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Assessment of chemical kinetic models on hypersonic flow heat transfer

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ABSTRACT

The objective of this study is to assess the performance of chemical kinetic model for heat transfer acting on the hypersonic vehicle. Four different chemical kinetic models, including Dunn Kang model, Gupta model, Park 87 model and Park 91 model, are implemented and assessed. The differences among these models are obvious, consisting of the elementary reactions, the method of evaluating backward rate coefficients and chemical kinetic rates. In order to further investigate the performance of these models for hypersonic aeroheating prediction, three typical test cases are employed: (1) the heat transfer acting on ELECTRE vehicle at Mach number 13, (2) the heat transfer acting on Apollo command module at Mach number 20.5 and (3) the heat transfer acting on Space Shuttle Orbiter at Mach number 20.985. Firstly, the behaviors of these models are demonstrated by comparing the numerical results with the flight data or experimental data in detail. Secondly, the reasons for the discrepancies of heat fluxes computed with these models are discussed. The results reveal that the heat fluxes acting on ELECTRE vehicle and the head of Space Shuttle Orbiter predicted by these chemical kinetic models are in good consistency and agree well with the flight or experimental data. With the increasing of complexity of the vehicle's geometry, the differences of heat flux, especially the peak heat flux, become more and more obvious, and the maximum difference among them may exceed 25%. The numerical results also indicate that the numerical prediction of heat transfer acting on complicated geometry exhibits a relatively strong sensitivity to the choice of chemical kinetic models. The difference of chemical kinetic rates and the complicated flow structure in the flowfield may be the primary reasons for the heat flux discrepancies.

1. Introduction

In recent years, many countries, such as the US, Europe, Russia, Japan and China, are developing hypersonic research and operational vehicles. As the vehicles fly in the atmosphere at hypersonic speed, the progressions of physical and chemical interactions ensue around the vehicles [1–3]. The air enveloping the vehicle is chemically reacted, vibrationally excited, and ionized. In addition, the time scales of these reactions and excitation processes are similar to the flow time scales, which results in a state of thermochemical non-equilibrium [1–3]. These complicated physical phenomena affect the aerodynamics and heat transfer acting on the vehicles significantly [1–3]. The aerodynamic drag force and severe heating are the major issues for the development of hypersonic vehicles [4]. Many new techniques, such as concentrated energy deposition along the stagnation streamline, aerodisk or aerospike ahead of the vehicle, counterflowing jet, as well as counterflowing jet combined with aerodisk, have been proposed and investigated by many researchers around the world for the drag and heating reductions [4–8]. Nowadays, computational fluid dynamics (CFD) has become an effective approach and played an important role in the predictions of aerodynamics and aerothermodynamics of the hypersonic entry vehicles.

The complex flowfields around the vehicle are described by augmented Navier-Stokes equations that consider the chemical reactions in the flow and non-equilibrium process of internal energy, such as transitional energy, rotational energy, vibrational energy and electronic energy [2,3]. Ultimately, the governing equations include species continuity equations, three momentum equations, and three energy equations describing vibrational, electronic, and total energies respectively [2,3]. Obviously, a qualified chemical kinetic model, including number of species, elementary reactions and relevant rate coefficients, are required to close the above governing equations [2,3]. So far, several different kinds of chemical kinetic models are developed for the hypersonic flow computations and heat transfer predictions. Blottner [9] develops a chemical kinetic model which contains 7 species and 7 elementary reactions, and indicates that the stagnation point heating rates predicted by the model are in reasonable agreement with Fay

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Nomenclature

c_{fr}	parameter of chemical reaction r
D_s	diffusion coefficient of species s
E	total energy
E_v	vibrational energy
E_{fr}	parameter of chemical reaction r
h_s	enthalpy per unit mass of species s
$h_{v,s}$	vibrational enthalpy per unit mass of species s
H	total enthalpy
k_{fr}	forward rate coefficient of chemical reaction r
k_{br}	backward rate coefficient of chemical reaction r
$K_{eq,r}$	equilibrium constant
M_s	molecular weight of species s
nr	total number of reactions
ns	total number of species
n_{fr}	parameter of chemical reaction r
p	pressure
R	the universal gas constant
T	transitional-rotational temperature
T_v	vibrational-electronic temperature
T_d	control temperature of chemical reaction
u_j	velocity vector
x_j	cartesian coordinates
y_s	mole fraction of species s

Greek symbols

α_{rs}	stoichiometric coefficient for reactant in the r reaction
β_{rs}	stoichiometric coefficient for product in the r reaction
δ_{ij}	Kronecker delta function
η_v	thermal conductivity for vibrational-electronic energy
η	thermal conductivity for translational-rotational energy
ρ	density
ρ_s	density of species s
τ_{ij}	viscous stress tensor
ω_s	mass rate of production of species s

Subscript

s	species
r	chemical reaction

Riddel formula for the case which the air is only slightly dissociated and ionized. Dunn and Kang [10] also proposes a chemical kinetic model, which contains 11 species and 26 elementary reactions. The species in their model include five neutral species (N_2, O_2, N, O, NO), five charged species (N_2^+, O_2^+, N^+, O^+, NO^+) and one electron (e-). The forward and backward reaction rate coefficients of the model are evaluated by Arrhenius formula. Afterwards, Gupta [11] proposes a chemical kinetic model by combining Blottner model [9] and Dunn Kang model [10]. Gupta model also contains 11 species, but the number of elementary reactions are reduced from 26 to 20. The first seven reaction reactions and corresponding reactions rates are taken from Blottner model, and the remaining elementary reactions and relevant rate coefficients are taken from Dunn Kang model [11]. The forward reaction rate coefficients of Gupta model are also given by Arrhenius formula. However, the methods of evaluating the backward rate coefficients are revised [11]. Gupta indicates that the Arrhenius form rate coefficients are appropriate for flow velocity below 8 km/s. For higher velocity, the backward rate coefficients should be obtained from the forward rate coefficients and equilibrium constants [11]. Many different kinds of chemical kinetic models are proposed by Park in 1980s and 1990s. Firstly, Park [12] proposes a kinetic model including 11 species and 17 elementary reactions in 1985. The forward chemical rate coefficients of the model are also obtained by Arrhenius form, and the backward rate coefficients are obtained by equilibrium constants that fitted by a fourth-order polynomial [12]. Afterwards, the chemical kinetic rates of some elementary reactions, the method of evaluating the equilibrium constants, even more the elementary reactions are changed and revised by Park [13–15] gradually. These models are named as Park 85 model [12], Park 87 model [13], Park 91 model [14] and Park 2000 models [15] respectively.

The chemical kinetic models discussed above are widely applied to predict the aerodynamics and aerothermodynamics of hypersonic vehicles, and widely adopted in some of the well-known CFD software, such as LAURA and FUN3D [16,17]. However, because of a poorly understanding of the intrinsic chemical kinetic mechanism, the reaction mechanism and their kinetic rates are a source of considerable uncertainty [3]. As mentioned above, large difference can be found among these chemical kinetic models and mainly show up as the number of the species, the elementary reactions and the kinetic rates. In order to provide a useful guideline for stimulating further research and engineering application, it is very necessary and important to investigate the performance of these chemical kinetic models on heat transfer acting on the hypersonic vehicles.

In the current study, four different chemical kinetic models, including Dunn Kang model, Gupta model, Park 87 model and Park 91 model, are utilized to predict the laminar heat flux of three typical hypersonic configurations. Firstly, the behaviors of these models are demonstrated by comparing the predicted results with the flight data or experimental data in detail. Secondly, the reasons for the discrepancies of heat fluxes predicted by these models are also explained and discussed.

2. Numerical methods

All the test cases in the current study are calculated by an in-house code developed by the authors [18]. Three dimensional Navier-Stokes equations with chemical non-equilibrium processes are solved by finite volume method on structured meshes [18]. The main algorithms are briefly described as follows.

2.1. Governing equations

The mass conservation for species is governed by [2,3]

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_s \frac{\partial y_s}{\partial x_j}\right) + \omega_s \tag{1}$$

where ρ_s is the density of species s for $s = 1,\ldots,ns$, ρ is the density, y_s is the mole fraction of species s, D_s is the diffusion coefficient of species s, ω_s is the mass production rate of species s due to the chemical reactions, u_j is the j^{th} component velocity, and ns is the total number of species.

The conservation of momentum is [2,3]

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

τ_{ij} is the viscous stress tensor and defined as