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Regarding Multispecies Diffusion and Gradient Driven Transport

ERIK VOLD, Los Alamos National Lab — A theoretical framework for multispecies fluid transport has been long established in the Maxwell-Stefan equations but interpretations and solution methods appear in the literature to be quite varied. A framework is summarized here for mass drift of species which can include ionized gases with large differences in atomic mass driven by temperature, pressure, and electric potential gradient forces in addition to the usual diffusion driven by concentration gradients. The zero sum over species of mass drift flux closes the $(n_s - -1)$ independent species drift equations for the n_s species and ensures a non-zero molar flux summed over species of different atomic mass. This non-zero species molar flux leads to pressure perturbations, which require a compressible fluids computation to correctly account for the mass average flow and density relaxation. Computations in an initially isothermal binary mixing case illustrate the relaxation of the interfacial density profile by the mass averaged velocity arising from a divergent velocity field. Pressure perturbations associated with boundary reflections and viscosity are shown to have a negligible contribution to the density relaxation compared to the non-zero velocity divergence due to the expansion of each gas during the diffusion. An energy flux, consistent with the species mass diffusion leads to a significant temperature perturbation dominated by a bulk fluid PdV work term rather than the sum over species enthalpy flux. An example for binary diffusion across an interface between species with a large atomic mass difference shows a large asymmetry in species concentration profile unless properly constrained to a net zero sum over species mass flux.

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