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Perspective

Reactive Multiphase Flows: Interfacial Chemistry in Dynamic Transport Systems

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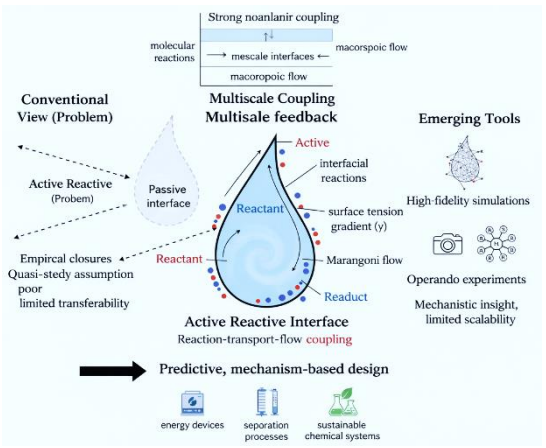
ABSTRACT

Reactive multiphase flows underpin a wide range of energy, environmental, and chemical technologies, yet their predictive description remains limited. Although interfaces are now widely recognised as chemically active, most theoretical and computational frameworks continue to treat them as quasi-steady boundaries or incorporate their effects through empirical closures. This Perspective argues that such approaches are fundamentally inadequate when reaction, transport, and hydrodynamic timescales become comparable and when reaction-driven interfacial forces actively restructure phase distributions. We critically examine the limitations of prevailing modelling paradigms using dimensionless reasoning and order-of-magnitude estimates, highlighting how coupled Damköhler, Marangoni, and capillary effects undermine model transferability across operating regimes. By synthesising advances in operando diagnostics, interface-resolved simulations, and physics-informed data-driven methods, we propose a unifying framework that treats interfaces as dynamically evolving, rate-determining subsystems. We further articulate a set of concrete, testable research challenges that define a forward-looking agenda for predictive design. This perspective aims to shift reactive multiphase flow research from descriptive integration toward quantitatively grounded, mechanism-based understanding across diverse application domains.



Keywords*:* Carbon capture; Electrochemical systems; Interfacial phenomena; Multiphase flow; Reactive transport; Sustainable chemical engineering

1. Introduction

Reactive multiphase flows are ubiquitous in natural and engineered systems, including gas–liquid reactors, liquid–liquid extraction processes, solid–fluid catalytic systems, and electrochemical energy devices [1],[2],[3],[4]. These systems involve the coexistence of multiple phases whose interactions are intrinsically coupled to chemical reactions. Although multiphase flow and reaction engineering have traditionally evolved as distinct disciplines, this separation rests on the implicit assumption that interfaces act primarily as passive boundaries enabling mass and heat transfer, as a comprehensive diagram of multiple coupling mechanisms can be seen in Figure 1. Increasing experimental and theoretical evidence now indicates that this assumption is fundamentally limiting for reactive systems.

At reactive interfaces, adsorption, desorption, and surface reactions can actively modify interfacial tension, wettability, and transport resistance on timescales comparable to, or faster than, fluid motion

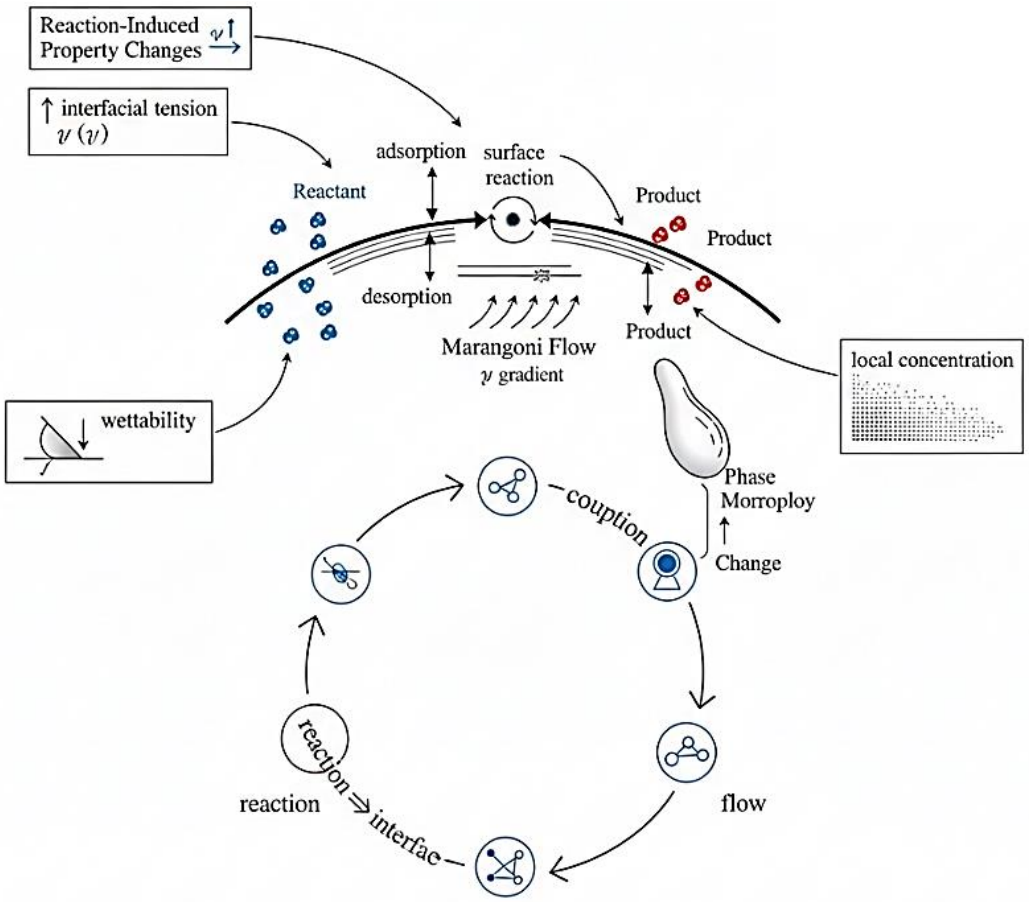


Figure 1: *Multiple coupling mechanisms in reactive multiphase flows. Reactive multiphase systems exhibit strong and simultaneous coupling between chemical reactions, interfacial properties, and hydrodynamic transport. Interfacial reactions modify surface tension, wettability, and local composition, which in turn generate Marangoni stresses and alter droplet or bubble dynamics. The resulting flow and phase redistribution feed back into species transport and reaction rates, creating a closed, multiscale coupling loop linking molecular-scale chemistry, interfacial dynamics, and macroscopic flow behavior.*

[5],[6],[7]. These reaction-driven changes generate surface tension gradients that induce Marangoni stresses, alter droplet and bubble stability, and continuously reshape phase morphology. In gas–liquid systems, chemical consumption or generation of interfacial species can directly control bubble growth and detachment, while in liquid–liquid systems, interfacial reactions may produce transient interphases with physicochemical properties distinct from either bulk phase [8],[9].

Such phenomena demonstrate that interfaces cannot be treated as static geometrical entities, but instead function as dynamic chemical environments that actively regulate transport and reaction pathways. Crucially, reactive multiphase flows are governed by strong, bidirectional coupling across length and time scales. Molecular-scale reaction kinetics influence mesoscale interfacial structure and phase distribution, which in turn determine macroscopic flow regimes, mass transfer efficiency, and overall reactor performance [10]. Reaction-induced restructuring of interfaces can redirect transport pathways and generate nonlinear feedback mechanisms, leading to oscillatory behaviour, hydrodynamic instabilities, or self-organised patterns. Under these conditions, classical distinctions between reaction-limited and transport-limited regimes lose validity, exposing the limitations of conventional modelling and scale-up strategies that rely on fixed interfaces and weakly coupled reaction–transport descriptions.

Despite broad recognition of interfacial activity, most existing theoretical and computational frameworks continue to treat interfacial effects as secondary corrections to bulk behaviour, often incorporated through empirical parameters or quasi-steady assumptions. This Perspective argues that such incremental extensions are insufficient. A predictive understanding of reactive multiphase systems requires a conceptual shift in which interfaces are treated as dynamically evolving, rate-determining subsystems that mediate coupling between chemistry, transport, and flow. Establishing this viewpoint is essential for developing modelling, experimental, and data-driven approaches capable of guiding the rational design of next-generation energy and chemical technologies.

1.1. Critical Analysis

Despite substantial progress, the predictive description of reactive multiphase flows remains quantitatively limited. Most continuum-scale multiphase frameworks, including volume-of-fluid and Euler–Euler models, rely on empirical closures for interfacial area density, mass transfer coefficients, and effective reaction rates. These closures implicitly assume quasi-steady interfaces and a separation of timescales between hydrodynamics, transport, and reaction. In many reactive systems, however, this separation does not hold. For example, characteristic reaction times at reactive interfaces ($\tau_r \sim 10^{-3}$–10^{-1} s) are often comparable to convective or diffusive transport times ($\tau_t \sim 10^{-2}$–1 s), yielding Damköhler numbers of order unity. Under such conditions, reaction-driven changes in interfacial properties directly feed back into flow and transport, violating the assumptions underlying standard closure relations and leading to poor model transferability across operating conditions [11],[12],[13].

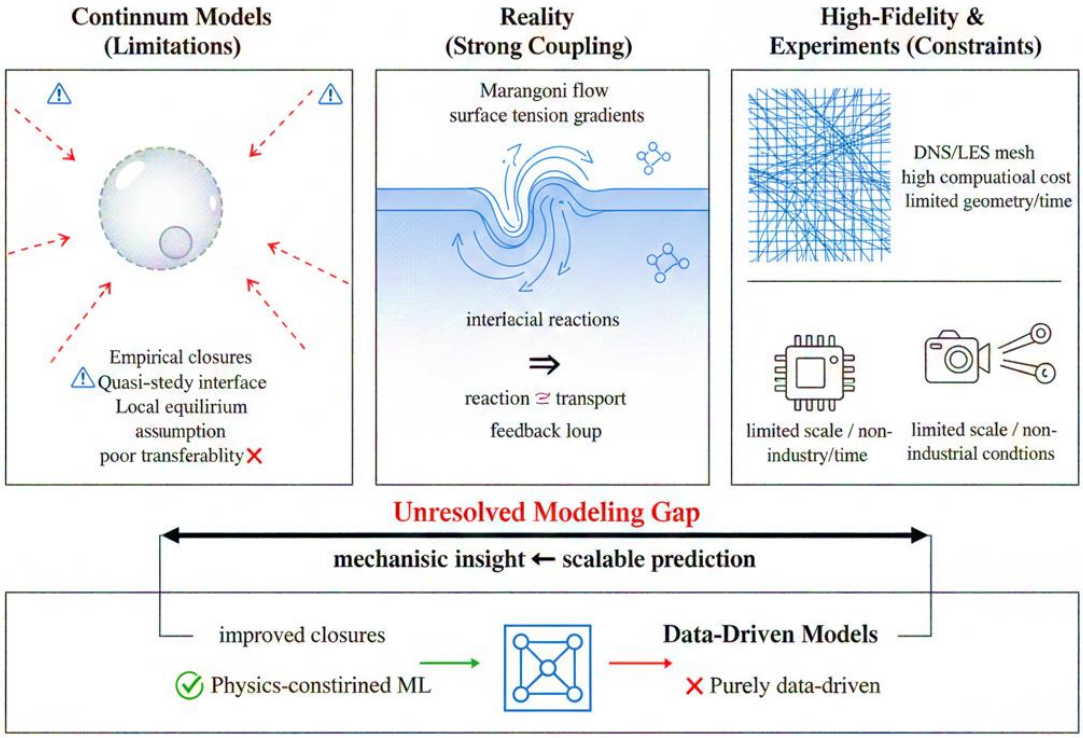


Figure 2: *Current limitations and modeling gaps in reactive multiphase flows. Continuum multiphase models rely on empirical closures that assume quasi-steady interfaces and local equilibrium, limiting their validity when reactions dynamically modify interfacial properties. High-fidelity simulations and advanced experiments provide detailed insight into coupled interfacial dynamics but are restricted to simplified geometries, short timescales, or non-industrial conditions. Data-driven approaches offer new opportunities to bridge these gaps; however, without strong physical constraints, they risk limited interpretability and generalization. Developing scalable, physically grounded predictive frameworks remains a central challenge.*

Interfacial force balances provide a further illustration of this limitation. Reaction-induced gradients in surface concentration or temperature can generate Marangoni stresses that compete with viscous and inertial forces. In many gas–liquid and liquid–liquid systems, estimated Marangoni numbers range from 102 to 104, indicating that interfacial stresses can dominate local flow near reacting interfaces [14],[15]. Yet most continuum models neglect such effects or subsume them into effective parameters, obscuring their impact on phase distribution, bubble or droplet dynamics, and mass transfer efficiency. As a result, predictions of key performance metrics, such as interfacial area, conversion rate, or pressure drop, can deviate by orders of magnitude when extrapolated beyond calibrated conditions.

High-fidelity numerical simulations have clarified the mechanistic origins of such behaviour by explicitly resolving reaction–transport–interface coupling. However, the computational cost of resolving interfacial thicknesses ($\sim 10^{-9}$–10^{-6} m) alongside device-scale flow domains ($\sim 10^{-2}$–1 m) imposes severe constraints on spatial resolution and simulation time [16],[17],[18]. Consequently, these approaches are typically restricted to idealised geometries, low Reynolds numbers, or short physical times, limiting their ability to predict long-term evolution or statistically steady operation. Experimental advances, including high-speed imaging, microfluidic platforms, and operando spectroscopy, have revealed similarly rich interfacial dynamics, but often at length scales, flow rates, or residence times that differ substantially from industrial systems. Quantitative links between these observations and macroscale performance metrics remain weak [19],[20].

Data-driven and machine-learning approaches are emerging as promising complements to traditional modelling. When constrained by physical laws, these methods can extract reduced-order representations and closure relations from high-dimensional datasets [21]. However, their success depends on data quality, interpretability, and integration with established transport theory. Without careful physical grounding, purely data-driven models risk obscuring causal mechanisms rather than clarifying them.

Taken together, these quantitative considerations indicate that the central limitation is not a lack of resolution or data, but the absence of frameworks that explicitly treat interfaces as dynamically evolving, rate-controlling subsystems. Progress will require models and experiments that resolve how competing dimensionless groups govern interfacial evolution and feed back into macroscopic performance. Establishing such quantitatively grounded frameworks is essential for advancing reactive multiphase flows from descriptive analysis toward predictive design. A critical picture is provided in Figure 2.

1.2. Outlook

Reactive multiphase flows are foundational to a wide range of energy conversion, storage, and chemical transformation technologies, yet their rational design remains limited by incomplete mechanistic understanding [22],[23]. In systems such as electrolysers, fuel cells, batteries, and reactive separation processes, performance and durability emerge from the dynamic coupling between multiphase transport, interfacial chemistry, and reaction-driven structural evolution. While recent studies have clarified individual aspects of these processes, progress toward predictive design requires a shift from descriptive frameworks to quantitatively testable, forward-looking research agendas as provided in Figure 3.

A first critical challenge concerns the dynamic coupling between reactions and interfacial evolution. Reactive interfaces are

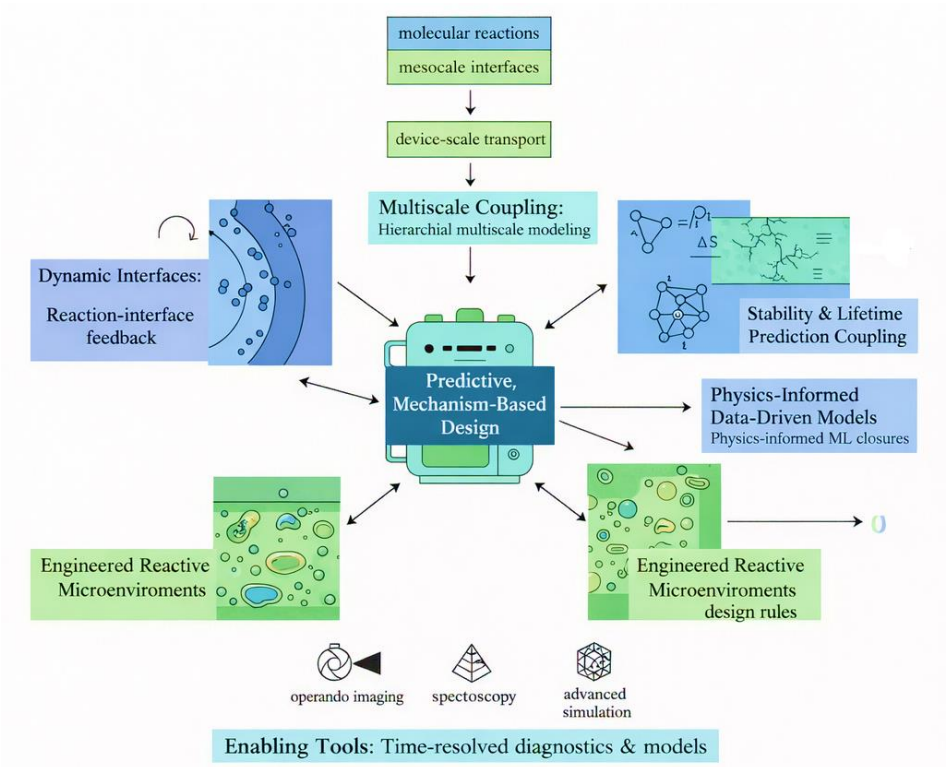


Figure 3: *Outlook and research roadmap for reactive multiphase systems. Future progress toward predictive design requires integrated advances in understanding dynamic reaction–interface coupling, bridging molecular kinetics with device-scale transport through multiscale frameworks, and developing physics-informed data-driven models. Engineering reactive microenvironments and quantitatively predicting stability and lifetime under coupled multiphase and reactive stresses are essential to move beyond empirical optimization. Together, these directions establish a pathway toward mechanism-based, predictive control of reactive multiphase processes in energy and chemical*

rarely static; instead, phase distributions, surface chemistry, and local curvature evolve continuously under operating conditions. A central scientific question is how such interfacial dynamics feed back into local reaction rates, mass transport resistances, and energy losses. Addressing this requires the combination of time-resolved operando diagnostics, such as advanced imaging and spectroscopy, with interface-resolved multiphase models that explicitly capture reaction-induced morphological change. Establishing causal links between interfacial evolution and macroscopic performance would enable predictive control strategies rather than post hoc optimisation.

A second unresolved challenge lies in bridging molecular-scale reaction kinetics with device-scale transport phenomena. Elementary reaction steps are governed by local chemical environments and atomic-scale energetics, whereas overall performance depends on mesoscale phase connectivity and macroscopic flow fields. The absence of robust multiscale frameworks limits the transferability of current models across materials and operating regimes. Future efforts must focus on hierarchical modelling approaches that consistently couple first-principles kinetics, mesoscale interface dynamics, and continuum transport descriptions. Such integration would allow quantitative predictions of performance trends and operating limits without reliance on system-specific empirical parameters.

Third, the growing availability of experimental and simulation data presents an opportunity to develop physics-informed data-driven methodologies tailored to reactive multiphase systems. However, the key scientific challenge is not data volume but data efficiency and physical fidelity. Learning frameworks must incorporate conservation laws, interfacial thermodynamics, and kinetic constraints to ensure robustness and interpretability. When properly constrained, physics-informed models could reduce uncertainty in parameter estimation, enable reliable extrapolation to untested conditions, and accelerate materials and reactor design.

A fourth priority direction involves the intentional engineering of reactive microenvironments. Local variations in wettability, pore geometry, and phase distribution can strongly influence reaction pathways and selectivity, yet these effects remain poorly quantified. Systematic studies combining micro- and nano-fabrication, controlled surface modification, and targeted simulations are needed to establish design rules that link microenvironmental control to measurable gains in efficiency and selectivity. Such insights are essential for translating process intensification concepts from laboratory demonstrations to scalable technologies.

Finally, predictive modelling of stability and lifetime under coupled multiphase and reactive stresses remains a largely open problem. Degradation processes are often driven by the same interfacial and transport phenomena that enable high performance, leading to complex trade-offs between efficiency and durability. Integrating reactive flow models with descriptions of material evolution, chemical ageing, and mechanical stress accumulation is necessary to establish quantitative relationships between operating conditions and long-term performance decay.

Collectively, addressing these challenges will enable a transition from empirical optimisation toward predictive, mechanism-based design of reactive multiphase systems. Such a shift is essential for achieving transformative advances in energy technologies, carbon management strategies, and intensified chemical processes.

4. Conclusion

Reactive multiphase flows represent a class of systems in which chemistry, transport, and morphology are fundamentally

inseparable. Moving beyond traditional decoupled descriptions requires recognising interfaces as active, evolving chemical entities. Advances in experimental observation, computational modelling, and data-driven methods are reshaping the field, yet significant challenges remain in achieving predictive and scalable frameworks. Addressing these challenges will be essential for the development of efficient, resilient, and sustainable multiphase technologies across energy, environmental, and chemical engineering applications.

Declaration

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