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Modeling of industrial multiphase reactors

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Industrial multiphase reactors remain among the most challenging systems to model due to their complexity, multiscale coupling, and persistent uncertainties in turbulence, interphase transport, and constitutive closures. While traditional approaches combining first-principles physics, empirical correlations, and numerical pragmatism have enabled substantial progress, fundamental limitations persist. This perspective outlines how advances in artificial intelligence (AI), high-performance computing, and, eventually, quantum computing (QC) can steer multiphase modeling toward industry-ready predictive capability with an accuracy unthinkable today.

AI enables more generalizable, physics-constrained closures, while graphics processing units (GPUs) and exascale platforms already enable industry-scale simulations at unprecedented fidelity. Although QC is a longer-term prospect, hybrid quantum–classical approaches offer pathways to address complexities beyond classical limits. These developments promise to transform modeling workflows and engineering practice, with direct implications for scale-up, reliability, sustainability, and cost reduction. We highlight key research priorities, including multiphase-aware turbulence models, AI-assisted closures, hybrid solvers, computing architectures, and rigorous verification, validation, and uncertainty quantification.

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Introduction/Motivation

George Box's remark — 'All models are wrong, but some are useful' — aptly captures the challenge of multiphase-reactor modeling. No model captures every physical detail: some remain elusive, others too complex or costly. Practical models, therefore, blend first principles with empirical and numerical pragmatism (Figure 1). This compromise has driven decades of progress, refined through improved measurements and closures, data-driven methods, and advanced computation architectures.

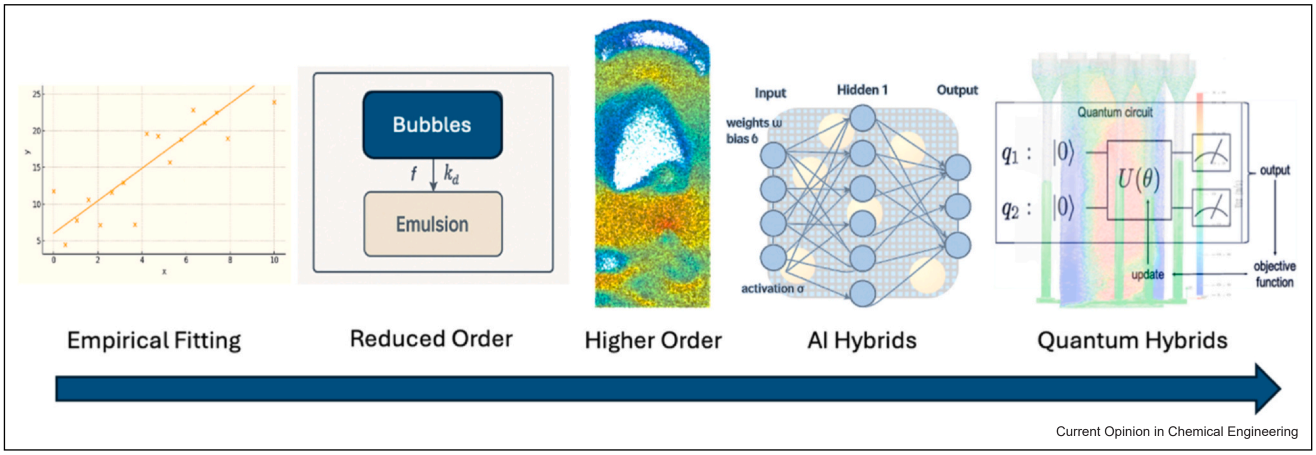
Physics-aware artificial intelligence (AI) is the near-term stimulus (Figure 2). It enriches constitutive models (drag, breakup, turbulence, heat/mass transfer) by fusing multidimensional data with mechanistic constraints, enhancing generalizability across chemistries, regimes, and equipment. AI is also reshaping workflows: (i) refining encoded physics; (ii) changing code development (e.g. auto-discovered closures, machine learning (ML)-assisted meshing/solvers); and (iii) transforming user interaction (e.g. explainable AI, digital twins). Graphics processing units (GPUs) enable high-fidelity, plant-scale simulations (Figure 3); quantum computing (QC), though still limited, targets specific bottlenecks that could yield transformative speedups (Figure 4). As these mature, models capturing detailed physics (e.g. free-surface dynamics, bubble interfaces, interparticle forces) and reactor-specific designs (e.g. distributors, baffles, geometries) could be solved in days rather than months.

Yet, faster tools make it easier to get plausible-looking wrong answers. Domain expertise — numerics, statistics, transport, kinetics, thermodynamics — remains non-negotiable, as do rigorous verification, validation, and uncertainty quantification (VVUQ) practices. Realizing the ultimate ambition is likely a decade or more away, but advances in hardware, algorithms, diagnostics, and datasets are steadily closing the gap. As in any discipline, progress will be iterative — advances, recalibrations, and the occasional step back — on the way to robust, reliable industrial-scale modeling.

Evolution of models

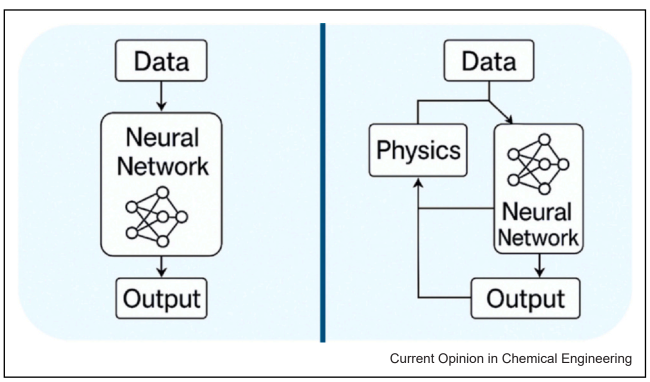
Figure 1 overviews the generalized evolution of multiphase reactor models — from early reliance on empirical and reduced-order approaches to today's dominance of

Figure 1



Evolution of multiphase-reactor modeling strategies from empirical correlations to reduced-order models, high-fidelity CFD, AI-augmented closures, and emerging quantum-hybrid approaches. Industrial-scale multiphase CFD employs meshes on the order of 10^9–10^{10} cells [1]. AI-based reduced-order models reported to achieve at least 3 orders-of-magnitude acceleration for multiphase flow prediction and parametric exploration while maintaining agreement with high-fidelity CFD [2]. Using physics-informed loss functions, speedups of 100 times over CFD and 10 times over CFD–DEM demonstrated [3]. Recent quantum-algorithm research, including Carleman-linearized lattice-Boltzmann formulations, suggests that quantum solvers may eventually reduce cost scaling from polynomial to logarithmic in system size, indicating potential orders-of-magnitude speedups for future quantum-native CFD [4].

Figure 2



Comparison of (black-box) AI and physics-aware (gray-box) AI for multiphase-flow modeling. NN provides 1000-fold speedup over conventional CFD; while physics-aware NN requires at least 15% more time than NN, they offer improved extrapolation capabilities [5].

higher-order models driven by computational advances — and highlights how emerging AI and QC are poised to further close the gap between modeling capability and engineering needs.

Empirical correlations

Early models relied on empirical/semi-empirical correlations, exemplified by the Ergun equation [10]. Parameters like holdup, pressure drop, dispersion, and mass transfer coefficients were obtained from lab-scale experiments and generalized for reactor design. While practical, these models offer limited predictive and scale-up reliability beyond the experimental scope.

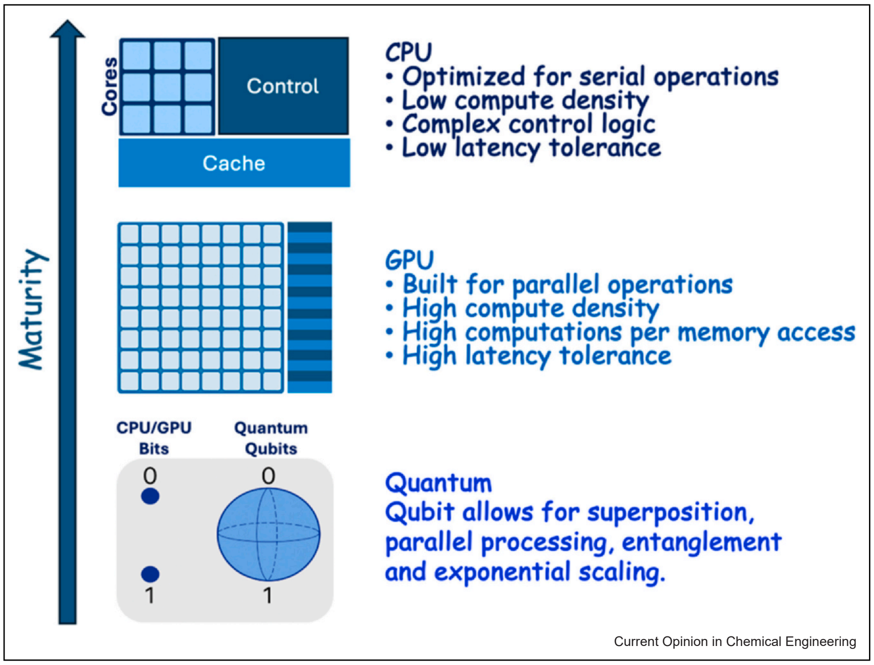
Reduced-order models

With advances in computation and experimentation, reduced-order model (ROM) sophistication grew. Reactors are idealized as networks of plug-flow, continuous-stirred-tank, and dispersion zones, with transport parameters inferred from residence-time measurements and tanks-in-series analogies. Population balance models (PBMs), using discretization or moments, capture droplet/bubble/particle size distributions to account for breakup/coalescence, aggregation, attrition, dissolution, and growth. Coupled with kinetics, these frameworks enable scale-up, optimization, and process development, delivering actionable engineering insights despite limited spatial resolution.

Computational fluid dynamics

Leveraging single-phase computational fluid dynamics (CFD), the third wave extended CFD to multiphase flows [11]. The Euler–Euler two-fluid model (TFM) became the workhorse, solving separate phase balances (mass/momentum/energy/species) coupled through interphase exchange (drag, stress, heat/mass transfer). For free-surface systems, volume of fluid (VOF) [12] and related interface-capturing methods advanced in parallel. Increasing computational power enabled Euler–Lagrange CFD–discrete element method (DEM) for particle-resolution dynamics, lattice-Boltzmann methods (LBMs) for complex boundaries and phase transitions, and CFD-PBM for dispersed-phase evolution. These

Figure 3



Evolution of high-performance computing hardware, highlighting increases in parallelism, memory bandwidth, and heterogeneous CPU–GPU–QC. Offloading between hardware is, in part, memory-bound, damping speedups. Speedups of two orders-of-magnitude have been enabled by GPU acceleration for multiphase systems [6,7]. Current quantum technology is still limited to comparatively small and noisy systems characterizing the NISQ era, so quantum algorithms that are forgiving to errors and use only hundreds of qubits may give a quantum advantage over conventional computing [8].

tools illuminated key phenomena (e.g. bubble dynamics, solids circulation), though predictive accuracy remains limited by non-universal closures, missing physics, and grid-resolution constraints. Meanwhile, high-performance cumputing (HPC) advances — commodity clusters, cloud computing, and open-source platforms — democratized access.

Multiscale and filtered models

Around the 2000s, advances in multiphase CFD began to translate into industrial practice. Large-scale reactors require massive grid numbers, making tractability and fidelity dependent on multiscale partitioning (micro/meso/macro) [13]. Three strategies are notable: (i) coarse-graining to reduce dispersed-phase cost [14]; (ii) filtered TFM (fTFM) embedding subgrid mesoscale effects into closures [15]; and (iii) energy-minimization multiscale (EMMS)-based closures for reactor-scale instabilities (e.g. clusters) [16]. In parallel, GPUs accelerate computation.

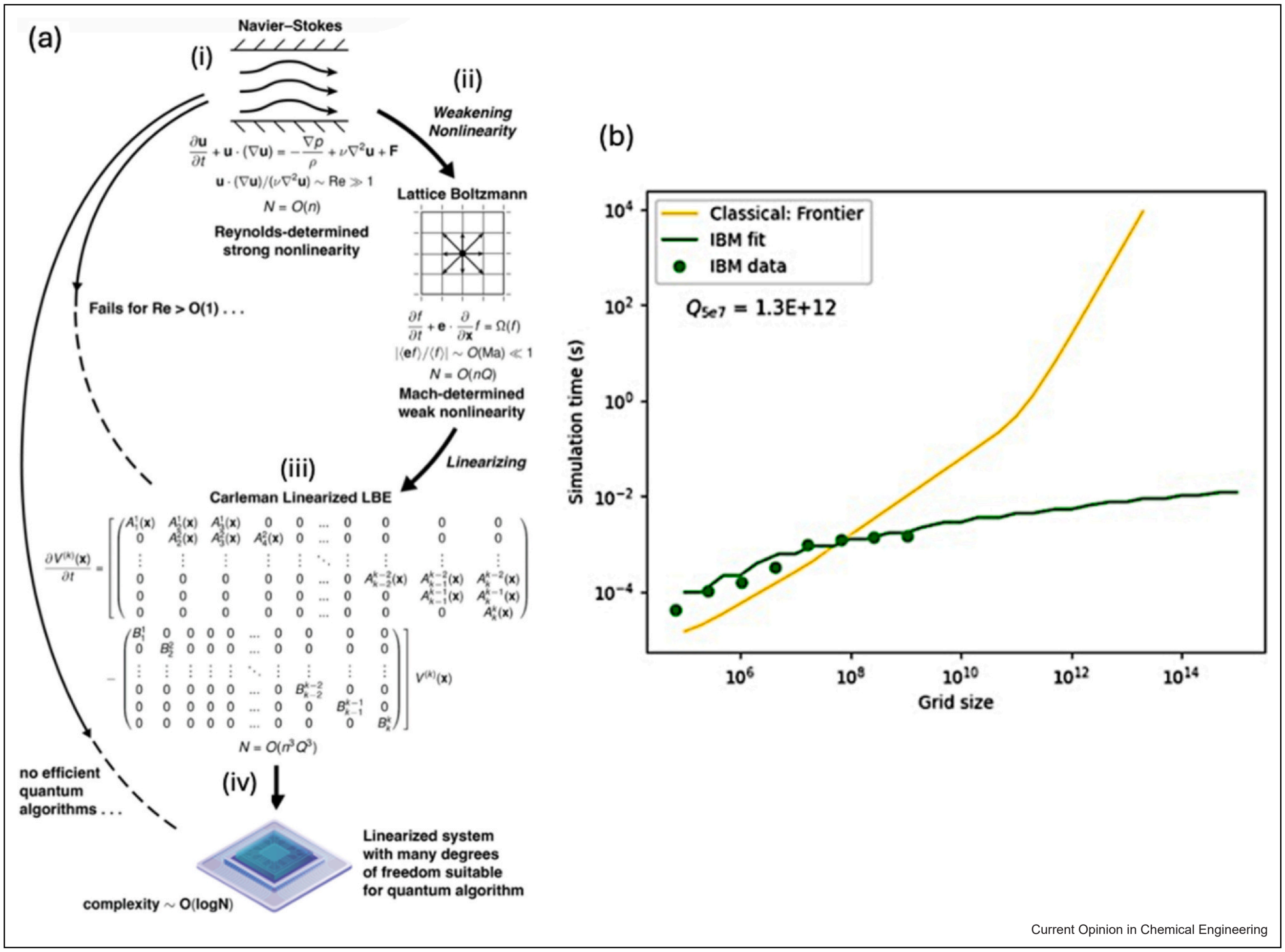
Artificial intelligence-driven models

AI augments classical modeling through physics-aware closures, surrogates, and digital-twin workflows. Physics-aware ML (Figure 2) enforces constraints (conservation, symmetries, bounds), improving robustness and generalization beyond empirical correlations [17]. In gas–solid systems, ML applied to fTFM learns subgrid drag and solids stress from fine-grid data, boosting coarse-grid accuracy across regimes [18]. Integrated pipelines combining CFD, data-driven surrogates, and statistical modules accelerate design and enable real-time digital-twin emulation [19].

Quantum computing

High-fidelity simulation of industrial-scale multiphase reactors is still not achievable [20]. NASA's CFD Vision 2030 cautions that large eddy simulation (LES) for industrial *single-phase* applications may remain impractical by 2030 [21]. Modern supercomputers face memory-bandwidth limits, with data movement dominating CFD runtime. QC offers a potential breakthrough, as quantum state spaces can handle and process large CFD datasets. Challenges remain — managing nonlinear calculations, data transfer to/from quantum processors, and quantum hardware noise — but progress is underway. Methods under study for Noisy Intermediate-Scale Quantum (NISQ) and forthcoming fault-tolerant devices [22] include Carleman linearization [4], variational approaches [9], and linearized Navier–Stokes reformulations [23].

Figure 4



While multiphase implementations remain a future opportunity, quantum-CFD demonstrations on current NISQ platforms have been achieved for single-phase flows. **(a)** Hybrid quantum-classical formulations recast selected linear components of the Navier–Stokes equations into quantum-solvable blocks, yielding costs that scale logarithmically with system size, in contrast to the polynomial scaling of classical solvers [4]. **(b)** Comparison of simulation times between classical CFD versus variational quantum-CFD (VQCFD) indicates speedups for the latter for higher grid resolution [9].

Outstanding gaps

The overarching goal is physics-consistent, tractable models that retain generality across operating regimes, equipment designs, and scales, while avoiding ad-hoc, case-specific tuning.

Multiscale coupling and mesoscale structures

Bridging particle-scale physics (e.g. collisions, wakes, bubble dynamics, interparticle forces) to industry-scale flow remains unresolved. Filtered and coarse-grained models still struggle to represent mesoscale structures (e.g. clusters, bubbles) without case-specific tuning [6,24], and many underlying assumptions remain to be verified (e.g. analytically or via direct numerical simulation (DNS)) [25]. Multiscale studies have demonstrated that coupling particle- and reactor-scale physics can improve predictions (e.g. heat transfer, conversion, overall reactor performance [6]).

Interphase momentum, heat, and mass transfer

Closures for interphase forces (e.g. drag, lift, virtual mass, stress) remain empirical and regime-specific, yielding wide variability among standard models [26]. Uncertainty is known to be acute near walls (lift-dispersion coupling), and in reactive systems (poorly characterized micromixing and interfacial heat transfer).

Bubble/droplet coalescence/breakup

Common coalescence/breakup kernels give markedly different size distributions and interfacial areas under identical conditions [27]. Mesoscale approaches (e.g. EMMS-informed PBM) still lack reliable extrapolation to industry-scale conditions.

Distinctions between bubble and droplet behaviors arise from interfacial boundary conditions — shear-free gas versus finite-shear liquid [28]. In bubbles, low density permits rapid internal motion and breakup into uneven fragments; in droplets, higher density restricts internal motion, producing more uniform sizes. DNS reveals multi-timescale, stochastic fragmentation with viscosity-ratio-controlled pathways beyond Hinze scaling [29].

Chemistry–hydrodynamics interaction

Highly exothermic/endothermic reactions, micromixing, catalyst deactivation, and fouling create two-way coupling between reaction and transport that current closures capture poorly, particularly when kinetics and hydrodynamics evolve on comparable timescales [30].

Phase transition

Phase-change impacts on hydrodynamics still rely heavily on empirical or semi-empirical forms that often omit Stefan flow and evolving interfacial topology [31], and recent work shows that such omissions can lead to unexpected behaviors like droplet levitation [32]. High-fidelity phase-field/phase-change, multiphase LBM, and CFD–DEM/VOF frameworks are available, but their stability/accuracy requirements (e.g. thin interfaces, large density ratios, particle-mesh coupling) make them computationally intensive, limiting industry-scale application [33,34].

Turbulence

Two-way coupling remains elusive: small St ~ O(1) inclusions enhance dissipation, while larger/heavier particles or high loadings augment turbulence [35]. Reynolds-Averaged Navier–Stokes and LES subgrid models adapted from single-phase turbulence often fail to account for this behavior. Bubble-induced or particle-induced turbulence source terms remain case-tuned, and particle-laden LES typically needs specialized subgrid-scale terms to represent unresolved momentum exchange and clustering.

Free surfaces

Most models assume a smooth interface, yet even then, it is smeared by numerical diffusion. Bubble collapse at the surface further complicates modeling and often relies on empirical observations. Even then, such observations are limited to the micro-scale hydrodynamics, ignoring the effects of the region around the collapsing bubble. Secondary physics, such as evaporation, condensation, melting, expansion, or solidification at the free surface, further increase this complexity, especially since most free-surface models (VOF/level set) fail to maintain phase-change consistency.

Internals and geometry effects

Industrial reactors have internals, distributors, and complex geometries that drive phase distribution and mixing. CFD optimization of proprietary distributor designs demonstrates how design details govern critical phenomena (e.g. gas–solid dispersion) [36]. Yet, most models are simplified, for example, applying a single drag for particles and internals despite differences in surface and shape. These omitted geometric features can promote small recirculation zones, eddies, and dead zones — often below grid resolution — causing numerical diffusion, erroneous pressure gradients, and instabilities.

Leveraging new tools

How to harness artificial intelligence?

AI is a strategic accelerator, not a replacement for mechanistic CFD. Building on kinetic theory of granular flow, EMMS, and fTFM, which revealed the limits of regime-specific closures, physics-AI hybrids can generalize closures, speed simulations, and enable digital twins across chemistries, regimes, and equipment. VVUQ must be upheld to prevent AI from becoming merely a data-fitting tool.

AI-assisted closures

Neural networks (NNs) trained on high-fidelity data (e.g. DNS, tomography) are replacing empirical drag and stress correlations in fTFM, enhancing generalizability across dilute and dense regimes [18,37]. For example, coarse-grid simulations (~30 times the particle diameter) using an artificial neural network (ANN)-augmented filtered-drag closure were shown to reproduce fine-grid trends [38]. Physics-informed neural networks (PINNs) enforce physical consistency through embedded constraints [39], enabling systematic augmentation of multiphase modeling across scales [19]. Universal differential equations (UDEs) couple known transport models with AI-discovered terms, balancing fidelity with flexibility [40]. Collectively, these advance AI-driven closures for drag, turbulence, breakup/coalescence, and kinetics, though challenges persist in data scarcity/quality, computational cost, and out-of-distribution generalization.

Surrogates and digital twins

AI enables reduced-order surrogates and digital twins for design, optimization, and control. Across multiphase reactors and related flow systems, surrogate models routinely deliver orders-of-magnitude speedups while retaining predictive accuracy, enabling design space exploration and digital-twin deployment that are inconceivable with CFD alone [19]. PINNs offer a physics-consistent alternative to conventional surrogate models, approximating solution spaces of PDE-governed systems, while preserving conservation laws and boundary conditions through their loss formulation [41].

Active learning strategies guide efficient data acquisition for closure development [42], while Bayesian ML provides for uncertainty quantification [43]. Surrogates (ROMs/ML) deliver significant speedups but can fail catastrophically under extrapolation, so credibility demands physics constraints and VVUQ before deployment [44].

AI-enabled reduced-order surrogates complement mechanistic CFD by delivering low-cost inference after training, albeit with significant upfront data needs; physics-aware architectures and active-learning approaches mitigate data demands while maintaining VVUQ robustness.

Strategic accelerator, not replacement

The consensus is that authoritative reviews and roadmaps converge on the view that AI will not replace mechanistic CFD; rather, it will accelerate and augment it by informing closures, speeding submodels, and enabling credible surrogates within VVUQ workflows [19,30,45]. Implementation guidelines are recommended in Box 1.

A practical path forward is a hybrid strategy that combines physics-aware frameworks with reactor-specific submodels, balancing computation efficiency, predictive fidelity, and data requirements.

How to exploit quantum computing?

Quantum CFD could revolutionize simulations of industrial-scale multiphase reactors through circuit-based QC. Rather than replacing classical HPC, QC is expected to complement it with hybrid quantum–classical HPC frameworks.

Traditional CFD algorithms were designed for classical computing architectures, with gains achieved by porting algorithms to new hardware generations — CPUs, GPUs, and distributed clusters — all rooted in the same computational model. This approach offers limited benefit for QC, whose architecture differs fundamentally, introducing foundational challenges [22]:

1. *Linearity versus Nonlinearity*: QC operates on intrinsically linear mathematical frameworks, contrasting with the nonlinear Navier–Stokes equations governing fluid flow.
2. *State Preparation and Readout Costs*: Preparing quantum states that encode physical flow fields and extracting useful results from quantum measurements remain computationally expensive.
3. *Hardware Limitations*: Current NISQ devices face decoherence, qubit dephasing, and high gate-error rates, limiting practical problem sizes and circuit depths.

Despite these challenges, the distinct computational paradigm of quantum mechanics offers quantum-native CFD formulations with transformative potential, motivating close collaboration across fluid dynamics, numerical analysis, and quantum information science. On current NISQ hardware, quantum CFD remains limited to small, low-Re test cases due to qubit and circuit-depth constraints, confining quantum methods to algorithm-development and hybrid-insert roles. Table 1 summarizes the main multiphase CFD approaches under investigation and distinguishes near-term hybrids from longer-term quantum-native strategies.

Quantum computing accelerating existing computational fluid dynamics algorithms (near-term)

Current quantum CFD research focuses on adapting classical algorithms for NISQ hardware, which accommodates only shallow circuits. In classical CFD, nonlinear terms are handled through discretization and iterative schemes, reducing the governing equations to large linear systems — the main computational bottleneck. Quantum linear solvers accelerate this step.

The Harrow–Hassidim–Lloyd (HHL) algorithm offers exponential speedup over classical solvers, but is impractical on today's quantum devices due to deep circuit requirements. More practical alternatives include the linear combination of unitaries (LCU) [46], variational quantum Eigensolver (VQE) [47], and variational quantum linear solver (VQLS) [48] — all suitable for NISQ hardware.

Box 1 Practitioner Guidelines for AI Implementation

- Physics integration
  Use PINNs/UDEs to embed constraints (conservation, symmetries, bounds) so AI augments — not overrides — governing equations.
- Guardrails via VVUQ
  Like any closure, verification (code), validation (data), UQ (epistemic/aleatory), and monitoring for drift are needed in AI deployment.
- Targeted acceleration
  Prioritize AI where it is most impactful, for example, drag/turbulence/breakup closures, ROM/surrogates for design space sweeps, and digital-twin emulation.
- Generalization discipline
  Enforce domain of applicability, out-of-distribution (OOD) checks, and active learning to expand coverage without overfitting.
- Human-in-the-loop
  Keep expert oversight for model selection, retraining triggers, and decision thresholds.

Table 1

Near-term quantum-classical hybrids versus long-term fully quantum CFD formulations.

Category	What it involves	Example methods
Near-term hybrid inserts (credible on NISQ)	Quantum routines accelerate specific linear substeps inside classical CFD loops (e.g. pressure/Poisson solves, implicit diffusion, PBM moment updates).	VQLS, VQE-based pressure solve, quantum-Krylov/LCU updates, truncated Carleman-linearized steps
Mid-term hybrid PDE solvers (early fault-tolerant quantum computers)	Larger PDE components offloaded to quantum hardware; nonlinear updates remain classical; potential for quantum-assisted subgrid models.	Hybrid HSE-inspired solvers, quantum-accelerated LBM, quantum-assisted turbulence/closure models
Long-term fully quantum CFD	Entire CFD system solved in a quantum-native formulation (full Navier–Stokes/HSE/Liouville dynamics) on fault-tolerant devices.	HSE formulations, Liouville-space solvers, deep-circuit quantum Navier–Stokes, fault-tolerant HHL-style solvers

Hybrid quantum-classical CFD frameworks have demonstrated that nonlinear updates can be recast as block-linear systems solvable by quantum linear solvers, improving efficiency without compromising accuracy [49]. Because quantum processing units are best suited for linear or block-linear subproblems that dominate runtime (e.g. pressure/Poisson solves, implicit diffusion), near-term hybrid workflows keep core Navier–Stokes updates, turbulence closures, and multiphase couplings on CPUs/GPUs.

Carleman linearization offers another route by replacing nonlinear terms (e.g. in LBM) with auxiliary variables yielding an expanded linear system [4]. Truncating the infinite-dimensional Carleman system makes it tractable, but current hardware cannot support the required circuit depth.

Variational Quantum Algorithms (VQAs), including VQE and VQLS, are promising for near-term CFD applications because of their shallow circuit depth and flexibility [8]. Song et al. [47] proposed a hybrid solver that uses a VQA for the pressure Poisson equation for incompressible Navier–Stokes flow, validated on a 2D lid-driven cavity via noise-free simulation and demonstrated on noisy quantum hardware. The fluid simulation is reformulated as an optimization task: a parameterized quantum circuit represents the flow field, and a cost function (e.g. residual error in governing equations) is iteratively minimized.

Discovering quantum-native computational fluid dynamics algorithms (longer-term)

In the longer-term, quantum-native CFD formulations could deliver breakthrough performance. One approach expresses fluid dynamics through the Liouville equation, which governs the probability distribution of flow configurations; although computationally infeasible on classical machines due to exponential trajectories, its linearity makes it amenable to quantum solvers. Succi et al. [50] highlight associated challenges, including the representation of nonlinear effects and numerical stability.

Another promising framework, the hydrodynamic Schrödinger equation (HSE), recasts Navier–Stokes dynamics into a unitary evolution [23], potentially enabling prediction-correction schemes for turbulence on fault-tolerant quantum hardware. HSE-inspired subroutines (e.g. quantum encodings of vorticity and enthalpy fields) may also enhance hybrid quantum–classical CFD workflows.

In principle, quantum-native formulations (such as HSE or Liouville-space approaches) could eventually probe flow-state manifolds far beyond classical computational limits, potentially revealing behavior in high-Re turbulence or strongly coupled multiphase regimes that is inaccessible today. Thus, long-term quantum CFD may contribute not only to accelerated computation but also to the discovery of new physical mechanisms.

Verification, validation, and uncertainty quantification checklist

Industry-ready modeling requires rigorous VVUQ, as summarized in Box 2. These elements provide a practical, defensible basis for determining whether a model is sufficiently credible for design, scale-up, and/or operational decision-making [51,52].

Effective integration points between AI or quantum and CFD can be identified through bottleneck profiling, error-sensitivity analysis, and multiscale partitioning that reveal where surrogate or accelerated evaluations offer genuine leverage. Performance gains can then be quantified through side-by-side benchmarking of augmented and baseline workflows (e.g. comparing computation time, memory, solver iterations, and scaling) together with VVUQ-based accuracy metrics to ensure predictive fidelity is maintained.

When predictions contradict physical intuition, interpretability can be supported through physics-aware architectures and diagnostic tools (e.g. saliency or sensitivity analyses, feature-attribution methods (e.g. shapley additive explanations (SHAP)), and residual-based error checks) to identify which inputs or terms

Box 2 VVUQ Checklist.

- Benchmarks
  Reproducible benchmark cases that capture key regimes and transitions (e.g. residence time distribution, liquid-liquid dispersion)
- Code Verification
  Conservation checks, spatial/temporal refinement, and regression tests for relevant solvers.
- Validation Metrics
  Validate against targeted reactor-scale observables (e.g. circulation flux, phase distribution).
- UQ protocols
  Assess sensitivity to closure parameters (e.g. drag, stress, turbulence), distinguish epistemic and aleatory sources, and define model assumptions and domains of applicability.

drive anomalous behavior and whether the issue stems from data limitations, extrapolation, or model-form error.

Needs in commercial software and architecture

Software

Industrial practice balances commercial CFD platforms (e.g. ANSYS Fluent, Simcenter STAR-CCM+, Flow Science Flow-3D, COMSOL Multiphysics, CPFD Barracuda) with open frameworks. Commercial software offers TFM, VOF, PBM, and hybrids through friendly graphical user interfaces and extensive model libraries. Their robustness and support appeal to engineers, but their partially closed architectures limit integration of new closures or mesoscale models. Popular open-source platforms include Keysight's OpenFOAM (Open Field Operation and Manipulation) and NETL's (U.S. National Energy Technology Lab) MFiX (Multiphase Flow with Interphase eXchanges), supporting TFM, CFD–DEM, and particle-in-cell (PIC) approaches.

Achieving reactor-scale fidelity, digital-twin coupling, and AI-assisted VVUQ requires synergizing the robustness of commercial platforms with the extensibility and performance portability of open, exascale-targeted frameworks (e.g. MFiX-Exa built on AMReX (adaptive mesh refinement in C++)) and interoperability standards (e.g. CAPE-OPEN (Computer-Aided Process Engineering Open Simulation Environment), FMI (Functional Mock-up Interface)).

GPU-acceleration

Modern GPUs now enable large-scale multiphase simulations, once limited by memory-bandwidth bottlenecks. A GPU-based multiphase solver achieved up to a 300-times speedup on a single NVIDIA A100 compared to an Xeon CPU core, and scaled efficiently across 13,824 GPUs on OLCF Summit (the leading computer) [7]. A notable open-source effort is FluTAS, a GPU-accelerated multiphase solver that achieves order-of-magnitude speedups using OpenACC on multi-GPU systems, although its FFT-based pressure solver limits strong-scaling efficiency [53]. For dense gas–solid systems, a GPU-accelerated CFD–DEM framework runs fluid solves on CPUs, while DEM and CFD–DEM coupling on GPUs, enabling a single GPU to match the efficiency of eight in earlier runs, while the CFD solver runs three times faster with fewer CPU cores [54]. Also, implementing dynamic CPU–GPU load balancing resulted in a further 2.3-times speedup [55]. Native multi-GPU solvers in commercial platforms now extend these gains to practical engineering applications, validated on both canonical and industrial benchmarks.

Exascale

Exascale supercomputing systems capable of at least 10^{18} floating-point operations per second marked a computing milestone in May 2022. However, pre-/post-processing, computation, storage, and data transfer remain key bottlenecks to achieving exascale performance [1]. The next-generation MFiX-Exa, a CFD–DEM/PIC code re-architected on AMReX, targets performance portability and exascale readiness [56]. OpenFPM offers enhanced particle and particle-mesh infrastructure with GPU portability and distributed memory support [57], well-suited for exascale multiphase solvers.

Interoperability standards such as CAPE-OPEN enable plug-and-play coupling of third-party closures, kinetics, or AI surrogates with CFD and process simulators. The path forward demands: (i) performance portability (CPU/GPU, vendor-neutral backends) with adaptive mesh refinement (AMR) and load balancing, (ii) scalable solvers and particle-mesh kernels (e.g. OpenFPM), (iii) amenable plugin points (for closures, AI modules, etc.), and (iv) coupling to process/digital-twin ecosystems (e.g. CAPE-OPEN).

Quantum

- Quantum-classical hybrid
  Treating QC as a co-processor, quantum linear solvers (e.g. pressure/Poisson, PBM moment/transport systems, and Carleman-linearized LBM) can be coupled to established CFD loops [4,47], directly analogous to CPU–GPU hybrids. On today's NISQ hardware, variational and quantum-Krylov solvers appear more amenable than deep HHL-style circuits, while preconditioning and error-mitigation are recommended.
- Credibility and performance
  VVUQ needs to be adopted rigorously, with runtime, accuracy, and reproducibility benchmarked against

best-in-class HPC baselines, and clear definitions of problem and domains of applicability. Failures and underlying reasons should also be openly reported.

- People, access, and integration
  Cross-trained teams (fluid mechanics, QC, etc.) need to be ready, cloud QC prototyped, and workflow integration (containers/continuous integration, scheduler hooks, data pipelines) ensured so quantum inserts are operationally viable.
- Hardware reality and expectations.

Fault-tolerant QC remains a later-decade milestone per the IBM roadmap. Quantum can be positioned as a strategic accelerator (once error correction, scale, and integration are resolved) inside hybrid workflows, expanding as devices mature.

Outlook and future directions

Decades of advances have progressively resolved various phenomena spanning various spatial-temporal scales. Adaptive, scale-bridging strategies outperform one-size-fits-all. Notably, faster tools can also accelerate failure. Domain expertise and VVUQ remain non-negotiable, as models become truly 'useful' (per George Box) and eventually sufficiently generalizable for industrial-scale implementation. The next phase likely hinges on four trends:

- **Learning from the past, building adaptive models**
  Coarse-grained/filtered formulations succeeded by pragmatically trading resolution for fidelity. Analogously, AI-assisted coarse-graining, adaptive layering/c, and regime-aware closures that retain physical structure while expanding applicability are advancing. Additionally, digital twins are maturing from pilots to tools for predictive maintenance, feed-forward control, and dynamic optimization [58].
- **Emerging computational architectures**
  GPU acceleration and exascale systems have redefined the computational landscape, delivering unprecedented speedups that brings previously intractable cases within reach [7,59]. For single-phase compressible flow, Wilfong et al. [60] demonstrated exascale CFD with over one quadrillion degrees of freedom, highlighting what is now achievable through integrated algorithm–hardware co-design. As CPU/GPU hybrids become mainstream, quantum-classical hybrids may become the next frontier. In parallel, cloud-based deployment democratizes access to HPCs.
- **Gray-box modeling: bridging physics and AI**
  Physics-aware ML (e.g. PINNs, UDEs) constrains learned closures (drag, turbulence, interfacial transfer) and supplies efficient surrogates, all within VVUQ scaffolding [18,39]. This results in faster, generalizable, and explainable models.
- **Quantum subroutines**
  Full quantum CFD is not ready, but hybrid implementations of quantum-classical routines are possible on NISQ devices [4,23,49]. Meanwhile, rigorous benchmarking to ascertain benefits and VVUQ are important steps. QC could unlock direct solutions of industry-scale multiphase reactors — far beyond current capabilities.

Data Availability

No data were used for the research described in the article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References and recommended reading

Papers of particular interest, published within the period of review, have been highlighted as:

- • of special interest
- •• of outstanding interest

1. • Neau H, Ansart R, Baudry C, Fournier Y, Mérigoux N, Koren C, Laviéville J, Renon N, Simonin O: **HPC challenges and opportunities of industrial-scale reactive fluidized bed simulation using meshes of several billion cells on the route of Exascale**. *Powder Technol* 2024, **444**:120018, https://doi.org/10.1016/j.powtec.2024.120018.
This paper maps the HPC bottlenecks and opportunities for simulating industrial reactive fluidized beds at extreme mesh sizes (billions of cells) on the path to exascale. Drawing on large-scale Eulerian multifluid simulations, the authors outline limits from memory footprint, load balancing, solver scalability, and I/O, and point to advances like GPU acceleration, improved partitioning, and algorithmic/physics co-design as the strategy for routine billion-cell runs for industry. In short, it's a roadmap showing what must change in codes and hardware to make credible, industry-scale CFD practical.

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The authors reformulate the Navier–Stokes nonlinearity into a lattice-Boltzmann form and then apply low-order Carleman linearization, demonstrating it is much more accurate than previously believed for these systems. This trades nonlinearity for extra degrees of freedom, allowing quantum algorithms for linear systems to tackle nonlinear fluid flows with logarithmic cost with respect to system size, compared to polynomial scaling classically. The result provides evidence of quantum speedups for simulating turbulent, multiscale fluid dynamics.

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