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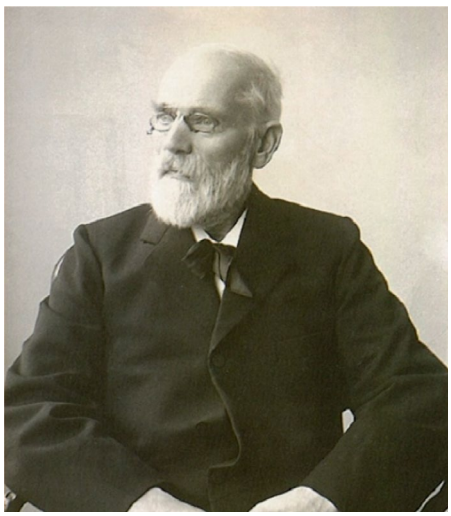
Encouraging activity in molecular thermodynamics

Molecular thermodynamics emerged from the convergence of classical thermodynamics with molecular chemistry and physics. In this Editorial, we reflect on the impact of molecular thermodynamics in chemical engineering and share our excitement for future developments in this field.

Classical thermodynamics is fundamental to nearly all areas of science. Indeed, the early work of pioneers like Carnot, Boltzmann, Clausius and Gibbs — who, coincidentally, was awarded the first Engineering PhD in the United States[1] — forms, in part, the foundation of introductory physics and chemistry courses to this day.

At the same time that researchers were uncovering the foundations of classical thermodynamics, their contemporaries were breaking new ground in molecular chemistry and physics. For example, just three years after Sadi Carnot published in 1824 what is today the Carnot cycle[2], another eponymous figure, Robert Brown, reported his observations of pollen particles undergoing what we now know as Brownian motion[3]. The parallel progress in these fields, although perhaps serendipitous in timing, was a necessary precursor to the late nineteenth-century rise of a new branch of thermodynamics: molecular thermodynamics.

Molecular thermodynamics connects molecular-scale behavior (such as finite molecule size and intermolecular forces) to classical thermodynamic observables (such as pressure, temperature and volume). One might recognize this example as the basis of the van der Waals equation of state, an improvement to the ideal gas law that contributed strongly to van der Waals' 1910 Nobel Prize in Physics. Building on this foundation, work in the field continued actively, with the introduction of new models such as the Redlich–Kwong equation in 1949, the Wilson equation in 1964, the non-random-two-liquid equation in 1968 and the Peng–Robinson equation in 1976 (ref. 2), to name just a few examples.



The application of these advances has naturally driven substantial scientific progress in chemical engineering. For instance, consider the industrial importance of polymer mixing. Flory–Huggins theory, which contributed to Paul J. Flory's 1974 Nobel Prize in Chemistry, provides a toy lattice model to understand the thermodynamics of polymer solutions and blends based on molecular sizes, volume fractions and characteristic interaction parameters[4]. Beyond its immediate applications, the legacy of Flory–Huggins established the beginnings of our contemporary view of key polymer-related chemical processes, including blending, dissolution and self-assembly.

Modern advances continue to refine the molecular picture of thermodynamics as it relates to chemical engineering. This progress has been enabled, in part, by the rapid development of powerful computational and experimental tools. Undeniably, the researcher's toolkit today looks vastly different from what it was in the days of van der Waals or even Flory. Software packages such as COSMO-RS now readily bridge thermodynamics with quantum chemistry, allowing users to rapidly access phase-equilibrium data and screen for optimal solvents or estimate partition coefficients[5]. Meanwhile, increased raw computing power and refined algorithms, along with the accessibility of atomistic and molecular simulations, have enhanced the accuracy and utility of multiscale chemical process modeling. For instance, the recent PrISMa platform integrates molecular-scale simulations with process modeling, techno-economic analysis and life-cycle assessment to identify promising case-specific CO_2 sorbents[6].

These developments are already transforming the use of molecular thermodynamics in chemical engineering, and exciting opportunities for further progress continue to emerge through the ongoing application of these tools. Our editorial team is eager to support the next wave of advances in molecular thermodynamics as they lead to practical engineering solutions. We view the opportunities as plentiful: holistic chemical process simulations require improved thermodynamic models and larger datasets; electrolyte design in batteries necessitates a detailed description of concentrated ion solvation dynamics and transport; stable multi-component catalyst design relies on a nuanced understanding of phase equilibria; and new selective molecular separation processes require quantitative molecular thermodynamic analyses.

These are, of course, just a few examples among many. At *Nature Chemical Engineering*, we hope to encourage further activity in molecular thermodynamics within the purview of chemical engineering science. To us, the potential is abundantly clear.

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