Investigation of the High-Energy Oxidation of FiberForm from DSMC Analysis of Molecular Beam Experiments


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Overview of the Effort
A collaborative effort between the University of Illinois at Urbana-Champaign (UIUC), NASA Ames Research Center (ARC) and Montana State University (MSU) succeeded at developing a new finite-rate carbon oxidation model [2] from molecular beam scattering experiments on vitreous carbon (VC) [1]. We now aim to use the direct simulation Monte Carlo (DSMC) code SPARTA to apply the model to each fiber of the porous fibrous Thermal Protection Systems (TPS) material FiberForm (FF). The detailed micro-structure of FF was obtained from X-ray micro-tomography and then used in DSMC. Both experiments and simulations show that the CO2 products ratio increased at all temperatures from VC to FF. We postulate this is due to the larger number of collisions: an O atom encounters inside the porous FF material compared to the flat surface of VC. For the simulations, we particularly focused on the lowest and highest temperatures studied experimentally, 1023 K and 1823 K, and found good agreement between the finite-rate DSMC simulations and experiments.

Molecular Beam Experiments
A hyperthermal O/O2 beam composed of approximately 90% O and 10% O2 is directed at a carbon sample at an incident angle of 45°. The number density as a function of arrival time at the detector, N(t), for the products exiting the surface was collected at various final angles that were in the plane of the beam and the surface normal. Angular flux distributions at each final angle can be obtained from the time-of-flight (TOF) distributions.

Finite-Rate Model from VC experiments [2]
The detailed TOF information of the scattered products was used to distinguish between the time scales of the various reaction mechanisms. In general, the Langmuir-Hinshelwood (LH) mechanism is a thermal surface mechanism consisting of 3 major steps: adsorption, formation and desorption. Since the reaction takes place on the surface, the reactants must first adsorb on surface sites. The second step is the formation step, in which the reactants interact with carbon to form products on the surface. Finally, these products are desorbed as gas-phase species. The LH mechanisms employed in this model are further classified as 3 different types (herein referred to as LH(1-3)) and are distinguished based on the time scales of the CO/CO2 formation and desorption processes:
• LH1. Rapid formation and desorption (prompt mechanism)
• LH2. Slow formation with rapid desorption (formation limited)
• LH3. Rapid formation with slow desorption (desorption limited)

A total of 9 reactions were inferred from analysis of the experimental data: adsorption, desorption of O, LH3 formation and desorption of 2 types of CD, and LH1 formation of O, CO and CO2. CO(a) is weakly bound and exits the surface quickly, while CO(b) is strongly bound to the surface and desorbs much more slowly.

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Reaction</th>
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<tbody>
<tr>
<td>Adsorption</td>
<td>O + (a) → O(a)</td>
</tr>
<tr>
<td>LH1 CO(a) formation</td>
<td>O*(a) + C*(b) → CO*(a) + O*(a)</td>
</tr>
<tr>
<td>LH1 CO(b) formation</td>
<td>O*(a) + C*(b) → CO*(a) + O*(a)</td>
</tr>
<tr>
<td>LH1 O formation</td>
<td>O*(a) + C*(b) → O*(a) + O*(b)</td>
</tr>
<tr>
<td>LH2 CO formation</td>
<td>O*(a) + O*(b) + CO*(a) + O*(b)</td>
</tr>
<tr>
<td>LH3 CO2 formation</td>
<td>O*(a) + O*(b) + CO2*(a) + O*(b)</td>
</tr>
<tr>
<td>Desorption</td>
<td>CO2*(a) → CO*(a) + O*(a)</td>
</tr>
<tr>
<td>LH3 CO2 desorption</td>
<td>CO2*(a) → CO*(a) + O*(a)</td>
</tr>
</tbody>
</table>

Results
Based on experimental results, it is assumed that O is non-reactive for the purpose of this work. Similarly, it is assumed that CO molecules formed as reactions products do not participate in subsequent reactions with the carbon surface.

In order to obtain the Thermal Desorption (TD) component of TOF signals, a Maxwell-Boltzmann at t=0 is fitted at the surface temperature.

Decomposition of the total TOF signal of O and CO at 1823 K from DSMC into three components: IS, TD and slow

FiberForm Microstructure
FiberForm is a rigid anisotropic material with an average porosity around 57%. We acquired micro-CT images of a 3 mm diameter cylindrical sample using a 3D X-ray microscope at Stanford University and extracted a 0.5 mm thick slab of material from the reconstructed dataset. The final voxel size of the sample used for the simulation was 3.302 mm, and the surface comprised of approximately 16 million triangles.

References

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