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Numerical simulations of high enthalpy flows around entry bodies

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Abstract Ablation flows around entry bodies are at highly nonequilibrium states. This paper presents comprehensive computational fluid dynamics simulations of such hypersonic flow examples. The computational scheme adopted in this study is based on the Navier–Stokes equations, and it is capable of simulating multiple-dimensional, non-equilibrium, chemically reacting gas flows with multiple species. Finite rate chemical reactions, multiple temperature relaxation processes, and ionizations phenomena with electrons are modeled. Simulation results of several hypersonic gas flows over axisymmetric bodies are presented and compared with results in the literature. It confirms that some past treatment of adopting less species for hypersonic flows is acceptable, and the differences from more species and more chemical reactions are not significant.

1. Introduction

Thermal protection systems (TPSs) are essential for the successful operation of space vehicles.[1] Simulating the hypersonic ablation flows around a TPS system involves many challenges which include, but not limited to, multiple species with chemical reactions and complex thermodynamics relations,[2,3] mechanical ablation,[4] thin shock waves with large gradients and interactions with boundary layers, multiple dimensions with possible surface recessions, multiple temperatures, radiations, and other multiple physics demanding careful modellings. Investigations with experiments are expensive and challenging; hence, we usually rely on computational fluid dynamics (CFD) simulations to investigate these flows.

In the literature, there are many investigations on hypersonic flows, and only some of them are listed here. Some concentrated on numerical scheme development and parameter effects.[5,6] Some adopted particle simulation methods, such as the direct simulation Monte Carlo (DSMC), which are quite flexible for rarefied hypersonic flows.[7–10] Zhong et al.[8] included 11 species and 31 reactions. Much other works during the past adopted the Navier–Stokes equations (NSEs). Gosse and Candler[2] modeled the gas flow over a sphere-cone vehicle coupling in the solution of the mass and energy balance with surface reactions at an altitude of 16 km. In that work, gas–surface reactions and surface sublimation were included, and it was found that the predicted surface recession rate for a validation case was lower than that from experimental measurement. Chen and Milos[11] studied a hypersonic flowfield over a dense carbon-phenolic heat shield under flow conditions typical for

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earth reentry from a plant-entry mission. The ablation surface conditions of oxidation irradiation and material sublimation were coupled with NSEs and it was found that the surface ablation had only a small impact on the predicted convective heat flux. Huang[12] concentrated on silicon-based materials, and it was found that the effects from resin materials on the ablation flowfield were appreciable.

This paper presents some hypersonic flow simulations with an NSE-based CFD solver which can serve as a foundation for further development. The next few sections are organized as follows: in Section 2, some details for the governing equations and numerical schemes are presented; in Section 3, some detailed thermodynamics relations and chemical reaction models are listed, Section 4 includes some simulation results with comparisons and discussions, and Section 5 draws several conclusions.

2. Governing equations and numerical schemes

The new CFD solver is based on NSEs. The axis-symmetric NSEs are listed as follows, including some chemical reaction source terms[13]:

$$\boldsymbol{U}_t + (\boldsymbol{E}_{\text{in}})_x + (\boldsymbol{F}_{\text{in}})_r + \boldsymbol{G} = (\boldsymbol{E}_{\text{v}})_x + (\boldsymbol{F}_{\text{v}})_r + \boldsymbol{G}_{\text{v}} + \boldsymbol{W} \tag{1}$$

where "in" and "v" represent inviscid and viscous properties; subscripts "x" and "r" represent partial derivatives along the x and r directions; and G_{v} is one source term related to axissymmetry:

$$\boldsymbol{U} = [\rho_1, \cdots, \rho_{n_s}, \rho u, \rho v, E, \rho e_{\text{v}}]^{\text{T}}$$

$$\boldsymbol{E}_{\text{in}} = [\rho_1 u, \cdots, \rho_{n_s} u, \rho u^2 + p, \rho uv, u(E+p), \rho u e_v]^{\text{T}}$$

$$\boldsymbol{F}_{\text{in}} = [\rho_1 v, \cdots, \rho_{n_s} v, \rho uv + p, \rho v^2 + p, v(E+p), \rho v e_v]^{\text{T}}$$

$$\boldsymbol{G} = [\rho_1 v, \cdots, \rho_{n_s} v, \rho uv, \rho v^2, v(E+p), \rho v e_v]^{\text{T}}/r$$

$$\boldsymbol{E}_v = [\rho D_1 X_{1x}, \cdots, \rho D_{n_s} X_{n_s,x}, \tau_{xx}, \tau_{xr}, u\tau_{xx} + v\tau_{xr} + q_x, q_{xv}]^{\text{T}}$$

$$\boldsymbol{F}_v = [\rho D_1 X_{1x}, \cdots, \rho D_{n_s} X_{n_s,x}, \tau_{xr}, \tau_{rr}, u\tau_{xr} + v\tau_{rr} + q_r, q_{rv}]^{\text{T}}$$

$$\boldsymbol{G}_v = \frac{[\rho D_1 X_{1x}, \cdots, \rho D_{n_s} X_{n_s,x}, \tau_{xr}, \tau_{rr} - \tau_{rx}, u\tau_{xr} + v\tau_{rr} + q_r, q_{rv}]^{\text{T}}}{r}$$

$$\boldsymbol{W} = [\dot{\omega}_1, \cdots, \dot{\omega}_{n_s}, 0, 0, 0, S_v]^{\text{T}}$$

where u and v are the velocity components along the x- and r-directions, ρ is the mixture density, ρ_i is the density for the ith species, p is the mixture gas pressure, E is the mixture total internal energy, e_{v} the specific vibrational energy, D the diffusion coefficient, X the species concentration, n_{s} the number of species, $\dot{\omega}$ the source terms for density, and S_{v} the source term for vibrational energy. The shear stress tensor τ and the heat flux q are:

$$\tau_{xx} = -\frac{2}{3}(\mu + \mu_{\text{t}})(2u_x - v_r - v/r)$$

$$\tau_{rr} = -\frac{2}{3}(\mu + \mu_{\text{t}})(2v_r - u_x - v/r)$$

$$\tau_{xr} = \tau_{rx} = (\mu + \mu_{\text{t}})(u_r + v_x)$$

$$\tau_{\theta\theta} = -\frac{2}{3}(\mu + \mu_{\text{t}})(u_x + v_r + v/r)$$

$$q_x = kT_x + k_v(T_v)_x + \sum_{i=1}^{n_s}(h_i \rho D_i (C_i)_x)$$

$$q_r = kT_r + k_v(T_v)_r + \sum_{i=1}^{n_s}(h_i \rho D_i (C_i)_x)$$

$$q_{xv} = k_v(T_v)_x + \sum_{i=\text{mol}}(e_{vi} \rho D_i (C_i)_x)$$

$$q_{\text{xr}} = k_v(T_v)_r + \sum_{i=\text{mol}}(e_{vi} \rho D_i (C_i)_r)$$

$$X_{ix} = (C_i)_x$$

$$X_{ir} = (C_i)_r$$

In the above expressions, k is the thermal conductivity, k_{v} is the vibrational energy conductivity, $e_{\text{v}i}$ is the specific vibrational energy for the ith species, D_i is the mass diffusion coefficient for the ith species, μ and μ_{t} are the laminar and turbulence viscosity coefficients, C_i is the mass fraction for the ith species, and $\sum_{i=\text{mol}}$ are the summations over molecule species.

The other symbols are listed as follows: h is the specific enthalpy, e is the specific mixture internal energy, $\bar{M}$ is the mixed molecular mass, Δh_i^0 is the formation heat for the ith species, h_0^i is the heat of formation, $e_{\text{t}i}$ and $e_{\text{r}i}$ are the specific internal translational and rotational energy, and R is the gas constant, MW_i is the molecular weight for the ith species, M is the averaged molecular weight:

$$\begin{cases} h = e + p/R \\ \rho = \sum_{i=1}^{n_s} \rho_i \\ \bar{M} = 1 \Big/ \sum_{i=1}^{n_s} (C_i/\text{MW}_i) \\ p = \rho RT/\bar{M} \\ E = \rho[e + (u^2 + v^2)/2] \\ e = \sum_{i=1}^{n_s} C_i(e_{\text{t}i} + e_{\text{r}i} + \Delta h_i^0) + \sum_{i=\text{mol}}(C_i e_{vi}) \end{cases} \tag{2}$$

Before solving Eq. (1), they are non-dimensionalized, and the coordinate system is mapped into a curvilinear system. For in-viscid flux computation, the coefficient matrix needs to be computed and decomposed into an eigenvalue matrix. The Sterge flux scheme is used to compute the fluxes, and the properties at the cell edge are computed with the Roe scheme.[14,15]

Once the fluxes across the cell interface are obtained, the source term W for chemical reaction and vibrational energy relaxation is evaluated. By solving a set of ordinary differential equations (ODEs), $\text{d}W_i/\text{d}t = S_i$, we can update the flowfield properties with these source term contributions. In summary, an update of the flowfield properties from time step n to $n+1$ is obtained by the following equation: