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Aerodynamic performance investigation through different chemistry modelling approaches for space re-entry vehicles using the DSMC method

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Abstract

High-speed flows with Mach numbers well above the hypersonic regime pose significant modelling complexities due to increased levels of thermal energy, which in turn result in a variety of chemical reactions that become dominant and thus have to be accurately modelled. Within Computational Fluid Dynamics (CFD), the Direct Simulation Monte Carlo (DSMC) method is commonly chosen here as it has shown superior performance over traditional Navier-Stokes-based solvers due to a breakdown in the continuum hypothesis. Space re-entering vehicles are commonly exposed to high Mach numbers when entering into earth's atmosphere and low density so that the mean free path of particles is comparable to the length of the vehicle itself. Thus, these types of applications require challenging modelling approaches which is the subject of this study. We use the open-source CFD solver OpenFOAM in this study, which comes prebuilt with the *dsmcFoam* solver. This implementation of the DSMC method lacks, however, the ability to model chemical reactions and thus is not equipped to predict aerodynamic coefficients for high-speed flows. Recently, the *dsmcFoam+* solver has been proposed [1] and implemented into OpenFOAM which features, among other things, the ability to model chemical reactions through the Quantum-Kinetic (QK) model. The aim of this study, then, is threefold; 1) Validate the new *dsmcFoam+* solver against available reference data from the literature and compare it to the default *dsmcFoam* solver, highlighting the importance of chemical modelling, 2) Publish all simulation and setup files through an online repository to facilitate an easy case setup for researchers wishing to evaluate or adopt the new *dsmcFoam+* solver, 3) Provide documentation for the new *dsmcFoam+* solver in the context of OpenFOAM where there is little documentation available. We investigate the flow of a re-entry vehicle with a freestream Mach number of 25.6 at different angle of attacks and find that the chemical modelling approach taken has a significant influence over the aerodynamic coefficients which are up to 24% apart. Similar results are obtained for the heat transfer coefficient, which shows differences of up to 28%. Based on our findings, we advocate that the *dsmcFoam+* solver should be used for aero-thermodynamic calculations as its ability to predict chemical reactions and thus changes in the flow field will significantly affect the overall solution accuracy compared to a non-reacting modelling approach.

Key words: *Computational Fluid Dynamics; Direct Simulation Monte Carlo; Quantum-Kinetic Model; Re-entry Vehicle; Aero-thermodynamics*

1 Introduction

Understanding the flow physics of re-entry vehicles into earth's atmosphere is of crucial importance as Mach number beyond the hypersonic regime may be achieved. To slow down the descent speed, blunt body shape configurations are used, which experience atmospheric friction leading to challenging surface heating rates, pressure loads and excessive level of chemical activities. Therefore, the chemical composition of the atmosphere that influences the flow field characteristics, the high temperature exposed surface and the bow shock properties must be studied thoroughly to get a good understanding of the real gas effects exerted by these flow conditions and the flow characteristics experienced by the vehicle's body. The impact of including chemical reactions with the application of the QK chemistry model in high-speed hypersonic rarefied aero-thermodynamics will be studied herein, where complex flow interactions are present such as strong fully detached bow shock formation, causing a large temperature rise and high vibrational excitation of air molecules inside. Molecular species dissociation and new species formation are also introduced, in addition to high surface heating rates, large pressure loads and high degree of gas rarefaction effect.
The Navier-Stokes equations are based on the continuum hypothesis and are valid for low-Knudsen number flows only. For Knudsen numbers approaching unity and above, the continuum hypothesis

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breaks down and particle-based method may provide a better description of a given flow field. The Knudsen number is defined as

$$Kn = \frac{\lambda}{L}. \tag{1}$$

DSMC is a stochastic probabilistic particle-based method. The fundamental DSMC approximation allows the decoupling of the molecular motion and inter-molecular collisions over a small time step.

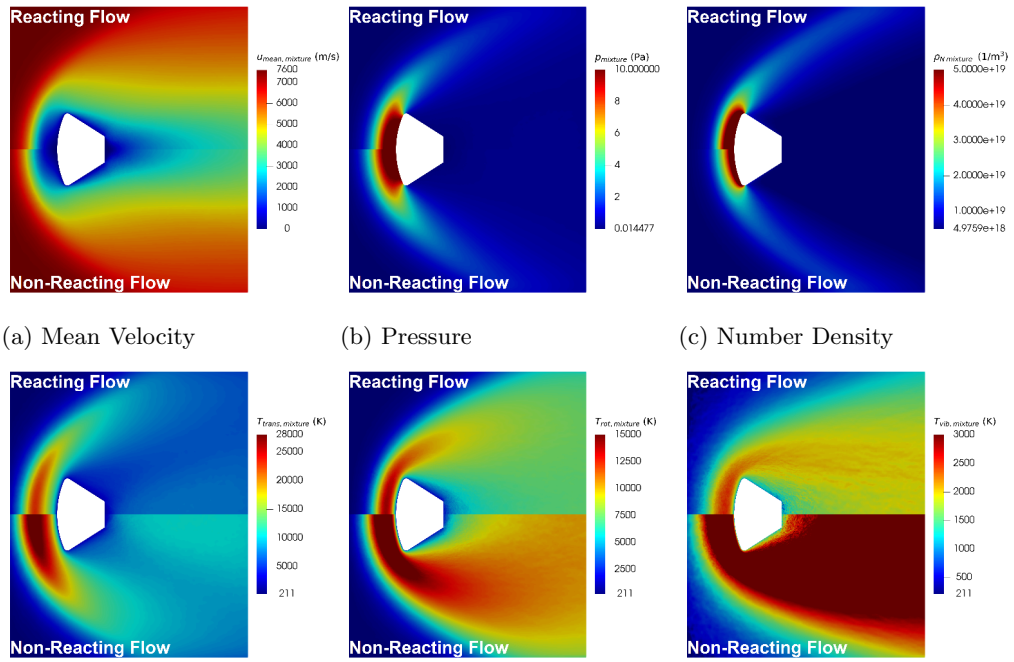
2 Problem Description

The DSMC method is able to capture non-equilibrium effects in high speed hypersonic rarefied flows by using a wide variety of chemistry models that were developed in the past. A traditional temperature-based rate model called the TCE model can be used for that purpose, where it applies the equilibrium kinetic theory to convert the Arrhenius rate coefficients, which are defined at a macroscopic level, to collision probabilities function of the collision energy at the microscopic level. The TCE is a phenomenological model, hence it is highly dependent on the availability of experimental data to fit the Arrhenius rate coefficient equation. A new collision-based chemical kinetics model, called the QK chemistry model [4] was developed, based on the primary properties of two colliding particles, that are, their total collision energy, quantized vibrational levels, and molecular dissociation energies. The QK model was recently implemented into the open-source OpenFOAM package and released through the newly developed *dsmcFoam+* [1] solver, which provides open-source access to the QK model within a general-purpose DSMC framework. The aim of this study is to compare the capability of the newly developed *dsmcFoam+* solver applied to the Orion Crew Module (OCM) [2], highlighting the importance of chemical modelling, and compare its aerodynamic performance characteristics to [2] which looked at the traditional rate-based method. For this study, a 5-species air model was used to model the reacting gas mixture of N_2, O_2, NO, N, and O. In total, for a 5-species air model, 34 chemical reactions will take place and they are split between 15 dissociation reactions (type I: $\mathbf{AB} + \mathbf{CD} \rightarrow \mathbf{A} + \mathbf{B} + \mathbf{CD}$ and type II: $\mathbf{AB} + \mathbf{C} \rightarrow \mathbf{A} + \mathbf{B} + \mathbf{C}$), 15 recombination reactions ($\mathbf{A} + \mathbf{B} + \mathbf{C} \rightarrow \mathbf{AB} + \mathbf{C}$), and 4 exchange reactions ($\mathbf{AB} + \mathbf{C} \leftrightarrow \mathbf{AC} + \mathbf{B}$). The recombination reaction at high altitudes and high temperatures can be neglected because their importance at low-density flow becomes negligible.

3 Numerical Results

In the following, we will investigate the wake structure of the OCM in order to get a better understanding of the different chemical modelling strategies. This will help forming an understanding of the wake region as well as the leading bow shock. Figure (1) shows the flow features around the OCM during re-entry into earth's atmosphere at an altitude of 105 km, with a re-entry speed of 7,600 m/s and an angle of attack equal 0°. We have split the contour plots at the module's symmetry axis, the top shows a reacting flow using the QK model in order to simulate the chemical activities occurring in the flow and at the bottom a non-reacting flow, i.e. without including any chemical reaction and model.

The first thing to notice is that the non-reacting case predicts a larger leading bow shock, which is evident from Fig. (1a). For the reacting case, energy is absorbed into chemical reactions leading to thinner shock wave structures. This influence is felt further downstream due to the hyperbolic nature of compressible flows which thus influences the wake region. The additional energy available for chemical reactions leads to the formation of additional atomic compositions which is supported by an increase of the number density over the bow shock as shown in Fig. (1c). The aforementioned excess energy for the non-reacting case and lack of a source to remove this energy leads to an overprediction of the temperature within the bow shock. In-fact, the temperature experiences the strongest difference to its reacting counterpart where the wake structure exhibits a vastly different distribution of temperature as detected in Fig. (1d, 1e, 1f) that shows the breakdown of temperature for all energy modes, i.e. translational, rotational, and vibrational temperatures. According to these results, a decrease in the bow shock temperature for all energy



(a) Mean Velocity (b) Pressure (c) Number Density

(d) Translational Temperature (e) Rotational Temperature (f) Vibrational Temperature

Figure 1: Flow field structures at a freestream of 0° angle of attack, for both the QK chemistry modelling approach (reacting flow) and a baseline case with no chemistry modelling (non-reacting flow).

modes is visualised for a reacting flow compared to a non-reacting one and the high distribution of the maximum temperatures values are located inside the shock layer in front of the OCM. This shows that the chemical reactions may not just change the thickness of the shock wave structures but also the distribution of thermodynamic properties throughout the domain. Similar observation to the above can be made for the pressure shown in Fig. (1b), however, the importance here being that any changes in pressure directly correlates to differences in the prediction of aerodynamic performance metrics. By just inspecting Fig. (1) we are able to qualitatively reason about the importance of incorporating chemical models into a DSMC simulation. Since the standard *dsmcFoam* solver shipped with the OpenFOAM distribution does not contain this capability, the presented results show a strong motivation to adopt the newly developed *dsmcFoam+* solver for similar flow condition investigations.

A series of simulations for angle of attacks equal 0°, −26°, −30°, −60° and −90° are performed with freestream conditions taken from [2]. In their work, they used the *DS3V* solver for an axisymmetric 3D grid of half the capsule. Since the DS3V uses the TCE chemical model, we are able to comment on the comparison between the different chemical reaction approaches taken.

The results obtained for the drag and lift forces coefficients from the *dsmcFoam+* simulations are shown in Tab. (1). We can see an initial good agreement between both the *dsmcFoam+* simulation results and those obtained in [2] using a simplified chemical modelling approach when the angle of attack is less than −30° and where the drag coefficient is considered. Here the differences between the reference data and our simulations are less than 1%. We have seen in Fig. (1) that the pressure field already exhibits differences around the OCM body which is further exacerbated with an increase in the angle of attack. In the absence of experimental validation data it is not possible to judge which of these results matches reality better, however, the simplifications made in the chemical model manifest themselves in a change of aerodynamic lift and drag forces and therefore careful consideration has to be given as to how chemical reactions need to be resolved.

	C_D		C_L		$C_{m,0}$	
AoA	DS3V [2]	dsmcFoam+	DS3V [2]	dsmcFoam+	DS3V [2]	dsmcFoam+
0°	1.709	1.724	0.000	0.000	0.000	0.000
-26°	1.464	1.499	0.350	0.433	0.114	0.113
-30°	1.390	1.434	0.369	0.463	0.129	0.128
-60°	0.972	1.073	0.196	0.191	0.225	0.198
-90°	0.918	1.116	-0.148	-0.338	0.218	0.190

Table 1: Comparison of the aerodynamic forces and moment coefficients for different values of the angle of attack (AoA) against the results obtained in [2].

Looking at the lift coefficient, for the angle of attacks tested in this study we can see a 24% difference at $-26°$ and a lift coefficient twice as big at $-90°$. The results obtained herein show a higher lift value. In [2], however, it was stated that an increased rarefaction (or decreased number density) results in a lower lift coefficient. As already shown in Fig. (1c), chemical reaction increase the number density which could explain the increase in lift as observed here. The pitching moment coefficient, on the other hand, showed good agreement throughout the tested angle of attacks and differences were at most 12% and seen in Fig. (1).

4 Conclusions

We can conclude here that the choice of chemical reaction modelling in DSMC computation for high speed hypersonic aero-thermodynamic applications, to model real gas effects for high Mach number flows using the molecular hypothesis, has a significant influence over its ability to predict the flow field both close to solid boundaries, as well as in the farfield of the domain of interest. The *dsmcFoam+* solver having the capability to model chemical reactions using the QK model has shown to capture these effects and we therefore recommend its usage over the default *dsmcFoam* solver shipped with OpenFOAM by default which lacks the ability to handle chemical reactions.

Data Access Statement

All simulation setup files and documentation underlying this paper can be accessed through a dedicated online repository which can be accessed at `https://doi.org/10.17862/cranfield.rd.14730483.v1` [5].

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