Simultaneous Determination of Thermal and Mutual Diffusivity of Binary Mixtures of $n$-Alkanes with Carbon Monoxide, Hydrogen, and Water by Dynamic Light Scattering

Andreas Heller
Erlangen Graduate School in Advanced Optical Technologies, University of Erlangen-Nuremberg, Erlangen, Germany

Michael H. Rausch
Erlangen Graduate School in Advanced Optical Technologies, University of Erlangen-Nuremberg, Erlangen, Germany

Institute of Engineering Thermodynamics, University of Erlangen-Nuremberg, Erlangen, Germany

Jiaqi Chen, Matthieu S. H. Fleys and Gerard P. van der Laan
Shell Global Solutions International B.V., Amsterdam, Netherlands

Zoi A. Makrodimitri
Molecular Thermodynamics and Modelling of Materials Laboratory, National Center for Scientific Research “Demokritos”, Aghia Paraskevi Attikis, Greece

Ioannis G. Economou
Chemical Engineering Program, Texas A&M University at Qatar, Doha, Qatar

Andreas P. Fröba
Erlangen Graduate School in Advanced Optical Technologies, University of Erlangen-Nuremberg, Erlangen, Germany

Institute of Engineering Thermodynamics, University of Erlangen-Nuremberg, Erlangen, Germany

apf@ltt.uni-erlangen.de

In the present study, it is demonstrated that thermal and mutual diffusivities of binary mixtures of the $n$-alkanes $n$-dodecane ($n$-C$_{12}$H$_{26}$), $n$-octacosane ($n$-C$_{28}$H$_{56}$), and $n$-tetracontane ($n$-C$_{40}$H$_{82}$) with carbon monoxide (CO), hydrogen (H$_2$), and water (H$_2$O) are simultaneously accessible by dynamic light scattering (DLS). As the light scattering signals originating from thermal and concentration fluctuations appear in similar time scales, different data evaluation strategies were tested to achieve minimum uncertainties in the resulting transport properties. To test the agreement of the respective theoretical model with the DLS signals in the regression, an improved multi-fit procedure is introduced. With the selected data evaluation strategy, expanded uncertainties ($k = 2$) of 4 to 15% and 4 to 30% in the thermal and mutual diffusivities could be obtained for the binary mixtures. The mutual diffusivities for the mixtures measured at temperatures ranging from 398 to 523 K and pressures of 5 to 30 bar at saturation conditions are in agreement with molecular dynamics (MD) simulations using atomistic models and with experimental data from literature.