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Comparison of transport properties models for numerical simulations of Mars entry vehicles

Jiaao Hao[a], Jingying Wang[b,*], Zhenxun Gao[a], Chongwen Jiang[a], Chunhian Lee[a]

[a] School of Aeronautical Science and Engineering, Beihang University, Beijing 10091, China
[b] School of Energy and Power Engineering, Shandong University, Jinan, Shandong 250100, China

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ABSTRACT

Effects of two different models for transport properties, including the approximate model and the collision integral model, on hypersonic flow simulations of Mars entry vehicles are numerically investigated. A least square fitting is firstly performed using the best-available data of collision integrals for Martian atmosphere species within the temperature range of 300–20,000 K. Then, the performance of these two transport properties models are compared for an equilibrium Martian atmosphere gas mixture at 10 kPa and temperatures ranging from 1000 to 10,000 K. Finally, four flight conditions chosen from the trajectory of the Mars Pathfinder entry vehicle are numerically simulated. It is indicated that the approximate model is capable of accurately providing the distributions of species mass fractions and temperatures in the flowfield. Both models give similar translational-rotational and vibrational heat fluxes. However, the chemical diffusion heat fluxes predicted by the approximate model are significantly larger than the results computed by the collision integral model, particularly in the vicinity of the forebody stagnation point, whose maximum relative error of 15% for the super-catalytic case. The diffusion model employed in the approximate model is responsible to the discrepancy. In addition, the wake structure is largely unaffected by the transport properties models.

1. Introduction

Robotic sample return and human exploration missions will be performed for future Mars exploration programs, which require the appropriate modeling of the multi-physicochemical phenomena and the accurate prediction of the aerothermodynamic environment including the hypersonic flowfield characteristics and the surface heat transfers of Mars entry vehicles [1].

In the literature of hypersonic numerical simulations, it was found that different models of transport properties can significantly affect the predicted flowfield and the surface heat transfers of planetary entry vehicles [2–4]. However, in these studies, the reentry conditions for the Earth atmosphere are evaluated with much more attention than the Mars entries. Chen et al. [5] simulated the nonequilibrium flowfield around the MESUR probe. The results demonstrated that the surface heat transfers are very sensitive to models selected for the transport properties. Papadopoulos et al. [6] performed a comparison study among different transport models in three codes, including GASP, GIANTS, and LAURA, for the Mars 2001 orbiter. The results indicated that the diffusion model can have a significant impact on the catalytic surface heating. Bose et al. [7] conducted a Monte Carlo sensitivity and uncertainty analysis for the predictions of laminar convective heat transfer over the Mars Pathfinder entry vehicle. It was found that the transport properties contributed a large portion of the uncertainty, especially in high catalytic regimes. The objective of the present paper is to extend the previous studies to more general Martian atmospheric entry conditions, and to make a deeper evaluation about the effects of transport properties models on flowfield characteristics and surface heat transfer for both the forebody and the afterbody of Mars entry vehicles. The past successful Mars entry vehicles include Viking I & II, Pathfinder, Mars Exploration Rover (MER) A & B, Phoenix, and Mars Science Laboratory (MSL). Pathfinder, MER A & B, and Phoenix share a similar forebody geometry, but their afterbodies are different with those of Viking I & II and MSL. To ascertain the range of effect of the transport properties models, the Mars Pathfinder vehicle is chosen as the test case due to the highest entry velocity [8] and the resulting intensive thermo-chemical nonequilibrium process.

In this study, hypersonic thermo-chemical nonequilibrium flows over Mars entry vehicles are numerically investigated using the two-temperature model and an 8-species finite rate chemical reaction model. Firstly, the performances of different transport properties models are compared for an equilibrium Martian atmosphere gas

* Corresponding author.
E-mail address: wjy_sdu@126.com (J. Wang).

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Table 1
Species vibrational energy data [11].

Species	g_r	$\theta_{v,r}$ (K)
CO_2 (bending)	2	945
CO_2 (symmetric)	1	1903
CO_2 (antisymmetric)	1	3329
CO	1	3074
O_2	1	2239
N_2	1	3395
NO	1	2817

mixture at 10 kPa and temperatures ranging from 1000 to 10,000 K. The MSL experimental model is then used as a test case to evaluate the capability of the present code to reproduce the surface heating experimental data. Finally, four flight conditions chosen from the trajectory of the Mars Pathfinder entry vehicle are numerically simulated with different transport properties models.

2. Thermo-chemical nonequilibrium model

The hypersonic thermo-chemical nonequilibrium flow of a Mars entry vehicle is described by Park's two-temperature model [9]. It is assumed that the translational-rotational energy mode is fully excited in terms of a translational-rotational temperature T_{tr}. The vibrational energy of molecules and the electron translational energy are in equilibrium corresponding to a vibrational-electron temperature T_{ve}. Among the chemical species considered in this paper, CO_2 is a linear triatomic molecule with three modes of vibration, namely, the doubly degenerate bending mode, the symmetric stretching mode, and the antisymmetric stretching mode [10]; the remaining molecular species are all diatomics with single vibration mode. Values for the species vibrational energy data are taken from Ref. [11] as listed in Table 1, where g_r and $\theta_{v,r}$ represent, respectively, the degeneracy and the characteristic vibrational temperature of each vibrational mode.

The energy transfer between the translational mode of heavy particles and the vibrational mode is obtained using the Landau–Teller model [12], with the vibrational relaxation time modeled by the Millikan–White expression [13]. The results of Camac [14] indicate that the energy transfer between the three vibrational modes of CO_2 is so fast that the translational-vibrational energy transfer can be characterized using a single vibrational relaxation time as given by

$$\tau_{v,CO_2}^{MW} = \frac{101325}{p}\cdot\exp[36.5T_{tr}^{-1/3} - 17.71] \quad (1)$$

To avoid the under-predicted relaxation time at high temperatures, Park's correction [9] is introduced. In addition, non-preferential model [15] is used to account for the added or removed vibrational energy due to chemical reactions.

In this paper, simulations are performed employing the 8-species (C, O, N, O_2, N_2, NO, CO, CO_2) finite rate chemical reaction model proposed by Micheltree and Gnoffo [16]. The Micheltree and Gnoffo model was originally reduced from the 18-species reaction model presented by Park et al. [17], while neglecting ionization reactions. Actually, the degree of ionization under the conditions of interest in this paper is expected to be small, and the Micheltree and Gnoffo model is capable of accurately predicting the surface heat fluxes under such conditions [7]. The vibrational-electron temperature T_{ve} degrades into a vibrational temperature T_v as a consequence.

The forward reaction rates are calculated by Arrhenius expressions, while the backward reaction rates are obtained via equilibrium constants. To consider the coupling effects between the thermal nonequilibrium and chemical reaction processes, a combination of the translational-rotational temperature and the vibrational temperature is implemented to define the reaction controlling temperature. For the Micheltree and Gnoffo model as given in Table 2, the first ten reactions are dissociation reactions controlled by the geometric average of T_{tr} and T_v, while the remaining reactions are controlled by T_{tr}.

Table 2
Reaction parameters for the Micheltree and Gnoffo reaction model [16].

No.	Reaction	A (cm^3/mol/s)	B	C (K)
1	CO + M ↔ C + O + M (M = atom)	3.4×10^{20}	−1.00	129,000
2	CO + M ↔ C + O + M (M = mol.)	2.3×10^{20}	−1.00	129,000
3	CO_2 + M ↔ CO + O + M (M = atom)	1.4×10^{22}	−1.50	63,275
4	CO_2 +M ↔ CO + O + M (M = mol.)	6.9×10^{21}	−1.50	63,275
5	O_2 + M ↔ O + O + M (M = atom)	1.0×10^{22}	−1.50	59,750
6	O_2 + M ↔ O + O + M (M = mol.)	2.0×10^{21}	−1.50	59,750
7	N_2 + M ↔ N + N + M (M = atom)	3.0×10^{22}	−1.60	113,200
8	N_2 + M ↔ N + N + M (M = mol.)	7.0×10^{21}	−1.60	113,200
9	NO + M ↔ N + O + M (M = C, N, O, NO, CO_2)	1.1×10^{17}	0.00	75,500
10	NO + M ↔ N + O + M (M = N_2, O_2, CO)	5.0×10^{15}	0.00	75,500
11	NO + O ↔ O_2 + N	8.4×10^{12}	0.00	19,450
12	N_2 + O ↔ NO + N	6.4×10^{17}	−1.00	38,370
13	CO + O ↔ O_2 + C	3.9×10^{13}	−0.18	69,200
14	CO_2 + O ↔ O_2 + CO	2.1×10^{13}	0.00	27,800

3. Transport properties models

The flowfields involved in this study are all assumed to be laminar. The viscous stresses are modeled assuming a Newtonian fluid and Stokes' hypothesis. Heat fluxes are modeled using Fourier's law for all energy modes. The species mass diffusion fluxes are modeled employing the modified Fick's law [3], which ensures that the sum of diffusion fluxes is zero. Two different models, namely, the approximate model and the collision integral model, for transport properties are considered in the present study.

3.1. Approximate model

The approximate model uses Blottner's curve fits [18] for the species viscosities with fitting coefficients listed in Table 3 [11,19] and Eucken's relation [12] for the species thermal conductivities. The viscosity and thermal conductivities of gas mixtures are then computed using Wilke's mixing rule [20]. In addition, the effective mass diffusion coefficients are obtained by the constant Lewis number model (CLN) [2], where the Lewis number is set to be 1.4. For air species, it has been shown that Blottner's curve fits can yield adequate values for temperatures ranging from 1000 to 30,000 K [18]; Eucken's relation matches accurate results at moderate temperatures up to 6000 K, but significantly under-predicts the thermal conductivities at higher temperatures [21]; Wilke's mixing rule is simplified first-order Chapman–Enskog relation, which is very inaccurate at temperatures above 7500 K [22]. In general, the approximate model is commonly employed for Earth entry velocities below 10 km/s, as suggested in Ref. [23]. Nevertheless, the application scope of the approximate model still remains unclear for Mars entries.

Table 3
Blottner's curve fit coefficients [11,19].

Species	A_s	B_s	C_s
C	−0.0052	0.7413	−12.8689
O	0.0205	0.4257	−11.5803
N	0.0120	0.5930	−12.3805
O_2	0.0484	−0.1455	−8.9231
N_2	0.0203	0.4329	−11.8153
NO	0.0452	−0.0609	−9.4596
CO	−0.0195	1.0133	−13.9787
CO_2	−0.0195	1.0478	−14.3221