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Review Article

Multiphase Flow Simulation in Energy Systems: A Review of Computational Fluid Dynamics (CFD) Techniques and Challenges

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Abstract

Multiphase flow phenomena underpin the performance of numerous energy technologies, including oil and gas production, nuclear reactors, thermal power systems, carbon capture processes, and emerging hydrogen energy applications. Computational fluid dynamics (CFD) has become an indispensable tool for investigating these complex flows by enabling detailed prediction of interfacial dynamics, phase interactions, heat and mass transfer, and transport behavior under diverse operating conditions. This review critically examines contemporary CFD techniques employed for multiphase flow simulation in energy systems, with emphasis on the strengths, limitations, and application domains of major modeling approaches. Eulerian–Eulerian and Eulerian–Lagrangian frameworks, interface-capturing methods such as the Volume of Fluid, Level Set, and Phase Field techniques, and emerging particle-based and Lattice Boltzmann methods are comparatively assessed. The review further discusses essential numerical modeling strategies, including turbulence modeling, interfacial force representation, mesh generation, discretization schemes, solver selection, convergence assessment, and model verification and validation. Recent applications across conventional and low-carbon energy systems are synthesized to illustrate the growing role of CFD in system design, performance optimization, and operational safety. Key challenges remain in accurately resolving complex interfaces, coupling multiscale and multiphysics phenomena, reducing computational cost, and improving predictive reliability through robust experimental validation and uncertainty quantification. Finally, emerging advances in artificial intelligence-assisted CFD, high-performance computing, physics-informed reduced-order models, and digital twin technologies are highlighted as promising directions for next-generation multiphase flow simulation. By integrating recent methodological developments with practical energy applications, this review provides a concise and comprehensive reference for researchers and engineers seeking to advance CFD-driven analysis and optimization of multiphase energy systems.

Keywords: Computational fluid dynamics (CFD), Multiphase flow simulation, Energy systems, Interface-capturing methods, Numerical modeling, and Digital twins

Introduction

Multiphase flows are integral to the operation of modern energy systems because they govern the transport of momentum, heat, and mass between interacting phases under complex thermofluid conditions. Such flows are encountered

in oil and gas production, nuclear reactor cooling, thermal power generation, carbon capture technologies, hydrogen production, and renewable energy systems, where their behavior directly influences process efficiency, operational safety, and equipment reliability (Yarahmadi *et al.*, 2025). Accurately predicting interfacial dynamics, phase interactions,

and transport phenomena remains a major engineering challenge due to the nonlinear nature of multiphase processes. Computational fluid dynamics (CFD) has consequently become an indispensable tool for investigating these phenomena by numerically resolving complex flow fields that are often difficult or impossible to characterize experimentally (Zhang *et al.*, 2025). Continuous improvements in computational algorithms and numerical methods have further strengthened the capability of CFD to simulate increasingly sophisticated multiphase systems relevant to both conventional and low-carbon energy technologies (Yarahmadi *et al.*, 2025).

The rapid evolution of CFD has led to the development of diverse numerical frameworks capable of representing different multiphase flow regimes with varying levels of accuracy and computational efficiency. Eulerian–Eulerian formulations are widely employed for dense multiphase systems because they efficiently model interactions between continuous and dispersed phases (Porombka and Schlottke, 2025), whereas Eulerian–Lagrangian approaches are particularly effective for tracking individual particles, droplets, and bubbles in dilute flows (Yarahmadi *et al.*, 2025). Interface-capturing methods, including the Volume of Fluid, Level Set, and Phase Field techniques, have significantly enhanced the prediction of moving interfaces, free-surface evolution, and phase transitions in complex engineering systems (Yarahmadi *et al.*, 2025). More recently, particle-based approaches and advanced computational strategies have expanded the capability of CFD to simulate multiphase flows involving thermochemical reactions and highly coupled transport processes, thereby improving its applicability to advanced energy technologies (Zhang *et al.*, 2025).

The increasing predictive capability of CFD has accelerated its adoption across a broad spectrum of energy applications. In oil and gas engineering, CFD has improved the design and optimization of separation devices such as hydrocyclones by accurately describing liquid–liquid flow behavior and separation efficiency (Oliveira *et al.*, 2025). In thermal and nuclear energy systems, advanced numerical models have enhanced the understanding of multiphase heat transfer, boiling, condensation, and two-phase transport processes that are essential for system performance and safety (Yarahmadi *et al.*, 2025). CFD has also been successfully applied to investigate two-phase separation in branching T-junctions relevant to industrial piping networks (Lu *et al.*, 2022) and ejector-based flow systems used in refrigeration and vacuum generation technologies (Sadeghiseraji *et al.*, 2024). Despite these advances, accurately resolving turbulent interfaces, multiphysics interactions, and multiscale transport processes while maintaining computational efficiency remains a persistent challenge, motivating continued methodological innovation and the integration of data-driven techniques such as physics-informed machine learning (Sharma *et al.*, 2023).

Although numerous review articles have examined specific aspects of multiphase CFD, the existing literature remains

fragmented. Recent reviews have focused on liquid–liquid hydrocyclone modeling (Oliveira *et al.*, 2025), thermochemical reactive multiphase simulations (Zhang *et al.*, 2025), Euler–Euler formulations for multi-regime flows (Porombka and Schlottke, 2025), multiphase heat transfer (Yarahmadi *et al.*, 2025), two-phase separation in branching T-junctions (Lu *et al.*, 2022), and ejector-based numerical simulations (Sadeghiseraji *et al.*, 2024). Likewise, emerging studies on physics-informed machine learning have primarily emphasized algorithmic development rather than its integration into multiphase CFD for energy applications (Sharma *et al.*, 2023). Consequently, there is a need for a comprehensive review that critically synthesizes contemporary CFD techniques, evaluates the numerical strategies underpinning their predictive capability, compares their applicability across diverse energy systems, and highlights the major computational challenges and emerging opportunities shaping future research.

The purpose of this review is to provide a comprehensive and critical synthesis of contemporary computational fluid dynamics techniques employed for multiphase flow simulation in energy systems. The review examines the principal numerical approaches used to model multiphase transport, including Eulerian–Eulerian, Eulerian–Lagrangian, interface-capturing, and particle-based methods, with emphasis on their underlying principles, strengths, limitations, and appropriate application domains. It further discusses the numerical modeling strategies that determine simulation accuracy, including turbulence modeling, interfacial force representation, mesh generation, discretization schemes, solver selection, convergence assessment, and verification and validation procedures. Representative applications in oil and gas systems, nuclear thermal hydraulics, renewable energy technologies, carbon capture processes, and hydrogen systems are synthesized to demonstrate the practical relevance of CFD in modern energy engineering. In addition, the review critically examines persistent challenges related to interface resolution, multiscale and multiphysics coupling, computational cost, scalability, and predictive uncertainty while highlighting emerging advances in artificial intelligence-assisted CFD, high-performance computing, physics-informed reduced-order modeling, and digital twin technologies. By integrating methodological developments with practical engineering applications, this review provides a coherent framework for understanding the current state of multiphase CFD and identifies future research directions that can support the development of more accurate, efficient, and reliable simulation tools for next-generation energy systems.

CFD Techniques for Multiphase Flow Simulation

Computational fluid dynamics (CFD) has evolved into a fundamental tool for simulating multiphase flows in energy systems by enabling detailed prediction of phase interactions, interface evolution, and coupled transport phenomena. Ongoing advances in numerical algorithms have led to the development of several modeling techniques, each offering

distinct capabilities depending on the flow regime, phase distribution, and computational requirements (Zhang *et al.*, 2025). Consequently, the choice of a CFD approach is governed by the complexity of the physical system, the desired level of accuracy, and the available computational resources (Yarahmadi *et al.*, 2025). The principal techniques include Eulerian–Eulerian and Eulerian–Lagrangian formulations, interface-capturing methods such as the Volume of Fluid (VOF), Level Set, and Phase Field models, as well as particle-based and Lattice Boltzmann methods. Each approach

possesses unique strengths and limitations in representing interfacial dynamics, dispersed phases, and multiphase transport processes, making them suitable for different energy applications (Ghannam *et al.*, 2025). The following subsections critically discuss these major CFD techniques, emphasizing their governing concepts, computational characteristics, and practical relevance to multiphase flow simulation in modern energy systems.

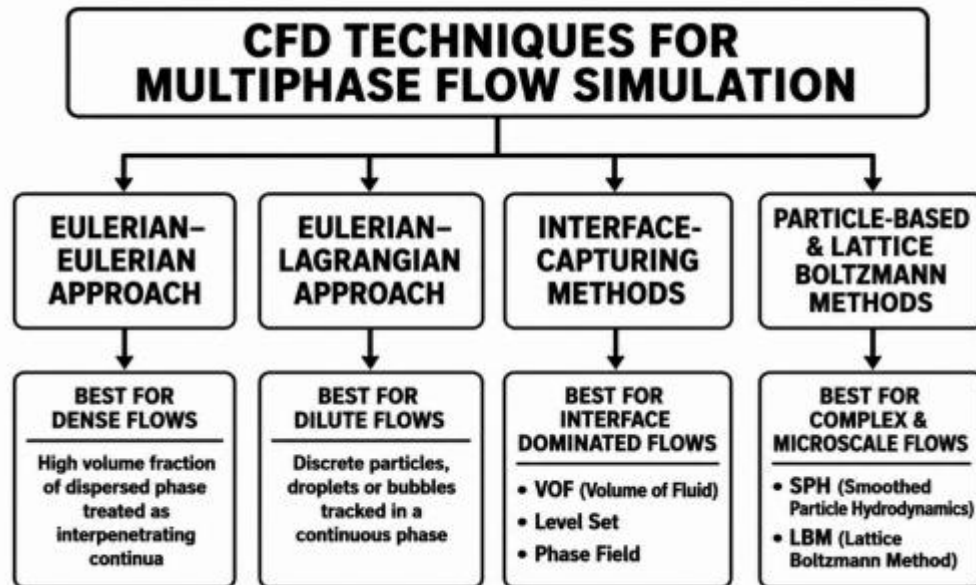


Figure 1. Classification of major CFD techniques for multiphase flow simulation. The figure classifies the principal CFD techniques for multiphase flow simulation based on their modeling principles and typical application domains in energy systems. Source: Modified from Ghannam *et al.* (2025)

Eulerian–Eulerian Approach

The Eulerian–Eulerian approach is a continuum-based computational fluid dynamics (CFD) technique in which all phases are treated as interpenetrating continua that simultaneously occupy the computational domain. Instead of tracking individual particles, droplets, or bubbles, each phase is represented by its own set of conservation equations for mass, momentum, and energy, while interactions between phases are described through interphase exchange models (Porombka and Schlottke, 2025). This formulation is particularly effective for simulating multiphase systems with high dispersed-phase concentrations, where tracking individual interfaces becomes computationally impractical (Zhang *et al.*, 2025). The method offers high computational

efficiency and can effectively represent complex interactions such as drag, lift, virtual mass, wall lubrication, and turbulent dispersion through appropriate closure models (Yarahmadi *et al.*, 2025). These capabilities have made the Eulerian–Eulerian framework widely applicable to gas–liquid, liquid–liquid, and gas–solid flows encountered in fluidized beds, hydrocyclones,

chemical reactors, pipelines, and thermal energy systems. Recent advances have further improved its ability to simulate multi-regime flows and thin liquid films, thereby enhancing prediction accuracy under realistic operating conditions (Porombka and Schlottke, 2025). In addition, the integration of lattice Boltzmann formulations with Eulerian–Eulerian Navier–Stokes equations has provided improved numerical stability and interface representation for complex multiphase simulations (Piredda and Asinari, 2025). Despite these advantages, the Eulerian–Eulerian approach is less effective in resolving sharp interfaces and tracking the motion of individual particles because all phases are treated as continuous media. Consequently, simulation accuracy depends heavily on the selection of constitutive equations and interphase closure models, particularly for highly transient or heterogeneous flows (Ghannam *et al.*, 2025). Nevertheless, its balance between computational efficiency and predictive capability continues to make it one of the most widely used CFD techniques for large-scale multiphase flow simulations in energy systems.

Eulerian–Lagrangian Approach

The Eulerian–Lagrangian approach combines continuum and particle-tracking formulations to simulate multiphase flows containing dispersed phases such as solid particles, liquid droplets, or gas bubbles. In this framework, the continuous phase is solved using the Eulerian formulation, whereas the dispersed phase is tracked individually using Lagrangian particle trajectories. The interaction between the two phases is represented through the exchange of momentum, heat, and mass, enabling detailed prediction of particle transport and dispersion (Yang *et al.*, 2024). This hybrid formulation is particularly suitable for dilute multiphase flows where individual particle behavior significantly influences the overall flow dynamics (Qian *et al.*, 2024). One of the major advantages of the Eulerian–Lagrangian approach is its ability to accurately capture particle trajectories, residence time, collision behavior, and particle–fluid interactions. These capabilities make it highly effective for investigating spray dynamics, pneumatic conveying, combustion systems, particle separation, and pollutant transport in energy-related processes (Yang *et al.*, 2024). The method also provides detailed information on localized transport phenomena that cannot be resolved by continuum-based models, making it valuable for optimizing process design and improving system performance (Ghannam *et al.*, 2025). Consequently, Eulerian–Lagrangian simulations have been widely adopted in process engineering and energy applications where dispersed-phase behavior governs heat and mass transfer. Despite its high predictive capability, the Eulerian–Lagrangian approach becomes computationally expensive as the number of dispersed particles increases because each particle must be tracked individually throughout the simulation domain. This limitation reduces its efficiency for dense multiphase systems, where continuum-based approaches are generally preferred (Ghannam *et al.*, 2025). In addition, simulation accuracy depends on appropriate models for particle collision, breakup, coalescence, and turbulence interactions, which may introduce additional uncertainties under complex flow conditions (Qian *et al.*, 2024). Nevertheless, the Eulerian–Lagrangian framework remains one of the most powerful CFD techniques for analyzing dilute multiphase flows that require detailed particle-scale resolution.

Interface-Capturing Methods (VOF, Level Set, Phase Field)

Interface-capturing methods are widely used in computational fluid dynamics (CFD) to simulate multiphase flows with distinct and deformable interfaces. Unlike Eulerian–Eulerian and Eulerian–Lagrangian formulations, these methods explicitly represent the interface separating different phases, enabling accurate prediction of interface evolution, deformation, breakup, coalescence, and surface tension effects (Li *et al.*, 2023). Consequently, they are particularly suitable for free-surface and immiscible multiphase flows encountered in energy systems, including bubble dynamics, liquid jets,

boiling, condensation, and fuel injection processes (Yarahmadi *et al.*, 2025). Among these techniques, the Volume of Fluid (VOF) method is the most widely adopted because it tracks the volume fraction of each phase within computational cells while ensuring excellent mass conservation. Its robustness and computational efficiency have made it the preferred approach for simulating large interface deformations and free-surface flows in industrial applications (Zhang *et al.*, 2025). The Level Set method, in contrast, represents the interface using a continuous signed-distance function, providing smoother interface reconstruction and more accurate curvature estimation. However, it is more susceptible to mass conservation errors and often requires reinitialization procedures to maintain interface accuracy (Li *et al.*, 2023). The Phase Field method describes the interface as a diffuse transition region governed by thermodynamic principles, making it particularly effective for modeling complex interface topologies, phase separation, and interfacial dynamics. Recent improvements, including conservative Allen–Cahn formulations, have significantly enhanced numerical stability and interface preservation during long-duration simulations (Aihara *et al.*, 2023). Although interface-capturing methods provide superior representation of moving interfaces, their computational cost generally increases with interface complexity and mesh refinement requirements. Accurate prediction also depends on the numerical treatment of surface tension, interface curvature, and discretization schemes, particularly in highly transient multiphase flows (Li *et al.*, 2023). Recent comparative studies have further demonstrated that coupling phase-field formulations with Lattice Boltzmann solvers improves interface resolution, numerical stability, and multiphase transport accuracy, thereby extending their applicability to complex engineering and energy systems (He *et al.*, 2024). Consequently, interface-capturing methods remain indispensable for CFD simulations where precise interface evolution is essential for reliable performance prediction.

Particle-Based and Lattice Boltzmann Methods

Particle-based and Lattice Boltzmann methods have emerged as powerful alternatives to conventional CFD techniques for simulating complex multiphase flows, particularly where interface dynamics, particle interactions, and microscale transport phenomena are difficult to resolve using continuum-based models. These approaches provide enhanced flexibility for modeling highly transient flows, irregular geometries, and multiphysics interactions, making them increasingly relevant to advanced energy applications (Ghannam *et al.*, 2025). Among particle-based techniques, Smoothed Particle Hydrodynamics (SPH) is the most widely applied mesh-free method. SPH represents fluids as discrete particles that move according to governing conservation laws, eliminating the need for computational meshes and allowing efficient simulation of large interface deformations, free-surface flows, fragmentation, and fluid–structure interactions (Pozorski and Olejnik, 2024). Owing to these advantages, SPH has been successfully applied to multiphase mixing, sloshing, impact

dynamics, and other complex engineering problems where conventional mesh-based methods may encounter numerical difficulties (Ghannam *et al.*, 2025). The Lattice Boltzmann Method (LBM) adopts a mesoscopic approach by describing fluid behavior through particle distribution functions rather than directly solving the Navier–Stokes equations. This formulation offers excellent numerical stability, efficient parallelization, and accurate representation of complex boundary conditions and interfacial phenomena (Piredda and Asinari, 2025). Recent developments in color-gradient LBM have significantly improved the simulation of immiscible multiphase flows in porous media by enhancing interface stability, viscosity treatment, and fluid acceleration modeling (Zahid and Cunningham, 2025). Likewise, coupling LBM with phase-field formulations has further improved interface

resolution and numerical accuracy for multiphase transport processes (He *et al.*, 2024). Despite their advantages, particle-based and Lattice Boltzmann methods generally require greater computational resources than conventional continuum-based approaches, particularly for large-scale industrial simulations. Their predictive performance is also influenced by model parameterization, numerical stability, and boundary condition implementation (Pozorski and Olejnik, 2024). Nevertheless, continued advances in high-performance computing and algorithm development are expanding their applicability, making these methods increasingly valuable for high-fidelity multiphase flow simulations in emerging energy systems.

Table 1. Comparison of major CFD techniques for multiphase flow simulation

Technique	Key features	Typical applications
Eulerian–Eulerian	Treats all phases as interpenetrating continua	Fluidized beds, reactors, hydrocyclones
Eulerian–Lagrangian	Tracks discrete particles within a continuous phase	Sprays, combustion, particle transport
Volume of Fluid (VOF)	Captures sharp moving interfaces with good mass conservation	Free-surface flows, boiling, condensation
Level Set	Represents interfaces using a signed-distance function	Bubble and droplet dynamics
Phase Field	Models interfaces as diffuse transition regions	Phase separation, microfluidics
Smoothed Particle Hydrodynamics (SPH)	Mesh-free particle-based simulation	Sloshing, impact, fluid–structure interaction
Lattice Boltzmann Method (LBM)	Mesoscopic approach for complex flows and geometries	Porous media, microscale and multiphase transport

Numerical Modeling Strategies

The accuracy and reliability of multiphase CFD simulations depend not only on the selected modeling technique but also on the numerical strategies adopted during model implementation. Appropriate turbulence and interfacial force models, mesh generation, numerical discretization, solver selection, and verification and validation procedures are essential for achieving stable, accurate, and computationally efficient solutions (Chen *et al.*, 2023; Yarahmadi *et al.*, 2025). Collectively, these strategies determine the predictive performance of CFD models and their applicability to complex multiphase flows in energy systems. The following subsections discuss the key numerical modeling strategies that underpin high-fidelity multiphase flow simulations.

Turbulence and Interfacial Force Modeling

Turbulence and interfacial force modeling are critical to the accuracy of multiphase CFD simulations because they govern momentum transfer, phase distribution, and interface evolution. Turbulence enhances mixing and transport

processes, whereas interfacial forces regulate the interactions between continuous and dispersed phases, thereby influencing overall flow behaviour (Ni, 2024). Consequently, appropriate modeling of these phenomena is essential for reliable prediction of multiphase flows in energy systems. Turbulence is commonly represented using Reynolds-Averaged Navier–Stokes (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS), with model selection depending on the required balance between computational efficiency and simulation accuracy. RANS models remain the preferred choice for most industrial applications due to their relatively low computational cost, whereas LES and DNS provide higher-fidelity predictions for complex turbulent flows but require substantially greater computational resources (Raje *et al.*, 2024). Interfacial interactions are typically described through drag, lift, virtual mass, wall lubrication, and turbulent dispersion forces, which are incorporated using appropriate closure models to improve prediction of phase transport and separation (Porombka and Schlottke, 2025). Recent studies have improved turbulence–interface coupling through advanced numerical formulations and refined interphase force models, resulting in more accurate predictions of bubble and droplet dynamics (Malikov *et al.*, 2024). Nevertheless, turbulence closure and interfacial force modeling remain

important sources of uncertainty in multiphase CFD, emphasizing the need for continued model development and validation to enhance predictive reliability across diverse energy applications (Ni, 2024).

Mesh Generation and Numerical Discretization

Mesh generation and numerical discretization are fundamental to the stability and accuracy of multiphase CFD simulations. The computational mesh defines the spatial resolution of the flow domain, while discretization schemes convert the governing conservation equations into algebraic forms that can be solved numerically. Appropriate mesh design is particularly important near phase interfaces, walls, and regions with steep velocity or pressure gradients, where inadequate resolution may lead to significant numerical errors (Yarahmadi *et al.*, 2025). Structured meshes generally provide higher numerical accuracy for simple geometries, whereas unstructured and hybrid meshes offer greater flexibility for complex engineering systems. Similarly, higher-order discretization schemes improve solution accuracy by reducing numerical diffusion and better preserving interface characteristics, although they often require additional computational effort (Muralha *et al.*, 2023). Consequently, mesh independence studies are routinely performed to ensure that simulation results are not influenced by mesh size or refinement level. Despite continuous advances in mesh generation techniques, achieving an optimal balance between computational cost and numerical accuracy remains a major challenge, particularly for transient and highly complex multiphase flows. Adaptive meshing and improved discretization strategies continue to enhance solution accuracy while reducing computational requirements, making them essential components of modern multiphase CFD modeling (Chen *et al.*, 2023).

Solver Selection and Convergence

Solver selection and convergence assessment play a crucial role in ensuring the stability, efficiency, and reliability of multiphase CFD simulations. Pressure-based solvers are commonly employed for incompressible and low-speed multiphase flows, whereas density-based solvers are generally preferred for highly compressible or high-speed flow applications. The choice of solver depends on the governing flow characteristics, numerical formulation, and desired level of computational accuracy (Muralha *et al.*, 2023).

Convergence is achieved when successive iterations produce negligible changes in residuals and key flow variables, indicating that a stable numerical solution has been obtained. In practice, convergence assessment should not rely solely on residual reduction but also consider the stability of physical quantities such as pressure drop, velocity, temperature, and phase volume fraction to ensure solution reliability (Chen *et al.*, 2023). Appropriate time-step selection, relaxation factors, and iterative control parameters further contribute to numerical stability and computational efficiency. Although advances in solver algorithms have improved the robustness of multiphase CFD simulations, convergence difficulties remain common in strongly coupled, transient, and interface-dominated flows. Careful solver selection, together with systematic convergence monitoring, therefore remains essential for obtaining accurate and physically meaningful simulation results (Arnold and Höhne, 2026).

Model Verification and Validation

Model verification and validation are essential for establishing the credibility and predictive reliability of multiphase CFD simulations. Verification determines whether the numerical model correctly solves the governing equations by assessing discretization errors, solver performance, and numerical consistency. Validation, in contrast, evaluates the accuracy of simulation results by comparing numerical predictions with experimental measurements or benchmark data (Chen *et al.*, 2023). Verification procedures commonly include mesh independence studies, time-step sensitivity analyses, and residual convergence assessments to ensure that numerical errors are minimized (Muralha *et al.*, 2023). Validation further confirms the capability of a CFD model to reproduce key physical parameters, such as velocity, pressure, temperature, and phase distribution, under realistic operating conditions (Kjeldsberg *et al.*, 2023). Recent studies have also demonstrated the importance of validating turbulence and interfacial force models to improve predictive accuracy in complex multiphase flows (Malikov *et al.*, 2024; Arnold and Höhne, 2026). Rigorous verification and validation enhance confidence in simulation outcomes and support the application of CFD as a reliable tool for the design, optimization, and safety assessment of multiphase energy systems. Consequently, they remain indispensable components of high-quality numerical modeling workflows.

Table 2. Summary of numerical modeling strategies in multiphase CFD

Strategy	Purpose	Outcome
Turbulence and interfacial force modeling	Represents turbulent flow and phase interactions	Improved prediction of multiphase flow behaviour
Mesh generation and numerical discretization	Defines spatial resolution and numerical accuracy	Reduced numerical errors and stable solution
Solver selection and convergence	Controls solution stability and computational efficiency	Reliable and converged CFD results
Model verification and validation	Assesses numerical correctness and physical accuracy	Increased confidence in simulation predictions

Applications in Energy Systems

Multiphase CFD has become an indispensable tool for analyzing complex fluid interactions across diverse energy systems. Its ability to predict phase distribution, heat and mass transfer, and interfacial dynamics supports the design, optimization, and safe operation of energy processes. From conventional oil and gas production to nuclear thermal

hydraulics, renewable energy technologies, and emerging carbon capture and hydrogen systems, multiphase CFD provides valuable insights that improve operational efficiency, system reliability, and sustainability. The following subsections highlight the major application areas and recent advances in the use of multiphase CFD across the energy sector.

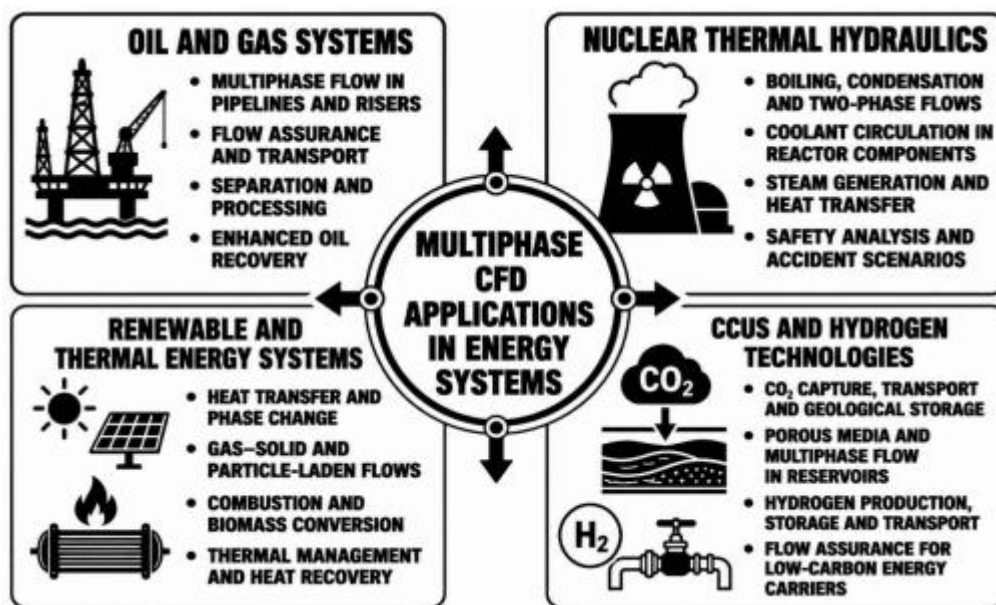


Figure 2. Major applications of multiphase CFD in energy systems. The figure summarizes the principal application domains of multiphase CFD in energy systems, highlighting its role in predicting complex flow behaviour, heat transfer, phase interactions, and transport phenomena to improve system performance, operational safety, and process optimization. Source: Modified from [Wu et al. \(2024\)](#)

Oil and Gas Systems

Multiphase flow is ubiquitous in oil and gas production, where the simultaneous transport of oil, gas, water, and solid particles significantly influences production efficiency, equipment integrity, and operational safety. Computational fluid dynamics (CFD) has become an indispensable tool for analysing these complex flow behaviours because it provides detailed insights into phase interactions that are often difficult

to obtain experimentally ([Zhang et al., 2025](#)). Consequently, multiphase CFD is widely employed to optimize production systems, improve flow assurance, and enhance hydrocarbon recovery. One of the major applications of multiphase CFD is the prediction of pressure drop, liquid holdup, slug formation, and phase separation in pipelines and processing facilities. Accurate simulation of these phenomena supports the design of separators, risers, and transport pipelines while minimizing operational risks associated with hydrate formation, wax deposition, sand production, and pipeline blockage ([Mahmoud et al., 2026](#)). Recent advances in AI-assisted CFD and high-

fidelity multiphase models have further improved the prediction of transient flow behaviour and complex fluid interactions under varying operating conditions ([Zhang et al., 2025](#)). Beyond conventional hydrocarbon production, multiphase CFD has become increasingly important in the energy transition. It is now applied to the transport of hydrogen, carbon dioxide, and ammonia, where reliable prediction of multiphase flow behaviour is essential for ensuring flow assurance, infrastructure integrity, and process safety ([Mahmoud et al., 2026](#)). Despite these advances, uncertainties associated with turbulence modeling, interfacial force prediction, and large-scale transient simulations remain important challenges, emphasizing the need for continued improvements in numerical models and computational efficiency ([Yarahmadi et al., 2026](#)).

Nuclear Thermal Hydraulics

Multiphase CFD has become an essential tool in nuclear thermal hydraulics, where accurate prediction of boiling, condensation, bubble transport, and two-phase coolant flow is critical to reactor performance and safety. Compared with

experimental investigations, CFD provides detailed visualization of complex flow phenomena under operating conditions that are often difficult to reproduce, thereby supporting reactor design, safety analysis, and performance optimization (Wu *et al.*, 2024). Current applications include the simulation of coolant circulation, critical heat flux, steam generation, and two-phase flow in reactor cores, steam generators, and cooling channels. Advanced Eulerian–Eulerian formulations and interface-capturing methods have significantly improved the prediction of interfacial dynamics, heat transfer, and phase distribution, enabling more realistic representation of nuclear thermal–hydraulic processes (Frederix, 2026). These advances contribute to improved assessment of reactor efficiency, operational stability, and accident scenarios under both normal and transient conditions (Wu *et al.*, 2024). Despite substantial progress, reliable simulation of nuclear multiphase flows remains challenging because of the strong coupling between turbulence, heat transfer, and interfacial phenomena. Consequently, ongoing research focuses on improving closure models, enhancing numerical accuracy, and strengthening model validation to increase the predictive capability of multiphase CFD for next-generation nuclear energy systems (Frederix, 2026; Yarahmadi *et al.*, 2026).

Renewable and Thermal Energy Systems

Multiphase CFD plays a vital role in the design and optimization of renewable and thermal energy systems by providing detailed analysis of fluid flow, heat transfer, and phase-change processes. It is extensively applied to solar thermal collectors, biomass combustion, geothermal systems, heat exchangers, and energy storage technologies, where multiphase interactions strongly influence system efficiency and thermal performance (Yarahmadi *et al.*, 2026). In renewable energy applications, CFD facilitates the simulation of boiling, condensation, particle transport, and gas–solid interactions, enabling improved prediction of heat transfer characteristics and optimization of operating conditions. Recent advances in high-fidelity multiphase models and AI-assisted CFD have further enhanced the accuracy of simulations involving thermochemical reactions and complex heat transfer processes, supporting the development of more efficient and sustainable energy technologies (Zhang *et al.*, 2025). In addition, CFD has become an important tool for improving thermal management and heat recovery in green hydrogen production systems, thereby contributing to enhanced energy efficiency and reduced operational losses (Cheng *et al.*, 2024). Although significant progress has been achieved, accurately modeling coupled heat transfer, turbulence, and phase interactions under transient operating conditions remains challenging. Continued improvements in numerical methods and computational efficiency are therefore

essential for expanding the application of multiphase CFD in next-generation renewable and thermal energy systems (Yarahmadi *et al.*, 2026).

Carbon Capture, Utilization, Storage (CCUS), and Hydrogen Technologies

Multiphase CFD has become increasingly important in the development of carbon capture, utilization, and storage (CCUS) and hydrogen technologies, where accurate prediction of multiphase transport is essential for process efficiency, infrastructure integrity, and operational safety. These technologies involve complex gas–liquid and gas–solid interactions during CO₂ capture, pipeline transport, geological storage, and hydrogen production, storage, and distribution (Liu *et al.*, 2025). CFD is widely applied to simulate CO₂ injection into geological formations, multiphase flow in porous media, and thermal–hydro–mechanical–chemical interactions that influence long-term storage security. These simulations improve understanding of fluid migration, pressure evolution, and trapping mechanisms, thereby supporting safer and more efficient carbon storage strategies (Liu *et al.*, 2025). Similarly, multiphase CFD has become an important tool for optimizing hydrogen production, thermal management, and transport systems, where accurate prediction of heat transfer and phase behaviour enhances system performance and energy efficiency (Cheng *et al.*, 2024). With the growing integration of low-carbon technologies, CFD is also being used to address flow assurance challenges associated with hydrogen, carbon dioxide, and ammonia transport. Recent advances in AI-assisted multiphase modeling have further strengthened the capability of CFD to predict complex transport phenomena and support the design of reliable energy infrastructure (Zhang *et al.*, 2025; Mahmoud *et al.*, 2026). Nevertheless, continued improvements in multiphysics coupling, numerical accuracy, and large-scale validation remain essential for the wider deployment of CCUS and hydrogen technologies.

Current Challenges in Multiphase CFD Simulation

Despite significant advances in numerical methods and computational capabilities, several challenges continue to limit the predictive accuracy and industrial applicability of multiphase CFD. Complex interface dynamics, multiscale interactions, high computational demands, and the need for rigorous experimental validation remain major barriers to reliable simulations across diverse energy systems. The following subsections discuss these key challenges and their implications for future model development.

Table 3. Contributions of multiphase CFD to energy systems

Energy system	Key multiphase phenomena	CFD contribution
Oil and gas	Gas–liquid–solid flow, slugging, separation	Optimizes flow assurance, equipment design, and production efficiency
Nuclear thermal hydraulics	Boiling, condensation, two-phase coolant flow	Improves reactor safety, cooling performance, and thermal analysis
Renewable and thermal energy	Heat transfer, phase change, particle transport	Enhances energy conversion, thermal management, and system efficiency
CCUS and hydrogen technologies	CO ₂ injection, porous media flow, hydrogen transport	Supports carbon storage, hydrogen infrastructure and process optimisation

Modified from [Wu et al. \(2024\)](#) and [Zhang et al. \(2025\)](#)

Interface Resolution and Phase-Change Prediction

Accurate resolution of fluid interfaces remains one of the most persistent challenges in multiphase CFD, particularly for flows involving bubble dynamics, droplet breakup, coalescence, boiling, and condensation. Although interface-capturing methods such as the Volume-of-Fluid, Level Set, and Phase-Field approaches have substantially improved interface representation, numerical diffusion and difficulties in preserving interface sharpness continue to affect prediction accuracy ([Li et al., 2023](#); [Kind et al., 2025](#)). These limitations become more pronounced when phase change is coupled with complex heat and mass transfer processes. Recent developments have integrated high-fidelity numerical formulations and AI-assisted modeling to improve interface tracking and phase-change prediction under complex operating conditions ([Zhang et al., 2025](#)). Nevertheless, achieving stable and accurate simulations across a wide range of flow regimes remains challenging, highlighting the need for more robust interface reconstruction algorithms and improved multiphysics coupling strategies ([Wang et al., 2023](#); [Yarahmadi et al., 2026](#)).

Multiscale and Multiphysics Coupling

Multiphase flows in energy systems involve the simultaneous interaction of fluid flow, heat transfer, mass transfer, chemical reactions, and phase transformation across multiple spatial and

temporal scales. Accurately coupling these processes remains a major challenge because the governing physical phenomena often exhibit different characteristic scales and require diverse numerical treatments ([Chew et al., 2026](#)). Consequently, simplifying assumptions are frequently introduced, which may compromise model fidelity under complex operating conditions. Recent advances in high-performance computing, hybrid numerical frameworks, and AI-assisted CFD have improved the integration of multiscale and multiphysics models, enabling more realistic simulation of coupled transport phenomena ([Zhang et al., 2025](#)). However, achieving

stable and computationally efficient coupling without sacrificing predictive accuracy remains an active area of research, particularly for highly transient and thermochemically reactive multiphase flows ([Yarahmadi et al., 2026](#)).

Computational Cost and Scalability

Multiphase CFD simulations are computationally demanding because they require the simultaneous solution of coupled governing equations while resolving complex interface dynamics and transient flow behaviour. The computational burden increases further with fine mesh resolution, advanced turbulence models, and high-fidelity interface-capturing techniques, limiting the application of detailed simulations to large-scale energy systems ([Yarahmadi et al., 2026](#)). Recent developments in parallel computing, adaptive mesh refinement, and AI-assisted CFD have improved computational efficiency and scalability, enabling faster simulations without substantially compromising accuracy ([Zhang et al., 2025](#)). Nevertheless, balancing computational cost with predictive fidelity remains a significant challenge, particularly for industrial-scale multiphase flows involving complex geometries and multiscale physical processes ([Chew et al., 2026](#)).

Experimental Validation and Uncertainty Quantification

Experimental validation and uncertainty quantification are essential for establishing the credibility and predictive capability of multiphase CFD models. Validation against high-quality experimental data ensures that numerical simulations accurately represent complex flow behaviour, while uncertainty quantification evaluates the influence of modeling assumptions, numerical errors, and input variability on simulation outcomes ([Shi et al., 2025](#)). However, obtaining reliable experimental data for complex multiphase flows remains difficult because of the challenges associated with measuring interfacial phenomena and transient flow characteristics ([Yarahmadi et al., 2026](#)). Recent advances in experimental diagnostics, benchmark databases, and data-driven techniques have strengthened model validation and improved confidence in CFD predictions ([Chen et al., 2023](#)). Nevertheless, standardized validation procedures and robust

uncertainty assessment frameworks are still needed to enhance the reliability and industrial adoption of multiphase CFD across diverse energy applications (Wang *et al.*, 2023; Zhang *et al.*, 2025).

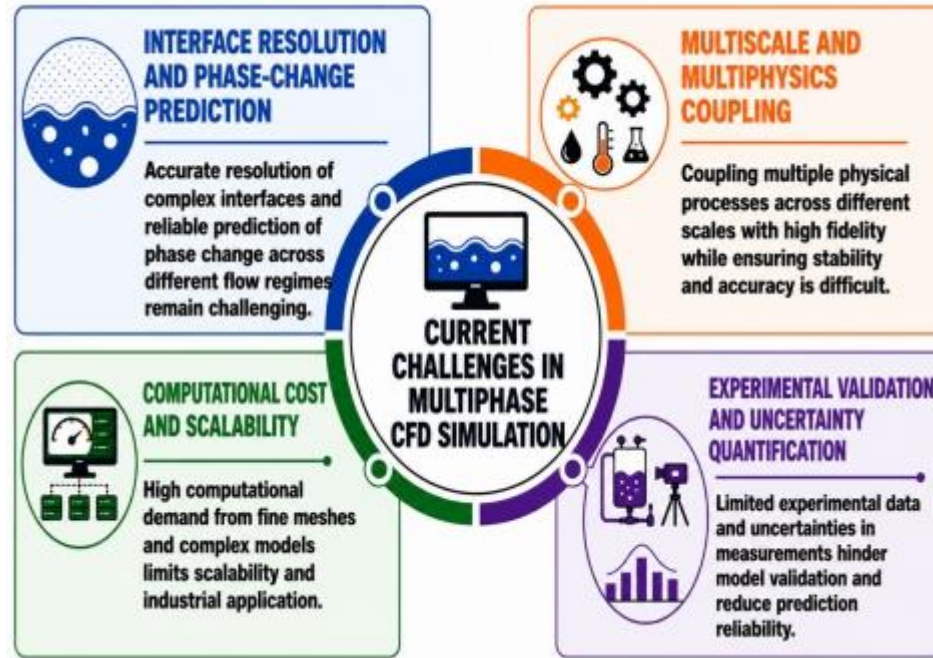


Figure 3. Current challenges in multiphase CFD simulation for energy systems. The figure summarizes the principal challenges that limit the predictive accuracy, computational efficiency, and industrial applicability of multiphase CFD in energy systems. Source: Modified from Yarahmadi *et al.* (2026)

Future Perspectives

The future of multiphase CFD lies in the convergence of artificial intelligence (AI), high-performance computing (HPC), physics-informed modeling, reduced-order techniques, and digital twin technologies. AI-assisted CFD is increasingly being adopted to automate mesh generation, optimize numerical solvers, improve turbulence closure, and develop surrogate models that significantly reduce computational time while maintaining predictive accuracy (Wang *et al.*, 2024). The integration of AI with conventional CFD is also facilitating rapid design optimization and real-time analysis for increasingly complex energy systems (Zhang *et al.*, 2025). Physics-informed neural networks and reduced-order models are expected to play a transformative role in next-generation multiphase simulations. By embedding governing physical laws into machine learning frameworks, physics-informed models improve robustness, reduce dependence on large datasets, and enhance the prediction of complex nonlinear flow phenomena (Luo *et al.*, 2025). Similarly, intrusive and

non-intrusive reduced-order modeling techniques provide computationally efficient alternatives for representing high-dimensional multiphase flows while preserving essential physical characteristics, making them attractive for uncertainty analysis, optimization, and real-time applications (Padula *et*

al., 2024; Wu *et al.*, 2026). Continued advances in HPC will further enable large-scale, high-fidelity simulations involving multiscale and multiphysics interactions, thereby extending the applicability of multiphase CFD to industrial-scale energy systems. Coupling these capabilities with digital twin platforms offers significant opportunities for real-time process monitoring, predictive maintenance, and operational optimization using continuously updated simulation models (Efa and Ifa, 2025). Future research should therefore prioritize the development of interpretable AI-CFD frameworks, scalable computing strategies, standardized validation protocols, and reliable digital twin architectures to accelerate the deployment of accurate, efficient, and intelligent multiphase simulations across conventional and emerging energy technologies (Liu *et al.*, 2025; Yarahmadi *et al.*, 2026).

Conclusion

Multiphase CFD has become an indispensable tool for understanding and optimizing complex flow phenomena across modern energy systems. Continuous advancements in numerical techniques, turbulence modeling, interface-capturing methods, and computational strategies have significantly improved the accuracy and applicability of multiphase simulations in conventional and emerging energy technologies. Despite these achievements, challenges related to interface resolution, multiscale coupling, computational

efficiency, and model validation continue to limit predictive capability under highly complex operating conditions. Emerging developments in artificial intelligence, high-performance computing, reduced-order modeling, and digital twin technologies offer promising pathways to overcome these limitations and enable more reliable, efficient, and real-time simulations. Continued integration of advanced computational methods with robust physical modeling and experimental validation will be essential for developing next-generation multiphase CFD frameworks that support sustainable, safe, and high-performance energy systems.

Authors' Contributions

The authors of this research have significantly contributed to the study's conception, data collection, and manuscript development. All authors were involved in writing the manuscript or critically reviewing it for its intellectual value. They have reviewed and approved the final version for submission and publication and accepted full responsibility for the content and integrity of the work.

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Conflict of Interest

The authors declared that there are no conflicts of interest.

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