International Journal of Heat and Mass Transfer 112 (2017) 533–543

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Uncertainty analysis of laminar and turbulent aeroheating predictions for Mars entry

Xiaoyong Wang [a], Chao Yan [a,*], Shengjun Ju [a], Yongkang Zheng [a,b], Jian Yu [a]

[a] National Key Laboratory of Computational Fluid Dynamics, Beihang University, Beijing 100191, China
[b] China Aerodynamics Research and Development Center, Mianyang 621000, China

ARTICLE INFO

Article history:
Received 23 January 2017
Received in revised form 27 April 2017
Accepted 27 April 2017
Available online 11 May 2017

Keywords:
Uncertainty analysis
Laminar
Turbulent
Aeroheating
Mars

ABSTRACT

Uncertainty analysis of laminar and turbulent aeroheating predictions of a 70° spherically blunted cone at peak heating condition during Mars entry is performed. Due to the difficulty in obtaining accurate chemical kinetic model, numerical aeroheating predictions possess significant uncertainties. In this study, 14 rates in Park 8-species 14-reaction model are treated as epistemic uncertain variables represented with intervals, meanwhile stochastic expansion based on point collocation non-intrusive polynomial chaos expansion, is utilized to represent and propagate the uncertainties. In particular, Sobol indices are used to rank the relative contribution of each rate. 240 CFD evaluations are employed to obtain the laminar and turbulent uncertainty results respectively. The results show that the top contributing parameters to turbulent heat flux are similar to those observed in the laminar case in the windside region. However, in the leeside region, the key parameters, which produce significant uncertainties in laminar and turbulent cases, are evidently different. The maximum uncertainty in laminar aeroheating prediction is about 6%. In the large region of leeside flank, the uncertainty in turbulent aeroheating prediction is above 7%. Moreover, the uncertainty interval is as wide as 32.4 W/cm^2, which is about 15% of the mean value.

1. Introduction

When the vehicles flying in Earth or Martian atmosphere at hypersonic speeds, strong shock waves are formed around and extremely high temperatures are generated in the shock layer [1,2], which excite the vibrational mode energies of the molecules in the air and change the thermal properties of the air. Furthermore, significant chemical reactions, including dissociation and ionization reactions, are induced [2–4]. In the recent years, with the enhancement of computational recourse, computational fluid dynamics (CFD) has become an effective approach and played an important role in analysis of the hypersonic reentry flows and prediction of the heat transfer acting on Earth or Mars entry vehicles involving these complex physical phenomena [1–4].

The numerical predictions of these complex physical and chemical phenomena, which are crucial for the design of suitable thermal protection system (TPS), show great difficulty in the complex physical governing, not only the fluid dynamics, but also the thermodynamics and chemical kinetics [1–4]. In order to predict the aeroheating environment accurately, a qualified chemical kinetics including sufficient number of species, chemical reactions and accurate chemical kinetic rates, is required [3,4]. Currently, the best available chemical kinetic models for Mars entries are proposed by Park [1]. Based on a mixture of the experimental data in shock tube and chemical reaction rates taken from the combustion literature, Park et al. [1,5] propose an 18-species 33-reaction chemical kinetic model, which considers the ionization reaction in the air and can be utilized for high velocity Mars entry. After that, a reduced 8-species 14-reaction chemical kinetic model neglecting the ionization reactions and several trace neutral species, is proposed by Mitcheltree and Gnoffo [1,6]. Note that all the chemical reactions and corresponding rates in 8-species model are directly taken from Park 18-species model [1,5,6]. Unfortunately for Mars entry, the existent flight and experimental data are comparatively inadequate to verify and validate these chemical kinetic models. Many of the chemical kinetic rates have not been directly measured at conditions relevant to Mars entry [1,5]. The chemical kinetic rates are estimated from either indirect observations or pure estimates, which make themselves significant sources of uncertainty [1]. This uncertainty is known as epistemic uncertainty, and comes from several potential sources, such as lacking of knowledge or incomplete information about chemical kinetics and ignorance or negligence with regard to the accurate treatment

* Corresponding author.
E-mail address: yanchao@buaa.edu.cn (C. Yan).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2017.04.126
0017-9310/

Nomenclature

$C_{f,r}$	parameter of chemical reaction r
D_s	diffusion coefficient of species s
E	total energy
$E_{f,r}$	parameter of chemical reaction r
h_s	enthalpy per unit mass of species s
H	total enthalpy
$k_{f,r}$	forward rate coefficient of chemical reaction r
$k_{b,r}$	backward rate coefficient of chemical reaction r
M_s	molecular weight of species s
$n_{f,r}$	parameter of chemical reaction r
nr	the number of reactions
ns	the number of species
p	pressure
R	the universal gas constant
T	temperature
T_d	control temperature
u_j	jth component velocity
Y_s	mass fraction of species s
α_{rs}	the stoichiometric coefficients for reactants in the r reaction
β_{rs}	the stoichiometric coefficients for products in the r reaction
δ_{ij}	Kronecker delta function
η	thermal conductivity of the mixture
μ	viscosity of the mixture
ρ	density
ρ_s	species density
τ_{ij}	viscous stress tensor
$\dot{\omega}_s$	mass rate of production of species s

Subscript

s	species
r	chemical reaction

of the parameters in chemical kinetic rates [7]. Therefore, numerical prediction of the aerothermodynamics for Mars entry contains significant uncertainty, and it is essential to investigate the uncertainty and identify the key parameters in the aeroheating prediction of Mars entry vehicle.

Bose and Wright [8] investigate the laminar aeroheating uncertainty of Mars Pathfinder from 130 parameters, including 47 chemical rates in Park 8-species kinetic model. In their study, the chemical kinetic rates are conservatively assigned with an order of magnitude uncertainty. They point out that only $O_2 + M \rightleftarrows 2O + M (M = O, CO)$ in Park 8-species model shows some sensitivity in laminar aeroheating prediction [8]. Brune et al. [9] perform uncertainty analysis of flowfield and aeroheating prediction over an axisymmetric aeroshell of hypersonic inflatable aerodynamic decelerator for Mars entry at peak stagnation point heating condition. 65 uncertainty parameters, including 25 chemical rates in 16-species 25-reaction kinetic model, are considered. The result shows that exothermic recombination reactions are more important at the shoulder, and CO_2 dissociation rates and CO heavy-particle excitation rates are the main contributors to the radiative heating at the nose and flank of the vehicle [9]. As mentioned above, a significant amount of uncertainties still exist in chemical kinetic models of Martian atmosphere. Previous researches mainly focus on the aeroheating uncertainty induced by the chemical rate uncertainty in the laminar flow. However, the uncertainty of the turbulent aeroheating predictions and its difference from laminar cases for the three dimensional Mars entry vehicle are not clearly known, and the relative research is insufficient. In order to provide a useful guideline for stimulating further research and engineering application, it is fairly necessary and important to investigate the uncertainties and identify the key parameters in chemical kinetic model for the laminar and turbulent aeroheating predictions of Mars entry vehicle.

In the recent years, stochastic expansion based on point collocation non-intrusive polynomial chaos expansion (NIPC), which needs no modification of original CFD code and treats CFD code as a black box, has been used as a means of uncertainty quantification (UQ) due to their high computational efficiency and utility for representing and propagating large uncertainties through complex models [7,9–12]. The NIPC method is based on a spectral representation of the uncertainty and more efficient than traditional methods, such as Monte Carlo method [12]. The theory behind the NIPC is well defined in Ref. [13], meanwhile the NIPC has been extensively applied for uncertainty quantification by Hosder et al. [7,9–10,14–18].

In this paper, the uncertainty analysis of laminar and turbulent aeroheating predictions on the surface of three dimensional 70° spherically blunted cone, which is a typical configuration of Mars entry vehicle, is performed at the peak convective heating condition during Mars entry. The 14 chemical kinetic rates in the Park 8-species 14-reaction model are treated as epistemic uncertain variables represented with intervals, meanwhile stochastic expansion based on point collocation NIPC as a means of efficient UQ, is utilized to represent and propagate the uncertainties in the chemical kinetic model. In particular, Sobol indices calculated by the expansion coefficients, are utilized to rank the relative contribution of each rate to the total uncertainty in laminar and turbulent heating predictions.

2. Numerical methods

In the current study, all the test cases are evaluated by an in-house code developed by the authors [22]. Three dimensional Navier-Stokes equations with chemical non-equilibrium processes are solved by finite volume method on structured meshes. The main algorithms of the code are presented as follow.

2.1. Governing equations

The conservation of mass for each species is [3,4]

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_s \frac{\partial Y_s}{\partial x_j}\right) + \dot{\omega}_s \tag{1}$$

where ρ_s is the density of species s for $s = 1, \ldots, ns$, ρ is the total density of all species, $Y_s = \rho_s/\rho$ is the mass fraction of species s, D_s is the diffusion coefficient of species s, $\dot{\omega}_s$ is the mass production rate of species s due to the chemical reactions, and u_j is the jth velocity component.

The conservation of momentum is [3,4]

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

in which, τ_{ij} is the viscous stress tensor and defined by

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} \tag{3}$$