

## Diffusion of Heat and Mass in a Chemically Reacting Mixture

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We report transport properties for the hydrogen dissociation reaction driven by a thermal force, at conditions where reactants and product concentrations are both sizable. The data are obtained for the first time from non-equilibrium molecular dynamics simulations of reactions far from chemical equilibrium. The results derived from the system's entropy production, show that the strongly endothermic reaction has a large impact on the transport coefficients. The thermal conductivity was found to be comparable to that of a medium dense gas at high temperature (1 W/mK), while the observed diffusion coefficient was small ( $10^{-7}$  m<sup>2</sup>/s). The coupling coefficient as expressed by the heat of transfer is was found to be in the same order of magnitude as earlier studies. This is at variance with the common perception that the Dufour effect is negligible in reacting mixtures.