Integrated Transport Property Program for Key Systems: Data, Models, and Simulation

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Efficient design of chemical processing equipment for various industrial sectors such as transportation, petroleum refining, energy, and refrigeration requires reliable values for the transport properties viscosity and thermal conductivity. The primary approach is the critical assessment of all available experimental data and their representation by correlations, incorporating theory when possible. Here we have extended the model base to the viscosity and thermal conductivity of the linear alkanes *n*-octane, *n*-nonane, *n*-decane, and *n*-dodecane. These are the first such models for the heavier alkanes commonly present in liquid-phase fuels. The development of these transport properties formulations was driven in part by the industrial need/demand for accurate knowledge of the properties of hydrocarbon mixtures, including economically important fluids such as natural gas and jet fuels.

CSTL researchers pursue an integrated strategy that combines experiment, theory and simulation in the development of advanced models for transport properties, leading to predictions of reliable information even when experimental data may be lacking.

M.L. Huber, A. Laesecke, R. Perkins, "*Transport Properties of n-Dodecane",* Energy & Fuels 18 (2004).
M.L. Huber, A. Laesecke, H.W. Xiang, "*Viscosity correlations for minor constituent fluids in natural gas: n-octane, n-nonane, and n-decane",* Fluid Phase Equilibria, 224 (2004).
M.L. Huber and R.A. Perkins, "*Thermal conductivity correlations for minor constituent fluids in natural gas: n-octane, n-nonane and n-decane",* Fluid Phase Equilibria, in press.

The new models represent the viscosity and thermal conductivity surfaces of these compounds over their entire fluid region, encompassing the dilute gas to the dense fluid and supercritical regions, at temperatures down to the triple point. They represent the available experimental data to within their experimental uncertainties and extrapolate in a physically meaningful manner. Our models for *n*-octane, *n*-nonane, *n*-decane, and *n*-dodecane have been presented in three manuscripts, and at the Properties and Phase Equilibria for Product and Process Design (PPEPPD) conference in Snowbird, Utah (May 16-21, 2004).

Complementing our experiment-based approach are computational studies of the properties of systems with model potentials. Such studies can improve fundamental understanding for conditions where measurements are not feasible. Results of high computational accuracy have been published for the shear viscosity, the self-diffusion coefficient, and the bulk viscosity. With comprehensive simulation data at over 350 state points, the temperature and density dependences of these properties of the Lennard-Jones potential are characterized for the first time over a wide range of fluid states. The simulation data for the bulk viscosity has revealed a large critical enhancement similar to that known for the thermal conductivity, but extending much farther into the supercritical region (it can be observed even at 4.5 times the critical temperature). From our simulations, the bulk viscosity is now known in a wider range of states for the Lennard-Jones model fluid than for any real fluid.

K. Meier, A. Laesecke, S. Kabelac, "*Transport coefficients of the Lennard-Jones model fluid. I. Viscosity",*,J. Chem. Phys., 121(2004)
K. Meier, A. Laesecke, S. Kabelac, "*Transport coefficients of the Lennard-Jones model fluid. II. Self-diffusion",* J. Chem. Phys.121 (2004)
K. Meier, A. Laesecke, S. Kabelac, *"Transport coefficients of the Lennard-Jones model fluid. III. Bulk viscosity",* J. Chem. Phys.122 (2005) in press.

The integrated program on transport properties represents a portion of our coordinated efforts on thermophysical properties. These are important to both our infrastructural work (information will be disseminated through such Standard Reference Databases as NIST REFPROP), and to the immediate needs of customers, such as a project on rocket propellant RP-1. The ongoing program will continue to focus on both immediate and specific demands for transport property information and on longer-term efforts to improve our predictive capabilities in these areas.