

MULTI-SCALE CFD/MD MODELLING OF HIGH-ENTHALPY FLOW/TPS INTERACTION AND ITS PRELIMINARY AERONAUTICAL APPLICATION

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Abstract

Multi-scale modelling of high-enthalpy flow/thermal protection system (TPS) interaction was performed to predict high-fidelity aerothermodynamics of high-speed spacecraft. Computational fluid dynamics and molecular dynamics techniques were integrated to simulate high-enthalpy flow and interfacial chemistry correspondingly. This joint model was preliminarily used to predict catalytic heating to TPS materials in aeronautical science. Joint simulation show that interface microscopic reaction rate determines the macroscopic species molar fluxes, which in turn generates a certain amount of catalytic heating.

Keywords: computational fluid dynamics, molecular dynamics, aerothermodynamics, high-temperature interface effects, multi-scale

1. General Introduction

High-speed spacecraft will encounter more remarkable high-temperature gas effect during hypersonic flight, leading to complex surface reactions, such as catalysis and oxidation [1]. The net heat flux experienced by a hypersonic spacecraft is the result of complex and dynamic interactions between flow field and thermal protection system (TPS) surface. Previous studies of theoretical computations, wind tunnel experiments and flight data all show that surface thermal load can vary sharply with the TPS material properties and surface reaction models. The scatter induced by material catalytic properties or surface modelling can be as large as 2~4 times on specific conditions [2]. Consequently, it is difficult to precisely predict aerothermodynamics using the single macroscopic numerical techniques, typically computational fluid dynamics (CFD), because the gas-solid interface chemistry need to be characterized or determined by microscopic numerical techniques, such as molecular dynamics (MD). It urges us to join MD into CFD for high-fidelity gas/material interaction prediction.

It is an effective way to solve the above-mentioned problems by describing the interface dynamics process through smaller-scale theoretical simulations and obtaining the interface parameters required by CFD. Norman et al. [3-5] established a computational chemistry method based on MD to describe the heterogeneous catalysis of high-temperature dissociated air on the SiO₂ surface for the high-speed reentry problem. However, the above method has not yet simulated the surface reaction influence on macroscopic flow. Marschall and Maclean et al. [6,7] tried to establish a cross-scale framework of joint CFD/MD simulation for the dynamic processes of air adsorption/desorption and recombination on the surface of carbon- or silicon-based materials. Such framework is difficult to realize for multi-scale computation. The well-known software DPLR has initially formed the framework to combine computational surface chemistry and CFD to realize the cross-scale characterization of wall heterogeneous catalysis [8]. In view of the endothermic/exothermic effects caused by the surface reaction, it is urgent to further carry out the joint investigation of the micro-scale simulation method and the macro-scale CFD method to realize the predictive ability of the cross-scale catalytic heat transfer process.

In this study, we established a multi-scale model to numerically predict the high-enthalpy flow/TPS

interaction. The overall chemical non-equilibrium flow field was obtained by the conventional CFD solver, while on the gas-solid interface an MD solver was used to generate a quantitatively CFD boundary condition for gas/TPS chemistry.

2. Joint CFD/MD Modelling

2.1 CFD Techniques

At the macroscopic level, the high-enthalpy flow/TPS interaction is an important physical and chemical phenomenon related with hypersonic chemical non-equilibrium flow field and thermal protection material. The surface catalytic heat transfer is one of the typical interaction processes. It describes the process of thermal protection material particles that stimulate or strengthen gas-phase particles to participate in the wall recombination reactions and thence produce chemical reaction heat release.

For the heterogeneous catalytic reaction on the wall, the particles (molecules or atoms) on the bulk surface only serve as hosts and do not exchange mass with the gas-phase particles, but heat transfer can occur. The recombination of gas-phase particles on the wall generates a large amount of chemical heat, which increases the heat flux onto the wall, thereby intensifying the thermal load on the TPS surface.

From the perspective of CFD, the surface catalytic heat transfer process mainly affects the surface heat flux and related heat transfer into the aircraft's TPS by affecting the boundary layer profiles (velocity, temperature, species mass fraction, etc.). The catalytic efficiency is usually used in CFD to characterize the surface catalytic properties of thermal protection materials by controlling the distribution of the wall species mass fraction. The catalytic efficiency is generally obtained by experimental measurement or microscopic theoretical simulation, such as MD.

CFD considers the hypersonic gas flow that follows the laws of conservation of mass, momentum and energy, which are the well-known Navier-Stokes (NS) equations. For the multi-species gaseous reacting system, in the density-based conservation formation, these extended equations can be written as

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot (\mathbf{F}_c - \mathbf{F}_v) = \mathbf{S} \quad (1)$$

where \mathbf{Q} is the array of conserved variables, \mathbf{F}_c and \mathbf{F}_v are the arrays of inviscid and viscous fluxes, and \mathbf{S} is source term induced by gaseous chemical reactions. Steady solution will be obtained with time marching method, which is related with time in iteration but ultimately tends to steady results. Specially the lower and upper symmetrical Gauss-Seidel (LUSGS) implicit algorithm was used in this paper. For the detailed numerical methods used in CFD to solve this problem, one can refer to previous literature [9].

As to viscous wall boundary conditions, the impingement of the gaseous particles on the solid-phase TPS brings gas-solid interaction and interface mass, momentum and energy transport behavior. The laws of conservation are locally reduced to the boundary condition on the viscous wall satisfying the surface mass, momentum and energy balance equations for the steady state as [9]

$$(\mathbf{J} - \rho \mathbf{Y}^T \mathbf{u}) \cdot \mathbf{n} = \mathbf{J}_{wn} \quad (2)$$

$$\nabla p \cdot \mathbf{n} = 0 \quad (3)$$

$$(\mathbf{q}^f + \mathbf{h} \cdot \mathbf{J}) \cdot \mathbf{n} = \mathbf{q}^s \cdot \mathbf{n} + q_w^r \quad (4)$$

where \mathbf{J} is mass flux matrix for all species in three directions, \mathbf{Y} is mass fraction array for all species, \mathbf{q} is heat flux array in three directions and \mathbf{h} is enthalpy array for all species.

The mass flux or molar flux I is driven by interface chemical reactions. The molar flux of specified reaction pathway is dependent on species molar concentration and reaction rate coefficients as follows [10]

$$I = k_f \prod_{i=1}^{N_s} X_i^{\nu_i'} - k_b \prod_{i=1}^{N_s} X_i^{\nu_i''} \quad (5)$$

The surface reaction rate coefficients are computed from kinetic theory with the following form

$$k_f = \gamma \left(\frac{1}{4\phi_s^{v_s}} \right) \bar{V} T'^{\beta} \exp \left(\frac{E_s}{R_0 T} \right) \quad (6)$$

These interface quantities, such as excitation energy, density of total/occupied adsorption sites and recombination efficiency, are obtained from MD simulation.

The above CFD algorithm has been coded and packaged in the fluid-thermal-structural coupling platform, named *Coupled Analysis Platform for Thermal Environment and structure Response* (CAPTER), developed by the authors' team [11].

2.2 MD Techniques

The catalytic heat transfer process for flow/TPS interaction in the chemical reaction boundary layer is mainly embodied in the microscopic MD process in the very near-wall region. Such process occurs within Knudsen layer, typically within about 1 μm from the solid surface. In details, the microscopic movements of adsorption, recombination, desorption and diffusion occur near the wall due to the existence of unsaturated bonds on the cutting surface of the material surface. At the microscale, only the diffusion process of gas can be considered, while the macroscopic flow process can be ignored. From this point of view, the surface catalyzed heat transfer process is different from the three-dimensional gas-phase reaction and diffusion. It produces local reaction and diffusion behaviors on the two-dimensional surface.

At the microscopic level, the flow/TPS interaction process with catalytic effects can be divided into five independent physical and chemical steps [12]:

- (1) Diffusion: The gas-phase particles in the high-enthalpy dissociated gas mixture move to the vicinity of the solid cutting surface according to the regular law of molecular thermal motion.
- (2) Adsorption: Due to the unsaturated bonds on the cutting surface or the van der Waals force (intermolecular force) of the solid molecules, the gas-phase particles are bound near the solid cutting surface of the wall. That is, the gas-phase particles undergo chemical adsorption or physical adsorption.
- (3) Recombination: The adsorbed particle is chemically recombined with gas-phase particles (Eley-Rideal mechanism, ER); or one adsorbed particle is chemically recombined with another adsorbed particle through surface migration (Langmuir-Hinshelwood mechanism, LH); or the adsorbed particle combines with the solid-phase particle at the adsorption site. The combination/recombination behaviors form diatomic or polyatomic molecules with stronger chemical bonds.
- (4) Desorption: The above mentioned bounded large particles get rid of the bondage of the chemical bond or van der Waals force at the adsorption site, and then leave the adsorption site. That is, the particle at the adsorption site is chemically or physically desorbed.
- (5) Diffusion: The desorbed gas-phase particles move far away from the vicinity of the solid cutting surface through conventional molecular thermal motion.

According to the microscopic dynamics of the gas-solid interface, an MD model with ReaxFF force field including diffusion, adsorption, recombination and desorption was established. The ER mechanism and LH mechanism were taken into account for simulation. In this model, processes such as adsorption, recombination and desorption must involve at least one adsorbed atom before they can take place. Along with these processes, energy transfer and conversion occur between the gas phase and the solid phase through the occupation and separation of adsorption sites.

According to the finite-rate reaction model, the number of adsorption sites on the solid surface is assumed to be limited, and the process of endotherm/exotherm at each site is regarded as a heat source on the solid surface. The adsorption process includes physical adsorption and chemical adsorption. Because physical adsorption only plays a leading role at low temperature, but under $Ma > 10$ environmental condition, the gas is in a high-temperature aerodynamic environment, so only the chemical adsorption process was considered in this model. For the case, only monolayer adsorption was considered.

In the process of flow/TPS interaction, the energy conservation including translational energy and internal energy (other internal energy except translational energy) is satisfied. The current MD method has been fully verified in the fields of interface heterogeneous catalysis [13].

2.3 Joint CFD/MD Framework

CFD and MD co-work for the flow/TPS interaction problem. CFD solver provides computation

environment for MD, while the boundary condition of CFD relies on MD statistical results. Figure 1 shows the sketch of joint CFD/MD simulation for hypersonic flow over blunt body.

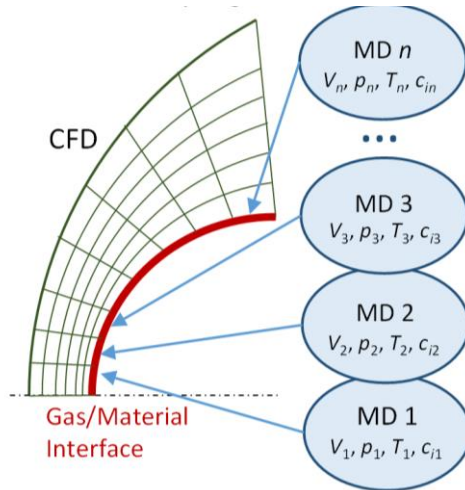


Figure 1 – Sketch of joint CFD/MD simulation framework for flow/TPS interaction simulation.

Based on the above overall framework, combined with the calculation capabilities of the existing CFD and MD methods, Figure 2 shows the flow chart of detailed procedure for CFD/MD joint simulation. The specific implementation steps are:

- (1) Run CFD solver for non-equilibrium flow with non-catalytic and adiabatic viscous wall boundary condition to obtain the macroscopic hypersonic flow field.
- (2) Determine the input parameters required for microscopic MD simulation from the wall pressure, temperature, density and species distribution of the flow field in aerodynamic environment.
- (3) Simulate the surface heterogeneous catalysis process with MD according to the microscopic catalytic properties of thermal protection materials.
- (4) Count the chemical reaction rate of the wall according to the MD simulation results, and update the wall thermal/chemical state.
- (5) Rerun CFD solver according to the wall thermal/chemical state from MD statistical data to obtain the updated macroscopic hypersonic flow field.
- (6) Proceed to step (2), until the wall thermal/chemical state keeps unchanged (the change is neglectably small), and finalize the joint simulation.

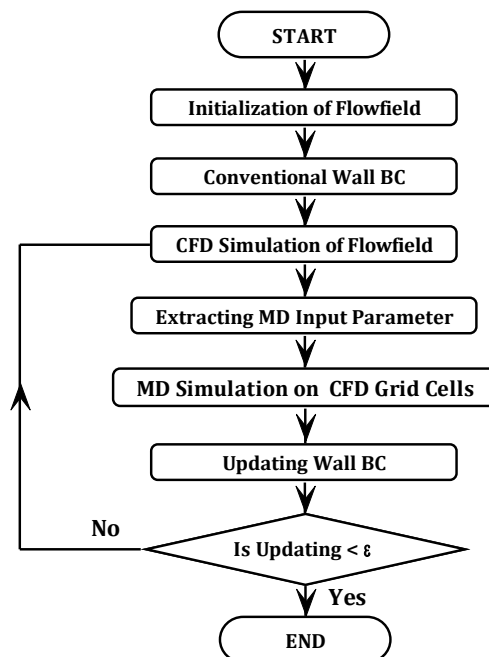


Figure 2 – Flow chart of CFD/MD joint simulation for flow/TPS interaction.

3. Preliminary Aeronautical Case

3.1 Simulation Case Settings

A simple aeronautical case was carried out to present the multi-scale CFD/MD joint simulation. It is a chemically reacting hypersonic flow over a cylindrical body made of chemically active silicon-based material. Simulation settings of both macroscopic CFD and microscopic MD were presented in details hereafter.

3.1.1 Macroscopic CFD simulation settings

(1) Geometry. The geometric model of the macroscopic calculation is a cylinder with a diameter of 90 mm, from the HEG hypersonic experiment [14].

(2) Mesh generation. The computational grid is a structured multi-block hexahedral grid, as shown in Figure 3. In this case, 4 blocks were divided for parallel acceleration with 4 processors. In order to more accurately simulate the boundary layer details and wall heat flux, the grid is properly refined in the wall normal direction and orthogonal enough. The Reynolds number of the wall normal first layer is on the order of $O(1)$.

(3) Gas model. The macroscopic CFD calculation uses the Gupta's model of 17 chemical reactions with 5 species (N, O, N₂, O₂, NO) [15].

(4) Boundary condition. Table 1 shows the hypersonic free flow conditions used in the macroscopic CFD simulation. Under the initial conditions, the wall is set to be adiabatic and non-catalytic conditions. In the simulation process, the wall temperature and reaction rate obtained by the MD simulation are used to close the CFD viscous wall boundary.

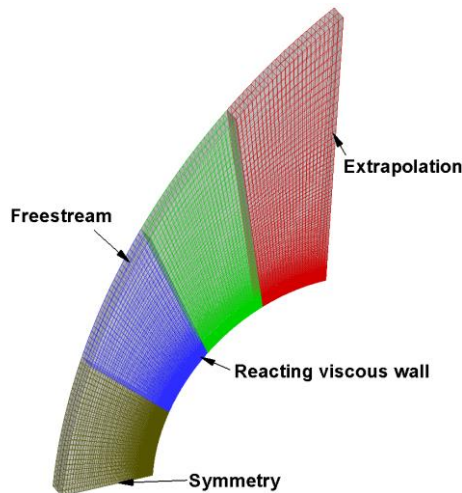


Figure 3 – Mesh generation and boundary conditions for chemically reacting hypersonic flow over a cylindrical body.

Table 1 – Computation condition for macroscopic CFD simulation.

| No. | Parameter | N ₂ | O ₂ | O | NO |
|-----|------------------------------|----------------|----------------|----------|----------|
| 1 | Speed/(m/s) | | 4776 | | |
| 2 | Mach number | | 8.78 | | |
| 3 | Pressure/Pa | | 687 | | |
| 4 | Temperature/K | | 694 | | |
| 5 | Density/(kg/m ³) | 0.002398 | 0.000437 | 0.000259 | 0.000166 |

3.1.2 Microscopic MD simulation settings

(1) Geometry. The simulated spatial scale is a hexahedral box of 20nm×20nm×20nm.

(2) Boundary condition. One of the sides (lower part $z = z_{\min}$) is a wall containing adsorption sites. Periodic boundary conditions were used in the x and y directions; and the lowest layer in the z direction was set as the solid phase with adsorption sites. The upper part of the z direction is the

species control zone, where the temperature and species concentration keep.

(3) Material settings. The solid material is silicon, with a limited number of 1208 adsorption sites, that is, the molar concentration is 5.015×10^{-6} mol/m². The total amount of simulated particles is determined according to the wall density and the mass fraction of each species.

(4) Adsorption site settings. The active sites are randomly distributed on the surface, and the number are 75% of the total grid number on the solid surface.

(5) Simulation parameters. The overall time for simulation is 13 ns. Table 2 shows the calculation parameters of the catalytic heat transfer process at the microscopic gas-solid interface.

Table 2 – Computation condition for microscopic MD simulation.

| No. | Parameter | Physical value | Value in MD simulation |
|-----|---------------------------|------------------------|-------------------------|
| 1 | Simulation time | 10 ns | 10 ⁷ steps |
| 2 | Dimension | 20 nm*20 nm*20 nm | 2000x2000x2000 |
| 3 | Initial wall temperature | 2000 K | 2000 |
| 4 | Bulk density | 2.34 g/cm ³ | 0.05031 |
| 5 | Bulk specific heat | 2000 J/(kg·K) | 2x10 ⁻⁷ |
| 6 | Bulk thermal conductivity | 150 W/(m·K) | 3.2247x10 ⁻⁸ |

3.2 Macroscopic Flow Field under Non-Catalytic Condition

Using CFD techniques, a numerical simulation of hypersonic non-equilibrium flow around a cylinder was carried out. The details of hypersonic non-equilibrium flow field and near-wall aerodynamic/aerothermodynamic environment were obtained.

Figure 4 shows the temperature field distribution contour of the hypersonic flow around a cylinder under non-catalytic wall condition. After the hypersonic air flow passes across a bow shock wave, the air speed drops, and both the pressure and temperature rise. At such local high temperature, the O₂ and N₂ gas mixture chemically reacts into atomic oxygen and nitrogen, forming a high-enthalpy dissociation aerodynamic environment.

After the normal shock wave, O₂ undergoes a large amount of dissociation reaction to generate O atoms; a small amount of N₂ is also dissociated into N atoms, and a certain amount of NO is generated in the high temperature region. Due to the chemical non-equilibrium effect, the gas passing through the vicinity of the shock wave has not yet dissociated. As a result, the local temperature is as high as 7000 K. After a very short period of relaxing process, the gas continues to dissociate, and the gas temperature drops to about 5000 K.

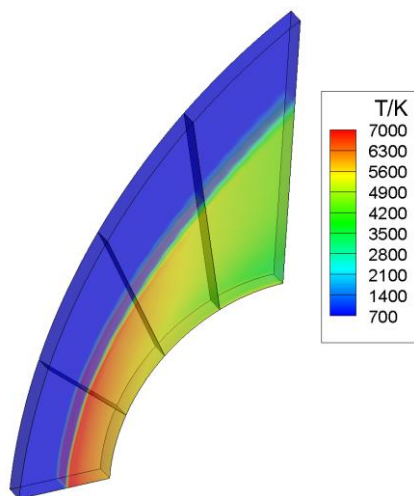


Figure 4 – Temperature field distribution contour of the hypersonic flow around a cylinder under non-catalytic wall condition.

Figure 5 shows the wall temperature, pressure and density distribution in the absence of chemical reactions on the wall. A temperature distribution from the stagnation point 5738 K to the side end 4369 K is formed near the wall. The pressure and density gradually decrease from a higher value at the stagnation point to a lower value at the end side.

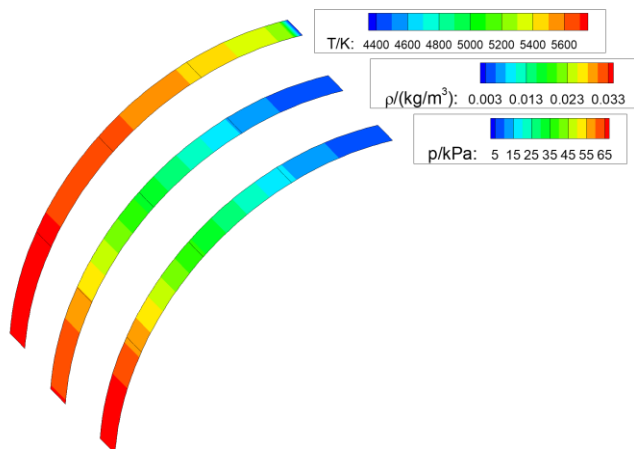


Figure 5 – Contour of surface temperature, density and pressure on the non-catalytic wall.

Figure 6 shows the mass fraction distribution of each species on the non-catalytic wall. On the wall, due to the high-temperature aerodynamic environment, the nitrogen element is mainly in the form of N_2 molecules, and the oxygen element is mainly in the form of O atoms, and there are a small amount of N atoms and NO molecules at the same time.

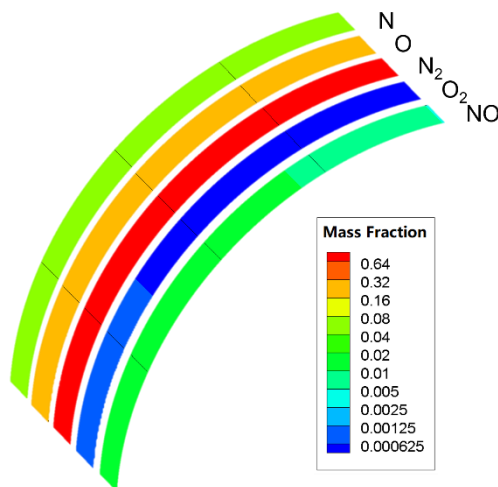


Figure 6 – Surface mass fraction distribution of each species on the non-catalytic wall.

3.3 Microscopic Wall Thermal State under Aerodynamic Environment

Based on the aerodynamic environment obtained by CFD simulation, the MD simulation of wall heterogeneous catalysis under the high-enthalpy aerodynamic environment was carried out. Statistical data of the surface coverage, molar flux of each reaction, reaction proportion, heating to the wall and other microscopic characteristic parameters were obtained.

The surface coverage is the ratio of the number of active sites occupied by adsorbed particles to the total number that can be theoretically occupied. The variation of surface coverage with time was obtained. After the simulation is stable, the surface coverage fluctuates around 0.0724, which is consistent with the low surface coverage at high temperature.

The MD simulation counts the changes over time in the number of different processes in the catalytic reaction, including ER and LH reaction, adsorption process, thermal desorption process, etc. It can be found that as the simulation progresses, the frequency of occurrence of each process tends to stabilize. The macroscopic rate of each reaction can be calculated by the number of occurrences of

the microscopic process, as shown in Table 3. According to calculations, on a gas-solid surface of 20nm×20nm, the adsorption reaction rate is $1.435 \times 10^9/s$, that is, $5.9607 \text{ mol}/(\text{m}^2 \cdot \text{s})$; the LH reaction rate is $1.5611 \text{ mol}/(\text{m}^2 \cdot \text{s})$; the ER reaction rate is $2.0105 \text{ mol}/(\text{m}^2 \cdot \text{s})$; the rate of desorption process is $0.90993 \text{ mol}/(\text{m}^2 \cdot \text{s})$.

The MD simulation counts the total number of adsorbed atoms participating in each process of the catalytic reaction as a percentage of the total number of adsorbed atoms, as shown in Table 3. When counting the number of adsorbed atoms involved, the ER reaction is 1, the LH reaction is 2 because two adsorbed atoms combine in each reaction process, and the thermal desorption reaction is 1. The results show that the number of adsorbed atoms participating in the LH process is dominant among the adsorbed atoms. The proportion of LH reaction is found to be higher than that of ER reaction, which is consistent with the scientific understanding that LH reaction is dominant at high temperature.

Table 3 – Statistical data of the surface reaction event.

| No. | Event | Microscopic reaction rate | Statistical molar flux | Proportion of adsorbed atoms |
|-----|-------------|---------------------------|---|------------------------------|
| 1 | Adsorption | $1.435 \times 10^9/s$ | $5.9607 \text{ mol}/(\text{m}^2 \cdot \text{s})$ | 100% |
| 2 | LH reaction | $3.758 \times 10^8/s$ | $1.5611 \text{ mol}/(\text{m}^2 \cdot \text{s})$ | 52% |
| 3 | ER reaction | $4.840 \times 10^8/s$ | $2.0105 \text{ mol}/(\text{m}^2 \cdot \text{s})$ | 36% |
| 4 | Desorption | $2.191 \times 10^8/s$ | $0.90993 \text{ mol}/(\text{m}^2 \cdot \text{s})$ | 12% |

The solid-phase surface catalytic efficiency is the ratio of the total number of atoms undergoing surface reactions to the total number of atoms colliding with the surface. In the simulation, the ratio of the total number of atoms in the LH reaction and the ER reaction and the total number of atoms colliding with the surface was counted. Finally, the surface catalytic efficiency does not exceed 0.002. From the current results, the material was believed to be low catalytic material.

3.4 Some Discussion about Follow-up Research

Multi-scale CFD/MD modelling can theoretically solve the problems of difficult surface reaction characterization and unclear formulation of key parameters under high-enthalpy airflow. Thereby, the prediction ability of hypersonic aircraft aerodynamic heating with surface catalytic effects was improved.

The computation results in this paper are generally preliminary, and more quantitative and accurate cross-scale numerical simulations are required in further research work. For possible application in aeronautical engineering, some future research perspectives should be noted as follows.

- Experimental verification with high-temperature intermediate measurement should be carried out in order to obtain the details of high-temperature interface parameter related with CFD and MD simulation, such as chemically reacting boundary layer profiles, surface adsorption sites, heat flux and species concentration at ultra-high temperature.
- In the framework of current high-performance computing, hyperscale ExaFlops computing, GPU acceleration algorithm, coding based on CPU/GPU heterogeneous system architecture should be seriously followed to overcome the time-consumption problems in cross-scale simulation.

4. Conclusion

A multi-scale CFD/MD modelling work was performed in this paper on the fluid-thermal-structural coupling platform CAPTER. A simple aeronautical application case describing the cross-scale dynamic process of surface heterogeneous catalysis on high-temperature TPS was preliminarily carried out, and typical computation results are obtained as follows.

- Studies show that in a typical hypersonic aerodynamic environment, adsorption, ER, LH and other reactions occur at a specific rate on the wall;

- The interface microscopic reaction rate determines the macroscopic species molar fluxes, which in turn generates a certain amount of catalytic heating.

Relevant modelling can solve the interface characterization problems under high-enthalpy aerodynamic environment. Thereby, the prediction ability of hypersonic aircraft aerodynamic heating with catalytic effects was extended from single macroscopic CFD to multi-scale CFD/MD coupling. For possible application in aeronautical science, some further research perspectives were finally put forwards.

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