New Method to Calculate the Self-Diffusion Coefficient in Fluid Systems

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A new method to calculate the self-diffusion coefficient is proposed. It is based on an integrated form of the diffusion equation giving the current of tagged particles in terms of its value at a reference point. Molecular dynamics simulations of fluid argon systems at two different densities have been performed to calculate the molar flow of particles. The resulting value of the self-diffusion coefficient shows an excellent agreement with the results obtained from the mean-square displacement. Simulations of equimolar binary mixtures of argon with neon and methane were performed. They also show very good agreement with the predictions of the model. The method presented enables one to analyze the formation of a diffusion regime and can therefore be useful for transport at meso and nano-scales.