Abstract

This work combines two major simulation techniques, the Molecular Dynamics and Computational Fluid Dynamics to gain further insight into nucleation phenomena, where experimental investigations fall short due to the spatial, analytical and visual limitations inherent to any physical measurement setup. As a good example for a case, where experimental data were scarce due to difficult handling conditions, homogeneous nucleation simulations of CO_2 were set from the ground up, based on the MOSCITO and LAMMPS program package and the potential model by *Zhang* and *Duan*. The analysis incorporated the *ten Wolde* and *Frenkel* cluster statistics, the Mean First-Passage Times and the *Yasuoka-Matsumoto* technique. The reported nucleation rates span a temperature and supersaturation range of $T = 200$ - 237 K and $S = 2.03$ - 9.89 with and without Argon as carrier gas, which were compared to the classical and most recent theoretical approaches from literature. Depending on the theory and the temperature, maximum deviations of up to three orders of magnitude were found. Additionally, the Molecular Dynamics simulations were employed to characterise the binary formation of *Janus* particles of two model substances with artificial non-wetting properties from the gas phase on the atomic scale, where time-resolved visual feedback is difficult to obtain in measurement apparatuses. The structural variations at different conditions were monitored for sub- and post-critical clusters and compared to structures found in experiments. In order to get a deeper understanding of the Nucleation Pulse Chamber, the experimental setup was virtually recreated to apply Computational Fluid Dynamics calculations. The simulations revealed the dynamic density, pressure and temperature profile of the whole geometry with and without heat influx via the chamber's walls during a typical pressure pulse experiment for a mixture of *n*-propanol with Helium and yielded novel insight on the Pressure Drop Magnitude Effect, which was first observed by *Viisanen*, *Strey* and *Reiss* in 1993.