

Workshop 1: All About Data

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Understanding how to incorporate a wide variety of information into a coherent analysis with an appropriate level of skepticism is of growing importance. As consumers of technical information, we scientists and engineers must know how and when to accept, modify, or reject new and available data, particularly for process and product design. How do we efficiently and reliably integrate property and phase equilibrium measurements and modeling results into our work? How should uncertainties in data measurement and reporting be translated into engineering tolerances for designing, monitoring, and controlling the behaviors of chemical systems and substances?

In this workshop, experts will guide participants to answer such questions by exploring cases involving the incorporation of published results into practical designs. Topics will include: tools and appropriate skepticism for extracting information from scientific papers; techniques for synthesizing experimental data, molecular modeling, and model predictions to establish reliable values and confidence intervals for basic properties; and considerations about data use in making robust design decisions.

The workshop will involve small groups working on cases with sample data for realistic outcomes. As data and software are essential to the types of information handling we will be discussing, a docker container will be made available for download prior to the workshop. Having a laptop for the workshop would be desirable, but not necessary.