Molecular simulation study of droplet thermodynamics under extreme ambient conditions

Droplets play an important role in nature, e.g. in the form of rain, clouds and fog. For energy applications, droplet evaporation is the dominant mechanism in spray atomization occurring in internal combustion and jet engines. In such cases, the liquid phase is immersed into extreme ambient conditions of high temperature and pressure. High pressures are favorable to be generated immediately after the injection of a fuel mixture into the engine in order to accelerate its atomization, which in turn creates much more interface area per volume and thus enhances the evaporation process. Although these processes are commonly used, their fundamental understanding is insufficient.

An advanced physical understanding of all processes involved is mandatory in order to optimize technological systems and increase their efficiency. This was the main motivation behind the creation of the “Sonderforschungsbereich” Transregio 75 (SFB-TRR 75), which brings together scientists from a variety of institutes from the universities in Stuttgart, Darmstadt and the DLR Lampoldshausen, as well as from diversified backgrounds, ranging from mathematics, physics, chemistry and computer to engineering science. The entire project is funded by grants of the Deutsche Forschungsgemeinschaft (DFG). According to each academic background, every member of this Transregio is assigned to one of the different sub-projects. It is this interdisciplinary combination of expertise, which allows achieving the ambitious goal to gain and extend a fundamental understanding of droplet dynamics.

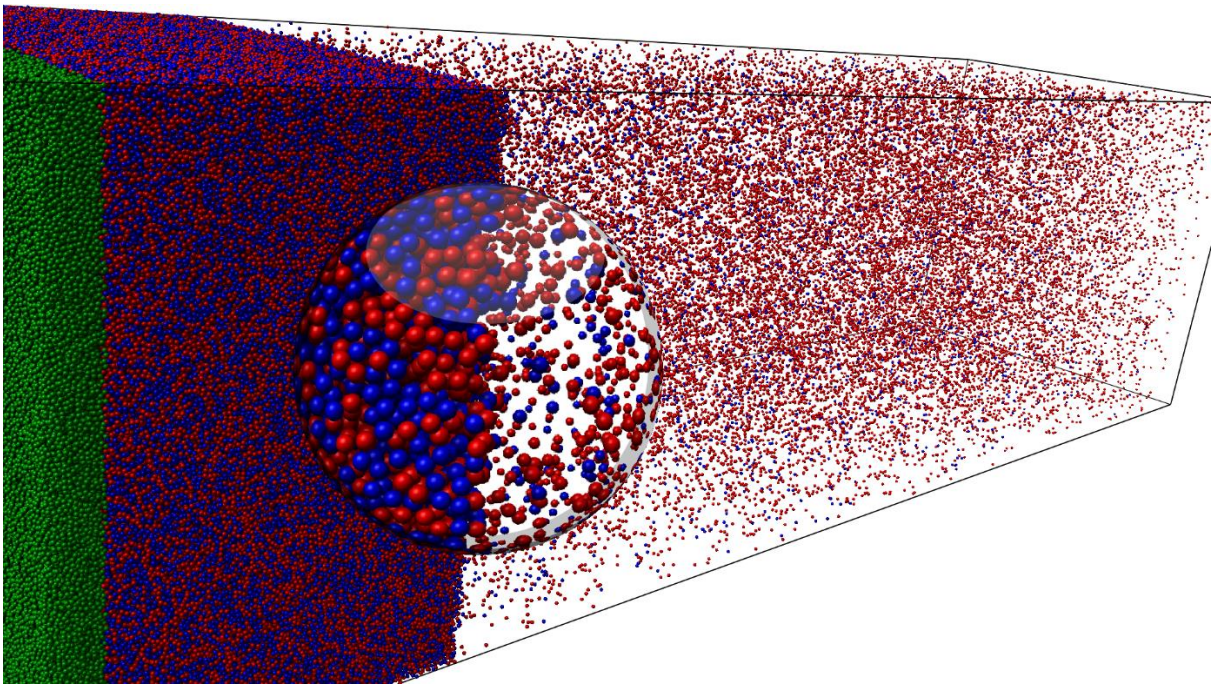

Fig. 1: Snapshot of a stationary simulation of evaporation into vacuum. The system consisted of a liquid and a vapor phase, connected through a planar interface. To the left, the liquid was extended by a reservoir, deployed for replenishment and thereby to attain stationary conditions. Particles constituting the reservoir, forward and backward particle flux are colored green, red and blue, respectively. The magnifying glass was added to support the visualization of the vapor-liquid interface.

The contributions of the group *Thermo* of TU Berlin are twofold, out of which one is to compute transport properties for relevant substances (e.g. acetone, oxygen, nitrogen) via equilibrium molecular dynamics simulations. Furthermore, the evaporation of nanoscale processes is modelled via appropriate methods using non-equilibrium molecular dynamics simulations.

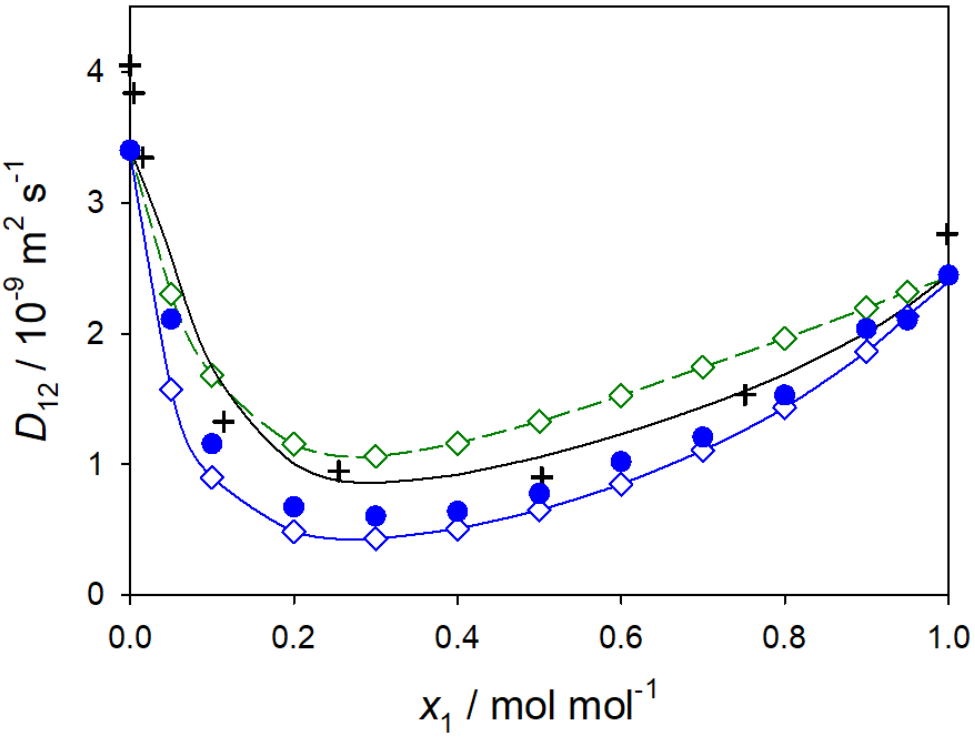

Fig. 2: Fick diffusion coefficient of the binary mixture methanol (1) + benzene at 298.15 K and 0.1 MPa. Simulation results (solid bullets) are compared with experimental data (crosses). The models by Li et al. (blue diamonds) and Zhou et al. (green diamonds) based on present simulation data are also shown.

SFB-TRR 75

Tropfendynamische Prozesse unter extremen Umgebungsbedingungen