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Striking a theoretical balance

Modeling chemical processes and systems underpins progress in chemical engineering science; we encourage submissions in this domain.

This journal's illustrative pre-launch image, included as this Editorial's figure, is emblematic of the multi-scale nature of chemical engineering: the discipline is concerned with designing macroscopic processes (a control volume around the network of pipes), applying microscopic physics (an infinitesimally small volume element within a single pipe), and connecting these scales. The Editorial in our February issue discussed the importance of macroscopic systems-level thinking in process engineering and our Analysis article format that showcases works in this area (*Nat. Chem. Eng.* **1**, 117–118; 2024). Here, we turn our attention to the continuum-level balances that form a key component of chemical engineering science.

Scientific advances are bolstered and often enabled by coordinated and concerted efforts in both experiment and theory. In the continuum limit, writing and solving mass, energy and momentum balances forms an important framework in chemical engineering for quantifying and advancing potentially practical devices, systems and processes. This framework not only allows one to explore regions of parameter space that may be challenging, costly or impossible to access otherwise, but also provides an avenue towards a complete picture of experimental findings through a quantitative evaluation of the physics that govern the system.

Despite its clear importance, we currently view research containing continuum modeling as underrepresented in submissions to the journal. *Nature Chemical Engineering* aims to support advances in both the applications and fundamentals of chemical engineering. As such, we are particularly interested in works that merge experimental efforts with theoretical analysis, especially in the continuum limit; this includes works that bridge molecular-scale phenomena with macroscopic processes (multi-scale modeling).

This interest is highlighted on the cover of the current issue and in an Article by Lees and co-workers reporting a continuum multiphysics model that guides the device-scale performance of a CO_2-to-CO electrolyzer. In this work, the researchers developed a one-dimensional model of a membrane electrode assembly (MEA) containing a Ag catalyst that was validated against their experimentally measured CO_2 crossover and CO formation rates. The modeling results show how electrolyzer performance is governed by coupled phenomena, for example, ion formation, ion transport, CO_2 solubility and water management.

As noted in an accompanying News & Views article by Ahmad Elgazzar and Haotian Wang, a key advance of the work stems from the choice of Marcus–Hush–Chidsey (MHC) theory to model reaction kinetics at the metal electrode. Lees and co-workers showed that the MHC-based model captured the experimental device performance, for example, the MEA polarization curve, CO_2 crossover, and CO and H_2 partial current densities. Conversely, they showed that the commonly used Tafel model overpredicted the CO partial currents at higher cell voltages since this model assumes that ion transfer limits the overall rate of the CO_2 reduction reaction.

At *Nature Chemical Engineering*, we are interested to hear about your research advances in chemical engineering science stemming from all theoretical approaches, not just those related to continuum modeling. Such developments may lie in, for example, microkinetic modeling, multi-scale modeling to bridge atomic, molecular, mesoscopic and macroscopic scales, integrating machine learning and data-driven approaches with physics-based modeling, and thermodynamic modeling.

As a journal focused on engineering, our interest in modeling is rooted in practicality. For example, we aim to publish research that enables a pathway to enhance the performance of particular processes or that has direct avenues towards applicability to a broad array of systems. In all cases, physically meaningful model validation and parameter estimation are crucial steps in model development; we also encourage sensitivity analyses to assess the impact of parameter choice on the resulting solution.

Today, physics-based modeling remains a cornerstone of chemical engineering training. We believe strongly that these frameworks will continue to enable future steps forward for chemical engineering science, theoretically speaking.

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