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Kinetic Modeling of Metal Oxide Chemistry and Particle Formation in a Plasma Flow Reactor¹ MIKHAIL FINKO, DAVIDE CURRELI, University of Illinois at Urbana-Champaign, BATIKAN KOROGLU, TIMOTHY ROSE, DAVID WEISZ, JONATHAN CROWHURST, HARRY RADOUSKY, Lawrence Livermore National Laboratory — Current understanding of metallic chemistry in extreme environments, such as nuclear fireballs, remains limited due to the challenging conditions present and the multitude of physical processes and timescales involved. In this work, we focus on the intermediate millisecond timescale of the problem by studying the evolution of metallic species in the rapidly cooling conditions of a plasma flow reactor. Using a global kinetic approach, we model the formation of molecular oxides as well as the nucleation, condensation, and coagulation processes that lead to nanoparticle formation and growth. In particular, the coupling between chemical kinetics and particle formation processes is implemented via the Simultaneous Particle and Molecule Modeling (SPAMM) approach of Pope and Howard. The resulting evolution of species concentrations and particle size distributions for iron, aluminum, and uranium is analyzed and compared with in situ and ex situ measurements. This work aims to bridge the gap between short timescale plasma chemistry and long timescale debris formation - a critical deficiency in current extreme environment models.

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