

## **475f Molecular Simulation of the Thermophysical Properties of Fluids: Phase Behavior and Transport Properties**

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Historically, reliable data for the thermophysical properties of fluids could only be obtained from accurate experimental measurement. The input from theory was, at best, limited to a supporting role by providing correlations. The large number of assumptions and approximations involved in theoretical tools such as equations of state meant that it was unrealistic to expect genuinely reliable predictions. More recently, the advent of powerful molecular simulation techniques has greatly enhanced the usefulness of thermophysical calculations, particularly in chemical engineering. Unlike conventional calculations, molecular simulation determines the properties of a fluid directly by evolving molecular coordinates in accordance with a rigorous calculation of intermolecular energies or forces. In this work, the application of molecular simulation to the prediction of the thermophysical properties of fluids relevant to chemical engineering applications is examined. Examples of both equilibrium and non-equilibrium phenomena such as viscosity are given. It is demonstrated, that in some cases, such as liquid-solid coexistence of fluids, molecular simulation can be more reliable than experimental measurements. This is particularly the case if the experimental conditions are physically onerous. Simulation can also provide unexpected insights into many thermophysical properties. For example, recent simulation results indicate that three-body interactions have an important influence on vapor-liquid coexistence and that considerable insights can also be gained by simulating rheological properties using non-equilibrium molecular dynamics techniques.