Proceedings of the Canadian Society for Mechanical Engineering International Congress 2021
CSME Congress 2021
June 27-30, 2021, Charlottetown, PE, Canada

ENGINEERING FOSSIL FUEL-DERIVED AROMATICS: FUNDAMENTALS AND NOVEL OPPORTUNITIES

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ABSTRACT

In order to develop green applications, we have been focused on understanding the conversions of fossil fuel-derived aromatics under high temperatures. As the starting point, the pyrolysis of small aromatics under controlled conditions was investigated using molecular dynamics (MD) techniques based on reactive force field. It was found that temperature can modulate the formation pathways of solid products. Specifically, at relatively low temperatures, solid cluster formation is mainly initiated through the direct combination of aryl radicals; in contrast, at relatively high temperatures, solid cluster formation is initiated by the assembly of chained radicals. However, at both temperatures, the final solid products are of reduced sp^2 fraction, as well as reduced number of rings, compared to the original reactants. Additional MD simulations confirmed the importance of pressure for solid carbon cluster formation, and verified the inhibiting effect of hydrogen on ring condensation from small aromatic molecules. We further probed the pyrolysis of heavy aromatics with different H:C ratios as well as different aromatic contents. It was observed that under processing temperature in the thousands of K, high initial H:C ratio in raw materials can lead to a significant dehydrogenation and a drastic increase in the sp^2 content. Contrarily, for raw materials with low initial H:C ratio, high-temperature treatment can result in that the final solid products are of decreased sp^2 fraction in comparison with its counterpart in reactants. Furthermore, the highest sp^2 fraction was achieved by using raw materials with large aromatic cores and intermediate H:C ratio, where the formation of graphitic stacking was also observed. Consistent with our simulation results, laser-ablated heavy aromatics produces a broad variety of carbon solids comparable to carbon black, amorphous carbon, and graphitic carbon. These products were subsequently used to fabricate prototype transparent heaters, supercapacitors, and strain sensors. Our work demonstrates the tunability of fossil fuel-derived aromatics, as well as their potential applications in electronics.