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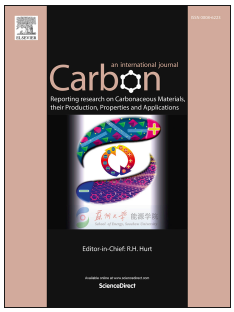

Development and validation of a finite-rate model for carbon oxidation by atomic oxygen

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Development and validation of a finite-rate model for carbon oxidation by atomic oxygen

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Abstract

Molecular beam experiments of hyperthermal oxygen atoms scattering from a vitreous carbon surface were simulated and analyzed using direct simulation Monte Carlo (DSMC). The purpose of this study was to construct and validate a surface chemistry model in DSMC by matching observed features in experimental time-of-flight (TOF) and angular distribution data. A variety of reaction mechanisms including adsorption, desorption, and several types of Langmuir-Hinshelwood (LH) reactions are used to characterize the surface processes in the DSMC surface chemistry framework. This framework is used to numerically simulate the beam-surface scattering experiments of oxygen on vitreous carbon with surface temperatures ranging from 600-2000 K. Detailed analysis of the experimental data including TOF and angular distributions, and product fluxes derived from these data, is used to propose modifications to the carbon surface oxidation model developed by Poovathingal *et al.* This revised model successfully captures the important features in the experimental TOF distributions, including: (i) the impulsively scattered and thermally desorbed components in the oxygen (O) TOF distributions, and (ii) the relatively slow long-tail components in the carbon monoxide (CO) TOF distributions. Comparisons between the simulated (DSMC) and experimental TOF and angular distributions, as well as product fluxes, show excellent agreement.

Keywords:
`Vitreous Carbon, Surface Chemistry, DSMC, Carbon Oxidation, Gas-Surface Interaction, Ablation`

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