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Numerical Analysis of Rarefied Hypersonic and Chemically Reacting Flow-field

Harshal Gijare
Research Scholar
IIT, Hyderabad
Sangareddy-502285
Email: me13m15p000002@iith.ac.in

Apurva Bhagat
Research Scholar
IIT, Hyderabad
Sangareddy-502285
Email: me13m15p000001@iith.ac.in

Nishanth Dongari
Assistant Professor
IIT, Hyderabad
Sangareddy-502285
Email: nishanth@iith.ac.in

Abstract
We have developed an open source CFD tool, which can simulate high temperature and chemically reacting flow-field in the rarefied regime. It is used to carry out simulations in the intermediate hypersonic flow regime (Mach number range from 8 to 15). Solver is tested with available data for high speed and rarefied flow applications. Heat load values for blunt conical surface and shock standoff distance for sphere are obtained with our solver and good agreement has been exhibited with the experimental data.

Keywords—Hypersonics; Rarefied; Air Chemistry; OpenFOAM

I. INTRODUCTION

Many approaches have been proposed to validate chemically reacting and rarefied flow-field solver [1]. One of the popular one is to measure heat load values , as their accurate prediction is imperative for re-entry applications to design the Thermal Protection System. Another approach is to measure shock stand-off distance [1], which is inversely proportional to optimally density of air in shock layer that in turn depends on degree of rarefaction and chemical reactions occurring in the flow-field.

When space vehicle re-enters at Mach number $(Ma) > 8$, the energy content and exchange between kinetic, internal and chemical modes in the flow precludes the otherwise common use of calorically perfect gas assumption. Calorically perfect gas assumption over-predicts the temperature values and design parameters [2]. The vibrational energy of components of molecules becomes pertinent for temperature above $800K$, while beyond $2500K$, the hot flow turns chemically reacting and it significantly changes the flow behavior. Typical re-entry vehicle follows the path where chemical reactions such as dissociation, and ionization occurs. We need to model air chemistry for accurate prediction of heat load and temperature as reactions will absorb considerable amount of heat. Various air chemical models are available in literature, but for current simulations 5 species model with 12 reactions including dissociation and exchange is imperative to model the flow-field [4].

Flow behaviour also changes with the degree of rarefaction, and this is defined using non-dimensional parameter, Knudsen number (Kn). It is the ratio of mean free path to the characteristic length scale which is directly proportional to the ratio of Ma to Reynolds number (Re).

$$Kn = \frac{Ma}{Re}\sqrt{\frac{\gamma\pi}{2}}. \tag{1}$$

If $Kn < 0.001$, standard compressible Navier Stoke's $(N-S)$ equations can be used to simulate the flow. However, majority of the hypersonic vehicles operate in the rarefied slip flow regime $(0.1 < Kn < 0.01)$, where N-S equations have to be implemented along with the non-equilibrium boundary conditions. In the current work, 1^{st} order velocity slip, temperature jump and thermal creep conditions are incorporated to extend solver's applicability to the slip flow regime.

The major objective of the current study is to develop an open source solver to optimize the aero-thermodynamic design of mid range hypersonic systems operating in rarefied flow regime.

II. OPENFOAM SOLVER

OpenFOAM (Open Source Field Operation and Manipulation) has various numerical solvers and schemes through a comprehensive C++ library, along with number of pre-processing and post-processing utilities [5]. It can be extended to add new features or modify existing subroutines. OpenFoam has *rhoCentralFoam*, which is a density-based N-S compressible flow solver based on central upwind schemes of Kurganov and Tadmor [6], [7]. The solver has been validated for compressible testcases, however limited to $(Ma < 10)$, $(T < 2000)$, single specie transport and chemically non-reacting flows.

New solver *hypersonicIITHFoam* is developed in the current work by utilizing the basic features of *rhoCentralFoam*. Additional features are incorporated to model air chemistry, species transport, and thermodynamic properties, which are computed using JANAF model. Coefficients for JANAF model are updated using Gordon and McBride[8] which provides polynomial fits for heat capacity, enthalpy and entropy as a function of temperature. 5 species and 12 reactions model of air is used and reaction rates are obtained from Gupta et.al [9]. Sutherland's model is used to compute transport properties such as viscosity, thermal conductivity and mass diffusivity (See Eqs 8-10).

Maxwell velocity slip and Smoluchowski temperature jump boundary conditions are incorporated in solver to extend its applicability to slip flow regime [10], [11]. Post-processing utility is used to compute heat flux to the wall. HPC facility available at IIT Hyderabad is used for parallelization, and each simulation is carried out using 32 Intel Hasaswell cores.

III. NUMERICAL METHODOLOGY

A. *Governing Equations*

In this section set of N-S compressible flow equation along with newly added equations to model chemically reacting flow field are presented. As gas mixture comprises of multiple species, specie's mass conservation equation is given as [12]

$$\frac{\partial \rho Y_s}{\partial t} + \nabla\cdot[\overrightarrow{u}\rho Y_i] - \nabla\cdot[\rho D_i \nabla Y_i] - \dot{w}_i = 0, \tag{2}$$

where Y_i is specie's mass fraction, D_i is diffusion of specie i in gas mixture, ρ is density and $\overrightarrow{u}$ is velocity vector. Eq 1 is solved for each specie where first term is rate of change of mass of specie per unit volume, second term is mass flux convected across cell faces, third term is mass diffusion due to concentration gradients and last term is rate of creation of specie due to chemical reaction. Last term is calculated from Arrhenius reaction rates, and the global mass conservation equation is written as:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot[\overrightarrow{u}\rho] = 0. \tag{3}$$

Conservation of momentum in vector form is written as:

$$\frac{\partial(\rho\overrightarrow{u})}{\partial t} + \nabla\cdot[\overrightarrow{u}(\rho\overrightarrow{u})] + \nabla p + \nabla\cdot\sigma = 0, \tag{4}$$

where σ is the viscous stress tensor.

$$\begin{aligned}\frac{\partial(\rho E)}{\partial t} + \nabla\cdot[\overrightarrow{u}(\rho H)] + \nabla\cdot(\sigma\cdot\overrightarrow{u}) - \nabla\cdot(k\nabla T) \\ -\nabla\cdot\Big[\rho\sum_i h_i D_i \nabla Y_i\Big] = 0,\end{aligned} \tag{5}$$

where, the primary variable (ρE) is total energy of the system, k is thermal conductivity , T is temperature and $E = e + \frac{|u^2|}{2}$, where $e = c_v T = (\gamma - 1)RT$ is the specific internal energy and $\gamma = \frac{c_p}{c_v}$ is the ratio of specific heats at constant pressure and volume. Total enthalpy is written as $\rho H = \rho E + p$. Additional term in the energy equation is due to diffusion of enthalpy driven by concentration gradients. The value of temperature is calculated as:

$$T = \frac{1}{c_v}\left(\frac{\rho E}{\rho} - \frac{|u^2|}{2}\right). \tag{6}$$

The above four equations are closed by the ideal gas equation of state and pressure is calculated as:

$$p = \rho RT. \tag{7}$$

B. *Transport Properties*

The viscosity μ is calculated using Sutherland's law [2], which is found to be accurate up to $6000K$. In intermediate hypersonic flow regime temperature is expected to stay below $6000K$.

$$\mu = \frac{A_s\sqrt{T}}{1 + \frac{T_s}{T}}, \tag{8}$$

where A_s and T_s are sutherland's coefficients. Thermal conductivity of mixture is calculated using Prandtl's number as below: Effective viscosity (μ_{eff}) is calculated from laminar and turbulent viscosity , and turbulence is modeled using Spalart Allmaras one equation model [2].

$$k_{eff} = \frac{C_p \mu_{eff}}{Pr}, \tag{9}$$

where C_p is heat capacity. Effective diffusivity (D_s) for mixture is calculated from Schmidt number(S_c) assuming it as a unity and using effective viscosity:

$$S_c = \frac{\mu_{eff}}{\rho D_s}. \tag{10}$$

C. *Chemical Kinetics*

In the Earth's atmosphere major composition of air is O_2 and N_2, which starts dissociating when temperature in shock layer reaches above $2500K$ and $4000K$ respectively to form O and N. Exchange reactions also take place to form specie NO, which also dissociates for $T > 3500$. It forms a mixture of 5 species: N_2, O_2, N, O and NO, and ionization of species can be neglected for intermediate hypersonic range, as temperature stays below $9000K$ [2]. Various reactions considered and their respective Arrhenius reaction rate parameters are provided in table I. Reaction rate is calculated as follows [9]:

$$r = AT^{\beta} exp\Big(\frac{E_a}{T}\Big). \tag{11}$$

A and β are arrhenius rate parameters, while E_a is ratio of activation energy $E(cal/mol)$ to universal gas constant. As all species are assumed to be in thermodynamic equilibrium, state of gas is governed by single equilibrium temperature.

TABLE I. **ARRHENIUS REACTION RATES FOR 5 SPECIES AIR MODEL**

Reaction	**Forward Reaction**		
	$A(cm^3/mol-sec)$	β	$E_a(K)$
$O2 + M \rightleftharpoons 2O + M$	3.61×10^{18}	-1.0	-5.94×10^4
$N_2 + M \rightleftharpoons 2N + M$	1.92×10^{17}	-0.5	-1.131×10^5
$N_2 + N \rightleftharpoons 2N + N$	4.15×10^{22}	-1.5	-1.131×10^5
$NO + M \rightleftharpoons N + O + M$	3.97×10^{20}	-1.5	-7.56×10^4
$NO + O \rightleftharpoons O_2 + N$	3.18×10^9	1	-1.97×10^4
$N_2 + O \rightleftharpoons NO + N$	6.75×10^{13}	0	-3.75×10^4
	Backward Reaction		
	$A(cm^3/mol-sec)$	β	$E_a(K)$
$2O + M \rightleftharpoons O2 + M$	3.01×10^{15}	-0.5	0
$2N + M \rightleftharpoons N2 + M$	1.09×10^{16}	-0.5	0
$2N + N \rightleftharpoons N_2 + N$	2.32×10^{21}	-1.5	0
$N + O + M \rightleftharpoons NO + M$	1.01×10^{20}	-1.5	0
$O_2 + N \rightleftharpoons NO + O$	9.63×10^{11}	1	-3.6×10^3
$NO + N \rightleftharpoons N_2 + O$	1.5×10^{13}	0	0

IV. RESULTS AND DISCUSSION

1st test case reported is ELECTRE test article consists of a blunt conical surface with total length of 0.4 m, semi aperture cone angle of 4.6 degree, and hemispherical nose with a radius of 0.035 m. For validation study free-stream conditions with 795K temperature 124.35 Pa pressure and freestream velocity 4930m/s is considered. Mesh is created using ICEM CFD tool. Mesh is refined manually in radial direction to capture boundary layer effects. Mesh is also refined adaptively based on high gradients present across shock layer. From refinement study it is observed that mesh near wall is sensitive to heat

load. Minimum cell thickness near wall $\Delta y = 0.00027m$. Figure 1 demonstrates the comparison of heat load values

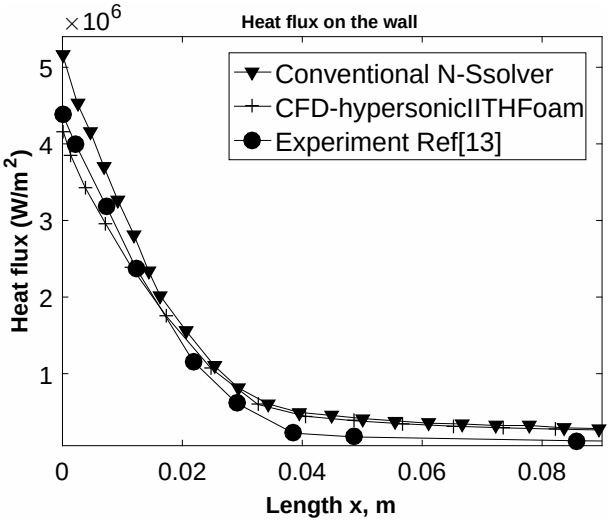

Fig. 1. **Heat flux on the blunt conical surface**

along arc length of blunt conical object with the experimental data and conventional CFD. As chemical reactions absorbs large amount of heat, heat load values are under-predicted near nose portion, where as deviation is much higher with conventional CFD solver. Deviation with the experimental data may be attributed to the fact that experiments are carried out in a old copper chamber which causes contamination effects[13], or it can be due to the constant diffusion coefficient for all species. They are over predicted in rare portion as density decreases away from the nose rarefaction effects are dominant in rare portion.

The second test case considered is hypersonic flow over a sphere of radius $200mm$. Free-stream conditions $293K$ ambient temperature and $1000K$ wall temperature. Shock standoff distance s is measured as thickness of shock layer at nose tip, which are compared with ballistic range experimental data for sphere [14]. We have carried out simulations for two conditions $\rho R = 1.7 \times 10^{-3}, 2 \times 10^{-4}$ (See Table II), which is hypersonic similarity condition. Hypersonic similarity means Mach number as well as Reynold number should be equal. Binary scaling parameter ρR identical to ballistic range experiments is used as similarity parameter, where ρ is density and R is Radius of sphere and it is inversely proportional to Kn.

TABLE II. **NORMALIZED SHOCK STANDOFF DISTANCE**

ρR	Velocity	Normalized Shock standoff distance s/R		
		C-CFD	H-CFD	Experimental Ref[14]
1.7×10^{-3}	2440	14.4	12.9	12.78
	2560	14	12.58	12.43
	3160	13.8	11.8	10.4
2×10^{-4}	2630	13.6	13.3	13.32
	3150	13.1	12.8	12.87
	3640	12.8	11.47	11.37

Table II gives comparison of normalized shock standoff distance (s/R), where $C-CFD$ indicates conventional solver and $H-CFD$ hypersonicIITHFoam solver. $\rho R = 1.7 \times 10^{-3}$ is the case in continuum regime and $\rho R = 2 \times 10^{-4}$ is in slip flow regime. Simulation data matches well with experimental data over conventional CFD solver, except for higher velocity near equilibrium case. Further study is needed to attribute this deviation.

V. CONCLUSIONS

We have developed an open source and parallel friendly non-equilibrium CFD solver to tackle mid range hypersonic flows in the rarefied regime by accurately modeling multi specie air chemistry, and slip/jump boundary conditions. Our results have exhibited good agreement with the experimental data and when compared shown significant improvement with the conventional high-speed compressible flow solver. In the future work, we will incorporate variable diffusion coefficients and higher order constitutive relations / boundary conditions to further improve the modeling of air chemistry and rarefaction effects, respectively.

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