Week 2

Thesis Study Report

Mehmet Furkan Tunç

25 February 2025

Contents

1. Current Timeline

2. Introduction

3. Overall Literature Review
   - 3.1. Flow Types
   - 3.2. Equilibrium Term
   - 3.3. Rarefication Degree

4. Selected Solvers
   - 4.1. hy2Foam
   - 4.2. Eilmer
   - 4.3. SU2-NEMO
   - 4.4. hyperReactingFoam
   - 4.5. Solver Comparisons

5. Test Cases
   - 5.1. Testing Timeline
   - 5.2. Adiabatic Heat Bath
   - 5.3. Blunted Cone
   - 5.4. Double Wedge

6. Future Work

Legend
Not Started
Currently
Completed
Incompleted within time limits

1. Current Timeline

Sub Task No	Main Task Description	Sub Task Description	Week 1	Week 2	Week 3	Week 4	Week 5	Week 6	Week 7	Week 8	Week 9	Week 10
1	Understanding the governing equations, and the required computational sub-modules	Overall literature study for relevant open source for hy2Foam										
2		Selection and compilation of the relevant open source hy2Foam										
3		Overall literature study for relevant open source Eilmer										
4		Selection and compilation of the relevant open source Eilmer										
5		Overall literature study for relevant open source SU2-NEMO										
6		Selection and compilation of the relevant open source SU2-NEMO										
7		Test Case Simulations for hy2Foam, Eilmer, SU2-NEMO										
8		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

Wenqing Zhang, Zhijun Zhang*, Xiaowei Wang and Tianyi Su

*Correspondence:
zhjzhang@mail.neu.edu.cn

School of Mechanical Engineering and Automation, Northeastern University, Shenyang 110819, China

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

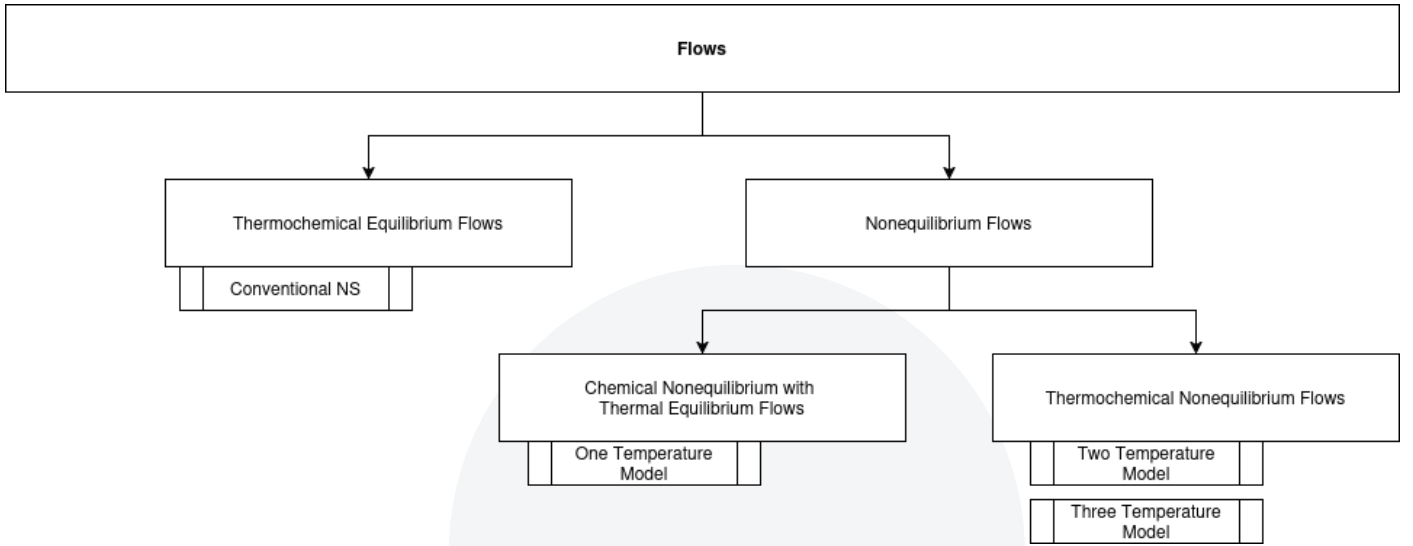
3. Overall Literature Review

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.

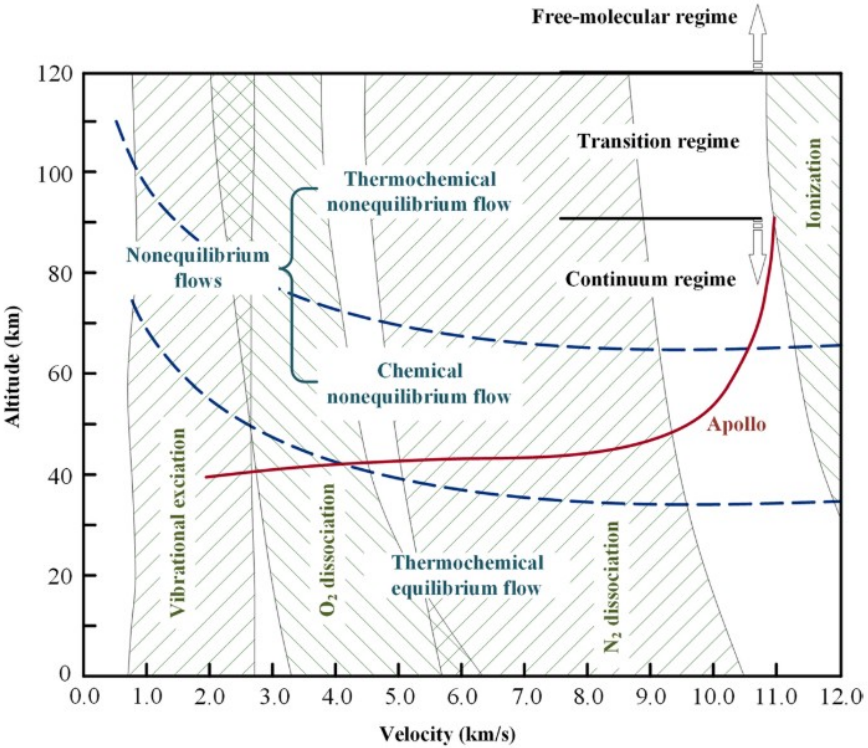
3.2. Equilibrium Term

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

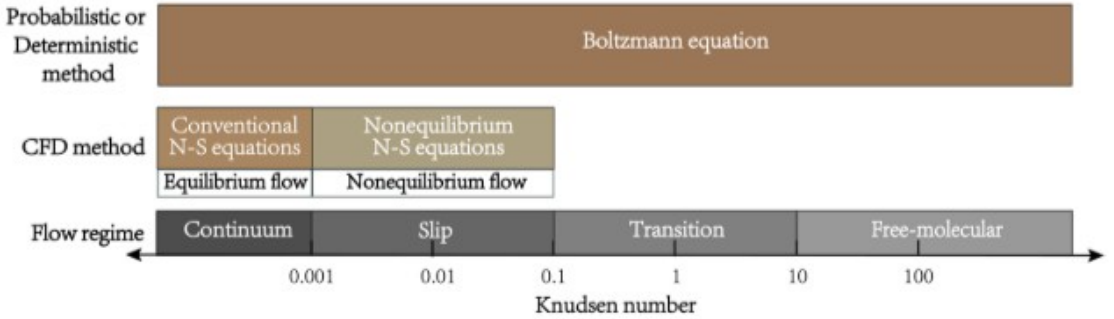
Relaxation: Physical relaxation refers to the process by which a system evolves toward equilibrium after being disturbed from its initial state.

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. Rarefication Degree



Since rarefication 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 rarefication 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. 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.

02 Eilmer

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

04 hyperReactingFoam

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

4.1. hy2Foam

hy2Foam(**Hy**personic 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 †

Vincent Casseau [1,2,*,‡], Rodrigo C. Palharini [3,‡], Thomas J. Scanlon [1,2,‡] and Richard E. Brown [2,‡]

[1] James Weir Fluids Laboratory, University of Strathclyde, Glasgow G1 1XJ, UK; tom.scanlon@strath.ac.uk
[2] Centre for Future Air-Space Transportation Technology, University of Strathclyde, Glasgow G1 1XJ, UK; richard.brown@strath.ac.uk
[3] Instituto de Aeronáutica e Espaço, Division of Aerodynamics (DCTA/IAE/ALA), Praça Mal. Eduardo Gomes, 50 Vila das Acácias, São José dos Campos 12215-904, Brazil; rophys@gmail.com
* Correspondence: vincent.casseau@strath.ac.uk; Tel.: +44-141-548-5096
† 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.
‡ These authors contributed equally to this work.

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 *dsmcFoam*. 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 †

Vincent Casseau [1,2,*,‡], Daniel E. R. Espinoza [1,2,‡], Thomas J. Scanlon [1,2,‡] and Richard E. Brown [2,‡]

[1] James Weir Fluids Laboratory, University of Strathclyde, Glasgow G1 1XJ, UK; daniel.espinoza@strath.ac.uk (D.E.R.E.); tom.scanlon@strath.ac.uk (T.J.S.)
[2] Centre for Future Air-Space Transportation Technology, University of Strathclyde, Glasgow G1 1XJ, UK; richard.brown@strath.ac.uk
* Correspondence: vincent.casseau@strath.ac.uk; Tel.: +44-141-548-5040
† 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.
‡ These authors contributed equally to this work.

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 *dsmcFoam* 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

4.1. hy2Foam

hy2Foam's general capabilities are shared below:

Language (Framework)	C++, OpenFoam
Temperature Model	One and Two-Temperature Model
Temporal Scheme	Explicit (because of rhoCentralFoam)
Based On	Density (compressible solver)
Continuum Assumption?	Yes
2D/3D?	2D/3D
Mesh Capabilities?	Structured/Unstructured
Flux Calculation Scheme?	Kurganov Central-Upwind Scheme

5. 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 H_2-I_2 Mixture
- Relaxation of a N_2
- Relaxation of a non-Reacting and Reacting N_2-N Mixture
- Relaxation of non-Reacting and Reacting Air (N_2-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 N_2-O_2 flow is sent upon double-wedge geometry.

5. 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
V-T and V-V Relaxation of N_2-O_2	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

5.1. Testing Timeline

Sub Task No	Main Task Description	Sub Task Description	Week 1	Week 2	Week 3	Week 4	Week 5	Week 6	Week 7	Week 8	Week 9	Week 10
1	Test Case Simulations for hy2Foam	Pre-processing of Test Cases										
2		Chemical Relaxation of H2-I2 Mixture in Adiabatic Heat-Bath										
3		Vibrational-Translational Relaxation of N2 in Adiabatic Heat-Bath										
4		Vibrational-Translational Relaxation of a non-Reacting N2-N Mixture in Adiabatic Heat-Bath										
5		Vibrational-Translational and Vibrational-Vibrational Relaxation of a non-Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
6		Relaxation of a Chemically Reacting N2-N Mixture in Adiabatic Heat-Bath										
7		Vibrational-Translational and Vibrational-Vibrational Relaxation of a Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
8		Vibrational-Translational Relaxation of non-Reacting N2 on Blunted Cone										
9		Relaxation of Chemically Reacting N2-O2 Mixture on Double-Wedge										

Legend
Not Started
Currently
Completed
Incompleted within time limits

5.1. Testing Timeline

Sub Task No	Main Task Description	Sub Task Description	Week 1	Week 2	Week 3	Week 4	Week 5	Week 6	Week 7	Week 8	Week 9	Week 10
10	Test Case Simulations for Eilmer	Pre-processing of Test Cases										
11		Chemical Relaxation of H2-I2 Mixture in Adiabatic Heat-Bath										
12		Vibrational-Translational Relaxation of N2 in Adiabatic Heat-Bath										
13		Vibrational-Translational Relaxation of a non-Reacting N2-N Mixture in Adiabatic Heat-Bath										
14		Vibrational-Translational and Vibrational-Vibrational Relaxation of a non-Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
15		Relaxation of a Chemically Reacting N2-N Mixture in Adiabatic Heat-Bath										
16		Vibrational-Translational and Vibrational-Vibrational Relaxation of a Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
17		Vibrational-Translational Relaxation of non-Reacting N2 on Blunted Cone										
18		Relaxation of Chemically Reacting N2-O2 Mixture on Double-Wedge										

Legend
Not Started
Currently
Completed
Incompleted within time limits

5.1. Testing Timeline

Sub Task No	Main Task Description	Sub Task Description	Week 1	Week 2	Week 3	Week 4	Week 5	Week 6	Week 7	Week 8	Week 9	Week 10
19	Test Case Simulations for SU2-NEMO	Pre-processing of Test Cases										
20		Chemical Relaxation of H2-I2 Mixture in Adiabatic Heat-Bath										
21		Vibrational-Translational Relaxation of N2 in Adiabatic Heat-Bath										
22		Vibrational-Translational Relaxation of a non-Reacting N2-N Mixture in Adiabatic Heat-Bath										
23		Vibrational-Translational and Vibrational-Vibrational Relaxation of a non-Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
24		Relaxation of a Chemically Reacting N2-N Mixture in Adiabatic Heat-Bath										
25		Vibrational-Translational and Vibrational-Vibrational Relaxation of a Reacting N2-O2 Mixture in Adiabatic Heat-Bath										
26		Vibrational-Translational Relaxation of non-Reacting N2 on Blunted Cone										
27		Relaxation of Chemically Reacting N2-O2 Mixture on Double-Wedge										

6. Future Work

- Thermochemical non-equilibrium flow’s governing equations and main models which are used for determining necessary terms on the modeling
- Adiabatic Heat Bath inputs, post-processing, computational cost, and literature comparison for hy2Foam
- Blunted Cone inputs, mesh conversion to SU2 and Eilmer frameworks