Abstract Submitted
for the DPP12 Meeting of
The American Physical Society

Estimation of Species Diffusivities in Dense Plasma Mixtures Modeled with the Yukawa Interionic Potential[1] TOMORR HAXHIMALI, ROBERT RUDD, JULIE JACKSON, MICHAEL SURH, WILLIAM CABOT, KYLE CASPERSEN, JEFFREY GREENOUGH, FRANK GRAZIANI, PAUL MILLER, Lawrence Livermore National Laboratory — We employ classical molecular dynamics (MD) to investigate species diffusivity in binary Yukawa mixtures. The Yukawa potential is used to describe the screened Coulomb interaction between the ions, providing the basis for models of dense stellar materials, inertial confined plasmas, and colloidal particles in electrolytes. We use Green-Kubo techniques to calculate self-diffusivities and the Maxwell-Stefan diffusivities, and evaluate the validity of the Darken relation over a range of thermodynamic conditions of the mixture. The inter-diffusivity (or mutual diffusivity) can then be related to the Maxwell-Stefan diffusivities through the thermodynamic factor. The latter requires knowledge of the equation of state of the mixture. To test these Green-Kubo approaches and to estimate the activity contribution we have also employed large-scale non-equilibrium MD. In these simulations we can extract the inter-diffusivity value by calculating the rate of broadening of the interface in a diffusion couple. We also explore thermodynamic conditions for possible non-Fickian diffusivity. The main motivation in this work is to build a model that describes the transport coefficients in binary Yukawa mixtures over a broad range of thermodynamic conditions up to 1keV.

[1]This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

Tomorr Haxhimali
Lawrence Livermore National Laboratory

Date submitted: 17 Jul 2012 Electronic form version 1.4