

Thermophysical Properties for Chemical Industry

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Experience of a lifetime is shared along with some real examples regarding the industrial expectations and importance of thermophysical properties throughout the lifecycle of a chemical beginning with the development of new chemical processes, design of chemical plants, plant troubleshooting and optimization to environmental purposes and product support. Good experimental data are a key input with good property models providing the ability to use these data. Each major equipment in any large chemical plant is unique and under-design due to inaccurate properties can lead to serious investment losses. Hence, good thermophysical properties including databases and models, that meet enterprise-wide quality needs and expectations, are a key technology asset for any chemical related enterprise. Modeling of hydrogen bonding through Wertheim Association Theory can overcome the serious deficiencies in the current models for chemical purification processes and significantly reduce the design risk. Association theory can help move into other applications such as purification of fermentation products, polymer blending, product formulations including micelles and surfactants, and in reducing the development cycle through better predictions. However, further developments are a must in this regard and while many great opportunities lie ahead, technical networking and collaboration between chemical industry and academia is a major gap and some suggestions are provided so that research can move from proof-of-concept to practical usage.