Laminar Reactive Boundary Layer Simulation of an Ablating Heated Carbon Surface

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Two-dimensional simulations were performed with applications to reactive boundary layers present over ablating surfaces. This work was performed in close coordination with experimentalists at the Air Force Institute of Technology (AFIT), where the simulations will be applied to the reactive boundary layer present on missile surfaces caused by laser induced ablation. Previously developed semi-global surface reaction models for both non-porous and porous carbon were used in a finite volume computational fluid dynamics (CFD) reacting flow solver. Detailed chemical kinetics, molecular transport and thermodynamic properties were implemented into the CFD code and the surface reaction was included as an external subroutine. A range of surface temperatures and free stream velocities were simulated using a 5 mm long reacting carbon plate. Results show that reaction layers and species present along the surface differ according to carbon surface porosity, surface temperature, and chemical residence time. These predicted structures expose what types of intricacies are to be expected in reacting boundary layers that will be investigated experimentally by AFIT.

I. Introduction

Ablating surfaces are currently investigated to understand a variety of physical phenomenon with applications including rocket nozzles, channel flows, soot growth, Thermal Protective Systems (TPS), and coal combustion. When the surfaces in these applications are subjected to a substantial amount of heating, a reaction process occurs between the material face and the neighboring gaseous molecules. Areas along the surface, known as active sites, absorb the gaseous molecules and quickly desorb them in some altered state. These altered, or excited, molecules then proceed to react with various other gaseous species. The physico-chemical processes involved are unique to not only the material’s molecular composition but also to the material’s structure. In the case of ablating surfaces, the material contributes a molecule to the gaseous reactant and, therefore, the material’s surface regresses as the reaction processes take place. For example, solid carbon oxidation reacts with oxygen, water, and other reactants to form carbon monoxide. The surface contributes its solid carbon molecules to the gaseous product and consequently the material regresses in size. Such physical processes of carbon can be observed on a daily basis, from the burning of wood in a fireplace to the hot coals in a charcoal grill. Additionally surface ablation can be found in extreme physical scenarios, such as the heat shields (TPS) used on hypersonic re-entry vehicles as well as in high energy laser (HEL) defense systems, where a laser is used to heat and terminate the exterior body of a threatening missile.

This investigation focuses on the development of a reactive boundary layer model for ablating surfaces. The physical-chemical model implemented depend on the specific ablation problem, which, in turn, requires a variety of modelling methodologies and assumptions. Early investigations of hypersonic re-entry vehicles were restricted by limited computational power, hence several analytical and self-similar solutions for ablating carbon materials were explored as reported in refs. These studies focused primarily on understanding surface recession rates for the Mercury, Apollo and Gemini re-entry capsules. In the years since, computational power has increased and the areas of research expanded.

Ablating surfaces are currently investigated in a variety of physical applications, with flow regimes ranging between the subsonic, continuum, to hyper-
sonic, rarefied, gas limits. Studies in surface reaction chemistry have proposed several semi-global reaction models for porous and nonporous graphite surfaces.\textsuperscript{7–11} These heterogeneous surface reaction models have since been implemented in various ablation models\textsuperscript{12–16} with applications including, but not limited to, rocket nozzles, channel flows, soot growth, and Thermal Protective Systems (TPS). Many of these models utilize various methods of Computational Fluid Dynamics (CFD), which solve the reacting Navier-Stokes equations for the gaseous phase to understand the interactions between the flow is both high-speed and rarefied and cannot be modelled using the continuum assumption. To address this regime, recent efforts have studied ablating carbon surfaces using Direct Simulation Monte Carlo (DSMC) to understand the interactions between the gas dynamics and surface reactions.\textsuperscript{17}

The surface reaction research has also focused on other topics, for example catalytic-combustion within monoliths in various simple geometries. These studies on the cracking of complex hydrocarbons were investigated in order to reduce unwanted emissions in industrial gas-turbine power generators.\textsuperscript{18} The physics involved is very similar to the aforementioned surface reaction applications, the flow is driven over a reacting surface. However, the fluid flows at a much lower speeds through a tube or channel and gaseous reactions are not present. Recent efforts have modelled the coupling between surface reactions and gas phase fluid using plug flow or boundary layer self-similar solution approximations.\textsuperscript{19–21} These approximations reduce computational cost but results have shown to be significantly different from full reacting Navier-Stokes solutions.\textsuperscript{22}

The work presented here is performed in close coordination with experimentalists at the Air Force Institute of Technology (AFIT),\textsuperscript{23} where the simulations will be applied to the reactive boundary layer present on missile surfaces caused by laser induced ablation. In particular, the initial work presented in this paper focuses on laminar, subsonic ($M < 0.3$) free-stream conditions. Simulations were done using the OpenFOAM\textsuperscript{24} Finite Volume Method (FVM) CFD package, where both detailed chemistry models and molecular transport libraries were implemented. A boundary condition was developed specifically to allow transport and reaction of species at a planar surface. This allows for a coupling between homogeneous gas phase and heterogeneous surface reaction models. Results show that that the presence of various species in the gas phase is strongly coupled with the flow residence time and the surface temperature. Interesting two-dimensional effects are identified due to oxygen depletion at the leading edge and carbon-dioxide formation in the gas-phase.

II. Heterogeneous Kinetic Model for Carbon Surface Ablation

In order to model the surface ablation, two sets of heterogeneous semi-global reaction models were used. The models include reaction with gaseous species $O_2$, $CO_2$, $H_2O$, $OH$, and $O$-atoms at the surface. These reactant species produce largely $CO$ and traces of $H_2$ and $H$-atoms. The first model used was developed by Bradley et al.\textsuperscript{10} and is meant for pure graphite surfaces (assumed non-porous). The specific reaction rate parameters used in this model are listed in Table 1.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$i$</th>
<th>$B_i$</th>
<th>$n_i$</th>
<th>$E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_s + OH \rightarrow CO + H$</td>
<td>1</td>
<td>$3.61 \times 10^2$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$C_s + O \rightarrow CO$</td>
<td>2</td>
<td>$6.65 \times 10^2$</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>$C_s + H_2O \rightarrow CO + H_2$</td>
<td>3</td>
<td>$4.80 \times 10^5$</td>
<td>0.0</td>
<td>68800</td>
</tr>
<tr>
<td>$C_s + CO_2 \rightarrow 2CO$</td>
<td>4</td>
<td>$9.00 \times 10^3$</td>
<td>0.0</td>
<td>68100</td>
</tr>
<tr>
<td>$C_s + \frac{1}{2}O_2 \rightarrow CO$</td>
<td>5</td>
<td>$2.40 \times 10^3$</td>
<td>0.0</td>
<td>30000</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>$2.13 \times 10^1$</td>
<td>0.0</td>
<td>-4100</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>$5.35 \times 10^{-1}$</td>
<td>0.0</td>
<td>15200</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>$1.81 \times 10^7$</td>
<td>0.0</td>
<td>97000</td>
</tr>
</tbody>
</table>

Table 1: The heterogeneous reaction rate parameters of non-porous carbon.\textsuperscript{10}

Knowing the specific reaction rate parameters listed in Table 1, the mass production rate ($w_i'$ is in units of $\text{kg/m}^2/\text{s}$) can be calculated by using the modified-Arrhenius expression,

$$k_i = B_i T^{n_i} \exp(-E_i/RT),$$

(1)
with following surface mass production rate relations:

\[
\begin{align*}
 w'_{OH} &= - (p_{OH}) k_1, \quad (2) \\
 w'_{O} &= - (p_{O}) k_2, \quad (3) \\
 w'_{H_2O} &= - (p_{H_2O})^{1/2} k_3, \quad (4) \\
 w'_{CO_2} &= - (p_{CO_2})^{1/2} k_4, \quad (5) \\
 Y &= \frac{1}{1 + k_6 p_{O_2} Y}, \\
 w'_{O_2} &= \left( - \frac{1}{2} \right) \left[ k_5 p_{O_2} + k_7 p_{O_2} Y \right], \quad (6) \\
 w'_{H} &= (p_{OH}) k_1 \frac{W_H}{W_{OH}}, \quad (7) \\
 w'_{H_2} &= (p_{H_2O}) k_3 \frac{W_{H_2}}{W_{H_2O}}, \quad (8) \\
 w'_{CO} &= w'_{OH} \frac{W_{CO}}{W_{OH}} + w'_{O} \frac{W_{CO}}{W_{O}} + w'_{H_2O} \frac{W_{CO}}{W_{H_2O}} + (2) w'_{CO_2} \frac{W_{CO}}{W_{CO_2}} + w'_{O_2} \frac{W_{CO}}{W_{O_2}}. \quad (9)
\end{align*}
\]

Here, \( p_i \) denotes partial pressure of species \( i \), in atmospheric pressure units. The second model was developed by Chelliah et al.\textsuperscript{7,8} and takes into account the bulk porosity of the graphite surface. The reaction rate parameters of this model are listed in Table 2.

<table>
<thead>
<tr>
<th>( k )</th>
<th>Reaction</th>
<th>( B_k )</th>
<th>( n_k )</th>
<th>( E_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( C_s + OH \rightarrow CO + H )</td>
<td>1.65</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>( C_s + O \rightarrow CO )</td>
<td>3.41</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>( C_s + H_2O \rightarrow CO + H_2 )</td>
<td>( 2.00 \times 10^8 )</td>
<td>0.0</td>
<td>64750</td>
</tr>
<tr>
<td>4</td>
<td>( C_s + CO_2 \rightarrow 2CO )</td>
<td>( 6.00 \times 10^7 )</td>
<td>0.0</td>
<td>64300</td>
</tr>
<tr>
<td>5</td>
<td>( C_s + \frac{1}{2}O_2 \rightarrow CO )</td>
<td>( 4.40 \times 10^6 )</td>
<td>0.0</td>
<td>43000</td>
</tr>
</tbody>
</table>

Table 2: The heterogeneous rate constants of porous carbon\textsuperscript{7,8}

Here, the mass production rate is calculated using the expression,

\[
 w'_i = \nu_{ik} W_i (\rho Y_i / W_i) B_k T^{n_k} \exp(-E_k / RT),
\]

where subscript \( i \) denotes the species of interest, while subscript \( k \) denotes the particular reaction step in Table 2. Specifically, \( W_i \) and \( Y_i \) are the molecular weight and mass fraction of species \( i \), respectively, and \( \nu_{ik} \) is the stoichiometric coefficient of species \( i \) in the \( k \)th reaction. The units of \( w'_i \) are in kg/m\(^2\)/s. It is clear that the surface reaction rates for these two models must be calculated differently, but the necessary parameters can be easily acquired within any simulation.

For a typical gas-phase species composition at the surface, Fig. 1 shows the calculated ratio of the porous to nonporous model’s reaction rates as a function of temperature, for major reactant species, \( H_2O, O_2, \) and \( CO_2. \)
These reaction rates were calculated using constant reference quantities for density, $\rho = 0.15 \text{ kg/m}^3$, and pressure, $p = 0.9 \text{ atm}$, which were taken from a non-reacting flat plate solution at a fixed temperature of $2200K$. Surface species concentrations for water and oxygen were the free-stream quantities of $Y_{H_2O} = 0.03$ and $Y_{O_2} = 0.20$. Carbon Dioxide was estimated based on past simulations at a value of $Y_{CO_2} = 0.035$, while the remainder was assumed to be nitrogen. According to these models, the porous carbon surface reaction rates for $O_2$ and $CO_2$ can be two orders of magnitude greater than the nonporous surfaces. This is expected, as a porous carbon material has more active sites per surface area.

**III. Numerical Approach**

An open-source computational fluid dynamics (CFD) package, OpenFOAM,$^{24}$ was used to solve the following conservation equations:

\begin{align}
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} &= 0, \\
\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \rho \vec{v} \nabla \vec{v} &= -\nabla p + \nabla \cdot \mathbf{T}, \\
\frac{\partial \rho h_s}{\partial t} + \nabla \cdot \rho \vec{v} \nabla h_s - \nabla \cdot \rho \alpha \nabla h_s &= -\sum_{i=1}^{N} h_i w_i, \\
\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \rho \vec{v} \nabla Y_i - \nabla \cdot \rho D_i \nabla Y_i &= w_i,
\end{align}

where $\vec{v}$ is the velocity vector, $p$ is pressure, $\rho$ is density, $D_i$ is mixture average diffusion coefficient of specie $i$, $T$ is the deviatoric stress tensor, $h_s$ is sensible enthalpy, $\alpha$ is the thermal diffusion coefficient, $\sum_{i=1}^{N} h_i w_i$ is heat release due to chemical reactions, $Y_i$ is mass fraction of species $i$, and $w_i$ is the mass production rate of species $i$. The aforementioned equations require an iterative process to solve for the pressure field. This code uses the Pressure Implicit Splitting of Operators (PISO) method$^{26}$ which is much like the widely used Semi Implicit Method of Pressure Linked Equations (SIMPLE)$^{27}$ The PISO method iterates between the solved velocity field and a guessed pressure field until a specified numerical tolerance is met. All transport and thermodynamic data were calculated using the same approach as the CHEMKIN Transport Package$^{28}$ and thermodynamic database, respectively.

Each conservation equation is solved in a segregated manner. The terms on the left hand side of each equation are treated implicit and the finite vol-
ume terms calculated using second-order accurate Total Variation Diminishing (TVD) Van-Leer schemes. The terms on the right hand side were calculated explicitly and taken to be source terms in each FVM iteration. The source terms, $\sum_{i=1}^{N} h_{i} w_{i}$ and $w_{i}$, come from the Arrhenius expression calculated from the chemical kinetic model. The equations are integrated in time using the first-order implicit, Eulerian method. Transport data, reacting surface boundary species flux rates, and thermodynamic properties are updated using external subroutines after each time integration. Each finite volume equation is solved until a user specified tolerance is met and simulations are run for a specific number of time integrations. Steady-state can be observed by analyzing the normalized residuals of each variable before and after the finite volume iteration.

III.A. Surface Reaction Boundary Condition

All surface reactions listed in Tables 1 and 2 were implemented using a derived boundary type feature in OpenFOAM based on reaction rates at the interface. The equation at this interface can be written as:

$$\frac{\partial (\rho Y_i)}{\partial t} + \rho Y_i v_y + \rho D_i \frac{\partial Y_i}{\partial y} - w_i = 0,$$

where $v_y$ is the blowing velocity normal to the surface ($y$-direction), $\rho'$ is the surface density, $D_i$ is the mixture average diffusion coefficient of species $i$, and $w_i'$ is the surface reaction source term of species $i$. The above species flux equation is solved explicitly using an external subroutine. A first-order, upwind scheme is used for the $\partial Y_i/\partial y$ term. The source term, $w_i'$ is calculated from an external dictionary, by using the porous or non-porous heterogeneous reaction model. The subroutine uses past values for velocity normal to the reacting surface, $v_y$, and then it is updated using,

$$v_y = \frac{\sum_{i=1}^{N} w_i'}{\rho},$$

which assures a unique value for blowing velocity.

Because it is decoupled from the other FVM equations, this boundary condition must be explicitly calculated. This results in restricting the entire simulation’s time step to be determined by the collective diffusion, convection, and mass production terms at the surface. As a result, these simulations become computationally expensive and must be decomposed into several domains. By decomposing the domain into 16 subdomains, each simulation can be finished in less than 24 hours. Extensive grid independence studies were performed.

III.B. Computational Domain and Test Simulations

An illustration of the two-dimensional computational domain selected is shown in Figure 2, with a length in the $x$-direction of 10 mm and height of 1 mm in $y$-direction. The open section of the lower boundary located from $x = -2$ mm to $x = -1$ mm allows outflow prior to the flat plate which requires a far-field pressure boundary condition and zero-gradient conditions for other variables. The remainder of the lower boundary, from $x = -1$ mm to $x = 8$ mm, is a flat plate that contains the reacting carbon surface. This boundary specifies both no-slip and surface temperature as fixed conditions. The left barrier is the upstream boundary where the free-stream values for velocity, air species concentrations and free-stream temperature are specified as fixed value conditions. The downstream and upper barriers of the domain specify pressure as a far-field boundary condition and all remaining variables are specified as zero-gradient. The specific values for these boundary conditions are listed in Table 3. Free-stream moist air composition were fixed according to mass concentration as $Y_{O_2} = 0.20$, $Y_{H_2O} = 0.03$ and $Y_{N_2} = 0.77$. At all other boundaries, excluding the reacting surface where concentrations are calculated, the species boundary conditions are set to zero-gradient. Not listed in this table are the value for free-stream velocity, $U_{\infty}$, and surface temperature, $T_{surf}$, which are the variable input parameters in this investigation.
Boundary Pressure Temperature Velocity,
\((\text{Pa})\) \((\text{K})\) \((\text{m/s})\)
\(y = [0\text{mm}, 1\text{mm}]; x = -2\text{mm}\) \(\frac{\partial p}{\partial x} = 0\) \(T = 320\) \(\vec{v} = (U_\infty, 0)\)
\(y = [0\text{mm}, 1\text{mm}]; x = 8\text{mm}\) \(p_{\text{far-field}} = 101,325\) \(\frac{\partial T}{\partial x} = 0\) \(\vec{v} = 0\)
\(x = [0\text{mm}, 10\text{mm}]; y = 1\text{mm}\) \(p_{\text{far-field}} = 101,325\) \(\frac{\partial T}{\partial y} = 0\) \(\vec{v} = 0\)
\(x = [-2\text{mm}, -1\text{mm}]; y = 0\text{mm}\) \(p_{\text{far-field}} = 101,325\) \(\frac{\partial T}{\partial y} = 0\) \(\vec{v} = 0\)

Table 3: Values of imposed boundary conditions in present simulations.

(Note: The \(y\)-direction velocity, \(v_y\), will change along the boundary: \(x = [0\text{mm}, 5\text{mm}]; y = 0\text{mm}\), from zero as the blowing velocity is calculated during the simulation.)

The finite volume cell thicknesses for the simulated domain was 10\(\mu\text{m}\) for both \(y\) and \(x\)-directions, which resulted in simulating 100,000 cells for each investigation. Chemical residence time effects were investigated by varying free-stream velocity from 30 to 50 m/s while keeping a fixed surface temperature of 1800\(K\). This was done for both non-porous and porous surface reaction models. Temperature effects were studied by varying the surface temperature from 1800 to 2600\(K\) for both non-porous and porous models with free-stream velocity of 40 m/s. The various simulations that were done in this investigation are listed in Table 4.

<table>
<thead>
<tr>
<th>(x) ([\text{mm}])</th>
<th>(y) ([\text{mm}])</th>
<th>(\frac{\partial p}{\partial y} = 0)</th>
<th>(T = T_{\text{surf}})</th>
<th>(\vec{v} = (0, 0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>([-2\text{mm}, -1\text{mm}])</td>
<td>(y = 0\text{mm})</td>
<td>(p_{\text{far-field}} = 101,325)</td>
<td>(\frac{\partial T}{\partial y} = 0)</td>
<td>(\vec{v} = 0)</td>
</tr>
<tr>
<td>([-1\text{mm}, 8\text{mm}])</td>
<td>(y = 0\text{mm})</td>
<td>(p_{\text{far-field}} = 101,325)</td>
<td>(\frac{\partial T}{\partial y} = 0)</td>
<td>(\vec{v} = 0)</td>
</tr>
</tbody>
</table>

Table 4: Investigated input values of free-stream velocities and surface temperatures.

IV. Results

Numerical results from the converged solution of the reacting boundary layer structure are presented here, for the range of physical parameters indicated in Table 4. Both models produce carbon monoxide along the reacting surface which then diffuse into the gas-phase. The penetration of this carbon monoxide flux is a strong function of the surface temperature and the imposed free-stream velocity. The diffused carbon monoxide can ignite in the high temperature region of the thermal boundary layer leading to the production of carbon dioxide. This homogeneous carbon monoxide consumption is described using a detailed CO kinetic model. Since both surface kinetic models include carbon dioxide reaction with free-carbon sites at the surface, the overall process leads to a unique coupling between the heterogeneous surface and homogeneous gas-phase reactions. The results will show that the two-dimensional reaction boundary layer structures depend strongly on porosity, temperature, and free-stream velocity.

IV.A. Reacting Boundary Layer Structures

Presented here are several reaction layer structures, plotted along a line normal (from \(y = 0\text{mm}\) to \(y = 0.8\text{mm}\)) to the reacting surface located at \(x = 4\text{mm}\). The results show the variation of these reaction structures due to temperature and surface reaction model. Figures 3(a) and 3(b) show the reaction layers of the non-porous models with free-stream velocity of 40 m/s at 1800\(K\) and 2600\(K\) respectively. As can be seen, the higher temperature results produce more carbon monoxide at the surface and the gaseous reactions consumes more oxygen. This supports the previously shown trends that oxygen presence in the non-porous model reduces with increase temperature due to gaseous consumption.
Figures 4(a) and 4(b) show the reaction layers of the porous models with freestream velocity of 40 m/s at 1800 K and 2600 K respectively. These layers differ from the non-porous solutions in that oxygen is nearly completely consumed at the reacting surface for both temperatures. Comparatively, this shows the strength of the oxygen consumption rate in the porous model simulations. Additionally, it is clear that the consumption rates for carbon dioxide are also higher than the non-porous model as the species is nearly fully consumed in the higher temperature case.

IV.B. Two-Dimensional Contour Plots

While results presented above give detailed information about the reacting boundary layer when the surface is heated by an external laser source, the two-dimensional contour plots presented in this section gives quick overview. Figures 5(a) and 5(b) show contour plots of oxygen, carbon monoxide, and carbon dioxide mole fractions for the non-porous model with surface temperature of 1800 K and 2600 K, respectively. These results clearly show the gaseous reaction and transport for oxygen, carbon monoxide and carbon dioxide throughout the simulated domain. The effect the surface temperature variation has on oxygen across the plate is evident as the contour plots show its consumption is increased for the
2600K solution. Likewise, the higher surface temperature creates larger amounts of both carbon dioxide and carbon monoxide. As previously mentioned, carbon dioxide is produced by the gas-phase reactions and its mole fraction is highest closest to the plate in the downstream, non-reacting region. At this location the no-slip boundary condition causes the residence time to increase, which allows longer production time of carbon dioxide. This, coupled with the fact this region does not have surface reactions, creates an area of high carbon dioxide concentration.

![Figure 5: Two-dimensional contour plots of non-porous carbon surface reaction with freestream velocity of 40 m/s](image)

(a) For surface temperature of 1800 K  
(b) For surface temperature of 2600 K

Figures 6(a) and 6(b) show contour plots of oxygen, carbon monoxide, and carbon dioxide mole fractions for the porous model with surface temperature of 1800K and 2600K respectively. The strong consumption rate for oxygen is clearly evident, as for both low and high temperature cases oxygen is nearly fully consumed along the plate. Similar to that of the non-porous model, carbon dioxide is highest in the location of the non-reacting downstream part of the flat plate. Unlike the solutions to the non-porous case, the 1800K and 2600K surface temperatures both produce comparatively close amounts of carbon dioxide. Overall, these results show the porous case having a larger amount of activity than the non-porous case.
Figures 7(a) and 7(b) show contour plots of oxygen, carbon monoxide, and carbon dioxide mole fractions for the porous model with the same surface temperature of 1800K but with varied free-stream velocity of 30m/s and 50m/s respectively. The presence of carbon dioxide is a clear indicator of the effect that the free-stream velocity has on these solutions. An increase in velocity decreases the residence time and not only spreads the carbon dioxide downstream but reduces its overall presence. Likewise, oxygen consumption and carbon monoxide production is reduced with the increase in velocity. Overall the increase in velocity reduces the activity along the flat plate.

Figure 7: Two-dimensional contour plots of non-porous carbon surface reaction at a with surface temperature of 1800K with varied velocity
V. Conclusion

A reacting carbon surface subjected to an external laser heating was simulated using both non-porous and porous heterogeneous surface reaction models. The inflow free-stream velocity and the surface temperatures were held constant for each simulation but varied to explore different heating levels and flow residence time effects. These results show that the reaction structures depend heavily on the modeled carbon porosity. In general, reacting boundary layer for the non-porous model were less pronounced than the porous model. This is expected, as the porous carbon model takes into account the larger number of active sites that promote reactivity. The reaction boundary layer thickness was roughly the same between both porous and non-porous cases, however, species composition varied greatly between the models. For the porous models, oxygen was rapidly consumed in the leading edge of the plate, whereas the non-porous case had considerably less oxygen depletion. Oxygen depletion at the surface is also coupled via gaseous reactions that produce carbon dioxide. The results show that, while carbon monoxide was produced at the surface, the flow residence time was long enough to be consumed in the homogeneous gas-phase reaction producing carbon dioxide. This homogeneous gaseous reaction also consumes oxygen, which lowers its concentration at the surface. Additionally, carbon dioxide formed in the gas-phase is diffused to the surface where it reacts to form carbon monoxide.

This unique coupling was shown to be a contributing factor in reaction structures for both porous and non-porous models.

The results also showed conclusively that the increase in temperature promoted reactivity along the flat plate as well as gaseous reactivity within the thermal boundary layer. Additionally, the results show that the decrease in residence time (by increasing free stream velocity) caused a delayed production of carbon dioxide in the gaseous phase, which effected the presence of carbon monoxide and reactant species along the flat plate. In actual experiments to be performed by AFIT by using high-energy laser source, the surface temperature will be a function of the laser intensity and may not be uniform across the surface. However, present results give a strong insight into species profiles and trends expected as a function of the imposed flow velocity, surface temperature, and porosity of the carbon samples to be used.

Acknowledgments

The authors would like to acknowledge the High-Energy Laser Joint Technology Office (HEL-JTO) for funding, HEL JTO MRI (AFOSR-BAA-2010-2). Ryan Johnson was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program and the Virginia Space Grant Consortium (VSGC) Graduate Fellowship Program.

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