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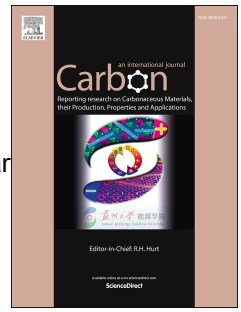

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Ablative Thermal Protection Systems: Pyrolysis Modeling by Scale-Bridging Molecular Dynamics

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Abstract

Pyrolysis of a phenolic polymer is a well-known heat removal mechanism in charring ablators, but the process has not been well-quantified. Here, we perform scale-bridging molecular dynamics (MD) simulations based on a reactive-force-field (ReaxFF) potential to elucidate the pyrolysis kinetics of a highly crosslinked phenolic formaldehyde resin. We show that bulk pyrolysis starts at temperatures of ~500 K, and exhibits a temperature dependence that follows the Arrhenius law. The pyrolysis process initiates with the removal of –OH functional groups and –H atoms from aromatic C rings within the bulk phenolic resin to release H_2O, followed by breaking of these C rings to release C-based fragments. Using the pyrolysis rates from MD simulations, we develop a thermal material response model applied to predict the heat transfer within a charring syntactic foam ablator. Our model predictions of the char thickness and temperature distributions, under a variety of heat loads, are in good agreement with prior experiments.

KEYWORDS: Thermal Protection System; Pyrolysis; Phenolic resin; Molecular dynamics; Syntactic foam ablator; AVCOAT