Diffusion of Gases in Binary Mixtures

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Established theory relating self- and mutual (binary) diffusion coefficients suggests that the self-diffusion coefficient of both components, at their respective infinite dilution, equals the mutual diffusion coefficient for a binary mixture. This has been studied for several liquid mixtures [e.g., 1] both via self-diffusion experiments and via models which describe the relationship between self-diffusion and composition. However, such models are not available for gaseous mixtures to the best of our knowledge, whilst self-diffusion measurements as a function of composition are sparse. In this work, we utilise pulsed field gradient (PFG) ^{1}H Nuclear Magnetic Resonance (NMR) to measure the self-diffusion coefficient of methane in three binary mixtures (methane-nitrogen, methane-helium, and methane-hydrogen) as a function of composition at pressures up to 100 bar and temperatures ranging from 28 to 40°C. An NMR-compatible sapphire glass cell capable of withstanding pressures up to 400 bar was designed and constructed to facilitate these measurements. The cell was successfully integrated into a benchtop NMR spectrometer for precise self-diffusion measurements using the pulsed field gradient (PFG) technique. The resultant apparatus enables accurate measurements of gaseous self-diffusion coefficients for compositions down to 0.5 mol% methane. This allows for extrapolation to infinite dilution in order to estimate the corresponding self-diffusion coefficient. Acquired data were consistently within 5% of literature values for the mutual diffusion coefficient and/or estimates based on Chapman-Enskog theory. In the case of methane-hydrogen we were able to explore the agreement between mutual diffusion and self-diffusion of both components at their respective infinite dilution. The acquired data are now available for the development of models to predict the self-diffusion as a function of composition in gaseous mixtures.

References

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