

**Molecular Dynamics Simulations of a Chemical Reaction; Conditions for Local Equilibrium in a Temperature Gradient**  
**- IACT Doctorate Award Presentation -**

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We have examined a simple chemical reaction,  $2F \rightarrow F_2$ , in various temperature gradients by using non-equilibrium molecular dynamic (NEMD) simulations. A mechanical model was used, based on Stillinger and Weber's 2- and 3-body potentials. Equilibrium and non-equilibrium molecular dynamics simulations showed that the chemical reaction is in local thermodynamic as well as in local chemical equilibrium  $\Delta_r G = 0$  in the supercritical fluid, for temperature gradients up to  $10^{12}$  K/m. The velocity distributions of both components were close to being Maxwellian. The peak distributions were shifted slightly up or down from the average velocity of all particles. The shift depended on the magnitude of the temperature gradient. A net reaction rate was observed much smaller than the forward and the backward reaction rates. The reaction was diffusion controlled as the reaction rate was controlled by the divergence of the component fluxes. The results support the assumption that the entropy production of the reacting mixture can be written as a product sum of fluxes and forces. The temperature gradient promotes interdiffusion of components in the stationary state, a small reaction rate and an accumulation of the molecule in the cold region and the atom in the hot region. The reaction enthalpy is important for the transport processes in the mixture.