



Week 8

Thesis Study Report

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10 April 2025

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Legend	
	Not Started
	Currently
	Completed
	Incompleted within time limits

1. Current Timeline

Sub Task Description	Week 1	Week 2	Week 3	Week 4	Week 5	Week 6	Week 7	Week 8	Week 9
Overall literature study for relevant open source for hy2Foam									
Selection and compilation of the relevant open source hy2Foam									
Overall literature study for relevant open source Eilmer									
Selection and compilation of the relevant open source Eilmer									
Overall literature study for relevant open source SU2-NEMO									
Selection and compilation of the relevant open source SU2-NEMO									
Test Case Simulations for hy2Foam, Eilmer, SU2-NEMO									
Examination of implementation of chemical reactions within the relevant solvers									

2. Introduction

In the current study, main goal is:

- Developing transient, compressible, two-temperature, 3D, Implicit semi-coupled, thermochemical non-equilibrium hypersonic CFD solver
- Continuum assumption should hold for the flows that the developed solver can solve ($Kn_{max} < 1$).

Main goal is divided into smaller tasks. For the semester, study milestones are:

- Studying literature of three selected non-equilibrium hypersonic CFD solvers
- Running tutorial cases in selected CFD solvers
- Examining implementation of governing equations and chemistry models in the selected CFD solvers

3. Overall Literature Review

REVIEW

Open Access

A review of the mathematical modeling of equilibrium and nonequilibrium hypersonic flows



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Abstract

This paper systematically reviews the mathematical modeling based on the computational fluid dynamics (CFD) method of equilibrium and nonequilibrium hypersonic flows. First, some physicochemical phenomena in hypersonic flows (e.g., vibrational energy excitation and chemical reactions) and the flow characteristics at various altitudes (e.g., thermochemical equilibrium, chemical nonequilibrium, and thermochemical nonequilibrium) are reviewed. Second, the judgment rules of whether the CFD method can be applied to hypersonic flows are summarized for accurate numerical calculations. This study focuses on the related numerical models and calculation processes of the CFD method in a thermochemical equilibrium flow and two nonequilibrium flows. For the thermochemical equilibrium flow, the governing equations, chemical composition calculation methods, and related research on the thermodynamic and transport properties of air are reviewed. For the nonequilibrium flows, the governing equations that include one-, two-, and three-temperature models are reviewed. The one-temperature model is applied to a chemical nonequilibrium flow, whereas the two- and three-temperature models are applied to a thermochemical nonequilibrium flow. The associated calculations and numerical models of the thermodynamic and transport properties, chemical reaction sources, and energy transfers between different energy modes of the three models are presented in detail. Finally, the corresponding numerical models of two special wall boundary conditions commonly used in hypersonic flows (i.e., slip boundary conditions and catalytic walls) and related research, are reviewed.

Keywords: Mathematical modeling, Hypersonic flows, Chemical nonequilibrium flow, Thermochemical nonequilibrium flow, Thermochemical equilibrium flow

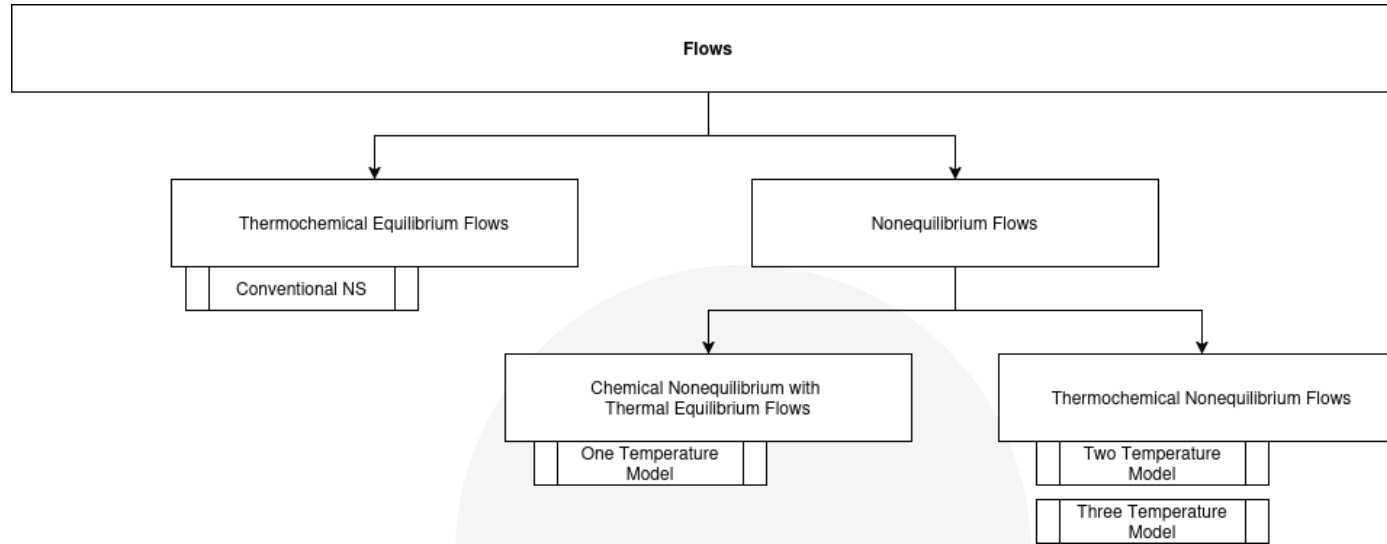
3. Overall Literature Review

Literature review and subsequent study of the literature is limited to solvers that are capable of:

- Solving compressible hypersonic flow
- Solving thermochemical non-equilibrium flow
- Employing two-temperature model

Main development platform is OpenFOAM, therefore two of the selected solvers are implemented within OpenFOAM framework. Also, outside of the hypersonic solvers, in order to understand and implement chemical reaction modeling, *reactingFoam* will be studied extensively.

3.1. Flow Types



Reacting flows can be separated into two main camp:

- 1) Equilibrium Flows: Internal energy modes are not considered and chemical reactions are independent of time, only depending pressure and temperature.
- 2) Non-equilibrium Flows: Flow is rarefied enough that internal energy modes are taken into account and chemical reactions cannot happen fast enough, so they must be modeled as time-dependent.

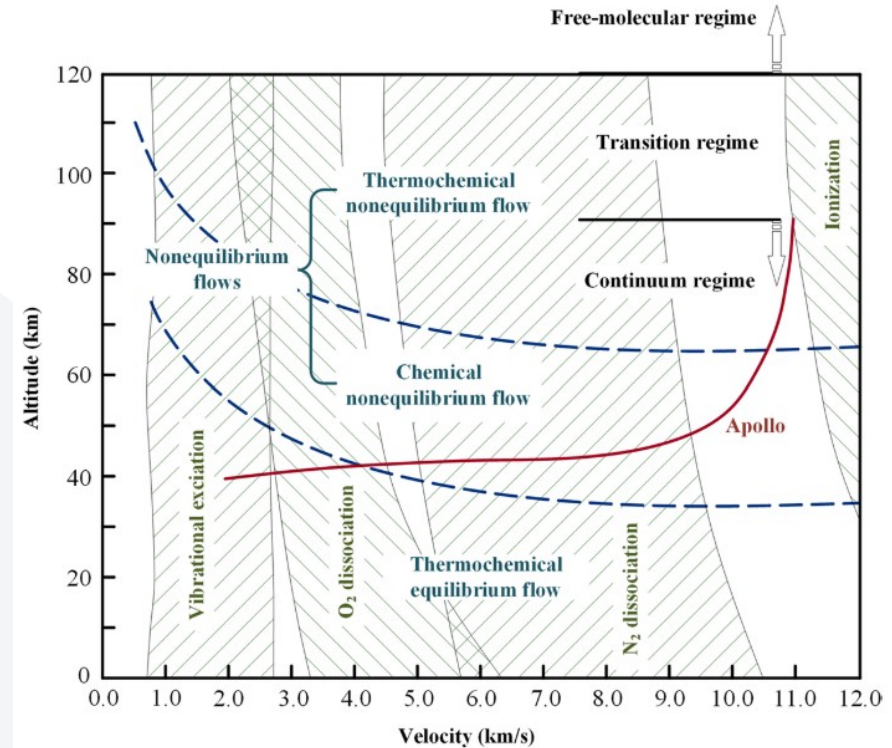
3.2. Equilibrium Term

Equilibrium: A system is in equilibrium when its macroscopic properties no longer change with time.

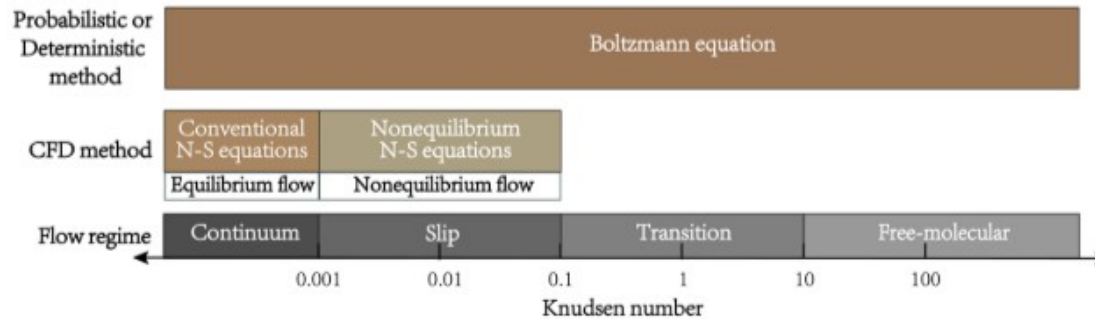
Relaxation: Physical relaxation refers to the process by which a system evolves toward equilibrium after being disturbed from its initial state.

Thus, a system is in non-equilibrium state if characteristic flow time is longer than relaxation times of the chemical reactions or internal energy modes.

$$\tau_{chemical} < \tau_{tr} < \tau_r < \tau_{vib}$$



3.3. Rarefaction Degree



Since rarefaction of a gas influences the characteristic flow time, that is mean collision time between fluid molecules, equilibrium of the flow is directly related to the rarefaction degree of the flow.

After 0.001 Kn, flow cannot be solved with conventional Navier-Stokes equations because heat transfer model of Fourier equation does not reflect the reality of the flow. According to non-equilibrium degree of the flow, chemical non-equilibrium and/or thermal non-equilibrium must be modelled with the governing equations using **two- or three-temperature** models which are collectively named as **non-equilibrium Navier-Stokes equations**.

4. Governing Equations

According to chemical equilibrium state of the flow, two sets of governing equations can be employed:

1. Conventional Navier-Stokes Equations
2. Non-equilibrium Navier-Stokes Equations

According to thermal equilibrium state of the flow, three different models of non-equilibrium Navier-Stokes equations can be employed:

1. One-temperature Model for thermal equilibrium flow
2. Two-temperatures Model for translational-rotational and vibrational-electronic coupling terms
3. Three-temperatures Model for translational-rotational, vibrational, and electronic terms

In the non-equilibrium flow models, there are several additional terms which are needed to be addressed with additional equations and empirical data. Limitations of these equations and limit conditions of the empirical data determines what are the extreme conditions that can be employed for the non-equilibrium flow models.

4.1. Conventional N-S Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (2)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} + \frac{\partial(p \delta_{ij})}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \quad (3)$$

$$\frac{\partial E}{\partial t} + \frac{\partial((E + p)u_j)}{\partial x_j} + \frac{\partial(\tau_{ij} u_i)}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = 0 \quad (4)$$

Conventional Navier-Stokes Equations:

(2) Continuity Equation

(3) Momentum Transportation Equation

(4) Energy Transportation Equation

Flows that are in the thermochemical equilibrium state can be handled by conventional Navier-Stokes equations.

$i (-)$	=	equation number
$j (-)$	=	variable number
$\rho (kg/m^3)$	=	density
$t (s)$	=	time
$u (m/s)$	=	velocity vector
$p (Pa)$	=	pressure
$\tau (Pa)$	=	shear stress tensor
$E (kg/(m \cdot s^2))$	=	total energy per unit volume
$q (W/m \cdot K)$	=	heat conduction vector
$\delta_{ij}(-)$	=	Kronecker Delta

4.2. Non-eq. N-S Equations

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_j + J_{s,j}) = \dot{w}_s \quad (5)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + p \delta_{ij} - \tau_{ij}) = 0 \quad (6)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left((E + p) u_j - \tau_{ij} u_i + q_j + \sum_{s=1}^{ns} J_{s,j} h_s \right) = 0 \quad (7)$$

$$\frac{\partial E_{ve}}{\partial t} + \frac{\partial}{\partial x_j} \left(E_{ve} u_j + q_{ve,j} + \sum_{s=1}^{ns} J_{s,j} h_{ve,s} \right) + p_e \frac{\partial u_j}{\partial x_j} = Q_{ve} \quad (8)$$

$$\frac{\partial E_v}{\partial t} + \frac{\partial}{\partial x_j} \left(E_v u_j + q_{v,j} + \sum_{s=1}^{ns} J_{s,j} h_{v,s} \right) = Q_v \quad (9)$$

$$\frac{\partial E_e}{\partial t} + \frac{\partial}{\partial x_j} \left((E_e + p_e) u_j + q_{e,j} + \sum_{s=1}^{ns} J_{s,j} h_{e,s} \right) - u_j \frac{\partial p_e}{\partial x_j} = Q_e \quad (10)$$

$i (-)$	= equation number
$j (-)$	= variable number
$e (-)$	= electronic
$v (-)$	= vibrational
$ve (-)$	= vibrational-electronic
$s (-)$	= specie
$\rho (kg/m^3)$	= density
$t (s)$	= time
$u (m/s)$	= velocity vector
$p (Pa)$	= pressure
$\tau (Pa)$	= shear stress tensor
$E (kg/(m^2 \cdot s^2))$	= total energy per unit volume
$q (W/m \cdot K)$	= heat conduction vector
$\delta_{ij} (-)$	= Kronecker delta
$\dot{w}_s (kg/(m^3 \cdot s))$	= chemical source
$J_{s,j} (mol/(m^2 \cdot s))$	= diffusion term
$h_s (kg/(m^2 \cdot s^2))$	= enthalpy of specie
$Q (kg/(m^3 \cdot s))$	= energy source

Non-equilibrium Navier-Stokes Equations:

(5) Specie Continuity Equation

(6) Momentum Transportation Equation

(7) Energy Transportation Equation

(8) Vibrational-Electronic Energy Transportation Equation

(9) Vibrational Energy Transportation Equation

(10) Electronic Energy Transportation Equation

One Temp. Model: (5)-(6)-(7)

Two Temp. Model: (5)-(6)-(7)-(8)

Three Temp. Model: (5)-(6)-(7)-(9)-(10)

We are going to employ (5)-(6)-(7)-(9), which is three-temp. model without electronic terms and equations because we will not deal with ions and electrons.

4.2. Non-eq. N-S Equations

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho_s u_j + J_{s,j}) = \dot{w}_s \quad (5)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + p \delta_{ij} - \tau_{ij}) = 0 \quad (6)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left((E + p) u_j - \tau_{ij} u_i + q_j + \sum_{s=1}^{ns} J_{s,j} h_s \right) = 0 \quad (7)$$

$$\frac{\partial E_{ve}}{\partial t} + \frac{\partial}{\partial x_j} \left(E_{ve} u_j + q_{ve,j} + \sum_{s=1}^{ns} J_{s,j} h_{ve,s} \right) + p_e \frac{\partial u_j}{\partial x_j} = Q_{ve} \quad (8)$$

$$\frac{\partial E_v}{\partial t} + \frac{\partial}{\partial x_j} \left(E_v u_j + q_{v,j} + \sum_{s=1}^{ns} J_{s,j} h_{v,s} \right) = Q_v \quad (9)$$

$$\frac{\partial E_e}{\partial t} + \frac{\partial}{\partial x_j} \left((E_e + p_e) u_j + q_{e,j} + \sum_{s=1}^{ns} J_{s,j} h_{e,s} \right) - u_j \frac{\partial p_e}{\partial x_j} = Q_e \quad (10)$$

Colored terms are the additional terms that must be dealt with additional equations and models where

- 1) ρ_s : Specie Density
- 2) $J_{j,s}$: Mass Diffusion
- 3) \dot{w}_s : Chemical Source Term
- 4) $\sum_{s=1}^{ns} J_{s,j} h_s$: Energy Change by Diffusion
- 5) E_v : Vibrational Energy
- 6) Q_v : Vibrational Energy Source Term

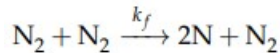
4.2.1. Chemical Source Term

$$\dot{\omega}_s = M_s \sum_{r_1}^{NR} (v''_{s,r} - v'_{s,r}) \left[k_{f,r} \prod_{n=1}^{NS} \left(\frac{\rho_n}{M_n} \right)^{v'_{n,r}} - k_{b,r} \prod_{n=1}^{NS} \left(\frac{\rho_n}{M_n} \right)^{v''_{n,r}} \right] \quad \text{where} \quad k_f = A_f \times T_{c,f}^{B_f} \exp\left(-\frac{T_a}{T_{c,f}}\right) \quad \text{and} \quad k_b = \frac{k_f}{K_{eq}}$$

For equilibrium constant calculation, Park and Gupta proposed two models:

according to Park: $K_{eq} = \exp(A_1/Z + A_2 + A_3 \ln Z + A_4 Z + A_5 Z^2)$ $Z = 10^4/T$

according to Gupta: $K_{eq} = \exp(A_1 Z^5 + A_2 Z^4 + A_3 Z^3 + A_4 Z^2 + A_5 Z + A_6)$ $Z = 10^4/T$



Reaction Rate	Arrhenius Law Constants		
	A	β	T_a
Park 1993	7.0×10^{21}	-1.6	113,200
QK	2.47×10^{18}	-0.62	113,500

Algorithm 1 Chemical Source Term Calculation Algorithm

- 1: Select reaction
- 2: Select chemistry model for reaction rate coefficients A_f, B_f, T_a (Park93, QK, Gupta)
- 3: Calculate controlling temperature $T_{c,f}$
- 4: Calculate forward reaction rate k_f using Eq. (14)
- 5: Calculate equilibrium constant K_{eq}
 - 5.1 Select necessary coefficients and model from reference works (Park, Gupta)
 - 5.2 Calculate equilibrium constant K_{eq} using Eq. (17)
- 6: Calculate backward reaction rate k_b using Eq. (16)
- 7: Calculate species chemical source term
 - 7.1 Select density (ρ_s) and molecular weight (M_s)
 - 7.2 Select product stoichiometric ($v''_{s,r}$) and reactant stoichiometric ($v'_{s,r}$) coefficients according to selected reaction
 - 7.3 Calculate final value using Eq. (13)

4.2.2. Mass Diffusion Term

1) Fick's Diffusion Model:

$$J_{s \neq e, j} = -\rho D_s \frac{\partial Y_s}{\partial x_j} \quad \text{and} \quad J_{e, j} = -\frac{1}{q_e} \sum_{s \neq e} q_s J_{s, j} \quad \text{where} \quad D_s = D = \frac{\kappa Le}{\rho C_p} \quad \text{or} \quad D_s = D = \frac{\kappa_{tr} Le}{\rho C_p}$$

Lewis Number is taken as 1.4

2) Modified Fick's Diffusion Model:

$$J_{s \neq e, j} = -\rho D_s \frac{\partial Y_s}{\partial x_j} - Y_s \sum_{r \neq e} \left(-\rho D_r \frac{\partial Y_r}{\partial x_j} \right) \quad \text{where} \quad D_s = D = \frac{\kappa Le}{\rho C_p} \quad \text{or} \quad D_s = D = \frac{\kappa_{tr} Le}{\rho C_p}$$

Lewis Number is taken as 1.4

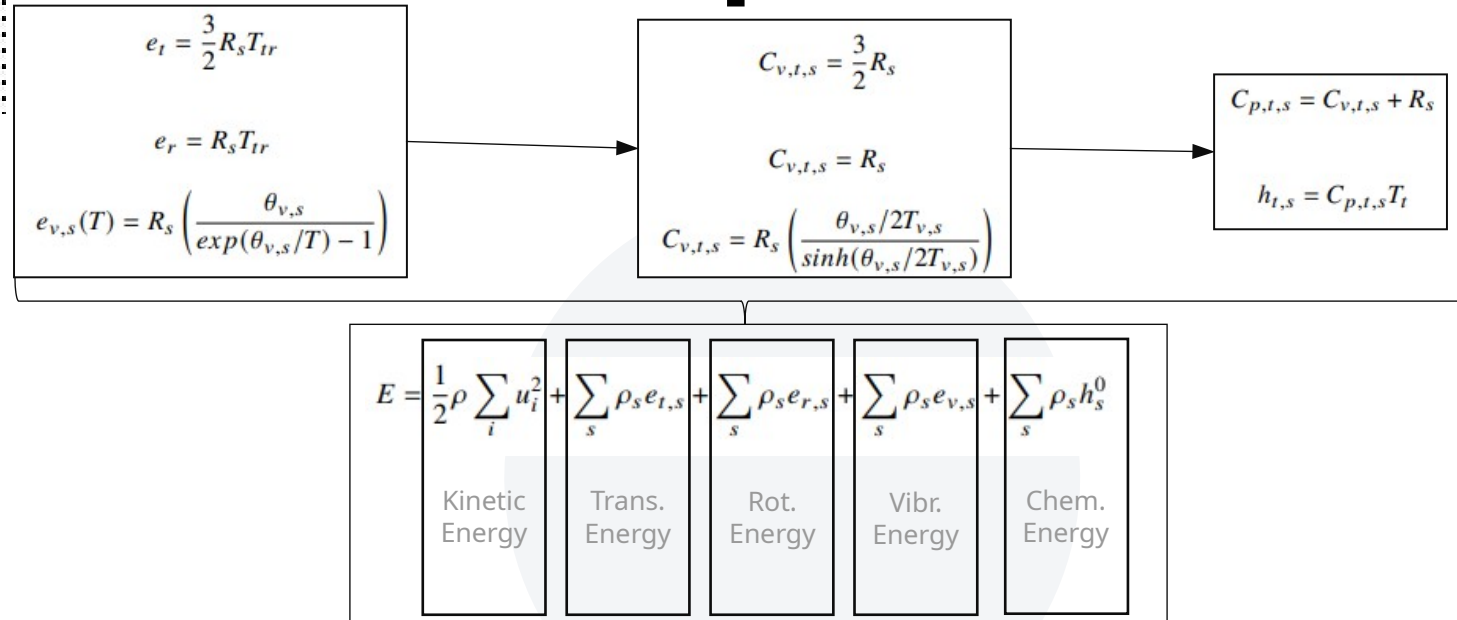
3) Stefan-Maxwell Diffusion Model:

$$J_{s, j} = -\rho D_s \frac{\partial Y_s}{\partial x_j} + \frac{Y_s}{(1 - X_s)} D_s \sum_{r \neq s} \left(\rho \frac{M}{M_r} \frac{\partial Y_r}{\partial x_j} + \frac{M}{M_r} \frac{J_r}{D_{s, r}} \right) \quad \text{where} \quad D_s = D = \frac{\kappa Le}{\rho C_p} \quad \text{or} \quad D_s = D = \frac{\kappa_{tr} Le}{\rho C_p}$$

Lewis Number is taken as 1.4

Thermal conductivity and special heat coefficient under constant pressure are calculated in thermodynamical and transport properties section.

4.2.3. Thermodynamic Properties



Energy of a mixture can be written as the sum of the different energy modes. In order to calculate these energy types, energy of each specie is calculated and added to total.

4.2.4. Transport Properties

Viscosity

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

according to Blottner:

$$\mu_s = 0.1 \times \exp((A_B \ln(T) + B_B) \ln(T) + C_B)$$

according to Gupta:

$$\mu_s = 0.1 \times [\exp(C_G)] T^{A_G \ln(T) + B_G}$$

Viscosity is calculated by curve-fitting formulas Blottner and Gupta gives. Reason for that approach is that curve-fitting is applied to experimental data and more accurate than theoretical models.

Thermal Conductivity

One-temperature model Fourier Eq. : $q_j = -(\kappa_t + \kappa_r + \kappa_v) \frac{\partial T}{\partial x_j} = -\kappa \frac{\partial T}{\partial x_j}$

Two-temperature model Fourier Eq. : $q_j = -(\kappa_t + \kappa_r) \frac{\partial T_{tr}}{\partial x_j} - \kappa_v \frac{\partial T_v}{\partial x_j} = -\kappa_{tr} \frac{\partial T_{tr}}{\partial x_j} - \kappa_v \frac{\partial T_v}{\partial x_j}$

$$\kappa_{tr} = \mu_s \left(\frac{5}{2} c_{v,t,s} + c_{v,r,s} \right) \quad \kappa_v = \eta_v \mu_s \quad , \quad \eta_v = 1.2$$

For the calculation of the heat conduction, Fourier equation is employed.

Thermal conductivity is calculated by Eucken's relationship as given above. Limit of this relationship is around 6000 K, after 6000 K relationship breaks down.

4.2.5. Mixing Rule

$$Q = \sum_s \frac{Q_s X_s}{\phi_s} \quad \leftarrow \quad \phi_s = X_s + \sum_{r \neq s} X_r \left[1 + \sqrt{\frac{\mu_s}{\mu_r}} \left(\frac{M_r}{M_s} \right)^{1/4} \right]^2 \left[\sqrt{8 \left(1 + \frac{M_s}{M_r} \right)} \right]^{-1}$$

where

Q is the quantity that belongs to the mixture

Q_s is the specie quantity,

X_s is the mass fraction,

ϕ_s is the scaling factor

Wilke's mixing rule is applied with the goal of determining mixture properties from the specie properties that belongs to the mixture.

It should be noted that Wilke's mixing rule is only applicable below 10000 K and is only valid for neutral gases.

4.2.6. Energy Source Terms

$$Q_V = \sum_{s=mol.} Q_{s,V-T} + \sum_{s=mol.} Q_{s,V-V} + \sum_{s=mol.} Q_{s,C-V}$$

Vibrational-Translational
Energy Source Term

- Millikan-White-Park Relaxation with classical/modified Landau-Teller formulation is employed for each specie.

Vibrational-Vibrational Energy
Source Term

- Knab's vibrational-vibrational energy transfer formulation is employed for each specie.

Chemical-Vibrational Energy
Source Term

- ParkTTv model is employed for each reaction.

There are more than one model for each energy mode, however simplicity and robustness is taken into the account.

4.2.6. Energy Source Terms

Classical Landau-Teller

$$Q_{s,V-T} = \rho_s \frac{e_{v,s}(T_t) - e_{v,s}(T_v)}{\tau_{s,V-T}} = \rho_s \frac{C_{V,v,s}(T_t - T_v)}{\tau_{s,V-T}}$$

Modified Landau-Teller

$$Q_{s,V-T} = \frac{T_t}{T_v} (T_t - T_v) \frac{C_{V,v,s} \rho_s}{\tau_{s,V-T}}$$

Relaxation time of the vibrational-translational energy mode $\tau_{s,V-T}$

$$\tau_{s,V-T} = \frac{\sum_{r=mol} X_r}{\sum_{r=mol} \frac{X_r}{\tau_{s-r,V-T}}}$$

Vibrational-translational relaxation time between species s and r $\tau_{s-r,V-T}$

$$\tau_{s-r,V-T} = \tau_{s-r,V-T}^{MW} + \tau_{s-r,V-T}^P$$

Millikan-White vibrational-translational relaxation time $\tau_{s-r,V-T}^{MW}$:

$$\tau_{s-r,V-T}^{MW} = \frac{1}{p} \exp \left[A_{s,r} \left(T_{tr}^{-1/3} - B_{s,r} \right) - 18.42 \right]$$

where

$$A_{s,r} = 1.16 \times 10^{-9/2} \sqrt{\frac{M_s M_r}{M_s + M_r}} \theta_{v,s}^{4/3}, \quad B_{s,r} = 0.015 \times 10^{-3/4} \left(\frac{M_s M_r}{M_s + M_r} \right)^{1/4},$$

$$\sigma_{v,s} = \sigma'_{v,s} \left(\frac{50000}{T} \right)^2$$

where $\sigma'_{v,s}$ is typically given as $3 \times 10^{-21} \text{ m}^2$ for N_2 , O_2 , and NO .

Park correction for vibrational-translational relaxation time

$$\tau_{s-r,V-T}^P = \frac{1}{\bar{c}_s \sigma_{v,s} n_{s,r}} \quad \bar{c}_s = \sqrt{\frac{8RT}{\pi M_s}}$$

Calculation
Sequence

4.2.6. Energy Source Terms

Knab V-V Formula

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

where

$$e_{v,s}(T) = R_s \left(\frac{\theta_{v,s}}{\exp(\theta_{v,s}/T) - 1} \right)$$

Park TTV Model

$$Q_{s,C-V} = \dot{w}_s \tilde{D}_s$$

where

$$\tilde{D}_s = \alpha_s \epsilon_{d,s}$$

Species s	\mathcal{M}_s (g·m ⁻³)	h_s° (J·kg ⁻¹)	$\theta_{v,s}$ (K)	D_s (J·kg ⁻¹)
N ₂	28.0134	0	3,371	3.36×10^7
O ₂	31.9988	0	2,256	1.54×10^7
NO	30.0061	3.04×10^6	2,719	2.09×10^7
N	14.0067	3.37×10^7	-	-
O	15.9994	1.56×10^7	-	-

where $\epsilon_{d,s}$ is the dissociation energy/potential of molecule s , and α_s is a constant typically set as 0.3.

4.2.6. Energy Source Terms

Algorithm 2 Vibrational Energy Source Term Calculation Algorithm

- 1: Calculate vibrational-translational energy source term Q_{V-T}
 - 1.1 Calculate Millikan-White coefficients $A_{s,r}$ and $B_{s,r}$ by Eqs. (54) - (56)
 - 1.2 Calculate Millikan-White relaxation time $\tau_{s-r,V-T}^{MW}$ by Eq. (53)
 - 1.3 Calculate average molecular speed \bar{c}_s by Eq. (58)
 - 1.4 Calculate limited collision cross-section $\sigma_{v,s}$ by Eq. (56)
 - 1.5 Calculate number density of the collision pair n_{s-r}
 - 1.6 Calculate Park relaxation time $\tau_{s-r,V-T}^P$ by Eq. (57)
 - 1.7 Calculate total relaxation time $\tau_{s-r,V-T}$ by Eq. (52)
 - 1.8 Calculate average relaxation time $\tau_{s,V-T}$ by Eq. (51)
 - 1.9 Calculate vibrational-translational energy exchange $Q_{s,V-T}$ by Eq. (49) or by Eq. (50)
 - 2: Calculate chemical-vibrational energy source term Q_{C-V} by Eq. (59)
 - 2.1 Find chemical source term \dot{w}_s using Algorithm 1.
 - 2.2 Find dissociation energy D_s for specie s
 - 2.3 Calculate coefficient D'_s
 - 2.4 Calculate chemical-vibrational energy source term $Q_{s,C-V}$
 - 3: Calculate vibrational-vibrational energy source term Q_{V-V} by Eq. (61)
 - 3.1 Find M_s, ρ_s, ρ_n given $n \neq s$
 - 3.2 Calculate internal vibrational energy of specie s with T_{tr} using Eq. (27)
 - 3.3 Calculate internal vibrational energy of specie s with T_v using Eq. (27)
 - 3.4 Calculate internal vibrational energy of specie $n \neq s$ with T_{tr} using Eq. (27)
 - 3.5 Calculate internal vibrational energy of specie $n \neq s$ with T_v using Eq. (27)
 - 3.6 Calculate vibrational-vibrational energy source term $Q_{s,V-V}$
 - 4: Calculate total vibrational energy source term Q_V by Eq. (33)
-

5. Selected Solvers

01

hy2Foam 

It is most commonly reviewed solver in this list. Navier-Stokes-Fourier equations are solved within OpenFOAM framework. Two-temperature model is employed.

03

SU2-Nemo 

It is the hypersonic and non-equilibrium solver of the SU2 framework. Two-temperature model is also employed.

02

Eilmer

It is selected for organized and easier to understand implementation. Navier-Stokes-Fourier equations are solved. Two-temperature model is employed.

04

hyperReactingFoam 

It has extensive documentation about implementation within OpenFOAM framework. After general literature review, this solver will be main focus.

5.1. hy2Foam

hy2Foam(**H**ypersonic flow with **2**-temperature model) is a two-temperature CFD solver which can handle 11 species air-mixture model.

Article

A Two-Temperature Open-Source CFD Model for Hypersonic Reacting Flows, Part One: Zero-Dimensional Analysis[†]

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[†] This paper is an extended version of our paper published in Casseau, V.; Scanlon, T.J.; Brown, R.E. Development of a two-temperature open-source CFD model for hypersonic reacting flows. In Proceedings of the 20th AIAA International Space Planes and Hypersonic Systems and Technologies Conference, Glasgow, UK, 6–9 July 2015.

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Academic Editors: Konstantinos Kontis and Mário M. G. Costa

Received: 2 August 2016; Accepted: 29 September 2016; Published: 18 October 2016

Abstract: A two-temperature CFD (computational fluid dynamics) solver is a prerequisite to any spacecraft re-entry numerical study that aims at producing results with a satisfactory level of accuracy within realistic timescales. In this respect, a new two-temperature CFD solver, *hy2Foam*, has been developed within the framework of the open-source CFD platform OpenFOAM for the prediction of hypersonic reacting flows. This solver makes the distinct juncture between the trans-rotational and multiple vibrational-electronic temperatures. *hy2Foam* has the capability to model vibrational-translational and vibrational-vibrational energy exchanges in an eleven-species air mixture. It makes use of either the Park TTV model or the coupled vibration-dissociation-vibration (CVDV) model to handle chemistry-vibration coupling and it can simulate flows with or without electronic energy. Verification of the code for various zero-dimensional adiabatic heat baths of progressive complexity has been carried out. *hy2Foam* has been shown to produce results in good agreement with those given by the CFD code LeMANS (The Michigan Aerothermodynamic Navier-Stokes solver) and previously published data. A comparison is also performed with the open-source DSMC (direct simulation Monte Carlo) code *dmcrFoam*. It has been demonstrated that the use of the CVDV model and rates derived from Quantum-Kinetic theory promote a satisfactory consistency between the CFD and DSMC chemistry modules.

Keywords: hypersonics; computational fluid dynamics; two-temperature solver; OpenFOAM; verification; direct simulation Monte Carlo

1. Introduction

The study of high-speed vehicles re-entering the Earth's atmosphere is of current interest as witnessed by the ongoing tests on the Orion capsule (see Figure 1a) [1,2]. Access to space continues to be a challenging area with significant economic and scientific implications in the near-future for the leading countries. Mastering the art of the high-speed regime is not solely limited to space missions though and new prospects may emerge such as those related to hypersonic civilian transportation. This future vision of air-space transportation is embodied by vehicles, such as the cFASTT-1 [3] shown

Article

A Two-Temperature Open-Source CFD Model for Hypersonic Reacting Flows, Part Two: Multi-Dimensional Analysis[†]

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[†] This paper is an extended version of our paper published in Casseau, V.; Scanlon, T.J.; John, B.; Emerson, D.R.; Brown, R.E. Hypersonic simulations using open-source CFD and DSMC solvers. In *DSMC and Related Simulations*, Proceedings of the 30th International Symposium on Rarefied Gas Dynamics, Victoria, BC, Canada, 10–15 July 2016; Ketsdever, A.; Struchtrup, H., Eds.; AIP Publishing, Melville, NY, USA; Volume 1786, 050006.

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Academic Editors: Konstantinos Kontis and Mário M. G. Costa

Received: 30 September 2016; Accepted: 8 December 2016; Published: 14 December 2016

Abstract: *hy2Foam* is a newly-coded open-source two-temperature computational fluid dynamics (CFD) solver that has previously been validated for zero-dimensional test cases. It aims at (1) giving open-source access to a state-of-the-art hypersonic CFD solver to students and researchers; and (2) providing a foundation for a future hybrid CFD-DSMC (direct simulation Monte Carlo) code within the OpenFOAM framework. This paper focuses on the multi-dimensional verification of *hy2Foam* and firstly describes the different models implemented. In conjunction with employing the coupled vibration-dissociation-vibration (CVDV) chemistry-vibration model, novel use is made of the quantum-kinetic (QK) rates in a CFD solver. *hy2Foam* has been shown to produce results in good agreement with previously published data for a Mach 11 nitrogen flow over a blunted cone and with the *dmcrFoam* code for a Mach 20 cylinder flow for a binary reacting mixture. This latter case scenario provides a useful basis for other codes to compare against.

Keywords: hypersonics; computational fluid dynamics; two-temperature solver; OpenFOAM; verification; direct simulation Monte Carlo

1. Introduction

The Knudsen number, defined as the ratio of the mean free path of the gas particles to the characteristic length of the problem, is commonly employed to gauge the degree of rarefaction of a gas. During the entry of a planetary atmosphere at hypervelocities, a craft will traverse the full range of the Knudsen number, from the free-molecular regime down to the continuum regime. Practically, this translates into the need for different numerical techniques to resolve the flow-field past such hypersonic bodies.

The direct simulation Monte Carlo (DSMC) method developed by Bird [1] is a particle-based methodology that is particularly well-suited for computing high Knudsen number flows, typically above 0.05, while the conventional computational fluid dynamics (CFD) approach that solves the Navier-Stokes-Fourier (NSF) equations is generally adopted for the lower range, below 0.005. In between lies an intermediate zone where DSMC is computationally prohibitive and where

5.1. hy2Foam

hy2Foam's general capabilities are shared below:

Framework?	OpenFOAM(C++)
Temperature Model?	One- and Two-temperatures
Reactions?	Yes
Temporal Scheme	Forward Euler(Explicit)
Rarefaction?	No, only continuum
Dimensions?	2D/3D
Mesh Structure?	Structured/Unstructured
Flux Calculation Scheme?	Central-Upwind Schemes (KT-KNP)
Turbulence Models?	SA, $k-\omega$ SST

Table 1 hy2Foam Summary

5.1.1. Governing Equations

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial (\mathcal{F}_{i,inv} - \mathcal{F}_{i,vis})}{\partial x_i} = \dot{\mathcal{W}}. \quad \text{where}$$

$$\mathcal{U} = (\rho, \rho_s, \rho u, \rho v, \rho w, E_{ve,m}, E)^T,$$

$$\mathcal{F}_{i,inv} = \begin{pmatrix} \rho u_i \\ \rho_s u_i \\ \rho u_i u + \delta_{i1} p \\ \rho u_i v + \delta_{i2} p \\ \rho u_i w + \delta_{i3} p \\ E_{ve,m} u_i \\ (E + p) u_i \end{pmatrix}, \quad \mathcal{F}_{i,vis} = \begin{pmatrix} 0 \\ -\mathcal{J}_{s,i} \\ \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ -q_{ve,i,m} - e_{ve,m} \mathcal{J}_{m,i} \\ \tau_{ij} u^j - q_{tr,i} - q_{ve,i} - \sum_{r \neq e} h_r \mathcal{J}_{r,i} \end{pmatrix}$$

Two-temperature model is given in flux-divergence form. It should be noted that mixture continuity equation is also included.

5.2. Eilmer

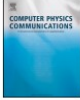

Eilmer is a general-purpose open-source compressible, hypersonic, non-equilibrium flow; two-temperature CFD solver.

Computer Physics Communications 282 (2023) 108551

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc



Eilmer: An open-source multi-physics hypersonic flow solver ☆, ☆

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ARTICLE INFO

Article history:
Received 23 May 2022
Received in revised form 10 September 2022
Accepted 19 September 2022
Available online 27 September 2022

Keywords:
Scientific computing
Computational fluid dynamics
Hypersonics
Parallel computing

ABSTRACT

This paper introduces Eilmer, a general-purpose open-source compressible flow solver developed at the University of Queensland, designed to support research calculations in hypersonics and high-speed aerothermodynamics. Eilmer has a broad userbase in several university research groups and a wide range of capabilities, which are documented on the project's website, in the accompanying reference manuals, and in an extensive catalogue of example simulations. The first part of this paper describes the formulation of the code: the equations, physical models, and numerical methods that are used in a basic fluid dynamics simulation, as well as a handful of optional multi-physics models that are commonly added on to do calculations of hypersonic flow. The second section describes the processes used to develop and maintain the code, documenting our adherence to good programming practice and endorsing certain techniques that seem to be particularly helpful for scientific codes. The final section describes a half-dozen example simulations that span the range of Eilmer's capabilities, each consisting of some sample results and a short explanation of the problem being solved, which together will hopefully assist new users in beginning to use Eilmer in their own research projects.

Program summary
Program Title: Eilmer
CPC Library link to program files: <https://doi.org/10.17632/gy2da2fyxm.1>
Developer's repository link: <https://github.com/gdtk-ua/gdtk>
Code Ocean capsule: <https://codeocean.com/capsule/7226427>
Licensing provisions: GPLv3
Programming language: D, Lua
Supplementary material: <https://gdtk.uqcloud.net>

Nature of problem: Eilmer solves the compressible Navier-Stokes equations with a particular emphasis on flows at hypersonic speeds. The code includes modelling for high-temperature gas effects such as chemical and vibrational nonequilibrium. Eilmer can be used for the simulation for unsteady and steady flows.

Solution method: The code is implemented in D [1] and built on a finite-volume formulation that is capable of solving the Navier-Stokes equations in 2D and 3D computational domains, discretised with structured or unstructured grids. Grids may be generated using a built-in parametric scripting tool or imported from commercial gridding software. The inviscid fluxes are computed using the reconstruction-evolution approach. In structured-grid mode, reconstruction stencils up to fourth-order spatial accuracy are available. In unstructured-grid mode, least-squares reconstruction provides second-order spatial accuracy. A variety of flux calculators are available in the code. Viscous fluxes are computed with compact stencils with second-order spatial accuracy. For unsteady flows, explicit time-stepping with low-order RK-family schemes are available, along with a point-implicit Backward-Euler update scheme for stiff systems of equations. For steady flows, convergence can be greatly accelerated using a Jacobian-free Newton-Krylov update scheme, which seeks a global minimum in the residuals using a series of large pseudo-timesteps. Domain decomposition is used for parallel execution using both shared memory and distributed memory programming techniques.

Additional comments including restrictions and unusual features: Eilmer provides a programmable interface for pre-processing, post-processing and user run-time customisations. The programmable interface

5.2. Eilmer

Eilmer's general capabilities are shared below:

Framework?	GD Tk(D,Lua)
Temperature Model?	One-, Two-, and Three-temperatures
Reactions?	Yes
Temporal Scheme	Runge-Kutta(Explicit), Backward Euler(Implicit)
Rarefaction?	No, only continuum
Dimensions?	2D/3D
Mesh Structure?	Structured/Unstructured
Flux Calculation Scheme?	Approx. Riemann Solvers
Turbulence Models?	SA, $k-\omega$ SST, IDDES

Table 2 Eilmer Summary

5.2.1. Governing Equations

$$\frac{\partial}{\partial t} \int_V \mathbf{U} dV = - \oint_S (\mathbf{F}_i - \mathbf{F}_v) \cdot \hat{n} dA + \int_V \mathbf{Q} dV$$

where

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \quad \mathbf{F}_i = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho vu \\ \rho wu \\ \rho Eu + pu \end{bmatrix} \hat{i} + \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho wv \\ \rho Ev + pv \end{bmatrix} \hat{j} + \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ \rho Ew + pw \end{bmatrix} \hat{k}$$

$$\mathbf{F}_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{zx} \\ \tau_{xx}u + \tau_{yx}v + \tau_{zx}w + q_x \end{bmatrix} \hat{i} + \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{zy} \\ \tau_{xy}u + \tau_{yy}v + \tau_{zy}w + q_y \end{bmatrix} \hat{j} + \begin{bmatrix} 0 \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ \tau_{xz}u + \tau_{yz}v + \tau_{zz}w + q_z \end{bmatrix} \hat{k}$$

For non-reacting, thermal equilibrium flow, governing equations are given as above.

5.2.1. Governing Equations

- For two-temperature and three-temperature models, extra terms are added to \mathbf{U} .
- For chemical reactions, a source term is added to continuity equation.
- For mixtures, alongside mixture mass conservation equation, specie conservation equations are added.
- For turbulence, RANS is employed:
 - Spalart-Allmaras
 - k-omega SST
 - LES

$$\begin{aligned}
 \mathbf{U} &= \begin{bmatrix} \vdots \\ \rho \hat{v} \end{bmatrix} && \text{Spalart-Allmaras} \\
 \mathbf{F}_i &= \begin{bmatrix} \vdots \\ \rho \hat{v} u \end{bmatrix} \hat{i} + \begin{bmatrix} \vdots \\ \rho \hat{v} v \end{bmatrix} \hat{j} + \begin{bmatrix} \vdots \\ \rho \hat{v} w \end{bmatrix} \hat{k} \\
 \mathbf{F}_v &= \begin{bmatrix} \vdots \\ \frac{\rho(v+\hat{v})}{\sigma} \frac{\partial \hat{v}}{\partial x} \end{bmatrix} \hat{i} + \begin{bmatrix} \vdots \\ \frac{\rho(v+\hat{v})}{\sigma} \frac{\partial \hat{v}}{\partial y} \end{bmatrix} \hat{j} + \begin{bmatrix} \vdots \\ \frac{\rho(v+\hat{v})}{\sigma} \frac{\partial \hat{v}}{\partial z} \end{bmatrix} \hat{k} \\
 \mathbf{Q} &= \begin{bmatrix} \vdots \\ \rho c_{b1}(1-f_{t2})\hat{S}\hat{v} - \rho \left[c_{w1}f_w - \frac{c_{b1}}{\kappa^2} f_{t2} \right] \left(\frac{\hat{v}}{d} \right)^2 + \\ \frac{1}{\sigma} \frac{\partial}{\partial x_j} \left(\rho(v+\hat{v}) \frac{\partial \hat{v}}{\partial x_j} \right) + \frac{c_{b2}}{\sigma} \rho \frac{\partial \hat{v}}{\partial x_i} \frac{\partial \hat{v}}{\partial x_i} \end{bmatrix}
 \end{aligned}$$

5.2.2. Discretization Process

$$\frac{\partial \vec{U}}{\partial t} = -\frac{1}{V} \sum_f^{faces} (\vec{F}_i - \vec{F}_v)_f \cdot \vec{n}_f A_f + \vec{Q} \quad \text{where}$$

\vec{U} is the conserved quantities

V is the volume,

\vec{F}_i is the inviscid flux,

\vec{F}_v is the viscous flux,

\vec{n}_f is the face normal vector,

A_f is the area of the face

\vec{Q} is the source vector.

- **Q** term includes chemical reaction terms which is solved with subcycles because of numerical stiffness.
- In implicit solutions, chemical reaction terms are included directly to the matrix.

5.2.3. Execution Sequence

Algorithm 3 Eilmer Execution Sequence Algorithm

1: Reconstruct the flow on the both sides of each face

1.1 Decide whether cells are structured or unstructured

1.2 Calculate left and right fluxes relative to interface

2: Compute the inviscid fluxes \vec{F}_i

2.1 Select an approximate Riemann Solver to find inviscid fluxes like Equilibrium-Flux-Method, Haenel or AUSMDV

3: Compute the gradients of the flow at each face by using a cell-centered least-squares gradient reconstruction

4: Compute the viscous fluxes \vec{F}_v

5: Compute the source terms \vec{Q}

5.1 Additional terms and models will be applied in here

6: Compute the rate of the change of the conserved variables \vec{R} by Eq. (62)

7: Advance the conserved quantities in time

7.1 Decide on using whether explicit(Runge-Kutta-Fehlberg) or implicit(Backward Euler) temporal schemes

5.5. Solver Comparisons

Framework?	OpenFOAM(C++)	Gas Dynamics Toolkit-GDTk(D,Lua)
Temperature Model?	One- and Two-temperatures	One-, Two-, and Three-temperatures
Reactions?	Yes	Yes
Temporal Scheme	Forward Euler(Explicit)*	Runge-Kutta(Explicit), Backward Euler(Implicit)
Rarefaction?	No, only continuum	No, only continuum
Dimensions?	2D/3D	2D/3D
Mesh Structure?	Structured/Unstructured	Structured/Unstructured
Flux Calculation Scheme?	Central-Upwind	Approx. Riemann Solvers
Turbulence Models?	SA, $k-\omega$ SST	SA, $k-\omega$ SST, IDDES

Table 4 Solver Comparisons

*Diffusive terms in hy2Foam and every rhoCentralFoam based solver are solved implicitly.

6. Test Cases

Three test cases are selected from literature:

Adiabatic Heat Bath(0-D): Thermochemical non-equilibrium flow is disturbed within a single cell. Relaxation phenomenon will be observed with:

- Relaxation of Reacting $\text{H}_2\text{-I}_2$ Mixture
- Relaxation of a N_2
- Relaxation of a non-Reacting and Reacting $\text{N}_2\text{-N}$ Mixture
- Relaxation of non-Reacting $\text{N}_2 - \text{O}_2$
- Thermal Eq. Reacting Air ($\text{N}_2\text{-O}_2$)

Blunted Cone(2-D): Hypersonic thermal non-equilibrium N_2 free-stream flow is sent upon blunted cone. No reactions are taking place.

Double Wedge(2-D): Thermochemical non-equilibrium $\text{N}_2\text{-O}_2$ flow is sent upon double-wedge geometry.

6. Test Cases

Case Name	Geometry	Reacting?	Mesh Convergence?	Mesh (OpenFOAM)	Mesh (Eilmer)	Mesh (SU2)	Timestep Convergence?
Single Temp. Relaxation of H_2-I_2	Heat Bath	Yes	No	Yes	No	No	No
V-T Relaxation of N_2	Heat Bath	No	No	Yes	No	No	No
V-T Relaxation of N_2-N	Heat Bath	No	No	Yes	No	No	No
V-T and V-V Relaxation of N_2-O_2	Heat Bath	No	No	Yes	No	No	No
Chemical Relaxation of Air	Heat Bath	Yes	No	Yes	No	No	No
V-T Relaxation of N_2-N	Heat Bath	Yes	No	Yes	No	No	No
V-T Relaxation of N_2	Blunted Cone	No	No	Yes	No	No	No
V-T and V-V Relaxation of N_2-O_2	Double Wedge	Yes	No	Yes	No	No	No

Legend	
	Not Started
	Currently
	Completed
	Incompleted within time limits

6.1. Testing Timeline

Legend	
Yellow	Not Started
Black	Currently
Green	Completed
Red	Incompleted within time limits

6.1. Testing Timeline



Legend	
	Not Started
	Currently
	Completed
	Incompleted within time limits

6.1. Testing Timeline



6.2. Adiabatic Heat Bath

In this case, several thermal non-equilibrium and chemical non-equilibrium mixtures are simulated.

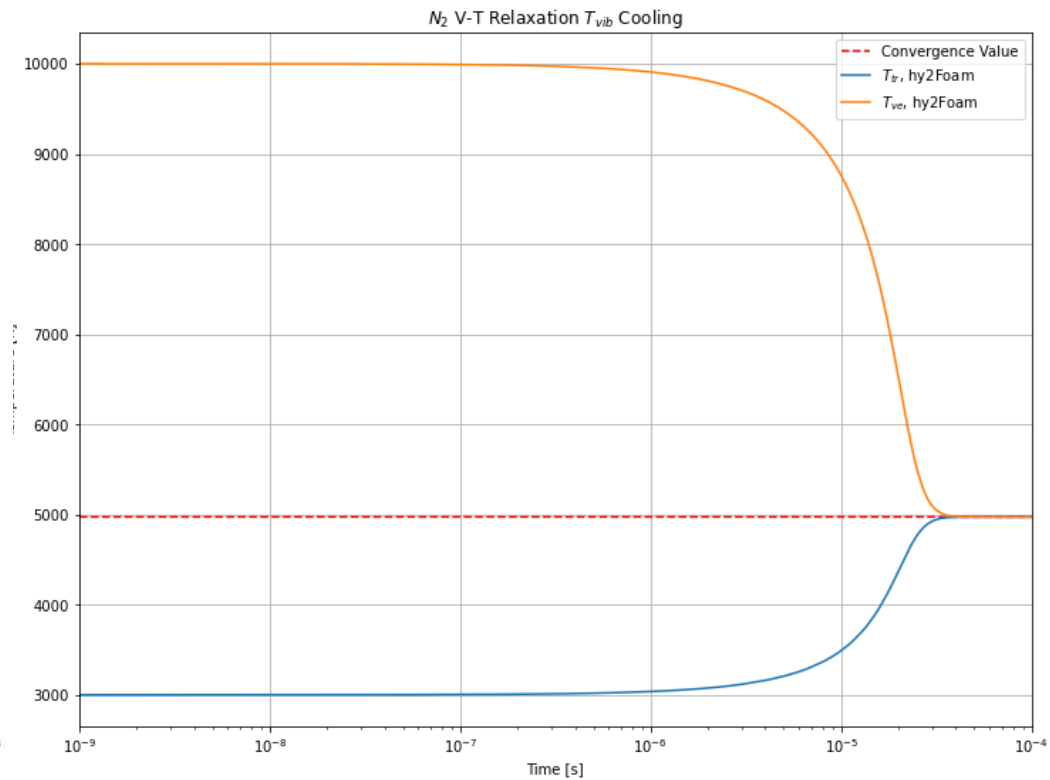
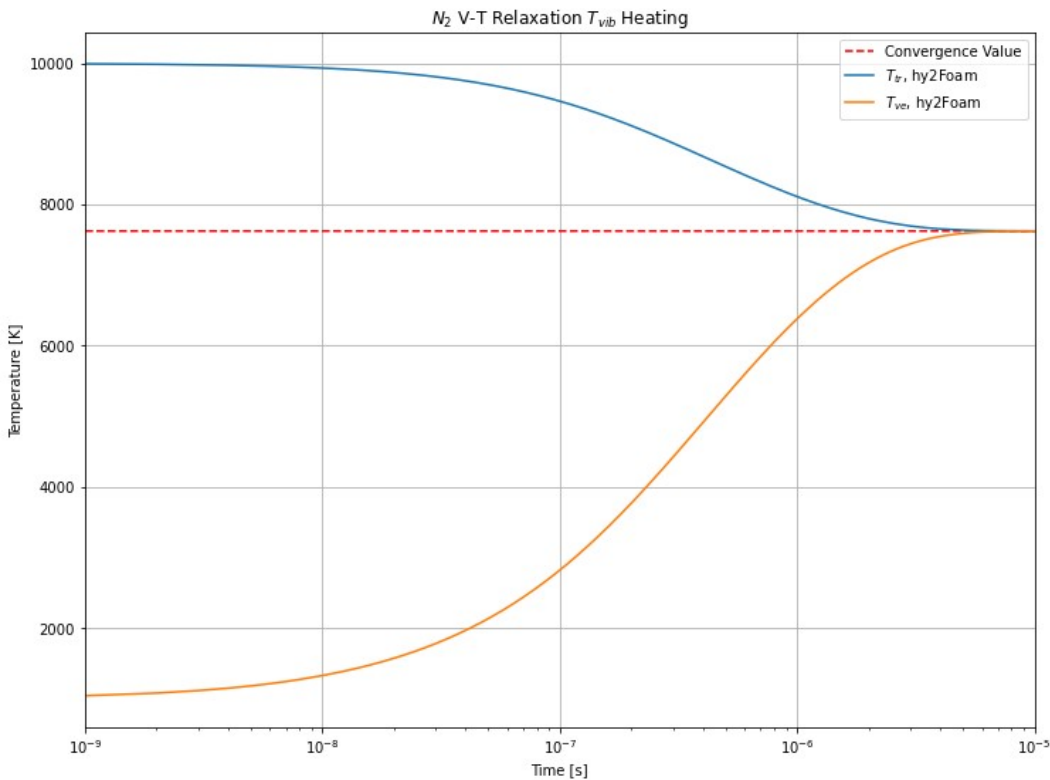
Case Name	Geometry	Reacting?	Thermal Equilibrium?
Single Temp. Relaxation of $\text{H}_2\text{-I}_2$	Heat Bath	Yes	Yes
V-T Relaxation of N_2	Heat Bath	No	No
V-T Relaxation of $\text{N}_2\text{-N}$	Heat Bath	No	No
V-T and V-V Relaxation of $\text{N}_2\text{-O}_2$	Heat Bath	No	No
Chemical Relaxation of Air	Heat Bath	Yes	Yes
V-T Relaxation of $\text{N}_2\text{-N}$	Heat Bath	Yes	No
V-T Relaxation of N_2	Blunted Cone	No	No
V-T and V-V Relaxation of $\text{N}_2\text{-O}_2$	Double Wedge	Yes	No

6.2. Adiabatic Heat Bath

Vibrational-Translational energy mode is going to be active for N_2 relaxation cases. No chemical reactions are active. There are two sub-cases to consider: Vibrational Heating and Vibrational Cooling.

Physical Inputs	Vibrational Heating	Vibrational Cooling
T_{Tr,N_2}	10000 K	3000 K
T_{V,N_2}	1000 K	10000 K
U	0 m/s	0 m/s
p	101325 Pa	101325 Pa
t	1e-9 s	1e-9 s
t_{end}	1e-5 s	1e-4 s
X_{N_2}	1	1

6.2. Adiabatic Heat Bath

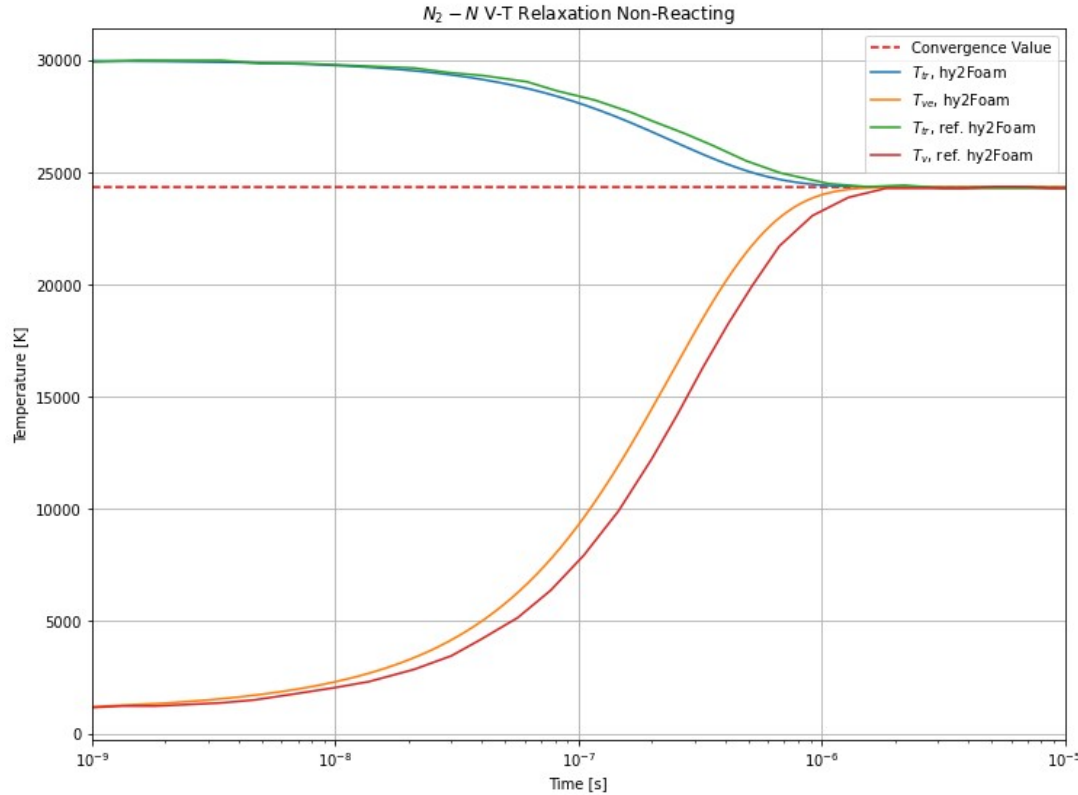


6.2. Adiabatic Heat Bath

Vibrational-Translational energy mode is going to be active for N_2 - N relaxation cases. No chemical reactions are active:

Physical Inputs	Vibrational Heating
$T_{Tr,N_2} - T_{Tr,N}$	30000 K
$T_{V,N_2} - T_{V,N}$	1000 K
U	0 m/s
p	41419.4 Pa
t	1e-9 s
t_{end}	1e-5 s
X_{N_2}	0.5
X_N	0.5

6.2. Adiabatic Heat Bath



6.2. Adiabatic Heat Bath

Vibrational-Translational energy mode is going to be active for N_2 - N relaxation cases. Chemical non-equilibrium is present in the flow. Only one reaction is taken into account:

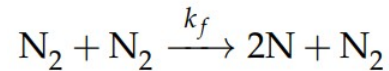
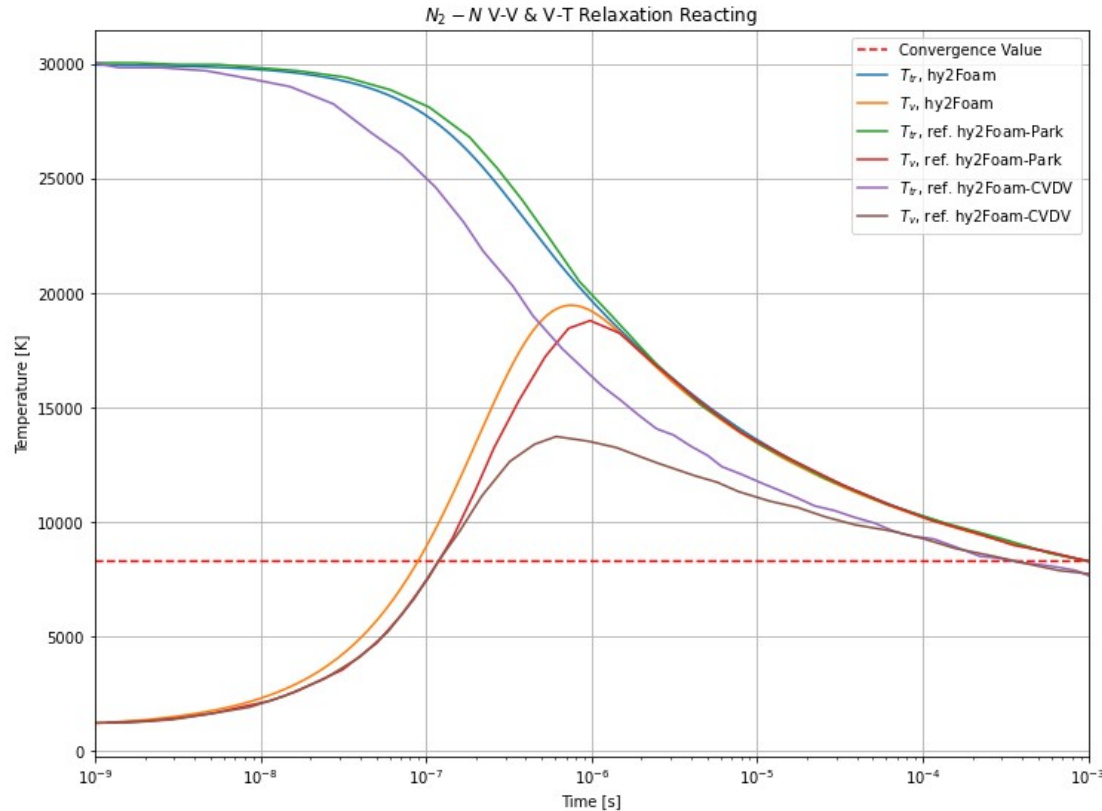


Table 2. Parameters for the evaluation of k_f .

Reaction Rate	Arrhenius Law Constants		
	A	β	T_a
Park 1993	7.0×10^{21}	-1.6	113,200
QK	2.47×10^{18}	-0.62	113,500

Physical Inputs	Vibrational Heating
$T_{Tr,N_2} - T_{Tr,N}$	30000 K
$T_{V,N_2} - T_{V,N}$	1000 K
U	0 m/s
p	41419.4 Pa
t	1e-9 s
t_{end}	1e-5 s
X_{N_2}	0.5
X_N	0.5

6.2. Adiabatic Heat Bath

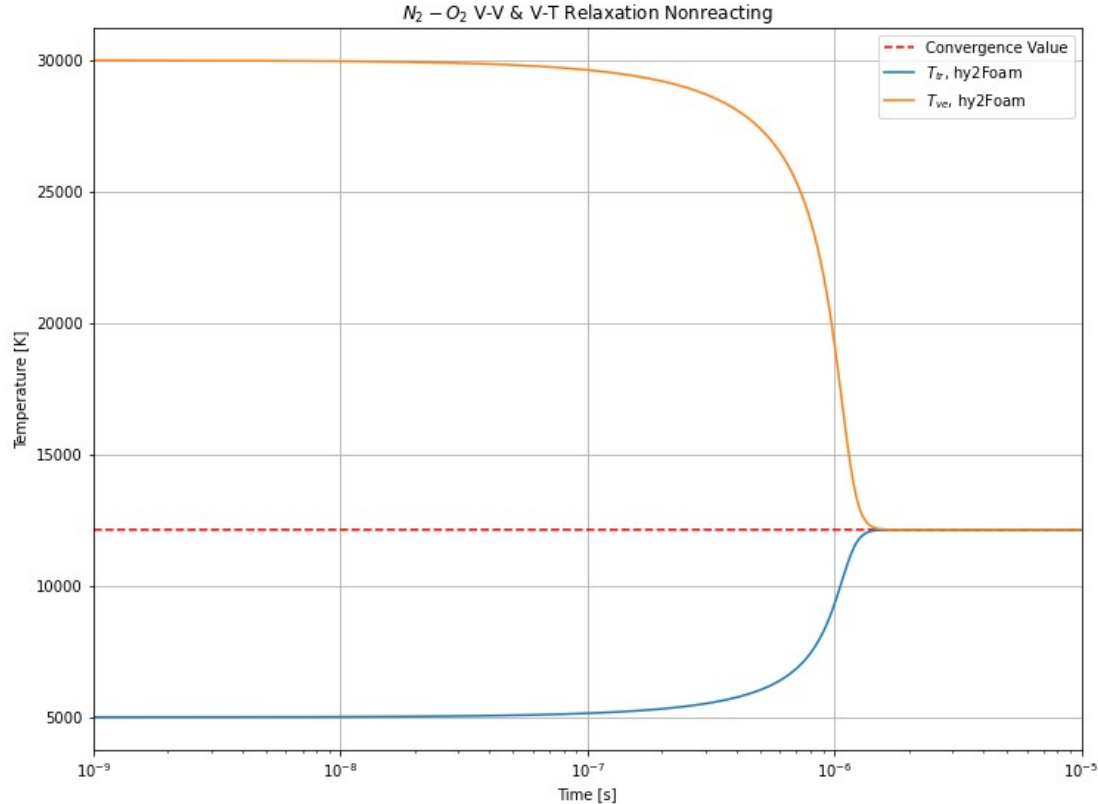


6.2. Adiabatic Heat Bath

Vibrational-Translational and Vibrational-Vibrational energy modes are going to be active for N_2 - O_2 relaxation cases. No chemical reactions are active:

Physical Inputs	Vibrational Heating
$T_{Tr,N_2} - T_{Tr,N}$	30000 K
$T_{V,N_2} - T_{V,N}$	5000 K
U	0 m/s
p	101325 Pa
t	1e-9 s
t _{end}	1e-5 s
X _{N2}	0.5
X _{O2}	0.5

6.2. Adiabatic Heat Bath



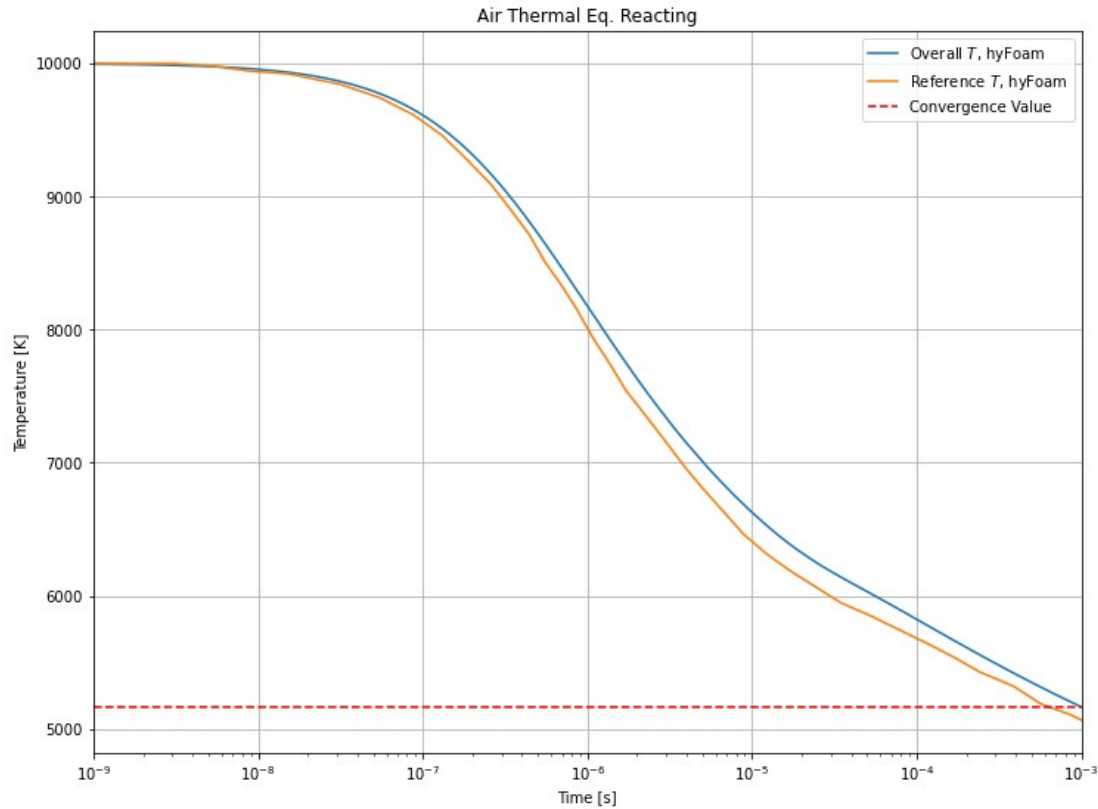
6.2. Adiabatic Heat Bath

No.	Reaction
1	$O_2 + N \rightarrow O + O + N$
2	$O_2 + NO \rightarrow O + O + NO$
3	$O_2 + N_2 \rightarrow O + O + N_2$
4	$O_2 + O_2 \rightarrow O + O + O_2$
5	$O_2 + O \rightarrow O + O + O$
6	$N_2 + O \rightarrow N + N + O$
7	$N_2 + O_2 \rightarrow N + N + O_2$
8	$N_2 + NO \rightarrow N + N + NO$
9	$N_2 + N_2 \rightarrow N + N + N_2$
10	$N_2 + N \rightarrow N + N + N$
11	$NO + N_2 \rightarrow N + O + N_2$
12	$NO + O_2 \rightarrow N + O + O_2$
13	$NO + NO \rightarrow N + O + NO$
14	$NO + O \rightarrow N + O + O$
15	$NO + N \rightarrow N + O + N$
16	$NO + O \rightarrow O_2 + N$
17	$N_2 + O \rightarrow NO + N$
18	$O_2 + N \rightarrow NO + O$
19	$NO + N \rightarrow N_2 + O$

Finally 5 species air relaxation case with thermal equilibrium is considered. Chemical non-equilibrium is present within flow field. 19 reactions are taken into account.

Physical Inputs	Vibrational Heating
T	10000 K
U	0 m/s
p	6383.475 Pa
t	1e-9 s
t _{end}	1e-3 s
X _{N2}	0.79
X _{O2}	0.21

6.2. Adiabatic Heat Bath



7. Future Work

- Additional equations and empirical data
-
- Blunted Cone inputs, post-processing, computational cost, and literature comparison for hy2Foam
-
- Double Wedge inputs, mesh conversion to SU2 and Eilmer frameworks