Wall temperature correlation for convective heating prediction of aircraft heat shield in high-enthalpy and chemically reacting flow

Xiaofeng Yang, Guangming Xiao, Lei Liu*, Yanxia Du and Yewei Gui
State Key Laboratory of Aerodynamics, China Aerodynamics Research and Development Center, Mianyang 621000, Sichuan, P. R. China

E-mail: leiliu@card.cn

Abstract. Hypersonic aircrafts and aero-engine combustion chambers both generate non-equilibrium and high-enthalpy flows and bring complex material-relied heat convection performance. The convective heating prediction is difficult due to unknown surface thermal state, leading to poor usability of wall temperature correlation method (WTCM). This paper aims at improving WTCM for convective heating prediction in chemically reacting flows through coupling computation of catalysis on thermal protection materials. Modified WTCM for chemically reacting flows accounts for two distinct physical events driven by temperature gradient and species reaction, which follow the Fourier’s and Fick’s laws, respectively. Preliminary validation testing demonstrates the feasibility of the modified WTCM to rapidly evaluate aerodynamic heating with limited deviation. The current research provides essential technical support for the evaluation and design of hypersonic aircrafts and aero-engine combustion chambers.

1 Introduction
Hypersonic aircrafts with high Mach number ($M_\infty > 10$) and aero-engine combustion chamber both generate non-equilibrium and high-enthalpy flows [1, 2]. The chemical non-equilibrium effect generated from high-speed/enthalpy gas flow and the gas/surface interaction bring more complex coupling heat convection performance. The evaluation of convective heat transfer over the thermal protection system (TPS) of heat shields at extremely high speed/enthalpy is of vital significance for the evaluation and design of hypersonic aircrafts or aero-engine combustion chambers [3].

Numerically, a coupling method of computational fluid dynamics (CFD) and computational heat transfer (CHT) can be used to solve the above problem. However, large computation cost may be taken for coupling simulation, especially for heat flux calculation from CFD. It urges the researchers to develop efficient or rapid methods for material-relied convective heating prediction to avoid time-consuming coupling computation.

For hypersonic or high-enthalpy perfect-gas flow, though aerodynamic heating level changes with wall temperature, the convection coefficient, or Stanton number ($St$), is usually invariant. $St$ is non-dimensionalized by mass flux at the edge of boundary layer $\rho_\infty u_\infty$ and wall enthalpy difference $h_{w,ad} - h_w$. Based on the above assumption, under the same free stream condition, when wall temperature changes, the variables at the edge of boundary layer remain unchanged. By additionally assuming specific heat nearly unchanged, wall temperature correlation method (WTCM) is therefore derived as
the description from Anderson [2]. By using WTCM, the heat flux distribution at given temperature can be fast predicted from the known heat flux data at other given temperature, such as the wall with room temperature $T_w = 300$ K.

When the flow is high-enthalpy or chemical non-equilibrium, the boundary layer flow becomes complicated due to processes with certain rate such as finite-rate chemical reactions [4]. Figure 1 presents the sketch of aerodynamic heating physics in high-enthalpy and chemical non-equilibrium flow over blunt body. The species concentration boundary layer and velocity/thermal boundary layer coexist, and surface catalysis brings additional diffusion in the boundary layer. The usability of WTCM for rapid evaluation of aerodynamic thermal environment deteriorates because of interface thermochemistry. As a result, the researchers should pay close attention to the improvement of WTCM in order to adapt chemically reacting flows.

Figure 1. Sketch of aerodynamic heating physics in high-enthalpy and chemical non-equilibrium flow over blunt body.

In order to deal with the above problem derived by WTCM, numerical simulation of heat flux considering catalysis on carbon-based materials in carbon-oxygen dissociated environment was performed in the current research work. According to the coupling simulation, WTCM was then modified and numerically tested preliminarily for high-enthalpy and chemical-nonequilibrium flows.

## 2 Methodology

### 2.1 Coupling simulation solvers

The numerical framework and coupling procedure were realized by programming and packaged into the in-house software platform CAPTER (*Coupled Analysis Platform for Thermal Environment and structure Response*), developed by the aircraft thermal science group of China Aerodynamics Research and Development Center (CARDC) [5].

The coupling simulation solvers include CFD for high-enthalpy and chemical nonequilibrium flow and CHT for TPS structural heat transfer. It is important to properly model the gas-solid interface, because the interface thermal state determines the aerodynamic heating and meanwhile is the input of structure energy. The interface balance equations (IBE) for mass, momentum and energy were established as [6, 7]

$$\left( \mathbf{m} - \rho Y^T \mathbf{u} \right) \cdot \mathbf{n} = \mathbf{m}_{w,n}$$

(1)
\[ \nabla p \cdot n = 0 \]  
(2)

\[ (q_s + h \cdot \dot{m}) \cdot n = q_s \cdot n + q_{wr} \]  
(3)

The above IBE connects the CFD and CHT solvers on the gas-solid interface, resulting in the closure of CFD/CHT coupling algorithm. Spatial interpolation was used to exchange data between the gas domain (CFD) and the solid domain (CHT).

### 2.2 Interface chemistry mechanism

Interface mass flux \( \dot{m} \) in IBE should be obtained from interface reaction rates, which is phenomenologically determined by the chemistry mechanism, that is, phenomenological catalytic (PC) model. On the gas-solid interface, the chemistry system is a multi-species and multi-reaction system. For specific reaction pathway, the mole flux is determined by the species concentration \( \bar{\rho}_i \) and reaction rate coefficient \( k_f \) as \[8\]

\[
\dot{M} = k_f \prod_{i=1}^{N_s} \bar{\rho}_i^{v'_i} - k_b \prod_{i=1}^{N_s} \bar{\rho}_i^{v''_i}
\]  
(4)

By summation of each species, the total mole flux for specific species \( s \) is

\[
\dot{M}_s = \sum_{i=1}^{N_s} (v''_s - v'_s) \dot{M}_i
\]  
(5)

At this point, the reaction rate coefficients \( k_f \) and \( k_b \) need to be determined.

Interface heterogeneous catalysis is the main phenomenon of gas/surface interaction, and Eley-Rideal (E-R) mechanism is one of typical recombination patterns that describe near-wall behaviours of atoms/molecules. The recombination is assumed to be irreversible, namely the surface backward reactions are neglected. The forward rate coefficient is \[9-11\]

\[
k_f = \gamma \frac{V_0}{\Phi_s^{v_s}} \exp \left( \frac{M \Delta E}{RT} \right)
\]  
(6)

where mean thermal speed of species \( s \) is \( V_0 = \sqrt{8RT/\pi M_s} \).

Since it is difficult to macroscopically obtained the exact values of recombination coefficients and site density, the effective recombination coefficient \( \bar{\gamma} = \gamma / \Phi_s^{v_s} \) with given values in advance is employed in the current simulation.

### 3 Computation models and conditions

Gas/surface interaction coupling simulation of high-enthalpy CO\(_2\) flow around carbon-based materials was intended to be performed to solve Mars entry problems. The settings of chemical reactions, heat shield properties and computational conditions are simply introduced hereafter.

#### 3.1 Gaseous and Surface chemical reactions

Six types of chemical reactions (\(2CO \leftrightarrow CO_2 + C, CO + O \leftrightarrow C + O_2, CO_2 + O \leftrightarrow CO + O_2, CO_2 + M \leftrightarrow CO + O + M, CO + M \leftrightarrow C + O + M\) and \(O_2 + M \leftrightarrow 2O + M\), where \(M\) is third body species) are included with five candidate species (C, O, O\(_2\), CO and CO\(_2\)). The rates of related chemical reactions are referred to from the work of Park et al [12].
For wall catalytic reactions, the recombination reactions of \( \text{O}_2 \) and \( \text{CO}_2 \) are considered, and the rates of chemisorption and E-R recombination are controlled. The chemisorption reactions of \( \text{O} \) and \( \text{CO} \) are considered [13], and three E-R recombination pathways are included as

\[
\text{O} + \text{O}(s) \rightarrow \text{O}_2(s) \\
\text{R1}
\]

\[
\text{CO} + \text{O}(s) \rightarrow \text{CO}_2(s) \\
\text{R2}
\]

\[
\text{O} + \text{CO}(s) \rightarrow \text{CO}_2(s) \\
\text{R3}
\]

where \( (s) \) denotes the particles adsorbed onto the surface empty chemisorption sites.

3.2 Heat shield properties
The multi-layer heat shield with 70-degree semi-conical blunt body shape is made of SLA-561V and aluminum honeycomb sandwiched between thin polyimide faceplate. The thermal properties of these materials are from Milos et al [14]. The main parameters of geometric configuration and TPS for current simulation are shown in Figure 2 from [15].

![Figure 2. Main parameters of geometric configuration and TPS for current simulation from [15].](image)

3.3 Computational conditions
The free stream condition for the current simulation is \( u_\infty = 4862 \text{ m/s} \), \( T_\infty = 173 \text{ K} \) and \( p_\infty = 27.4 \text{ Pa} \) for \( \text{CO}_2 \) related gaseous dissociated mixture from the work of Mitcheltree and Gnoffo [16]. Interface chemical condition includes non-catalytic (NC), fully catalytic (FC) and PC walls. For detailed geometry model, computational grid, solver settings and further validation investigation, one can refer to the previous work of Yang et al [6, 7].

4 Coupling results
4.1 Coupling evolution
The structure is aerodynamically heated by such high-speed flow, and the temperature in the structure gradually rises during the coupling process.
Figure 3 presents the initial temperature contour in the gas and solid domains. The inviscid flow field keeps nearly unchanged with the coupling process, the changes only exist in the boundary layer. Figure 3 also presents temperature distribution details in the stagnation region at the coupling time \( t = 0, 2, 4, 6 \text{ s} \). Under continuous aerodynamic heating, the structure is gradually heated to the final quasi-radiation-equilibrium state.

![Figure 3](image1.png)

**Figure 3.** Initial temperature contour in the gas and solid domains and temperature distribution details in the stagnation region at \( t = 0, 2, 4, 6 \text{ s} \).

The influence of interface catalysis on coupling heating evolution is shown in Figure 4, and different catalysis models generate different ascent/decent patterns of interface heatflux. FC generates the highest coupling heat flux owing to high heat release from interface reaction, while NC leads to the lowest heat flux due to no heat release. The PC result varies with the activation energy \( \Delta E \). At weak activation state (\( \bar{M} \Delta E / \bar{R} = 700 \text{K} \)), the evolution trend keeps the same as that of NC and FC.

When the activation state gets strong (\( \bar{M} \Delta E / \bar{R} = 2800 \text{K} \)), however, the above trend no longer remains. The heat flux rises at the initial stage (\( t < 0.05\text{s} \)), and then returns to the conventional downtrend. The types of interface catalysis mentioned above are believed to have great influence on surface temperature evolution as shown in Figure 5. The key reason is that the chemical heating rises with the increase of local temperature. In turn, chemical heating additionally enhances the local temperature.

4.2 Stagnation \( q_w - T_w \) correlation

The determination of correlation between stagnation heat flux \( q_w \) and local temperature \( T_w \) during the coupling process is the core of WTCM, which is presented in Figure 6 under the conditions of NC, FC and PC (\( \bar{M} \Delta E / \bar{R} = 2800 \text{K} \)).
The $q_w - T_w$ correlation with no interface chemistry (NC) keeps good linearity, while the $q_w - T_w$ linearity for PC turns to be the worst. From the comparison in Figure 6, one can observe that such linearity is weakened by the introduction of chemical heating due to interface thermochemistry. Separately, Figure 7 presents the stagnation $q_w - T_w$ correlation dominated by Fourier’s law (the heat transfer driven by temperature gradient) and Fick’s law (the heat exchange induced by concentration gradient from interface chemistry). The component of chemical heatflux ($F_i$) mainly contributes to the deterioration of $q_w - T_w$ linearity, while the conventional temperature-gradient component ($F_o$) still maintains high linearity during the coupling process.

![Figure 4](image1.png) \hspace{1cm} ![Figure 5](image2.png)

**Figure 4.** Influence of interface catalysis on heatflux evolution.  
**Figure 5.** Influence of interface catalysis on temperature evolution.

![Figure 6](image3.png) \hspace{1cm} ![Figure 7](image4.png)

**Figure 6.** Stagnation $q_w - T_w$ correlation for various interface conditions.  
**Figure 7.** Stagnation $q_w - T_w$ correlation dominated by Fourier’s and Fick’s laws.
5 Discussion on wall temperature correlation

5.1 WTCM improvement

Through in-depth investigation of boundary layer behaviours, we found that the heatflux described by Fourier’s law \( q_{f0} \) generally obeys the conventional WTCM, while the heatflux described by reacting diffusion (Fick’s law) \( q_{f1} \) is almost independent of boundary layer profiles such as velocity. Therefore, the conclusion can be drawn that \( q_{f1} \) can be simply dealt with by computing the chemical reaction rates from sole chemistry mechanism, eliminating the need for fully CFD/CHT coupled computation.

On the assumption mentioned above, only \( q_{f0} \) is considered with WTCM. The modified WTCM (M-WTCM) then has the following form

\[
\frac{q_{f0,1}}{q_{f0,0}} = \frac{T_{ad,T1}}{T_{ad,T0}}
\]

where “0” denotes the known heat flux at given temperature \( T_0 \), while “1” denotes the unknowns at other temperature \( T_1 \).

In other words, only the temperature-gradient part described by Fourier’s law (\( F_0 \)) is corrected due to wall temperature change. The total heatflux is the summation of temperature-gradient part (\( F_0 \)) and chemical-reaction part (\( F_1 \)) as

\[
q = q_{f0} + q_{f1}(T,Y)
\]

In weak or moderate chemistry condition (commonly for typical TPS materials), the diffusion rate is positively related to wall reaction rate. The heatflux induced by diffusion \( q_{f1} \) can be calculated from local reaction concentration, rather from CFD results. The temperature-gradient part \( q_{f0} \) can be obtained from WTCM based on the cold-wall result. The decomposition of temperature-gradient heating and chemical heating forms the fundamental of M-WTCM.

Based on the above idea of WTCM improvement, Figure 8 describes the details of flow chart of M-WTCM procedure for convection heating prediction. Using the known information of flow field data at room temperature \( T_0 \) and adiabatic temperature \( T_{ad} \) (computed from adiabatic simulation with \( q_w = 0 \)), the total heat flux at other temperature will be obtained by adding the heat flux from temperature gradient and that from chemical reaction.

5.2 Uncoupled validation with M-WTCM

Applying the M-WTCM procedure for convection heating prediction in Figure 8, a simple uncoupled case with rapid M-WTCM approach was carried out based only on the numerical results on room-temperature-wall ( \( T_w = 300 \text{K} \) ), adiabatic-wall ( \( q_w = 0 \) ) and radiation-equilibrium ( \( q_w = \varepsilon \sigma (T_w^4 - T_\infty^4) \) ) conditions.

Two assumptions are proposed for diffusion heatflux calculation: (1) the near-wall species concentration changes linearly with temperature; (2) reaction induced diffusion is limited by near-wall flow transport capability. The species mass fraction at given temperature is obtained by linear interpolation between cold-wall and radiation-equilibrium results. Since the near-wall flow transport capability is limited, the surface species cannot infinitely react. Wall diffusion is assumed to be limited to the level of 0.0007 kmol/m²s in this case.
Figure 8. Flow chart of M-WTCM procedure for convection heating prediction.

With the above WTCM settings, the heat flux results corrected by high-temperature walls covering the full coupling process were obtained. Figure 9 presents the stagnation \( q_w - T_w \) correlation from M-WTCM and its comparison with conventional WTCM and coupling result. The M-WTCM result keeps the same trend with the coupling one, and the \( q_w - T_w \) curve is closer to the coupling one than conventional WTCM. For detailed discussion, \( q_w \) is separated into temperature-gradient heating (Fo) and chemical heating (Fi) parts as shown in Figure 10. The original linearity of the former (Fo) gets slightly weak due to interface thermochemistry. The consistency of chemical heating (Fi) has some deviation at the whole temperature ranges and an accurate determination of interface reaction rates needs to be closely focused on.

Figure 9. Comparison of \( q_w - T_w \) correlation from conventional WTCM, current M-WTCM and coupling simulation.

Figure 10. Comparison of \( q_w - T_w \) correlation from M-WTCM dominated by the Fourier’s (Fo) and Fick’s (Fi) laws.
The result from this preliminary testing demonstrates the feasibility of M-WTCM in dealing with chemical convective heat transfer problems though some deviation exists between the coupling simulation and M-WTCM prediction.

6 Conclusion
This paper proposed a modified approach for WTCM through the understanding of CFD/CHT coupling simulation. This M-WTCM is capable of simulating aerodynamic heating considering surface thermochemistry with limited deviation, and can effectively support rapid assessment and design of high-speed aircrafts and aero-engine combustion chambers.

The characterization of interface thermochemistry and the calculation of its rate are found to be of vital importance for the further modification and application of the current M-WTCM approach. Future work for M-WTCM improvement includes but not limited to: (1) accurate determination of the near-wall species concentration at given temperature; (2) quantitative modelling of the near-wall flow transport limitation.

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