed exchange probability constant, $P_{m,l}$, is recommended as 10^{-2} [43]. $\sigma_{m,l}$ is defined as the collision cross-section of the collision pair (m, l). The cross sectional area of collision is calculated by considering the diameters of the respected molecules. Park TTV model [44] is selected in order to represent the chemistry-vibrational coupling term $Q_{m,C-V}$ as follows:

$$Q_{m,C-V} = \dot{w}_m D'_m \quad (2.21)$$

where a preferential model [45] predicts the coefficient D'_m :

$$D'_m = \alpha_m D_m \quad (2.22)$$

where the dissociation potential, D_m , is a thermodynamic property defined for each molecule “ m ” in the mixture while the coefficient for dissociation energy, α_m , is typically chosen as 0.3 [33]. The net mass production rate of each specie is calculated according to the following expression:

$$\dot{w}_s = M_s \sum_{r=1}^{N_r} (v''_{s,r} - v'_{s,r}) \times \left[k_{f,r} \prod_{k=1}^{N_r} \left(\frac{\rho_k}{M_k} \right)^{v'_{k,r}} - k_{b,r} \prod_{k=1}^{N_r} \left(\frac{\rho_k}{M_k} \right)^{v''_{k,r}} \right] \quad (2.23)$$

In this equation, forward and backward stoichiometric coefficients are represented by $v''_{s,r}$ and $v'_{s,r}$, respectively. N_R symbolizes the number of total reactions. The calculation of forward and backward reaction rates needs the employment of Arrhenius law:

$$k_{f,r} = A \times T_{tr}^{\beta} \times \exp\left(-\frac{T_a}{T_{tr}}\right) \quad (2.24)$$

where forward rate constants T_a , A and β denote activation temperature, pre-exponential factor and temperature exponent of the r^{th} reaction, respectively. In the primitive vector, the total energy term, E , consists of the sum of kinetic, translational, rotational, vibrational, and chemical energies as shown below:

$$E = \frac{1}{2} \rho \sum_i u_i^2 + \sum_s E_{t,s} + \sum_s E_{r,s} + \sum_s E_{v,s} + \sum_s \rho_s h_s^o \quad (2.25)$$

Each of the energy modes in this equation is expressed by a specific temperature. Nonetheless, rotational and translational modes are specified by a single temperature, T_{tr} , since rotational energy mode relaxes quickly such that it can be assumed in thermal equilibrium with translational mode [46]. The energy per unit mass of any specie in the mixture can be related to total energy of a particular mode as following:

$$E_v = \sum_s E_{v,s} = \sum_s \rho_s e_{v,s} \quad (2.26)$$

The distinct internal energies per unit mass of species can be written as:

$$e_t = \frac{3}{2} R_s T_{tr} \quad (2.27)$$

$$e_r = R_s T_{tr} \quad (2.28)$$

$$e_{v,s} = R_s \left(\frac{\theta_{v,s}}{\exp\left(\frac{\theta_{v,s}}{T_{v,s}}\right) - 1.0} \right) \quad (2.29)$$

where vibrational characteristic temperature, $\theta_{v,s}$ is found from the use of simple harmonic oscillator model [46]. Adding up translational and rotational internal energies reorders equation (2.25) as:

$$E = \frac{1}{2} \rho \sum_i u_i^2 + E_{tr} + \sum_s E_{v,s} + \sum_s \rho_s h_s^o \quad (2.30)$$

where h_s^o shows the formation of standard enthalpy for s^{th} specie.

2.2 Flow Equations For Thermal Equilibrium

In opposition to thermal non-equilibrium, all of the internal energy modes are assumed to be specified by a single temperature in thermally equilibrium state. Therefore, rather than rewriting the whole set of equations, only some modifications and reductions are required to obtain the governing equations for thermally equilibrium flow.

First, vibrational energy equation, which is represented in the sixth row of primitive, flux and source vectors in equation (2.1), is eliminated. Second, the vibrational and trans-rotational heat conduction terms depicted in the last row of equation (2.3) is removed and the heat conduction is specified by the equilibrium temperature only, such that:

$$\mathbf{q}_i = \sum_s \mathbf{q}_{i,s} = \sum_s -\kappa_s \frac{\partial T}{\partial x_i}, \quad (2.31)$$

The calculation of thermal conductivity coefficient, κ , is derived from the definition of the Prandtl number. Thus, thermal conductivity coefficient is calculated according to:

$$\kappa_s = \frac{c_{p,s} \mu_s}{Pr} \quad (2.32)$$

Equation (2.9) is still valid to obtain specie viscosity, μ_s . Nevertheless, the calculation of heat capacity at constant pressure, $c_{p,s}$, is entirely different due to the fact that the internal energies in equations (2.27, 2.28 and 2.29) can no longer be used in thermal equilibrium conditions. Therefore, depending on the type of problem, $c_{p,s}$ should be taken as a constant or be related to temperature increasement. In this study, most of the validations and analyses were performed by considering JANAF thermodynamic package that can calculate thermodynamic properties in the temperature range of 200K – 20000K [47]. The set of properties, heat capacity, enthalpy and entropy, employed in JANAF package can be stated as below:

$$\frac{c_p^o(T)}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (2.33)$$

$$\frac{H^o(T)}{RT} = -a_1 T^{-2} + \frac{a_2 \ln T}{T} + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{b_1}{T} \quad (2.34)$$

$$\frac{S^o(T)}{R} = -\frac{a_1 T^{-2}}{2} - \frac{a_2}{T} + a_3 \ln T + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + b_2 \quad (2.35)$$

Finally, because the internal energies of distinct modes are in equilibrium, conventional form of internal energy definition is inserted into equation (2.30) and the total energy equation (2.37) for thermal equilibrium is obtained as follows:

$$e_s = c_{v,s} T \quad (2.36)$$

$$E = \frac{1}{2} \rho \sum_i u_i^2 + \sum_s \rho_s e_s + \sum_s \rho_s h_s^o \quad (2.37)$$

3. SOLVER DEVELOPMENT

The new solver, *hyperReactingFoam*, was created with the help of two built-in standard solvers within the framework of OpenFOAM. OpenFOAM, written in C++ programming language, takes advantage of finite volume numerics to solve the partial differential equations for any unstructured mesh. Even though all the default solvers within OpenFOAM generate three-dimensional solution, one or two dimensional analyses can also be performed by the application of required boundary conditions. Shock wave boundary layer interactions for non-reacting high speed flows can be resolved by *rhoCentralFoam*, which is a density based, open-source, cell centered, finite volume Navier-Stokes solver within OpenFOAM. *rhoCentralFoam* is able to produce non-oscillatory solutions in the presence of discontinuities such as shock waves and contact surfaces. In *rhoCentralFoam*, an operator splitting method is applied in order to solve momentum and energy transport equations. In this splitting method, the convection of conserved variables are represented by an “explicit predictor equation” whereas the diffusion of primitive variables are described by an “implicit corrector equation”. In this method, the solution of convection component part with a diagonal solver provides fast convergence, while implicitly solved diffusion component part assists in terms of stability. The finite volume discretization used by *rhoCentralFoam* solver consists of semi-discrete, non-staggered central schemes for collocated variables assigned on polyhedral cells. Central-upwind scheme of Kurganov, Noelle and Petrova implemented in *rhoCentralFoam* produced successful results when validated against to analytical, numerical and experimental data in different type of problems [48].

Basic chemistry capabilities from *reactingFoam* solver are very helpful since the influence of chemical reactions in re-entry problems cannot be ignored in high temperature conditions. *reactingFoam* solver can store the specie properties in a pointer array, through which the development process of the new solver is tremendously eased. Nevertheless, *reactingFoam* can only produce low speed

solutions and the numerics of the solver are not suitable for capturing shock wave interactions at high speeds.

In essence, *hyperReactingFoam* was developed by combining these two standard OpenFOAM solvers on which some additional implementations performed. On the solver level, *hyperReactingFoam* contains a specie transport equation and "m" number of additional vibrational energy equations. Mass fraction of each specie in the mixture can be determined from the former equation while vibrational temperature of each molecule can be obtained through the additional vibrational equations. Equation (2.30) was employed to modify the default energy equation in *rhoCentralFoam*. By subtracting equation (2.26) from equation (2.30), *hyperReactingFoam* is able to calculate the trans-rotational temperature for thermal non-equilibrium conditions. Central-upwind interpolation scheme of Kurganov, Noelle and Petrova [15] was utilized for the discretization of additional vibrational energy equations. These vibrational energy equations, just as standard energy equation, are solved in two steps, which are composed of explicit predictor equation and implicit corrector equation.

The calculation of reaction sources written in equation (2.23) is already present in the *reactingFoam* solver. In order to calculate reaction sources, the list of species in *reactingFoam* is introduced through a Chemkin Interpreter input file. Chemkin is a widely used software tool for solving chemical kinetics problems ranging from combustion, chemical processing, atmospheric entries etc. [50]. In addition to the reactants list, the chemical reactions and the Arrhenius reaction rate parameters in equation (2.24) can also be introduced to the solver through the Chemkin file. The integration of reacting capabilities into *rhoCentralFoam* requires a library linking process. After linking the reaction libraries to the *rhoCentralFoam* solver, the capabilities of *reactingFoam* solver is thus activated and a combined solver, *hyperReactingFoam* can be generated.

Standard JANAF package in OpenFOAM libraries for the calculation of thermodynamic properties was altered for the applicability of a greater temperature range (200K - 20000K) to obtain solution that is more accurate because the temperatures can exceed the default maximum limit provided in the library. The extended JANAF package contains polynomial functions with 9 coefficients as can be observed in equations (2.33, 2.34 and 2.35). However, in unmodified state,

JANAF package uses polynomial functions with 7 coefficients, which are only valid between 200 K – 6000 K. Moreover, thermodynamic properties such as viscosity and thermal conductivity was added to the solver as shown in equations (2.8 and 2.9). Furthermore, the mixture value of thermo-physical properties is calculated by Wilke's mixing rule through equations (2.10 and 2.11). Figure 3.1 and Table 3.1 show general schematic diagram and algorithm of *hyperReactingFoam* solver for thermally non-equilibrium flows, respectively.

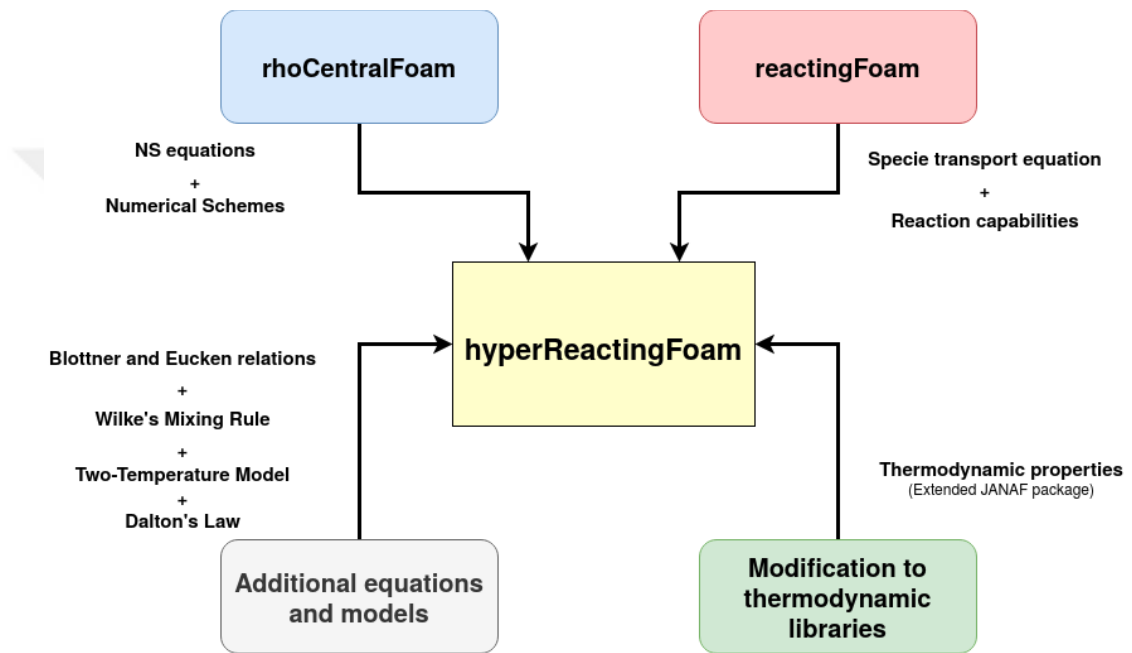


Figure 3.1 : *hyperReactingFoam* schematic diagram for thermal non-equilibrium.

Table 3.1 : *hyperReactingFoam* solution algorithm for thermal non-equilibrium.

Algorithm : <i>hyperReactingFoam</i> Solver
--

while $t < t_{end}$ do • set $t = t + \Delta t$ • include viscosity / thermal conductivity model and Wilke's mixing rule • evaluate surface fluxes for continuity, momentum and trans-rotational energy equations • solve continuity • solve explicit predictor equation for momentum • update velocity field • solve implicit corrector equation for momentum • solve "s" number of specie transport equations for mass fractions • solve explicit predictor equation for trans-rotational energy • update trans-rotational temperature field • solve implicit corrector equation for trans-rotational energy • solve equation of state by Dalton's Law • calculate the relations required for the Two-Temperature Model • evaluate surface fluxes for vibrational energy equations • solve "m" number of explicit predictor equations for vibrational energy • update vibrational temperature field of each specie • solve "m" number of implicit corrector equations for vibrational energy end while
--

Thermally non-equilibrium solver can be easily reduced to the equilibrium flow solver by deactivating some specific parts of the code. In order to obtain the equilibrium temperature, vibrational equations and relations required for the two-temperature model were removed from the algorithm. Additionally, the equilibrium temperature was obtained from equation (2.37) instead of equation (2.30). Heat conduction term written in equation (2.31) was replaced with equations (2.6 and 2.7). Besides, internal fluid energy was computed by the help of equation (2.36), in which the heat capacity at constant volume was found out from the JANAF polynomials. The solution of algorithm of *hyperReactingFoam* solver for thermally equilibrium flows can be seen from Table 3.2:

Table 3.2 : *hyperReactingFoam* solution algorithm for thermal equilibrium.

Algorithm : *hyperReactingFoam* Solver

while $t < t_{end}$ **do**

- set $t = t + \Delta t$
- include viscosity model and mixing rule
- evaluate surface fluxes for continuity, momentum and energy equations
- solve continuity
- solve explicit predictor equation for momentum
- update velocity field
- solve implicit corrector equation for momentum
- solve “s” number of specie transport equations for mass fractions
- solve explicit predictor equation for energy
- update temperature field
- solve implicit corrector equation for energy
- solve equation of state by Dalton’s Law

end while



4. SOLVER VALIDATION

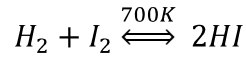
In this chapter, validation stages of *hyperReactingFoam* solver for both thermal equilibrium and non-equilibrium conditions were presented. For this purpose, three benchmark cases; an adiabatic heat bath, a double cone and a blunted cone model were selected. The test of *hyperReactingFoam* solver followed a validation process starting from simple to more complex cases and physics. The testing of each feature and assumptions were explained in each subsection. The numerical solutions obtained from *hyperReactingFoam* for these benchmark models were compared against to the other hypersonic codes; *LEMANS*, *MONACO*, *dsmcFoam* and *hy2Foam*, whose features were explained in Chapter 1. An analytical solution and experimental studies were also taken as references for comparison purposes.

For stagnant conditions, an heat bath model which is represented by a cubic geometry whose each side is equal to 1×10^{-5} m was chosen. Computational domain for heat bath model consists of one cell only. Time step for each calculation in heat bath problems was set to be 1×10^{-9} s. Both reacting and non-reacting computations were conducted on this model. The relaxation process between vibrational and trans-rotational energy modes was analyzed for single species and two species mixture. In addition to vibrational-translational relaxation, the vibrational energy transfer among distinct molecules was also taken into account by using the two-temperature model. In the case of momentum flux, a double cone and a blunted cone model were investigated for hypersonic conditions. Reacting and non-reacting solutions were obtained on the double cone while only non-reacting computations were performed on the blunted cone. In all of reacting case validations in thermal non-equilibrium, the term regarding chemistry-vibration coupling, $Q_{m,C-V}$, was activated in the vibrational energy equations.

4.1 Adiabatic Heat Bath Case

4.1.1 One step reversible reaction for single temperature

As a first validation case, a reversible reaction of hydrogen and iodine to form hydrogen-iodine is considered. This reaction is assumed to be taking place at a constant equilibrium temperature of 700 K with an initial pressure of 0.528 atm. The initial molar concentrations for the reactants are set to be $C_{I_2}^0 = C_{H_2}^0 = 4.54 \text{ mol/m}^3$.



The forward and backward reaction rates must be different from each other due to the fact that the chemical reaction is not in equilibrium state. The ratio between the forward and backward reaction rates is defined by an equilibrium constant, K_{eq} . This constant is a function of temperature and its calculation abide by the following formula [40]:

$$K_{eq} = \exp \left[A_1 \left(\frac{T}{10000} \right) + A_2 + A_3 \ln \left(\frac{10000}{T} \right) + A_4 \left(\frac{10000}{T} \right) + A_5 \left(\frac{10000}{T} \right)^2 \right], \quad (4.1)$$

By choosing the appropriate values for coefficients of “ A_i ” from the reference [44], K_{eq} can be calculated as 54.37 at 700 K. The analytical solution of time variations of reactants and product can easily be derived from [50]. Under the light of this information, the agreement between *hyperReactingFoam* solver and analytical solution is clear from Figure 4.1.

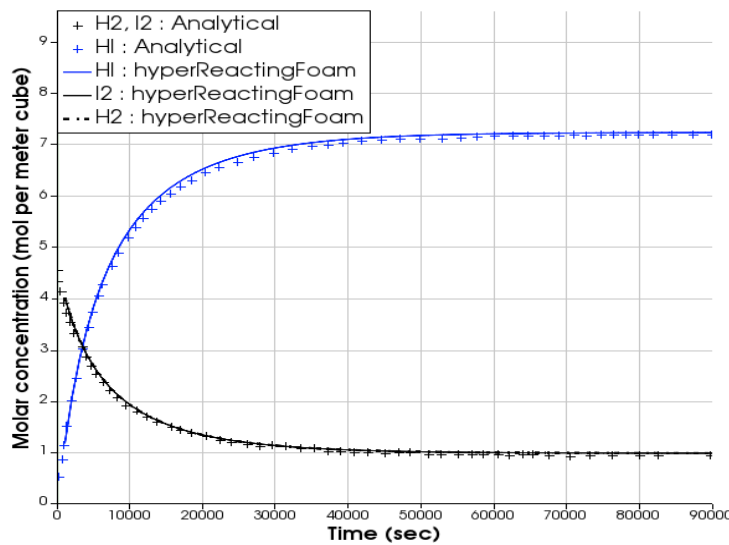


Figure 4.1 : Time variation of species molar concentration for H_2 - I_2 reacting mixture.

4.1.2 V-T relaxation of non-reacting nitrogen molecule

This case tests the non-equilibrium capability of *hyperReactingFoam* for the simplest state, in which only vibrational-translational term, Q_{V-T} is active without any chemical reactions. For this purpose, relaxation behavior of nitrogen gas in two particular conditions, namely vibrational heating and vibrational cooling, is examined. In the first process, N_2 reaches the equilibrium temperature with a lower initial vibrational temperature while in the other with a lower initial trans-rotational temperature. Initial conditions assigned to these two processes can be checked from Table 4.1.

Table 4.1 : Initial conditions for V-T relaxation of non-reacting N_2 .

Variable	Vibrational Heating	Vibrational Cooling
Vibrational Temperature : $Tv_{N_2}^0$	1000 K	10000 K
Trans-rotational temperature : Ttr^0	10000 K	3000 K
Velocity : U^0	0 m/s	0 m/s
Pressure : p^0	1 atm	1 atm

Figure 4.2 and 4.3 show that thermal equilibrium at 7623 K is achieved after nearly 10 μs in vibrational heating process while the relaxation time for vibrational cooling process to reach 4972 K takes at least 30 μs . It is obvious that the results obtained from *hyperReactingFoam* overlap with those of *MONACO* solver [51] for both vibrational heating and cooling conditions.

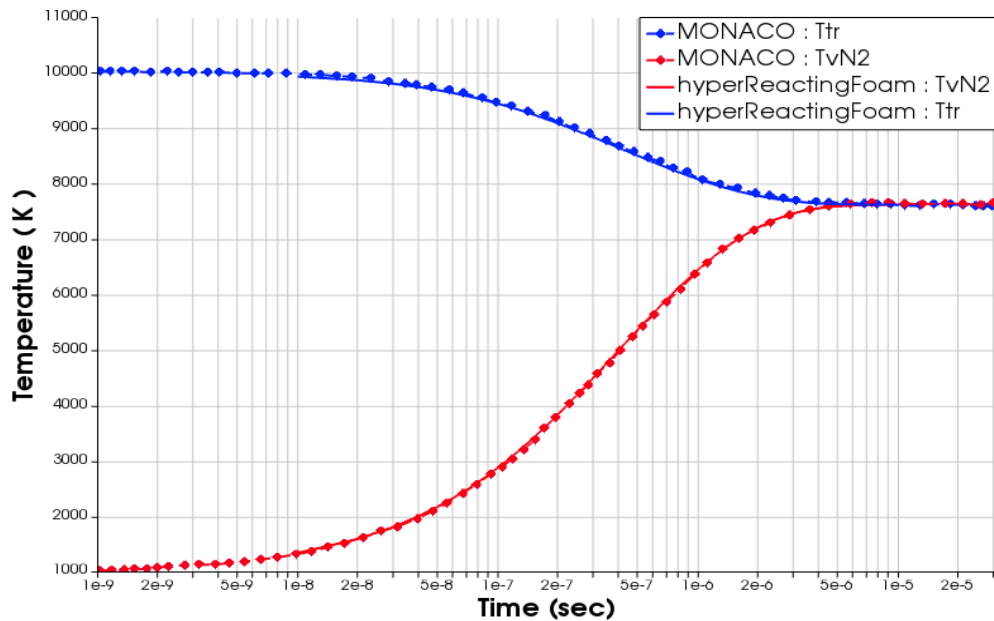


Figure 4.2 : V-T relaxation of N_2 for vibrational heating.

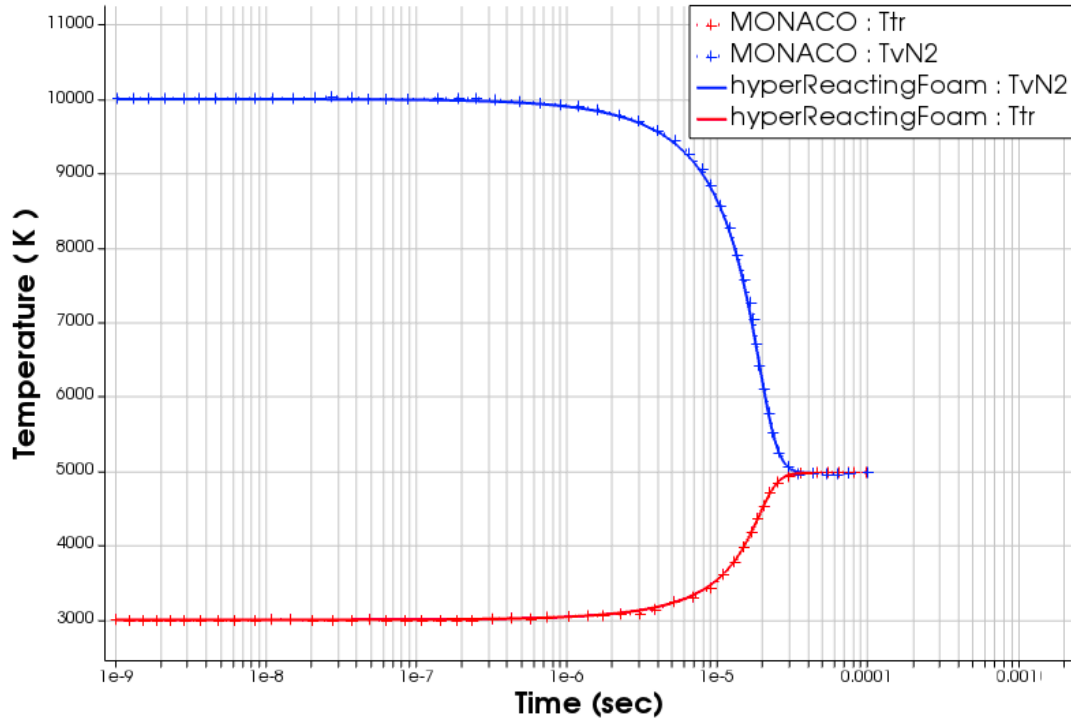


Figure 4.3 : V-T relaxation of N_2 for vibrational cooling.

4.1.3 V-T relaxation of non-reacting two-species mixture

Unlike the relaxation process of pure N_2 mixture, now nitrogen atoms, N , are also existent in this problem. Again, the energy transfers only between vibrational and trans-rotational modes because there is no any other molecule type aside from N_2 in the mixture. An equal initial amount of N_2 and N , in the measure of number density, are present in the heat bath, whose initial conditions are listed in Table 4.2. The number density for s^{th} specie in the mixture can be defined as:

$$n_s = \frac{N_A}{M_s} \rho_s \quad (4.2)$$

Table 4.2 : Initial conditions for V-T relaxation of non-reacting N_2 - N mixture.

Variable	Value	Unit
Vibrational Temperature : $Tv_{N_2}^0$	1000	K
Trans-rotational temperature : Ttr^0	30000	K
Number density of N_2 : $n_{N_2}^0$	5×10^{22}	m^{-3}
Number density of N : n_N^0	5×10^{22}	m^{-3}
Pressure : p^0	0.409	atm
Velocity : U^0	0	m/s

LEMANS and *hy2Foam* solvers was considered for this validation stage of *hyperReactingFoam*. *hy2Foam* solver was also verified its result against to *LEMANS* solver in this case. The researchers in [14] clarify why their result differs from the solution [51] of *LEMANS* solver. As they explain, they utilize a different type of convention to implement the second term of equation (2.19) in their study. Figure 4.4 illustrates that the data *hyperReactingFoam* provides overlaps with those of *hy2Foam* and *LEMANS* solvers. It is obvious that the relaxation process lasts at least 2 μ s, reaching an equilibrium temperature of 24350 K.

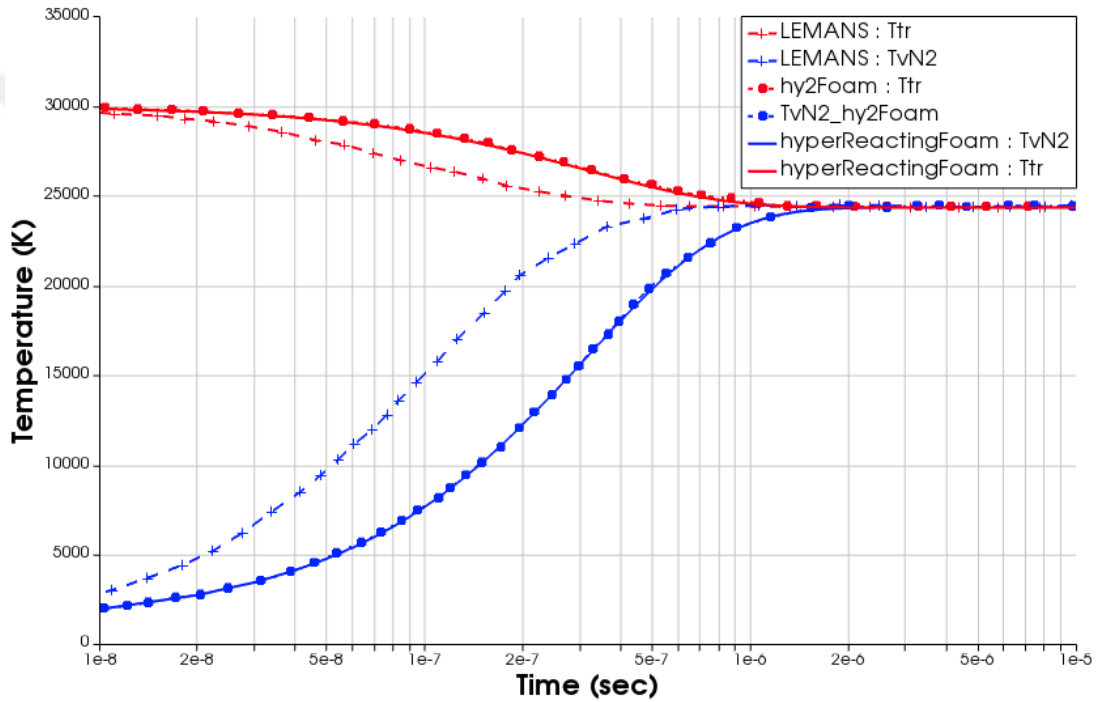


Figure 4.4 : V-T relaxation of non-reacting N_2 -N mixture.

4.1.4 V-T and V-V relaxation of non-reacting two-species mixture

Along with vibrational-translational relaxation, the test of energy exchange among various vibrationally excited species should also be included in the validation. This requires that in equation (2.16), the term $Q_{m,V-V}$ as well as $Q_{m,V-T}$ must be activated in order to allow two different type of energy exchanges. For this purpose, another vibrational cooling process, in which N_2 and O_2 molecules participate, is chosen. It is assumed that there are initially equal amount of mass fractions of N_2 and O_2 molecules. Initial mixture has an equal vibrational temperature for both N_2 and O_2 molecules.

whereas the trans-rotational temperature of these molecules has a much lower value. The details about initial conditions for this case are provided in Table 4.3.

Table 4.3 : Initial conditions for V-T and V-V relaxations of non-reacting N_2 - O_2 mixture.

Variable	Value	Unit
Vibrational Temperature of N_2 : $Tv_{N_2}^0$	30000	K
Vibrational Temperature of O_2 : $Tv_{O_2}^0$	30000	K
Trans-rotational Temperature : Ttr^0	5000	K
Mass Fraction of N_2 : $Y_{N_2}^0$	0.5	-
Mass Fraction of N : $Y_{O_2}^0$	0.5	-
Pressure : p^0	1	atm
Velocity : U^0	0	m/s

Temperature variations in Figure 4.5 depict that the required time for relaxation process of O_2 molecules is shorter than that of N_2 molecules. It is clear that a thermal equilibrium at around 12000 K is achieved after around 0.5 μs for the mixture. It is seen that the results of *hyperReactingFoam* solver is closer to *hy2Foam* solver than *LEMANS* solver in this case because both *hy2Foam* and *hyperReactingFoam* can compute “m” number of vibrational temperatures whereas *LEMANS* includes single vibrational temperature only.

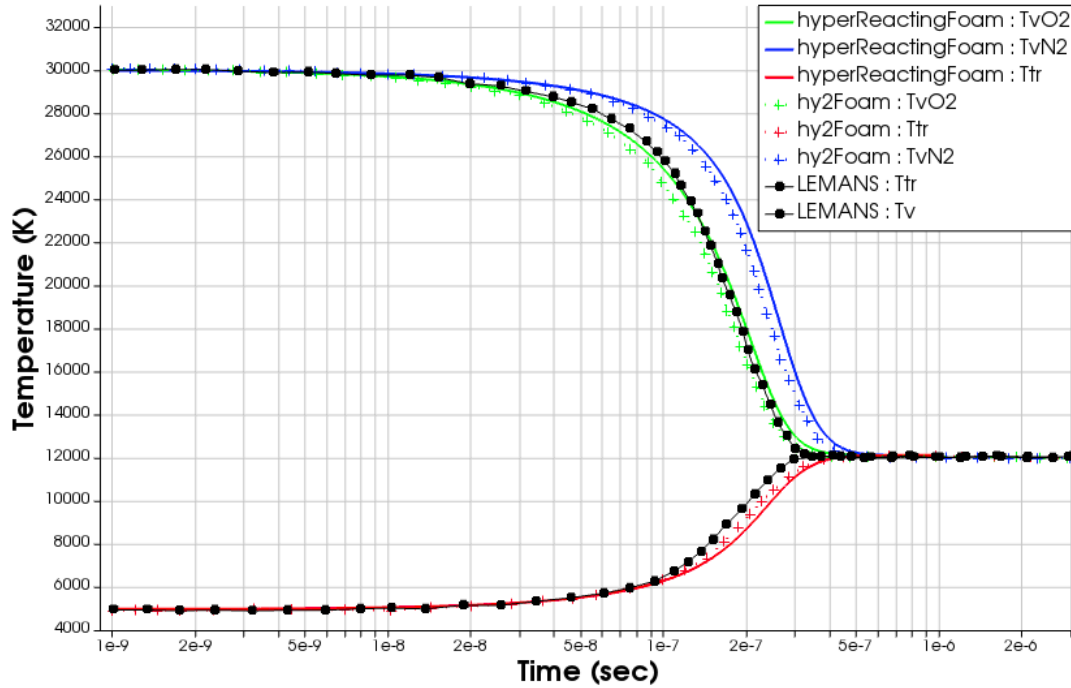
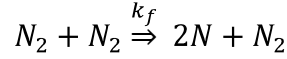


Figure 4.5 : V-T and V-V relaxations of non-reacting N_2 - O_2 mixture.

4.1.5 V-T relaxation of reacting two-species mixture

In this section, the effect of chemistry-vibration coupling term, $Q_{m,C-V}$, is tested as well as $Q_{m,V-T}$. In this way, only the term $Q_{m,V-V}$ is deactivated in the vibrational energy equation for this case. For the sake of simplicity, one-step irreversible reaction of nitrogen dissociation is considered as follows:



Arrhenius parameters of this chemical reaction are acquired from Park's two temperature model [40] and Quantum Kinetic theory [52]:

Table 4.4 : Arrhenius parameters for reaction rates.

Arrhenius constant	A	β	T_a
Unit	$\text{m}^3\text{mol}^{-1}\text{s}^{-1}$	-	K
Value	7.0×10^{-21}	-1.6	113200

The initial conditions provided in this case are identical to those of provided in Table 4.2. By including the chemistry effects to the case presented in section 4.1.3, the behavior of relaxation process changes drastically, as can be seen in Figure 4.6 below.

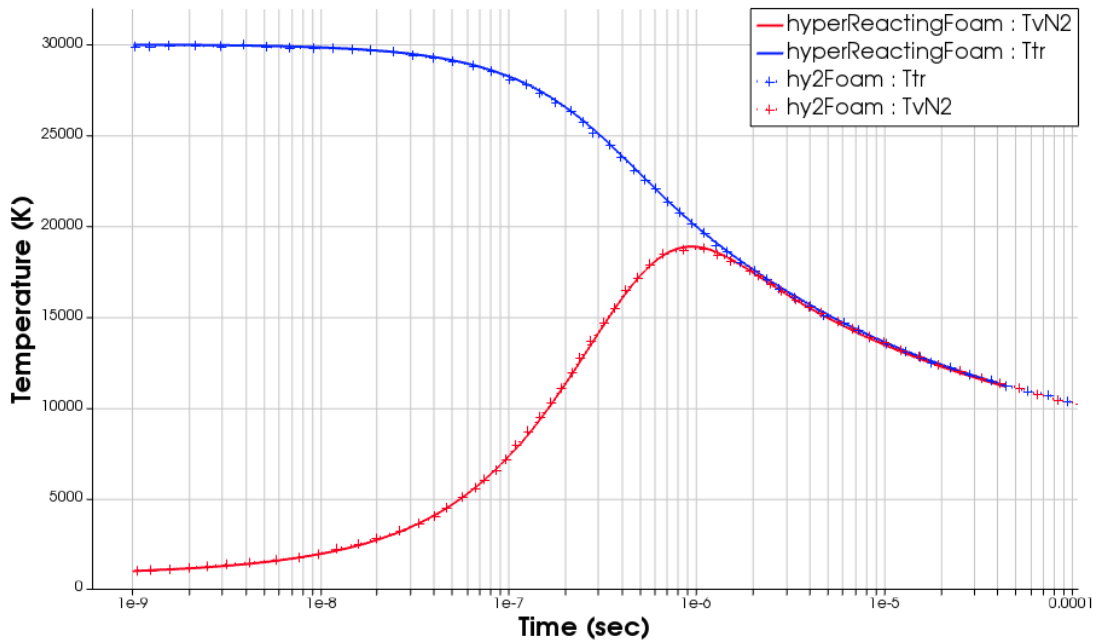


Figure 4.6 : Temperature variation for V-T relaxation of reacting N_2 -N mixture.

The chemistry capability of *hyperReactingFoam* is compared against to *hy2Foam* solver, which adopts Park TTV model for the chemistry-vibration coupling. The comparison of Figure 4.4 and Figure 4.6 shows that even though the required time to reach thermal equilibrium for both cases is the same, the values of equilibrium temperature differ from each other. In the reacting case, the equilibrium temperature is in a decreasing trend due to the chemistry-vibration coupling while the final temperature in the non-reacting case stays at a constant value even after thermal equilibrium is satisfied. In addition to temperature variation, the amounts of change of reacting species are also plotted in Figure 4.7. Number densities of the reacting species are normalized with respect to the initial mixture number density, which can be derived from Table 4.2. It is obvious that the number densities of the reacting species still change even after thermal relaxation is completed. This points to the fact that N_2 molecules still keep dissociating irreversibly to produce N atoms.

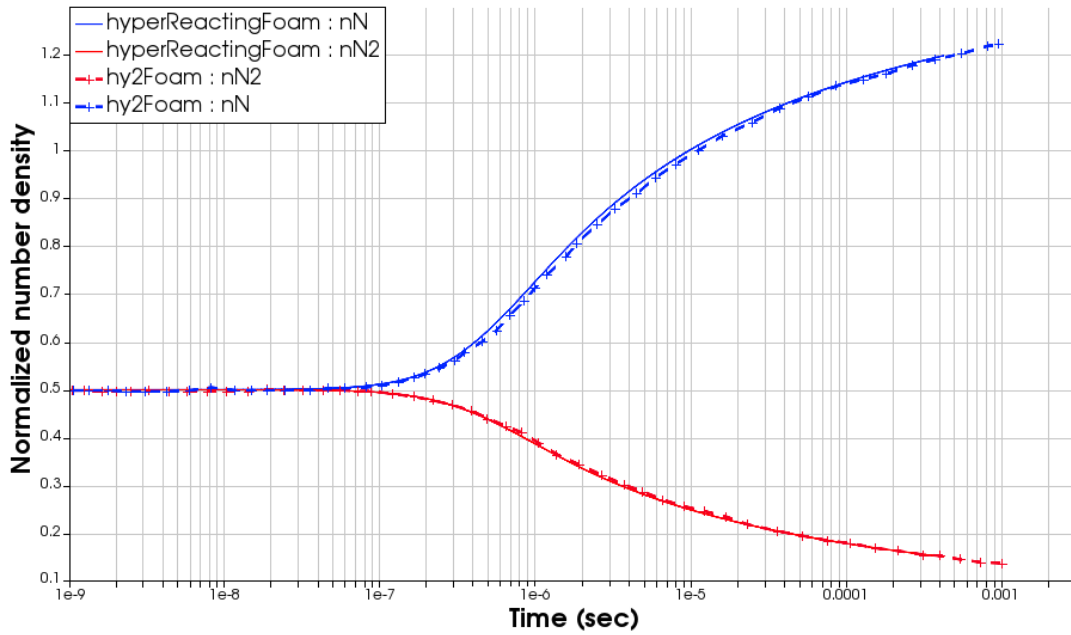


Figure 4.7 : Number density variation for V-T relaxation of reacting N_2 -N mixture.

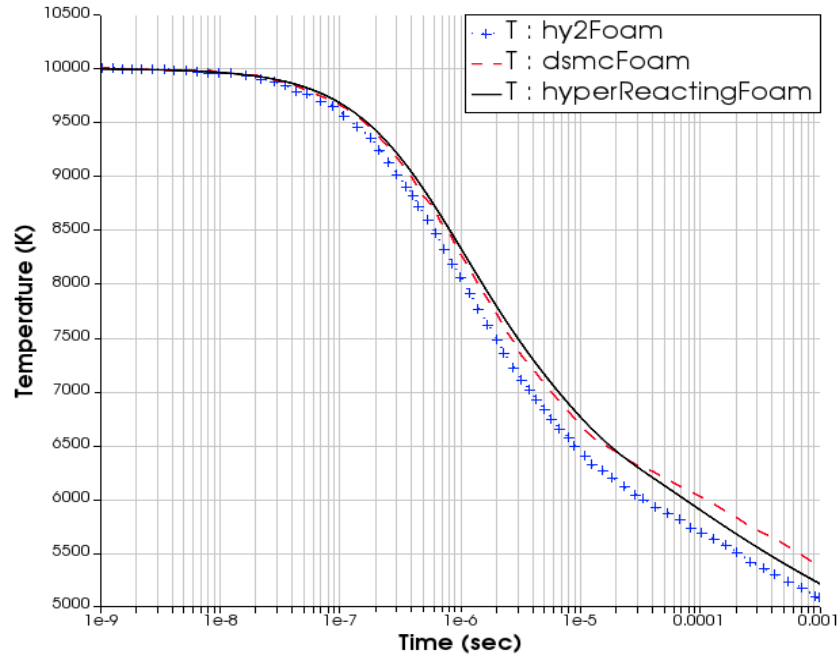
4.1.6 Chemically reacting air for single temperature

For the last stage of validation processes on adiabatic heat bath problem, a chemically reacting air is to be considered for the single temperature model. The air, which is composed of %79 N_2 and %21 O_2 in terms of volumetric fractions, is initially kept at 10000 K and 0.063 atm.

Table 4.5 : Initial conditions for reacting air.

Variable	Value	Unit
Temperature : T^0	10000	K
Mass Fraction of N_2 : $Y_{N_2}^0$	0.767	-
Mass Fraction of O_2 : $Y_{O_2}^0$	0.233	-
Mass Fraction of NO: Y_{NO}^0	0	-
Mass Fraction of N : Y_N^0	0	-
Mass Fraction of O : Y_O^0	0	-
Pressure : p^0	0.063	atm
Velocity : U^0	0	m/s

An air model [52] comprising 5 species (N_2 , O_2 , NO, N and O) with 19 chemical reactions, whose Arrhenius parameters are provided in Table A.1 in Appendix, are selected to investigate thermo-chemical behavior of the reacting mixture. Of these 19 reactions, the first 15 reactions are classified as dissociation reactions while the last four are known as exchange reactions. The thermodynamic properties of the reacting air are computed according to the extended JANAF relations provided in equations (2.33, 2.34 and 2.35). The results of *hyperReactingFoam* are validated against to *hy2Foam* and *dsmcFoam* solvers as can be seen in Figure 4.8 and 4.9 below.

**Figure 4.8** : Temperature variation for the reacting air.

In the case of chain reactions, unlike the overlapping results from the case with one-step reaction of hydrogen and iodine, there exists a deviation between the temperature graphs of *hyperReactingFoam* and *hy2Foam* solvers. Nevertheless, *dsmcFoam* result seems closer to *hyperReactingFoam* than *hy2Foam*. The difference between temperature variations directly reflects to the composition of the species since temperature is a direct function for the calculation of reaction rates.

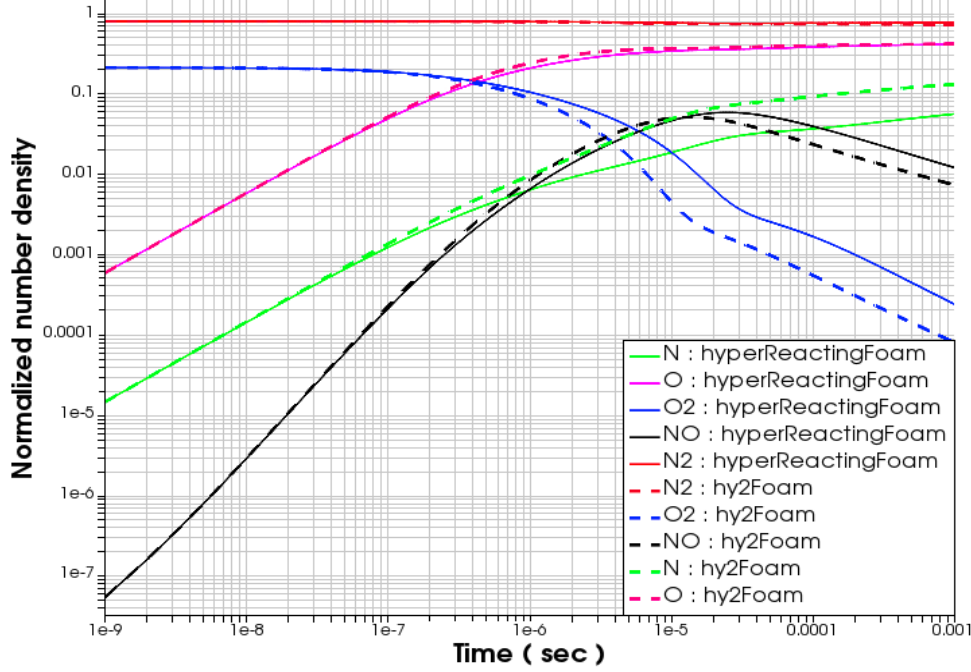


Figure 4.9 : Number density variations of the reacting species.

The left axis specifies the number density of each specie normalized with respect to the air number density at the initial state. Even though the number density variations of N₂ and O agree with *hy2Foam*, the differences in O₂, NO and N are noticeable.

4.2 Blunted Cone

In section 4.1, all the analyses were realized assuming a stagnant air in the computational domain. After this section, the rest of the validation studies, however, are to be conducted with free-stream conditions. Thermal non-equilibrium relaxation between vibrational-transrotational energy modes of N₂ is investigated over the blunted cone model with non-reacting assumption. The computational domain comprises 600 and 200 structural elements in stream-wise and normal directions,

respectively. The nose of cone has a radius of 6.35 mm and is extended by a flat plate, which has a length of 50 mm in the stream-wise direction. The cone surface makes 25° angle with free-stream direction. The distance of the first layer from the wall is measured as 10 μm in the wall normal direction. Figure 4.10 shows computational domain of the blunted cone model.

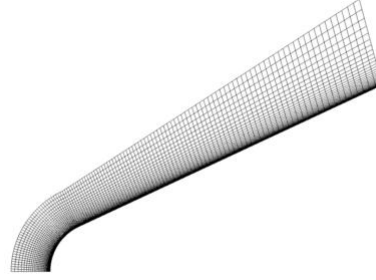


Figure 4.10 : Blunted cone [53].

The free-stream flow is composed of N_2 gas only. The initial conditions of free-stream nitrogen flow is given in Table 4.6. On the cone surface, Maxwell velocity slip [54] and Smoluchowski temperature jump [55] for transrotational and vibrational temperatures are applied. An initial thermal equilibrium at $t=0$ for N_2 molecules is assumed. The maximum time step for the iterations is derived from the maximum Courant number, which is equal to 0.5. The quantities obtained from the stagnation line and the cone surface are compared against to those of *hy2Foam* solver [53].

Table 4.6 : Free-stream conditions of non-reacting N_2 over blunted cone.

Variable	Value	Unit
Free-stream velocity : U_∞	2764.5	m/s
Free-stream pressure : p_∞	21.9139	Pa
Free-stream density : ρ_∞	5.113×10^{-4}	kg/m^3
Free-stream temperature : T_∞	144.4	K
Free-stream mean free path : λ_∞	1.01×10^{-4}	m
Overall Knudsen number : Kn_{ov}	0.002	-
Wall temperature : T_w	297.2	K

The definitions of pressure and friction coefficients are given by:

$$C_p = \frac{p - p_\infty}{0.5 \rho_\infty U_\infty^2} , \quad (4.3)$$

$$C_f = \frac{\tau}{0.5 \rho_\infty U_\infty^2} , \quad (4.4)$$

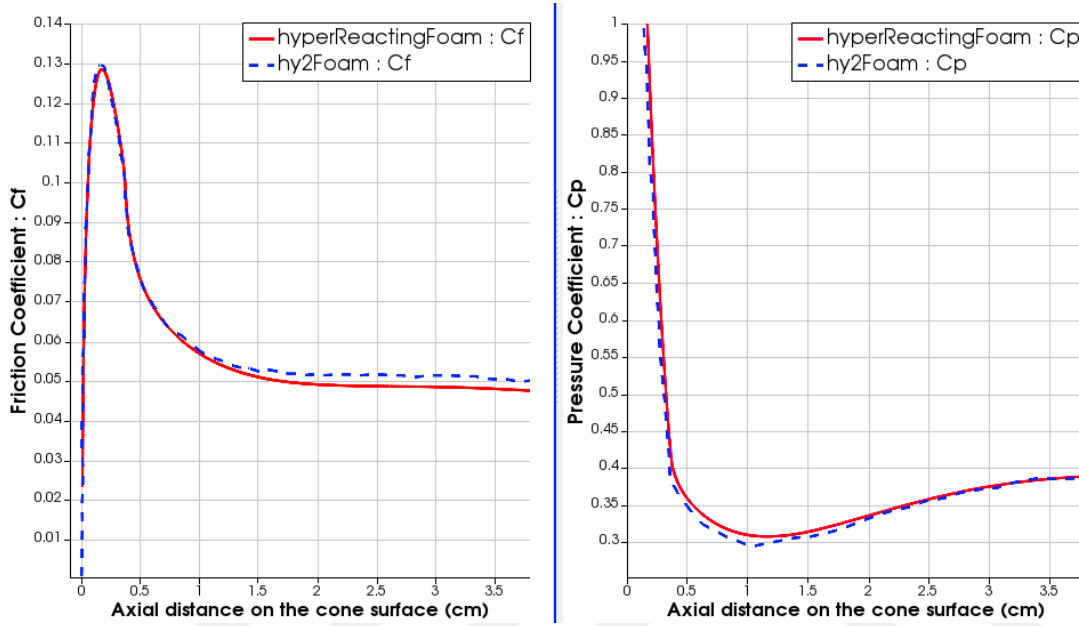


Figure 4.11 : Pressure and friction coefficients comparison on the surface of blunted cone.

Surface pressure and friction coefficient variations fairly agree with the solutions of *hy2Foam* solver even though the friction coefficient starts to differ at the downstream locations on the surface. Figure 4.12 also provides some useful stagnation line data such as velocity, density and temperature. All of the parameters plotted in Figure 4.12 are normalized with respect to their free-stream conditions given in Table 4.6. In Figure 4.12, x-axis specifies the locations of the stagnation line, whose endpoint is at $x=0$. This endpoint location on the nose of the blunted cone, where the velocity goes to zero, is called as “stagnation point”. At a shock standoff distance of 1.1 mm, a detached bow shock occurs in front of the blunted cone. It is understood that the thickness of the shock is approximately 0.3 mm as there are steep increase and decline in the density and velocity distributions within the interval of $-1.1 < x < -0.8$ mm. The temperature variation graph shows that the thermal equilibrium between trans-rotational and vibrational energy modes disrupts

after passing through the normal shock. This is expected since when a flow passes through strong discontinuities such as normal shocks; a great deal of its kinetic energy is converted to translational motion. This translational motion then exchanges its energy with rotational, vibrational and chemical energies within a certain number of collisions [33]. It is also interesting to see that transrotational and vibrational energy modes are in thermal equilibrium at the stagnation point.

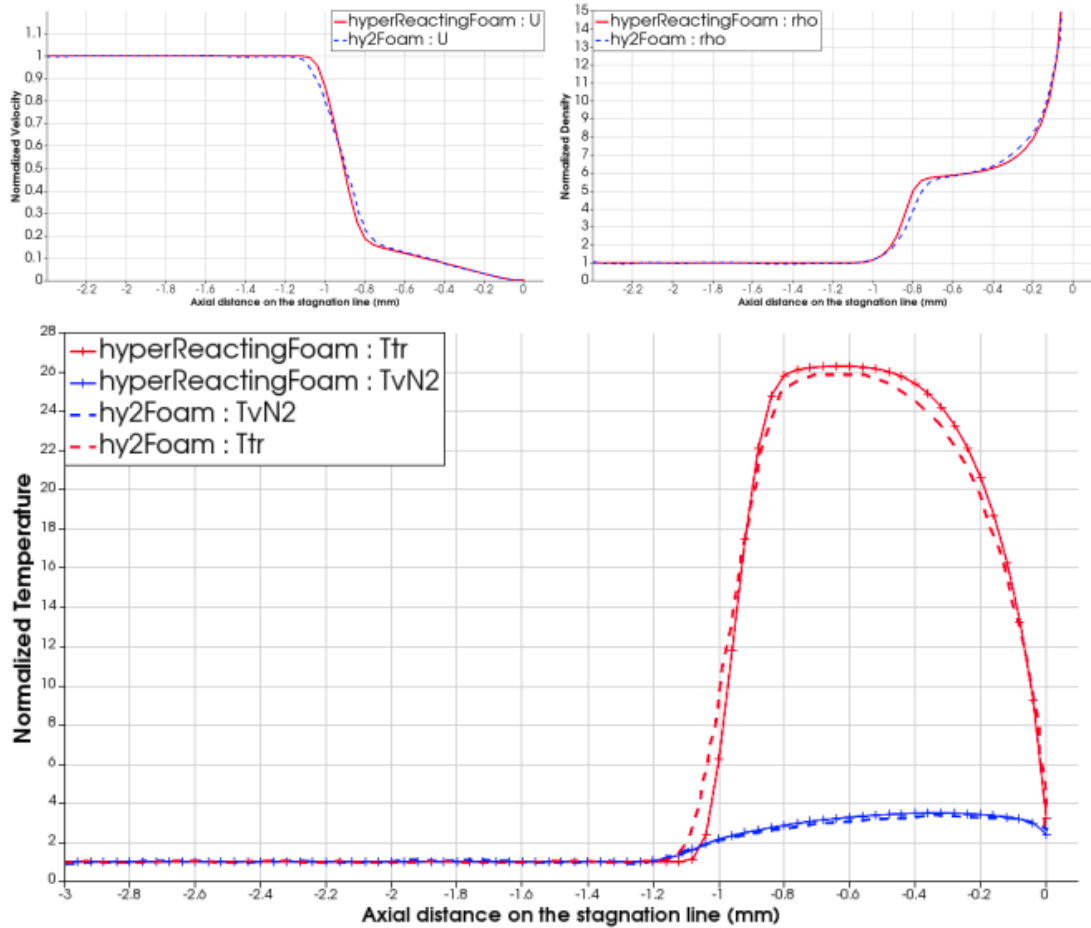


Figure 4.12 : Velocity (top-left), density (top-right) and temperature (bottom) comparison on the stagnation line.

4.3 Double Cone

Another model to verify *hyperReactingFoam* solver for thermally equilibrium and non-equilibrium flow is a double cone geometry on which both low and high enthalpy experiments [18] performed at Calspan University of Buffalo Research Center (CUBRC)'s LENS XX expansion tunnel. Only the low enthalpy experiment is taken to test the degree of accuracy of the solver in both non-reacting and reacting conditions. In addition to the experiment, a numerical solution on the double cone

model published by Kianvashrad & Knight is also used to validate *hyperReactingFoam*. Surface heat flux and pressure distributions are used to compare the differences between experimental and numerical solutions.

The picture of the experimental model and geometric dimensions can be seen in Figure 4.13. The first and second cone surfaces of the model have angles of 25° and 55° with free-stream direction, respectively.

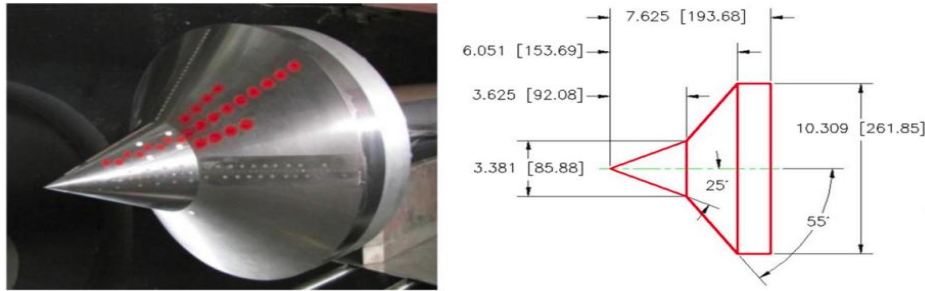


Figure 4.13 : The double cone model (left) and its sketch view with geometric dimensions in mm [56].

The inflow gas is in thermochemical and chemical equilibrium with the mass fractions provided in Table 4.7. The wall is kept isothermally at 300 K during the experiment. The Reynolds number, which is based on the flow conditions in Table 4.7 and the length of the first surface, for the low enthalpy experiment assures a fully laminar flow.

Table 4.7 : Low enthalpy conditions for the double cone experiment.

Total enthalpy	Pitot Pressure	Unit Reynolds, $10^6 / m$	Velocity	Density	Temperature	Y_{N_2}	Y_{O_2}
MJ/kg	kPa	m^{-1}	m/s	g/m^3	K	-	-
9.65	17.5	0.19	4303	0.984	389	0.765	0.235

Figure 4.14 shows the close-up picture of compression corner and boundary surfaces for the computational domain. The mesh is composed of 32385 structural hexahedral elements.

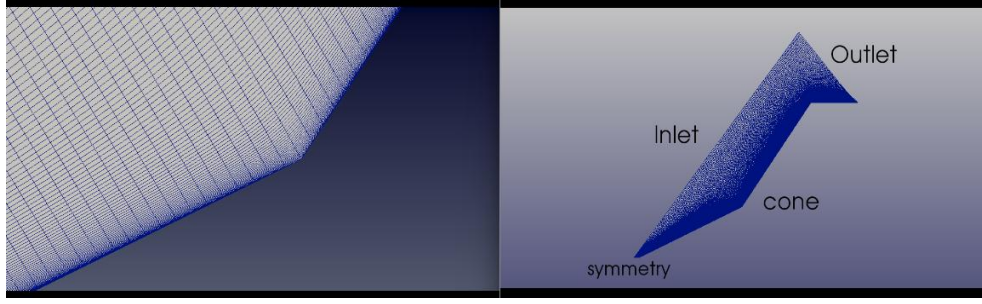


Figure 4.14 : Compression corner elements (left) and boundary condition types (right) on the surfaces for the double cone model.

Due to non-catalytic assumption on the cone surface, surface normal gradients of mass fractions are accepted as zero ($\frac{\partial y_i}{\partial n} = 0$). On the wedge surface, constant temperature condition for T_{tr} and adiabatic condition for T_{vi} are applied. The transrotational wall temperature is assumed to be equal to the isothermal wall temperature (300 K) at all times. Free-stream flow conditions given in Table 4.7 are assigned as boundary conditions at Inlet surface whereas at Outlet surface, Neumann type boundary conditions are given for all type of variables. Other types of boundary conditions, including Inlet and Outlet, can be checked from Table 4.8.

Table 4.8 : Boundary condition types assigned on boundary surfaces (FV: Fixed Value, ZG: Zero Gradient).

Boundary surface	Velocity	Pressure	Temperature	Mass fractions
Inlet	FV	FV	FV	FV
Outlet	ZG	ZG	ZG	ZG
cone	No slip	ZG	FV (T_{tr}) , ZG (T_{vi})	ZG
symmetry	symmetry	symmetry	symmetry	symmetry
wedge1	wedge	wedge	wedge	wedge
wedge2	wedge	wedge	wedge	wedge

wedge1 and wedge2 surfaces are the front and back sides of the computational domain. "wedge" and "symmetry" boundary condition types specify rotational symmetry of flow and the symmetry of flow with respect to the horizontal axis, respectively. Specie mass fractions at the start of the computation are set to be $Y_{N_2} = 0.76$, $Y_{O_2} = 0.23$, $Y_{NO} = 0.01$, $Y_N = 0.0$ and $Y_O = 0.0$ for each cell in the computational domain. Prandtl and Le numbers are equal to 0.736 and 1.4, respectively [56].

4.3.1 Reacting flow for thermal equilibrium

Firstly, the reacting capability of the solver is investigated on the double cone. In section 4.1, the reacting capability of the solver was tested with the zero-dimensional heat bath case only, in which any free-stream flow does not exist at all. For this validation stage, an air model composed of 5 species (N_2 , O_2 , NO , N and O) with 17 chemical reactions, whose reaction list is provided in the first seventeen row in Table A.1 in Appendix, is selected. Steady-state behavior of the reacting solution for thermal equilibrium is presented in Figure 4.15.

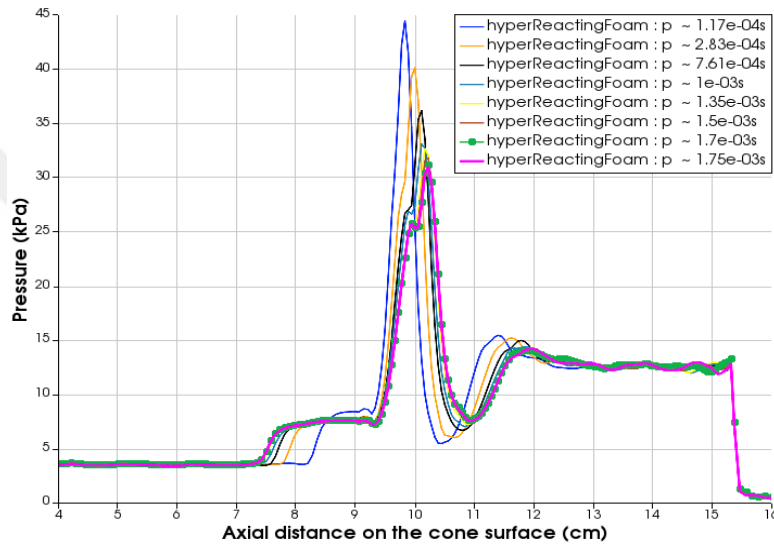


Figure 4.15 : Time variation of surface pressure distribution for reacting thermally equilibrium flow.

Obviously, the solution is converged to the steady state nearly after $1700 \mu s$ even though there are some observable oscillations on the second surface after this time step. The sharp decrease in the pressure after $x=15$ cm corresponds to the expansion waves over the expansion corner whereas pressure jumps between $x=7$ cm and $x=12$ cm are results of shock waves. In Figure 4.16 and 4.17, the steady state pressure and heat flux distributions are compared against to the experimental findings and the numerical study conducted by Kianvashrad & Knight [56].

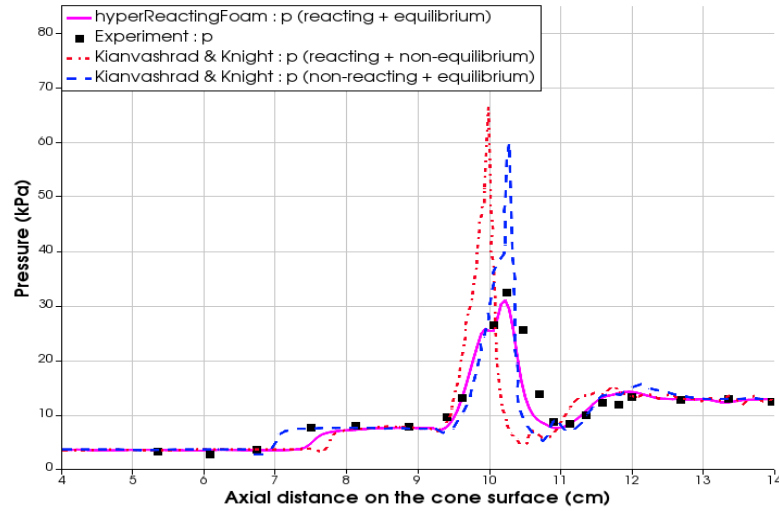


Figure 4.16 : The comparison of surface pressure distribution for reacting thermal equilibrium solution.

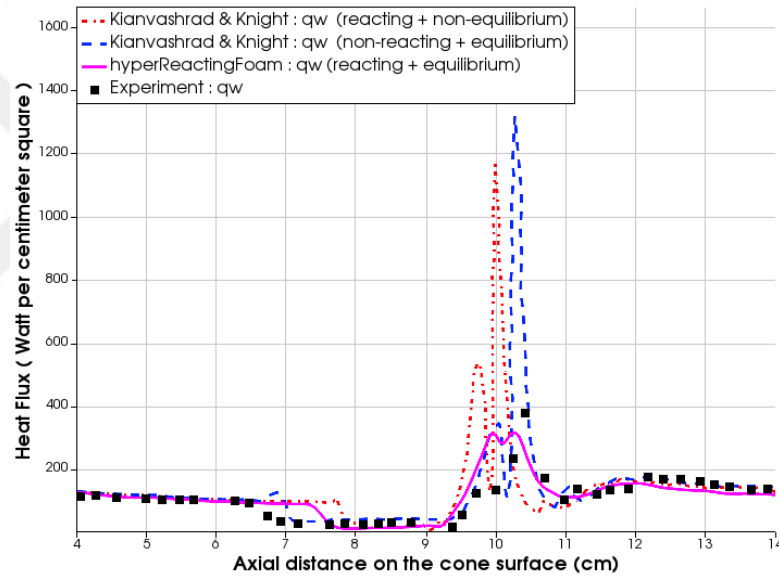


Figure 4.17 : The comparison of surface heat flux distribution for reacting thermal equilibrium solution.

The study of Kianvashrad and Knight does not have reacting solution for single temperature model. For this reason, the *hyperReactingFoam* solver was compared with non-reacting thermal equilibrium and reacting thermal non-equilibrium analyses of Kianvashrad and Knight. It is seen that both pressure and heat flux distributions, in terms of the magnitude and the locations of peak values, are better predicted by *hyperReactingFoam*. The analysis of Kianvashrad and Knight is able to pinpoint the peak locations in spite of overpredicting the magnitudes. Yet, the authors state that

these overpredictions are irrelevant since the experimental gauge spacing is as much as 50 times of the computational grid spacing near the peak location.

4.3.2 Non-reacting flow for thermal non-equilibrium

When turned the chemistry off, the effect of chemistry-vibrational energy exchange vanishes from the two-temperature model. Steady state analysis reveals that the solution converges to steady state after 800 μ s, which is far less than the time required for reacting thermal equilibrium flow. Moreover, the converged value of the maximum pressure obtained with this condition is higher than that of previous case.

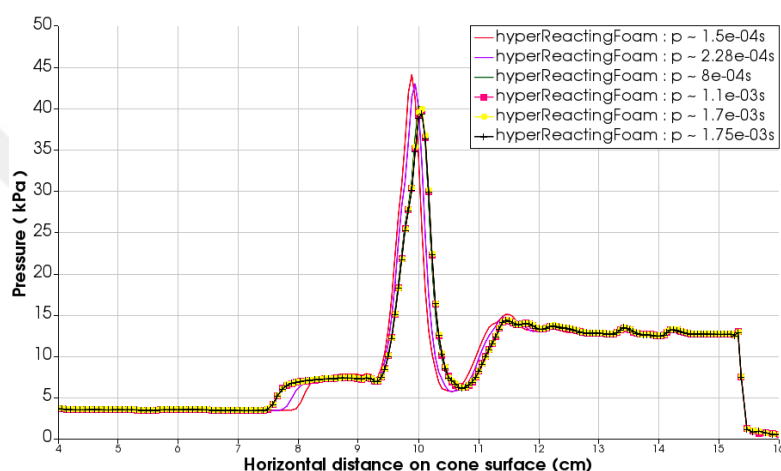


Figure 4.18 : Time variation of surface pressure distribution for non-reacting thermally non-equilibrium flow.

Pressure distribution plotted in Figure 4.19 depicts that non-reacting with thermal non-equilibrium analysis underpredicts the location of the experimental pressure peak while it overpredicts the magnitude. Similarly, the location of maximum heat flux goes upstream when compared to reacting flow with thermal equilibrium. It is also noticeable that the value of maximum heat flux at the surface exceeds that of reacting thermal equilibrium case.

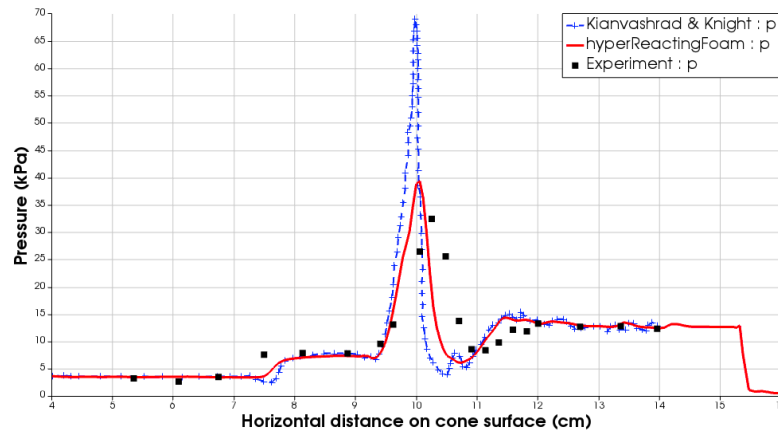


Figure 4.19 : The comparison of surface pressure distribution for non-reacting thermal non-equilibrium solution.

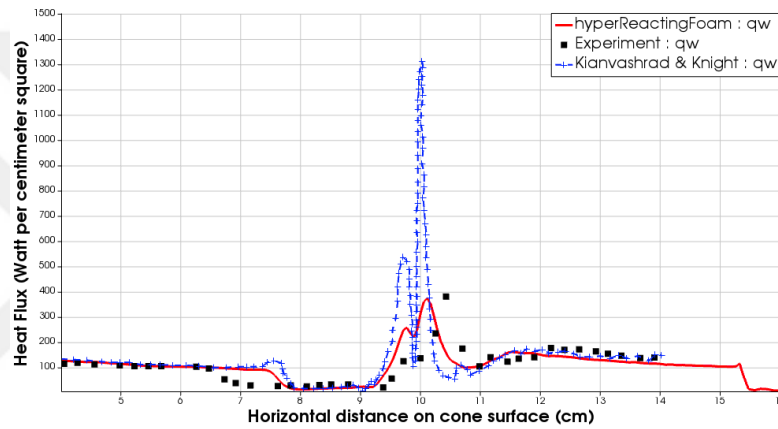


Figure 4.20 : The comparison of surface heat flux distribution for non-reacting thermal non-equilibrium solution.

4.3.3 Reacting flow for thermal non-equilibrium

For this case, the thermo-chemistry model explained in section 4.3.1 is again used for the comparative analysis in this section. Differently from the previous section, the activation of chemical reactions allows the energy exchange between vibrational and chemistry modes. Steady state convergence is achieved after 1710 μ s, which is more or less at the same order with other reacting case. Therefore, the time required to achieve steady state on the double cone is much longer if the chemistry plays a role in the flow. It is also clear that the behavior of the converged pressure distribution in Figure 4.22 is almost the same with that in Figure 4.16. Although displaying the same trend with reacting thermal equilibrium flow, the magnitude of heat flux distribution obtained with the two-temperature model is always lower than that of the case with thermal equilibrium.

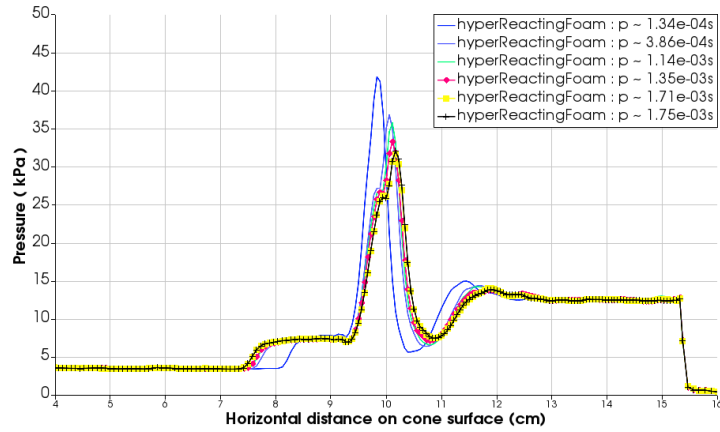


Figure 4.21 : Time variation of surface pressure distribution for reacting thermally non-equilibrium flow.

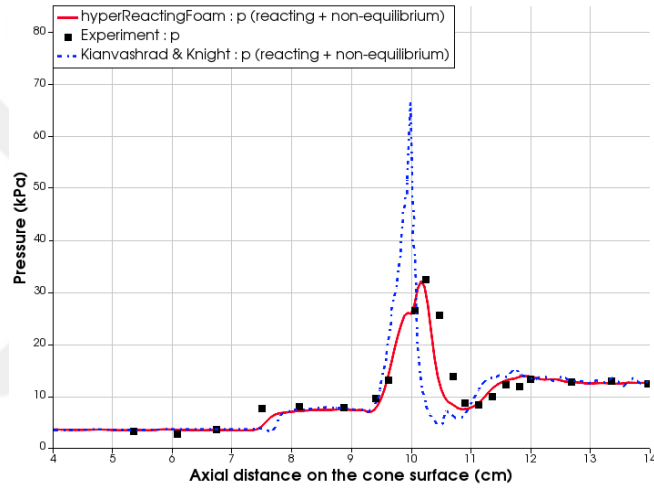


Figure 4.22 : The comparison of surface pressure distribution for reacting thermal non-equilibrium solution.

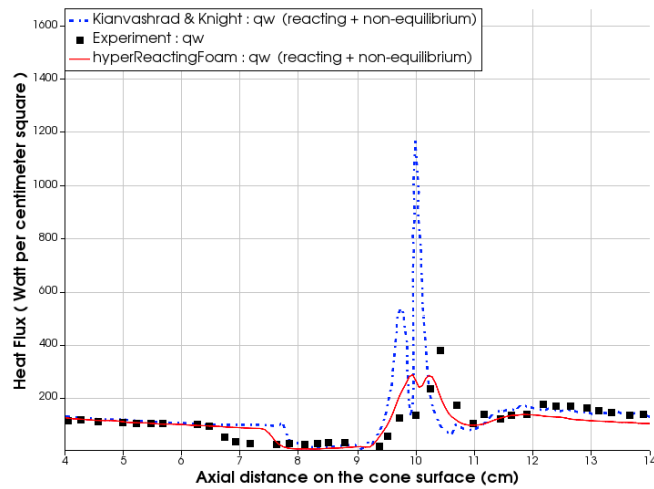


Figure 4.23 : The comparison of surface heat flux distribution for reacting thermal non-equilibrium solution.

5. DOUBLE WEDGE ANALYSES

One of the most interested subjects in the hypersonic community is the study of double wedge flows. The number of numerical and experimental studies on the double wedge geometry has increased considerably in the recent years. Swantek and Austin [57] have conducted a number of high-speed experiments on a 30° - 55° double wedge for both high and low enthalpy flows. For high enthalpies, they focused on the interaction and shock-establishment mechanism up to $242\ \mu\text{s}$. From their experiments, they provided Schlieren images as well as surface heat flux distribution along the surface of the double wedge. Figure 5.1 presents the picture of this experimental model and its dimensions with sketch view.

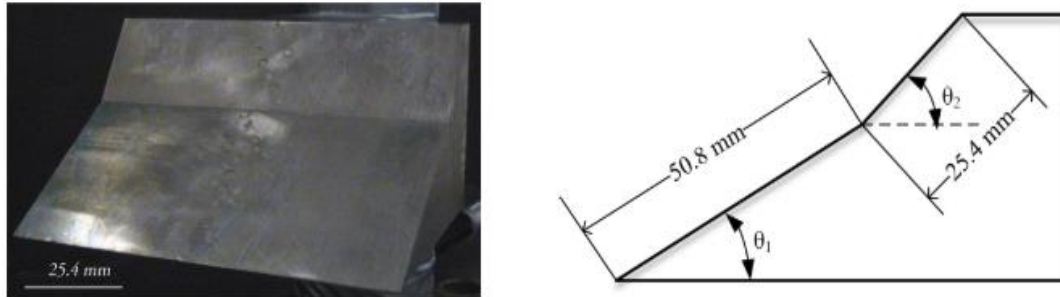


Figure 5.1 : Double wedge model studied by Swantek [57] (left) and its sketch view (right).

The fore angle, θ_1 , of the first surface is 30° and the aft angle, θ_2 , makes a 55° angle with the free-stream flow. The lengths of the first and second surfaces are 50.8 mm and 25.4 mm, respectively. Along the spanwise direction, the double wedge has a width of 101.6 mm.

In this section, thermal equilibrium and non-equilibrium reacting flow analyses by *hyperReactingFoam* solver was realized based on the double wedge model of Swantek and Austin. In addition to 30° - 55° double wedge, three other configurations with fixed fore and different aft angles were also analyzed. By fixing the fore angle

at 30°, other double wedge configurations with aft angles of 45°, 50° and 60° were generated.

5.1 Computational Domain

5.1.1 2-D computational domain

2-D and 3-D computational domains for our studies were presented in this section. Both 2-D and 3-D computational domains were constructed by Durna et. al. [29, 58], who also conducted non-reacting thermally equilibrium analyses on the same model. For 2-D mesh, the computational domain they created consists of 24 different blocks and these blocks contain 0.296 million structured elements. The numbers of maximum cells are 780 and 500 in streamwise and wall normal directions, respectively. The construction of the domain was realized by extending the mesh in the streamwise direction around the corners on the surface. blockMesh utility provided in OpenFoam software enabled the generation of 2-D mesh. In order to capture the boundary layer influences on the flow, a finer mesh resolution along the wall normal direction near the wedge surface was obtained. In this way, keeping y^+ below 1.0 was achieved. Figure 5.2 illustrates the view of blocks and the computational domain near the compression corner.

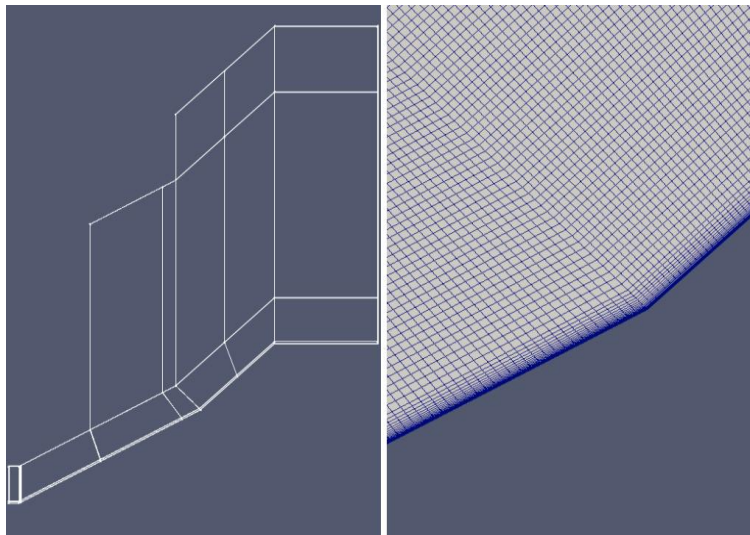


Figure 5.2 : Computational domain for 2-D model [29].

5.1.2 3-D computational domain

Unlike 2-D mesh generation technique presented above, for 3-D computations a different technique by Durna was adopted to achieve a high quality mesh. 3-D mesh was constructed by generating a non-conformal, body fitted, unstructured mesh with hexahedral elements. HEXPRESS software, which was used in the 3-D mesh generation, allowed a top-to-bottom grid generation technique. HEXPRESS software is able to generate boundary layer mesh and a smooth transition from boundary layer mesh to outer mesh is possible. The distances from sidewalls to the outer surface of computational domain along the spanwise direction are 0.4 and 0.6 times of the width of solid wedge for $\theta_2 = 45^\circ - 50^\circ$ and $\theta_2 = 55^\circ - 60^\circ$, respectively. The boundary faces for 3-D computational domain can be seen in the Figure 5.3.

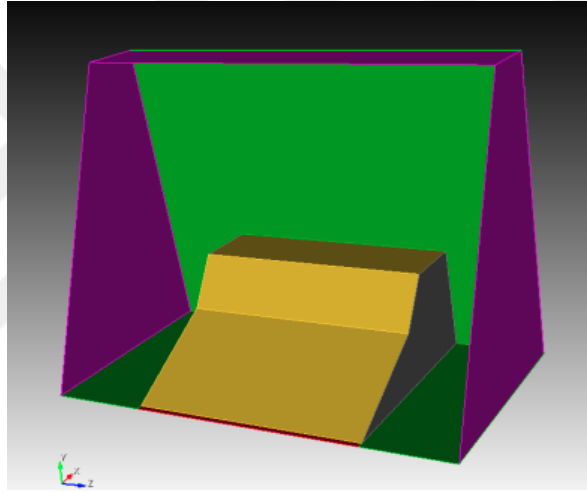


Figure 5.3 : Boundary faces for 3-D computational domain [58].

In order to resolve the boundary layer, aspect ratios near the first wedge surface might be too high due to the shortness of first cell thickness normal to the wedge surface. To avoid this, the maximum aspect ratio was set to be 122. With a general refinement level of 6, there are approximately 32 million of cells in the computational domain for $\theta_2 = 55^\circ$. The total cell number is slightly different for various aft angles. Before obtaining high resolution in the computational domain, other meshes which had 4.6 and 15 million cells with general refinement levels of 4 and 5 were also tried. The first cell thickness in the boundary layer mesh is 2.2×10^{-6} and the growth rate in the wall normal direction was set to be 1.18.

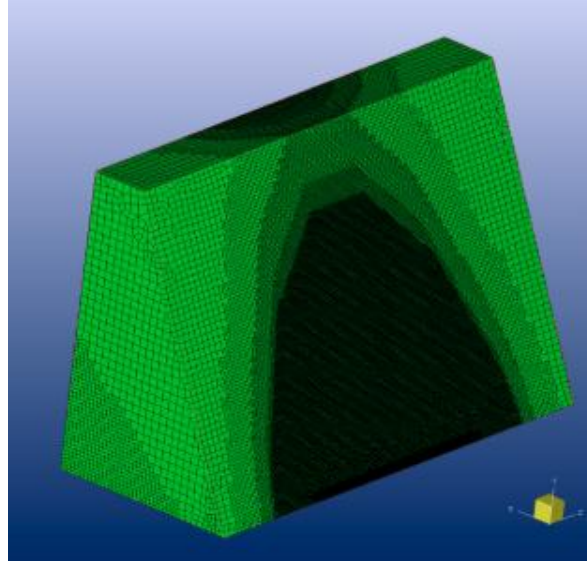


Figure 5.4 : The outer region of 3-D computational domain [58].

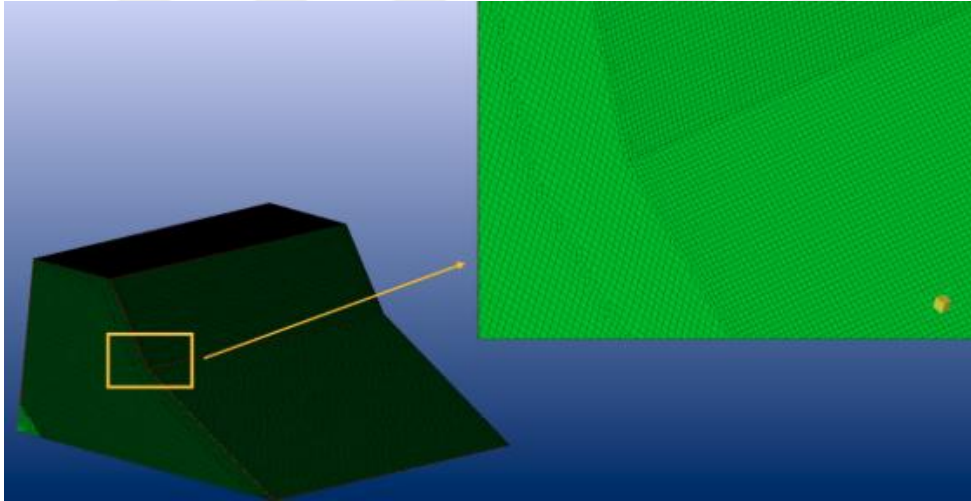


Figure 5.5 : The mesh on solid wedge and near the compression corner [58].

5.2 Free-stream and Boundary Conditions

High enthalpy flow conditions of Swantek and Austin [20] provided in Table 5.1 were taken as reference for boundary conditions of 2-D and 3-D computational domains at free-stream surfaces. At $t=0$, by impulsive start assumption, interior values of the computational domain were assigned to the free-stream conditions of the experiment. The flow is assumed as fully laminar, Prandtl number is set to 0.736, and Le number is accepted as 1.4.

Table 5.1 : High enthalpy flow conditions for double wedge experiments of Swantek and Austin [20].

Mach Number	Static Temperature	Unit Reynolds, $10^6 / m$	Velocity	Density	Static Pressure	Test Time	Stagnation Enthalpy
-	K	m^{-1}	m/s	kg/m^3	kPa	μs	MJ/kg
7.14	710	0.44	3812	0.004	0.78	242	8.0

5.2.1 Boundary conditions for 2-D computational domain

Figure 5.6 shows the boundary surfaces of 2-D computational domain. The wall is composed of two surfaces of the wedge and an expansion surface extended horizontally after EC. In front of the leading edge, there is a symmetry plane, which represents the symmetry of the flow with respect to the horizontal direction. The left and top surfaces are the part of Inlet boundary whereas the right surface forms Outlet boundary.

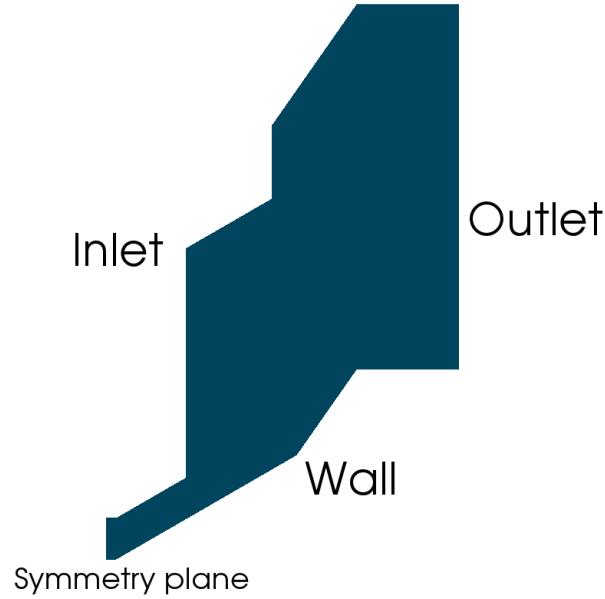


Figure 5.6 : Boundary faces for 2-D computational domain.

Chemically reacting air model presented in section 4.1.6 is selected with the same initial mass fractions for thermally equilibrium and non-equilibrium analyses. Free-stream conditions given in Table 5.1 are assigned as boundary conditions on the inlet surface for U , p , T . The initial mass fractions of $Y_{N_2} = 0.767$, $Y_{O_2} = 0.233$, $Y_{NO} =$

0.00, $Y_N = 0.0$ and $Y_O = 0.0$ are given for thermal equilibrium flow whereas the fractions are accepted as $Y_{N_2} = 0.78$, $Y_{O_2} = 0.209$, $Y_{NO} = 0.001$, $Y_N = 0.0$ and $Y_O = 0.01$ for thermal non-equilibrium flow. At the outlet surface, zero gradient conditions are applied for velocity, pressure, temperature and mass fractions. No-slip condition for velocity and isothermal wall temperature of 298K are imposed on the Wall boundary. Due to non-catalytic wall assumption, species diffusion fluxes across the wall are eliminated by assuming zero gradient conditions for mass fraction values. For thermally non-equilibrium cases, the free-stream vibrational temperatures are assumed to be equal to each other at a temperature of 1086 K. Furthermore, the wall is assumed as adiabatic for vibrational heat fluxes. The types of boundaries mentioned so far are listed in Table 5.2.

Table 5.2 : Boundary condition types applied on the boundary surfaces of 2-D model (FV : Fixed Value, ZG: Zero Gradient).

Boundary surface	Velocity	Pressure	Temperature	Mass fractions
Inlet	FV	FV	FV	FV
Outlet	ZG	ZG	ZG	ZG
Wall	No slip	ZG	FV (T_w) , ZG (T_{vi})	ZG
Symmetry plane	symmetry	symmetry	symmetry	symmetry

5.2.2 Boundary conditions for 3-D computational domain

Similar to 2-D model, the flow conditions in Table 5.1 are used for the boundary conditions on the front, top and outer side surfaces (colored with purple in Figure 5-2). No slip velocity conditions on the wedge surfaces are given while slip condition on the wedge sides (colored with grey in Figure 5-2) are imposed. The wedge surfaces are kept at a constant temperature value of 298 K whereas they are assumed adiabatic for vibrational heat fluxes. Red area in front of the leading edge specifies the symmetry boundary condition. 3-D boundary condition types according to the surface colors shown in the Figure 5-2 are presented in Table 5.3.

Table 5.3 : Boundary condition types applied on the boundary surfaces of 3-D model (sym: symmetry).

Boundary surface	U	p	T	Yi	Color
Wedge top surfaces	No slip	ZG	FV (T_w) , ZG (T_{vi})	ZG	Yellow
Wedge side surfaces	slip	ZG	FV (T_w) , ZG (T_{vi})	ZG	Grey
Top, front and outer sides	FV	FV	FV	FV	Purple
Symmetry plane	sym	sym	sym	sym	Red
Bottom and back side	ZG	ZG	ZG	ZG	Green

5.3 Grid and Time Convergence Studies

Grid convergence studies were conducted by Durna for 2-D and 3-D thermally equilibrium non-reacting analyses [58]. Due to limited computational resources available for the current research, it is impossible to conduct grid convergence study for 3-D mesh considering the fact that thermally equilibrium and non-equilibrium analyses for 3-D meshes took at least one month and three months, respectively. Therefore, this study relies on grid convergence study of Durna even though his works considerably differ in terms of flow physics. Nevertheless, time convergence study of 2-D mesh for the current research was performed in order to choose the most efficient time step for a fast convergence.

CFL condition is a convergence criterion for obtaining numerical solutions for partial differential equations. The choose of proper time step according to CFL number is important to achieve stability and convergence for explicit numerical solutions. CFL condition assures that the maximum distance that information can travel should be less than the grid lengths in a time step. For a simple 1-D case, the CFL defined as:

$$CFL = u \frac{\Delta t}{\Delta x} \quad (5.1)$$

where u , Δt and Δx represents velocity magnitude in a cell, the time step and the edge length of a particular cell in the computational domain, respectively. Generally, CFD solutions require the condition of $CFL_{max} < 1$. Considering this maximum CFL requirement, time independence of 2-D computational domain is investigated for three distinct time step values. As seen in Table 5-4, CFL condition is satisfied for all the time steps chosen.

Table 5.4 : Time step values for time independence study.

Time step	CFL_{max}
5e-11s	0.12
1.5e-10s	0.35
3.0e-10s	0.70

Figure 5-7 illustrates three different distributions ($t = 190\mu s$) obtained for three different time steps. It is seen that even though the time step is increased up to 3e-10s, wall pressure and heat flux distributions, excluding the small deviations at peak

values, do not change with increasing CFL number. This assures that the solution is independent of time step.

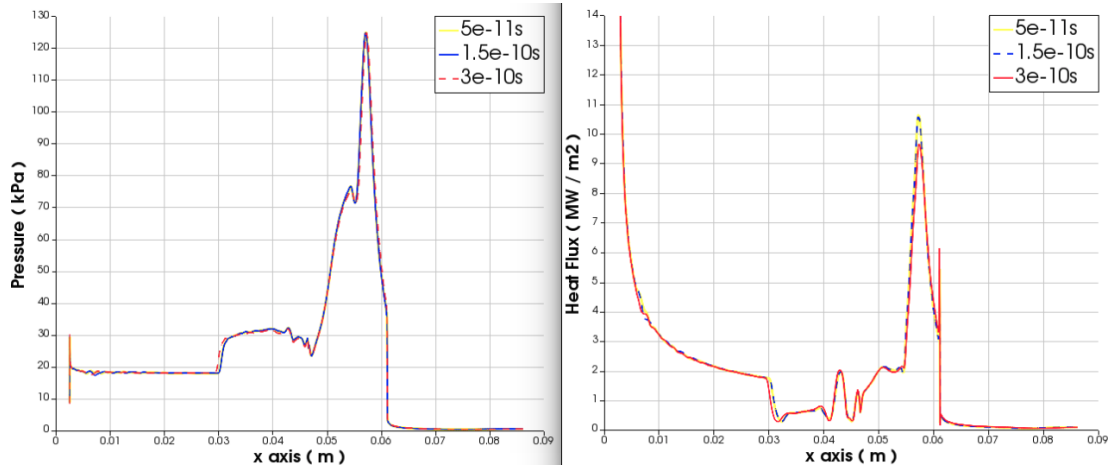


Figure 5.7 : Influence of time step on the 2-D computational domain.

5.4 Thermally Equilibrium Analyses

5.4.1 Shock structures

In Chapter 1, a brief theoretical introduction regarding shock wave – boundary layer interactions was presented. In this section, the interaction mechanisms of numerical solutions obtained for both 2-D and 3-D computational domains are introduced. Figure 5.8 depicts basic features of shock interactions over 30° - 55° double wedge model for 2-D computational domain at $242 \mu\text{s}$. The left hand side figure provides streamlines of flow field colored by Mach contours whereas the figure on the right illustrates the subsonic flow regions, which are confined by the sonic line.

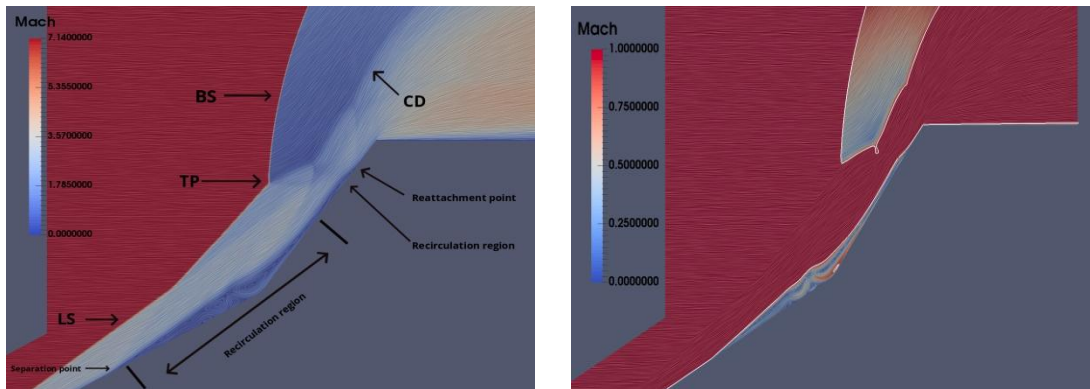


Figure 5.8 : Shock interactions (left) and subsonic regions (right) for reacting thermally equilibrium flow over 30° - 55° double wedge.

It is obvious that the flow is always supersonic apart from the near wall regions, recirculation regions and the flow field behind BS. In addition to the one around CC, there is observably another recirculation region on the second surface close to EC. The formation of another shock, which interacts with BS at TP, is the result of interaction of LS and a separation shock coming from the separation point. The right hand side figure indicates that the flow decelerates to the minimum speed downstream of TP and BS, where BS exhibits almost a normal shock behavior. The presence of CD and the supersonic region downstream of EC are other remarkable features.

Figure 5.9 presents the time evolution and comparison of 2-D and 3-D numerical Schlieren images for $\theta_2 = 55^\circ$ between 30 μs and 242 μs . The green lines represent 3-D density gradient fields taken from the mid-span of the double wedge whereas the red lines show the density gradient fields obtained from 2-D solution. In each frame, a sonic line belonging to the 3-D solution is also drawn for comparison purposes. It is obvious that there are no distinguishable differences between 2-D and 3-D shock structures up to 30 μs . After 60 μs , however, the separation line near CC starts to appear and the distance between SS and RS increases. At the same time, the area of 3-D subsonic region confined by BS, TP and CD grows considerably when compared to that at 30 μs . Another important feature is that after 60 μs , the expansion waves formed at EC start to interact with the reflected shocks impinging over EC. When the flow reaches to 120 μs , the locations of BS, TP and SS begin to differ from each other, resulting to upstream positioning of 2-D shocks. It should be noted that after this time, we start to observe extra shock waves near CC in 2-D solution due to shear layer deformations in this region. Nevertheless, these extra shock waves are not clearly observable in 3-D solution since the relaxation in spanwise direction might have played an important role in the absence of shear layer deformations. During the simulation time, the separation line always stretches both in upstream and downstream directions. It is also seen that the distances between BS and TP of 2-D and 3-D solutions reach to the maximum at the end of simulation while the strengths of bow shocks keep nearly the same at 242 μs .

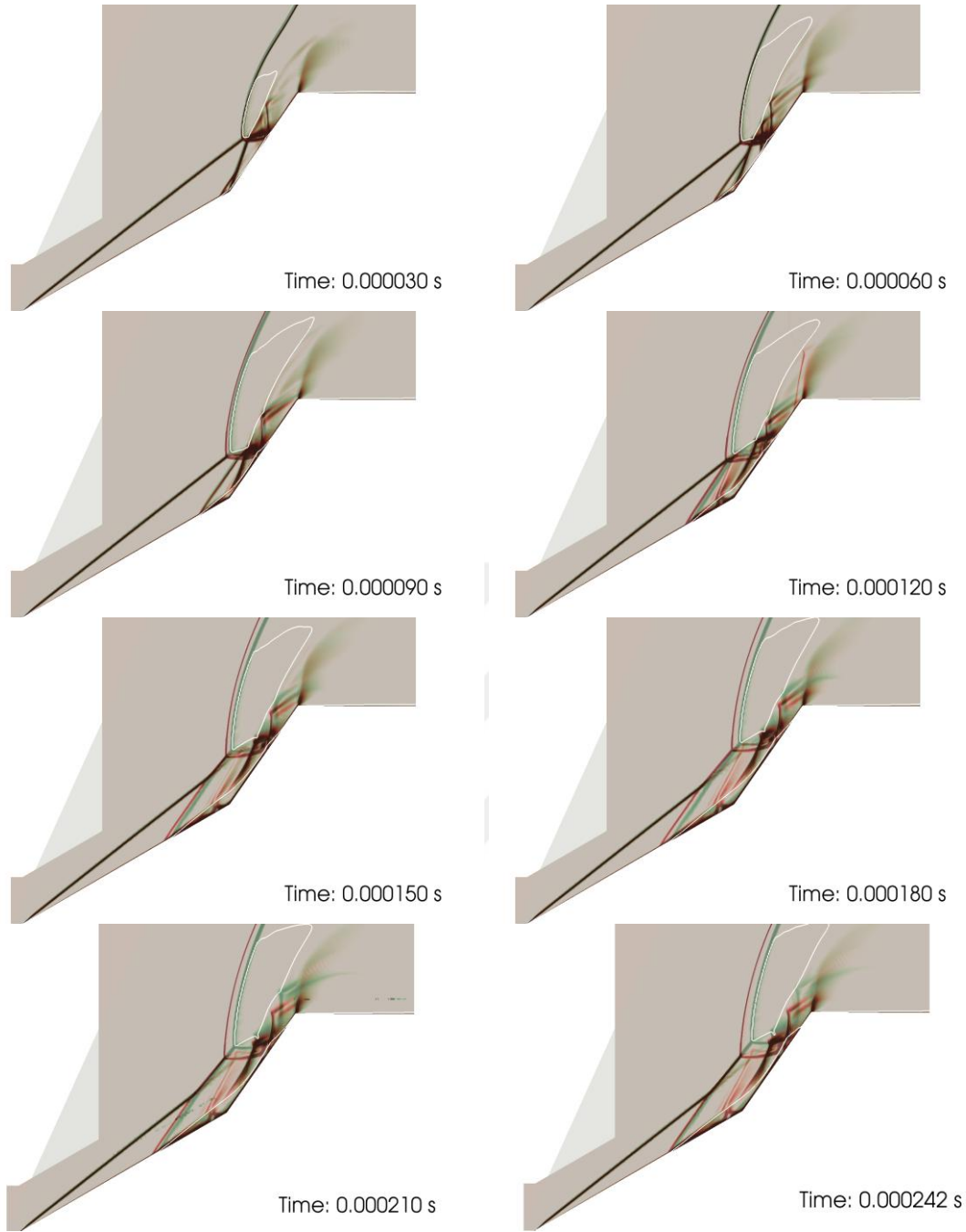


Figure 5.9 : Time evolution of overlapped density gradients of 2-D (red) and 3-D (green) solutions for thermally equilibrium reacting flow over 30°-55° double wedge.

Figure 5.10 compares the numerical Schlieren images of the double wedges with four different aft angles at 242 μ s. Obviously, as the angle of the second surface increases, the shock – shock and shock wave - boundary layer interactions become more complex. For $\theta_2 = 45^\circ$, we do not see any subsonic flow field apart from the near wall regions because $\theta_2 = 45^\circ$ is clearly not high enough for a strong bow shock

formation, rather an oblique shock forms as seen in the Figure 5.10. Nonetheless, an increase of 5° in θ_2 causes a bow shock formation and subsonic flow field behind it.

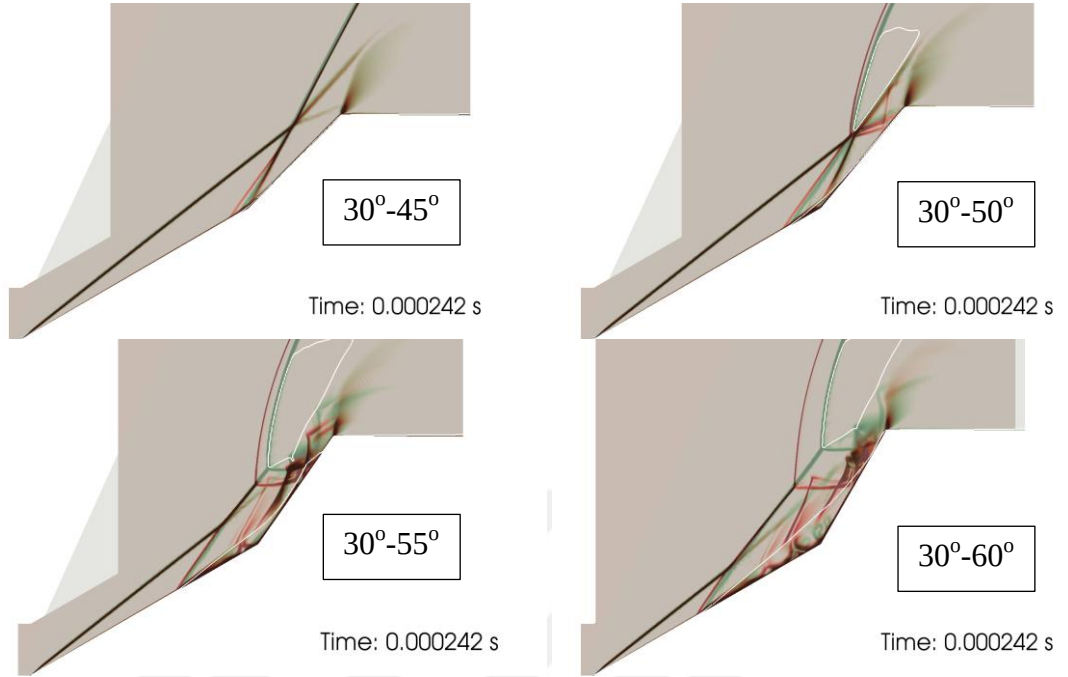


Figure 5.10 : Comparison of 2-D and 3-D overlapped density gradients at four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$) for thermally equilibrium reacting flow.

It is evident that the subsonic flow region contains a larger area as θ_2 further increases. Difference between 2-D and 3-D shock structures becomes more visible for $30^\circ - 60^\circ$ wedge flow, in which the distances between TP and BS of 2-D and 3-D solutions are longer when compared to other smaller angles. Additionally, the bottom-right frame shows that when $\theta_2 = 60^\circ$, LS and SS interacts at further upstream location, from which the separation line extends towards the end of the second surface. Moreover, the thickness of the recirculation region gradually grows as the inclination angle increases. It is also noticeable that the strength of BS both in 2-D and 3-D solutions enhances for higher angles of θ_2 . Related to bigger rate of shear layer deformations for higher aft angles, formation of extra shocks in 2-D solutions are only observable for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$ in the Figure 5.10.

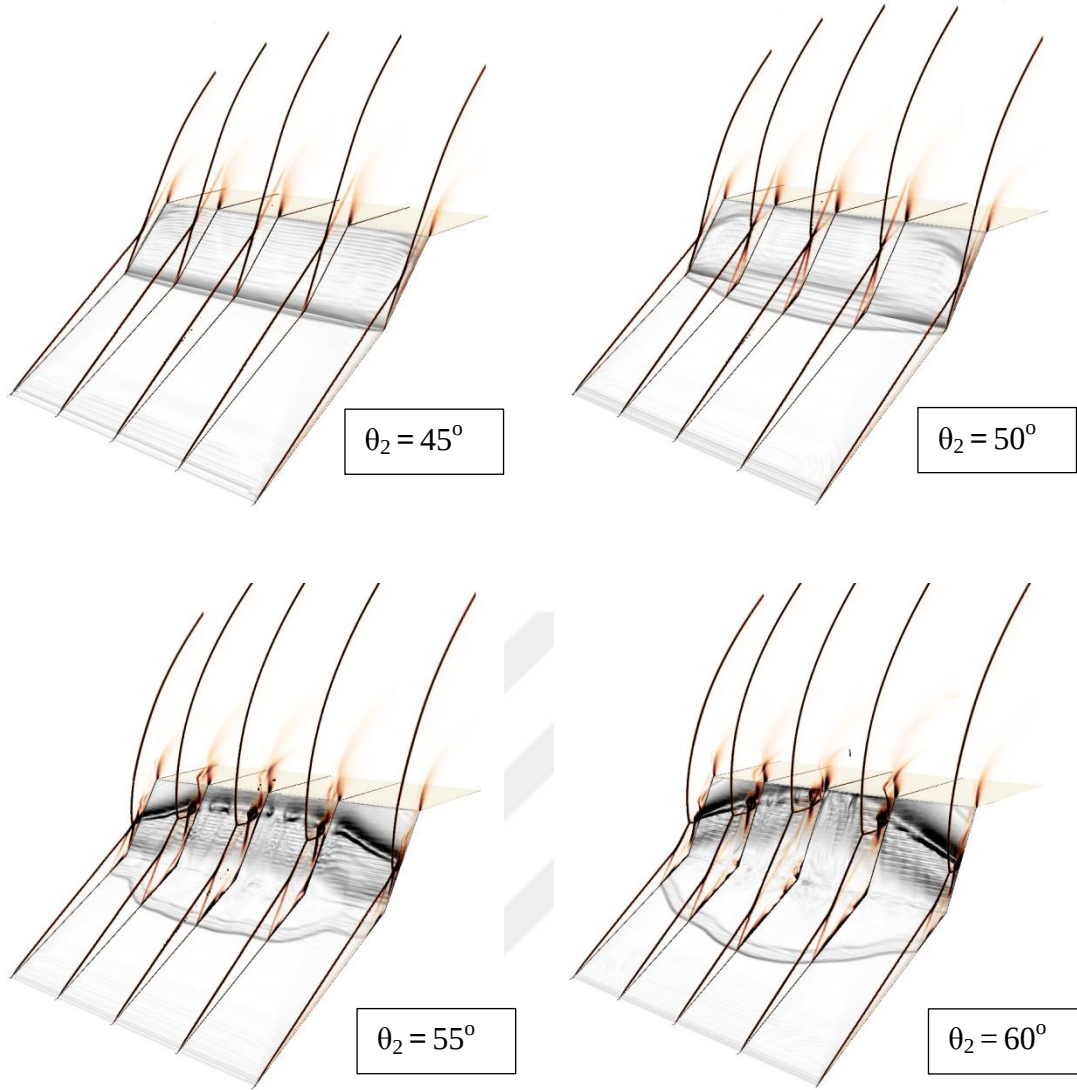


Figure 5.11 : 3-D density gradient contours plotted at the double wedge surface and at five different sections ($z = 0$, $z = 0.25$, $z = 0.5$, $z = 0.75$ and $z = 1.0$) for thermally equilibrium reacting flow.

In order to show the correlations between recirculation region and shock structures, four different images that contain surface density gradient distribution on the wedge and the shock structures obtained at five different spanwise stations, $z = 0.0$, $z = 0.25$, $z = 0.50$, $z = 0.75$ and $z = 1.0$, were generated as can be seen in the Figure 5.11. Even though it may be barely observable for $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$, each frame has a separation line (SL), a secondary shock line (SSL), an impingement line of TS and a reattachment line (RL) on the wedge surface. SL and SSL are the first two lines on the first surface of the wedge, respectively. Impingement line of TS and RL are divided by a separation region, colored by white, on the second surface of the wedge. Figure 5.11 shows that as the interaction becomes more severe, that is when the aft

angle increases, the total recirculation region occupies a larger area on the wedge surface. For stronger interactions at higher aft angles, the location of SL and SSL moves upstream whereas the location of impingement line of TS and RL moves downstream.

5.4.2 Specie concentrations

It is known that shock interactions have great influences on the change of air composition through chemical reactions triggered by temperature jumps across the shock waves. In order to observe the characteristics for variation of air composition, surface distributions of N, O, NO and O₂ mass fractions on the double wedge are obtained for all aft angles. The left column in the Figure 5.12 shows the variations of forming species, N, O and NO while the right column depicts the dissociating specie O₂ in the mixture. 2-D and 3-D mid-span distributions in each column are represented by solid lines and dashed lines, respectively. It is conspicuous that the amount of N available in the air mixture is negligible for all θ_2 . The most important feature observed from the graphs is that the rate of creation and destruction, that is the reaction rate, increases as the interactions become more severe with higher θ_2 . For example, the amount of O₂ dissociation for $\theta_2 = 45^\circ$ is around 0.002 in terms of mass fraction, while the dissociation in the case of $\theta_2 = 60^\circ$ goes up to as much as 0.09. Similarly, the maximum mass fraction of O is about % 0.08 for the highest aft angle, whereas the amount is limited to % 0.002 at most for the lowest aft angle. We also see that the reaction rates obtained from 3-D wedge surfaces are faster than those of 2-D wedges for $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$. Nevertheless, as the interactions become stronger for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$, the reaction rates are slower on the midspan of 3-D wedges than on 2-D wedges. It is also noticeable that the variations of mass fractions over 30° - 55° and 30° - 60° wedges show oscillatory behaviors along the surface.

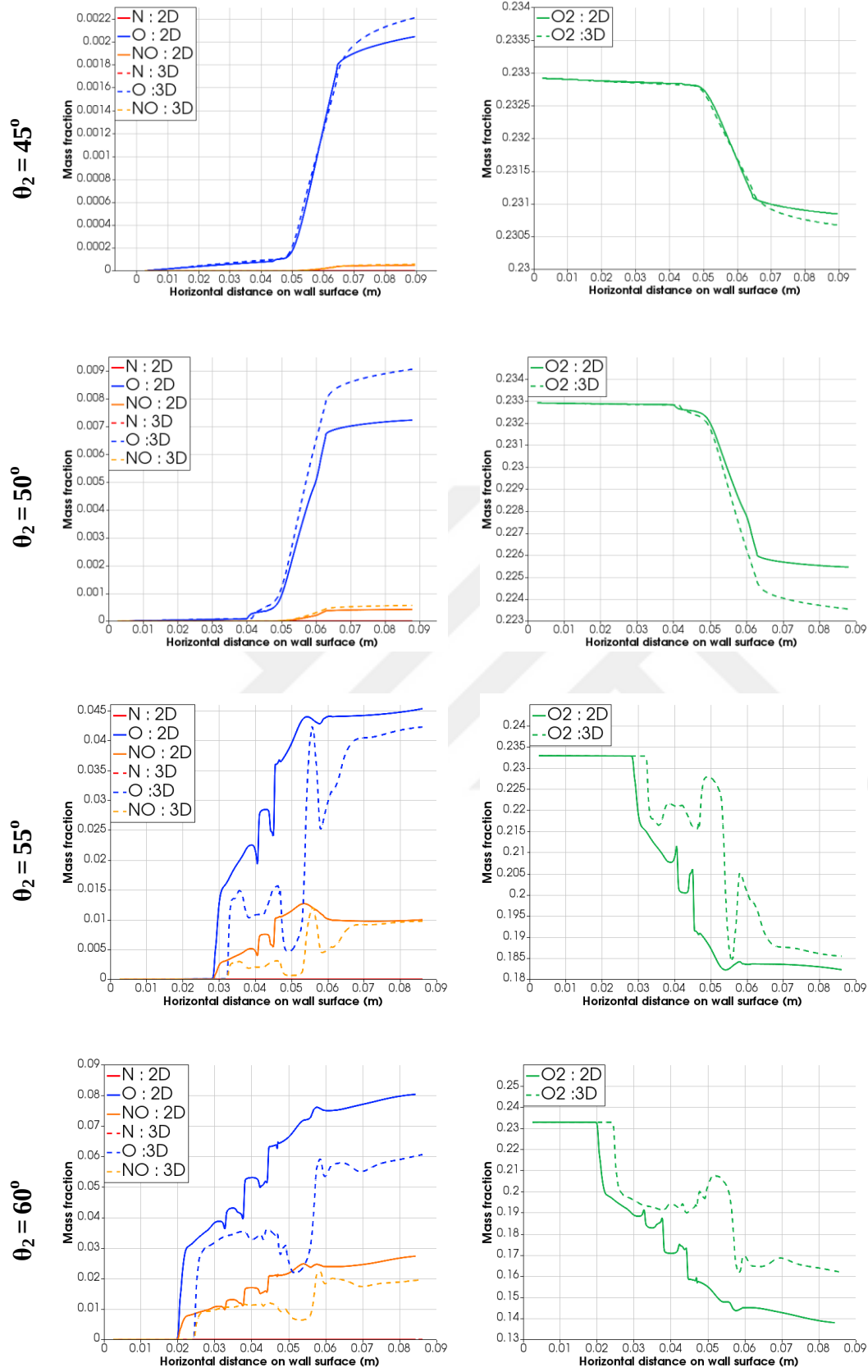


Figure 5.12 : Specie mass fraction comparisons between 2-D and 3-D (mid-span) for thermally equilibrium reacting flow.

5.4.3 Wall heat flux

Wall heat flux distributions of 2-D and 3-D solutions at three different span stations of the wedge surface were plotted and compared in Figure 5.13 for four different aft angles. It is seen that in all of the cases, the magnitudes of wall heat fluxes in 2-D are always less than those of 3-D solutions until the separation point, which is represented by a sudden drop in the heat flux magnitude, on the first surface. Additionally, 2-D separations on the first surface always occur earlier than 3-D separations for all θ_2 angles. By increasing the second angle, the location of the separation point moves upstream direction as can be understood by 2-D and 3-D sudden drops in heat flux values.

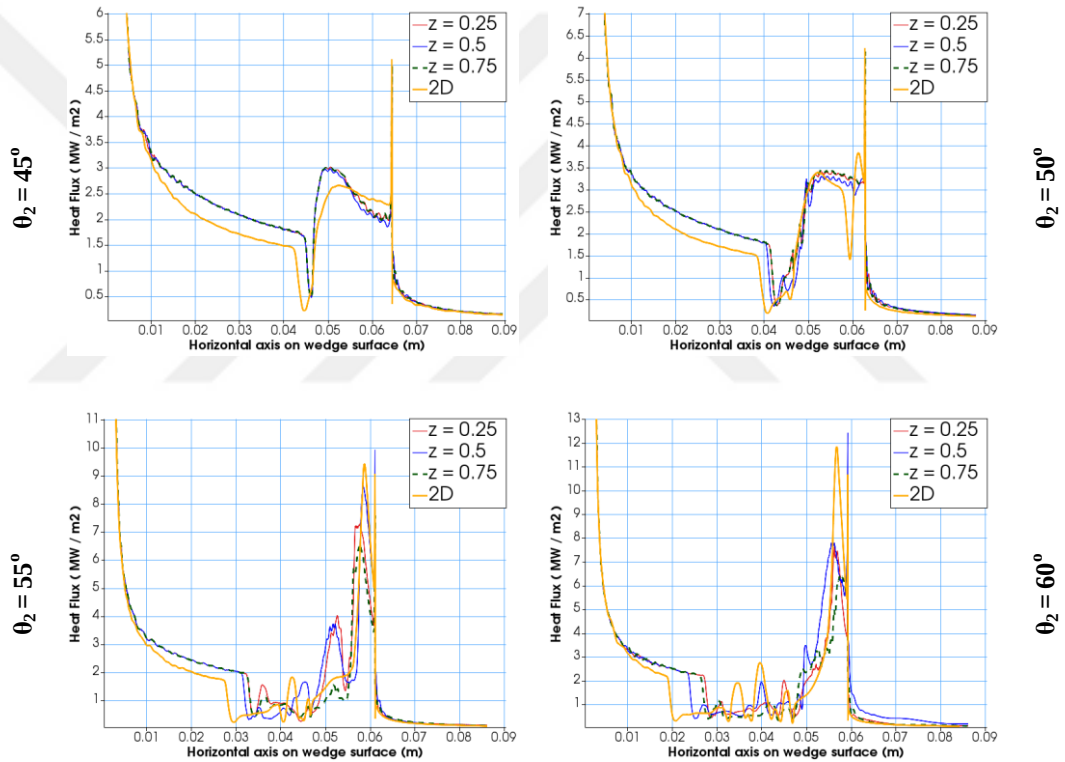


Figure 5.13 : Wall heat flux comparisons between 2-D and 3-D at three different sections ($z = 0.25$, $z = 0.5$ and $z = 0.75$) for thermally equilibrium reacting flow.

The magnitude of peak heat flux is larger for 2-D solutions for all the cases. As the severity of interactions goes up, both peak and overall magnitudes of heat flux increase considerably. For example, the maximum heat flux goes from 5 MW/m^2 to 12 MW/m^2 as θ_2 is increased from 45° to 60° . We should also note that for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$ there are observable oscillations of heat fluxes in the separated region

for both 2-D and 3-D solutions although these oscillatory behaviors are absent for the angles $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$. An almost overlapped distributions are obtained at three different stations for $\theta_2 = 45^\circ$ whereas this feature starts to disrupt after $\theta_2 = 50^\circ$. For the case of $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$, however, the heat flux distributions do not overlap even though they are taken from geometrically symmetric stations, $z=0.25$ and $z=0.75$.

5.4.3.1 Comparison with numerical studies and the experiment

Figure 5.14 compares numerical studies [59] with the experiment of Swantek and Austin. While Badr and Knight, Reimann and Rosa et al. presented their steady state results, Komives et al., Lani et al. and *hyperReactingFoam* performed time accurate solutions. Although there are significant differences among the outcomes of CFD studies and the experiment, there is reasonable accuracy for the location and magnitude of experimental peak heat transfer. Besides, all of numerical studies have a certain degree of oscillatory behavior in the separated region, which is absent in experiment. It should also be noted that the difference between 2-D and 3-D thermal equilibrium solutions of *hyperReactingFoam*, as shown in the previous section, are obvious. This is definitely a result of three dimensionality of the flow.

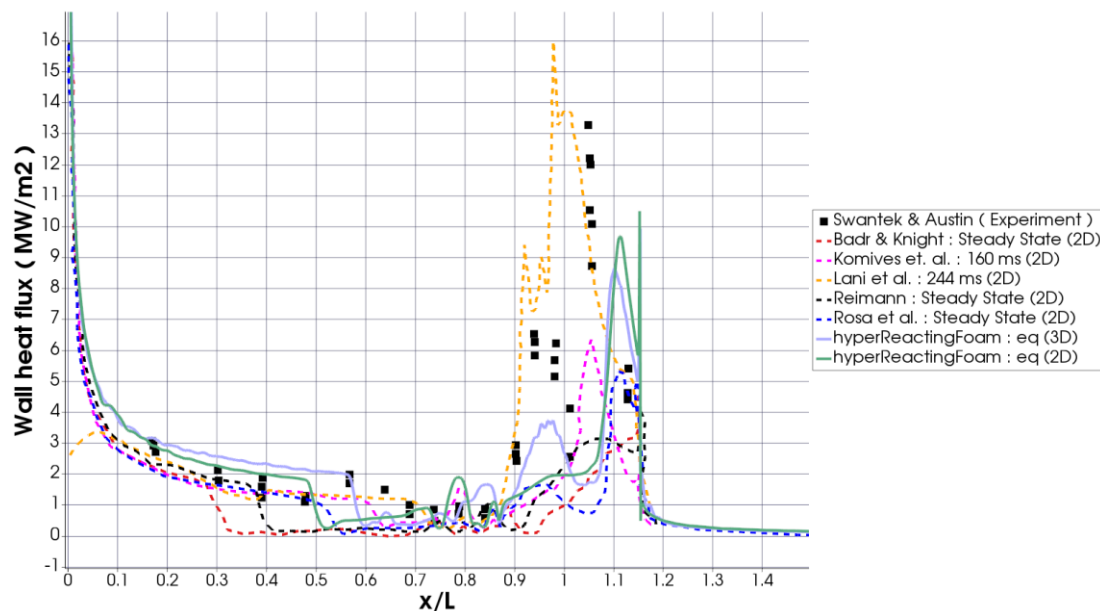


Figure 5.14 : Comparison of thermal equilibrium analyses with other numerical studies and the experiment.

5.4.4 Distributions on the 3-D wedge surface

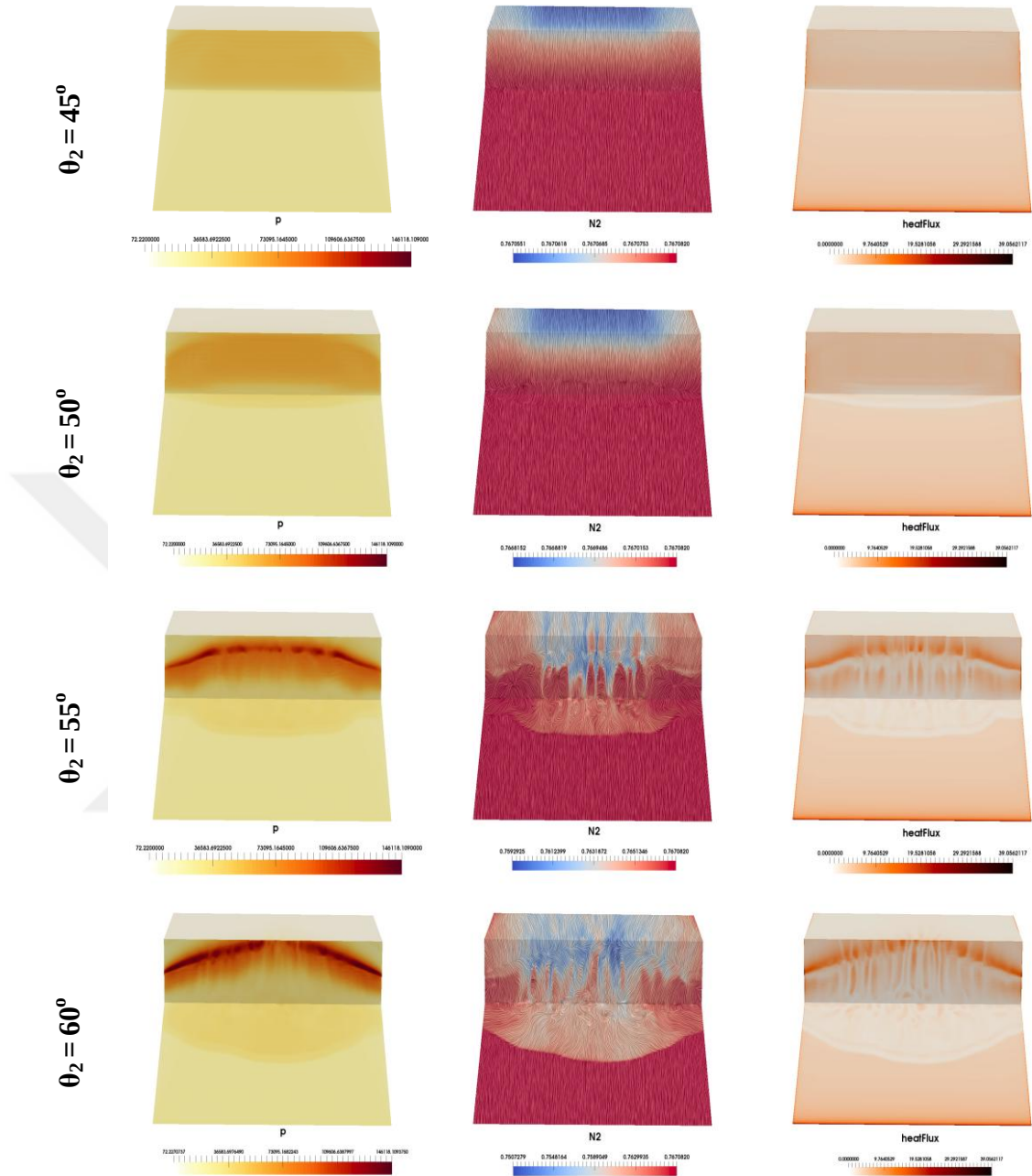


Figure 5.15 : Surface distributions of pressure, N_2 mass fraction and heat flux variables on the 3-D double wedge for four different aft angles.

Pressure distribution, surface streamlines colored by N_2 mass fraction and heat flux distribution contours for four θ_2 values are compared as shown in Figure 5.15 below. In compatible with the heat flux graphics, 30° - 45° double wedge has a uniform surface heat flux distribution in spanwise direction. For $\theta_2=45^\circ$, the streamlines are aligned in the free-stream direction over the wedge surface. However, as a result of

increased aft angle, three-dimensionality effects for surface streamlines become more obvious, especially in the recirculation region, where many nodes and saddle points form. From the second column, we see that the spanwise variation of N_2 is not uniform for all the aft angles. The first and third columns illustrate that the peaks in pressure and heat flux overlap with the reattachment line on the second surface. N_2 contours show that the dissociation of nitrogen gas is at most for $\theta_2=60^\circ$ with a maximum consumption mass fraction of 0.17 in comparison to an amount of 0.00003 for $\theta_2=45^\circ$. It is not surprise that the maximum dissociation rates of N_2 are reached within the second surface, in which heat flux rates are much higher as can be observed both in Figure 5.13 and in Figure 5.15.

5.5 Thermally Non-Equilibrium Analyses

5.5.1 Shock structures

Figure 5.16 compares the shock structures of thermally equilibrium and non-equilibrium analyses on 2-D wedges. The density gradient contours colored by red represent thermal non-equilibrium results while the green colors show the shock structures of thermal equilibrium solution. The figure also contains sonic lines in the flow field, in which blue and white isocontour lines depict sonic fields of thermal non-equilibrium and thermal equilibrium flows, respectively. It is conspicuous that the angles of LS and SS of non-equilibrium flow are higher than the ones of equilibrium flow for all cases. More upstream positioning of BS in all cases for thermal equilibrium condition is another obvious feature observed from this figure. We see that LS and SS of non-equilibrium flow position more upstream locations up to an aft angle increase of $\theta_2 = 55^\circ$, from which further increase in angle leads to a downstream positioning of LS and SS of non-equilibrium flow. It should be noted that the area encircled by sonic line behind BS is larger for thermal equilibrium flow in all aft angles. The difference, however, is the largest for $\theta_2 = 50^\circ$. Although there are some minor distances between each other, the separation lines of thermally equilibrium and non-equilibrium flows almost overlap in all θ_2 angles, apart from the subsonic region near CC for $\theta_2 = 60^\circ$, in which the sonic line of non-equilibrium flow is confined by the sonic line of equilibrium flow, leading to a smaller subsonic field near this region for thermal non-equilibrium flow. The existence of an enclosed sonic

line of thermal equilibrium flow close to EC for $\theta_2 = 60^\circ$ points to a Mach stem, which is clearly not observable for thermal non-equilibrium flow.

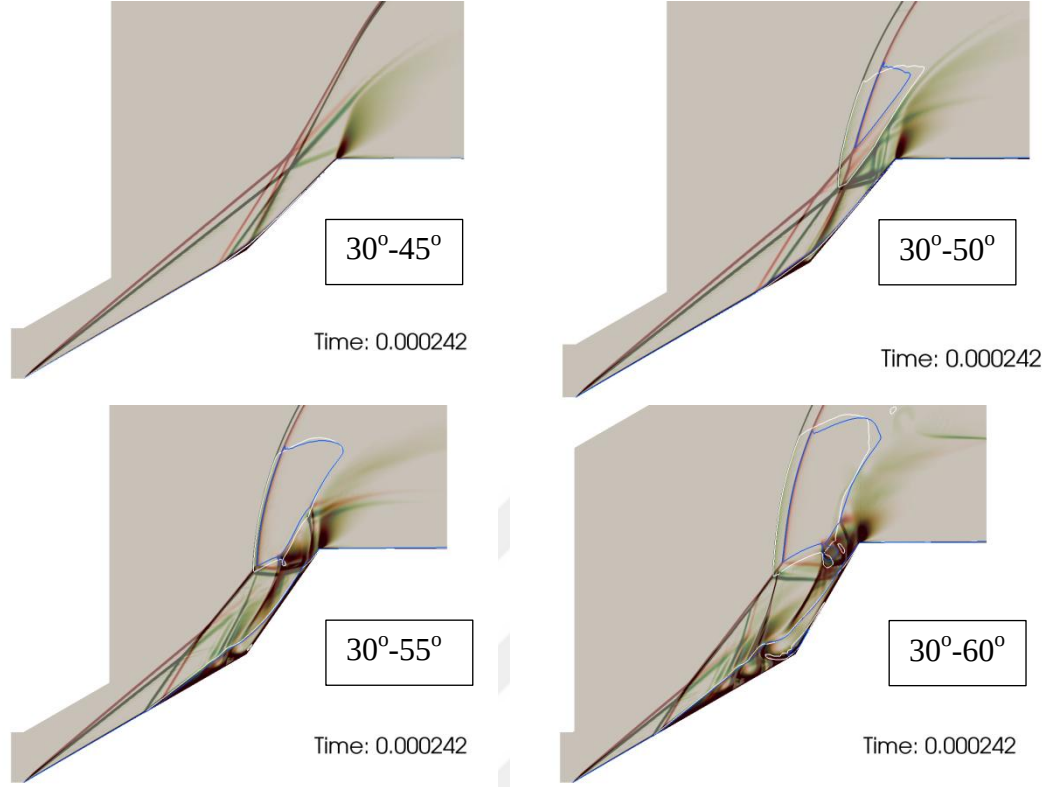


Figure 5.16 : Overlapped density gradient comparisons of 2-D thermally equilibrium and non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

In Figure 5.17 we see the time accurate solution of 3-D thermally non-equilibrium shock interaction mechanism at five different sections over the double wedge for four different aft angles. As it was observed earlier in 2-D solutions, the severity and complexity of interactions gradually increase in 3-D solutions as well when θ_2 is changed to 60° . For $\theta_2 = 45^\circ$, the strength of BS at all of the sections is considerably weaker than those of other higher aft angles, such that, in this angle, BS nearly behaves as an oblique shock. The area of separated region in 45° , as observed from the variation of surface density gradient, is very small in comparison to 55° and 60° . Besides, there is no observable TS impinging upon the second surface of the wedge for $\theta_2 = 45^\circ$. Nevertheless, as the angle is increased to 50° , an impingement line of TS starts to emerge on the second surface, especially between the sections $z=0.0 - z=0.25$ and $z=0.75 - z=1.00$. Apart from this, even though the area of separated region is still quite small, the difference with $\theta_2 = 45^\circ$ is clearly observable. The further increase in aft angle also shows that shock waves start to interact with the

expansion fan, especially at the sections $z=0.25$, $z=0.50$ and $z=0.75$. Furthermore, the surface density gradients for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$ show the three dimensionality of the flow, more clearly. As opposed to a straight line along the spanwise direction, SL, SSL, impingement line of TS and RL exhibit curvilinear distributions on the wedge surface. We should also mention that the interactions observed from the sections $z=0.0$ and $z=1.0$ are less complex when compared to other mid-sections.

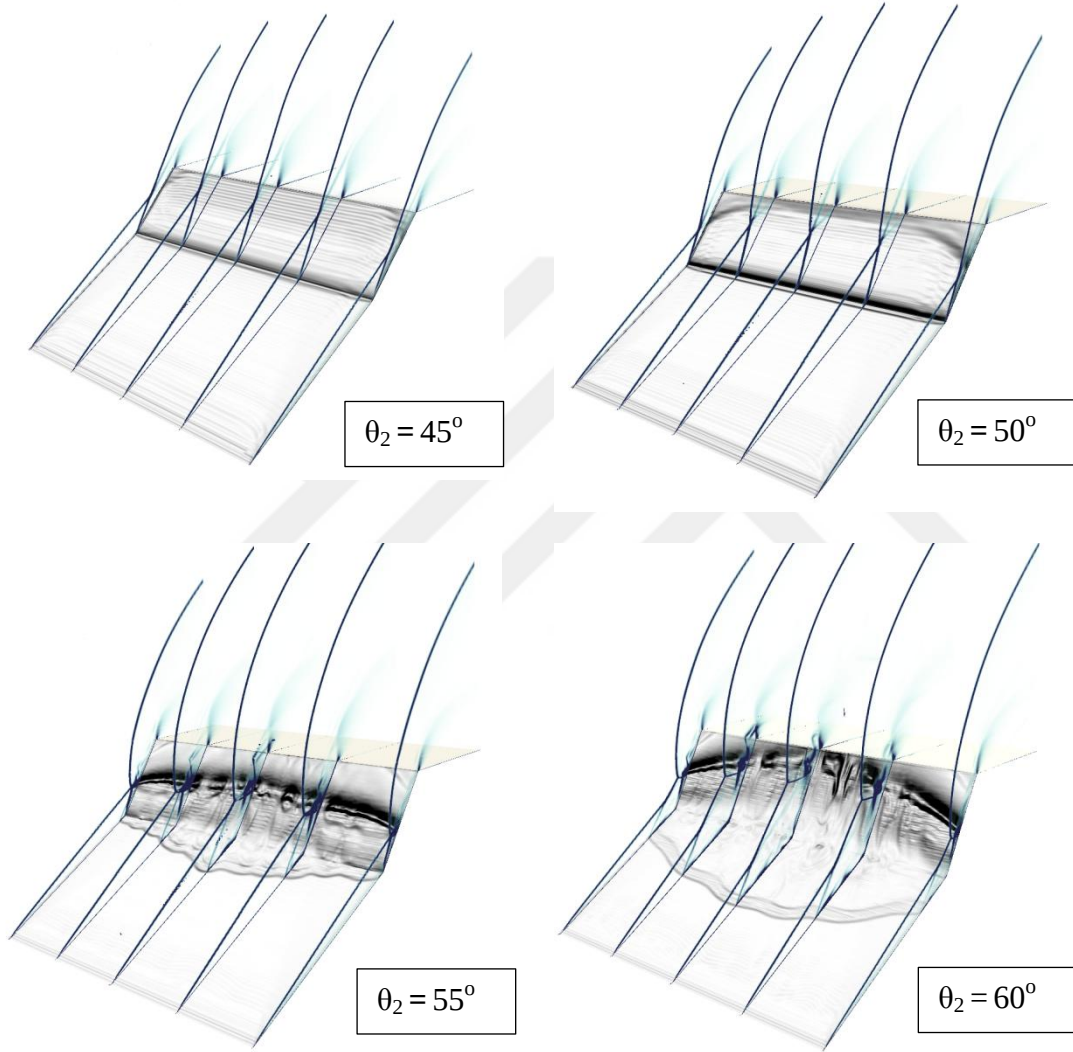


Figure 5.17 : 3-D density gradient contours for 242 ms plotted at the double wedge surface at five different sections ($z = 0.0$, $z = 0.25$, $z = 0.5$, $z = 0.75$ and $z = 1.0$) for thermally non-equilibrium reacting flow.

Figure 5.18 shows the time evolution of 3-D thermally non-equilibrium shock interaction mechanism at five different sections over the double wedge for $\theta_2 = 55^\circ$ between $40 \mu s$ and $233 \mu s$. It is seen that as the time evolves, both the area of separated region and the strength of interaction over the separated region gradually

increases. Between 40 μs and 78 μs , the surface density gradient over the second surface between CC and the impingement line of TS is observed to be considerably less than in magnitude when compared to later time steps. It should also be noted that after 160 μs , the distributions of SL and SSL along the spanwise direction changes from straight to curvilinear distributions.



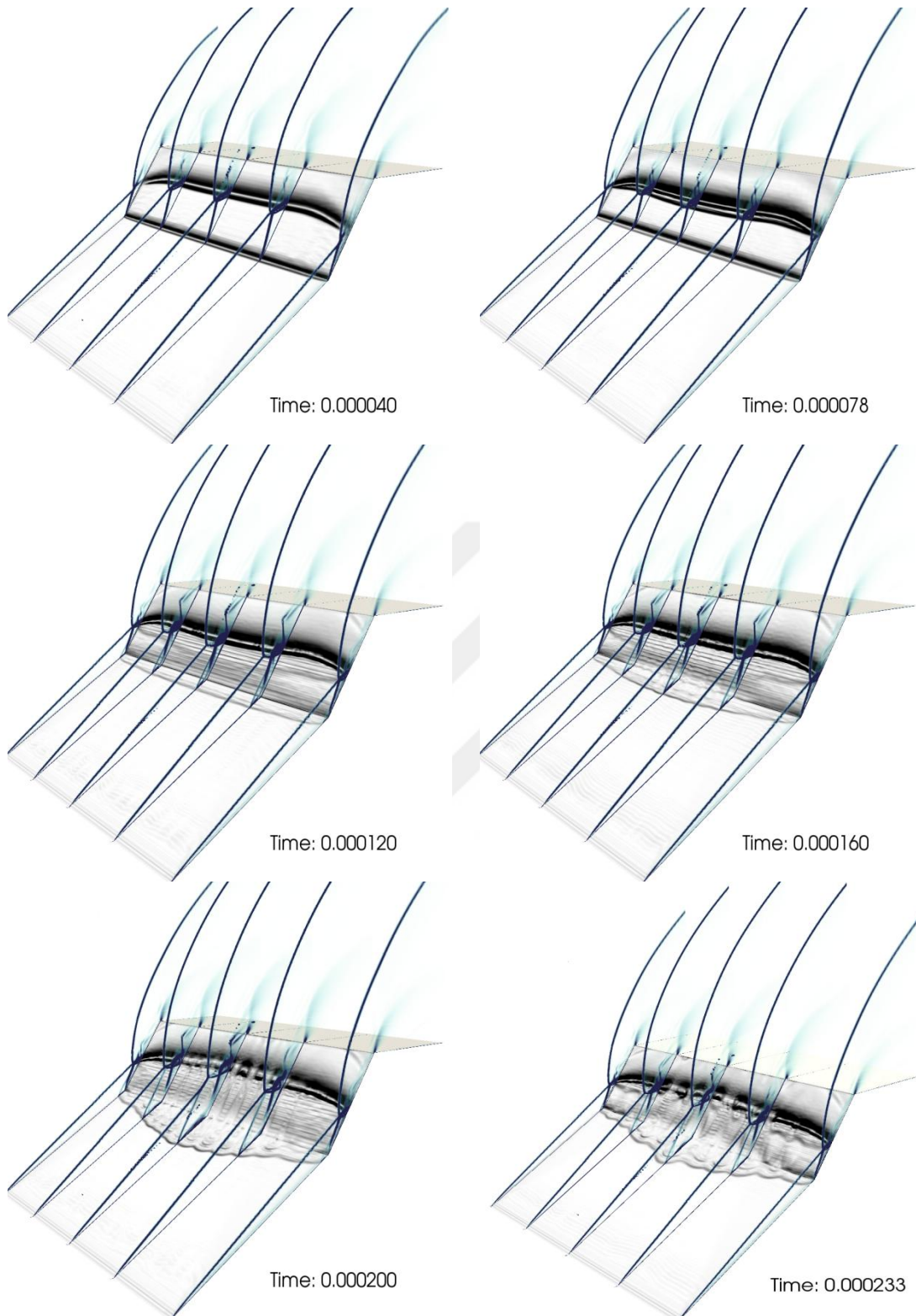


Figure 5.18 : 3-D density gradient contours for six different time steps (40ms, 78ms, 120ms, 160ms, 200ms and 233ms) plotted at the double wedge surface at five different sections ($z = 0.0$, $z = 0.25$, $z = 0.5$, $z = 0.75$ and $z = 1.0$) for thermally non-equilibrium reacting flow.

5.5.2 Specie concentrations

5.5.2.1 Comparison between 2-D equilibrium and non-equilibrium flows

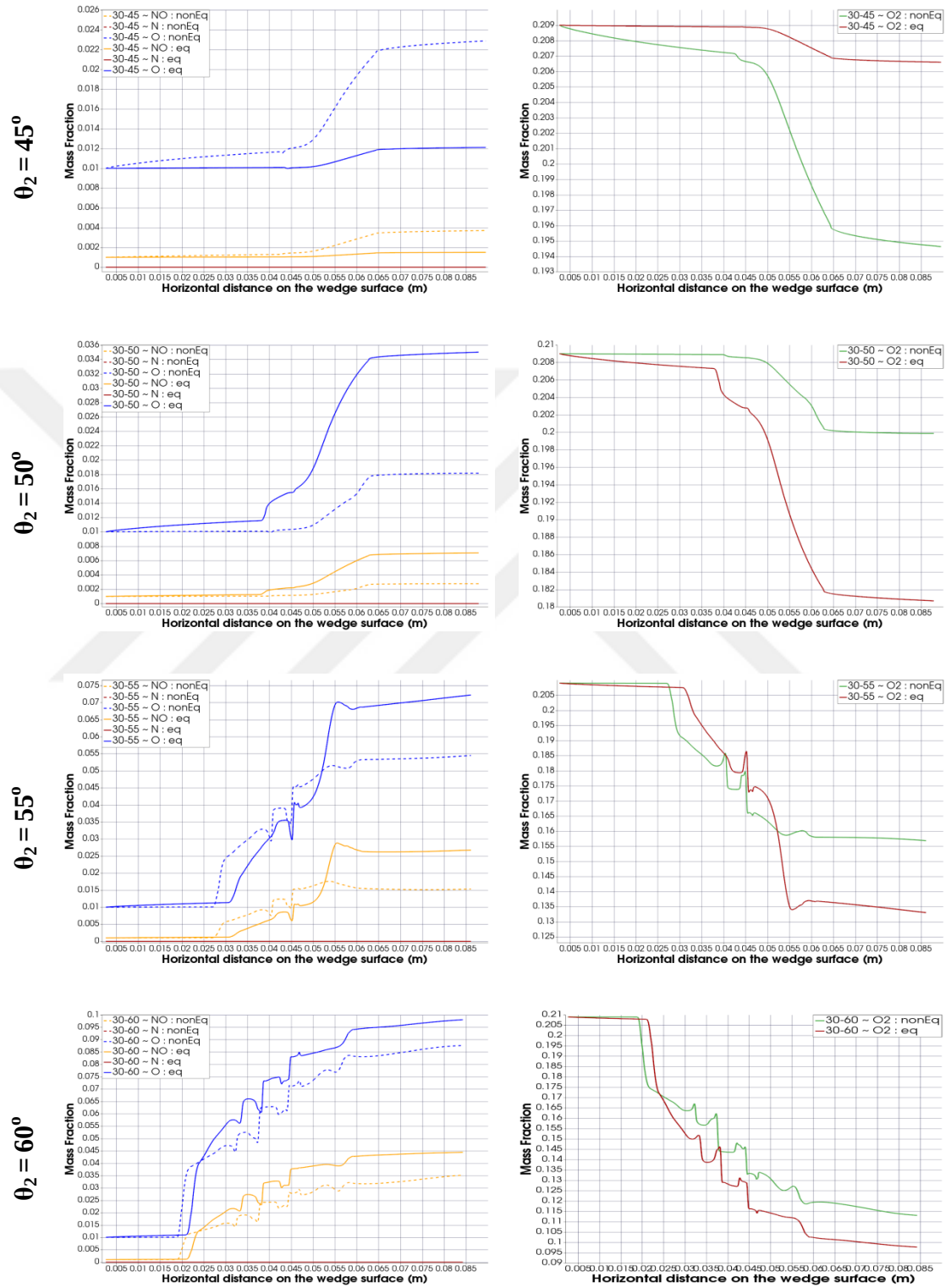


Figure 5.19 : Specie concentration comparisons of 2-D thermally equilibrium and non-equilibrium analyses for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$) for reacting flow.

Figure 5.19 shows the variations of specie mass fractions (N, O, NO and O₂) obtained by 2-D thermal equilibrium and thermal non-equilibrium analyses. It is seen that the minimum and maximum amount of species are observed over the expansion surface for all cases. The observation of mass fractions shows that the reaction rates are faster in thermal non-equilibrium flow for $\theta_2 = 45^\circ$, whereas the reaction rates of non-equilibrium flow become slower in comparison to equilibrium flow for other aft angles. Even though there exist considerable differences in mass fractions between the two conditions in all cases, the fastest reaction rates take place at the aft angle of $\theta_2 = 60^\circ$ for both conditions. We should also mention that in accordance with the shock structures in Figure 5.16, considerable differences in reaction rates are observed after SS for thermally equilibrium and non-equilibrium flows. It is also seen that the reactions over the expansion surface are almost frozen for the cases $\theta_2=45^\circ$ and $\theta_2=50^\circ$ whereas for $\theta_2=55^\circ$ and $\theta_2=60^\circ$, the reaction rates over the expansion surface are still non-negligible.

5.5.2.2 Comparison among all aft angles for 2-D non-equilibrium flows

Figure 5.20 presents the dissociation of O₂ and the production of N, O and NO in terms of mass fractions for four different aft angles in 2-D thermally non-equilibrium flow. It is clear that for all cases the production of N atom is negligible on the wedge surface, with a maximum mass fraction as low as $2.4e-7$. The dissociation of O₂ molecules and the production of NO and O becomes faster as the second angle of wedge increases up to 60° . Having reached the end of the wedge surface, nearly % 50 of O₂ molecules decompose to other species for $\theta_2 = 60^\circ$ while this ratio is only about % 7 for $\theta_2 = 45^\circ$. It is noticeable that reactions start at an upstream location, $L=0.02m$ on the first surface, for $\theta_2 = 60^\circ$ in comparison to a downstream location, $L=0.045m$ for $\theta_2 = 45^\circ$. Also, as the second angle increases up to 60° , the slope of the mass fraction curves becomes more steep, apart from the local oscillatory behaviors along the wall.

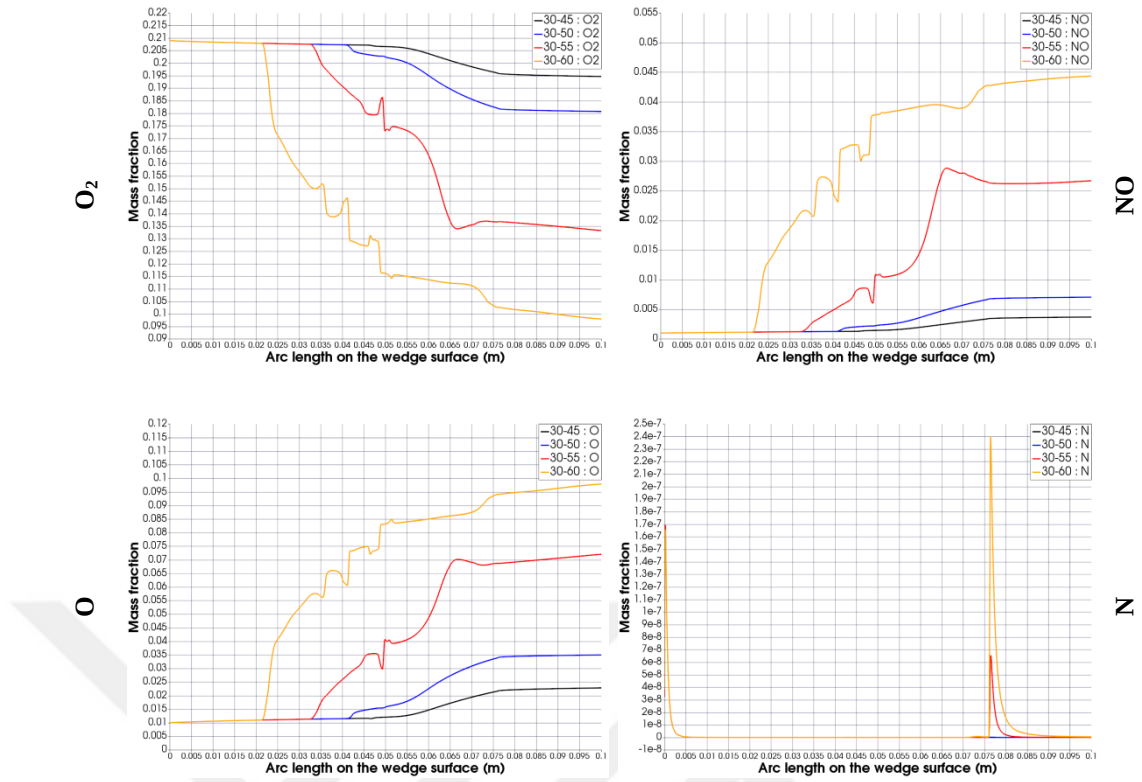


Figure 5.20 : Specie mass fraction comparisons of 2-D thermally non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

5.5.3 Wall heat flux

5.5.3.1 Comparison between 2-D equilibrium and non-equilibrium flows

Figure 5.21 presents the comparison of variations of wall heat flux distribution of 2-D thermal equilibrium and non-equilibrium flows. Even though the graphs have common and similar characteristics, considerable differences exist between equilibrium and non-equilibrium analyses. For instance, up to $\theta_2 = 50^\circ$, due to SS, there is an earlier sudden drop in heat flux for non-equilibrium flow. Nevertheless, as further increase of aft angle shifts this characteristic in favor of equilibrium flow. It is obvious that thermal non-equilibrium analyses provide higher magnitude of oscillations in the separated region especially for the cases of $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$. Additionally, the magnitudes of peak heat flux on the second surface, which are around 9.5 and 11.5 MW/m², obtained by equilibrium analyses are considerably higher than those of non-equilibrium flow for these two aft angles. On the other hand, the characteristics of heat flux distributions after the expansion fan are identical for all angles of θ_2 .

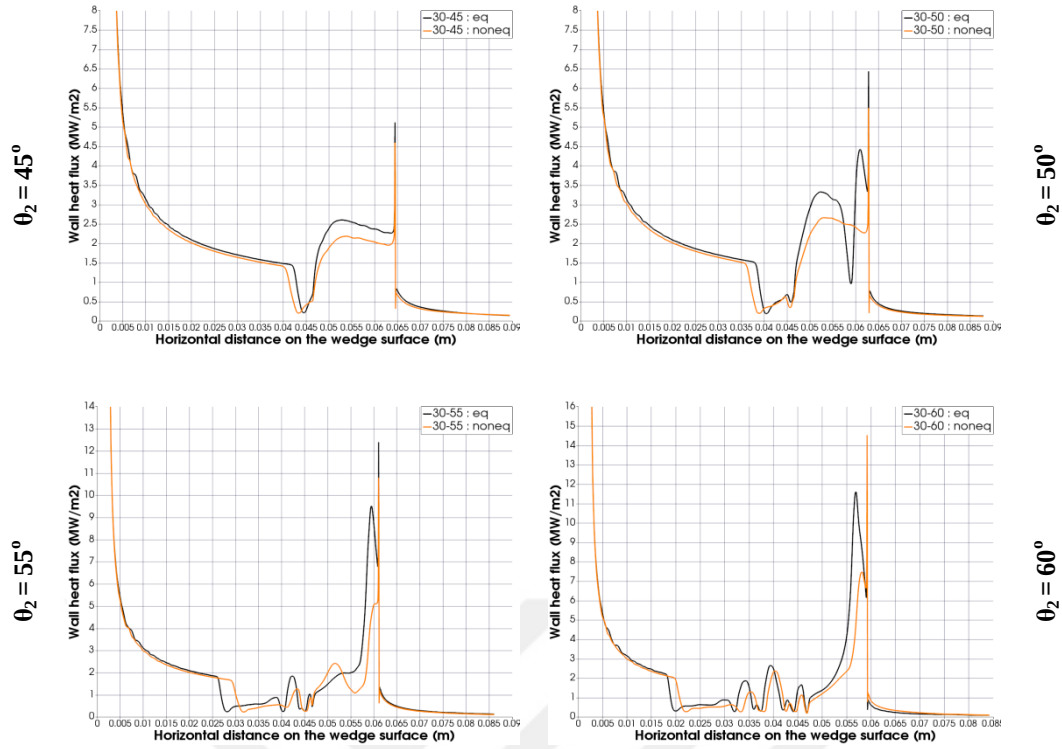


Figure 5.21 : Wall heat flux comparisons of 2-D thermally equilibrium and non-equilibrium reacting flows for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

5.5.3.2 Comparison among all aft angles for 2-D non-equilibrium flows

Figure 5.22 depicts the distribution of surface heat flux for four different aft angles in 2-D thermally non-equilibrium flow. There is a sudden drop in heat flux on the first surface which takes place at an earlier location as θ_2 is systematically increased to 60° . We see that, with the same increment, the magnitude of peak heat flux rises from 2.0 MW/m^2 to 7.5 MW/m^2 , although the location of the peak stays at the same location, which is around at 0.074 m . Likewise, heat flux curves plotted on the expansion surface show that increase in the angle of the second surface causes more heat transfer rates within this region. Moreover, the strength of interactions can be understood by the amplitudes of the oscillations within the separated region as θ_2 is increased to 60° . It is noticeable that these oscillations do not actually exist for the cases of $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$.

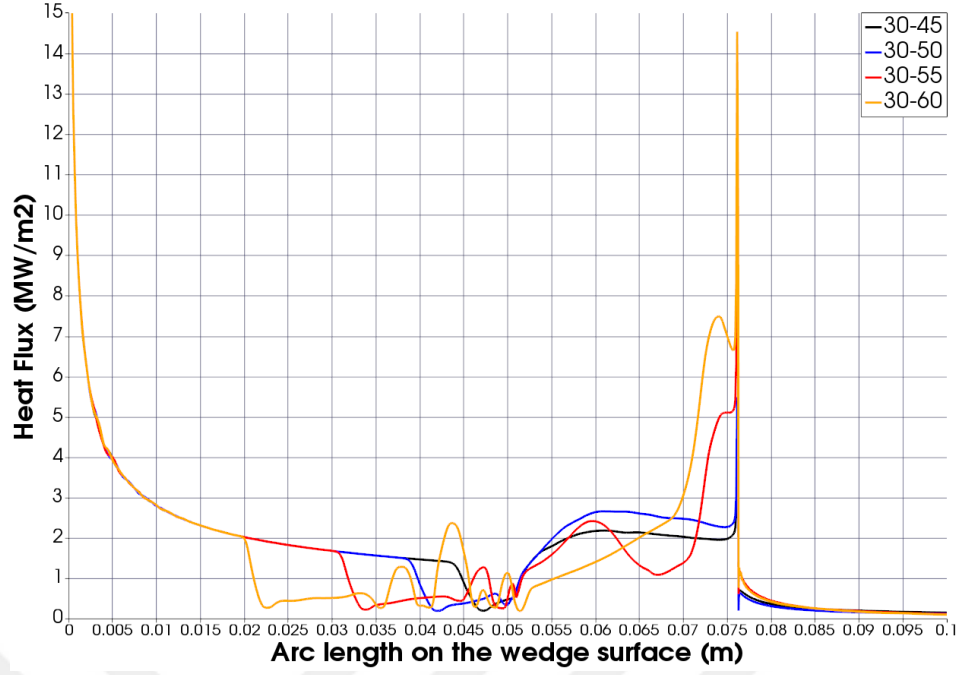


Figure 5.22 : Wall heat flux comparisons of 2-D thermally non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

Figure 5.23 shows the time evolution of surface heat flux distributions for four different aft angles in 2-D thermally non-equilibrium flow. It is seen that the maximum amount of wall heat transfer for $\theta_2 = 60^\circ$ is higher than those of other aft angles at all-time steps. We observe that, even at $80 \mu s$, the maximum local heat transfer for $\theta_2 = 60^\circ$ is larger than the maximum heat transfer of other aft angles obtained at $240 \mu s$. It should be mentioned that the changes in heat flux distribution for $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$ after $160 \mu s$ is miniscule as opposed to the significant changes observed for higher aft angles. The common thing among distinct θ_2 angles is that the separated region is the most time dependent area in terms of heat transfer distribution on the double wedge surface. Also, both for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$, as the time marches, the location of local maximum heat transfer on the second surface moves downstream with a decrease in the magnitude.

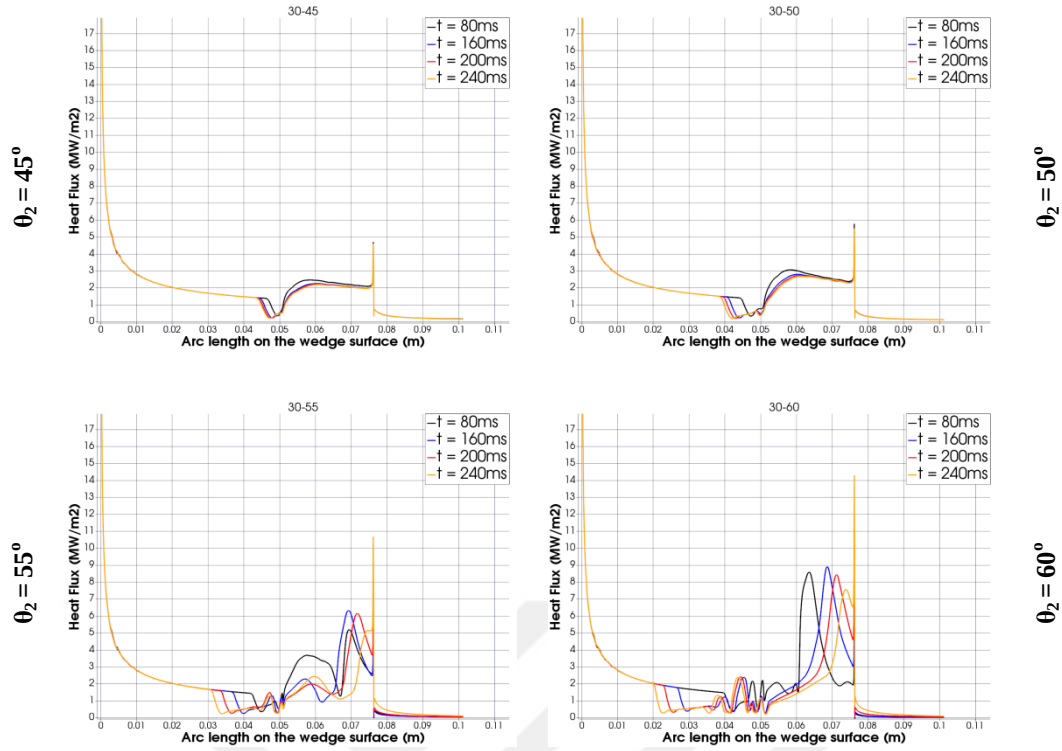


Figure 5.23 : Time marching of wall heat flux distribution of 2-D thermally non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

5.5.4 Wall pressure

5.5.4.1 Comparison between 2-D equilibrium and non-equilibrium flows

Figure 5.24 provides the comparison of wall pressure distributions of 2-D thermal equilibrium and non-equilibrium flows. We observe that thermal equilibrium analyses yield higher pressure in the separated region for all aft angles. This difference is especially more conspicuous given the higher peak values of thermal equilibrium pressures on the second surface. When compared carefully, it is seen that the location of peak pressure shifts to a downstream position for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$ if the analyses are conducted by thermal non-equilibrium conditions. It should also be noticed that the differences in pressure are observable in the first surface, including the locations up to the formation of SS. Compatible with the shock structure comparison in section 5.5.1, pressure jumps due to SS formation on the first wall starts to occur at an earlier location for thermal equilibrium flow when θ_2 is increased to 55° .

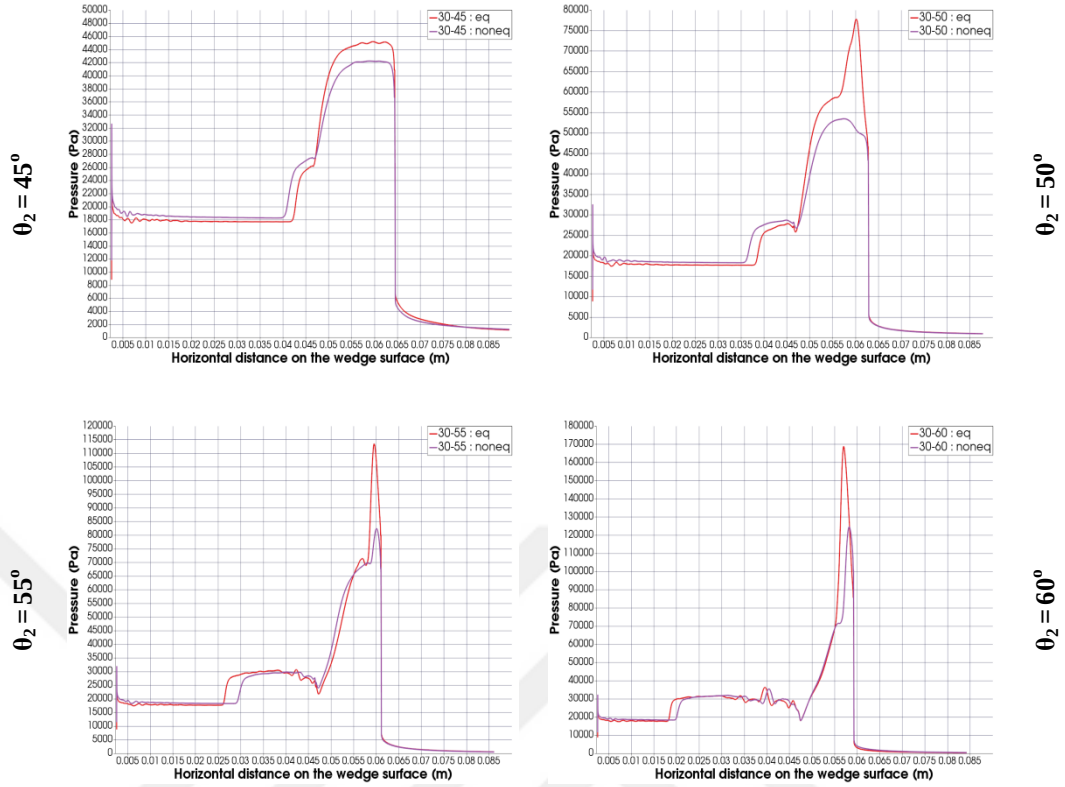


Figure 5.24 : Wall pressure comparisons of 2-D thermally equilibrium and non-equilibrium reacting flows for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

5.5.4.2 Comparison among all aft angles for 2-D non-equilibrium flows

Figure 5.25 presents the distribution of surface pressure for four distinct θ_2 angles in 2-D thermally non-equilibrium flow. The comparison shows that increase in the aft angle raises the pressure values in the separation region, especially the peak value, even though the location of maximum pressure within this region does not change at all. Similar to the trend of heat transfer and specie concentration parameters, pressure rises due to SS on the first surface starts to occur more upstream locations as θ_2 is gradually changed to 60° . We should also note that as the aft angle becomes 60° , there occur some oscillations in the separated region, where only gradual increases are present for the other three cases. The severity of the interactions for higher aft angle can be observed from the peak pressure ratio of $\theta_2=60^\circ$ to 45° , which is around 3.0 for thermal non-equilibrium flow.

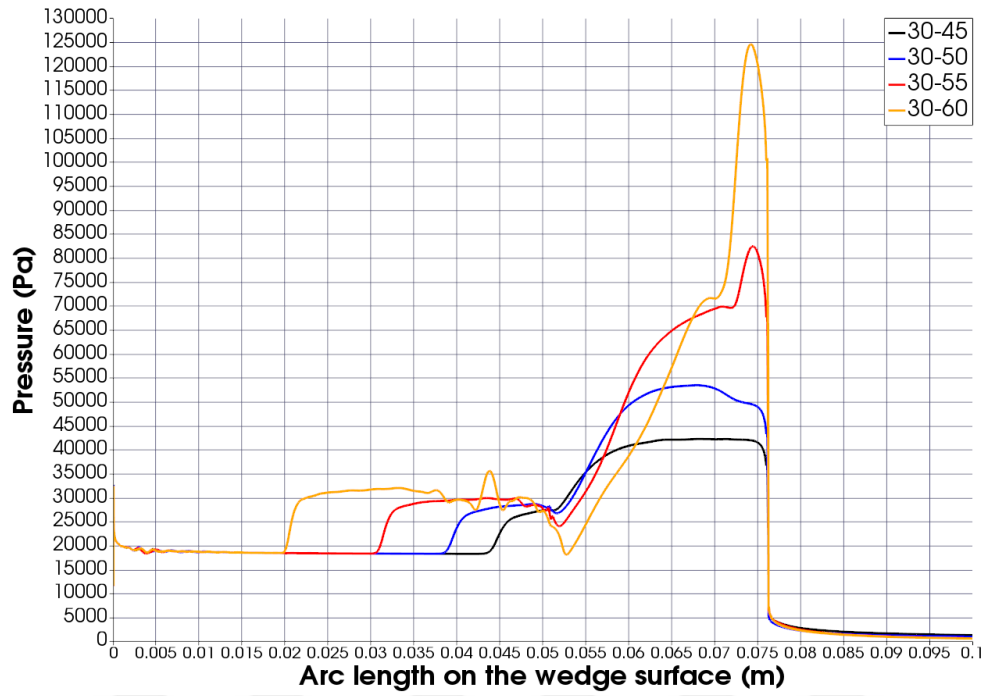


Figure 5.25 : Wall pressure comparisons of 2-D thermally non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

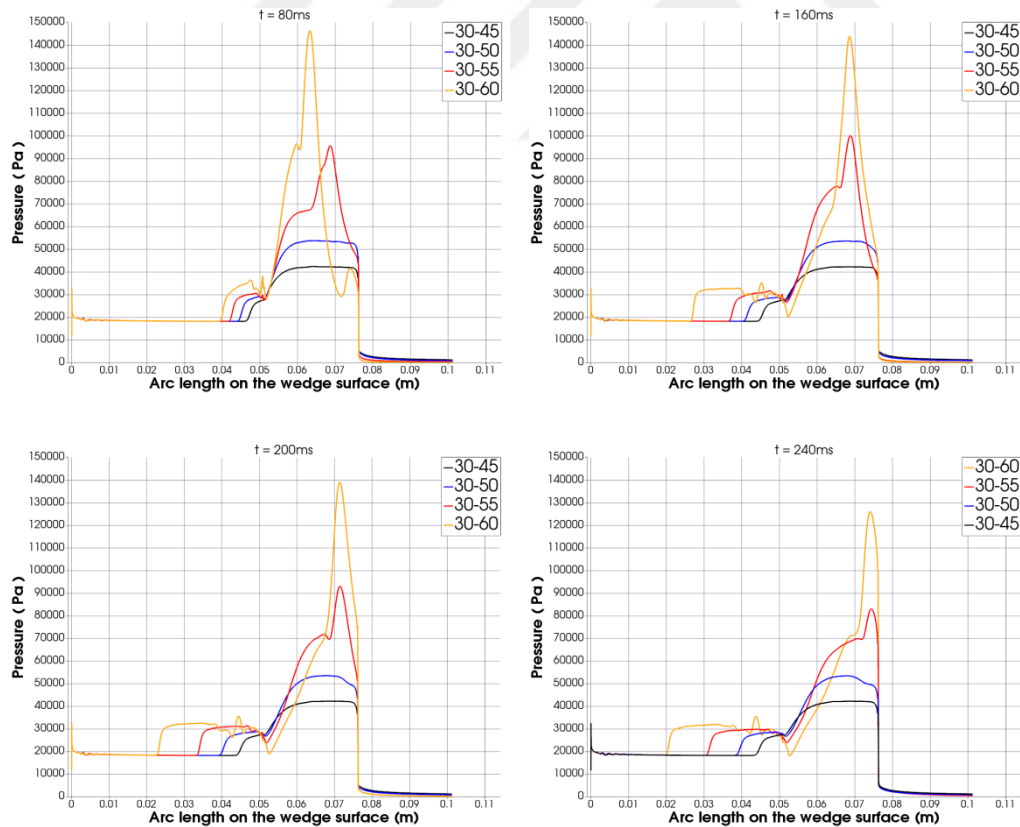


Figure 5.26 : Time marching of wall heat flux comparisons of 2-D thermally non-equilibrium reacting flow for four different aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

Figure 5.26 illustrates the time marching of surface pressure distributions for four different aft angles in 2-D thermally non-equilibrium flow. We should say that the wall pressure distributions for $\theta_2 = 45^\circ$ and 50° slightly changes as the flow develops. Nonetheless, after 160 μs there are significant drops on the wall pressure for the aft angles $\theta_2 = 55^\circ$ and 60° , with a decrease of peak pressure value by 10000 Pa and 15000 Pa, respectively. It is also seen that the local pressure peak on the second surface moves downstream after 160 μs . Besides, the locations of pressure peak of $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$ coincide at all times after 160 μs . Furthermore, for $\theta_2 = 60^\circ$, there is a local minimum of wall pressure around the wedge surface at $L=0.052\text{m}$, which stays at the same location after 160 μs .

5.5.5 Vibrational temperature

5.5.5.1 Comparison among all aft angles for 2-D non-equilibrium flows

Figure 5.27 provides the surface distributions of vibrational temperatures (T_{vN_2} , T_{vO_2} and T_{vNO}) of non-equilibrium analyses. It is clear that the equilibrium temperature at the leading edge starts to disrupt on the wedge surface and different distributions are observed along the wall. The vibrational temperature of NO molecules seems to be under around the equilibrium temperature for all aft angles and shows a constant distribution for the cases $\theta_2 = 45^\circ$ and 50° . The vibrational temperature of O_2 molecules on the wall is always higher than those of N_2 molecules for the aft angles 45° and 50° . Nonetheless, this characteristic considerably changes after 55° , which leads to a greater temperature of N_2 molecules over the expansion surface. We should also mention that as the interaction becomes more severe with the increment of θ_2 , vibrational temperature of N_2 rises all over the wedge surface, as can be seen from Figure 5.28. The figure also shows that the equilibrium temperature disrupts earlier on the wedge surface if the second angle is gradually increased from 45° to 60° .

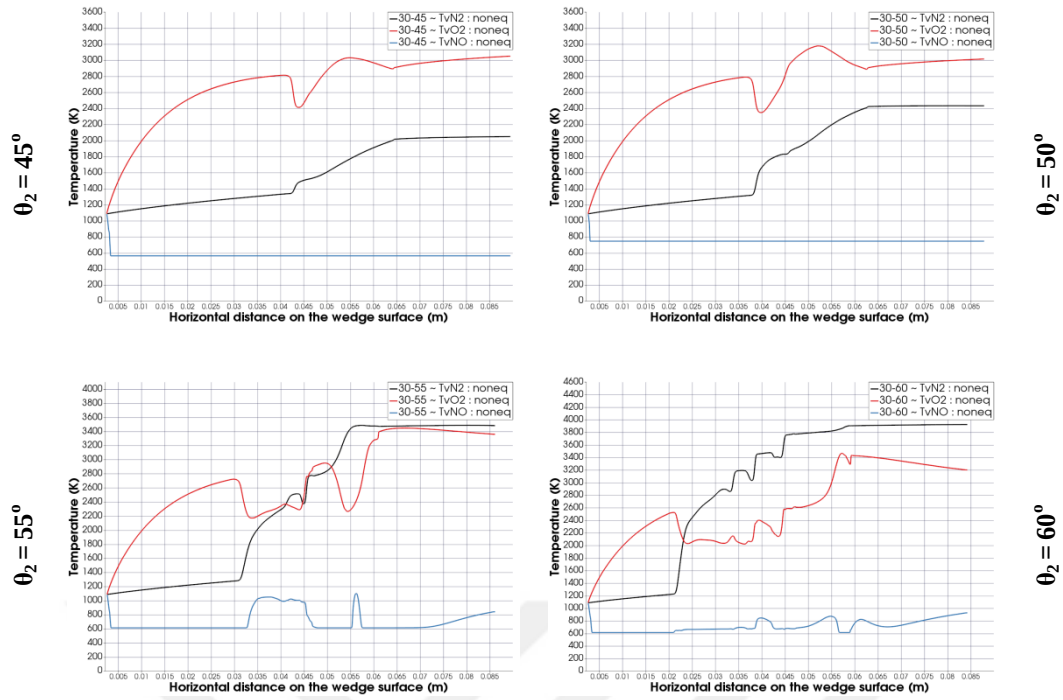


Figure 5.27 : Vibrational temperature comparisons of 2-D non-equilibrium reacting flows with respect to aft angles ($\theta_2 = 45^\circ, 50^\circ, 55^\circ, 60^\circ$).

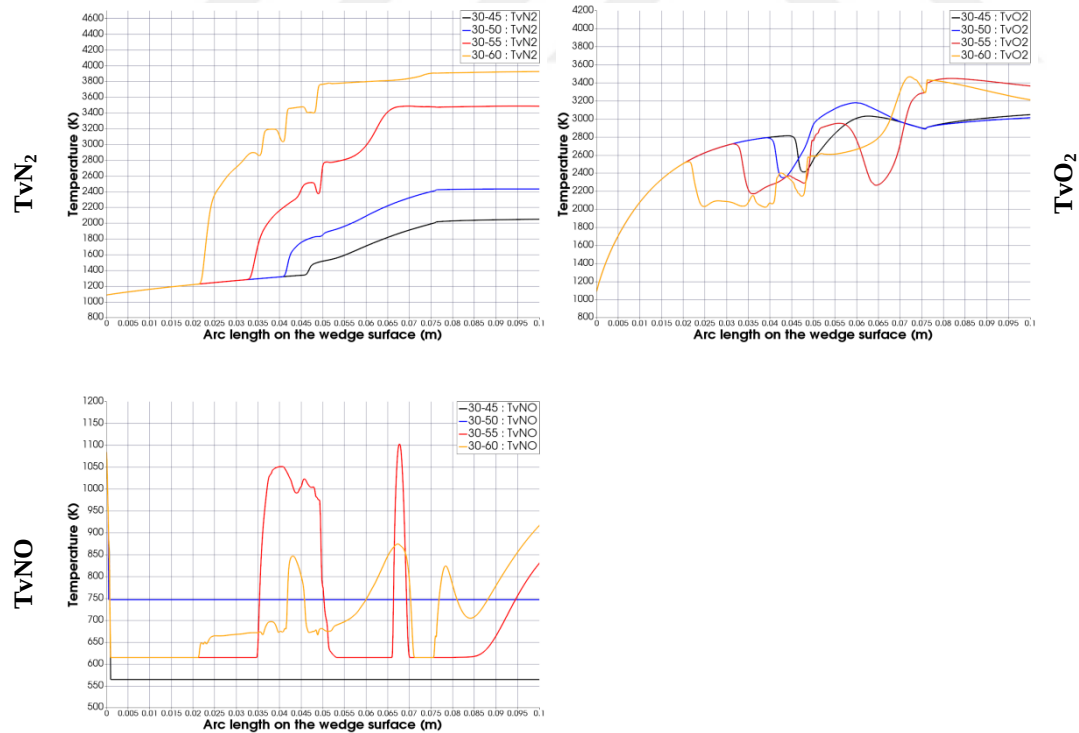


Figure 5.28 : Vibrational temperature comparisons of 2-D non-equilibrium reacting flows with respect to vibrational temperatures (TvN_2 , TvO_2 , $TvNO$).

5.5.5.2 Spanwise variations on 3-D wedge

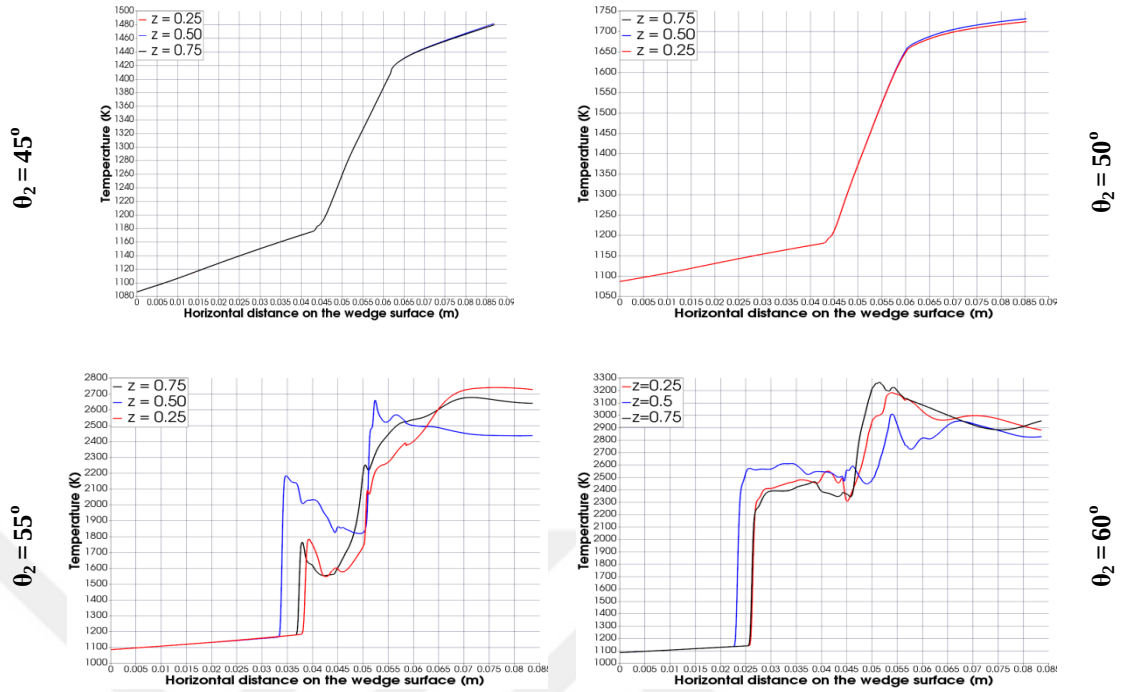


Figure 5.29 : Vibrational temperature of N_2 molecules obtained from 3-D wedge surface at three different sections ($z = 0.25, z = 0.5$ and $z = 0.75$) for thermally non-equilibrium reacting flow.

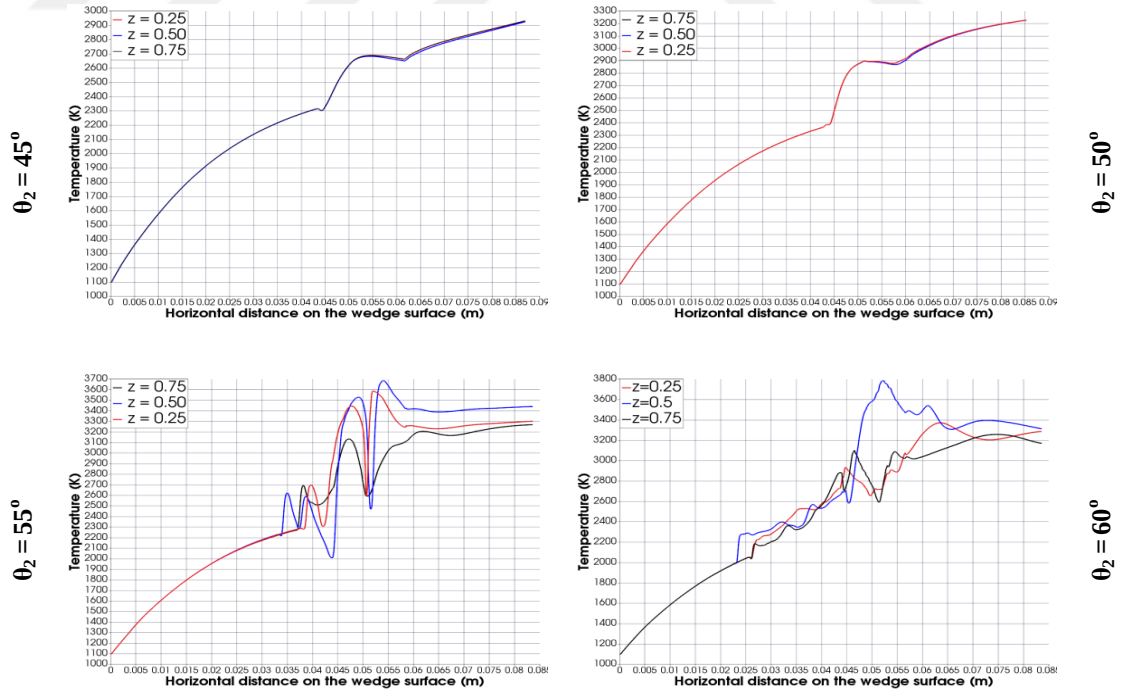


Figure 5.30 : Vibrational temperature of O_2 molecules obtained from 3-D wedge surface at three different sections ($z = 0.25, z = 0.5$ and $z = 0.75$) for thermally non-equilibrium reacting flow.

Figure 5.29 and Figure 5.30 compare the distributions of vibrational temperatures of N_2 and O_2 molecules at three different sections on the double wedge for all aft angles at 240 μs . Both figures show that the symmetry on $z=0.25$ and $z=0.75$ sections start to disrupt after $\theta_2 = 55^\circ$. The distributions of T_{vN_2} and T_{vO_2} exhibit a symmetric behavior for $\theta_2 = 45^\circ$ and $\theta_2 = 50^\circ$. The increase in the aft angles directly enhances the magnitude of vibrational temperatures at all three sections irrespective of whether the flow is symmetric. Both T_{vN_2} and T_{vO_2} show oscillatory behaviors on the separated region of all sections for $\theta_2 = 55^\circ$ and $\theta_2 = 60^\circ$. The temperature distributions of both figure provide that the vibrational temperatures of N_2 and O_2 molecules are not in thermal equilibrium at all sections for all θ_2 . Similar to other wall parameters, the characteristic of vibrational temperatures is directly influenced by the location of SS on the first surface, where increase in the second angle leads to an upstream movement of the location of temperature jump. Nevertheless, this temperature jump occurs earlier on the mid-section than the other symmetric slice pairs of $z=0.25$ and $z=0.75$. We should also mention that as opposed to separated region, T_{vN_2} and T_{vO_2} distributions on the expansion surface do not present oscillatory behaviors due to the absence of complex shock interactions on this surface.

Figure 5.31 presents the time evolution of the surface distributions of T_{vN_2} at three different sections for the aft angle $\theta_2 = 55^\circ$. It is clear that the distributions at the symmetric slice pairs of $z=0.25$ and $z=0.75$ are equal to each other at 80 μs . Even though the symmetry of the flow starts to be disrupting after 160 μs , the vibrational temperature distributions at three different sections are quite close to each other. However, after 200 μs , three dimensionality of the flow become more obvious as the distribution on the mid-section considerably diverges from the symmetric slice pairs. Until 160 μs , the mid-section contains the highest magnitude of T_{vN_2} distribution, however, this trend clearly changes after 200 μs , at which some portions of $z=0.5$ distribution on the wall are lower than those of $z=0.25$ and $z=0.75$.

Quite a similar variation for the time evolution of O_2 mass fractions obtained from the same three surface sections can also be observed from Figure 5.32.

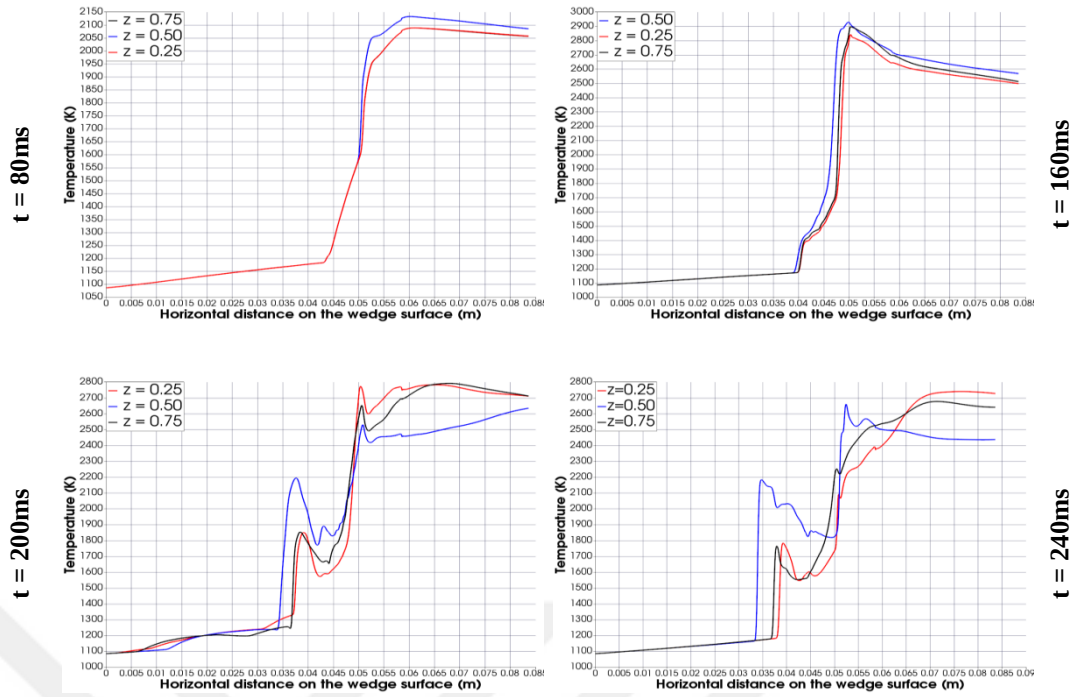


Figure 5.31 : Time marching of vibrational temperature of N_2 molecules obtained from $30^\circ\text{-}55^\circ$, 3-D wedge surface at three different sections ($z = 0.25$, $z = 0.5$ and $z = 0.75$) for thermally non-equilibrium reacting flow.

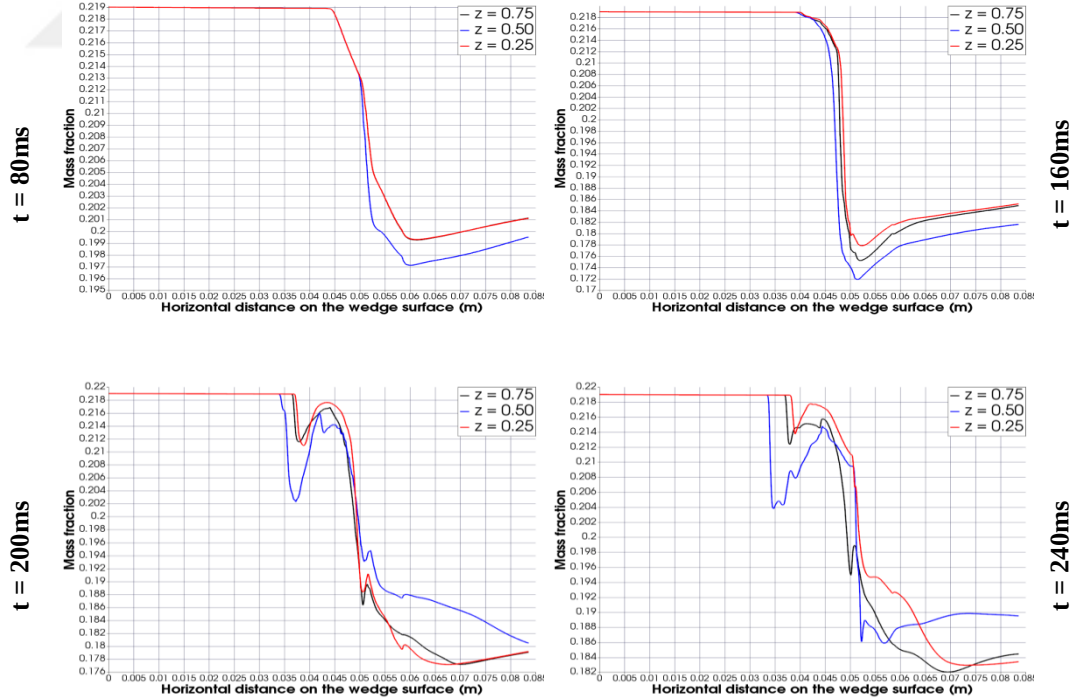


Figure 5.32 : Time marching of O_2 mass fraction obtained from $30^\circ\text{-}55^\circ$, 3-D wedge surface at three different sections ($z = 0.25$, $z = 0.5$ and $z = 0.75$) for thermally non-equilibrium reacting flow.

5.5.6 Distributions on the 3-D wedge surface

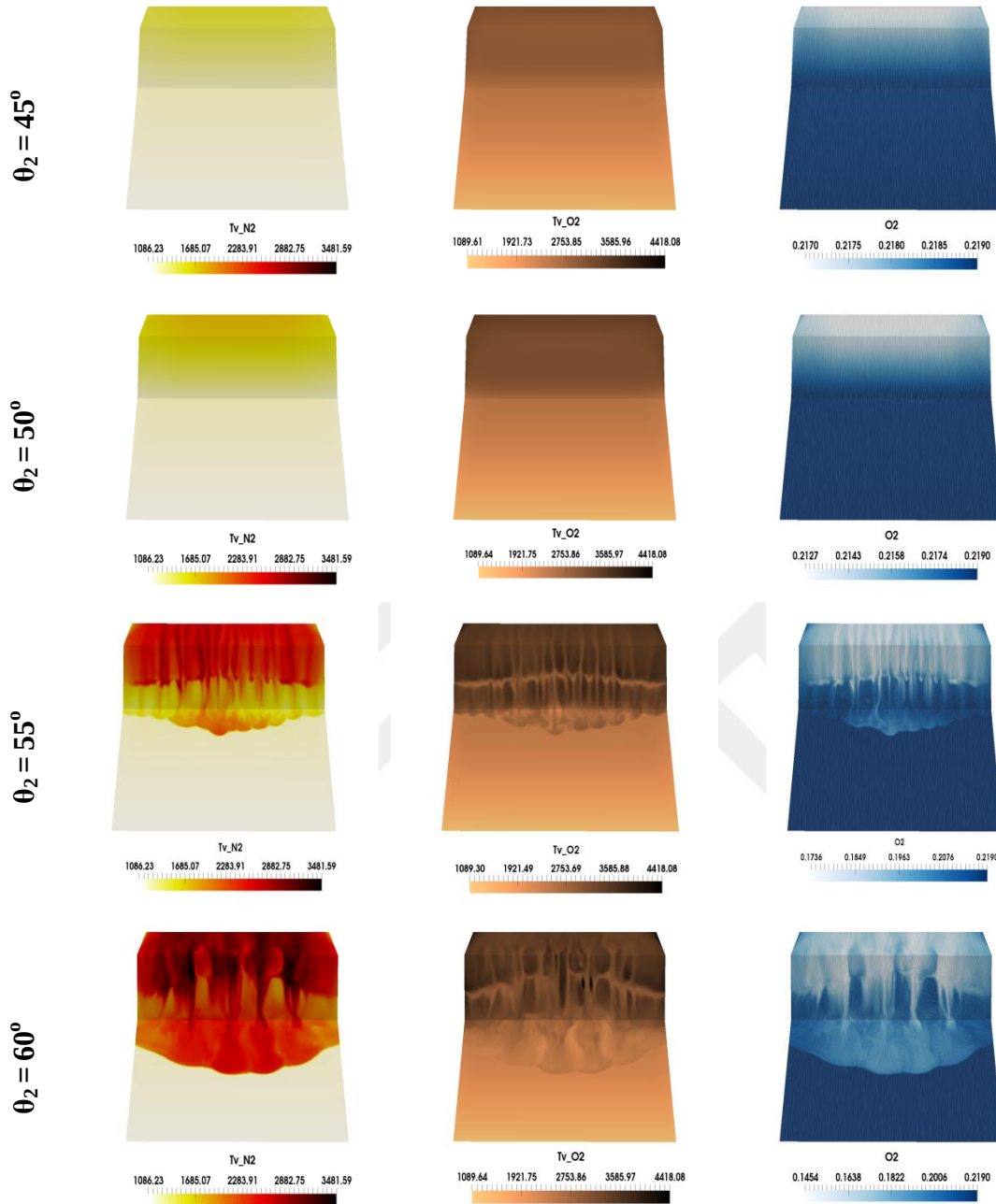


Figure 5.33 : Surface distributions of Tv_{N_2} , Tv_{O_2} and O_2 mass fraction on the 3-D double wedge for four different aft angles.

Vibrational temperature distributions of N_2 and O_2 molecules, in addition to O_2 mass fraction distributions are compared for four different θ_2 values as illustrated in Figure 5.33. It is clear that the surface distributions of these parameters share many similarities with the shock structures investigated earlier. In compatible with the distributions obtained in the previous figures, 30° - 45° double wedge has a uniform

vibrational temperature distribution in the spanwise direction. As the second angle increases, we see that the effective area of which the vibrational excitations influence becomes larger over the 3-D wedge. It is observed that even though there is a leading edge shock over the first surface, the equilibrium temperature is mostly disrupted after another shock, when the flow passes through SL over the surface. We see that for all angles, the dissociation rate of oxygen gas reaches its maximum after the flow passes through RL. The maximum dissociation of oxygen in terms of mass fraction is computed to be 0.002 for $\theta_2 = 45^\circ$ while this ratio goes up to as much as 0.0736 for $\theta_2 = 60^\circ$.





6. CONCLUSIONS

Within the scope of this study, a hypersonic solver was developed by blending two standard OpenFOAM solvers, *rhoCentralFoam* and *reactingFoam*. Reacting and non-reacting validation studies of the newly-developed code, *hyperReactingFoam*, were conducted on heat bath, blunted cone and double cone models. The results of validation tests showed a good agreement both for thermally equilibrium and non-equilibrium flows.

Thermally equilibrium and non-equilibrium analyses were performed on both 2-D and 3-D double wedge models for four distinct aft angles. Shock structures obtained from numerical Schlieren images showed that the interactions become stronger as the second angle of the wedge is systematically increased. The increase in the aft angle directly influenced the reaction rates, thermal equilibrium nature of the flow, pressure and wall heat flux distributions on the wedge surface. The differences between 2-D and 3-D analyses as well as the differences between thermal equilibrium and non-equilibrium solutions were reported in the relevant sections. Three-dimensionality of the flow was clearly observable from the spanwise variations of the flow parameters. The surface heat flux comparison with other numerical studies and the experiment presented a reasonable accuracy, even though there are significant deviations between all of the numerical studies and the experiment.

In future works, the same solver will also analyze the double cone model for different aft angles. The capability of the solver is to be extended to include rarefied regions for higher Kn numbers. The electronic states and ionization physics of high speed flows might also be included into the solver. A hybrid solver can be developed by coupling CFD and DSMC techniques in order to analyze the continuum – transition flow regime.



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APPENDICES

APPENDIX A: Reaction list



APPENDIX A

Table A.1 : Thermo-chemistry model for the reacting air

Index	Reaction	A $\text{m}^3 \text{kmol}^{-1} \text{s}^{-1}$	β -	T_a K
1	$\text{O}_2 + \text{N}_2 \rightarrow 2\text{O} + \text{N}_2$	7.829e16	-1.0	59370.6
2	$\text{O}_2 + \text{N} \rightarrow 2\text{O} + \text{N}$	6.624e16	-1.0	59370.6
3	$\text{O}_2 + \text{NO} \rightarrow 2\text{O} + \text{NO}$	6.624e16	-1.0	59370.6
4	$\text{O}_2 + \text{O}_2 \rightarrow 2\text{O} + \text{O}_2$	3.210e16	-1.0	59370.6
5	$\text{O}_2 + \text{O} \rightarrow 2\text{O} + \text{O}$	9.033e16	-1.05	59370.6
6	$\text{N}_2 + \text{O} \rightarrow 2\text{N} + \text{O}$	2.409e15	-0.54	113497.4
7	$\text{N}_2 + \text{O}_2 \rightarrow 2\text{N} + \text{O}_2$	9.033e15	-0.68	113497.4
8	$\text{N}_2 + \text{NO} \rightarrow 2\text{N} + \text{NO}$	9.033e15	-0.68	113497.4
9	$\text{N}_2 + \text{N}_2 \rightarrow 2\text{N} + \text{N}_2$	2.469e15	-0.62	113497.4
10	$\text{N}_2 + \text{N} \rightarrow 2\text{N} + \text{N}$	6.022e15	-0.68	113497.4
11	$\text{NO} + \text{N}_2 \rightarrow \text{N} + \text{O} + \text{N}_2$	1.265e17	-1.0	75544.2
12	$\text{NO} + \text{O}_2 \rightarrow \text{N} + \text{O} + \text{O}_2$	1.204e17	-1.0	75544.2
13	$\text{NO} + \text{NO} \rightarrow \text{N} + \text{O} + \text{NO}$	6.022e16	-1.0	75544.2
14	$\text{NO} + \text{O} \rightarrow \text{N} + 2\text{O}$	2.409e17	-1.1	75544.2
15	$\text{NO} + \text{N} \rightarrow \text{O} + 2\text{N}$	2.409e17	-1.1	75544.2
16	$\text{NO} + \text{O} \rightarrow \text{O}_2 + \text{N}$	1.385e8	0.5	19693.6
17	$\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N}$	4.818e10	0.0	37482.4
18	$\text{O}_2 + \text{N} \rightarrow \text{NO} + \text{O}$	2.409e12	-0.39	1448.6
19	$\text{NO} + \text{N} \rightarrow \text{N}_2 + \text{O}$	3.011e11	-0.35	1448.6

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