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The Role of Experimental Data in the Development of Thermodynamic Modeling and Process Simulation

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Abstract

Thermodynamic modeling and process simulation form the backbone of modern chemical and energy industries, enabling the design, optimization, and safe operation of complex processes. Despite rapid advances in computational power and theoretical frameworks, experimental data remain indispensable to the credibility and usefulness of these tools. This editorial discusses how experimental measurements have shaped the evolution of thermodynamic models and process simulators, why they continue to be essential in the era of digitalization and machine learning, and how future progress depends on a balanced integration of experiments, theory, and computation.

Introduction

Thermodynamics provides the language through which engineers and scientists describe phase behavior, energy transfer, and chemical equilibrium. Process simulation translates this language into practical decision-making tools used in plant design, scale-up, optimization, and control. At the heart of both fields lies a critical dependency: reliable experimental data. While equations of state, activity coefficient models, and molecular simulations offer predictive power, they are ultimately grounded, calibrated, and validated through experimental observation.

In recent years, the growing sophistication of modeling techniques has sometimes led to the perception that experiments are becoming less central. This editorial argues the opposite. Experimental data are not merely supportive inputs; they actively guide model development, reveal limitations in theoretical assumptions, and ensure that simulations remain connected to physical reality.

Experimental Data as the Foundation of Thermodynamic Models

Thermodynamic models aim to describe real systems using mathematical relationships. Whether one considers classical cubic equations of state, excess Gibbs energy models, or advanced molecu-

lar-based approaches, each relies on experimental data at multiple stages of development.

First, experimental measurements define the phenomena that models must capture. Phase equilibrium data, calorimetric measurements, density, viscosity, and transport properties reveal non-idealities and complex interactions that purely theoretical reasoning may overlook. Historically, the recognition of deviations from ideal gas or ideal solution behavior emerged directly from experimental inconsistencies, motivating the creation of improved models.

Second, experiments provide parameter values that give models quantitative meaning. Many thermodynamic formulations contain adjustable parameters representing molecular size, interaction energy, or association strength. These parameters cannot be inferred reliably without experimental benchmarks. The quality, range, and internal consistency of experimental datasets directly influence the predictive performance of the resulting models.

Third, experimental data serve as an objective test of model validity. A thermodynamic model that fits a narrow dataset but fails under different temperatures, pressures, or compositions offers limited practical value. Systematic experimental validation exposes weaknesses and guides iterative refinement, leading to more robust and transferable formulations.

Driving Process Simulation Accuracy and Reliability

Process simulation depends on thermodynamic models to predict material and energy balances across unit operations. Errors in thermodynamic property estimation propagate through simulations, potentially leading to flawed design decisions, economic losses, or safety risks. Experimental data play a decisive role in minimizing these risks.

Property packages embedded in simulators are typically developed and tested against extensive experimental databases. Vapor–liquid equilibrium data, heat capacities, enthalpies of mixing, and reaction equilibria are essential for ensuring that simulations reflect realistic process behavior. In separation processes such as distillation, absorption, or extraction, small inaccuracies in phase equilibrium predictions can lead to significant errors in equipment sizing and energy consumption estimates.

Moreover, experimental pilot-scale data provide a bridge between laboratory thermodynamics and industrial-scale simulation. These data capture real-world effects such as impurities, non-equilibrium behavior, and operational constraints that are difficult to model from first principles alone. Incorporating such insights improves simulator credibility and user confidence.

Experimental Data in Model Selection and Applicability

An often-overlooked contribution of experimental data is their role in guiding model selection. No single thermodynamic model is universally superior; each has a domain of applicability. Experimental comparisons reveal where a model performs well and where it fails.

For example, systems involving strong hydrogen bonding, electrolytes, or associating fluids often challenge simple equations of state. Experimental observations highlight these challenges and justify the adoption of more specialized models. In this sense, experimental data act as a decision-making compass, preventing the indiscriminate application of models beyond their reliable limits.

The Interplay with Molecular Simulation and Machine Learning

Modern thermodynamics increasingly incorporates molecular simulation and data-driven approaches. While these methods reduce dependence on traditional correlations, they do not eliminate the need for experimental data. On the contrary, experiments remain critical for validation and calibration.

Molecular simulations rely on force fields whose parameters are frequently derived from or tested against experimental properties. Without experimental reference points, simulated predictions risk becoming internally consistent yet physically inaccurate. Similarly, machine learning models trained on experimental datasets inherit both the strengths and limitations of the underlying measurements.

High-quality, diverse experimental data are therefore essential to avoid biased or misleading predictions.

Experimental data also play a strategic role in identifying where advanced methods add value. Discrepancies between model predictions and experimental results often signal complex physics or chemistry, motivating deeper investigation rather than blind reliance on computational output.

Challenges and Responsibilities in Experimental Data Generation

Despite their importance, experimental data face challenges related to cost, time, and reproducibility. High-pressure or high-temperature measurements, multicomponent systems, and reactive mixtures require specialized equipment and expertise. As a result, experimental datasets may be sparse or unevenly distributed across conditions of interest.

This reality places a responsibility on the scientific community to prioritize data quality, transparency, and accessibility. Careful uncertainty analysis, standardized reporting, and open databases enhance the value of experimental work beyond individual studies. When experimental data are treated as shared infrastructure rather than isolated results, their impact on modeling and simulation is amplified.

Future Perspectives

Looking ahead, the role of experimental data is likely to evolve rather than diminish. Automated experimentation, high-throughput measurements, and advanced sensors promise to expand the quantity and diversity of available data. When coupled with real-time process monitoring, experimental data can continuously inform and update simulation models, enabling adaptive and resilient process design.

At the same time, experimental insight will remain essential for interpreting model predictions, especially in emerging areas such as sustainable energy systems, carbon capture, and bio-based processes. These systems often involve novel materials and conditions where historical data are limited, reinforcing the need for targeted experimental investigation.

Conclusion

Experimental data are the cornerstone upon which thermodynamic modeling and process simulation are built. They define physical reality, enable parameter estimation, validate predictive tools, and guide model selection. Even as computational methods grow more powerful, experiments remain the ultimate reference against which theories and simulations are judged.

An effective future for thermodynamic modeling and process simulation depends on maintaining a strong, collaborative relationship between experimentalists and modelers. By valuing experimental data not as a constraint but as a catalyst for innovation, the field can continue to deliver reliable, efficient, and sustainable solutions to complex engineering challenges.