Coupled simulation for reentry ablative behavior of hypersonic vehicles

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Abstract. Numerical analyses of hypersonic vehicles ablative behaviors focus on the accurate models of the thermochemical reaction flow field. The assumptions of chemical equilibrium and non-catalytic wall cannot meet the ablative behavior prediction requirements for high Mach number flights with multiphase materials. In this paper, the numerical analysis of hypersonic vehicle reentry involves the nonequilibrium thermochemical flow field and thermodynamic structure with moving boundary. Two surface models, finite rate catalysis model and Park finite rate surface interaction model were applied into the flow field simulation. And the reentry ablative behaviors of two hypersonic vehicles were simulated by the partitioning methods using the computational fluid dynamics code Fluent and the material thermal and structural response code Abaqus with user defined codes. And the two codes were loosely coupled in time to exchange the data. The structural temperature, surface shape change at the wall under different reentry altitudes and various angles of attack were obtained. The validity and reliability of frame work set up were validated with previous work.

1. Introduction
Numerical analyses of reentry ablative behaviors of hypersonic vehicles become more and more important with the application of new materials and increasing flight speed. Taking the chemical reactions into Considerations in the flow field simulation are necessary practices. It was assumed early that those surface reactions were chemical equilibrium. But the flight data showed that the equilibrium hypothesis caused the predicted ablative surface recession to be too large [1], while predicted values of surface recession with chemical nonequilibrium models could be reduced. According to the idea of chemical nonequilibrium, the finite rate surface interaction model was developed, which mainly considered the oxidation, sublimation and nitridation of carbonaceous materials [2-4]. A diffusion flame model established by Li [5] was used to characterize the combustion reactions between pyrolysis gases which injected to materials’ surface and oxidative gases in boundary layer. When the flight speed is subsonic and wall temperature lower than 1400K, the material such as silica is difficult to be oxidized and reactions between the material and oxidative gases are generally not considered, but the catalytic reactions at the wall need to be modeled. Bourdon [6] established a simplified catalytic model and found that the occurrences of the catalytic reactions were strongly dependent on the wall temperature, the concentration of the different species close to the wall, and the free sites available on the surface. When the wall temperature up to 1400K, the catalytic properties of the wall increase. For
higher temperatures, thermal desorption becomes very efficient and the catalytic properties of the wall decrease.

For aeroheating/ablation coupling analysis with chemical reactions, various numerical programs have been developed, such as the commercial CFD program Fluent, STAR-CD, CFX and FEM programs LS-DYNA, ABAQUS [7-8], etc. In order to improve the calculational efficiency and enhance specific functions, many capable research institutions and individuals develop their own calculation programs. The combination of MASCC and CMA simulated the ablative behaviors of the 3D missile in a predetermined trajectory [9], in which CMA solved the internal energy balance, the surface recession and the thermal decomposition coupled with surface energy balance to simulate the response of pyrolyzing and ablating heatshield in hypersonic flows. The program FIAT [10] similar with CMA, is a standard finite-difference code developed by NASA that simulates thermal conduction, kinetic control pyrolysis, pyrolysis gas injection, and thermochemical surface recession in porous materials. In recent years, with the need to characterize ablative thermal response with more and more complex ablative mechanisms, the COMSOL program that can customize mathematical models has been greatly developed [11-13]. Compared with the common finite element programs ABAQUS and LS-DYNA, its flexible formula editing ability deserves more applications and attempts by researchers.

In this paper, the thermochemical flow field and thermo-mechanical temperature field were calculated with Fluent and ABAQUS respectively using loosely coupled method. The ablative behaviors of materials at different reentry heights were simulated, and the influences of different attack angles were analyzed on the surface species concentration, wall temperature and surface recession of ablating composites.

2. The model

The supersonic flow field around an aircraft was divided into two parts: the inviscid outer-flow and the viscous boundary layer flow [14]. Two types of thermochemical reactions occurred at different locations in the viscous flow. The reactions occurred between the bow shock and boundary layer edge were characterized by the aerodynamic models. And the reactions occurred between boundary layer edge and wall were characterized by the surface chemistry models.

2.1. Aerodynamic model

Due to the presence of kinetic energy dissipation and shock waves, the flow field temperature around the vehicles was very high that caused gases to be dissociated and even ionized. So thermochemical reactions needed to be calculated. In addition to the general conservation equations of mass, momentum and energy, a species conservation equation is needed and can be obtained as [8]:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho v_i Y_i) + \nabla \cdot J_i = R_i$$

(1)

Because of the existence of chemical reactions, the reaction heat is added into the conservation of energy which was depicted as [8]:

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \left[ \nu (\rho E + P) \right] = \nabla \cdot \left[ \lambda \nabla T - \sum_i h_i J_i + (\overline{\nabla \cdot \nu}) \right] + S_e$$

(2)

In this paper, the gas-phase reactions were characterized by 11-species (O, N, NO, O2, N2, CO, CO2, CN, C2, C3, C), 17-reaction model [15] with assumption of chemical non-equilibrium and thermal equilibrium, which include eight dissociation/recombination reactions and nine exchange reactions. The forward rate constants for reaction $r$ are expressed in the form of Arrhenius equations [16]:

$$k_{f,r} = A_r T^\beta \exp\left[-\left(E_r / RT\right)\right]$$

(3)

The backward rate constant is calculated by the forward rate constant and the equilibrium constant for the $r$ reaction.
2.2. The surface chemistry model

Considering the consumption and production of the species for carbonaceous ablating materials, the mass fraction of the species at the wall can be calculated by the species mass conservation equation [17]:

$$-\rho_w D_i \frac{\partial Y_i}{\partial n} + \rho_w v_{i,w} Y_{i,w} = M_i \dot{\omega}_i$$ (4)

Where the first term denotes the diffusion of the gas species and the second term denotes the mass flux away from surface into gas-phase interior. While the last one denotes the production or consumption rate due to surface reactions. The mass loss rate of ablating materials can be expressed as [18]:

$$\dot{m}_b = \rho_w v_w = -\sum_{i=1}^{n_b} M_i \dot{\omega}_i$$ (5)

Various kinetics models can be used to characterize the surface chemical reactions at the wall between the ablating materials and oxidative gases which mainly dependent on reentry conditions and materials ablative mechanisms. There are two surface reaction models involved in this paper, namely surface catalysis model and Park finite rate surface model.

2.2.1. Catalytic wall.

For the non-ablating structure materials, a surface catalysis model studied by Sorensen and Schwartzentruber [19] was employed in this paper. Different from simplified catalysis model [20], this surface catalysis model is characterized by finite rate method. There are 11 reactions occurred in this model as shown in Table 1. Diffusion has been modelled by using Fickian diffusion, which set a common definition of constant Lewis number of 1.4 to compute the diffusion coefficient.

| reaction type | reaction | $S_0/\gamma_{ER}/\gamma_{LH}/\gamma$ | $E(kJ/mol)$ |
|---------------|----------|----------------------------------|--------------|
| 1             | O+(s1)→O(s1) ads                     | .05            | 0            |
| 2             | N+(s1)→N(s1) ads                     | .05            | 0            |
| 3             | O+O(s1)→O2+(s1) ER                   | .001           | 9            |
| 4             | N+N(s1)→N2+(s1) ER                   | .001           | 9            |
| 5             | O+N(s1)→NO+(s1) ER                   | .001           | 9            |
| 6             | N+O(s1)→NO+(s1) ER                   | .001           | 9            |
| 7             | 2O(s1)→O2+2(s1) LH                   | .1             | 300          |
| 8             | 2N(s1)→N2+2(s1) LH                   | .1             | 300          |
| 9             | N(s1)+O(s1)→NO+2(s1) LH              | .2             | 300          |
| 10            | O(s1)→O+(s1) des                     | $1\times10^{12}$ | 350          |
| 11            | N(s1)→N+(s1) des                     | $1\times10^{12}$ | 350          |

2.2.2. The finite rate surface chemistry model.

The surface reactions between oxidative gases and ablating materials are applicable to the Eley-Rideal recombination and carbon sublimation in Park surface model. The forward reaction rates for E-R reaction mechanisms are shown in Eq.6 [17]. And the sublimation forward reaction rates are given in Arrhenius form as shown in Eq.3.

$$k_f = \frac{V}{4\phi_i} \gamma_i T^{-\phi_i \phi} \exp\left(-\frac{E_{ER}}{RT}\right)$$ (6)

where the parameters in the equations are shown in Table 2 [18]. Calculation of the net production rate also requires a backward rate coefficient. The backward rate coefficient is computed from the forward rate coefficient and the concentration-based equilibrium constant [17].
Table 2. Park’s surface reaction model.

| Model  | \( N_r \) | Reaction | Type | \( S_0/\gamma_0/A \) | \( \beta_i \) | \( E(\text{kJ/mol}) \) |
|--------|--------|----------|------|----------------|---------|----------------|
| Park   | 1      | \( \text{O}^+(s)+\text{C}(b)\leftrightarrow\text{CO}^+(s) \) | ER   | 0.63           | 0       | 9.644          |
|        | 2      | \( \text{O}_2+2(s)+2\text{C}(b)\leftrightarrow2\text{CO}+2(s) \) | ER   | 0.50           | 0       | 0              |
|        | 3      | \( \text{N}^+(s)+\text{C}(b)\leftrightarrow\text{CN}^+(s) \) | ER   | 0.30           | 0       | 0              |
|        | 4      | \( 3(s)+3\text{C}(b)\leftrightarrow\text{C}_3+3(s) \) | Sub  | \( 5.19 \times 10^{13} \) | 1       | 775.81         |
|        | 5      | \( \text{C}_3+3(s)\leftrightarrow3(s)+3\text{C}(b) \) | ER   | 0.10           | 0       | 0              |

2.3. Material thermal response model

The energy conservation of gas phase reactions and surface reactions are shown in Figure 1. The energy conservation of gas-phase reactions interior is written by,

\[
\frac{\partial \left( \rho_s E \right)}{\partial t} + \nabla \left[ \rho_s \left( u S + P \right) \right] = \nabla \left[ \lambda \left( \nabla T - \sum_i \bar{h}_i \mathbf{n}_i \right) \right] + S_h + S_w
\]

where \( S_h \) is the release heat due to gas-phase reactions and \( S_w \) is the release heat due to surface reactions. Energy balance on an ablative surface is given by,

\[
\dot{q}_{\text{CONV}} + \dot{q}_{\text{DIFF}} + \dot{q}_{\text{RAD-OUT}} = \dot{m} (h_w - h_s) + \dot{q}_{\text{RAD-OUT}} + \dot{q}_{\text{COND}}
\]

In this balanced system, the leaving energy fluxes include the radiation \( \dot{q}_{\text{RAD-OUT}} \) away from the surface and the conduction \( \dot{q}_{\text{COND}} \) into the materials. The inputting energy fluxes involve the conduction \( \dot{q}_{\text{CONV}} \), the inward radiation \( \dot{q}_{\text{RAD-OUT}} \) and the species diffusion \( \dot{q}_{\text{DIFF}} \). The remaining two terms \( \dot{m} h_s \) and \( \dot{m} h_w \) represent the reaction enthalpy flux and ablation mass ejector heat flux due to surface reactions.

2.4. Mesh movement algorithm in Abaqus

According to Eq.5, the mass loss rate of ablating materials was obtained as \( \dot{m}_b \). To make the material density \( \rho_s \), the surface recession rate can be obtained from:

\[
\dot{S} = \frac{\dot{m}_b}{\rho_s}
\]

The new spatial position of each node on the surface moving boundary at the end of each step can be expressed as:

\[
x = x - \dot{S} \Delta t \cdot n_x
\]
\[
y = y - \dot{S} \Delta t \cdot n_y
\]
Using the ALE adaptive mesh method, the UMESHMOTION subroutine in Abaqus is programmed to embed the surface recession formula into the finite element thermodynamic calculation to achieve thermal conduction, moving boundary, and thermal stress-strain coupling analysis.

In this paper, the CFD code Fluent is used for hypersonic flow field of thermal equilibrium, chemical nonequilibrium while the FEM code Abaqus is used to calculate the structural heat conduction and surface recession. The ablative behaviors of the hypersonic vehicles of some reentry altitudes and various angles of attack were studied.

2.5. Interaction between the CFD and FEM codes
Coupling analyses of hypersonic flow, heat transfer and material response were achieved by the partition method. The multi-field coupling analysis model can be divided into fluid part and solid part according to physical mechanisms and spatial locations, as shown in Figure 2. In this model, the flow field was simulated by CFD code to obtain the heat flux $q_w$ and the pressure $p_w$. The FEM code for the structural field was used to obtain the wall temperature $T_w$ and the structural displacement $u_s$. These two codes characterized the coupling interactions between hypersonic flow and thermal response of ablating materials through exchanging parameters in real time on the fluid-solid coupling interface. The calculation data required in next step by each solver were repeatedly exchanged on the coupling interface.

The calculation data required in next step by each solver were repeatedly exchanged on the coupling interface.

![Figure 2. Multiphysics coupled calculation model.](image)

For the complex multiphysics coupling calculations of hypersonic flow-heat transfer and material response, it was important to use reasonable time coupling strategies and schemes in the calculation to improve the calculation accuracy and reduce the computation time. In this paper, the loose coupling scheme is adopted which is shown in Figure 3. Compared with close coupling strategy, loose coupling has advantages in computational efficiency and complex flow field calculation, but the coupling time step needs to be carefully selected.
3. Result and discussion

Corresponding to two different surface reactions models, there were two different materials, ZrB₂ and C/C composite materials studied in the paper.

3.1. Finite rate catalytic model

The IRV-2 [22] structure was modeled with catalytic reactions at the wall in this section. IRV-2 is a sphere-biconic-cylinder with a nose cone radius of 0.01905m and a total length of 1.386m. The biconic angles are 8.42° and 6.10° with a break at 0.1488m. The calculation model with $64 \times 64$ grid created by ICEM are shown in Figure 4. In this paper, four points: point1~point4 at the beginning of the flight path are selected as the boundary conditions of the fluid calculation. The parameters of the four points are shown in Table 3 [22]:

![Figure 4. IRV-2 warhead model and computational grid.](image)

![Figure 5. Heat flux at trajectory Point 1 with various time step.](image)

The laminar finite-rate model in Fluent was used for gas-phase chemistry model as this model can ignore the effects of turbulent fluctuations. Surface catalytic reactions were programmed by UDF for using species concentrations as boundary conditions for wall species. The Axis boundary condition was specified at the centerline of the axisymmetric geometry.

| Point No. | Time (sec) | Altitude (m) | Temperature (K) | Pressure (Pa) | Mach No. | Velocity (m/s) |
|-----------|------------|--------------|-----------------|--------------|----------|----------------|
| 1         | 0          | 66935        | 227.81          | 8.1757       | 22.41    | 6780.6         |
| 2         | 4.25       | 55842        | 258.02          | 37.362       | 21.08    | 6788.3         |
| 3         | 6.75       | 49290        | 270.65          | 88.118       | 20.58    | 6785.2         |
| 4         | 8.75       | 44042        | 261.40          | 169.50       | 20.90    | 6773.0         |

The structural material simulated by catalytic reactions at the surface with non-ablating wall was ZrB₂[23], and the density, specific heat, thermal conductivity is taken as 6000kg/cm³, 628J/(kgꞏK), and 66W/(mꞏK), respectively. The emissivity is set to 0.8 with ambient temperature 190K.

A study of coupling time increment was conducted at trajectory Point No.1 to ensure adequate prediction of convective heat flux and the results were shown in Figure 5. Compared with those data obtained by 0.01s, the convective heat flux obtained by 0.001s and 0.0001s are more similar with the Tabiei’s. Considering the balance between the amount of CPU time and calculation accuracy, 0.001s was adapted as the coupling time increment in this paper.

The coupling simulation results are shown in Figure 6. The trend of change and the magnitude of the calculation values are close to those in the literature [15,22,23].
As can be seen in Figure 7, the results from Sockalingam, Tabiei and this paper are almost the same, but they are quite different from Hassan’s, this is because the materials used in the first three are ZrB$_2$, and the materials used by Hassan are C/C composites. The surface reaction is also different from the first three, which is Park finite rate surface chemical reaction. Among the first three, the structural thermal response codes used by the first three are all finite element codes, of which Tabiei considered the boundary retreat in the thermal response. For gas-phase reactions, the first two used the 5-species,5-reaction model, while in this paper, the 11-species,17-reaction model is used, and the mass concentration boundaries of species are all catalytic reactions. This shows that the choice of gas-phase reactions and the consideration of boundary recession have little effect on the flow field heat flow and wall temperature, but the choice of surface reactions model and material properties have a greater impact on the results.

3.2. The Park surface chemistry model
A leading-edge structure was modeled in this section with the schematic diagram of the model shown in Figure 8. The nose cone radius is 25.40mm with a half cone angle 12.5°, and the total length of the leading edge is 200mm. The material was selected from C/C composites with density of 2.798 g/cm$^3$, specific heat of 860 J/(kg·K), thermal conductivity of 18 W/(m·K), and emissivity of 0.8. The inflow velocity is 15 Mach with the pressure of 1137 Pa, and various angles of attack (AOA) of 0°, 10°, 20°, and 30°, respectively.
The temperature distributions of the structure surface were shown in Figure 9. It can be seen that the position of the maximum temperature moves toward the windward side with the increase of the angle of attack. The maximum temperature of different angles of attack was basically the same, and the temperature difference increased between the windward and leeward with the increasing AOA. The temperature difference between the two sides of the AOA of 0°, 10°, 20°, and 30° is 39K, 749K, 1385K, and 1829K, respectively.

When the AOA is greater than 10°, the temperature of the windward surface is significantly larger than that of the leeward side, which causes the surface recession depths on both sides to be very different. As shown in Figure 10, the maximum ablative recession depth of the structure increases with the increasing AOAs. And the position of the maximum recession is moving to the windside with increasing AOAs, which is the same trend as the temperature distribution.

The surface recession depth of the structure under different AOAs was shown in Figure 11. The windward side with the AOA of 30° has the largest depth of recession, which is 5.657mm, and the
AOA of 0° has the smallest depth of recession 5.456mm; the trend of the leeside recession depth changing is opposite to windward side.

![Graph](image1)

**Figure 11.** The surface recession of different AOAs at 20s: (a) Windside; (b) Leeside.

The ablative recession rates of the structure were shown in Figure 12. In the aspect of moving direction, the change trends of recession rates for different AOAs were consistent with the change of temperature distributions.

![Graph](image2)

**Figure 12.** Radial recession rate with different AOAs.

4. Conclusion

In this paper, the fluid/thermal/ablation coupled simulation were established by partition coupling method. The flow field data were loosely coupled with the structure data in real time, in order to simulate the ablative behavior of hypersonic reentry realistically. The established procedure was validated with the IRV-2 reentry vehicle and leading-edge structure. Results from IRV-2 indicated that surface chemistry model and material properties had a significant impact on the surface heat flux and wall temperature. The behavior of leading-edge vehicle was studied under different angles of attack. The stagnation temperature does not change with the increasing angle of attack. The position of the maximum temperature zone moves toward the windward side. The magnitude of the final surface recession was mainly determined by the wall temperature.

References

[1] Beerman 2009 Significance of nonequilibrium surface interactions in stardust return capsule ablation modeling *Journal of Thermophysics and Heat Transfer* **23** 425-432

[2] Park 2007 Calculation of stagnation-point heating rates associated with stardust vehicle *Journal*
of Spacecraft and Rockets 44 24-32
[3] Chen Y. K. and Milos F. S. 2004 Finite-rate ablation boundary conditions for a carbon-phenolic heat-shield 37th AIAA Thermophysics Conference 2004-2270
[4] Alba C. R. 2007 Development of a nonequilibrium finite-rate ablation model for radiating earth reentry flows Journal of Spacecraft and Rockets 35 1-23
[5] Li W.J. 2016 Protection of pyrolysis gases combustion against charring materials’ surface ablation International Journal of Heat and Mass Transfer 102 10-17
[6] Bourdon A. 2008 numerical simulation of stagnation line nonequilibrium airflows for reentry applications Journal of Thermophysics and Heat Transfer 22 168-177
[7] Yin T.T. and Zhang Z.W. 2014 Modeling ablative behavior and thermal response of carbon/carbon composites Computational Materials Science 95 35-40
[8] Meng S.H. and Zhou Y.J. 2016 Multiphysics coupled fluid/thermal/ablation simulation of carbon/carbon composites Journal of Spacecraft and Rockets 53 1-6
[9] Murray A.L. 2002 Coupled aeroheating/ablation analysis for missile configurations Journal of Spacecraft and Rockets 39 501-507
[10] Dec J. A. and Braun R. D. 2012 Ablative thermal response analysis using the finite element method Journal of Thermophysics and Heat Transfer 26 201-212
[11] Li Wei and Zhang Jun 2019 Evaluation of numerical ablation model for charring composites Sci China Tech Sci 62 1323-1330
[12] Zhang B. and Li X. 2018 Numerical simulation of ablation behavior of carbon/phenolic thermal protection system composite Acta Materiae Compositae Sinica 35 2786-2792
[13] Zhang B., Li X. 2018 Numerical simulation of thermal response and ablation behavior of a hybrid carbon/carbon composite Applied Composite Materials 25 675-688
[14] Wang J. F. 2008 Numerical method of carbon-based material ablation effects on aero-heating for half-sphere Modern Physics Letters B 32 1840011.1-184011.5
[15] Hassan, B. 1998 Coupled fluid/thermal prediction of ablating hypersonic vehicles 36th AIAA Aerospace Sciences Meeting and Exhibit 98-0168
[16] Alba C. R. and Greedyke 2016 Development of a nonequilibrium finite-rate ablation model for radiating earth reentry flows Journal of Spacecraft and Rockets 53 1-23
[17] Marschall, J. and Maclean M. 2011 Finite-rate surface chemistry model, I: formulation and reaction system examples 42nd AIAA Thermophysics Conference 2011-3783
[18] Maclean M. and Marschall J. 2011 Finite-rate surface chemistry model, II: coupling to viscous Naver-stokes code 42nd AIAA Thermophysics Conference 2011-3784
[19] Sorensen C. and Schwartzentruber T. 2011 Sensitivity analysis of reaction rates in a finite rate surface catalysis model 42nd Thermophysics Conference 27-30
[20] Sarma G. S. R. 2000 Physio-chemical modelling in hypersonic flow simulation Progress in Aerospace Sciences 36 281-349
[21] Bentley J L.1975 Multidimensional binary search trees used for associative searching Communications of the ACM 18 509-517
[22] Sockalingam S. and Tabiei A. 2009 Fluid/thermal/chemical non-equilibrium simulation of hypersonic reentry vehicles Int. Jnl. of Multiphysics 3 293-306
[23] Tabiei A. 2012 Multiphysics coupled fluid/thermal/structural simulation for hypersonic reentry vehicles Journal of Aerospace Engineering 25 273-281