
An investigation of a Mach 15 flow over a blunt wedge using first-principles potential energy surfaces: influence of wall temperature

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I. Introduction

The development of reliable models for the aerothermochemistry of the air flow surrounding a hypersonic vehicle still remains a difficult challenge due to the complex nonlinear couplings between internal energy relaxation, chemistry, transport phenomena, and fluid motion [1]. Due to their extreme cruise speeds, physically realistic simulations of these vehicles require finite-rate equations for free stream enthalpy redistribution into internal energy as well as chemical reactions. Further, a separate description of the average energy content contained in each of the internal energy modes of the gas is needed (thermal nonequilibrium). A single, local thermodynamic temperature becomes inaccurate, as local energy distributions may deviate from equilibrium Boltzmann distributions. While relatively small, these deviations have a significant impact on finite-rate processes in the gas [2–8]. The precise chemical state of the gas in the shock layer, generally a mixture of both molecular and atomic species, cannot be obtained by assuming local thermodynamic equilibrium, but it is the result of finite-rate chemical processes.

Based on these physical considerations, thermochemical nonequilibrium models were initially formulated using a simple, yet rather accurate, multi-temperature approximation. The local thermodynamic temperature of the gas is replaced by various temperatures corresponding to the average energy of each internal energy mode (rotational, vibrational, and electronic). Then, relaxation equations, e.g., the Jeans equation for rotation [9] and the Landau–Teller equation for vibration [10], are used to compute the net transfer of energy between external and internal energy modes. A key to the success of such a simplified description primarily relied on a physically realistic description of vibrational nonequilibrium, together with computational efficiency and ease of calibration against shock tunnel data [11]. Unfortunately, these models tend to have a worsening predictive capability outside the range of conditions of the experimental data used to calibrate them. In many scenarios, their formulation is inherently too simplistic to account for the subtle, yet important, non-Boltzmann effects present in regions of the flow that are in strong thermochemical nonequilibrium.

A much researched alternative to multi-temperature models is represented by state-to-state (StS) formulations. State-to-state models are an accurate, but more expensive alternative to a multi-temperature description, because molecular distributions are explicitly tracked via a master equation [12, 13] that takes as inputs all transition rates between each and every internal molecular state. Such distributions need not be assumed to be equilibrium Boltzmann distributions, but are the result of the local thermochemical state of the gas. If these transition rate coefficients are obtained from first-principles [14], this method removes any empiricism. However, due to the very large number of transitions that must be accounted for with adequate statistical uncertainty [15], the StS formulation quickly becomes computationally intractable for systems comprising more than three particles (e.g., N_2+N_2). Approximations to reduce the computational cost have been thoroughly investigated and, to simplify, are aimed at binning energy states together [16]. The inevitable loss of accuracy from these model reductions should then be estimated via a comparison with results obtained without such biases [17]. Recently, several authors [18–22] have conducted computational fluid dynamics (CFD) studies of high-enthalpy flows using StS models for air species. In all results, it was observed that the StS models provide better predictions for shock stand-off distances [18, 21] for air flows over spheres [23] compared

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to the results obtained from two-temperature models. Discrepancies in heat flux predictions between the StS and two-temperature models were also observed, with the former predicting a lower heat transfer rate [21]. For some flows [22], such differences were shown to be relatively minor. The improved accuracy of StS models is attributed to their ability to describe nonequilibrium vibrational energy distributions throughout the flow [18].

In this work, we discuss the Direct Molecular Simulation (DMS) of a two-dimensional, reactive 5-species (N_2 , O_2 , NO, N, and O) air flow over a blunt wedge at conditions where significant thermal and chemical nonequilibrium is observed in the shock layer.

Derived from the direct simulation Monte Carlo (DSMC) method of Bird [24] each DMS particle undergoes a sequence of collisions while transiting in the flow domain or for the duration of the simulation while in the simulation box. The post-collision states are all the internal atomic coordinates (position and velocities in the center of mass reference frame) and the center of mass velocity at the end of each trajectory. These post-collision states in turn become the initial conditions needed to time propagate the successive trajectory, or next collision, that the particle undergoes in the simulation domain. Bound-bound transitions, bound-free transitions, or exchange reactions are all possible outcomes of each trajectory. No electronic excitation is permitted and, thus, the gas mixture remains in its electronic ground state, i.e., so-called 5-species air.

Like DSMC, a time-accurate gas flow simulation is possible, and the steady-state nonequilibrium molecular energy and velocity distributions can be obtained at each point in the flow [25, 26]. No decoupling or grouping of states is necessary because trajectories determine the state transition, without *a priori* restrictions, solely as a function of the local gas microscopic state and the PES on which the interaction occurs. This feature makes the DMS method essentially assumption-free, and thus, DMS solutions have been used to benchmark reduced-order models, for example coarse grained StS models [17], phenomenological DSMC [25], and, more recently, CFD multi-temperature models [26].

The work presented here represents a continuation of our previous efforts to obtain the entire hypersonic aerothermodynamic field around a two-dimensional (or axisymmetric) body at near-continuum conditions that are physically representative of hypersonic laminar flow conditions. Here, we extend the investigation to multiple wall temperatures. This approach provides solutions where the coupling between the gas flow mechanics, the local gas-phase thermochemical nonequilibrium, and the diffusive mechanisms for mass, momentum, and energy are all obtained within a consistent, empiricism-free framework. Select comparisons with state-of-the-art computational fluid dynamic solutions obtained with NASA Fun3D [27] will be detailed.

II. Molecular interaction models: *ab initio* potential energy surfaces

The DMS method requires interaction potentials between the various gas particles present in the flow. As we only consider 5-species air, potential energy surfaces (PESs) for N_2 , O_2 , NO, N, and O in their ground electronic state are needed. In general, for a chemically reacting air mixture, molecular collisions occur between two diatomic molecules (e.g., N_2+O_2), between a diatomic molecule and an atom (e.g., $\text{NO}+\text{O}$), or between two atoms (e.g., $\text{O}+\text{N}$). For flows around an object, all these interactions must be included.

In this work, we utilize *ab initio* surfaces for nearly all interactions, with only two notable exceptions, namely N_2+NO and O_2+NO trajectories. Within a first-principles description of ground-electronic-state air, each interaction may be described by multiple surfaces, which are the result of spin and spatial degeneracies. All *ab initio* PESs are found in Potlib [28], an open-source repository maintained by the Theoretical and Computational Chemistry group at the University of Minnesota.

As of the preparation of this abstract, a full or partial *ab initio* treatment for N_2+NO and O_2+NO interactions is still unavailable. At typical shock layer temperatures, reaching as high as 10,000 K, nearly no oxygen remains in a molecular form [29], whereas only marginal molecular nitrogen dissociation occurs [2]. Therefore, with the exception of very high Mach regimes, for example for planetary entry, the mass fraction of molecular nitrogen would be quite close to the free stream value, whereas abundant atomic oxygen would be present. Due Zeldovich processes, collisions between O and N_2 produce a significant amount of NO, which in turn would readily collide with the similarly abundant N_2 . Hence, $\text{NO}+\text{N}_2$ and, to a lesser extent, $\text{NO}+\text{O}_2$ collisions are expected to be important as far as mass, momentum, and energy diffusion mechanisms are concerned. For this reason, these interactions cannot be omitted. So, we decided to use semi-empirical surfaces for these interactions [30]. Although not first-principles, these surfaces were built using sound physical considerations. The $\text{NO}+\text{N}_2$ and $\text{NO}+\text{O}_2$ surfaces have a simple analytic form. Nonetheless, they were shown to well-reproduce NO vibrational relaxation times and provide reasonable results for NO dissociation.

A summary of the PESs used in this work is contained in Table 1 with the corresponding references. Note that for

Table 1

Interaction	Reference	No. of PESs
$N_2 + N_2$	Bender et al. [15]	1
$N + N_2$	Varga and Truhlar [31]	1
$N + N$	Li et al. [32]	1
$N_2 + O_2$	Varga et al. [33]	1
$N_2 + O$	Lin et al. [34]	2
$N_2 + NO$	Andrienko and Boyd [30]	1*
$N + O_2$	Varga et al. [35]	3
$N + O$	Varga et al. [33]	1
$N + NO$	Lin et al. [34]	2
$O_2 + O_2$	Paukku et al. [36] Paukku et al. [37]	3
$O_2 + O$	Varga et al. [38]	9
$O_2 + NO$	Andrienko and Boyd [30]	1*
$O + NO$	Varga et al. [35]	2
$O + O$	Paukku et al. [37]	1
$NO + NO$	Varga et al. [33]	1

Table 2 Free stream conditions.

Mach	ρ_∞ [g/m ³]	T_∞ [K]	v_∞ [m/s]	$[O_2]_\infty$	$[N_2]_\infty$
15.	1.0	250	4955	0.2	0.8

some of the listed PESs, neural network fits were also provided in Potlib [28]. In this work, however, all PESs were based on permutation-invariant polynomial fits.

III. Simulation details

A Mach 15 air flow over a blunt wedge is presented in this work. The free stream conditions are listed in Tab. 2. The blunt wedge has a leading edge radius of 1 cm, a half angle of 15°, and a total length of 5 cm. A schematic of the geometry and boundary conditions is shown in Fig. 1. In particular, particles are injected into the flow domain across a parabolic inflow surface. This was done to minimize the extent of the *free stream* region in order to reduce the computational resources needed. The simulation domain box was likewise sized so that the bow shock would not impinge on the upper specular wall. The outflow is considered supersonic, i.e., there is no back pressure.

At variance with our previous study [39], the wall is modeled using a viscous boundary condition. Particles impinging on the wedge surface are reflected diffusely with both internal and external modes fully accommodated with the wall temperature. We extended our previous analysis [40] to consider two wall temperatures, namely 1000 K and to 2000 K. Energies for the scattered molecules were distributed according to equilibrium distributions, namely Maxwell-Boltzmann for the external modes and Boltzmann for the internal modes.

Finally, based on the free stream mean free path, we estimated a Knudsen number of $\sim 10^{-3}$ based on the wedge leading edge radius. Considering the density jump across the bow shock, this flow can be considered at near-continuum conditions in the shock layer.

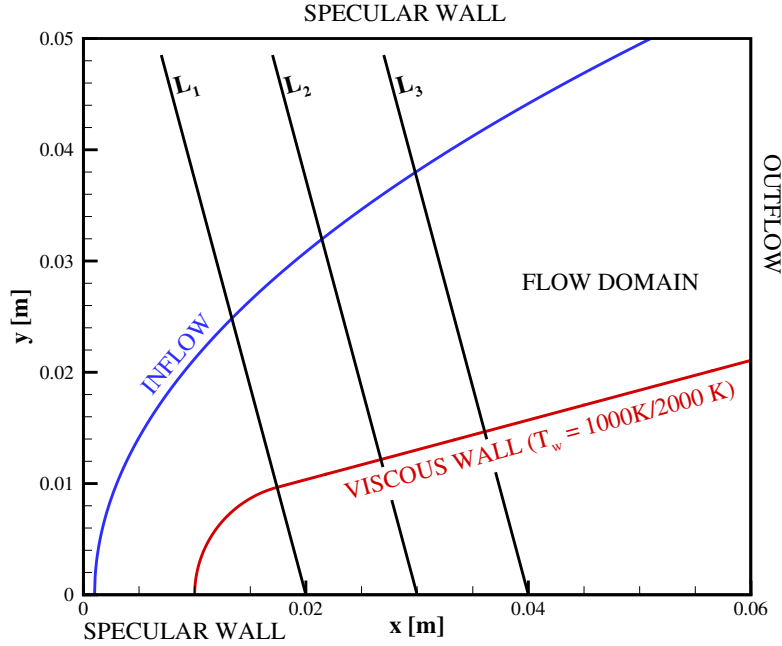


Fig. 1 Simulated geometry and boundary conditions.

IV. Results

An overview of the flowfield is shown in Fig. 2 where the ro-translational temperature T_{t-r} across the simulation domain is shown. The Mach 15 air flow is compressed by the blunt wedge, resulting in the formation of a bow shock, where temperatures exceed 12000 K. The hot gas then cools down to the imposed wall temperature set to 1000 K. The comparison between the DMS and CFD solutions, illustrated in Fig. 2, reveals similar qualitative features, where the most evident difference is the larger shock stand-off distance seen in the DMS result.

In Fig. 3, we show the vibrational thermal nonequilibrium parameter, defined as [26]:

$$\eta_{vib} = \frac{T_{t-r} - T_{vib}}{T_{t-r}}, \quad (1)$$

which reduces to zero under local thermal equilibrium, where the rotranslational (T_{t-r}) and vibrational (T_{vib}) temperatures coincide. As evidenced by both the DMS and CFD solutions, the slow relaxation rate of vibrational modes leads to significant vibrational nonequilibrium throughout the shock layer. The vibrational temperature significantly *lags* the translational one throughout most of the shock layer. Near the nose-wall junction, it can be seen that $\eta_{vib} < 1$ and remains negative along the flat wedge surface, due to the rapid expansion that produces a vibrationally frozen flow. This internal energy *freezing* is more pronounced in the DMS result, thus suggesting a slower relaxation process than predicted by CFD.

This qualitative difference between DMS and CFD is clearly revealed by the stagnation-line profiles, shown in Fig. 4, where it can also be seen that the DMS predicted shock layer temperatures remain substantially higher than those predicted by CFD before equilibration with the wall temperature, set to 1000 K.

The chemical activity in the flow is shown in Fig. 5, where the mass fractions for each air component (N_2 , O_2 , NO, N, and O) are plotted. Both molecular oxygen and nitrogen undergo dissociation in the hot shock layer near the stagnation point. As shown in Fig. 5, O_2 nearly completely dissociates, whereas N_2 dissociation is also significant, but more modest. The availability of atomic oxygen in the presence of relatively abundant molecular nitrogen is responsible for the production of NO seen in Fig. 5. The first Zeldovich reaction $N_2 + O \rightarrow NO + N$ is likely to be primarily responsible for the NO formation in the vicinity of the stagnation point. The second Zeldovich reaction $O_2 + N \rightarrow NO + O$ is likely to be secondary, as the availability of molecular oxygen quickly reduces along the stagnation streamline, whereas the availability of atomic nitrogen is limited. Nonetheless, both reactions are likely to take place

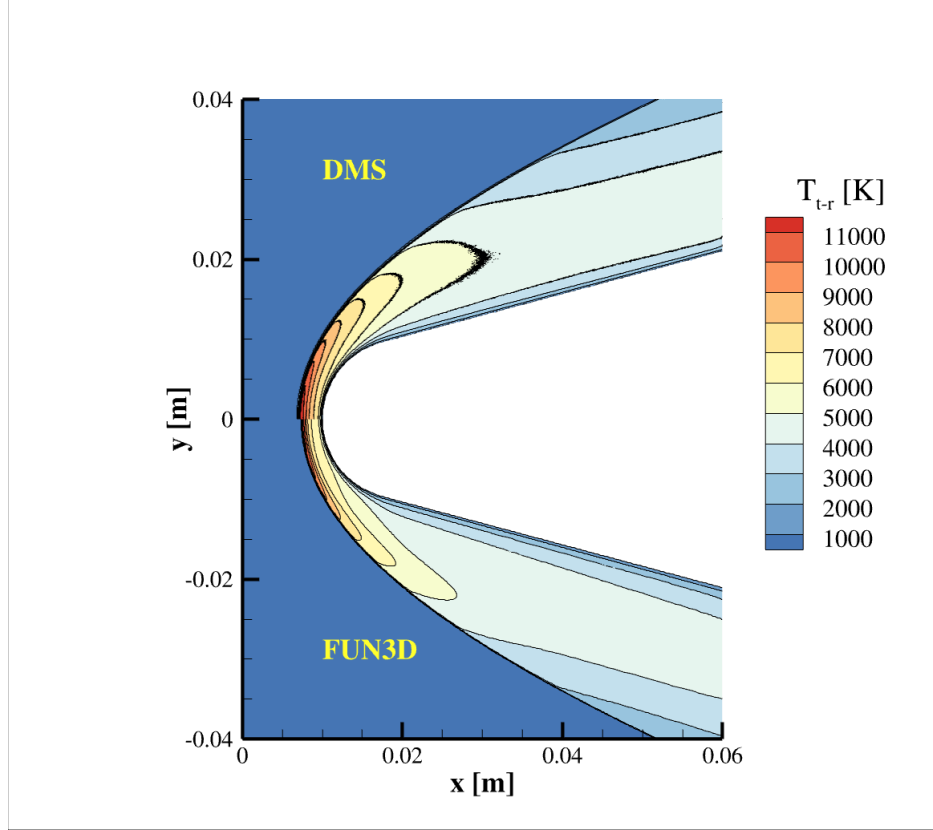


Fig. 2 Rotranslational temperature variation across the flowfield around the blunt wedge.

in the DMS simulation, albeit at reactant-limited speeds. Atomic nitrogen reaches concentrations around 2-3% near the stagnation point, whereas atomic oxygen is much more abundant ($\sim 10\%$) due to the near-complete dissociation of molecular oxygen.

The stagnation streamline profiles for O, NO, and N are shown in Fig. 6, where the wall temperature is set to 1000 K or 2000 K. Quite interestingly, the CFD results for the chemical makeup of the gas along the stagnation streamline almost negligibly affected by the wall temperatures, particularly at the wall. The DMS profiles, on the other hand, exhibit a more significant dependence on wall temperature, particularly near the wall, where the mass fractions of atomic oxygen and nitric oxide are significantly lower for the colder wall test case.

V. Conclusions and Future Work

The simulations that we will present at Scitech 2026 represent a fundamental description of high-temperature air thermochemistry in a hyper-velocity flow. All the newest and most accurate *ab initio* PESs available to describe molecular-level interactions among air species were used. The conference article will present a detailed analysis of the results extracted from simulations at various wall temperatures, together with comparisons with CFD results along various extraction lines across the flow field. The objective of the work is to provide a near-assumption-free, continuum-level test case useful to enhance the fidelity of reduced-order descriptions used in CFD, like the increasingly popular modified Marrone and Treanor model (MMT) [41].

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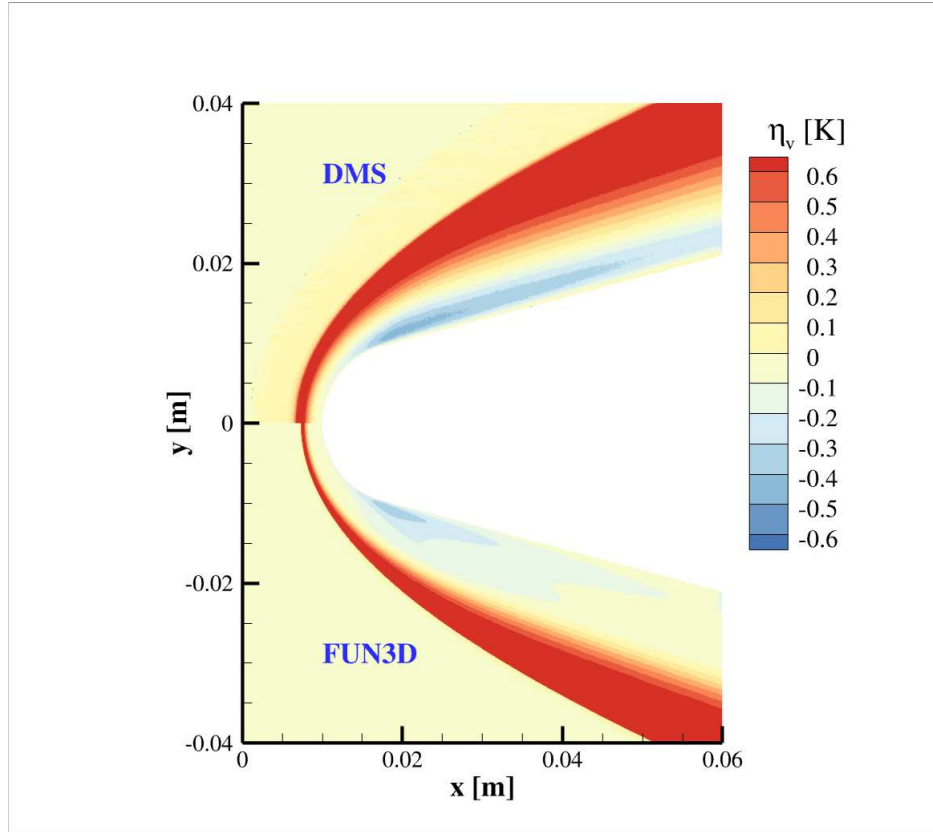


Fig. 3 Vibrational nonequilibrium parameter across the flowfield around the blunt wedge.

the Department of Defense, or the U.S. government.

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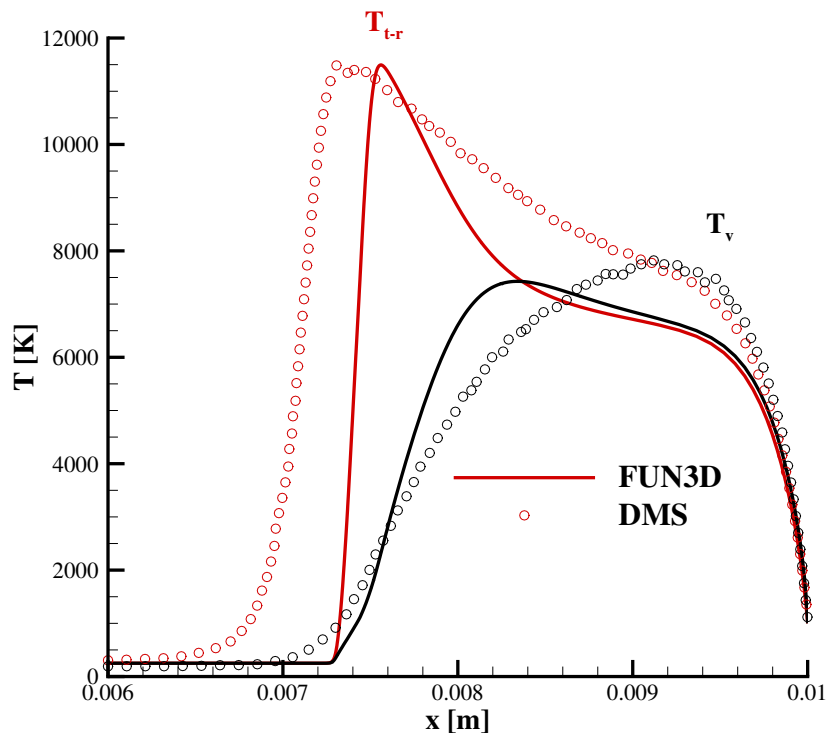


Fig. 4 Rotranslational and vibrational temperature profiles along the stagnation line as predicted by DMS and CFD for a wall temperature set to 1000 K.

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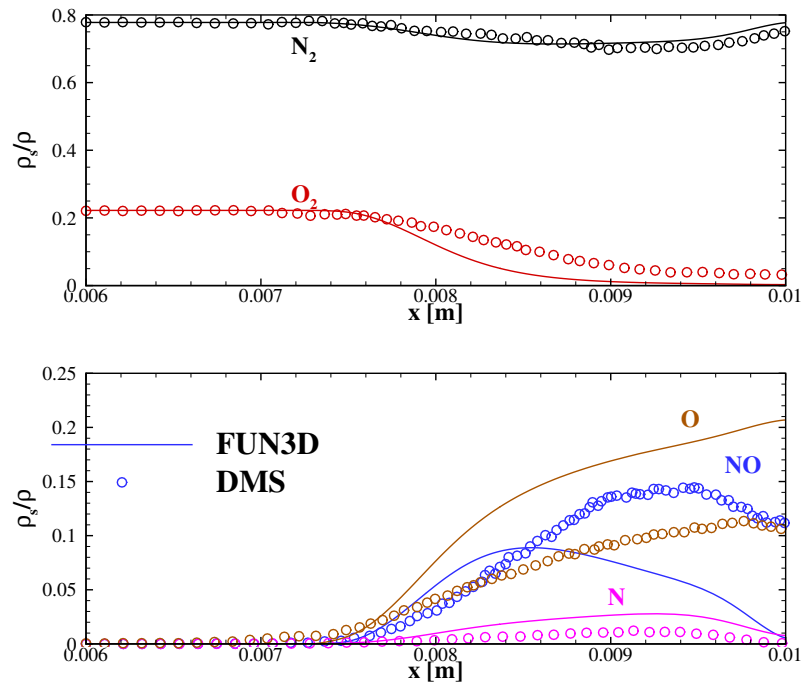


Fig. 5 Flow field mass fractions predicted by DMS and CFD for a wall temperature set to 1000 K.

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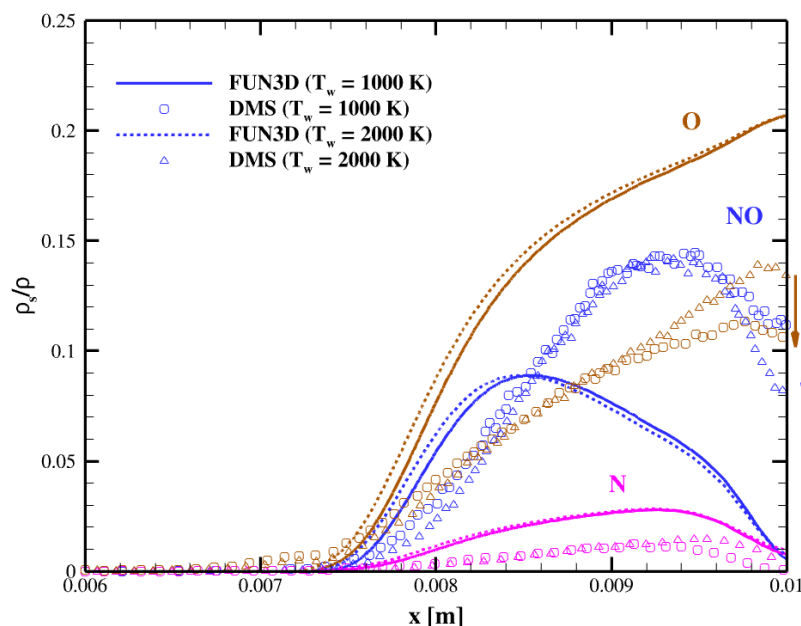


Fig. 6 Flow field mass fractions for O, NO, and N predicted by DMS and CFD.

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