

Abstract Submitted  
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**Hydrocarbon and water desorption from oxide surfaces using non-reactive and reactive molecular dynamics** JASON KOSKI, MATTHEW LANE, Sandia National Labs — Hydrocarbon and water desorption from oxide surfaces can significantly influence the performance of high-voltage pulsed power machines, such as Sandia’s Z-machine. The extreme temperatures and field strengths present in the Z-machine form plasmas and result in overall current loss. Previously, we have studied the desorption of water from a Fe<sub>2</sub>O<sub>3</sub> (0001) surface and fit the desorption profiles to Temkin isotherm models using non-reactive molecular dynamics (MD). Here, we expand on that work by analyzing hydrocarbon/water mixtures and comparing both non-reactive and reactive MD simulations. The reactive MD allows for bond breaking and ionization; phenomena that are present in the extreme environments of pulsed power machines. Specifically, we look at the desorption of hydrocarbon molecules of different chain lengths and chain architectures (i.e. linear or branched) as well as hydrocarbon/water mixtures of varying concentrations. Finally, we look at the effect of uniform external electric fields of varying strength and direction on the desorption profiles. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525.

Jason Koski  
Sandia National Labs

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