Abstract Submitted
for the DPP16 Meeting of
The American Physical Society

A molecular dynamics approach to barrodiffusion JAMES COOLEY, MATHIEU MARCIANTE, MICHAEL MURILLO, Los Alamos National Laboratory — Unexpected phenomena in the reaction rates for Inertial Confinement Fusion (ICF) capsules[**?**] have led to a renewed interest in the thermo-dynamically driven diffusion process for the past 10 years, often described collectively as barodiffusion[**?**]. In the current context, barodiffusion would manifest as a process that separates ions of differing mass and charge ratios due to pressure and temperature gradients set-up through shock structures in the capsule core. Barrodiffusion includes additional mass transfer terms that account for the irreversible transport of species due to gradients in the system, both thermodynamic and electric e.g, $\mathbf{i} = -\rho D[\nabla c + k_p \nabla ln(p_i) + k_T^{(i)} \nabla ln(T_i) + k_t^{(e)} \nabla ln(T_e) + \frac{e k_e}{T_i} \nabla \phi]$. Several groups have attacked this phenomena using continuum scale models and supplemented with kinetic theory to derive coefficients for the different diffusion terms based on assumptions about the collisional processes[**?**]. In contrast, we have applied a molecular dynamics (MD) simulation to this system to gain a first-principle understanding of the rate kinetics and to assess the accuracy of the differin

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Date submitted: 15 Jul 2016 Electronic form version 1.4