

Evaluation of SPARTA DSMC tool for Chemistry modeling in high temperature flows

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Abstract—The evaluation of open-source implementation of Direct Simulation Monte Carlo (DSMC) tool, SPARTA for chemistry modeling in high temperature flows is presented. The chemistry modeling is carried out using total collision energy method. The chemical non-equilibrium conditions occurring such as dissociation of N_2 and O_2 , exchange reactions and combined reactions in air are simulated in an adiabatic box with an initial temperature and pressure. The results such as the time variation of temperature and total number of particles are presented and discussed in this paper.

I. INTRODUCTION

In the hypersonic flow, the geometry of the body is a critical consideration in design. The main objective of the shape design is to reduce the surface heating by increasing the heating of air in the upstream of flow. Such intense heating will lead air to become chemically unstable. The resulting dissociation and exchange reactions are endothermic and cause a reduction in the temperature. The bluntness (the radius at stagnation point) of the shape is an important parameter which influences the aerodynamic heating in the surface [1].

In rarefied hypersonic flows the continuum concept is not valid especially in the near wall region. The ratio of mean free path of the gas molecule and characteristic length (Knudsen number) is the parameter which defines range of rarefaction in a flow. The solution of Navier-Stokes equation becomes invalid in the rarefied regimes ($Kn_\infty > 0.1$). The solution of Boltzmann equation is valid in all flow regimes. The complexity in the solution of Boltzmann equation led to the development of a simple and computationally affordable technique called Direct Simulation Monte Carlo (DSMC) Method [2] to predict the flow. DSMC method is a statistical approach which emulate the physical processes modeled by Boltzmann equation. DSMC is practically feasible as compared to the molecular dynamics simulation.

II. COMPUTATIONAL METHOD

DSMC method is a particle based simulation in which a simulated molecule, represent a much larger ensemble of molecule tracked through space and time. The movement of particle and collision between particles are computationally decoupled. The movement of each particle is linear in nature as prescribed by its velocity vector and time-step increment. The reorientation in the particle trajectory occurs as a result of collision with wall and intermolecular collisions. The particle motion and surface collision are deterministic and

intermolecular collisions are probabilistic. The collision rate is set based on kinetic theory of gas and probability of collision between collision pairs is found out by acceptance-rejection method. The collision and chemistry can be approximate using available phenomenological models. The macroscopic properties is found out from ensemble average of the properties of the particles.

III. SPARTA

SPARTA (Stochastic PARallel Rarefied-gas Time-accurate Analyzer) is an open-source Direct Simulation Monte Carlo (DSMC) code developed by Sandia National Laboratories [4], [3]. The first public release of SPARTA DSMC code is done on 29th July 2014 under GNU license.

The features of SPARTA includes 2d, 3d and axisymmetric geometric capability, steady as well as unsteady simulation capability, hierarchical Cartesian grid with multiple levels of local refinement, ability to define symmetric, thermal wall and free stream boundary conditions, parallel processing with message-passing techniques and a spatial-decomposition of the simulation domain and capable of easy modification and extending with new functionalities. The grid is used to group particles by grid cell for performing collisions and chemistry computations. Physical objects with triangulated surfaces can be embedded in the Cartesian grid by creating cut and split on grid cells. The grid is also used to compute particle/surface collisions.

SPARTA includes Variable Hard Sphere (VHS) [2] and Variable Soft Sphere (VSS) [6] models for approximation of molecular interaction and Total Collision Energy (TCE) model for handling chemistry.

IV. THERMOCHEMISTRY EFFECTS

The gas in the Earth atmosphere may be assumed to be a binary mixture of oxygen (O_2) and nitrogen (N_2). In the DSMC methodology, particles must be provided with the correct properties to capture kinetic and rotational modes of energy storage. Vibrational excitation of the gas molecules as well as dissociation of both oxygen and nitrogen are likely to be important features of the flow around any hypersonic vehicle at the higher altitudes such as (80 – 120 km). Even at lower speeds and altitudes vibrational excitation and limited dissociation of oxygen are likely to be important [1]. Such

real-gas effects need to be properly accounted for. The DSMC technique normally models air as either a 5-species mixture using dissociation, recombination and exchange reactions, or as a mixture of 11-species including ionization. In conventional CFD, reaction rates are calculated according to the Arrhenius law [1]. However, this relies on data sourced from equilibrium conditions, which may be inappropriate for rarefied hypersonic flows. In contrast, the DSMC method, with its particulate approach, is able to capture successfully the thermo-chemical non-equilibrium effects encountered in high speed rarefied gas environments [5], [7].

V. CHEMICAL REACTIONS

Chemical reactions in SPARTA code is handled by means of the Total Collision Energy (TCE) model [2]. The TCE model determine the reaction probabilities based on the defined reaction rate. This model treats the ratio of the cross-section for a given reaction to the total collision cross-section as a function of the total energy (translational and internal) of the two colliding particles. Bird [2] lays out the process for determining the reaction cross-section as a function of the collision energy, and for determining the parameters of this function based on the parameters of an Arrhenius-type rate equation. An Arrhenius-type rate equation has the form

$$k(T) = \Lambda T^\eta e^{E_a/k_b T} \quad (1)$$

where Λ and η are reaction-specific constant, E_a is the activation energy for the reaction, k_b is the Boltzmann constant, and T is the temperature of the gas. This form is not directly useful in DSMC because reactions and collisions in DSMC are handled by means of cross-sections, and so the Arrhenius parameters (Λ , η and E_a) must be used to obtain an equation for the cross section. Two such equations are derived in Bird [2], one for two body reactions such as exchange and dissociation reactions, and second one for three body reactions such as recombination reactions. The equation for two-body reactions is

$$\frac{\sigma_R}{\sigma_T} = \frac{\pi^{1/2} \varepsilon \Lambda T_{ref}^\eta}{2\sigma_{ref} (k_b T_{ref})^{\eta-1+\omega_{AB}}} \frac{\Gamma(\bar{\zeta} + 5/2 - \omega_{AB})}{\Gamma(\bar{\zeta} + \eta + 3/2)} \left(\frac{m_r}{2k_b T_{ref}}\right)^{1/2} \frac{(E_c - E_a)^{\eta+\bar{\zeta}+1/2}}{E_c^{\bar{\zeta}+3/2-\omega_{AB}}} \quad (2)$$

The equation for three-body reactions is

$$\frac{\sigma_R}{\sigma_T} = \frac{\pi^{1/2} n_T \varepsilon \Lambda T_{ref}^\eta}{2\sigma_{ref}} \frac{\Gamma(5/2 - \omega_{AB})}{\Gamma(\eta + 3/2)} \left(\frac{m_r}{2k_b T_{ref}}\right)^{1/2} \left(\frac{E_c}{k_b T_{ref}}\right)^{\eta-1+\omega_{AB}} \quad (3)$$

where $\frac{\sigma_R}{\sigma_T}$ is the ratio of cross-section for the given reaction to the total cross-section intensification between the two particles. A and B are the main reacting species, ε is a symmetry factor which is equal to 1 if $A \neq B$ and 2 if $A = B$. σ_{ref} , T_{ref} and ω_{AB} are VHS parameters for collisions between species A and species B, $\bar{\zeta}$ is the average number of degrees of freedom which contribute to the collision energy, n_T is the number density of the third body, m_r is the reduced mass of species A and B, E_c is the total collision energy (translational+internal),

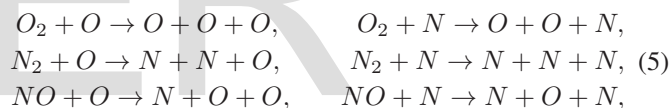
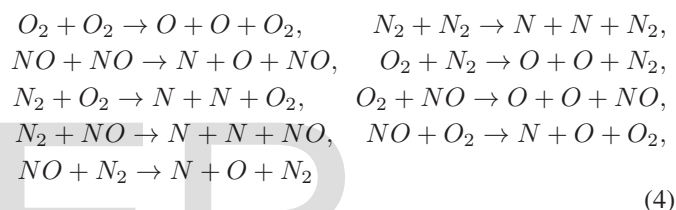
and Γ is the gamma function. The above equation for three-body reactions assumes that the activation energy for these reactions is zero, which is the case for all recombination reactions relevant to five-species air chemistry.

Bird [2] assumes that the reaction cross-section will be small relative to the VHS collision cross-section, which allows for the VHS collision cross-section to be treated as the total cross-section for use in the above equations. The advantage of this assumption is that reaction cross-sections only need to be calculated after a pair has been accepted for collision, rather than when the pair is initially selected.

Arrhenius rates for the reactions of different species of air have been reported in number of publications such as Gupta et al. [8] and Scanlon et al. [9]. In this work, Arrhenius rates provided by Scanlon et al. is used.

VI. AIR CHEMISTRY

The details of chemical reactions and molecular properties of different species of air is taken as given in the following. Chemical reactions in air includes nine molecule-molecule dissociations as in equation 4 and six molecule-atom dissociations as in equation 5.



The table I shows the molecular properties of species associated with the reactions in air. The reaction specific constant and activation energy of reactions are taken as per Scanlon [9].

TABLE I. MOLECULAR PROPERTIES OF SPECIES IN AIR

ID	Mol. weight	Mol. mass (kg)	Rot. dof.	Rot. rel. no.	Vib. dof.	Vib. reln. no.	Vib. temp. (K)
O2	32.00	5.31E-26	2	0.2	2	5.58659E-5	2256
N2	28.016	4.65E-26	2	0.2	2	1.90114E-5	3371
O	16.00	2.65E-26	0	0	0	0	0
N	14.008	2.325E-26	0	0	0	0	0
NO	30.008	4.98E-26	2	0.2	2	7.14285E-4	2719
O2+	32.00	5.31E-26	2	0.2	2	5.58659E-5	2256
N2+	28.016	4.65E-26	2	0.2	2	1.90114E-5	3371
O+	16.00	2.65E-26	0	0	0	0	0
N+	14.008	2.325E-26	0	0	0	0	0
NO+	30.008	4.98E-26	2	0.2	2	7.14285E-4	2719
e	0.001	9.109E-31	0	0	0	0	0

VII. RESULTS AND DISCUSSION

A cubical box of sides 1×10^{-5} m with six reflective surfaces is considered for the simulation. A total of 23,100 simulated particles with initial temperature of 20,000 K and a pressure of 0.063 atm is taken for the simulation. The computation is carried out for a total physical time of 1×10^{-4} s using a time-step of 1×10^{-10} s.

A. Non equilibrium dissociation of Oxygen (O_2)

Forward reactions on non equilibrium dissociation of Oxygen considered are $O_2 + O_2 \rightarrow O + O + O_2$ and $O_2 + O \rightarrow O + O + O$. The other reactions and recombination are not accounted. The value of initial species fraction of 1 is taken for O_2 species. The figure 1 shows the time variation of total number of particles. Figure 2 shows the variation of temperature with time. As dissociation reaction continues, due to endothermic nature of dissociation reaction the temperature reduces. The rate of reduction of temperature is same as the rate of increase of number of total particle as expected. The temperature reduced from initial 20,000 K to approximately 6,300 K at $1 \times 10^{-5} s$. The temporal variation of temperature of non-equilibrium dissociation of Oxygen obtained from the present computation is found to be in close agreement with that of the results of Scanlon et al. [9] as shown separately in figure 3. This results shows the importance of including chemistry in the flows which involves high temperatures such as hypersonic flow. This results also demonstrate the capability of opensource DSMC tool SPARTA for handling chemistry enabled flows.

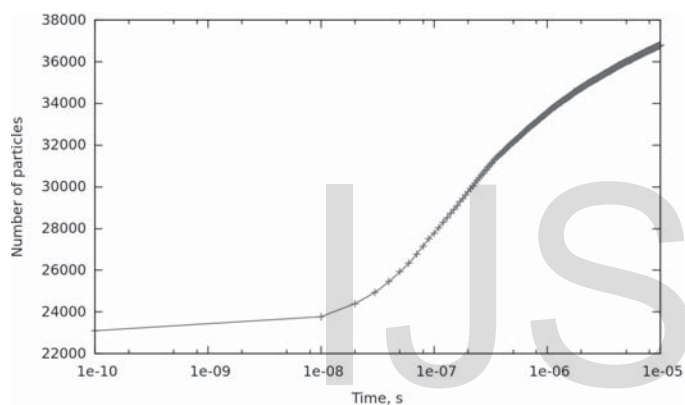


Fig. 1. The variation of number of particles with time for $O_2 \Rightarrow O$

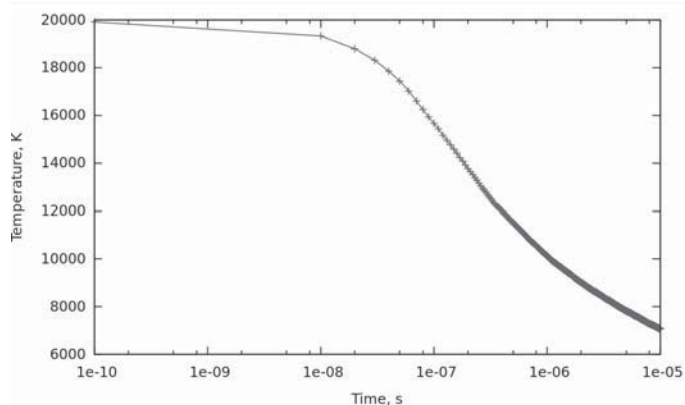


Fig. 2. The variation of temperature with time for $O_2 \Rightarrow O$

B. Non equilibrium exchange reaction

In this case forward exchange reaction between N_2 and O such as $N_2 + O \rightarrow NO + N$ is considered for simulation. All other reactions and backward reactions are not accounted. An equal initial species fraction is used for N_2 and O species. The initial temperature and pressure is set same as the previous

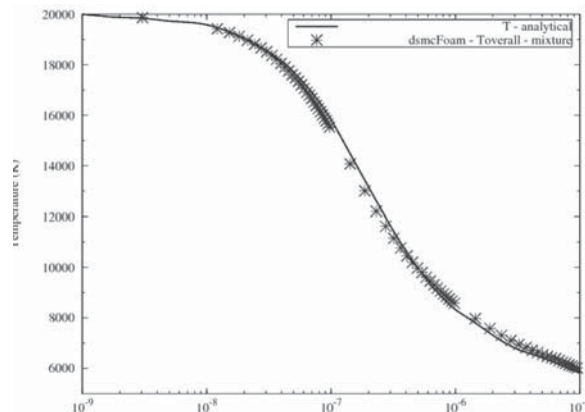


Fig. 3. The variation of temperature with time from Scanlon et al. [9] for $O_2 \Rightarrow O$

case. Figure 4 shows the variation of total number of particles during the reaction time. The decline of temperature from 20,000 K to approximately 13,250 K at $1 \times 10^{-4} s$ indicate endothermic nature of reaction and is shown in figure 5.

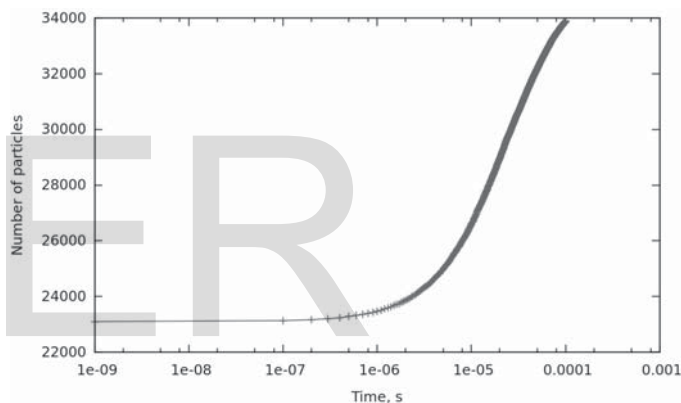


Fig. 4. The variation of number of particles with time for $N_2 + O \rightarrow NO + N$

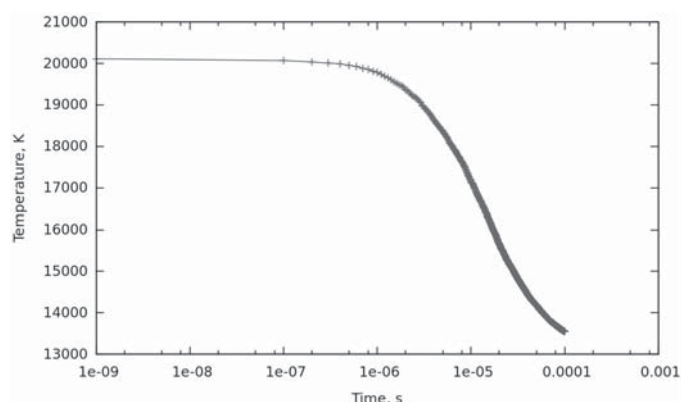


Fig. 5. The variation of temperature with time for $N_2 + O \rightarrow NO + N$

C. Air reactions

The complete set of reactions shown in equations 4 and 5 are considered in an adiabatic box filled with air at 0.063

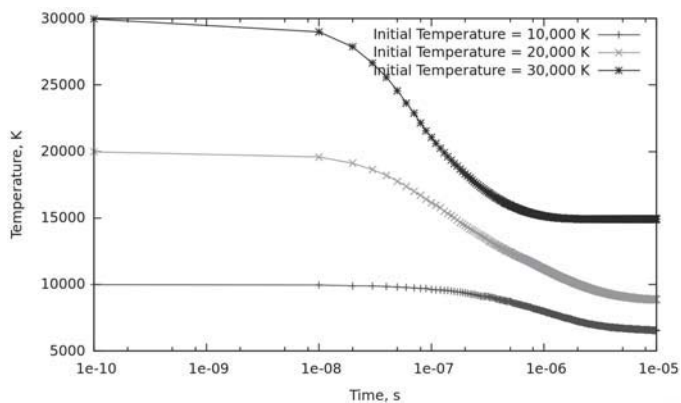


Fig. 6. The variation of temperature with time for reactions in air

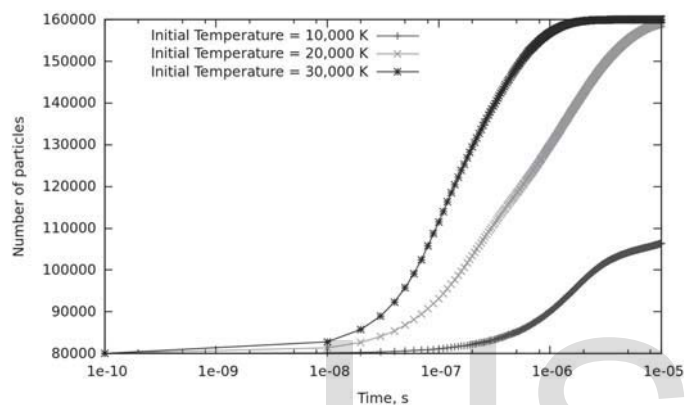


Fig. 7. The variation of number of particles with time for reactions in air

atm pressure with an initial composition of 79% of N_2 and 21% of O_2 . The simulation is carried out using a total number of 80,000 simulated particles for three different initial temperatures such as 10,000 K, 20,000 K and 30,000 K. The transient variation of temperature obtained is shown in figure 6. The declination of temperature is observed in the all initial values of temperature. After a physical time of $1 \times 10^{-5} s$ a temperature drop of 15,000 K, 11,000 K and 3,500 K is observed for case with initial temperature of 30,000 K, 20,000 K and 10,000 K simultaneously. Figures 7, 8 and 9 show the transient variation of total number of particle, number of collisions per time step and reactions per time step. It can be observe that after approximately $8 \times 10^{-6} s$ the variation of parameters are negligible, which indicate that the domain is approaching equilibrium condition.

VIII. CONCLUSIONS

An open source tool SPARTA having DSMC chemistry model based on the TCE approach has been evaluated for different chemical non-equilibrium conditions associated with air reactions. The code is validated for dissociation of O_2 from an initial temperature and pressure. The simulation is extended for forward exchange reaction and combined air reactions. The reduction in temperature due to endothermic nature of reactions, and the change in total number of particles are obtained. The air reactions are carried out with three different values of initial temperatures such as 10,000 K, 20,000 K and 30,000 K and results obtained are presented. The present

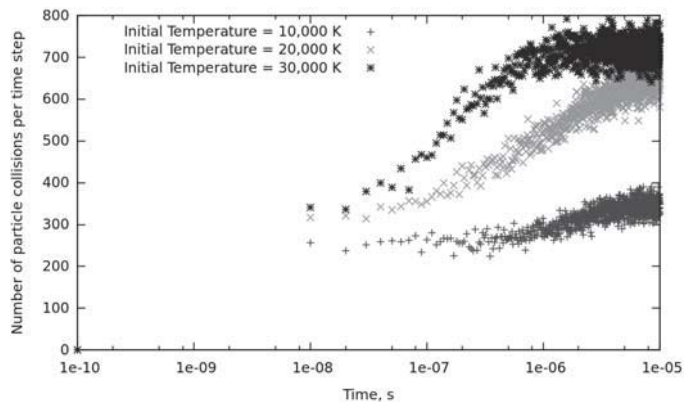


Fig. 8. The variation of number of collisions with time for reactions in air

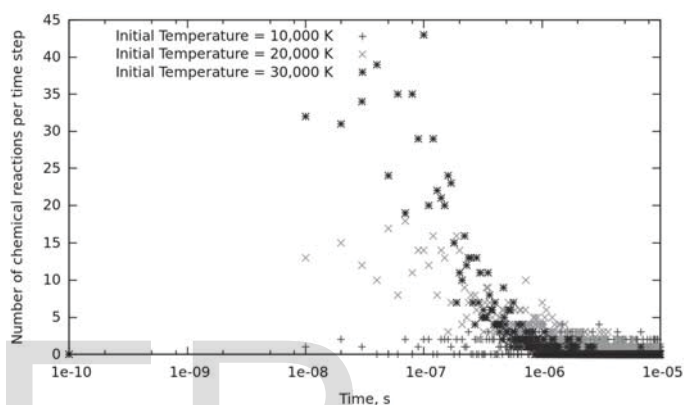


Fig. 9. The variation of number of reactions with time for reactions in air

study establishes the capability of SPARTA DSMC tool to handle hypersonic flow simulation by incorporating chemical kinetics. This study also point out the necessity of including chemistry in the high temperature flow simulation.

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