Comparison of Experimental Densities of Synthetic Air with Values Predicted by Molecular Simulation in the Temperature Range from (100 to 298) K at Pressures up to 8 MPa

Philipp Eckmann [S], Reiner Kleinrahm, Roland Span and Markus Richter [C]
Thermodynamics, Ruhr-University Bochum, Bochum, Germany
m.richter@thermo.rub.de

The accuracy of the prediction of thermophysical properties by the use of molecular simulation is attaining a comparable magnitude as existing experimental data. Simulations may be primarily used in the future when experiments are too expensive, time consuming or too dangerous. However, today results from simulations still must be validated with accurate experimental data to prove the claimed accuracy. Against this background, the (p, ρ, T, x) behavior of synthetic air was investigated in the temperature range from (100 to 298) K at pressures up to 8 MPa utilizing a single-sinker magnetic suspension densimeter for cryogenic liquid mixtures. Furthermore, densities were simulated with the molecular simulation tool ms2 [1]. Due to the supercritical liquefaction procedure and the integration of a special VLE-cell, all densities were measured without changing the sample composition. The relative combined expanded uncertainty (k = 2) in density considering all effects, including the correction of the uncertainty in composition, is presently estimated to be approximately 0.1 % for all measurements. The largest source of uncertainty is the value of the magnetic susceptibility of oxygen, which is necessary for the calculation and correction of the force transmission error of the magnetic suspension coupling. The relative deviations of the simulated density values from the experimental density values are between 1.4% and −5.6%. At T = 100 K the agreement of the simulated values with the experimental values is better than −0.13%. In comparison, the relative deviations of the experimental values from values calculated with the GERG-2008 equation are within ±0.48%. In conclusion, the relative deviations between the results of simulation and experiment are particularly for liquid densities at low temperatures smaller.

References:

[1] G. Rutkai, A. Köster, G. Guevara-Carrion, T. Janzen, M. Schappals, C.W. Glass, M. Bernreuther, A. Wafai, S. Stephan, M. Kohns, S. Reiser, S. Deublein, M. Horsch, H. Hasse, J. Vrabec, Comput. Phys. Commun. 221 (2017) 343–351. doi:10.1016/j.cpc.2017.07.025.