Abstract Submitted
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Calculation of diffusivity and viscosity of Al-Cu molten mixtures using molecular dynamics[1] ROBERT RUDD, WILLIAM CABOT, KYLE CASPERSEN, JEFF GREENOUGH, TOMORR HAXHIMALI, PAUL MILLER, DAVID RICHARDS, FREDRICK STREITZ, Lawrence Livermore National Lab — We use equilibrium classical molecular dynamics and Green-Kubo techniques to calculate the diffusivity and viscosity of Al-Cu molten mixtures. We calculate both the self-diffusivities and the Maxwell-Stefan diffusivities, and evaluate the validity of the Darken relation for this system. We compare the results with those from experiments reported in the literature. We have constructed an analytic model that is fit to the MD results. This transport model has been implemented in a continuum hydrodynamics code. Both the continuum code and extremely large-scale molecular dynamics have been used to simulate the development of vortices due to the Kelvin-Helmholtz instability in a shear layer, and we discuss the results of that comparison.

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