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Molecular dynamics for homogeneous nucleation of water and carbon dioxide in different carrier gases

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We evaluate the feasibility of the natural gas liquefaction process with very limited gas treatment or heavy carbons removal. Such reduction in system processing would significantly reduce treatment steps and thus also maintenance costs. Phase transitions in a binary gas mixture of carbon dioxide and methane need be determined. In order to do so, we first focus on homogeneous nucleation phenomena constituting the fundamental process in phase transitions from vapour to liquid. Molecular Dynamics (MD) is a promising technique to study this. It was previously successfully used for single component systems like Argon [1]. We first compare and validate cluster dynamics and nucleation rates from a mixture of water (as condensate) and argon (as carrier gas) with existing results available in literature [2]. Promising results were already found. The applied methodology allows us to investigate also other mixture systems such as with helium as a carrier gas. In this case nucleation rates are compared with experimental data found from shock-tube measurements as well [3] in order to demonstrate the versatility of the method. Moreover, preliminary results based on homogeneous nucleation simulations in carbon dioxide are presented and directly compared with experiments from our laboratory expansion cloud chamber set-up.

[1] T. Kraska, J. Chem. Phys. 124, 054507 (2006)
[2] K. Yasuoka and M. Matsumoto, J. Chem. Phys. 109, 8463 (1998)
[3] Vincent Holten, Water Nucleation: Wave Tube Experiments and Theoretical Considerations (2009)

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