

Simulation of multiphase flow with thermochemical reactions: A review of computational fluid dynamics (CFD) theory to AI integration

Dongkuan Zhang ^{a,b}, Tanzila Anjum ^a , Zhiqiang Chu ^c, Jeffrey S. Cross ^{b,*}, Guozhao Ji ^{a,**} 

^a Key Laboratory of Industrial Ecology and Environmental Engineering, School of Environmental Science & Technology, Dalian University of Technology, Dalian, 116024, China

^b Department of Transdisciplinary Science and Engineering, School of Environment and Society, Institute of Science Tokyo, 2-12-1, O-okayama, Meguro-ku, Tokyo, 152-8550, Japan

^c Fuxin Huanfa Waste Disposal Co., Ltd, Fuxin, 123000, China



ARTICLE INFO

Keywords:

Computational fluid dynamics(CFD)
Artificial intelligence(AI)
Surrogate modeling
Machine learning
Multiphase flow

ABSTRACT

This review explores the integration of Computational Fluid Dynamics (CFD) and Artificial Intelligence (AI) in the modeling of multiphase flows and thermochemical systems, which have the characteristics of nonlinear interactions, complex geometries, and high computational costs. These systems, found in diverse applications such as chemical reactors, energy production, and environmental modeling, present significant challenges in accurately simulating dynamic fluid behaviors. Traditional CFD approaches, while mathematically rigorous, often struggle with convergence efficiency, mesh sensitivity, and physical boundary constraints in high-dimensional or reactive flow environments. Recent developments in machine learning (ML), particularly deep learning (DL) and physics-informed neural networks (PINNs), have catalyzed a paradigm shift in fluid dynamics modeling. Data-driven models now enable real-time inference, surrogate modeling, and multiscale learning, surpassing the conventional limitations of CFD solvers. These techniques leverage vast datasets, often generated by simulations or experiments, to develop models capable of making accurate predictions without the need for extensive computational resources. Frameworks such as neural operators and hybrid physical-statistical models offer not only improved scalability but also enhanced robustness across diverse flow regimes, from turbulent flows to complex reactive systems. Despite this promise, AI-enhanced CFD still faces key challenges. Many AI models depend heavily on empirical data rather than physics-based simulations, limiting their generalizability and physical consistency. Inverse modeling techniques, such as reinforcement learning, remain in their early stages, reducing their effectiveness for parameter optimization in heat transfer and fluid flow. Additionally, AI models often struggle to generalize across unfamiliar flow regimes—such as transitions from laminar to turbulent or reactive flows—restricting their broader applicability. These challenges highlight the need for more robust and interpretable AI-CFD frameworks. Nonetheless, promising results have been achieved. For instance, PINNs applied to the lid-driven cavity flow problem demonstrated a maximum mean squared error of 7.38×10^{-4} in the horizontal and 5.99×10^{-4} in the vertical direction compared to OpenFOAM solutions. Furthermore, inference cost scales linearly with grid resolution, and computational speed exceeds that of traditional solvers by factors ranging from 12 to 626, showcasing substantial gains in efficiency, scalability, and accuracy. The integration of AI into CFD holds the potential to revolutionize simulation capabilities, opening new frontiers for industrial applications and scientific research involving complex fluid systems.

Abbreviation

AI	Full Term Artificial Intelligence
----	--------------------------------------

(continued on next column)

(continued)

AMR	Adaptive Mesh Refinement
ANSYS	ANSYS
BDF	Backward Differentiation Formula

(continued on next page)

* Corresponding author.

** Corresponding author.

E-mail addresses: cross.j.aa@m.titech.ac.jp (J.S. Cross), guozhaoji@dlut.edu.cn (G. Ji).

(continued)

CFD	Computational Fluid Dynamics
CFDEM	Computational Fluid Dynamics - Discrete Element Method
CFL	Courant–Friedrichs–Lowy
CO	Carbon Monoxide
CP	Control Point
CPFD	Computational Particle Fluid Dynamics
CPU	Central Processing Unit
DEM	Discrete Element Method
DES	Detached Eddy Simulation
DL	Deep Learning
DNS	Direct Numerical Simulation
DPM	Discrete Phase Model
EDQNM	Eddy Damped Quasi-Normal Markovian Approximation
EMMS	Energy Minimization Multi-Scale
ENO	Essentially Non-Oscillatory
FDM	Finite Difference Method
FEM	Finite Element Method
FGM	Flamelet Generated Manifold
FNO	Fourier Neural Operator
FVM	Finite Volume Method
GAN	Generative Adversarial Network
GPR	Gaussian Process Regression
GPU	Graphics Processing Unit
JS	Jensen-Shannon (Divergence)
LBM	Lattice Boltzmann Method
LES	Large Eddy Simulation
LHS	Latin Hypercube Sampling
LSTM	Long Short-Term Memory
MIX	MIX + GAN (Mixture Generative Adversarial Networks)
ML	Machine Learning
MP	Multiprocessing
MPI	Message Passing Interface
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PDF	Probability Density Function
PIC	Particle-in-Cell (Method)
PIML	Physics-Informed Machine Learning
PINN	Physics-Informed Neural Networks
PINO	Physics-Informed Neural Operators
PISO	Pressure Implicit with Splitting of Operators
PR	Pressure
QHD	Quasi-Hydrodynamic
RANS	Reynolds-Averaged Navier-Stokes
RBDO	Reliability-Based Design Optimization
RL	Reinforcement Learning
RSM	Reynolds Stress Model
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
SVM	Support Vector Machine
TFM	Two-Fluid Model
TVD	Total Variation Diminishing
UQ	Uncertainty Quantification
VOF	Volume-of-Fluid
WENO	Weighted Essentially Non-Oscillatory
WMLES	Wall-Modeled Large Eddy Simulation

Symbols in
equations

Symbol	Meaning	Unit
$\frac{\partial U}{\partial y}$	velocity gradient	1/s
l_m	mixing length	m
C_{w1}	Model constant	
P_k	Production of k due to shear	m^2/s^3
\tilde{v}	Modified turbulent kinematic viscosity	m^2/s
C_{b1}, C_{b2}	Model constants	
f_{t2}	Transition-related damping function	
\tilde{S}	Modified vorticity magnitude	1/s
$f_w(\frac{\tilde{v}}{d})$	Wall damping function	
d	Distance to the nearest wall	m
C_{1e}, C_{2e}	Model constants	
C_μ	Model constant for ν_t	
ν	Laminar kinematic viscosity	m^2/s
U_j	Velocity in direction j	m/s
x_j	Spatial coordinate in direction j	m
P_k	Production of turbulent kinetic energy	m^2/s^3
σ_k, σ_ω	Turbulent Prandtl numbers	
β^*, β, α	Model constants	

(continued on next column)

(continued)

σ_k, σ_ω	Turbulent Prandtl numbers	
ω^2	Specific dissipation squared	$1/s^2$
$\frac{\omega}{k} P_k$	Production of ω	$1/s^2$
ν_t	Turbulent viscosity	m^2/s
a_1	Model constant	
ω	Specific dissipation rate	1/s
SP_2	Strain rate-related limiter function	1/s
α_k	Volume fraction of phase k	
ρ_k	Density of phase k	kg/m^3
\tilde{v}_k	Velocity of phase k	m/s
t	Time	s
p	Pressure	Pa
τ_k	Stress tensor of phase k	Pa
\vec{g}	Gravitational acceleration	m/s^2
\vec{F}_{int}	Internal force between phases	N
C_d	Drag coefficient	
ρ_f	Density of the fluid	kg/m^3
A_p	Cross-sectional area of particle	m^2
\vec{u}_f	Fluid velocity	m/s
\vec{u}_p	Particle velocity	m/s
C_d	Drag coefficient	
Re_p	Particle Reynolds number	
e_f	Fluid phase volume fraction	
μ	Dynamic viscosity	Pa·s
τ_{ij}	Stress tensor	Pa
u_i, u_j	Velocity components	m/s
δ_{ij}	Kronecker delta	
$\nabla \cdot$	Divergence operator	
R_{ij}	Reynolds stress tensor	Pa
$u'_i u'_j$	Fluctuating velocity components	m/s
μ_t	Turbulent viscosity	m^2/s
S_{ij}	Strain rate tensor	1/s
ρ	Density	kg/m^3
Y_i	Mass fraction of species i	
v	Velocity vector	m/s
J_i	Diffusion flux of species i	$kg/(m^2·s)$
R_i	Source term for species i	$kg/(m^3·s)$
A	Pre-exponential factor	
E_a	Activation energy	J/mol
R	Universal gas constant	J/(mol·K)
T	Temperature	K
ν	Kinematic viscosity	m^2/s
Y_R, Y_O, Y_P	Mass fractions of reactants, oxygen, and products	
B	Constant	
ϵ	Turbulent dissipation rate	m^2/s^3
k	Turbulent kinetic energy	m^2/s^2
a, c	Stoichiometric coefficients	
$[A], [C]$	Concentration of species A and C	mol/m ³

1. Introduction

Multiphase flows involve the interaction of different phases of matter, such as liquids, gases, and solids, within a single system [1,2]. Thermochemical reactions encompass chemical transformations, heat, and mass transfer processes [3,4]. The interplay between these phenomena is fundamental to numerous engineering applications, particularly in energy conversion, chemical manufacturing, and environmental systems [5,6]. Computational Fluid Dynamics (CFD) has become a powerful tool for simulating complex, heterogeneous systems, offering detailed insights into key physical fields. CFD simulates combustion, gasification, and multiphase flows in biomass reactors [7], electrolyzers [8], solar thermal systems [9–12], and carbon capture processes by modeling complex fluid dynamics, heat transfer, and chemical reactions, thereby aiding in their design and optimization. [1,2,13]. These insights are essential for optimizing reactor design, enhancing operational performance, and guiding process intensification strategies.

However, as the urgency of transitioning to low-carbon and sustainable energy systems intensifies, traditional CFD alone faces increasing limitations in addressing the nonlinear, dynamic, and

coupled behaviors present in renewable energy devices, such as biomass combustors [14], electrolyzers [15], solar receivers [5,10,16–18], and carbon capture systems [19,20]. These systems often operate under variable and uncertain conditions, where high-resolution simulation is needed to optimize efficiency, minimize emissions, and ensure safety. As shown in Fig. 1, integrating AI into CFD offers a transformative opportunity to accelerate these simulations, enable real-time control, and improve the scalability of optimization frameworks. By leveraging data-driven models trained on experimental and high-fidelity simulation data, researchers can achieve accurate predictions even in previously uncharted parameter spaces—essential for guiding the design and operation of next-generation sustainable energy infrastructure.

Simulating reactive multiphase flows is one of the most challenging tasks in CFD. It requires resolving chemical stiffness, multiscale turbulent structures, and complex interfacial dynamics [21,22]. As dictated by Arrhenius kinetics, the exponential dependence of reaction rates on temperature imposes minimal time step requirements for numerical integration [23,24]. Simultaneously, the wide range of turbulence length scales—from millimeters to microns—demands excellent spatial resolution. Furthermore, interfacial phenomena such as breakup, coalescence, and phase change in gas–liquid, gas–solid, or liquid–solid systems introduce additional nonlinear transport complexities. Coupling these three aspects within a unified simulation framework makes it exceedingly difficult to maintain physical fidelity while keeping computational costs within practical limits—an ongoing core challenge in high-fidelity CFD [25–28].

During the 1970s–1990s, engineering applications predominantly relied on RANS (Reynolds-averaged Navier–Stokes) models coupled with eddy dissipation concepts or $k-\epsilon$ turbulence models, often combined with single- or two-step global reaction mechanisms [29,30]. These approaches treated turbulent mixing as the rate-limiting step of combustion, thereby significantly relaxing chemical stiffness and allowing simulations to run on relatively coarse meshes. However, this came at the cost of losing detailed information on intermediate species such as NOx and CO, and failing to capture the influence of transient eddy structures on local reaction rates [31,32].

By the early 2000s, advancements in LES (Large Eddy Simulation) and DNS (Direct Numerical Simulation) enabled researchers to incorporate detailed chemical kinetics, such as Zeldovich NOx formation, Soret diffusion, and multispecies transport, on highly refined meshes [33–40]. In parallel, interface-capturing techniques like Volume-of-Fluid (VOF), Level-Set, Discrete Element Method (DEM), and Discrete Phase Model (DPM) were employed to track dynamic phase boundaries explicitly [27,41–43]. While this period saw significant improvements in grid and temporal resolution, the fundamental breakthrough was the transition from brute-force refinement toward more structured and efficient modeling architectures—integrating hybrid closure models, precomputed chemical manifolds, and scalable parallel algorithms [44,45].

Today, the mainstream strategy no longer focuses solely on refining meshes or shrinking time steps. Instead, it emphasizes co-optimization across spatial resolution, chemical simplification, numerical methods, and parallel execution [46–48]. Hybrid RANS–LES frameworks apply RANS modeling in near-wall regions for efficiency, reserving LES to resolve large-scale turbulence in the core flow [49,50]. Concurrently, reduced-order chemistry techniques—such as the Flamelet Generated Manifold (FGM), multidimensional intrinsic coordinate tabulation—transform high-dimensional reaction kinetics into low-dimensional look-up tables, replacing stiff integration with efficient interpolation [51–57]. In multiphase flows, combinations of Eulerian–Lagrangian PDF methods and interface-tracking algorithms enable high-fidelity descriptions of droplet evaporation, bubble collapse, and interfacial transport [31,58–61]. Operator splitting approaches further decouple fluid dynamics, chemical reactions, and heat/mass transfer into independently solvable steps [62,63]. Adaptive mesh refinement (AMR) and dynamic time stepping respond to local error estimates, while GPU acceleration and in-situ data analysis greatly enhance feasibility for large-scale industrial problems [63–65]. Overall, the evolution of reactive multiphase flow modeling reflects not merely a push for higher mathematical resolution but a shift toward architectural innovation that balances computational feasibility with physical accuracy.

Traditional CFD methods face challenges handling complex multiphase flow systems due to high computational demands, slow convergence, and instability, especially as reactor scales increase. Researchers have introduced machine learning (ML) techniques, starting with simple models like artificial neural networks (ANNs) for small-scale problems, such as flow field prediction and turbulence model optimization [66–68]. Later, regression models like support vector machine (SVM) and Kriging partially replaced CFD calculations, reducing time costs but remaining limited for complex flows [69]. Advances in deep learning, including convolutional neural networks (CNNs) and recurrent neural networks (RNNs), enabled more sophisticated applications like turbulence reconstruction [70–72]. Physics-informed neural networks (PINNs) further integrated physical laws into ML, improving accuracy and reducing reliance on data for tasks like turbulence and chemical reaction simulation [73–75]. Supported by graphics processing units (GPUs) and distributed computing, AI is now advancing towards real-time predictions for large-scale fluid systems [76].

Existing reviews on CFD application mainly focus on CFD models' accuracy and stability [77]. Reviews on AI in this area typically concentrate on its application in optimizing fluid dynamics and reaction modeling [78–80]. While these studies provide valuable insights into the respective fields, they lack a systematic discussion on the CFD and AI. A comprehensive and in-depth review exploring the potential and future development of CFD and AI integration in multiphase flow thermochemical reactions is of significant academic and practical importance. This review summarizes research on the numerical simulation of multiphase flow and thermochemical reactions in the past decade, focusing on the last five years, and delves into the integration of CFD with AI in this field. It aims to provide theoretical support for optimizing and simulating complex physicochemical processes in energy, chemical, and environmental engineering. It also offers new methodologies for efficient industrial process design and operational parameter optimization.

2. CFD theory and solving techniques

2.1. Fundamentals and computational challenges in CFD simulation

While experimental techniques and analytical modeling remain valuable in fluid dynamics research, CFD has emerged as a critical approach for investigating complex flow phenomena—particularly when traditional methods are limited by scale, precision, or feasibility. Compared to these alternatives, CFD offers superior flexibility and resolution, making it especially effective for simulating multi-scale, non-

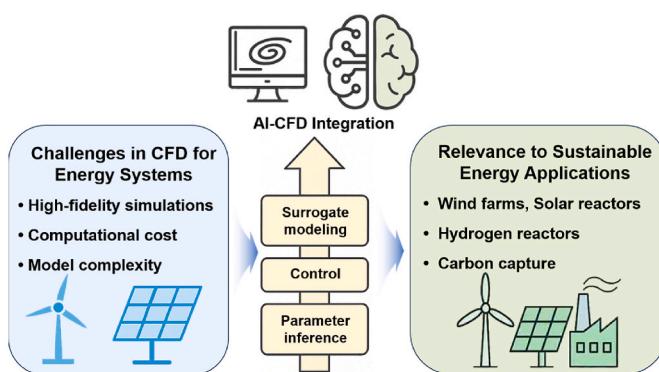


Fig. 1. AI-CFD integration for sustainable energy applications.

linear, and reactive flow systems [10,17]. At its core, a typical CFD simulation can be divided into three tightly interlinked stages—pre-processing, solving, and post-processing, as illustrated in Fig. 2, each presenting its own computational and methodological challenges. To ensure accurate and stable simulations, addressing the intricate issues that arise at every step, from mesh generation and boundary condition treatment to numerical discretization and result interpretation, is essential. This section delves into the latest advances and persistent hurdles associated with each stage, highlighting ongoing efforts to enhance robustness, efficiency, and fidelity in CFD simulations.

2.1.1. Challenges in pre-processing

In the pre-processing stage of CFD simulation, significant challenges remain in handling complex geometries and dynamic problems [21,81]. Current methods require substantial manual grid generation intervention, limiting efficiency. Traditional static grid methods struggle with dynamic phenomena, such as bubble breakup or droplet evaporation, as they fail to adapt to a changing interface [82]. High-resolution grids capture critical regions, such as turbulence cores or interface gradients, but at a prohibitively high computational cost [83,84]. In addition, high-resolution grids can also introduce numerical instabilities. When the grid becomes excessively refined, steep local gradients and extreme values in the discretization process may lead to numerical oscillations and error amplification. This can ultimately result in undefined solutions, compromising the accuracy of the simulation and, in some cases, causing the computation to fail [85,86].

Researchers transitioned from static mesh strategies to more adaptive refinement techniques to address these limitations. Early CFD simulations typically employed uniform grids to solve governing equations. While this approach theoretically improved global resolution, it often triggered numerical instabilities in regions exhibiting sharp physical variations. Excessively refined uniform grids in such areas could intensify oscillations and destabilize the solution [87,88]. To mitigate this, researchers began employing local mesh refinement in critical areas, such as flame fronts, phase interfaces, and turbulent zones [89,90]. Although this strategy aimed to balance computational cost and resolution, it remained susceptible to instability due to grid discontinuities and cross-scale coupling issues. In recent years, the introduction of adaptive mesh refinement (AMR) and dynamic time-stepping techniques has enabled a more effective balance between resolution and numerical

stability. Current research increasingly prioritizes maintaining numerical robustness alongside achieving high spatial resolution [91–94]. Advanced high-order numerical schemes—such as Weighted Essentially Non-Oscillatory (WENO), Total Variation Diminishing (TVD), and Essentially Non-Oscillatory (ENO) methods—are now widely used to enhance accuracy in localized regions while suppressing spurious oscillations [95,96]. Dynamic time-stepping ensures strict compliance with CFL conditions and reaction rate constraints in highly resolved zones, reducing instability risks associated with small time steps [97–99]. Additional stabilization techniques, including preprocessing methods, artificial viscosity, and robust solvers, have also been applied to alleviate localized instabilities and prevent the occurrence of undefined solutions [86,96,100].

2.1.2. Boundary condition treatment

Boundary conditions play a vital role, ensuring the solution adheres to physical constraints at the domain boundaries. Boundary conditions are typically defined based on empirical observations or experimental conditions, yet they may require mathematical adjustments during the solving process to ensure numerical stability and convergence [101]. This raises a fundamental question: boundary conditions are not always defined consistently with the physical system and may need to be modified for practical applications [102]. Moreover, the choice and adjustment of boundary conditions directly influence the resolution of the equations and the accuracy of the solutions, thereby significantly affecting the outcomes of CFD simulations [103].

Early CFD efforts involved researchers importing observed boundary conditions from physical systems into numerical models, such as fixed temperature, fixed pressure, or no-slip conditions [104]. While this approach seemed straightforward, it quickly revealed numerical instability and convergence difficulties in complex flows or multiphysics coupling scenarios. As CFD theory advanced, scholars recognized the necessity for boundary conditions in mathematical models to satisfy specific requirements, such as continuity, smoothness, and differentiability, to guarantee the stability and precision of numerical discretization. Consequently, researchers began exploring mathematical adjustments to the original physical boundary conditions, employing techniques like buffer zones, weighting functions, and smoothing processes to ensure continuous transitions at the boundaries and mitigate numerical oscillations caused by discontinuities [105,106].

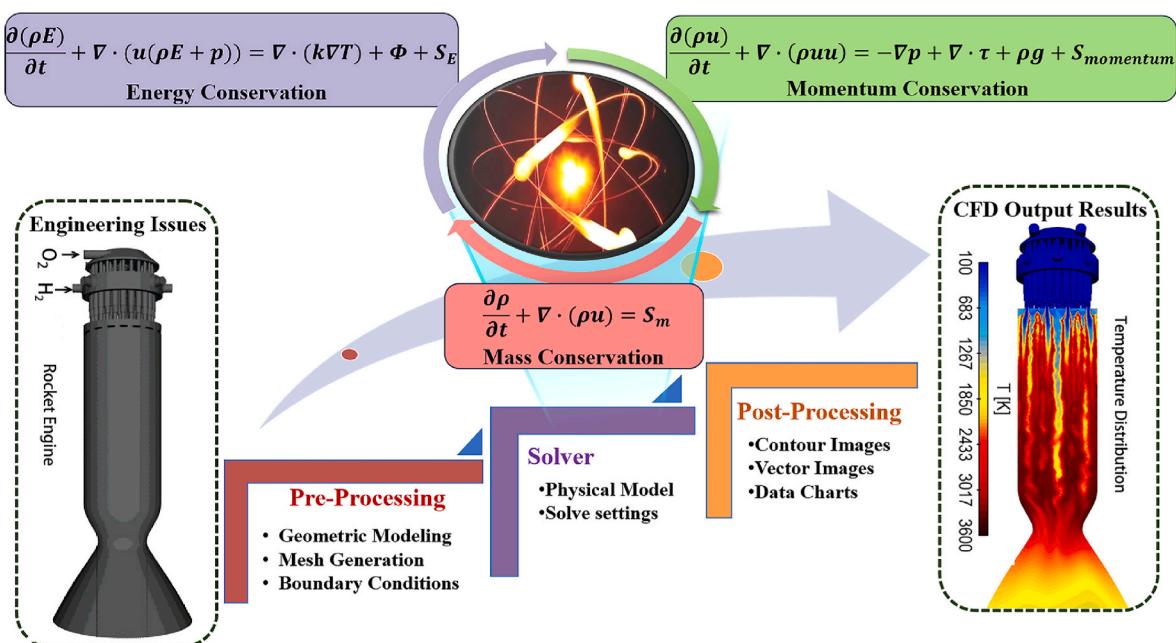


Fig. 2. CFD workflow for multiphase flow and thermochemical reaction simulation.

The CFD field has developed a relatively mature system for handling boundary conditions. Researchers establish boundary conditions based on physical experimental data and adjust them according to the characteristics of numerical methods. For instance, mixed boundary conditions are often employed when addressing turbulence, heat transfer, or multiphase flow problems [107]. These may strictly limit certain variables physically while enhancing numerical stability through added smoothing conditions or artificial diffusion terms. Furthermore, using high-resolution grids has made the impact of boundary conditions on the solution significantly more sensitive [108]. To prevent sharp gradients at the boundaries from causing numerical instability, researchers frequently utilize locally adaptive meshes and dynamic time-step control methods, ensuring that the discretization of boundary regions maintains sufficient detail while effectively alleviating discontinuity issues from boundary condition adjustments [109].

2.1.3. Numerical methods for solving governing equations

The core of CFD involves solving the partial differential equations of fluid mechanics across space and time using numerical methods. The control volume's values are continuously updated until the convergence criteria are satisfied [110]. Spatial and temporal discretization are key steps in numerical solving, converting PDEs (partial differential equations) into discrete forms. As illustrated in Fig. 3, the finite volume method (FVM) is widely applied in engineering for spatial discretization due to its adaptability to complex geometries [111]. In contrast, the finite difference method (FDM) is preferred for structured grids due to its simplicity [112]. The finite element method (FEM) is suited for high-accuracy solutions in problems with complex boundaries. Additionally, the spectral method uses global functions, such as the Fourier series, to represent the overall solution, indirectly achieving spatial discretization. It is well-suited for problems with periodic or smooth solutions [113]. The lattice Boltzmann method (LBM) is a numerical approach based on microscopic particle distributions, directly relying on grid-based discretization to simulate fluid flow [41,114,115].

For temporal discretization, explicit methods are computationally simple but constrained by stability conditions, while implicit methods are more stable but computationally intensive. Semi-implicit methods balance efficiency and stability [63]. These methods are well-developed and widely applied to simulate turbulent flows, multiphase flows, and chemical reactions. Current research mainly focuses on improving high-order methods like weighted essentially non-oscillatory (WENO) and spectral methods for turbulence and multiphase flows, optimizing

them for unstructured grids to reduce dissipation, and developing efficient time integration schemes to address nonlinear effects [116].

2.1.4. Acceleration techniques

With the advancement of computer hardware, CFD acceleration has increasingly shifted towards utilizing graphics processing units (GPUs). As illustrated in Fig. 4, unlike distributed computing based on central processing units (CPUs) combined with parallel programming frameworks such as message passing interface (MPI) and open multi-processing (OpenMP), GPUs improve computation speed significantly by distributing matrix-vector computations across individual GPU cores, thereby avoiding inter-cell communication and leveraging the parallel processing capabilities of GPUs [117]. Cooper-Baldock Z et al. [118] evaluated different CPU architectures and GPUs and demonstrated that GPUs significantly outperform CPUs in computational speed. Yu J et al. [119] proposed a GPU-accelerated discrete element method (DEM) that effectively leverages the parallel architecture of GPUs. The GPU-accelerated parallel algorithm for particle collisions significantly reduced computation time, demonstrating excellent performance in terms of acceleration and stability. However, a key challenge is that traditional algorithms, such as finite difference and finite element methods, were not initially designed for parallel architectures. These algorithms must be redesigned to adapt to highly parallel architectures like GPUs [120].

2.2. Turbulence modeling in CFD

In turbulence and multiphase flow simulations, modeling complex turbulent phenomena relies on simplifying and approximating the governing equations, as shown in Table 1. Nonlinear terms, such as convective and interaction, are central to fluid dynamics but often introduce numerical dissipation, leading to deviations from real-world behavior [21,121,122]. One of the fundamental challenges in turbulence modeling lies in achieving accurate closure of the RANS equations, which typically relies on a series of simplifying assumptions [123,124]. Traditional models, such as zero-equation or single-equation formulations, estimate turbulent stresses using empirical relationships or transport equations for a single turbulent property [125]. More advanced two-equation models, like the widely adopted $k-\epsilon$ and $k-\omega$ formulations, solve transport equations for turbulent kinetic energy and its dissipation rate (or specific dissipation rate), enabling more accurate estimation of turbulent viscosity and Reynolds stresses. However, these models often rely on assumptions such as flow isotropy and linear eddy viscosity, which limit their ability to capture transient features and anisotropic structures, especially in flows involving separation, adverse pressure gradients, or rotation [126]. To address these deficiencies, Reynolds Stress Models (RSM) introduce separate transport equations for each of the six Reynolds stress components, significantly improving anisotropy representation at the cost of greater computational complexity [127–129].

LES has evolved significantly since introducing the classical Smagorinsky model with fixed coefficients. Subsequent developments—such as the Germano dynamic procedure and hybrid spectral approaches—have greatly improved its ability to represent subgrid-scale stress accurately. Nevertheless, LES remains computationally expensive for high-Reynolds-number flows due to its satisfactory near-wall resolution requirements [130]. Traditional log-law-based wall functions struggle with low-Reynolds-number effects, strong pressure gradients, and flow separation [131]. Generalized wall functions incorporating pressure-gradient and heat-flux corrections have been proposed to overcome these limitations. Wall-Modeled LES (WMLES) has emerged as a practical solution, applying simplified RANS or enhanced wall-function models near walls while resolving large eddies in the outer flow region, typically keeping y^+ between 30 and 100 to balance resolution and cost [132]. Adaptive mesh refinement (AMR) techniques enhance simulation fidelity by dynamically increasing resolution in

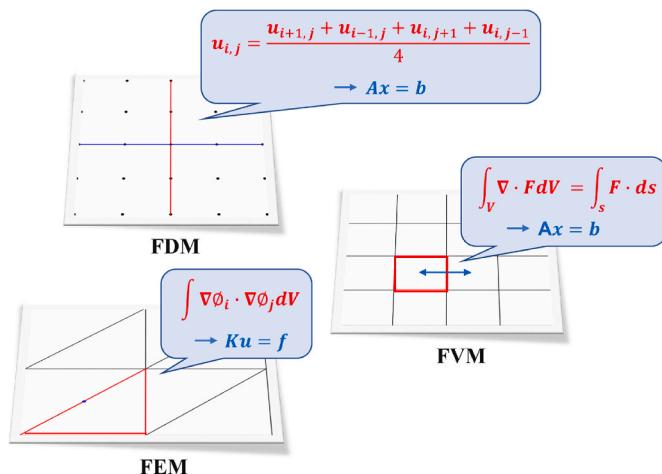


Fig. 3. Illustration of numerical methods: FDM, FVM, and FEM for solving partial differential equations (Each method transforms the continuous PDEs into algebraic equations, like $Ax = b$ or $Ku = f$, making them solvable on a computer. These approaches are essential for simulating complex physical processes).

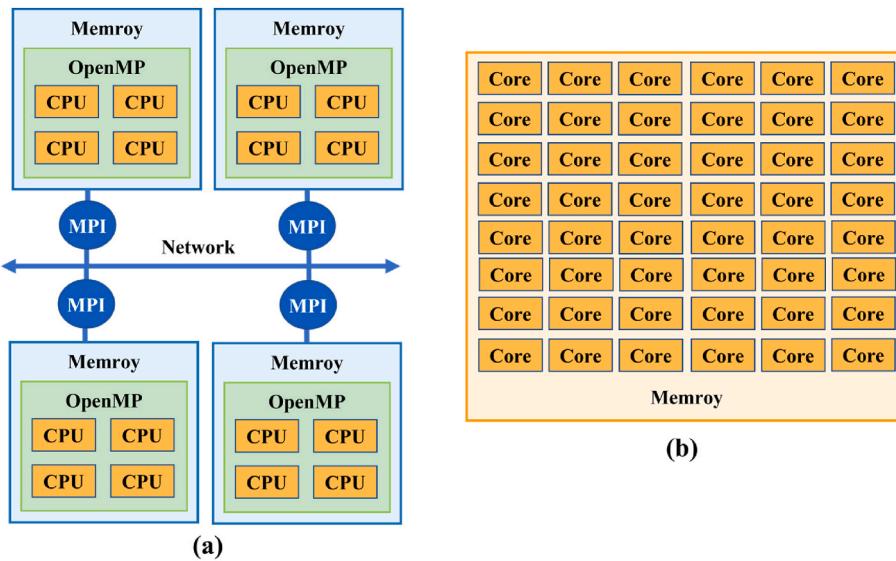


Fig. 4. CPU-based parallel computing (a) vs. GPU-accelerated computing (b) in CFD simulations.

Table 1
Empirical closure formulas in turbulence models (CFD).

Model	Governing equations
Mixing-Length Model	$\nu_t = l_m^2 \left \frac{\partial U}{\partial Y} \right $
Spalart-Allmaras model	$\frac{D\tilde{\nu}}{Dt} = C_{b1}(1 - f_{12})\tilde{\nu} + \frac{1}{\sigma} \left[\nabla \cdot ((\nu + \tilde{\nu})\nabla \tilde{\nu}) + C_{b2} \nabla \tilde{\nu} ^2 \right] - C_{w1}f_w \left(\frac{\tilde{\nu}}{d} \right)^2$
Standard k-ε Model	$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \epsilon + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]$ $\frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = C_{1\epsilon} \frac{\epsilon}{k} P_k - C_{2\epsilon} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right]$ $\nu_t = C_\mu \frac{k^2}{\epsilon}$
Standard k-ω Model	$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta^* k \omega + \frac{\partial}{\partial x_j} \left[(\nu + \sigma_k \nu_t) \frac{\partial k}{\partial x_j} \right]$ $\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha \frac{\omega}{k} P_k - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[(\nu + \sigma_\omega \nu_t) \frac{\partial \omega}{\partial x_j} \right]$ $\nu_t = \frac{k}{\omega}$
SST k-ω Model (Shear Stress Transport)	$\nu_t = \frac{a_1 k}{\max(a_1 \omega, SF_2)}$
Reynolds Stress Model (RSM)	$\frac{\partial R_{ij}}{\partial t} + U_k \frac{\partial R_{ij}}{\partial x_k} = P_{ij} + \Phi_{ij} - \epsilon_{ij} + D_{ij}$ $R_{ij} = u'_i u'_j$

regions with high flow gradients, avoiding unnecessary refinement elsewhere and optimizing computational resources [133]. These developments have shifted industrial CFD practices toward hybrid RANS-LES frameworks.

With the development of computer technology, particularly the advancement of computational capabilities, Direct Numerical Simulation (DNS) has gradually become an essential tool in turbulence research. DNS solves the Navier-Stokes equations directly, without relying on turbulence models, and can capture all turbulence scales, from large-scale to small-scale energy transfers. This capability allows DNS to provide unprecedented accuracy in simulating turbulent flows. However, despite its high precision, DNS faces significant limitations due to its computational cost [134]. The resolution required to simulate turbulence accurately increases exponentially with the Reynolds number, making DNS impractical for high Reynolds number flows and complex boundary conditions commonly encountered in engineering applications. As a result, DNS is primarily applicable to low Reynolds

number turbulence where the computational demand is more manageable.

Significant advancements in turbulence modeling have emerged in recent years, primarily focusing on data-driven methods and machine learning (ML) applications [135–142]. Traditional turbulence models, such as Reynolds-averaged Navier-Stokes (RANS), have been enhanced using neural networks and reinforcement learning techniques, improving the accuracy of turbulence predictions by capturing complex nonlinear behaviors. Hybrid models like Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) have seen increased use in simulations involving complex geometries, offering better accuracy than traditional approaches [143]. These innovations have provided more precise predictions in both engineering and scientific applications, particularly for turbulent flows in intricate systems. However, these advancements also bring forth debates, especially regarding the trade-off between model accuracy and computational efficiency. While ML techniques promise to improve predictive accuracy, concerns about the computational cost and model generalization remain. Future research is expected to focus on integrating experimental data with simulation models to refine turbulence predictions and enhance the generalization capabilities of machine learning-based models. It is also important to note that the enhancement of traditional RANS models through neural networks represents a key development in this area, and this topic will be explored in detail in a subsequent chapter, highlighting the synergy between traditional and data-driven approaches in advancing turbulence modeling.

2.3. Multiphase flow simulation

2.3.1. Methodological system: across micro, Meso, and macro scales

As shown in Fig. 5, multiphase flow simulations can be categorized into three primary levels—micro-scale, mesoscale, and macro-scale—based on the scale of the system and the modeling framework. At the micro-scale, particle-resolved direct numerical simulation (PR-DNS) offers the highest accuracy by directly resolving detailed interactions between individual particles and the surrounding fluid. Tenneti S et al. [144] reviewed the use of PR-DNS for understanding gas-solid flow physics, addressing challenges in model development across scales, and summarizing recent insights into momentum, energy, and heat transfer in such flows. Kravets B et al. [145] study compares PR-DNS with non-resolved DEM/CFD simulations, highlighting the limitations of the latter in accurately capturing drag, lift, and heat transfer for non-spherical particles, while providing valuable insights for improving

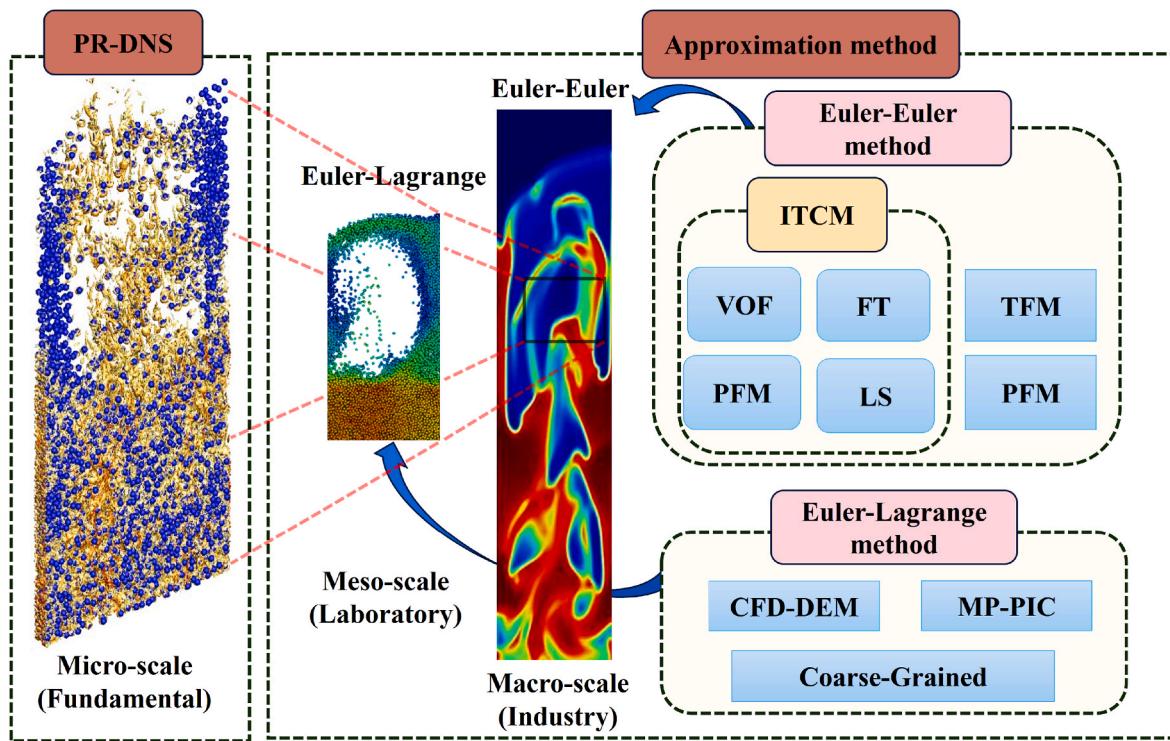


Fig. 5. Different methods for high-phase fraction multiphase flow simulation.

closure relations and particle-fluid interaction models in future simulations. Summarizing the existing research, it is shown that this method is invaluable for studying the fundamental mechanisms of multiphase flows but is limited to small-scale systems due to its extremely high computational cost.

At the mesoscale, the Euler-Lagrange method balances accuracy and

efficiency. It combines the Eulerian framework for solving fluid dynamics with the Lagrangian framework for tracking discrete particles or bubbles, making it suitable for low-to-medium concentration particle systems [146]. Common extensions include CFD-DEM, which integrates computational fluid dynamics with the discrete element method for simulating medium-concentration particle flows [147]. In this context, a

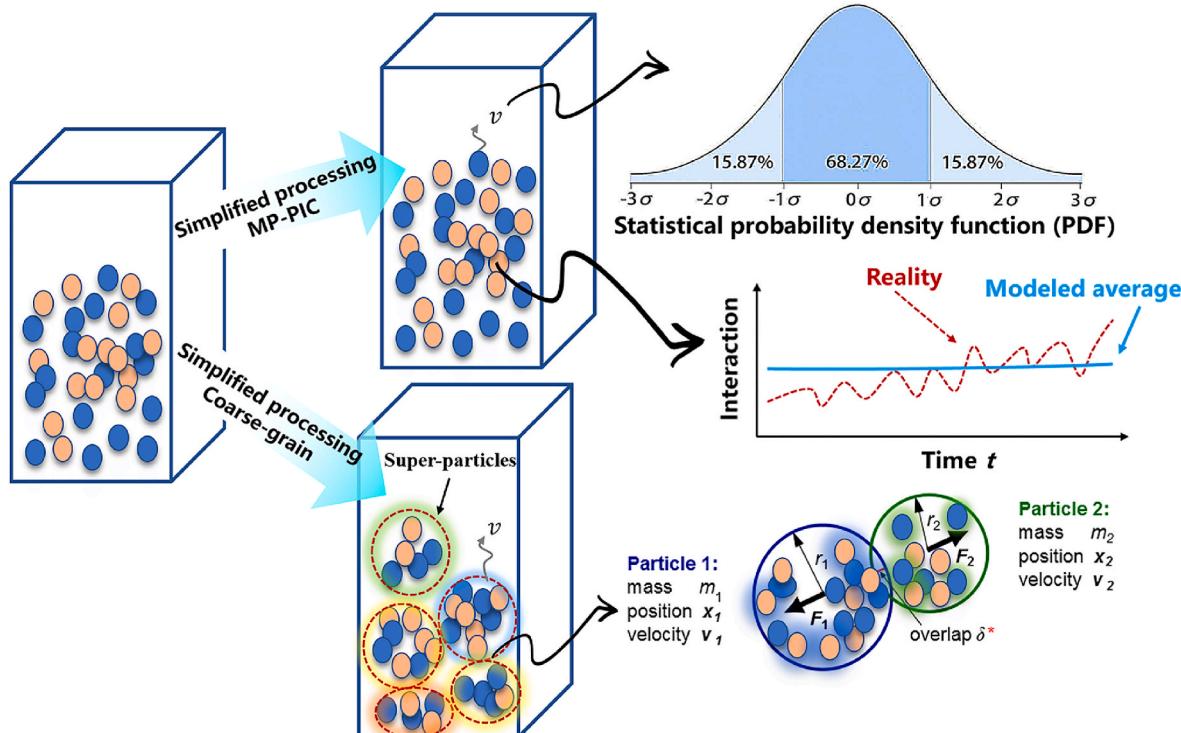


Fig. 6. Comparison of MP-PIC and coarse-grained models in particle simulation.

fluidized bed reactor is a typical area of research and application. Zhao et al. [148] reviewed recent progress in CFD-DEM simulations for fluidized beds, showcasing the method's ability to accurately predict particle flow behavior and its potential to be applied to multiphase flow simulations involving complex geometries. Wang et al. [149] pointed out that dense gas-solid reactive flows, where the number of particles can be huge, cannot be modeled using traditional CFD-DEM methods. Methods such as multiphase particle-in-cell (MP-PIC) and Coarse-Grained models have been developed to address these challenges, trading off some accuracy in particle-particle interactions to enable the simulation of ultra-large-scale systems, as shown in Fig. 6. MP-PIC employs volume-averaging to handle large-scale particle flows efficiently at the cost of reduced particle-particle interaction accuracy. As studied by Feng et al. [150] in their parametric investigation of MP-PIC simulation of bubbling fluidized beds, it was revealed that a threshold exists for grid size; below this threshold, grid-independent results can be achieved. Coarse-grained models, which simplify computations by grouping particles into clusters, enable simulations of ultra-large-scale systems with reduced precision [151–153]. Kaiwei et al. investigated the applicability of the coarse-grained CFD-DEM model in dense medium cyclones, and the results showed that the method's error is negligible for dilute flows and acceptable for dense flows, demonstrating that this approach can effectively balance computational efficiency and accuracy [153]. Recently, some popular commercial software such as CFD-Barracuda and ANSYS-Rocky have embedded coarse-grain models, significantly reducing the computation cost of tracking individual particles, making the cases with massive particle numbers possible to be modeled [154–157]. These advancements in mesoscale modeling methods demonstrate the growing capability to tackle the computational challenges associated with low-to-medium multiphase flows.

At the macro-scale, the Euler-Euler method treats all phases as interpenetrating continua and solves their governing equations using conservation laws. This method is highly efficient for simulating high-concentration systems in large-scale industrial applications. For multiphase flows with clear interfaces, the Euler-Euler method can be coupled with interface tracking models such as VOF, a grid-based interface capturing method that tracks the interface position by using a scalar function representing the ratio of fluid volume within a computational cell, which is suitable for large-scale interface capturing [43,158]. Based on this concept, Mathur et al. [159] proposed a Euler-Euler two-fluid solver for multi-scale two-phase flows, demonstrating its modeling capabilities for segregated and dispersed flow regimes. Building on this, the Level Set method offers an alternative approach for interface tracking, utilizing a signed distance function to represent the interface, which provides higher precision for capturing complex and dynamically evolving interfaces in multiphase flows. Kan et al. [160] developed a novel immersed boundary method based on the Level Set function to simulate geometrically complex pumps, achieving simulation results that showed excellent agreement with experimental data. The Phase-Field method uses a diffuse interface model controlled by a phase-field variable. It is well-suited for capturing micro-scale interface changes and complex topological transitions in multiphase flows [161]. Mao et al. [162] developed a time-dependent mobility phase-field model for accurate surface tension calculations. The model demonstrated excellent applicability for addressing complex topological changes of interfaces on unstructured grids and practical problems involving intricate dynamics, such as bubble-bubble and bubble-surface interactions. The Two-Fluid Model (TFM) models fluid and particle phases as continua for dense particle flows, offering high computational efficiency but limited resolution of particle-particle interactions [163]. This method avoids the intensive computational load from tracking particles. It can be regarded as one of the most efficient model frames in computing multiphase flow, but at the expense of the realism of the actual process. Adnan et al. [164] utilized the TFM method to simulate a 3D conical fluidized bed reactor and enhanced its performance through

sensitivity analysis-based optimization. Their evaluation demonstrated that this optimization approach improves the alignment between experimental data and model results, highlighting the potential to achieve a balance between computational efficiency and accuracy. These methods emphasize the importance of selecting and optimizing appropriate modeling approaches to address the trade-offs between computational efficiency, accuracy, and the specific requirements of complex multiphase flow simulations in industrial applications.

2.3.2. Industrial application example: fluidized bed reactor

Despite the theoretical advantages of various multiscale modeling approaches—each tailored to different particle concentrations and system scales—significant challenges persist in their application to complex industrial environments. Fluidized bed reactors serve as a representative example, where highly coupled gas-solid interactions, turbulent structures, and particle agglomeration coexist with intense heat and mass transfer and chemical reaction processes. These complexities impose stringent requirements on computational models' spatiotemporal resolution and physical fidelity. In particular, the interplay between gas turbulence and particle dynamics gives rise to transient mesoscale structures—such as clusters, collisions, and agglomeration-deagglomeration phenomena—strongly influencing local drag, mixing behavior, and reaction kinetics. Additionally, exothermic or endothermic reactions generate steep gradients in temperature and species concentration, further complicating the flow field [165]. While conventional macroscopic models such as the Eulerian–Eulerian two-fluid model offer computational efficiency, their reliance on empirical closures, as shown in Table 2, assumes local homogeneity and neglects critical feedback mechanisms between mesoscale dynamics and turbulence [166]. Consequently, these models often fail to deliver reliable predictions under conditions of high solids loading or vigorous reaction activity. This highlights the pressing need for the continued evolution of multiscale modeling approaches that can resolve particle-level behavior, robustly couple multiphysics phenomena, and remain computationally tractable for large-scale industrial applications.

Over the past decades, modeling approaches have evolved from purely empirical two-fluid models toward hybrid Eulerian–Lagrangian frameworks and multi-physics coupling strategies that explicitly resolve particle-scale dynamics. Early efforts enhanced two-fluid formulations with semi-empirical corrections derived from cluster-scale experiments or energy-minimization multi-scale (EMMS) theory, improving solids distribution and pressure drop predictions [167]. The advent of

Table 2
Governing equations and empirical closure models for multiphase flows.

Model	Governing equations
Conservation of mass	$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k) = 0$
Conservation of momentum	$\frac{\partial(\alpha_k \rho_k \vec{v}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k \vec{v}_k) = -\alpha_k \nabla p + \nabla \cdot \vec{F}_k + \alpha_k \rho_k \vec{g} + \vec{F}_{int}$
General Form of Drag Force	$\vec{F}_d = \frac{1}{2} C_d \rho_f A_p \vec{u}_f - \vec{u}_p (\vec{u}_f - \vec{u}_p)$
Stokes' Law	$C_d = \frac{24}{Re_p}, Re_p < 1$
Schiller–Naumann	$C_d = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}), Re_p < 1000$
Gidaspow Model	Combines Ergun (dense) + Wen – Yu (dilute) regions
Wen–Yu Model	$C_d = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) \epsilon_f^{-2.65}$
Newtonian Fluid Stress Tensor	$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \nabla \cdot \vec{u}$
Reynolds Stress Tensor (Turbulent Flows):	$R_{ij} = u'_i u'_j$
Closure required using models (e.g., Boussinesq approximation)	$-\rho R_{ij} = 2\mu_t S_{ij} - \frac{2}{3} \rho k \delta_{ij}$

CFD-DEM coupling marked a paradigm shift: by integrating a discrete element method (DEM) solver—often employing the Cundall–Strack soft-sphere contact model—with a CFD solver, researchers could directly compute inter-particle forces, collision histories, and local heat and mass exchange. To mitigate the prohibitive computational cost of full-scale DEM, coarse-grained DEM and multiscale population-balance approaches were introduced, alongside GPU acceleration, enabling simulations of industrially relevant reactor volumes [149].

State-of-the-art simulations routinely employ high-fidelity CFD-DEM platforms like CFDEM and MFix-DEM, augmented with coarse-graining and GPU-based parallelism to capture cluster formation, segregation, and fluid-solid exchange within acceptable runtimes. Concurrently, EMMS-informed multi-fluid models have matured, embedding locally varying drag and solids-stress corrections to reconcile two-fluid predictions with discrete-particle behavior [168]. Multi-physics coupling has been extended to include detailed chemical kinetics and radiative/conductive heat transfer, thereby enabling accurate prediction of temperature profiles, local ignition or extinction events, and pollutant formation. Moreover, large eddy simulation (LES) techniques tailored for multiphase flows—incorporating subgrid cluster models—have emerged to resolve the interaction between unresolved turbulent eddies and particulate structures, furnishing unprecedented insight into transient mixing and reaction phenomena.

2.4. CFD-coupled chemical reactions: applications and challenges

As the world shifts toward renewable energy to address climate change and rising energy demands, accurately modeling complex chemical reactions—central to processes like biomass gasification, water electrolysis, and CO₂ reduction—is essential for optimizing efficiency and reducing emissions. Coupling Computational Fluid Dynamics (CFD) with chemical kinetics enables detailed simulations of these systems, capturing interactions between flow, heat transfer, and reaction dynamics. However, challenges such as turbulent mixing, multiphase flows, multiscale kinetics, high computational costs, and limited validated data hinder widespread application, despite the method's transformative potential in virtual prototyping and system design.

2.4.1. Evolution of CFD-chemistry coupling in energy systems

As shown in Fig. 7, CFD-based chemical reaction modeling began in the mid-20th century, initially focusing on simplified, one-dimensional laminar combustion with global kinetics. As computational capabilities improved, these models evolved to handle multi-species, multi-step reactions in complex geometries.

From the 1960s–1980s, core numerical methods such as finite difference and finite volume were established, while chemical kinetics, grounded in transition state theory and Arrhenius expressions, became integrated into engineering simulations. A key milestone was the development of the KIVA code, which enabled combustion and spray modeling in engines, marking one of the earliest practical CFD-

chemistry couplings.

The 1990s saw major progress with the incorporation of turbulence-chemistry interaction models like the Eddy Dissipation Concept (EDC), allowing more realistic simulation of flames, combustion instabilities, and pollutant formation. Increasing computational power enabled the use of detailed kinetic mechanisms in turbulent reacting flows.

In the 2000s, the rise of high-performance computing (HPC) allowed CFD to expand into multiphase and porous media systems, such as fluidized beds and catalytic reactors. New solvers were developed to handle the stiffness of complex chemical kinetics, establishing CFD as a core design tool in the chemical and energy industries.

Since the 2010s, the focus has shifted toward renewable energy systems. Integrating AI and machine learning has introduced powerful tools for mechanism reduction, surrogate modeling, and real-time simulation. Modern CFD is now central to creating digital twins—virtual replicas of physical systems—for performance monitoring, fault prediction, and system optimization in clean energy applications.

2.4.2. Current technical landscape and core challenges

Modeling chemically reactive flow systems through CFD presents a formidable computational challenge due to the intricate and nonlinear coupling of three fundamental processes: fluid dynamics, heat transfer, and chemical kinetics. These processes interact across a wide spectrum of spatial and temporal scales. Chemical reaction rates often vary exponentially with temperature, especially in exothermic systems governed by Arrhenius kinetics. This leads to strong numerical stiffness in the governing equations and necessitates extremely small time steps or implicit solution schemes to maintain numerical stability. At the same time, turbulent flows introduce a broad range of length and time scales, requiring fine spatial resolution and advanced turbulence models to capture relevant transport phenomena accurately. Furthermore, in many renewable energy applications, reactive systems are also multiphase in nature—e.g., gas-solid in biomass gasification or gas-liquid in electrolyzers—which adds spatially dynamic interfaces that critically influence interphase mass and heat transfer [111].

The governing equations in multiphase CFD simulations typically include the Navier–Stokes equations for momentum, an energy conservation equation, and species transport equations for all reactive components, as shown in Table 3. These are accompanied by closure models that account for turbulence (e.g., RANS, LES), interphase interactions, and reaction kinetics. Depending on the combustion or reaction regime, several chemical models are used: the laminar finite-rate model for simple systems with negligible turbulence, the eddy dissipation model for turbulence-dominated non-premixed combustion, and the eddy dissipation concept (EDC) for simulations that incorporate detailed kinetic mechanisms in turbulent flames. These models are widely used in industry-standard solvers such as ANSYS Fluent and OpenFOAM. However, none of these models can fully overcome the fundamental challenge posed by multi-scale, nonlinear feedback loops that exist in high-temperature, stiff-reacting systems [169].

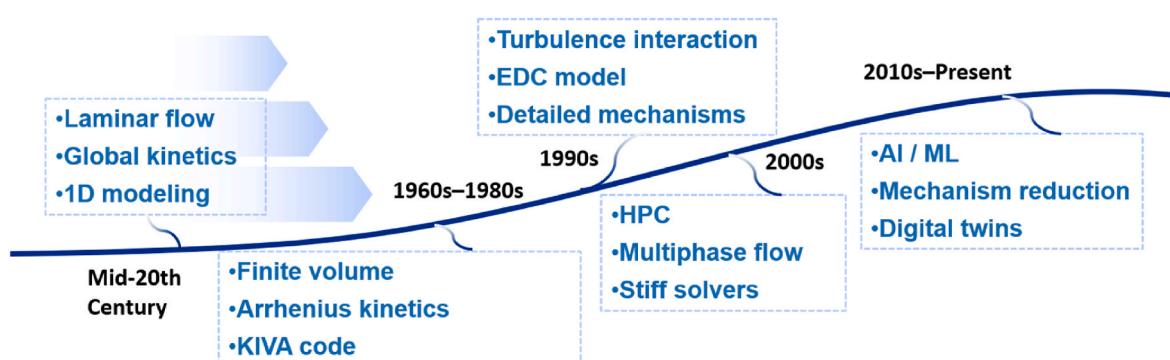


Fig. 7. Evolution of CFD-Coupled chemical reaction modeling.

Table 3
Governing equations and closure models in multiphase reactive flow in CFD.

Model name	Main formulas	Scenarios
Navier-Stokes	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$ $\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = - \nabla p + \nabla \cdot \tau + \mathbf{S}_m$ $\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = - \nabla p + \nabla \cdot \tau + \mathbf{S}_m$	Modeling fluid flow in areas like aviation, weather, oceans, and engineering.
Species transport equation	$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = - \nabla \cdot \vec{J}_i + R_i$	Multi-species flows, combustion, and chemical reaction simulations
Laminar finite rate model	$k = A \exp\left(-\frac{E_a}{RT}\right)$, $R_i = \sum R_{i,r}$	Laminar conditions, low turbulence
Eddy dissipation model	$R = \rho \frac{\epsilon}{k} \min\left(Y_R, \frac{Y_O}{\nu}, B \frac{Y_P^{1.5}}{Y_R^{0.5}}\right)$	Turbulent conditions, non-premixed combustion
Eddy dissipation concept	Depending on detailed chemical mechanisms	Complex turbulence, premixed/diffusion combustion,
General reaction rate expression	$-\frac{1}{a} \frac{d[A]}{dt} = \frac{1}{c} \frac{d[C]}{dt}$	Any reaction, based on stoichiometry

Traditionally, segregated solvers were used, where the fluid flow equations were solved independently of the heat and species equations, and reaction kinetics were often applied in post-processing. While this approach significantly reduces computational cost, it neglects crucial feedback mechanisms—such as heat release from exothermic reactions affecting local fluid velocity and turbulence structure—that are pivotal in accurately simulating combustion or other highly reactive systems. In response to these limitations, modern solvers have transitioned toward fully coupled, implicit solution frameworks. These solvers simultaneously resolve momentum, energy, species, and reaction source terms, enabling accurate modeling of tightly coupled feedback processes and significantly improving numerical stability [170].

The mathematical stiffness introduced by detailed chemical kinetics remains one of the most severe challenges. Complex reaction networks often result in stiff ordinary differential equations (ODEs), where characteristic timescales can differ by several orders of magnitude. To address this, implicit time integration schemes such as Gear's method or backward differentiation formulas (BDF) are commonly adopted. Moreover, solver architectures now include adaptive mesh refinement (AMR) to selectively increase spatial resolution near reaction fronts or steep thermal gradients, as well as local time-stepping to avoid unnecessary computational load in regions of slow dynamics [90].

To further improve efficiency and convergence, numerical methods such as preconditioned finite volume schemes, multigrid solvers, and Laplace transformation techniques are employed, especially in regimes dominated by stiffness or tight coupling [171–173]. For large-scale simulations, parallel computing frameworks based on MPI (distributed memory) and OpenMP (shared memory) are used to distribute workload across high-performance computing clusters [174–176]. These strategies have enabled full 3D simulations of industrial-scale reactors within feasible runtimes. Nevertheless, such simulations still demand significant computational resources and specialized knowledge of solver configuration and convergence behavior [177–179].

As the demand for high-throughput design and simulation grows, researchers increasingly turn to reduced-order models and mechanism reduction techniques to manage complexity without sacrificing accuracy in critical regions. Techniques like Flamelet Generated Manifolds (FGM) and reaction progress variable tabulation allow for fast lookup of precomputed reaction states, eliminating the need to solve stiff ODEs at every grid point and time step. These methods are especially useful in large combustion systems where only a few chemical pathways dominate. Additionally, operator-splitting approaches decouple the physical

sub-processes—fluid flow, transport, and reaction—so that each can be solved using the most appropriate numerical scheme. This hybrid solution strategy enables flexible, modular simulation workflows that are easier to optimize and parallelize [180–182].

Finally, uncertainty quantification (UQ) and global sensitivity analysis are increasingly integrated into CFD workflows to account for modeling uncertainties, kinetic parameter variability, and the influence of boundary condition assumptions. These tools help quantify the reliability of simulation outcomes, identify key parameters affecting performance, and guide experimental design. They are particularly valuable in systems involving novel feedstocks, catalysts, or operational modes—common in renewable energy technologies—where empirical data is limited and model extrapolation is unavoidable [183].

In summary, while CFD-coupled reactive flow modeling has made remarkable strides, it remains one of the most challenging areas in numerical simulation due to the simultaneous presence of stiff kinetics, turbulent transport, multiphase interactions, and dynamic feedback mechanisms. Continued advances in solver architecture, numerical schemes, kinetic databases, and high-performance computing are essential to further push the boundaries of accuracy, scalability, and practical applicability in real-world energy systems.

2.4.3. Applications in renewable energy systems

The integration of CFD with detailed chemical reaction models has opened up new opportunities in the design, analysis, and optimization of renewable energy systems. These applications are not limited to traditional fuel combustion but span a wide range of clean energy technologies, including biomass gasification, catalytic upgrading of biofuels, electrochemical energy conversion, and photobioreactor systems. In each case, CFD serves as a virtual laboratory for testing design hypotheses, understanding internal physical-chemical phenomena, and optimizing system parameters—often in ways that are impractical or too costly to achieve through experiments alone.

One of the most mature applications of CFD-coupled chemistry in renewable energy is biomass gasification [184]. In this process, solid organic feedstocks such as wood chips, agricultural waste, or municipal solid waste are thermochemically converted into a mixture of CO, H₂, CH₄, and CO₂ under limited oxygen or steam conditions. The process involves a complex sequence of devolatilization, char oxidation, and gas-phase reactions, each with different thermal and kinetic characteristics. CFD simulations can model the interplay between particle heating, volatile release, homogeneous and heterogeneous reactions, and syngas formation. For example, by simulating the temperature distribution and residence time within a downdraft gasifier, engineers can identify cold spots that hinder conversion or hot zones that cause slagging, enabling better control over the air-steam feed rate or insulation strategy [185].

Another major area of application is in heterogeneous catalytic reactors, particularly for upgrading bio-derived intermediates like bio-oil, syngas, or volatile fatty acids into fuels and chemicals. These reactors often involve porous catalytic beds or coated surfaces, where reaction rates are sensitive to temperature gradients, diffusion limitations, and local flow non-uniformity. CFD models allow for the incorporation of surface reaction kinetics, often based on Langmuir–Hinshelwood or microkinetic frameworks, into the simulation of transport phenomena. A representative example is the work by Hafeez et al. [186], who employed CFD modeling to systematically investigate the influence of channel geometry, wall temperature, and catalyst distribution on product selectivity in microchannel reactors for hydrodeoxygenation. These insights are essential not only for maximizing yield but also for avoiding catalyst deactivation due to hotspot formation or uneven fouling.

CFD-coupled chemical modeling also plays a vital role in the development of low-emission combustion systems using renewable fuels such as biodiesel, ethanol, and synthetic gases [187]. Unlike fossil fuels, many biofuels have high oxygen content, low volatility, and complex ignition

behavior, which significantly affects flame structure and pollutant formation. Using CFD, combustion chambers and burners can be evaluated in terms of flame stability, NOx and CO emission characteristics, and ignition delay times. The use of detailed chemical mechanisms, sometimes coupled with multi-fuel surrogate models, helps predict real fuel behavior under varying pressure, equivalence ratio, and exhaust gas recirculation (EGR) conditions. This modeling capability is especially important for the design of hybrid dual-fuel engines or biofuel-compatible gas turbines, where performance depends heavily on transient combustion dynamics.

In the field of electrochemical energy systems, including fuel cells and electrolyzers, CFD-chemical coupling offers a multidimensional view into device operation. Solid oxide fuel cells (SOFCs), for instance, require simulation of porous media transport, ionic conduction, and electrochemical reactions at the anode and cathode interfaces [188]. Similarly, proton exchange membrane (PEM) electrolyzers involve multiphase flows of water, hydrogen, and oxygen, where CFD is used to optimize channel geometry, flow field design, and gas-liquid separation efficiency [189]. In both cases, CFD allows engineers to simulate current density distribution, temperature gradients, and reactant utilization, thereby improving durability, efficiency, and safety of the device. When combined with experimental electrochemical impedance data, these models can also be used to calibrate degradation models and forecast long-term performance.

A rapidly growing area is the application of CFD in photobioreactor design for algal biomass production [190]. Microalgae cultivation systems are used to convert CO₂ and sunlight into lipids or carbohydrates, which are then processed into biofuels. CFD simulations are particularly valuable in modeling light distribution, nutrient transport, and hydrodynamic stresses inside the reactor. These factors directly affect growth rates, lipid accumulation, and even cell viability. For instance, simulations can reveal how internal mixing affects light/dark cycles for cells suspended in dense cultures, or how bubble sparging creates shear forces that may damage delicate algal strains. By optimizing reactor geometry, bubble size, or agitation rates, productivity can be significantly enhanced without increasing operational energy input [191]. As large-scale algal systems become more economically viable, CFD will play a crucial role in scaling up laboratory designs to commercial-scale

cultivation.

Through these diverse examples, it becomes clear that CFD-coupled chemical reaction modeling is not merely a theoretical tool, but a critical enabler of innovation in renewable energy systems. It helps bridge the gap between molecular-level understanding and system-scale design, offering insights that are otherwise inaccessible by purely experimental or purely empirical approaches.

In summary, while recent advances have greatly improved the simulation of reactive flows, challenges related to multi-scale coupling, stiffness, and turbulence modeling remain. These issues motivate the exploration of hybrid approaches and AI-driven frameworks discussed in the following sections.

3. AI revolutionizes CFD simulations

Traditional CFD methods often suffer from several key limitations, as shown in Fig. 8. First, achieving accurate results typically requires excellent computational grids, significantly increasing computational cost and simulation time [192]. Second, the accuracy of numerical methods is highly sensitive to the quality of the computational mesh [193]. In addition, setting appropriate boundary conditions can be difficult and lead to unstable or failed solutions [194]. These problems become even more severe when multiple physical phenomena are coupled, often causing numerical instability and convergence issues. As a result, CFD simulations can become both time-consuming and error-prone, especially for real-world engineering problems. Artificial intelligence (AI) has emerged as a powerful tool to address these challenges in recent years [195]. By integrating multiple data sources, improving model adaptability, reducing grid dependency, and accelerating prediction processes, AI offers promising new ways to enhance CFD simulations' efficiency, robustness, and scalability [196,197]. This review explores how AI transforms traditional CFD workflows and highlights its potential to overcome long-standing limitations in the field.

Fig. 9 presents a conceptual framework for integrating CFD with AI-based modeling to address the challenges inherent in multiphase flows with thermochemical reactions. It illustrates the synergy between simulation data, surrogate modeling, and core transport phenomena.

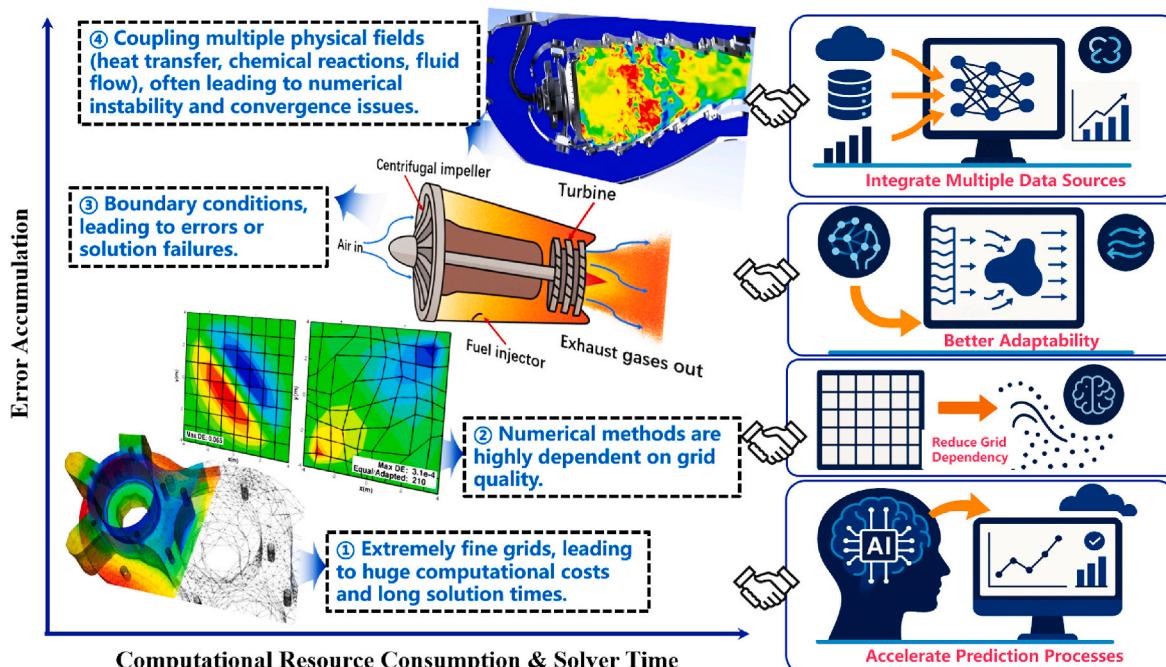


Fig. 8. Challenges in physics-based simulations and AI-Driven solutions for enhanced computational efficiency.

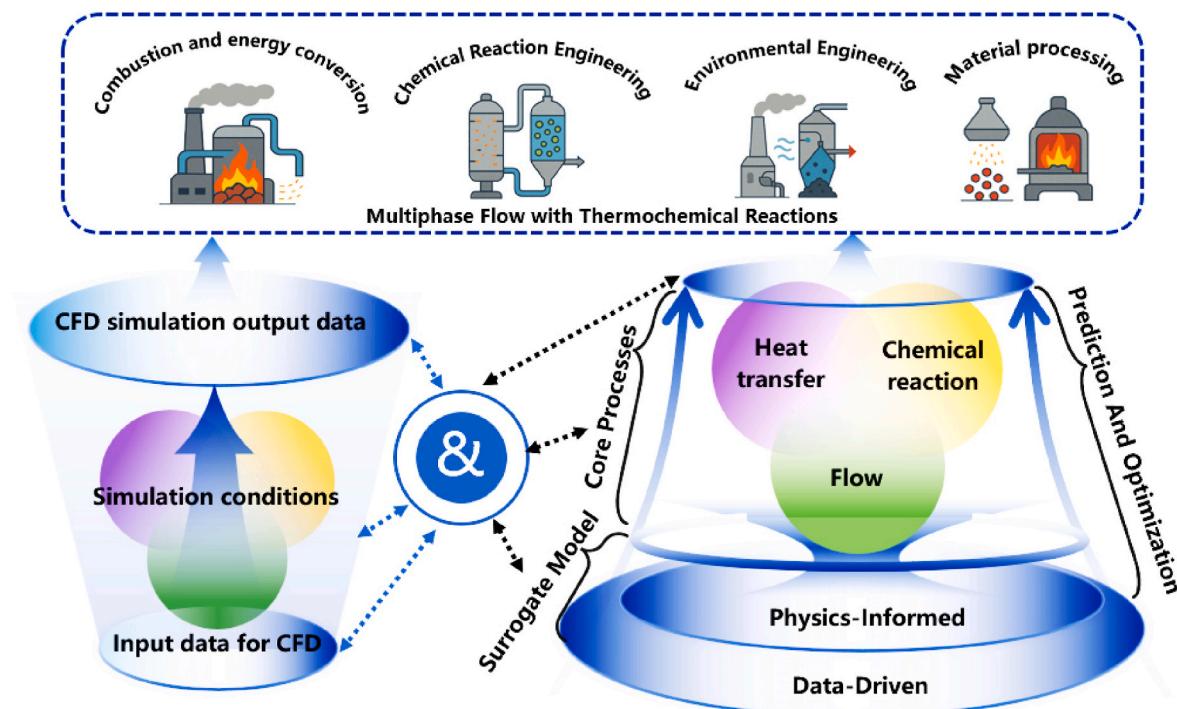


Fig. 9. Conceptual framework for integrating CFD simulation with AI.

This integrated approach enables efficient prediction and optimization across diverse application domains, including combustion, chemical processing, and environmental engineering. Building on this framework, current research in AI-enhanced CFD can be broadly categorized into four key directions. The first involves AI-assisted CFD solving, where machine learning techniques are applied to accelerate convergence, enhance solver robustness, and reduce computational cost [198,199]. The second focuses on data-driven turbulence modeling, in which AI models learn from high-fidelity datasets to replicate complex turbulent behaviors in reactive and multiphase environments. Since turbulence directly influences mixing, reaction rates, and interfacial dynamics, accurate modeling of turbulent transport is essential for predictive reliability [70]. The third direction is the development of surrogate models, which serve as fast and efficient approximations of full CFD simulations. These models facilitate rapid design optimization, uncertainty quantification, and real-time prediction, significantly expanding the practical applicability of CFD in engineering workflows [200]. Lastly, physics-informed modeling has gained increasing attention, wherein machine learning architectures are constrained by governing physical laws—such as conservation of mass, momentum, and energy—to ensure physically consistent and generalizable predictions [74, 201]. These research directions reflect a paradigm shift in CFD methodologies, emphasizing hybrid modeling strategies that unify data-driven learning with domain knowledge to enable scalable, accurate, and interpretable simulation of complex reactive multiphase systems.

3.1. Fundamentals of machine learning

3.1.1. Evolution of machine learning in CFD applications

Artificial Intelligence (AI) aims to create intelligent systems, while Machine Learning (ML), a subset of AI, focuses on enabling systems to learn from data without explicit programming [202]. ML is typically categorized into three types based on learning objectives, as shown in Fig. 10: Supervised learning, where the model learns from labeled data to predict outputs [203]; unsupervised learning, where the model identifies patterns in unlabeled data; and reinforcement learning, where the

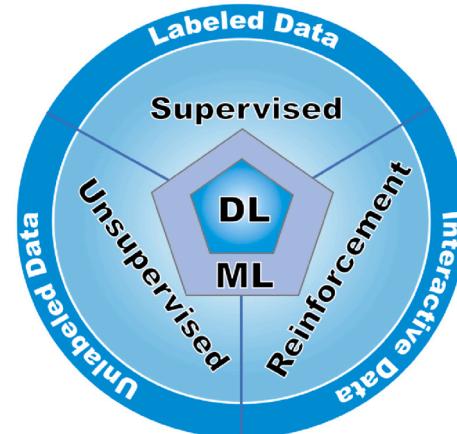


Fig. 10. Classification of ML approaches based on data type.

model learns through trial and error by receiving feedback from an environment [204]. Data plays a crucial role in ML, and models are trained using training data and evaluated using testing data to ensure they generalize well to new, unseen examples [205]. The success of machine learning models depends on optimizing algorithms to minimize errors and avoid issues like overfitting or underfitting [206,207]. Evaluation metrics such as accuracy, precision, recall, and F1 score are used to assess performance [208]. Deep learning, a subset of ML, uses complex neural networks to learn highly intricate patterns, making it especially effective in tasks like image recognition and natural language processing [209–211].

The development of ML in CFD has evolved from auxiliary modeling to deep integration, as shown in Fig. 11. In the early stages, simple statistical methods and techniques were used to improve turbulence closure models and data fitting [212]. For instance, the statistical theory of turbulence, which began in the early 1920s with G.I. Taylor's analysis of turbulence's "diffusing power," laid the foundation for statistical

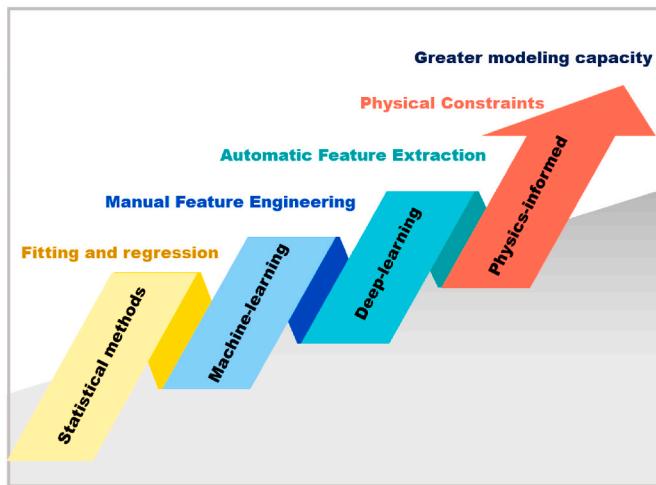


Fig. 11. Evolution of computational techniques in CFD

approaches in turbulence modeling. Additionally, researchers' development of the eddy damped quasi-normal Markovian (EDQNM) approximation in the 1970s applied statistical methods to turbulence modeling, improving the accuracy of closure models [213]. Subsequently, data-driven modeling gained prominence, leveraging high-fidelity simulation data to optimize parameter prediction and reduce computational complexity in turbulence and multiphase flow simulations [214]. Zhu et al. developed a data-driven approach for turbulence modeling that utilizes DNS data to train machine learning models, enhancing the accuracy of Reynolds stress predictions in various flow scenarios [215]. Bode et al. explored deep learning techniques for subgrid modeling in turbulent flows, demonstrating that neural networks trained on DNS data can effectively capture small-scale turbulence effects, thereby improving LES predictions while maintaining computational efficiency [216]. The introduction of deep learning further advanced flow field prediction, turbulence modeling, and real-time optimization, with techniques like CNNs and reinforcement learning widely applied to complex flow and multiphase interface modeling [217]. More recently, PINNs have combined machine learning with the fundamental equations of fluid dynamics, significantly enhancing the efficiency and accuracy of multi-scale coupling simulations and industrial CFD applications [110]. This progression reflects the transition of ML from purely data-driven approaches to

physics-integrated solutions, offering efficient methods for tackling complex fluid dynamics problems.

3.1.2. Overview of neural network architectures and working principles

Artificial Neural Networks (ANNs) in CFD has become a cornerstone of AI-enhanced workflows, facilitating the development of efficient, scalable, and accurate models for turbulence prediction, surrogate simulations, and physics-constrained inference. By learning complex nonlinear mappings from data, neural networks address critical challenges in CFD, offering innovative solutions for high-dimensional flow modeling, time-dependent dynamics, and unstructured mesh processing. This section presents an overview of the neural network architectures commonly employed in CFD applications, as shown in Fig. 12, providing the necessary theoretical foundation for subsequent methods explored in this work.

Multilayer Perceptrons (MLPs), or feedforward neural networks, serve as the basic neural network architecture. These networks consist of interconnected layers of neurons, where each layer performs a linear transformation followed by a nonlinear activation function (such as ReLU, sigmoid, or tanh). Trained via gradient-based optimization using backpropagation, MLPs are capable of universal function approximation. However, their dense connectivity and lack of spatial or temporal priors often limit their scalability for high-dimensional CFD problems, where data sparsity and computational demands are significant.

Convolutional Neural Networks (CNNs) are widely adopted in CFD to handle spatial complexity. CNNs introduce local receptive fields and weight sharing, which makes them particularly effective at capturing spatial correlations in structured data such as velocity or pressure fields. Their ability to extract multi-scale features from flow images or CFD grids has led to their extensive application in flow reconstruction, interface detection, and subgrid turbulence modeling.

For time-dependent flows, Recurrent Neural Networks (RNNs), particularly their variant Long Short-Term Memory (LSTM) networks, are employed to model temporal dependencies. These networks can maintain memory of past inputs, enabling dynamic sequence modeling. RNNs and LSTMs are thus ideal for time-resolved simulations, adaptive solvers, and real-time control systems, making them critical for unsteady flow simulations.

Another important aspect of CFD involves dimensionality reduction for high-dimensional simulation outputs. Autoencoders (AEs) and Variational Autoencoders (VAEs) are frequently used to compress flow field data into low-dimensional latent spaces. This compression facilitates efficient surrogate modeling, visualization, and uncertainty

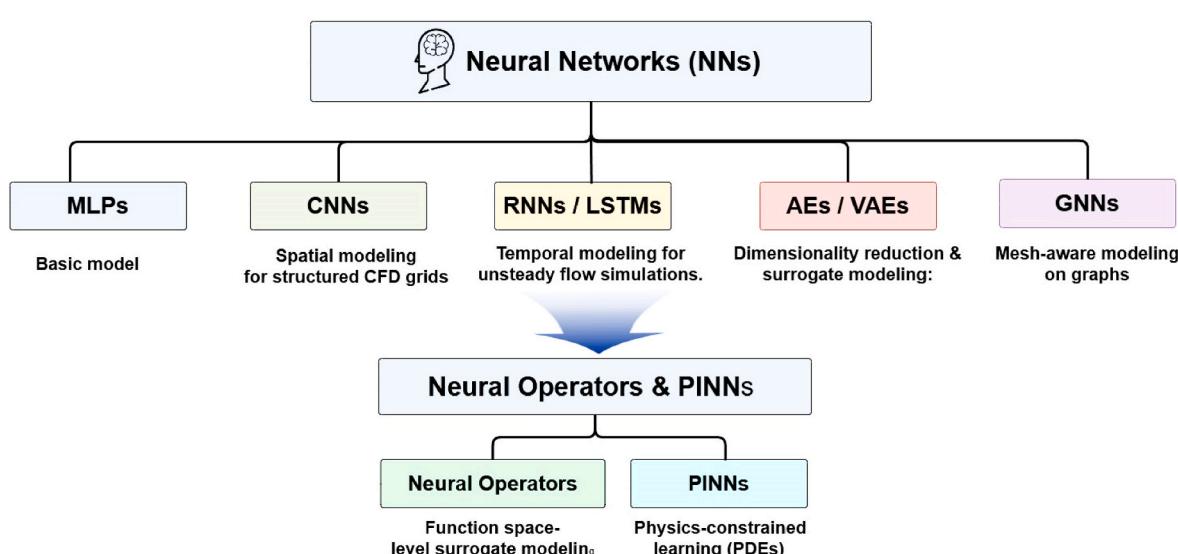


Fig. 12. Neural network family tree.

quantification, enabling the handling of large-scale data typical of CFD simulations.

In the case of unstructured meshes, Graph Neural Networks (GNNs) provide an efficient approach for processing data defined on graphs. By treating mesh nodes as graph nodes and encoding relationships between elements as edges, GNNs facilitate information propagation across mesh-like structures. This makes GNNs particularly useful for CFD simulations involving unstructured grids and mesh-adaptive learning tasks.

Neural Operators, such as the Fourier Neural Operator (FNO) and DeepONet, have emerged as a promising alternative to traditional surrogate models. Unlike conventional neural networks that map finite-dimensional vectors, neural operators directly learn solution mappings between infinite-dimensional function spaces, enabling mesh-independent surrogate modeling. This capability allows them to generalize across varying boundary and initial conditions, providing a versatile and efficient solution to complex PDEs (discussed in Section 3.4.2).

Finally, A more recent advancement in neural network architectures is the development of Physics-Informed Neural Networks (PINNs). These models directly incorporate physical constraints—such as partial differential equations (PDEs) and boundary conditions—into the loss function during training. This integration ensures that the solutions learned by the network are data-efficient and physically consistent. PINNs are particularly advantageous in scenarios with limited labeled data or complex multi-physics interactions, as detailed in Section 3.5.

Recent advancements have demonstrated the effectiveness of artificial neural networks (ANNs) in modeling complex thermochemical reaction systems in real-world applications. For instance, Irfan et al. [218] developed an ANN model to predict NO removal efficiency during the NH₃–NO–SCR process over a CuO/γ-Al₂O₃ catalyst in a bubbling fluidized bed reactor. The study showed that the ANN model provided more accurate and generalized predictions across varying operating conditions, such as reaction temperature, gas velocity, and NH₃/NO ratio compared to a mechanistic kinetic model. This demonstrates the ANN's capacity to handle non-linear dynamics in industrial-scale catalytic reactors. In another case, Liou et al. [219] employed an ANN-based regression model to predict nitrogen oxide emissions from Taiwan's Taichung thermal power plant. Their model incorporated both fuel characteristics and boiler operation parameters and achieved a high R² value of 0.97. This highlights the ANN's potential for real-time environmental monitoring and emission control in coal-fired power generation. These examples underscore the practical applicability of AI-based modeling in thermochemical systems, validating the feasibility and accuracy of such approaches under realistic industrial conditions.

3.2. AI-assisted CFD solving

The traditional process of solving CFD problems involves key stages, such as geometric discretization, time integration, and the selection and optimization of solving algorithms. These stages' accuracy, efficiency, and stability depend heavily on the appropriate choice and tuning of several critical parameters. These parameters, including geometric discretization parameters, time integration parameters, and solving algorithm parameters, significantly influence the results of CFD simulations [220]. Zhu et al. [221] highlighted that complex flow simulations, particularly those involving high Reynolds numbers, unsteady flows, and multiphase systems, face significant challenges in selecting appropriate parameters. This issue is compounded by the difficulties in accurately predicting multiphase flow dynamics, which require advanced techniques like machine learning to enhance model robustness and computational efficiency.

Geometric discretization parameters refer to how the physical domain is divided into small cells or meshes. This division has a direct impact on both the solution accuracy and computational resource consumption. Xu et al. [222] explored the effect of geometric discretization

in mesh-based modeling and proposed conditionally-parameterized neural networks (CP-Nets) to improve mesh-based simulations of physical systems. They demonstrated that CP-Nets effectively captured the hierarchical relationships between the physical quantities and the discretization parameters by incorporating mesh-specific discretization features directly into the neural network architecture. This approach significantly enhanced model performance, especially in complex simulations such as unsteady flows with chemical reactions. Wu et al. [223] developed a regression model-guided moving mesh method that combines machine learning with variational adaptation techniques, significantly improving flow feature resolution while maintaining mesh topology and reducing reliance on traditional iterative CFD solvers.

AI has also enabled adaptive mesh refinement, where the mesh resolution is adjusted dynamically based on flow characteristics. This approach ensures that critical regions of the flow field receive higher resolution for greater accuracy, while areas with less significant impact on the overall result maintain lower computational cost. Zhu et al. [224] proposed a physics-informed neural network (PINN)-based adaptive mesh refinement strategy that utilizes PDE residuals to identify regions needing higher resolution, achieving comparable or improved solution accuracy with significantly fewer mesh cells than traditional refinement indicators. By automating these processes, AI contributes to a more efficient and precise CFD analysis, reducing the need for manual intervention and improving the overall performance of CFD simulations.

The choice of time integration parameters, particularly the time step, is crucial for ensuring computational stability and precision. Han et al. [225] introduced an AI-enhanced adaptive time stepping algorithm that dynamically optimizes the time step size by learning from system states, significantly improving efficiency while maintaining high accuracy. In addition, the selection of solving algorithm parameters pertains to the numerical methods employed, such as turbulence modeling or the methods for solving the Navier-Stokes equations. These factors directly affect the efficiency and accuracy of the CFD solving process. Sousa et al. [226] proposed a hybrid solver architecture incorporating machine learning-based surrogate models into the PISO algorithm to optimize pressure-momentum coupling, significantly reducing computation time without compromising solution accuracy. In complex flow simulations, particularly those involving high Reynolds numbers, unsteady flows, multiphase flows, or complicated geometries, selecting appropriate parameters remains a significant challenge [227]. Kim et al. [228] developed a convolutional neural network model to predict turbulent heat transfer based solely on wall-shear stress and pressure data, achieving a correlation coefficient of 0.98 with DNS results and demonstrating robustness across varying Reynolds numbers. This reduces the number of iterations required in the traditional solving process, thus speeding up the overall computation.

Despite the substantial gains in accuracy and automation offered by AI-assisted CFD solvers, it is important to acknowledge that these methods often come with significant computational costs during the training phase. Neural networks, particularly deep architectures used in surrogate modeling, adaptive meshing, and time stepping, require extensive high-fidelity datasets and may take hours or even days to train, depending on the problem scale and network complexity. This presents a critical trade-off: while training can be computationally intensive, once trained, these models enable rapid inference, support real-time optimization, and reduce the need for repeated manual tuning across different simulation scenarios. With the growing availability of GPU acceleration, parallel computing, and transfer learning techniques, the training burden is being mitigated, making AI-based methods increasingly viable for industrial-scale applications. As the following sections demonstrate, this paradigm—front-loaded training with long-term computational benefits—is a recurring theme across AI-enhanced turbulence modeling and multiphysics simulation.

3.3. Data-driven turbulence modelling

3.3.1. Enhancing and developing turbulence models

Conventional turbulence models rely on empirical closures and assumptions. Data-driven turbulence modeling leverages large datasets of high-fidelity turbulence data, such as Direct Numerical Simulation (DNS), to enhance traditional turbulence models or develop entirely new closure models [229].

Enhance traditional turbulence models. This approach seeks to improve the accuracy of Reynolds-Averaged Navier-Stokes (RANS) or other turbulence simulation methods by utilizing machine learning (ML) and deep learning (DL) techniques. Eddy-viscosity models, commonly used in RANS simulations, offer a computationally efficient means of representing turbulence by relating viscosity to flow characteristics, such as velocity gradients [230]. However, these models often fail to capture the full complexity of turbulent flows due to their oversimplified nature. Data-driven techniques, intense neural networks (DNNs), present a promising solution for improving eddy viscosity predictions by learning directly from high-fidelity data. This approach can adaptively adjust turbulence viscosity based on local flow features, thus enhancing the accuracy of RANS predictions, especially in cases involving complex or unsteady turbulence. Zhang et al. [70] reviewed recent advances in ML-based turbulence modeling and underscored how deep neural networks can enhance eddy viscosity predictions, especially by learning from high-fidelity data, while also noting challenges such as data quality, physical interpretability, and generalization to unseen flow regimes.

Beyond improving existing models, data-driven techniques offer the potential to develop new closure models that do not rely on empirical assumptions. By learning directly from high-fidelity turbulence data, entirely data-driven models can predict Reynolds stresses and other turbulence quantities based on flow features. Zhu et al. [215] proposed a data-driven turbulence modeling framework that directly learns Reynolds stress from DNS data using Gaussian process regression, with RANS flow features as inputs. Their method improved both Reynolds stress prediction and the propagated velocity fields, demonstrating its potential to enhance RANS accuracy in canonical turbulent channel flows. This approach provides a more flexible and accurate means of representing turbulence, bypassing the need for traditional closure models and offering insight into the nonlinear relationships between turbulence quantities that conventional models cannot capture. Fiore et al. [231] introduced a hybrid training framework that integrates DNS and RANS data to improve the generalizability of data-driven thermal closures. By enabling the model to detect input fidelity and adjust accordingly, their approach reduces sensitivity to Reynolds stress inconsistencies and improves predictive robustness in RANS environments.

In Large Eddy Simulation (LES), subgrid-scale turbulence is not directly resolved, requiring models to predict the unresolved effects. Traditional subgrid-scale models often rely on heuristic formulations, which can be inaccurate, particularly in flows with strong anisotropy or high turbulence intensity. Data-driven surrogate models, trained on DNS or LES data, have shown promise in providing more accurate predictions of these unresolved effects. Shin et al. [232] proposed a deep learning-based subgrid-scale model, trained on filtered DNS data, to predict flame surface density using only local inputs. Their model outperforms traditional algebraic models in LES of premixed turbulent combustion, demonstrating the potential of deep learning to improve subgrid-scale modeling. Maulik et al. [233] proposed a physics-informed deep learning framework for LES closures, where artificial neural networks are trained to learn optimal convolution and deconvolution maps between coarse-grained and DNS data. Their approach bypasses explicit eddy-viscosity modeling and blends structural and functional modeling concepts, achieving accurate and stable subgrid-scale predictions for Kraichnan turbulence. This combination of reliability and flexibility offers a balanced solution for turbulence modeling.

3.3.2. Uncertainty quantification and generalization

One of the advantages of data-driven methods is their potential to improve uncertainty quantification in turbulence modeling. Traditional models often struggle to quantify the uncertainty in their predictions, which is crucial for engineering applications where variability in flow conditions must be considered. This capability is particularly valuable in design and decision-making processes, where it is essential to assess the reliability of simulation results under varying conditions. Sudharsun et al. [234] developed a neural network-based framework to model pressure-strain correlations and quantify uncertainty in the Reynolds stress model. By training on high-fidelity DNS data, their model accurately predicted both isotropic and anisotropic components of the pressure-strain tensor, and used a binary classifier to identify error-prone regions in RANS simulations with up to 95 % accuracy across various Reynolds numbers. Integrating uncertainty quantification into turbulence modeling allows engineers to make more informed decisions, particularly in complex scenarios where traditional models fall short. As these data-driven methods evolve, they promise to improve the robustness and reliability of turbulence predictions in practical applications, such as aerodynamic design, weather forecasting, and industrial flow simulations.

Despite the promise of data-driven turbulence modeling, significant challenges persist, particularly concerning overfitting and generalization. Several strategies have been proposed to address these challenges. Kraposhin et al. [235] proposed a regularized quasi-hydrodynamic (QHD) numerical framework for incompressible viscous flows, implemented in OpenFOAM. Their approach introduces a tunable regularization parameter to enhance numerical stability and reduce spurious oscillations, acting similarly to regularization in machine learning. The QHD algorithm demonstrated robust performance across various benchmark cases, showing good accuracy and mesh-independence without the need for additional iterative corrections used in traditional PISO or SIMPLE solvers. This regularization technique not only improves the stability of simulations but also helps mitigate overfitting, enhancing the generalization ability of turbulence models in diverse flow regimes. Combining physical-based regularization with machine learning strategies provides a promising avenue for developing more reliable and adaptable turbulence models that can perform well under various conditions.

Generative Adversarial Networks (GANs) and Physics-Embedded GANs (Phy-GANs), which consist of two main components: a generator and a discriminator, present a promising approach for enhancing the generalization capability of turbulence models. GANs, by their nature, enable the model to learn from a broader spectrum of turbulence behaviors, as they generate synthetic flow data across various conditions. This synthetic data generation allows the model to encounter a wider array of scenarios, ultimately enhancing its ability to generalize to unseen turbulence states. On the other hand, Physics-Embedded GANs further improve this process by incorporating physical constraints, such as the Navier-Stokes equations, into the adversarial training mechanism. This incorporation ensures that the generated synthetic data is diverse and physically consistent with the underlying laws of fluid dynamics. Arora et al. [236] explored the theoretical foundations of GAN generalization and equilibrium, shedding light on the limitations of standard metrics, such as Jensen-Shannon (JS) divergence and Wasserstein distance. While these traditional metrics do not guarantee generalization when using finite samples, the authors highlighted a weaker yet more reliable measure—neural network distance—as a better predictor of generalization performance. Moreover, they proposed the MIX + GAN framework, which utilizes a finite mixture of generators and discriminators to stabilize the training process and enhance overall performance. This novel approach achieved empirical improvements on benchmark datasets, illustrating the potential of combining mixture models with adversarial training for superior generalization and robustness in turbulence modeling.

Reinforcement learning (RL) has emerged as a powerful tool to

enhance the generalization capabilities of turbulence models, complementing the progress made through Generative Adversarial Networks (GANs) and Physics-Embedded GANs. Unlike traditional machine learning approaches that rely on static datasets, RL optimizes model parameters through iterative interactions with the environment. This dynamic learning approach allows turbulence models to adapt to varying flow conditions, improving their robustness and applicability in complex real-world scenarios. By leveraging continuous feedback from model predictions, RL enables turbulence models to self-adjust in response to changing flow characteristics. This adaptability is particularly crucial for applications involving real-time flow control and optimization, where maintaining model accuracy across diverse conditions is essential. Moreover, integrating deep neural networks with RL further enhances the model's ability to generalize across a wide range of flow regimes without requiring extensive retraining. Duraisamy et al. [237] provided a comprehensive review of machine learning-enhanced Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) models, highlighting RL as an innovative and effective framework for data-driven flow control. The review emphasized the importance of incorporating physics-informed constraints, model-consistent training, and interdisciplinary collaboration in developing accurate and generalizable turbulence models. Through its feedback-driven learning mechanism, RL offers a powerful tool for improving model fidelity and ensuring consistent performance in dynamically changing environments.

3.4. Construct the surrogate models

In complex multiphase and thermochemical simulations, the computational cost associated with traditional high-fidelity models can be prohibitively expensive, especially when repeated simulations are required for optimization or design exploration. Surrogate modeling, powered by machine learning, offers a promising solution to this challenge by creating reduced-order models that approximate the behavior of the system with far fewer computational resources. These surrogate models can provide rapid predictions after an initial training phase, drastically reducing the time and cost of simulating complex physical systems. The training phase, which involves learning from high-fidelity simulation data, can require substantial computational effort, particularly when dealing with large, multi-physics systems. The system's complexity and the data quality are key factors influencing the overall training time. Despite these initial costs, once trained, surrogate models can offer dramatic reductions in computational time for subsequent simulations, making them invaluable tools for real-time prediction and iterative processes in multiphysics modeling.

3.4.1. Data-based surrogate models

Developing efficient and accurate surrogate models has become a pivotal focus in CFD and reaction engineering in reactive multiphase flows involving complex thermochemical processes. These systems are often characterized by strongly coupled physical phenomena—mass, momentum, and energy transport intricately interacting with multiple chemical reactions—resulting in highly nonlinear and computationally expensive models. While accurate, direct numerical simulations (e.g., CFD or DNS) are prohibitively costly for iterative tasks such as design optimization, uncertainty quantification, or real-time control. In this context, surrogate modeling has become a strategy to reduce computational burden while retaining predictive fidelity significantly.

Surrogate models are constructed from a limited set of high-fidelity simulation data, experimental observations, or measured responses to capture the input-output relationship through a mathematical mapping. A typical surrogate modeling workflow involves four key stages: sampling the input parameter space, conducting simulations or experiments, training the model, and evaluating and deploying it. In thermochemical multiphase flows, input parameters may include temperature, pressure, velocity, species concentrations, and reaction rate constants—variables

that exhibit high-dimensional, nonlinear couplings. These complexities impose stringent requirements on the model's generalization and representational capabilities.

One of the primary challenges in this domain is high dimensionality. A representative case might involve tens of input variables spanning broad numerical ranges. Classical design-of-experiment methods such as Latin Hypercube Sampling (LHS) or Sobol sequences become ineffective in high dimensions due to their inability to cover the parameter space adequately. Furthermore, many samples in high-dimensional space may be redundant, which contributes little to capturing system behavior and degrades model robustness and accuracy. Ling et al. [238] conducted a comprehensive review on adaptive-surrogate-model-assisted RBDO methods and emphasized that classical DoE techniques such as LHS and Sobol sequences are often inadequate in high-dimensional settings, as they can lead to redundant sampling and inefficient surrogate model training. To address this, the authors proposed adaptive and sequential sampling strategies, which leverage prediction uncertainty to improve sampling efficiency and model accuracy across the design space.

To address this, adaptive sampling strategies have been proposed. These leverage preliminary surrogate models to identify regions with steep response gradients or high predictive uncertainty, thereby guiding additional sampling efforts. For instance, Gaussian Process Regression (GPR) naturally quantifies predictive uncertainty, which can inform variance-based adaptive sampling strategies. Minh et al. [239] developed a two-stage framework combining multiplicative dimensional reduction and GPR to perform global sensitivity analysis and uncertainty quantification on a crude distillation unit, demonstrating that predictive variance from GPR enables efficient surrogate modeling with significantly reduced simulation cost—up to 95 % less than traditional methods—while preserving accuracy. These active learning or information-based sampling approaches aim to extract maximal information from minimal samples, thereby enhancing modeling efficiency and expressiveness. This methodology has demonstrated superior performance over classical LHS in process simulation, catalytic reactor design, and combustion system optimization.

Deep learning techniques have also found increasing application in surrogate modeling of multiphase thermochemical systems. Compared to traditional response surface models or GPR, deep neural networks (DNNs) offer significantly enhanced expressiveness for highly nonlinear mappings. The effectiveness of deep neural networks as surrogate models has been extensively demonstrated in recent studies. Notably, Kochkov et al. [240] showcased that deep learning-based surrogates could reproduce high-fidelity fluid dynamics at a fraction of the computational cost traditional solvers require. Fig. 13(A) shows that their results revealed that the AI model maintained physical accuracy across various test conditions even with coarse input resolutions. Such findings highlight the transformative potential of AI-enabled surrogate modeling in achieving efficient, real-time CFD simulations. As a representative example, as shown in Fig. 13(B), Le et al. [241] developed a deep U-Net-based surrogate model for predicting steady-state incompressible laminar flows around 2D obstacles. Their method transforms CFD solutions into interpolated mesh-aligned features and learns to reconstruct velocity and pressure fields using an encoder-decoder architecture. The model demonstrated high accuracy across various shapes with significant speed-up over traditional solvers.

Architectures such as Convolutional Neural Networks (CNNs), Graph Neural Networks (GNNs), and Long Short-Term Memory networks (LSTMs) have been used to model spatial structures, temporal dynamics, and multi-physics interactions in these systems. A representative example is MeshGraphNets, proposed by Pfaff et al. [242], as shown in Fig. 13(C), which models physical dynamics on irregular meshes via message-passing GNNs. Separating mesh-space and world-space interactions and incorporating a learned remeshing module enables resolution-adaptive simulation across fluids, cloth, and structural systems. Zhou et al. [243] reviewed recent advances in uncertainty quantification for structural response and system identification, emphasizing

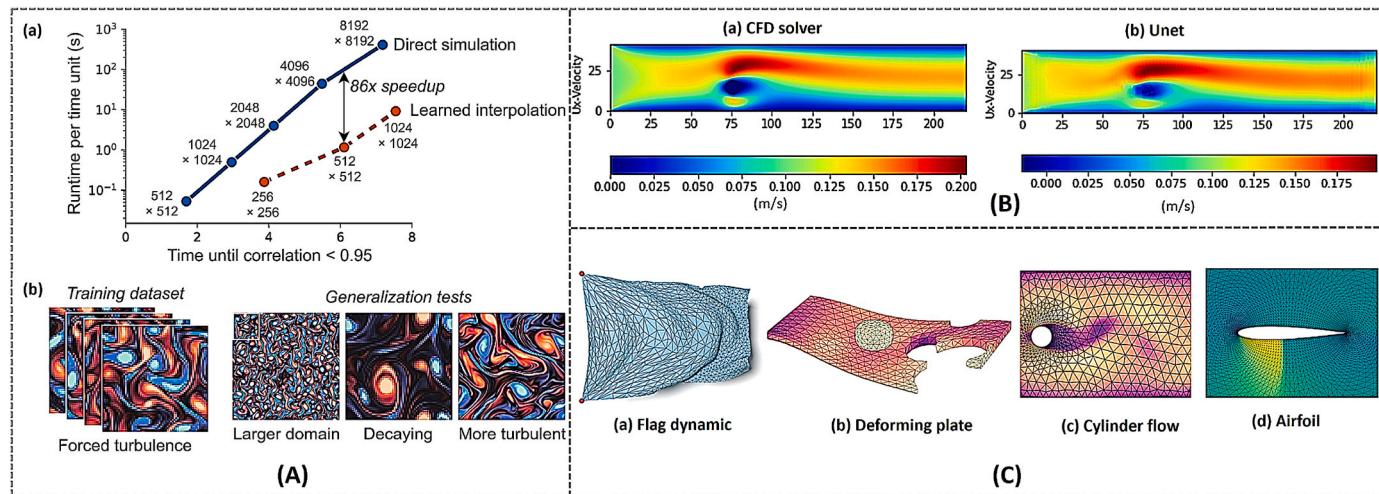


Fig. 13. (A) Deep learning-based correction enables accurate simulation of 2D Kolmogorov flow at significantly coarser resolutions. (a) Runtime vs. time until decorrelation shows that learned interpolation achieves up to 86 × speedup over direct simulation. (b) Model trained on forced turbulence generalizes to larger domains, decaying flows, and more turbulent regimes. [240]. (B) Comparison of velocity field predictions between a traditional CFD solver (a) and a UNet-based deep learning model (b). The UNet accurately reproduces key flow features with significantly reduced computational cost [241]. (C) Examples of physical systems simulated using message-passing GNNs on irregular meshes, including cloth (a), deformable structures (b), fluid around a cylinder (c), and airfoil flow (d). The model separates mesh- and world-space interactions and leverages a learned remeshing module for resolution-adaptive simulation [242].

how deep learning architectures such as CNNs, ResNets, and LSTMs have been increasingly adopted to capture complex spatial and temporal patterns in structural dynamics, especially under uncertain conditions. These architectures enable surrogate modeling and inverse identification with improved efficiency and robustness. Recent research has explored multiscale modeling by combining DNNs at different hierarchical levels—for example, capturing species diffusion and reaction kinetics at the microscale, and thermal convection or velocity fields at the macroscale—leading to more accurate and computationally efficient surrogate models. Wang et al. [110] provided a comprehensive and up-to-date survey on machine learning techniques in CFD, highlighting multiscale modeling with deep neural networks (DNNs) across hierarchical levels. They emphasized how DNNs have successfully captured microscale chemical kinetics and macroscale flow features, such as thermal convection, enabling more accurate, generalizable, and efficient surrogate models across complex CFD tasks.

Incorporating physical laws is another crucial development aimed at mitigating overfitting and alleviating data scarcity. Within the GPR framework, physical constraints such as conservation laws (mass, energy, momentum) can be embedded into the model architecture or objective function. One approach involves embedding partial differential equations (PDEs) directly into the loss function, or modifying kernel functions to reflect spatial correlation and boundary condition information. These physics-informed machine learning (PIML) methods have become central in modeling complex thermochemical systems, increasing model credibility and extrapolation capacity in undersampled regions. Farrag et al. [244] comprehensively reviewed PIML approaches in metal additive manufacturing, categorizing them into domain knowledge integration, simulation-based data usage, and physics-guided model training. They highlighted the unique advantages of PINNs in embedding governing physical laws into neural networks to enhance both model interpretability and predictive robustness, even under data-scarce and noisy conditions.

Another key application of surrogate models is uncertainty quantification (UQ). In thermochemical systems, many parameters are inherently uncertain—reaction rate constants may be estimated empirically, and species concentrations may be prone to measurement error [245]. Surrogate models enable efficient propagation of such uncertainties through fast prediction of response distributions. For example, GPR's predictive variance, combined with Monte Carlo simulations, facilitates

sensitivity analysis and robust optimization with substantially reduced computational cost. Minh et al. [239] proposed a two-stage uncertainty quantification framework combining multiplicative dimensional reduction and Gaussian process regression (GPR), which enabled accurate sensitivity analysis and surrogate-based optimization for crude distillation units (CDUs), while reducing the computational cost by over 95 % compared to conventional Quasi-Monte Carlo methods.

Despite recent progress, the construction of high-accuracy, generalizable surrogate models remains highly dependent on expensive high-fidelity simulation data. Strategies such as transfer learning, data augmentation, and multi-fidelity modeling have been proposed to address this limitation. The latter approach builds correlations between low-fidelity, low-cost models and a limited number of high-fidelity models to maintain accuracy while reducing computational expense. This technique is particularly effective for modeling multistage reaction systems, such as those involving localized hotspots in catalytic reactors or post-flame regions in combustion processes. Wang et al. [246] systematically reviewed recent advances in CFD-DEM modeling of dense gas-solid reacting flows, highlighting how emerging techniques such as data-driven closure models, multi-fidelity simulation frameworks, and physics-informed learning approaches have been integrated to tackle multi-scale and multi-physics challenges. They emphasized that incorporating methods like transfer learning and model acceleration techniques can significantly improve computational efficiency without sacrificing physical accuracy.

3.4.2. Neural operator-based surrogate models

In recent years, Neural Operators have emerged as a promising paradigm for learning mappings between infinite-dimensional function spaces, as shown in Table 4, with notable applications in computational physics, material science, and reactive multiphase flows [247]. Unlike traditional surrogate models that map from finite-dimensional parameter spaces to responses, neural operators learn function-to-function mappings—transforming input functions like initial or boundary conditions directly into solution fields such as temperature, velocity, or species distributions. This allows for mesh-free, end-to-end learning of the solution operator for PDEs, offering both high expressiveness and significantly faster inference.

Initially introduced by Lu et al. (2021), the concept was further advanced by Li et al. with the Fourier Neural Operator (FNO), which

Table 4
Comparison of representative neural operators.

Operator	Mechanism	Applications	References
FNO	Performs kernel convolution in the Fourier domain, then applies inverse transform to return to spatial domain.	Fluid dynamics, material simulations, CO ₂ sequestration.	[248–250]
DeepONet	Branch-trunk network structure encoding input functions and query locations separately.	Multiphase reaction modeling, physical control systems.	[251,252]
GNO	Extends operators to graph structures using graph convolution kernels.	Packed-bed reactors, multiphase systems.	[253,254]
PINO	Combines data loss with PDE-based physics loss in training.	Turbulence, inverse problems.	[252,255]
Transformer-based NO	Uses attention mechanism to model non-local relationships via variable kernels.	Mesh-independent modeling, unstructured geometry tasks.	[256,257]
Generative NO	Learns probabilistic mappings using GANs, diffusion models, or VAEs in function space.	Stochastic PDE modeling.	[258,259]

leverages Fourier transforms to capture global patterns in the frequency domain [260]. This structure provides intrinsic scale-invariance and is well-suited for predicting field evolution in complex physical systems. Zhu et al. [261] introduced the use of the Fourier Neural Operator (FNO) for the transient analysis and control of supercritical CO₂ cycles. By leveraging the FNO, the study significantly improved computational efficiency, drastically reducing memory and time consumption while accurately predicting the system's dynamics. This novel approach offers a promising alternative to traditional numerical methods, offering superior speed and precision in solving complex physical systems.

Another influential architecture is the DeepONet, which combines a trunk network that encodes spatial locations with a branch network that encodes sampled input functions [262]. This framework is beneficial for modeling coupled responses from multiple input fields, such as jointly predicting reaction rates from temperature and concentration fields. Recent extensions, such as Graph Neural Operators (GNOs) proposed by Li Z et al. [254], have further expanded applicability to unstructured meshes and complex geometries. This is crucial for systems with irregular multiphase boundaries, such as packed-bed reactors or turbulent combustion zones.

A key advantage of neural operators lies in their superior generalization capabilities. Traditional surrogate models often struggle with out-of-sample generalization, particularly under novel boundary conditions or geometrical configurations [263]. Neural operators, by training in function space, can extrapolate to unseen domains, as demonstrated in studies of combustion processes with variable reaction kinetics, inlet compositions, and boundary perturbations.

However, practical deployment of neural operators still faces several challenges. First, due to the high-dimensional output (entire fields), the models tend to be large and require substantial computational resources for training. Second, they are typically trained in a supervised manner, relying heavily on data from expensive CFD or numerical solvers, and can yield physically inconsistent solutions without constraints. This has led to the development of Physics-Informed Neural Operators (PINO), where physical laws (e.g., conservation equations) are incorporated into the training loss. Zhao et al. [264] provide a comprehensive review of advances in Physics-Informed Neural Networks (PINNs) and their applications in solving complex fluid dynamics problems. They discuss the challenges and improvements in using PINNs, particularly in modeling turbulence, multiphase flows, and multiscale systems, and highlight how integrating physical laws into the neural network architecture

enhances the accuracy and efficiency of the models.

Representative applications of neural operators in thermochemical systems include modeling surface reaction kinetics, predicting thermal runaway thresholds, and reconstructing multiphase turbulent combustion flows. These models enhance prediction efficiency and enable real-time feedback in control and design processes. Future research directions are expected to focus on architectural improvements (e.g., transformer-based neural operators), integration with multi-fidelity modeling (to enhance generalization under data scarcity), and probabilistic extensions (e.g., Bayesian Neural Operators) to support robust and trustworthy surrogate modeling frameworks for complex reactive multiphase systems.

3.5. Physics-informed modeling

3.5.1. Physics-informed neural networks

Physics-informed neural networks (PINNs) are a modeling framework that integrates physical laws, such as the Navier–Stokes equations, energy conservation, and mass conservation, directly into the neural network training process for efficient solving of partial differential equations (PDEs), as shown in Fig. 14. Unlike traditional numerical methods, which rely on mesh discretization and precise initial and boundary conditions [265], PINNs avoid high computational costs and boundary specification challenges. While deep learning and neural operator methods are more efficient in learning function space mappings, they often lack an intrinsic mechanism to enforce physical consistency, leading to physically unrealistic solutions that can reduce model stability and generalization. By incorporating physical constraints, PINNs bridge the gap between data-driven methods and physical laws, enhancing both stability and physical reliability while maintaining flexibility. This makes PINNs a promising solution for scientific computing, offering an accurate and efficient approach to solving complex, unseen flow scenarios.

The core idea of PINNs is to approximate physical field variables using a neural network, with the network's output constrained by both data fitting and the residuals of the underlying partial differential equations (PDEs). Automatic differentiation allows for the computation of these residuals, which are integrated into the overall loss function. This composite loss includes data errors (such as discrepancies in measured velocities or temperatures), equation residuals (e.g., from Navier–Stokes or reaction-diffusion equations), and constraints from initial and boundary conditions. The training process minimizes the PDE residuals in unsupervised or weakly supervised settings, making PINNs particularly effective for problems like heat conduction and steady-state flows. For instance, Xu et al. [266] employed PINNs to study heat conduction in porous media, demonstrating that the network could accurately learn temperature and heat flux distributions by minimizing the PDE residuals, achieving high accuracy and substantial speedups compared to traditional methods.

In the context of thermo-chemical reactive multiphase flows, Physics-Informed Neural Networks (PINNs) offer a powerful and unified modeling framework capable of simultaneously capturing the complex interactions among multiple interdependent physical variables. By directly embedding the governing equations of energy conservation, species transport, and chemical reaction kinetics into the learning process, PINNs can infer temperature distributions, reaction rates, and interfacial dynamics even without comprehensive labeled data. This makes them particularly well-suited for data-scarce scenarios where traditional modeling approaches struggle. For example, Jalili et al. [267] proposed a PINN-based model to investigate film boiling heat transfer, which involves strong coupling between thermal and multiphase flow fields. Without relying on observational data, their framework leveraged the inherent structure of the physical laws and transfer learning techniques to predict the underlying thermo-fluid behavior accurately. The study demonstrated the high fidelity and generalization capability of PINNs in capturing complex multiphase dynamics, thereby

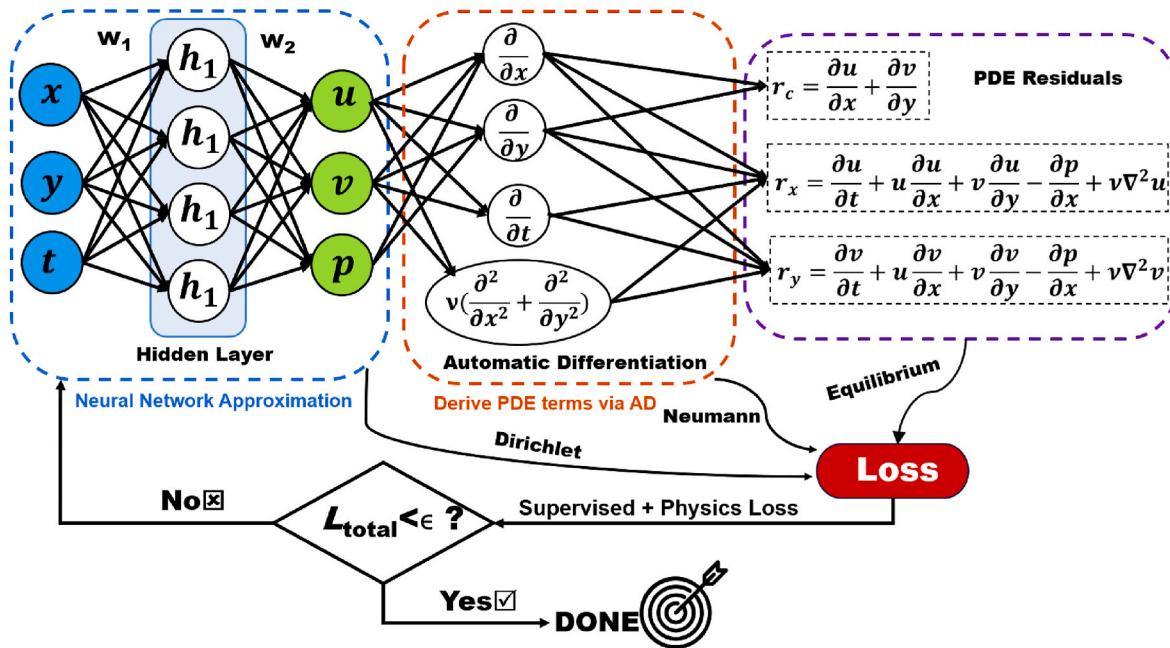


Fig. 14. Schematic of a Physics-Informed Neural Network (PINN) framework for solving incompressible Navier–Stokes equations. The network takes spatial and temporal coordinates (x, y, t) as input and outputs flow variables (u, v, p). PDE residuals are computed via automatic differentiation and incorporated into the loss function and boundary conditions. The total loss guides the training process until convergence.

underscoring their potential for advancing modeling and simulation in reactive and data-limited thermo-chemical systems. Similarly, Darlik and Peters [268] developed a PINN-based surrogate to reconstruct flow fields of dense biomass particles in a moving grate combustion chamber, as shown in Fig. 15. Their method bypasses traditional CFD-DEM coupling by treating the granular medium as a quasi-continuum. It accurately recovers velocity, pressure, and density fields using only CFD-mapped data and physical constraints.

3.5.2. Challenges and advances of PINNs

Despite the potential advantages of Physics-Informed Neural Networks (PINNs), several significant challenges persist, which limit their applicability to complex real-world problems. One of the primary challenges is the occurrence of vanishing gradients, especially in systems governed by stiff equations [269]. This issue can severely hinder the convergence during training, making it challenging to optimize the network effectively. Additionally, in coupled multiphysics problems, there is often a dynamic range discrepancy among different physical quantities, complicating the assignment of uniform weights to various components of the loss function.

Recent advancements have focused on refining the network architecture and implementing strategies such as adaptive weighting techniques to overcome these challenges [270]. For example, Maddu et al. [271] identified scale imbalances as a significant source of optimization bias in PINNs. They proposed an inverse Dirichlet weighting strategy, which dynamically adjusts the loss gradients across different objectives based on their residual magnitudes. This approach helps mitigate the problem of vanishing gradients, especially in multiscale issues, by ensuring that each physical variable contributes to the loss function in proportion to its scale. Such strategies have proven effective in improving convergence and stability, particularly in problems involving disparate physical quantities or extreme conditions.

Another critical innovation in overcoming the limitations of PINNs in complex systems is the implementation of domain decomposition techniques [264,272]. Traditional PINN architectures may struggle to handle systems with complex geometries or multiple coupled physical fields. To address this, domain decomposition PINNs partition the

physical domain into smaller subdomains, each independently trained. The interactions between subdomains are managed through network interfaces that connect the boundaries of each subdomain. This approach not only enhances computational efficiency by mitigating issues such as vanishing gradients in large-scale problems but also improves the stability of the training process by localizing complexity within each subdomain. For example, Dolean et al. [273] proposed a multilevel domain decomposition approach, extending the finite basis physics-informed neural networks (FBPINNs) concept. This method significantly improves performance when solving high-frequency and multiscale problems by facilitating better communication between subdomains, thus enhancing accuracy and computational efficiency.

Finally, developing multi-network collaborative training strategies, exemplified by eXtended PINNs (XPINNs), represents a notable advancement for systems characterized by multiple scales or coupled physical processes. In this approach, the overall model comprises multiple sub-networks, each dedicated to optimizing the residuals of a specific physical field, such as heat conduction, reaction-diffusion, or fluid dynamics. These sub-networks communicate through shared layers or interface modules, enabling the model to capture complex nonlinear interactions between physical processes. Jagtap et al. [274] introduced XPINNs as a generalized domain decomposition method, where the physical domain is divided into smaller subdomains, each handled by an independently trained PINN. This approach addresses challenges like vanishing or exploding gradients in large-scale problems by enhancing parallelization and computational efficiency. By applying simple interface conditions, XPINNs effectively stitch together the subdomains, allowing for the resolution of complex multiphysics problems with improved stability and reduced computational cost.

Physics-informed Neural Networks (PINNs) represent a significant advancement in the ability to solve complex multi-physics problems by effectively integrating physical laws with machine learning models. This innovative approach enables the models to leverage governing equations during the training process, which enhances their ability to generate valuable and accurate results. However, similar to other machine learning techniques, the training time for PINNs can be considerable, particularly when addressing large-scale systems. Given the

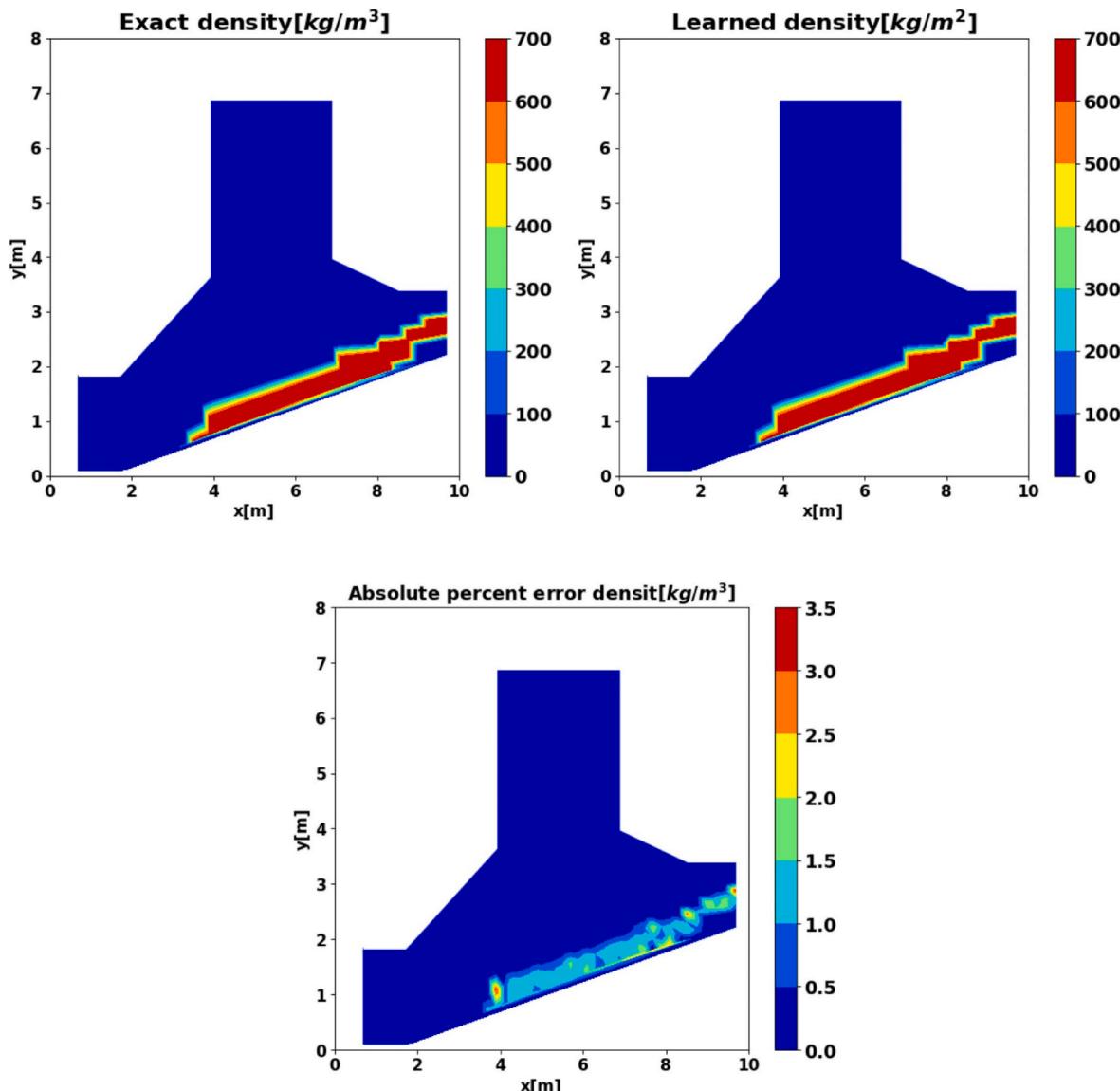


Fig. 15. Comparison between the ground truth and PINN-predicted density fields for biomass particle flow in a moving grate furnace. The top-left panel shows the exact particle density field obtained from high-fidelity CFD simulations. In contrast, the top-right panel presents the density field predicted by the physics-informed neural network (PINN). The bottom panel illustrates the absolute percent error between the two fields, demonstrating that the PINN achieves high accuracy with errors mostly below 2 %. This result highlights the capability of PINNs to reconstruct particle-resolved fields in quasi-continuum granular systems without relying on coupled CFD-DEM models [268].

substantial computational effort required for training these models, it is vital to consider the efficiency of the training processes. Recent developments in the field have made notable strides in addressing the challenges inherent in applying PINNs to intricate multi-physics and multiscale problems. Innovations such as dynamic loss weighting, domain decomposition, and multi-network collaborative training have significantly improved the stability, efficiency, and accuracy of PINNs. Together, these advancements facilitate the application of PINNs to a broader array of real-world scientific and engineering challenges, paving the way for their use in increasingly complex scenarios. By balancing the integration of physical principles with the demands of computational efficiency, PINNs hold the potential to revolutionize problem-solving across various domains.

4. Conclusion and perspectives

The integration of AI with Computational Fluid Dynamics (CFD) has already made significant strides in advancing multiphase flow

simulations and thermochemical reaction modeling, providing new pathways for solving complex engineering challenges. Looking ahead, the synergy between AI and CFD promises to play a pivotal role in accelerating the development of renewable and sustainable energy technologies. As the world moves towards cleaner energy solutions, AI-CFD integration offers unique opportunities to optimize processes in biomass energy, solar thermal systems, wind energy, and carbon capture and storage. AI models, with their ability to learn from large datasets and adapt to complex, nonlinear systems, could enhance the design and performance of these technologies, making them more efficient and cost-effective.

While AI-CFD integration holds immense promise, it also raises ethical considerations that must be addressed to ensure responsible implementation. Two major concerns are data privacy and model interpretability. More research is needed to develop explainable AI methods that enhance model transparency and provide users with insights into how AI models arrive at their predictions. Besides, current research in this area is disproportionately concentrated on simplified,

canonical benchmarks—such as flow around circular cylinders, NACA airfoils, Rayleigh–Bénard convection, and natural convection in square cavities. While these test cases are essential for validation, they lack real-world systems' geometric and physical complexity. Consequently, many AI-CFD frameworks exhibit limited generalizability and often struggle in turbulent, multiphase, or dynamically evolving environments. Besides, the training time of the neural network is affected by many factors, including the size of the data set, the complexity of the model, and the parameter adjustment during the training process, so AI-CFD frameworks require a lot of training time at the start. It is important to manage this training time effectively to ensure the process remains practical and efficient.

Several challenges must be addressed to realize the potential of AI-enhanced CFD fully.

- (1) Data and Generalization: AI models typically require extensive high-fidelity training data, which can be costly or impractical to obtain in complex systems. Extrapolation to unseen flow conditions and geometries remains a core issue.
- (2) Physical Consistency: Even with physics-informed architectures, models can exhibit instability or convergence issues in stiff or ill-posed problems.
- (3) Computational Cost: Training deep learning models comes with high computational demands, which may cancel out the speed improvements gained during inference.
- (4) Ethical and Interpretability Concerns: The increasing use of black-box AI models in CFD necessitates careful consideration of transparency, fairness, and data privacy, particularly in safety-critical applications.

Specific Areas for Future Research.

- (1) AI-enhanced Thermochemical Reaction Modeling: Further development is needed in integrating AI-driven approaches like Physics-Informed Neural Networks (PINNs) for high-fidelity simulations of combustion, gasification, and pyrolysis processes in renewable energy applications.
- (2) Optimization of Energy Storage Systems: AI-CFD models could play a crucial role in the optimization of energy storage systems (e.g., batteries, supercapacitors) by simulating thermal, chemical, and flow interactions, which are vital for the stability and efficiency of storage solutions.
- (3) Power networks Integration of Renewable Energy: AI-CFD simulations could provide insights into the dynamic behavior of energy power networks with a high penetration of renewable sources, addressing challenges related to energy distribution, storage, and power networks stability.
- (4) AI for Sustainable Manufacturing: AI-CFD could be used to optimize manufacturing processes for renewable energy technologies, reducing energy consumption and material waste in the production of solar panels, wind turbines, and battery systems.

In conclusion, the integration of AI with CFD opens a vast array of possibilities in advancing renewable energy technologies, driving us toward a more sustainable and energy-efficient future. The next decade will likely see groundbreaking advancements in this area, requiring interdisciplinary collaboration and innovation to address the growing demands of global energy systems. While AI introduces new challenges in data quality, generalization, and physical consistency, its integration with traditional numerical methods opens new avenues for model acceleration, hybrid learning, and adaptive computation. Future progress will rely on advances in interpretable AI, scalable computing infrastructure, and domain-informed datasets to fully realize the transformative potential of AI-assisted CFD.

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.

Acknowledgments

This work was supported by the Liaoning Provincial Science and Technology Plan Project (2023JH1/10400007) and the Fundamental Research Funds for the Central Universities (DUT24ZD103), and the China Scholarship Council (202406060182). The authors thank the Liaoning Provincial Department of Science and Technology for its support and all collaborators involved in the research.

Data availability

Data will be made available on request.

References

- [1] Wang FZ, Animasaun IL, Muhammad T, Okoya SS. Recent advancements in fluid dynamics: drag reduction, lift generation, computational fluid dynamics, turbulence modelling, and multiphase flow. *Arabian J Sci Eng* 2024;49:10237–49. <https://doi.org/10.1007/s13369-024-08945-3>.
- [2] Zhu LT, Chen XZ, Bo OY, Yan WC, Lei H, Chen Z, et al. Review of machine learning for hydrodynamics, transport, and reactions in multiphase flows and reactors. *Ind Eng Chem Res* 2022;61:9901–49. <https://doi.org/10.1021/acs.iecr.2c01036>.
- [3] Dogu O, Pelucchi M, Van de Vijver R, Van Steenberge PHM, D'Hooge DR, Cuoci A, et al. The chemistry of chemical recycling of solid plastic waste via pyrolysis and gasification: state-Of-The-Art, challenges, and future directions. *Prog Energy Combust Sci* 2021;84. <https://doi.org/10.1016/j.pecs.2020.100901>.
- [4] Jin HF, Yuan WH, Li W, Yang JZ, Zhou ZY, Zhao L, et al. Combustion chemistry of aromatic hydrocarbons. *Prog Energy Combust Sci* 2023;96. <https://doi.org/10.1016/j.pecs.2023.101076>.
- [5] Guene Lougou B, Wu L, Ma D, Geng B, Jiang B, Han D, et al. Efficient conversion of solar energy through a macroporous ceramic receiver coupling heat transfer and thermochemical reactions. *Energy (Calg)* 2023;271:126989. <https://doi.org/10.1016/j.energy.2023.126989>.
- [6] Wang Z, Wu C, Wang X, Xie M, Li Y, Zhan Z, et al. Ultra-durable solar-driven seawater electrolysis for sustainable hydrogen production. *Adv Funct Mater* 2025;35:2416014. <https://doi.org/10.1002/adfm.202416014>.
- [7] Wang Z, Li Y, Zhan Z, Xie M, Li Y, Zhang C, et al. Biomimetic inner helicoidal microfluidics with enhanced capillary rise for step liquid lifting mimicking transpiration. *Int J Extrem Manuf* 2025;7:025505. <https://doi.org/10.1088/2631-7990/ad9672>.
- [8] Zhong Y, He X, Wang W, Xu Y, Wang Y, Shuai Y. Performance enhancement of graphite-based flexible composite phase change materials and heat dissipation characteristics of electronic devices. *Appl Therm Eng* 2025;263:125393. <https://doi.org/10.1016/j.applthermaleng.2024.125393>.
- [9] Guene Lougou B, Geng B-X, Pan R-M, Wang W, Yan T-T, Li F-H, et al. Solar-driven photothermal catalytic CO₂ conversion: a review. *Rare Met* 2024;43:2913–39. <https://doi.org/10.1007/s12598-024-02638-4>.
- [10] Wu L, Guene Lougou B, Jiang B, Zhang H, Guo Y, Geng B, et al. Experimentally validated numerical model of multi-spectral bands radiative transport in solar receiver/reactor with photo-active porous absorber reacting media. *Energy Convers Manag* 2023;278:116740. <https://doi.org/10.1016/j.enconman.2023.116740>.
- [11] Ye Y, Yu B, Ai Q, Liu M, Shuai Y. A study on full-domain transient temperature reconstruction and backward sensor placement for distributed heat source systems. *Int J Therm Sci* 2025;213:109823. <https://doi.org/10.1016/j.ijthermalsci.2025.109823>.
- [12] Pan R, Yang Y, Lougou BG, Wu L, Wang W, Guo Y, et al. Thermal performance evaluation of a novel solar-driven pyrolysis reactor. *Energy (Calg)* 2024;313:134051. <https://doi.org/10.1016/j.energy.2024.134051>.
- [13] Allobaid F, Almohammed N, Farid MM, May J, Rossger P, Richter A, et al. Progress in CFD simulations of fluidized beds for chemical and energy process engineering. *Prog Energy Combust Sci* 2022;91. <https://doi.org/10.1016/j.pecs.2021.100930>.
- [14] Khodaei H, Alvarez-Bermudez C, Chapela S, Olson C, MacKenzie MD, Gómez MA, et al. Eulerian CFD simulation of biomass thermal conversion in an indirect slow pyrolysis rotary kiln unit to produce biochar from recycled waste wood. *Energy (Calg)* 2024;288:129895. <https://doi.org/10.1016/j.energy.2023.129895>.
- [15] Wang J, Bo L, Liu J, Wang L, Luo X, Liu Z, et al. A CFD model-based design optimization for flow field enhancement in lithium electrolyzer. *Chem Eng Res Des* 2025;214:390–402. <https://doi.org/10.1016/j.cherd.2025.01.014>.
- [16] Wang F, Shuai Y, Tan H, Yu C. Thermal performance analysis of porous media receiver with concentrated solar irradiation. *Int J Heat Mass Tran* 2013;62:247–54. <https://doi.org/10.1016/j.ijheatmasstransfer.2013.03.003>.

- [17] Geng B, Guene Lougou B, Shuai Y, Zhang H, Pan Q, Han D, et al. Design of gas-liquid two-phase separation device with application in solar hydrogen production system. *Renew Sustain Energy Rev* 2023;175:113169. <https://doi.org/10.1016/j.rser.2023.113169>.
- [18] Zhang Y, Xu P, Liang S, Liu B, Shuai Y, Li B. Exergy analysis of hydrogen production from steam gasification of biomass: a review. *Int J Hydrogen Energy* 2019;44:14290–302. <https://doi.org/10.1016/j.ijhydene.2019.02.064>.
- [19] Esmaili Rad F, Abbasian J, Arastoopour H. CFD simulation of a circulating fluidized bed carbon capture system using a solid-supported amine sorbent. *Powder Technol* 2024;434:119358. <https://doi.org/10.1016/j.powtec.2023.119358>.
- [20] Lei B, Fu Y, Cadena J, Saini A, Hu Y, Yao J, et al. Accelerating computational fluid dynamics simulation of post-combustion carbon capture modeling with MeshGraphNets. *Frontiers in Artificial Intelligence* 2025;7:1441985. <https://doi.org/10.3389/frai.2024.1441985>.
- [21] Wang FZ, Animasaun I, Muhammad T, Okoya S. Recent advancements in fluid dynamics: drag reduction, lift generation, computational fluid dynamics, turbulence modelling, and multiphase flow. *Arabian J Sci Eng* 2024;49: 10237–49. <https://doi.org/10.1007/s13369-024-08945-3>.
- [22] Li S-J, Zhu L-T, Zhang X-B, Luo Z-H. Recent advances in CFD simulations of multiphase flow processes with phase change. *Ind Eng Chem Res* 2023;62: 10729–86. <https://doi.org/10.1021/acs.iecr.3c00706>.
- [23] Staszak M. Artificial intelligence in the modeling of chemical reactions kinetics. *Physical Sciences Reviews* 2023;8:51–72. <https://doi.org/10.1515/psr-2020-0079>.
- [24] Batiot B, Rogaume T, Richard F, Luche J, Collin A, Guillaume E, et al. Origin and justification of the use of the arrhenius relation to represent the reaction rate of the thermal decomposition of a solid. *Appl Sci* 2021;11:4075. <https://doi.org/10.3390/app1109075>.
- [25] Khater MM. Unraveling dynamics: analytical insights into liquid-gas interactions. *Chaos Solitons Fractals* 2024;184:114977. <https://doi.org/10.1016/j.chaos.2024.114977>.
- [26] Lu H, Liu G, Zhang Q, Jiang X, Pang B, Cai W. Computational transport phenomena of multiphase systems and fluidization. <https://doi.org/10.1007/978-981-96-0698-6>.
- [27] Jain N, Le Moine A, Chaussonnet G, Flatau A, Bravo L, Ghoshal A, et al. A critical review of physical models in high temperature multiphase fluid dynamics: turbulent transport and particle-wall interactions. *Appl Mech Rev* 2021;73: 040801. <https://doi.org/10.1115/1.4051503>.
- [28] Lu P, Zhao L, Zheng N, Liu S, Li X, Zhou X, et al. Progress and prospect of flow phenomena and simulation on two-phase separation in branching T-junctions: a review. *Renew Sustain Energy Rev* 2022;167:112742. <https://doi.org/10.1016/j.rser.2022.112742>.
- [29] Choudhary MK. Mathematical modeling of rate phenomena in glass melting furnaces. Fiberglass science and technology: chemistry, characterization, processing, modeling, application, and sustainability. 2021. p. 483–539. https://doi.org/10.1007/978-3-030-72200-5_8.
- [30] Wang T, Zhong W, Qian Y, Zhu C. Fundamentals of computational fluid dynamics. Wind turbine aerodynamic performance calculation. Springer; 2023. p. 175–91. <https://doi.org/10.1007/978-3-662-04654-8>.
- [31] Yang T, Yin Y, Zhou H, Ren Z. Review of Lagrangian stochastic models for turbulent combustion. *Acta Mech Sin* 2021;1–22. <https://doi.org/10.1007/s10409-021-01142-7>.
- [32] Yao N, Pan W, Zhang J, Wei L. The advancement on carbon-free ammonia fuels for gas turbine: a review. *Energy Convers Manag* 2024;315:118745. <https://doi.org/10.1016/j.enconman.2024.118745>.
- [33] Ferrari S, Rossi R, Di Bernardino A. A review of laboratory and numerical techniques to simulate turbulent flows. *Energies* 2022;15:7580. <https://doi.org/10.3390/en15207580>.
- [34] Domingo P, Vervisch L. Recent developments in DNS of turbulent combustion. *Proc Combust Inst* 2023;39:2055–76. <https://doi.org/10.1016/j.proci.2022.06.030>.
- [35] Wan T, Zhou M, Zhao P, Wang X. Challenges in the modeling and simulation of turbulent supercritical fluid flows and heat transfer. *Propulsion and Energy* 2025; 1:6. <https://doi.org/10.1007/s44270-024-00005-3>.
- [36] Drubetskoi E, Eckart S, Krause H. Short overview on combustion systems scale-up with emphasis on NOx emissions of gas-fired furnaces. *Energy Sci Eng* 2022;10: 621–9. <https://doi.org/10.1002/ese3.1028>.
- [37] Rueda-Vázquez JM, Serrano J, Pinz S, Jiménez-Espadafor FJ, Dorado M. A review of the use of hydrogen in compression ignition engines with dual-fuel technology and techniques for reducing NOx emissions. *Sustainability (Basel)* 2024;16:3462. <https://doi.org/10.3390/su16083462>.
- [38] Bakhchin D, Ravi R, Douadi O, Faqir M, Essadiqi E. Integrated catalytic systems for simultaneous NOx and PM reduction: a comprehensive evaluation of synergistic performance and combustion waste energy utilization. *Environ Sci Pollut Control Ser* 2024;31:46840–57. <https://doi.org/10.1007/s11356-024-34287-6>.
- [39] Köhler W, Mialdin A, Bou-Ali M, Shevtsova V. The measurement of sorbet and thermodiffusion coefficients in binary and ternary liquid mixtures. *Int J Thermophysics* 2023;44:140. <https://doi.org/10.1007/s10765-023-03242-x>.
- [40] Ershkov SV, Prosviryakov EY, Burmasheva NV, Christianto V. Solving the hydrodynamical system of equations of inhomogeneous fluid flows with thermal diffusion: a review. *Symmetry* 2023;15:1825. <https://doi.org/10.3390/sym15101825>.
- [41] Pozorski J, Olejnik M. Smoothed particle hydrodynamics modelling of multiphase flows: an overview. *Acta Mech* 2024;235:1685–714. <https://doi.org/10.1007/s00707-023-03763-4>.
- [42] Adebayo EM, Tsoutsanis P, Jenkins KW. A review of diffuse interface-capturing methods for compressible multiphase flows. *Fluids* 2025;10:93. <https://doi.org/10.3390/fluids10040093>.
- [43] Mohan A, Tomar G. Volume of fluid method: a brief review. *J Indian Inst Sci* 2024;104:229–48. <https://doi.org/10.1007/s41745-024-00424-w>.
- [44] Wang H, Yan H, Rong C, Yuan Y, Jiang F, Han Z, et al. Multi-scale simulation of complex systems: a perspective of integrating knowledge and data. *ACM Comput Surv* 2024;56:1–38. <https://doi.org/10.1145/365466>.
- [45] Sanderse B, Stinis P, Maulik R, Ahmed SE. Scientific machine learning for closure models in multiscale problems: a review. <https://doi.org/10.3934/fods.2024043>.
- [46] Parker A, Agrawal A, Bittle J. Representative phenomena of cyclic turbulent combustion in high-pressure fuel sprays. *Flow Turbul Combust* 2023;111:675–96. <https://doi.org/10.1007/s10494-023-00432-3>.
- [47] Roos WA, Zietsman JH. Accelerating complex chemical equilibrium calculations—A review. *Calphad* (N Y) 2022;77:102380. <https://doi.org/10.1016/j.calphad.2021.102380>.
- [48] Taylor CJ, Pomberger A, Felton KCG, Grainger R, Barecka M, Chamberlain TW, et al. A brief introduction to chemical reaction optimization. *Chem Rev* 2023;123: 3089–126. <https://doi.org/10.1021/acs.chemrev.2c00798>.
- [49] Menter F, Hüppe A, Matyushenko A, Kolmogorov D. An overview of hybrid RANS-LES models developed for industrial CFD. *Appl Sci* 2021;11:2459. <https://doi.org/10.3390/app11062459>.
- [50] Heinz S, Fagbade A. A critical review of hybrid RANS-LES concepts: Continuous eddy simulation versus classical methods. *AIAA SCITECH*; 2025. p. 2214. <https://doi.org/10.2514/6.2025-2214>. Forum2025.
- [51] Nejaamtheen MN, Choi J-Y. A comprehensive review of flamelet methods: future directions and emerging challenges. *Energies* 2024;18:45. <https://doi.org/10.3390/en18010045>.
- [52] Tao T, Zhenguo W, Mingbo S, Hongbo W, Guoyan Z, Jiangfei Y. Flamelet-like models applied in scramjet combustors: a state of art and prospect. *Chin J Aeronaut* 2023;36:24–43. <https://doi.org/10.1016/j.cja.2023.07.036>.
- [53] Mutto M. Tabulated chemistry models for Numerical simulation of combustion flow field. *Fluids* 2025;10:83. <https://doi.org/10.3390/fluids10040083>.
- [54] Kumar R, Sikander A. Review and analysis of model order reduction techniques for high-dimensional complex systems. *Microsyst Technol* 2024;30:1177–90. <https://doi.org/10.1007/s00542-023-05605-8>.
- [55] Lu K, Zhang K, Zhang H, Gu X, Jin Y, Zhao S, et al. A review of model order reduction methods for large-scale structure systems. *Shock Vib* 2021;2021: 6631180. <https://doi.org/10.1155/2021/6631180>.
- [56] Cavallotti C. Automation of chemical kinetics: status and challenges. *Proc Combust Inst* 2023;39:11–28. <https://doi.org/10.1016/j.proci.2022.06.002>.
- [57] Shejan ME, Bhuiyan SMY, Schoen MP, Mahamud R. Assessment of machine learning techniques for simulating reacting flow: from plasma-assisted ignition to turbulent flame propagation. *Energies* 2024;17:4887. <https://doi.org/10.3390/en17194887>.
- [58] Zhou L. An eulerian-eulerian-lagrangian modeling of two-phase combustion. *Theor Comput Fluid Dynam* 2023;37:767–80. <https://doi.org/10.1007/s00162-023-00666-x>.
- [59] Chen H, Wei S, Ding W, Wei H, Li L, Saxén H, et al. Interfacial area transport equation for bubble coalescence and breakup: developments and comparisons. *Entropy* 2021;23:1106. <https://doi.org/10.3390/e23091106>.
- [60] Rashid FL, Al-Obaidi MA, Hussein AK, Ahmad S, Alildeiri MS, Mujtaba IM. Bubble dynamics in sustainable technologies: a review of growth, collapse, and heat transfer. *Processes* 2024;13:38. <https://doi.org/10.3390/pr13010038>.
- [61] Li X, Wang S, Yang S, Qiu S, Sun Z, Hung DL, et al. A review on the recent advances of flash boiling atomization and combustion applications. *Prog Energy Combust Sci* 2024;100:101119. <https://doi.org/10.1016/j.pecs.2023.101119>.
- [62] Li J, Zheng D, Zhang W. Advances of phase-field model in the numerical simulation of multiphase flows: a review. *Atmosphere* 2023;14:1311. <https://doi.org/10.3390/atmos14081311>.
- [63] Zhang A, Guo Z, Jiang B, Xiong S, Pan F. Numerical solution to phase-field model of solidification: a review. *Comput Mater Sci* 2023;228:112366. <https://doi.org/10.1016/j.commatsci.2023.112366>.
- [64] Grave M, Coutinho AL. Comparing the convected level-set and the Allen–Cahn phase-field methods in AMR/C simulations of two-phase flows. *Comput Fluid* 2022;244:105569. <https://doi.org/10.1016/j.compfluid.2022.105569>.
- [65] Daiß G, Diehl P, Yan J, Holmen JK, Gayatri R, Junghans C, et al. Asynchronous-many-task systems: challenges and Opportunities—Scaling an AMR astrophysics code on exascale machines using Kokkos and HPX. *arXiv preprint arXiv: 241215518* 2024. <https://doi.org/10.48550/arXiv.2412.15518>.
- [66] Majchrzak M, Marciniak-Lukasiak K, Lukasiak P. A survey on the application of machine learning in turbulent flow simulations. *Energies* 2023;16:1755. <https://doi.org/10.3390/en16041755>.
- [67] Abuwafaa WH, AlSawaftah N, Darwish N, Pitt WG, Husseini GA. A review on membrane fouling prediction using artificial neural networks (ANNs). *Membranes* 2023;13:685. <https://doi.org/10.3390/membranes13070685>.
- [68] Kang M, Bian J, Li B, Fan X, Xi Y, Wang Y, et al. Advanced progress of numerical simulation in drum drying process: gas–Solid flow model and simulation of flow characteristics. *Int Commun Heat Mass Tran* 2024;157:107758. <https://doi.org/10.1016/j.icheatmasstransfer.2024.107758>.
- [69] Panchigar D, Kar K, Shukla S, Mathew RM, Chadha U, Selvaraj SK. Machine learning-based CFD simulations: a review, models, open threats, and future

- tactics. *Neural Comput Appl* 2022;34:21677–700. <https://doi.org/10.1007/s0521-022-07838-6>.
- [70] Zhang Y, Zhang D, Jiang H. Review of challenges and opportunities in turbulence modeling: a comparative analysis of data-driven machine learning approaches. *J Mar Sci Eng* 2023;11:1440. <https://doi.org/10.3390/jmse11071440>.
- [71] Lino M, Fotiadis S, Bharath AA, Cantwell CD. Current and emerging deep-learning methods for the simulation of fluid dynamics. *Proceedings of the Royal Society A* 2023;479:20230058. <https://doi.org/10.1098/rspa.2023.0058>.
- [72] Yang G, Xu R, Tian Y, Guo S, Wu J, Chu X. Data-driven methods for flow and transport in porous media: a review. *Int J Heat Mass Tran* 2024;235:126149. <https://doi.org/10.1016/j.ijheatmasstransfer.2024.126149>.
- [73] Sharma P, Chung WT, Akoush B, Ihme M. A review of physics-informed machine learning in fluid mechanics. *Energies* 2023;16:2343. <https://doi.org/10.3390/en16052343>.
- [74] Cai S, Mao Z, Wang Z, Yin M, Karniadakis GE. Physics-informed neural networks (PINNs) for fluid mechanics: a review. *Acta Mech Sin* 2021;37:1727–38. <https://doi.org/10.1007/s10409-021-01148-1>.
- [75] Farea A, Yli-Harja O, Emmert-Streib F. Understanding Physics-Informed Neural Networks: Techniques, Applications, Trends, and Challenges. *AI* 2024;5:1534–57. <https://www.mdpi.com/2673-2688/5/3/74>.
- [76] Gauthu S. High-performance computing and big data: emerging trends in advanced computing systems for data-intensive applications. *Journal of Advanced Computing Systems* 2024;4:22–35. 10.69987.
- [77] Chowdhury IA. State-of-the-Art CFD simulation: a review of techniques, validation methods, and application scenarios. *Journal of Recent Trends in Mechanics* 2024;45–53. <https://doi.org/10.46610/jortm.2024.v09i02.005>.
- [78] Yuan S, Ajam H, Sinnah ZAB, Altalabwy FM, Ameer SAA, Husain A, et al. The roles of artificial intelligence techniques for increasing the prediction performance of important parameters and their optimization in membrane processes: a systematic review. *Ecotoxicol Environ Saf* 2023;260:115066. <https://doi.org/10.1016/j.ecoenv.2023.115066>.
- [79] Sofos F, Stavrogiannis C, Exarchou-Kouveli KK, Akabua D, Charilas G, Karakasidis TE. Current trends in fluid research in the era of artificial intelligence: a review. *Fluids* 2022;7:116. <https://doi.org/10.3390/fluids7030116>.
- [80] Al-Othman A, Tawalbeh M, Martis R, Dhou S, Orhan M, Qasim M, et al. Artificial intelligence and numerical models in hybrid renewable energy systems with fuel cells: advances and prospects. *Energy Convers Manag* 2022;253:115154. <https://doi.org/10.1016/j.enconman.2021.115154>.
- [81] Kodman JB, Singh B, Murugaiah M. A comprehensive survey of open-source tools for computational fluid dynamics analyses. *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* 2024;119:123. <https://doi.org/10.37934/afmts.119.2.123148>.
- [82] Lerotholi L, Everson R, Koech L, Neomagus H, Rutto H, Branken D, et al. Semi-dry flue gas desulphurization in spray towers: a critical review of applicable models for computational fluid dynamics analysis. *Clean Technol Environ Policy* 2022;24:2011–60. <https://doi.org/10.1007/s10098-022-02308-y>.
- [83] Mukherjee S, Lu D, Raghavan B, Breitkopf P, Dutta S, Xiao M, et al. Accelerating large-scale topology optimization: state-of-the-art and challenges. *Arch Comput Methods Eng* 2021;1–23. <https://doi.org/10.1007/s11831-021-09544-3>.
- [84] Neau H, Ansart R, Baudry C, Fournier Y, Mérigoux N, Koren C, et al. 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;120018. <https://doi.org/10.1016/j.powtec.2024.120018>.
- [85] Xu S, Zhao J, Wu H, Zhang S, Müller J-D, Huang H, et al. A review of solution stabilization techniques for RANS CFD solvers. *Aerospace* 2023;10:230. <https://doi.org/10.3390/aerospace10030230>.
- [86] Lv Y, Ekaterinaris J. Recent progress on high-order discontinuous schemes for simulations of multiphase and multicomponent flows. *Prog Aero Sci* 2023;140:100929. <https://doi.org/10.1016/j.paerosci.2023.100929>.
- [87] Xu X, Gao Z, Zhang M. A review of simplified numerical approaches for fast urban airflow simulation. *Build Environ* 2023;234:110200. <https://doi.org/10.1016/j.buildenv.2023.110200>.
- [88] Jeong S-J. CFD simulation of pre-chamber spark-ignition engines—A perspective review. *Energies* 2024;17:1–39. <https://doi.org/10.3390/en17184696>.
- [89] Li Z, Zhou T, Lu W, Yang H, Li Y, Liu Y, et al. Computational fluid dynamics (CFD) technology methodology and analysis of waste heat recovery from high-temperature solid granule: a review. *Sustainability (Basel)* 2025;17:480. <https://doi.org/10.3390/su17020480>.
- [90] Shi QY, Zhuang CJ, Lin B, Wu D, Li L, Zeng R, et al. Adaptive local mesh refinement for steady state and transient simulation of semiconductor devices. *IEEE 21st Biennial Conference on Electromagnetic Field Computation (IEEE CEFC)* 2024. <https://doi.org/10.1109/cefc61729.2024.10585921>. Jeju, SOUTH KOREA.
- [91] Cary AW, Chawner J, Duque EP, Gropp W, Kleb WL, Kolonay RM, et al. Cfd vision 2030 road map: progress and perspectives. *AIAA aviation* 2021;2726. <https://doi.org/10.2514/6.2021-2726>. forum2021.
- [92] Dbouk T. A computational framework with an adaptive mesh refinement technique for concentrated suspension flows. *Part Sci Technol* 2020;38:782–91. <https://doi.org/10.1080/02726351.2019.1624663>.
- [93] Mucha P, Jiang M, Bay RJ, Amer Soi Mechanical E. Enhancements of computational fluid dynamics analysis of air entrapment and fluid-structure interaction during plate entry to water through VOF-slip and adaptive discretization schemes. *ASME 41st International Conference on Ocean, Offshore and Arctic Engineering (OMAE)* 2022. <https://doi.org/10.1115/OMAE2022-80796>. Hamburg, GERMANY.
- [94] Philip B, Wang Z, Berrill MA, Birke M, Pernice M. Dynamic implicit 3D adaptive mesh refinement for non-equilibrium radiation diffusion. *J Comput Phys* 2014;262:17–37. <https://doi.org/10.1016/j.jcp.2013.12.058>.
- [95] Bozorgpour R, Darian HM. Recent advancements in fluid flow simulation using the WENO scheme: a comprehensive review. *J Nonlinear Math Phys* 2025;32:1–56. <https://doi.org/10.1007/s44198-025-00269-6>.
- [96] Fu L. Review of the high-order TENO schemes for compressible gas dynamics and turbulence. *Arch Comput Methods Eng* 2023;30:2493–526. <https://doi.org/10.1007/s11831-022-09877-7>.
- [97] Teixeira F, Sarris C, Zhang Y, Na D-Y, Berenger J-P, Su Y, et al. Finite-difference time-domain methods. *Nature Reviews Methods Primers* 2023;3:75. <https://doi.org/10.1038/s43586-023-00257-4>.
- [98] Van Hoecke L, Boeije D, Gonzalez-Quiroga A, Patience GS, Perreault P. Experimental methods in chemical engineering: computational fluid dynamics/finite volume method—CFD/FVM. *Can J Chem Eng* 2023;101:545–61. <https://doi.org/10.1002/cjce.23686>.
- [99] Dadi VS, Veluru S, Tanneri HK, Busigari RR, Potnuri R, Kulkarni A, et al. Recent advancements of CFD and heat transfer studies in pyrolysis: a review. *J Anal Appl Pyrolysis* 2023;175:106163. <https://doi.org/10.1016/j.jaap.2023.106163>.
- [100] Lyu H-G, Sun P-N, Huang X-T, Zhong S-Y, Peng Y-X, Jiang T, et al. A review of SPH techniques for hydrodynamic simulations of ocean energy devices. *Energies* 2022;15:502. <https://doi.org/10.3390/en15020502>.
- [101] Chouly F. A review on some discrete variational techniques for the approximation of essential boundary conditions. *Vietnam J Math* 2024;1–43. <https://doi.org/10.1007/s10013-024-00702-1>.
- [102] Folkner D, Katz A, Sankaran V. Design and verification methodology of boundary conditions for finite volume schemes. *Comput Fluid* 2014;96:264–75. <https://doi.org/10.1016/j.compfluid.2014.03.028>.
- [103] Pan K-Q, Liu J-Y. Investigation on the choice of boundary conditions and shape functions for flexible multi-body system. *Acta Mech Sin* 2012;28:180–9. <https://doi.org/10.1007/s10409-011-0527-8>.
- [104] Nobili C. The role of boundary conditions in scaling laws for turbulent heat transport. *arXiv preprint arXiv:211215564* 2021. <https://doi.org/10.48550/arXiv.2112.15564>.
- [105] Yang Y, Yan H, Li S, Song W, Li F, Duan H, et al. Development of pipeline transient mixed flow model with smoothed particle hydrodynamics based on preissmann slot method. *Water (Lond 1974)* 2024;16:1108. <https://doi.org/10.3390/w16081108>.
- [106] Song W, Yan H, Tao T, Guan M, Li F, Xin K. Modeling transient mixed flows in drainage networks with smoothed particle hydrodynamics. *Water Resour Manag* 2024;38:861–79. <https://doi.org/10.1007/s11269-023-03689-5>.
- [107] Vasilev A, Sukhanovskii A. Turbulent convection in a cube with mixed thermal boundary conditions: low rayleigh number regime. *Int J Heat Mass Tran* 2021;174:121290. <https://doi.org/10.1016/j.ijheatmasstransfer.2021.121290>.
- [108] Manueco L, Weiss P-É, Deck S. On the coupling of wall-model immersed boundary conditions and curvilinear body-fitted grids for the simulation of complex geometries. *Comput Fluid* 2021;226:104996. <https://doi.org/10.1016/j.compfluid.2021.104996>.
- [109] Grigoriev SK, Zakharov DA, Kornilina MA, Yakobovskiy MV. Dynamic load balancing using adaptive locally refined meshes. *Mathematical Models and Computer Simulations* 2024;16:280–92. <https://doi.org/10.1134/S2070048224020091>.
- [110] Wang H, Cao Y, Huang Z, Liu Y, Hu P, Luo X, et al. Recent advances on machine learning for computational fluid dynamics: a survey. <https://doi.org/10.48550/arXiv.2408.12171>; 2024.
- [111] Wang F, Shuai Y, Tan H, Zhang X, Mao Q. Heat transfer analyses of porous media receiver with multi-dish collector by coupling MCRT and FVM method. *Sol Energy* 2019;133:158–68. <https://doi.org/10.1016/j.solener.2019.04.004>.
- [112] Liszka T, Orkisz J. The finite difference method at arbitrary irregular grids and its application in applied mechanics. *Comput Struct* 1980;11:83–95. [https://doi.org/10.1016/0045-7949\(80\)90149-2](https://doi.org/10.1016/0045-7949(80)90149-2).
- [113] Mahian O, Kolsi L, Amani M, Estellé P, Ahmadi G, Kleinstreuer C, et al. Recent advances in modeling and simulation of nanofluid flows—Part II: applications. *Phys Rep* 2019;791:1–59. <https://doi.org/10.1016/j.physrep.2018.11.003>.
- [114] Delavar MA, Wang J. Chapter 18 – lattice boltzmann method and its applications. In: Eslamian S, Eslamian F, editors. *Handbook of hydroinformatics*. Elsevier; 2023. p. 289–319. <https://doi.org/10.1016/B978-0-12-821285-1.00001-4>.
- [115] Moradi J, Andwari AM, Konné J. Numerical methods for the flow fields: A comparative review. *Scandinavian Simulation Society* 2025:472–80. <https://doi.org/10.3384/ecp212.064>.
- [116] Castro M, Costa B, Don WS. High order weighted essentially non-oscillatory WENO-Z schemes for hyperbolic conservation laws. *J Comput Phys* 2011;230:1766–92. <https://doi.org/10.1016/j.jcp.2010.11.028>.
- [117] Yang C-T, Huang C-L, Lin C-F. Hybrid CUDA, OpenMP, and MPI parallel programming on multicore GPU clusters. *Comput Phys Commun* 2011;182:266–9. <https://doi.org/10.1016/j.cpc.2010.06.035>.
- [118] Cooper-Baldock Z, Almirall BV, Inthavong K. Speed, power and cost implications for GPU acceleration of computational fluid dynamics on HPC systems. *arXiv preprint arXiv:240402482*. 2024. <https://doi.org/10.48550/arXiv.2404.02482>.
- [119] Yu J, Wang S, Luo K, Fan J. GPU-accelerated discrete element simulation of granular and gas-solid flows. *Powder Technol* 2024;437:119475. <https://doi.org/10.1016/j.powtec.2024.119475>.
- [120] Zhang W, Zhong Z-h, Peng C, Yuan W-h, Wu W. GPU-accelerated smoothed particle finite element method for large deformation analysis in geomechanics. *Comput Geotech* 2021;129:103856. <https://doi.org/10.1016/j.compgeo.2020.103856>.

- [121] Tregnago G. Biphasic turbulence. *Nat Energy* 2019;4:629. <https://doi.org/10.1038/s41560-019-0454-7>.
- [122] Wang Z, Mathai V, Sun C. Self-sustained biphasic catalytic particle turbulence. *Nat Commun* 2019;10:3333. <https://doi.org/10.1038/s41467-019-11221-w>.
- [123] Mishra B, Rai S, Gavhane K, Deshpande M. Turbulence modeling in navier-stokes equations: challenges and approaches. *International Research Journal of Modernization in Engineering Technology and Science* 2024;6:964. <https://doi.org/10.56726/IRJMET53610>.
- [124] Blaisdell GA, Spyropoulos ET, Qin JH. The effect of the formulation of nonlinear terms on aliasing errors in spectral methods. *Appl Numer Math* 1996;21:207–19. [https://doi.org/10.1016/0168-9274\(96\)00005-0](https://doi.org/10.1016/0168-9274(96)00005-0).
- [125] Deng X. A mixed zero-equation and one-equation turbulence model in fluid-film thrust bearings. *J Tribol* 2024;146:034101. <https://doi.org/10.1115/1.4063945>.
- [126] Toubiana E, Russeil S, Bougeard D, François N. Large Eddy simulation and Reynolds-averaged navier-stokes modeling of flow in staggered plate arrays: Comparison at various flow regimes. *Appl Therm Eng* 2015;89:405–20. <https://doi.org/10.1016/j.applthermaleng.2015.06.025>.
- [127] Liu Y, Zhou Z, Zhu L, Wang S. Numerical investigation of flows around an axisymmetric body of revolution by using Reynolds-stress model based hybrid Reynolds-averaged Navier-Stokes/large eddy simulation. *Phys Fluids* 2021;33. <https://doi.org/10.1063/5.0058016>.
- [128] Mathur A, Roelofs F, Fiore M, Koloszar L. State-of-the-art turbulent heat flux modelling for low-Prandtl flows. *Nucl Eng Des* 2023;406:112241.
- [129] Sandberg RD, Zhao Y. Machine-learning for turbulence and heat-flux model development: a review of challenges associated with distinct physical phenomena and progress to date. *Int J Heat Fluid Flow* 2022;95:108983. <https://doi.org/10.1016/j.ijheatfluidflow.2022.108983>.
- [130] Gopalan H, Heinz S, Stöllinger MK. A unified RANS–LES model: computational development, accuracy and cost. *J Comput Phys* 2013;249:249–74. <https://doi.org/10.1016/j.jcp.2013.03.066>.
- [131] Knopp T, Spallek F, Frederich O, Rapin G. Application of numerical Wall functions for boundary layer flows with separation and reattachment. In: Dillmann A, Heller G, Krämer E, Wagner C, Breitsamter C, editors. *New results in numerical and experimental fluid mechanics X*. Cham: Springer International Publishing; 2016. p. 145–55. https://doi.org/10.1007/978-3-319-27279-5_13.
- [132] Fazeli M, Emdad H, Mehdi Alishahi M, Rezaeiravesh S. Wall-modeled large eddy simulation of 90° bent pipe flows with/without particles: a comparative study. *Int J Heat Fluid Flow* 2024;105:109268. <https://doi.org/10.1016/j.ijheatfluidflow.2023.109268>.
- [133] Cam RS, Ahmed U, Fang J, Chakarborty N, Nivarti G, Moulinec C, et al. An unstructured adaptive mesh refinement approach for computational fluid dynamics of reacting flows. *J Comput Phys* 2022;468:111480. <https://doi.org/10.1016/j.jcp.2022.111480>.
- [134] Alves Portela F, Sandham ND. A DNS/URANS approach for simulating rough-wall turbulent flows. *Int J Heat Fluid Flow* 2020;85:108627. <https://doi.org/10.1016/j.ijheatfluidflow.2020.108627>.
- [135] Bae HJ, Koumoutsakos P. Scientific multi-agent reinforcement learning for wall-models of turbulent flows. *Nat Commun* 2022;13:1443. <https://doi.org/10.1038/s41467-022-28957-7>.
- [136] Kan K, Zhao F, Xu H, Feng J, Chen H, Liu W. Energy performance evaluation of an axial-flow pump as turbine under conventional and reverse operating modes based on an energy loss intensity model. *Phys Fluids* 2023;35. <https://doi.org/10.1063/5.0132667>.
- [137] Shu D, Li Z, Barati Farimani A. A physics-informed diffusion model for high-fidelity flow field reconstruction. *J Comput Phys* 2023;478:111972. <https://doi.org/10.1016/j.jcp.2023.111972>.
- [138] Eivazi H, Tahani M, Schlatter P, Vinuesa R. Physics-informed neural networks for solving Reynolds-averaged navier-stokes equations. *Phys Fluids* 2022;34. <https://doi.org/10.1063/5.0095270>.
- [139] Marusic I, Chandran D, Rouhi A, Fu MK, Wine D, Holloway B, et al. An energy-efficient pathway to turbulent drag reduction. *Nat Commun* 2021;12:5805. <https://doi.org/10.1038/s41467-021-26128-8>.
- [140] Xu Q, Zhuang Z, Pan Y, Wen B. Super-resolution reconstruction of turbulent flows with a transformer-based deep learning framework. *Phys Fluids* 2023;35. <https://doi.org/10.1063/5.0149551>.
- [141] Zhou Y. Turbulence theories and statistical closure approaches. *Phys Rep* 2021;935:1–117. <https://doi.org/10.1016/j.physrep.2021.07.001>.
- [142] Yousif MZ, Yu L, Hoyas S, Vinuesa R, Lim H. A deep-learning approach for reconstructing 3D turbulent flows from 2D observation data. *Sci Rep* 2023;13:2529. <https://doi.org/10.1038/s41598-023-29525-9>.
- [143] Spalart PR. Detached-Eddy simulation. *Annu Rev Fluid Mech* 2009;41:181–202. <https://doi.org/10.1146/annurev.fluid.010908.165130>.
- [144] Tenneti S, Subramaniam S. Particle-Resolved direct numerical simulation for gas-solid flow model development. *Annu Rev Fluid Mech* 2014;46:199–230. <https://doi.org/10.1146/annurev-fluid-010313-141344>.
- [145] Kravets B, Schulz D, Jasevičius R, Reinecke SR, Rosemann T, Krugel-Emden H. Comparison of particle-resolved DNS (PR-DNS) and non-resolved DEM/CFD simulations of flow through homogenous ensembles of fixed spherical and non-spherical particles. *Adv Powder Technol* 2021;32:1170–95. <https://doi.org/10.1016/j.apt.2021.02.016>.
- [146] Tian B, Huang B, Li L, Wu Y. Eulerian–Lagrangian multiscale numerical analysis of multimodal partial shedding dynamics. *Int J Multiphas Flow* 2024;178:104876. <https://doi.org/10.1016/j.ijmultiphaseflow.2024.104876>.
- [147] Ren B, Zhong W, Jin B, Yuan Z, Lu Y. Computational fluid dynamics (CFD)–Discrete element method (DEM) simulation of gas–solid turbulent flow in a cylindrical spouted bed with a conical base. *Energy Fuel* 2011;25:4095–105. <https://doi.org/10.1021/ef200808v>.
- [148] Zhao Z, Zhou L, Bai L, Wang B, Agarwal R. Recent advances and perspectives of CFD–DEM simulation in fluidized bed. *Arch Comput Methods Eng* 2024;31:871–918. <https://doi.org/10.1007/s11831-023-10001-6>.
- [149] Wang S, Shen Y. Coarse-grained CFD–DEM modelling of dense gas–solid reacting flow. *Int J Heat Mass Tran* 2022;184:122302. <https://doi.org/10.1016/j.ijheatmasstransfer.2021.122302>.
- [150] Feng M, Li F, Wang W, Li J. Parametric study for MP-PIC simulation of bubbling fluidized beds with Geldart A particles. *Powder Technol* 2018;328:215–26. <https://doi.org/10.1016/j.powtec.2018.01.024>.
- [151] Xiong Z, Xu J, Liu C, Ge W. A sub-grid gas–solid interaction model for coarse-grained CFD–DEM simulations. *Chem Eng J* 2024;498:155042. <https://doi.org/10.1016/j.cej.2024.155042>.
- [152] Zhou L, Zhao Y. CFD–DEM simulation of fluidized bed with an immersed tube using a coarse-grain model. *Chem Eng Sci* 2021;231:116290. <https://doi.org/10.1016/j.ces.2020.116290>.
- [153] Chu K, Chen J, Yu A. Applicability of a coarse-grained CFD–DEM model on dense medium cyclone. *Miner Eng* 2016;90:43–54. <https://doi.org/10.1016/j.mine.2016.01.020>.
- [154] Córcoles J, Acosta-Iborra A, Almendros-Ibáñez JA, Sobrino C. Numerical simulation of a 3-D gas–solid fluidized bed: Comparison of TFM and CPFD numerical approaches and experimental validation. *Adv Powder Technol* 2021;32:3689–705. <https://doi.org/10.1016/j.apt.2021.08.029>.
- [155] Domínguez-Coy P, Córcoles J, Almendros-Ibáñez JA. Review on erosion of horizontal tubes immersed in fluidized beds of Geldart B particles. *Renew Sustain Energy Rev* 2024;196:114359. <https://doi.org/10.1016/j.rser.2024.114359>.
- [156] Motaln M, Lerher T. Numerical simulation of conveying fine powders in a screw conveyor using the discrete element method. *Tehnicki glasnik* 2023;17:338–45. <https://doi.org/10.31803/tg-20230513115809>.
- [157] Asylbekov E, Poggemann L, Dittler A, Nirschl H. Discrete element method simulation of particulate material fracture behavior on a stretchable single filter fiber with additional gas flow. *Powders* 2024;3:367–91. <https://doi.org/10.3390/powders3030021>.
- [158] Gopala VR, Van Wachem BG. Volume of fluid methods for immiscible-fluid and free-surface flows. *Chem Eng J* 2008;141:204–21. <https://doi.org/10.1016/j.cej.2007.12.035>.
- [159] Mathur A, Dovizio D, Frederix E, Komen E. A Hybrid dispersed-large Interface Solver for multi-scale two-phase flow modelling. *Nucl Eng Des* 2019;344:69–82. <https://doi.org/10.1016/j.nucengdes.2019.01.020>.
- [160] Kan K, Yang Z, Lyu P, Zheng Y, Shen L. Numerical study of turbulent flow past a rotating axial-flow pump based on a level-set immersed boundary method. *Renew Energy* 2021;168:960–71. <https://doi.org/10.1016/j.renene.2020.12.103>.
- [161] Roccon A, Zonta F, Soldati A. Phase-field modeling of complex interface dynamics in drop-laden turbulence. *Physical Review Fluids* 2023;8:090501. <https://doi.org/10.1103/PhysRevFluids.8.090501>.
- [162] Mao X, Joshi V, Jaiman R. A variational interface-preserving and conservative phase-field method for the surface tension effect in two-phase flows. *J Comput Phys* 2021;433:110166. <https://doi.org/10.1016/j.jcp.2021.110166>.
- [163] Adnan M, Sun J, Ahmad N, Wei JJ. Comparative CFD modeling of a bubbling bed using an Eulerian–Eulerian two-fluid model (TFM) and a eulerian-lagrangian dense discrete phase model (DDPM). *Powder Technol* 2021;383:418–42. <https://doi.org/10.1016/j.powtec.2021.01.063>.
- [164] Adnan M, Sun J, Ahmad N, Wei JJ. Validation and sensitivity analysis of an Eulerian–Eulerian two-fluid model (TFM) for 3D simulations of a tapered fluidized bed. *Powder Technol* 2022;396:490–518. <https://doi.org/10.1016/j.powtec.2021.08.057>.
- [165] Chang J, Zhao J, Zhang K, Gao J. Hydrodynamic modeling of an industrial turbulent fluidized bed reactor with FCC particles. *Powder Technol* 2016;304:134–42. <https://doi.org/10.1016/j.powtec.2016.04.048>.
- [166] Chahed J, Roig V, Masberrat L. Eulerian–Eulerian two-fluid model for turbulent gas–liquid bubbly flows. *Int J Multiphas Flow* 2003;29:23–49. [https://doi.org/10.1016/S0301-9322\(02\)00123-4](https://doi.org/10.1016/S0301-9322(02)00123-4).
- [167] Liu X, Hu S, Jiang Y, Li J. Extension and application of energy-minimization multi-scale (EMMS) theory for full-loop hydrodynamic modeling of complex gas–solid reactors. *Chem Eng J* 2015;278:492–503. <https://doi.org/10.1016/j.cej.2014.11.093>.
- [168] Yang Z, Lu B, Wang W. Coupling Artificial Neural Network with EMMS drag for simulation of dense fluidized beds. *Chem Eng Sci* 2021;246:117003. <https://doi.org/10.1016/j.ces.2021.117003>.
- [169] Wang F, Shuai Y, Wang Z, Leng Y, Tan H. Thermal and chemical reaction performance analyses of steam methane reforming in porous media solar thermochemical reactor. *Int J Hydrogen Energy* 2014;39:718–30. <https://doi.org/10.1016/j.ijhydene.2013.10.132>.
- [170] Xie Q, Liu Y, Yao M, Zhou H, Ren Z. A fully coupled, fully implicit simulation method for unsteady flames using Jacobian approximation and clustering. *Combust Flame* 2022;245:112362. <https://doi.org/10.1016/j.combustflame.2022.112362>.
- [171] Abdellatif HH, Ambrosini W, Arcilesi D, Bhowmik PK, Sabharwall P. Flow Instabilities in boiling channels and their suppression methodologies—A review. *Nucl Eng Des* 2024;421:113114. <https://doi.org/10.1016/j.nucengdes.2024.113114>.
- [172] Fang Z-W, Zhang J-L, Sun H-W. A fast finite volume method for spatial fractional diffusion equations on nonuniform meshesImage 1. *Comput Math Appl* 2022;108:175–84. <https://doi.org/10.1016/j.camwa.2022.01.015>.

- [173] Neau H, Ansart R, Baudry C, Fournier Y, Mérigoux N, Koren C, et al. 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>.
- [174] Eddelbuettel D. Parallel computing with R: a brief review. *WIREs Computational Statistics* 2021;13:e1515. <https://doi.org/10.1002/wics.1515>.
- [175] Fakhry D, Abdelsalam M, El-Kharashi MW, Safer M. A review on computational storage devices and near memory computing for high performance applications. *Memories - Materials, Devices, Circuits and Systems* 2023;4:100051. <https://doi.org/10.1016/j.memori.2023.100051>.
- [176] Maksum Y, Amiri A, Amangeldi A, Inkarkov M, Ding Y, Romagnoli A, et al. Computational acceleration of topology optimization using parallel computing and machine learning methods – analysis of research trends. *Journal of Industrial Information Integration* 2022;28:100352. <https://doi.org/10.1016/j.jii.2022.100352>.
- [177] Kit Windows-Yule CR, Benyahia S, Toson P, Che H, Nicușan AL. Numerical modelling and imaging of industrial-scale particulate systems: a review of contemporary challenges and solutions. *KONA Powder and Particle Journal* 2025;42:15–36. <https://doi.org/10.14356/kona.2025007>.
- [178] Attanayake DD, Sewerin F, Kulkarni S, Dernbecher A, Dieguez-Alonso A, van Wachem B. Review of modelling of pyrolysis processes with CFD-DEM. *Flow, Turbulence and Combustion* 2023;111:355–408. <https://doi.org/10.1007/s10494-023-00436-z>.
- [179] Novia N, Hasanudin H, Hermansyah H, Fudholi A, Pareek VK. Recent advances in CFD modeling of bioethanol production processes. *Renew Sustain Energy Rev* 2023;183:113522. <https://doi.org/10.1016/j.rser.2023.113522>.
- [180] Gupta H, Teerling OJ, van Oijen JA. Effect of progress variable definition on the mass burning rate of premixed laminar flames predicted by the Flamelet Generated Manifold method. *Combust Theor Model* 2021;25:631–45. <https://doi.org/10.1080/13647830.2021.1926544>.
- [181] Descombes S, Duarte M, Massot M. Operator splitting methods with error estimator and adaptive time-stepping. Application to the simulation of combustion phenomena. Splitting methods in communication, imaging, science, and engineering. Springer; 2017. p. 627–41. https://doi.org/10.1007/978-3-319-41589-5_19.
- [182] Cai K, Huang G, Song Y, Yin J, Wang D. A sub-grid scale model developed for the hexahedral grid to simulate the mass transfer between gas and liquid. *Int J Heat Mass Tran* 2021;181:121864. <https://doi.org/10.1016/j.ijheatmasstransfer.2021.121864>.
- [183] Rezaeivash S, Vinuesa R, Schlatter P. An uncertainty-quantification framework for assessing accuracy, sensitivity, and robustness in computational fluid dynamics. *Journal of Computational Science* 2022;62:101688. <https://doi.org/10.1016/j.jocs.2022.101688>.
- [184] Padoin N, Matiazzo T, Riella HG, Soares C. A perspective on the past, the present, and the future of computational fluid dynamics (CFD) in flow chemistry. *Journal of Flow Chemistry* 2024;14:239–56. <https://doi.org/10.1007/s41981-024-00313-4>.
- [185] Naaz Z, Ravi MR, Kohli S. Modelling and simulation of downdraft biomass gasifier: issues and challenges. *Biomass Bioenergy* 2022;162:106483. <https://doi.org/10.1016/j.biombioe.2022.106483>.
- [186] Hafeez S, Aristodemou E, Manos G, Al-Salem SM, Constantinou A. Computational fluid dynamics (CFD) and reaction modelling study of bio-oil catalytic hydrodeoxigenation in microreactors. *React Chem Eng* 2020;5:1083–92. <https://doi.org/10.1039/DORE00102C>.
- [187] Wijeyakulasuriya S, Kim J, Probst D, Srivastava K, Yang P, Scarcelli R, et al. Enabling powertrain technologies for Euro 7/VII vehicles with computational fluid dynamics. *Transport Eng* 2022;9:100127. <https://doi.org/10.1016/j.treng.2022.100127>.
- [188] Wu Z, Zhu P, Huang Y, Yao J, Yang F, Zhang Z, et al. A comprehensive review of modeling of solid oxide fuel cells: from large systems to fine electrodes. *Chem Rev* 2025;125:2184–268. <https://doi.org/10.1021/acs.chemrev.4c00614>.
- [189] Rivera FH, Pérez T, Castañeda LF, Nava JL. Mathematical modeling and simulation of electrochemical reactors: a critical review. *Chem Eng Sci* 2021;239:116622. <https://doi.org/10.1016/j.ces.2021.116622>.
- [190] Ranganathan P, Pandey AK, Sirohi R, Tuan Hoang A, Kim S-H. Recent advances in computational fluid dynamics (CFD) modelling of photobioreactors: design and applications. *Bioresour Technol* 2022;350:126920. <https://doi.org/10.1016/j.biortech.2022.126920>.
- [191] Amanna B, Bahri PA, Moheimani NR. Application of computational fluid dynamics in optimizing microalgal photobioreactors. *Algal Res* 2024;83:103718. <https://doi.org/10.1016/j.algal.2024.103718>.
- [192] Oluwasakin E, Torku T, Tingting S, Yinusa A, Hamdan S, Poudel S, et al. Minimization of high computational cost in data preprocessing and modeling using MP4Py. *Machine Learning with Applications* 2023;13:100483. <https://doi.org/10.1016/j.mlwa.2023.100483>.
- [193] Secco NR, Kenway GK, He P, Mader C, Martins JR. Efficient mesh generation and deformation for aerodynamic shape optimization. *AIAA J* 2021;59:1151–68. <https://doi.org/10.2514/1.J059491>.
- [194] Cengizci S, Öztop HF, Müläyim G. Stabilized finite element simulation of natural convection in square cavities filled with nanofluids under various temperature boundary conditions. *Int Commun Heat Mass Tran* 2024;156:107655. <https://doi.org/10.1016/j.icheatmasstransfer.2024.107655>.
- [195] Yulia F, Chairina I, Zulya A, Nasrullah. Multi-objective genetic algorithm optimization with an artificial neural network for CO₂/CH₄ adsorption prediction in metal-organic framework. *Therm Sci Eng Prog* 2021;25:100967. <https://doi.org/10.1016/j.tsep.2021.100967>.
- [196] Chen X, Wang Z, Deng L, Yan J, Gong C, Yang B, et al. Towards a new paradigm in intelligence-driven computational fluid dynamics simulations. *Engineering Applications of Computational Fluid Mechanics* 2024;18:2407005. <https://doi.org/10.1080/19942060.2024.2407005>.
- [197] Rahman MS, Hazra S, Chowdhury IA. Advancing computational fluid dynamics through machine learning: a review of data-driven innovations and applications. *Journal of Fluid Mechanics and Mechanical Design* 2024;42–51. <https://doi.org/10.46610/JFMMD.2024.v06i02.005>.
- [198] Zheng T, Meng F, Fan W, Liu M, Lu D, Luan Y, et al. AI-Assisted flow field design for Proton exchange membrane fuel cells: progress and perspective. *JBE* 2025;22:47–64. <https://doi.org/10.1007/s42235-024-00607-2>.
- [199] Filo G, Lempa P, Wisowski K. Review of deterministic and AI-Based methods for fluid motion modelling and sloshing analysis. *Energies* 2025;18:1263. <https://doi.org/10.3390/en18051263>.
- [200] Forrester AJ, Bressloff NW, Keane AJ. Optimization using surrogate models and partially converged computational fluid dynamics simulations. *Proc R Soc A* 2006;462:2177–204. <https://doi.org/10.1098/rspa.2006.1679>.
- [201] Choi S, Jung I, Kim H, Na J, Lee JM. Physics-informed deep learning for data-driven solutions of computational fluid dynamics. *Kor J Chem Eng* 2022;39:515–28. <https://doi.org/10.1007/s11814-021-0979-x>.
- [202] Kühl N, Schemmer M, Goutier M, Satzger G. Artificial intelligence and machine learning. *Electron Mark* 2022;32:2235–44. <https://doi.org/10.1007/s12525-022-00598-0>.
- [203] Rani V, Nabi ST, Kumar M, Mittal A, Kumar K. Self-supervised learning: a succinct review. *Arch Comput Methods Eng* 2023;30:2761–75. <https://doi.org/10.1007/s11831-023-09884-2>.
- [204] Matsuo Y, LeCun Y, Sahani M, Precup D, Silver D, Sugiyama M, et al. Deep learning, reinforcement learning, and world models. *Neural Netw* 2022;152:267–75. <https://doi.org/10.1016/j.neunet.2022.03.037>.
- [205] Zhou L, Pan S, Wang J, Vasilakos AV. Machine learning on big data: opportunities and challenges. *Neurocomputing* 2017;237:350–61. <https://doi.org/10.1016/j.neucom.2017.01.026>.
- [206] Montesinos López OA, Montesinos López A, Crossa J. Overfitting, model tuning, and evaluation of prediction performance. *Multivariate statistical machine learning methods for genomic prediction*. Springer; 2022. p. 109–39. https://doi.org/10.1007/978-3-030-89010-0_4.
- [207] Aliferis C, Simon G. Overfitting, underfitting and general model overconfidence and under-performance pitfalls and best practices in machine learning and AI. *Artificial intelligence and machine learning in health care and medical sciences: Best practices and pitfalls* 2024:477–524. https://doi.org/10.1007/978-3-031-39355-6_10.
- [208] Naidu G, Zuva T, Sibanda EM. A review of evaluation metrics in machine learning algorithms. *Computer science on-line conference*. Springer; 2023. p. 15–25. https://doi.org/10.1007/978-3-031-35314-7_2.
- [209] Sarker IH. Deep learning: a comprehensive overview on techniques, taxonomy, applications and research directions. *SN computer science* 2021;2:1–20. <https://doi.org/10.1007/s42979-021-00815-1>.
- [210] Taye MM. Understanding of machine learning with deep learning: architectures, workflow, applications and future directions. *Computers (Basel)* 2023;12:91. <https://doi.org/10.3390/computers12050091>.
- [211] Gheisari M, Ebrahimpour M, Rahimi M, Moazzamigodarzi M, Liu Y, Dutta Pramanik PK, et al. Deep learning: applications, architectures, models, tools, and frameworks: a comprehensive survey. *CAAI Transactions on Intelligence Technology* 2023;8:581–606. <https://doi.org/10.1049/cit2.12180>.
- [212] Girimaji SS. Turbulence closure modeling with machine learning: a foundational physics perspective. *New J Phys* 2024;26:071201. <https://doi.org/10.48550/arXiv.2312.14902>.
- [213] Fouquet A, Lesieur M, André JC, Basdevant C. Evolution of high Reynolds number two-dimensional turbulence. *J Fluid Mech* 1975;72:305–19. <https://doi.org/10.1017/S0022112075003369>.
- [214] Iskhakov AS, Dinh NT, Leite VC, Merzari E. Machine learning from RANS and LES to inform coarse grid simulations. *Prog Nucl Energy* 2023;163:104809. <https://doi.org/10.1016/j.pnucene.2023.104809>.
- [215] Zhu Y, Dinh N. A data-driven approach for turbulence modeling. *arXiv preprint arXiv:200500426* 2020. <https://doi.org/10.48550/arXiv.2005.00426>.
- [216] Bode M, Gauding M, Kleinheinz K, Pitsch H. Deep learning at scale for subgrid modeling in turbulent flows. <https://doi.org/10.48550/arXiv.1910.00928>; 2019.
- [217] Basha N, Arcucci R, Angelici P, Anastasiou C, Abadie T, Casas CQ, et al. Machine learning and physics-driven modelling and simulation of multiphase systems. *Int J Multiphas Flow* 2024;179:104936. <https://doi.org/10.1016/j.ijmultiphaseflow.2024.104936>.
- [218] Irfan MF, Mjalli FS, Kim SD. Modeling of NH₃-NO-SCR reaction over CuO/γ-Al₂O₃ catalyst in a bubbling fluidized bed reactor using artificial intelligence techniques. *Fuel (Guildf)* 2012;93:245–51. <https://doi.org/10.1016/j.fuel.2011.09.043>.
- [219] Liou J-L, Liao K-C, Wen H-T, Wu H-Y. A study on nitrogen oxide emission prediction in Taichung thermal power plant using artificial intelligence (AI) model. *Int J Hydrogen Energy* 2024;63:1–9. <https://doi.org/10.1016/j.ijhydene.2024.03.120>.
- [220] Martins JR. Aerodynamic design optimization: challenges and perspectives. *Comput Fluid* 2022;239:105391. <https://doi.org/10.1016/j.compfluid.2022.105391>.
- [221] Zhu L-T, Chen X-Z, Ouyang B, Yan W-C, Lei H, Chen Z, et al. Review of machine learning for hydrodynamics, transport, and reactions in multiphase flows and reactors. *Ind Eng Chem Res* 2022;61:9901–49. <https://doi.org/10.1016/j.iecr.2c01036>.

- [222] Xu J, Pradhan A, Duraisamy K. Conditionally parameterized, discretization-aware neural networks for mesh-based modeling of physical systems. *Adv Neural Inf Process Syst* 2021;34:1634–45. <https://doi.org/10.48550/arXiv.2109.09510>.
- [223] Wu T, Liu X, An W, Huang Z, Lyu H. A mesh optimization method using machine learning technique and variational mesh adaptation. *Chin J Aeronaut* 2022;35: 27–41. <https://doi.org/10.1016/j.cja.2021.05.018>.
- [224] Zhu Y, Zhao S, Zhou Y, Liang H, Bian X. An unstructured adaptive mesh refinement for steady flows based on physics-informed neural networks. arXiv preprint arXiv:241119200 2024. <https://doi.org/10.48550/arXiv.2411.19200>.
- [225] Han C, Zhang P, Bluestein D, Cong G, Deng Y. Artificial intelligence for accelerating time integrations in multiscale modeling. *J Comput Phys* 2021;427: 110053. <https://doi.org/10.1016/j.jcp.2020.110053>.
- [226] Sousa P, Rodrigues CV, Afonso A. Enhancing CFD solver with Machine Learning techniques. *Comput Methods Appl Mech Eng* 2024;429:117133. <https://doi.org/10.1016/j.cma.2024.117133>.
- [227] Breuer M. A challenging test case for large eddy simulation: high reynolds number circular cylinder flow. *Int J Heat Fluid Flow* 2000;21:648–54. [https://doi.org/10.1016/S0142-727X\(00\)00056-4](https://doi.org/10.1016/S0142-727X(00)00056-4).
- [228] Kim J, Lee C. Prediction of turbulent heat transfer using convolutional neural networks. *J Fluid Mech* 2020;882:A18. <https://doi.org/10.1017/jfm.2019.814>.
- [229] Duraisamy K, Iaccarino G, Xiao H. Turbulence modeling in the age of data. *Annu Rev Fluid Mech* 2019;51:357–77. <https://doi.org/10.1146/annurev-fluid-010518-040547>.
- [230] Plaut E, Heinz S. Exact eddy-viscosity equation for turbulent wall flows—Implications for computational fluid dynamics models. *AIAA J* 2022;60: 1347–64. <https://doi.org/10.2514/1.J060761>.
- [231] Fiore M, Saccaggi E, Koloszar L, Bartosiewicz Y, Mendez MA. Data-driven turbulent heat flux modeling with inputs of multiple fidelity. *Physical Review Fluids* 2025;10:034606. <https://doi.org/10.1103/PhysRevFluids.10.034606>.
- [232] Shin J, Ge Y, Lampmann A, Pfitzner M. A data-driven subgrid scale model in large eddy simulation of turbulent premixed combustion. *Cambust Flame* 2021;231: 111486. <https://doi.org/10.1016/j.combustflame.2021.111486>.
- [233] Maulik R, San O, Rasheed A, Vedula P. Data-driven deconvolution for large eddy simulations of Kraichnan turbulence. *Phys Fluids* 2018;30. <https://doi.org/10.1063/1.5079582>.
- [234] Sudharun G, Warrior HV. Enhancing turbulence modeling: machine learning for pressure-strain correlation and uncertainty quantification in the reynolds stress model. *Phys Fluids* 2023;35. <https://doi.org/10.1063/5.0177438>.
- [235] Kravoshin MV, Ryazanov DA, Elizarova TG. Numerical algorithm based on regularized equations for incompressible flow modeling and its implementation in OpenFOAM. *Comput Phys Commun* 2022;271:108216. <https://doi.org/10.1016/j.cpc.2021.108216>.
- [236] Arora S, Ge R, Liang Y, Ma T, Zhang Y. Generalization and equilibrium in generative adversarial nets (gans). International conference on machine learning. PMLR; 2017. p. 224–32. <https://doi.org/10.48550/arXiv.1703.00573>.
- [237] Duraisamy K. Perspectives on machine learning-augmented Reynolds-averaged and large eddy simulation models of turbulence. *Physical Review Fluids* 2021;6: 050504. <https://doi.org/10.1103/PhysRevFluids.6.050504>.
- [238] Ling C, Kuo W, Xie M. An overview of adaptive-surrogate-model-assisted methods for reliability-based design optimization. *IEEE Trans Reliab* 2023;72:1243–64. <https://doi.org/10.1109/TR.2022.3200137>.
- [239] Minh LQ, Duong PLT, Lee M. Global sensitivity analysis and uncertainty quantification of crude distillation unit using surrogate model based on gaussian process regression. *Ind Eng Chem Res* 2018;57:5035–44. <https://doi.org/10.1021/acs.iecr.7b05173>.
- [240] Kochkov D, Smith JA, Alieva A, Wang Q, Brenner MP, Hoyer S. Machine learning-accelerated computational fluid dynamics, 118. Proceedings of the National Academy of Sciences; 2021, e2101784118. <https://doi.org/10.1073/pnas.2101784118>.
- [241] Le T-T-H, Kang H, Kim H. Towards incompressible laminar flow estimation based on interpolated feature generation and deep learning. *Sustainability (Basel)* 2022; 14:11996. <https://doi.org/10.3390/su141911996>.
- [242] Pfaff T, Fortunato M, Sanchez-Gonzalez A, Battaglia P. Learning mesh-based simulation with graph networks. International conference on learning representations. 2020. <https://doi.org/10.48550/arXiv.2010.03409>.
- [243] Zhou K, Wang Z, Gao Q, Yuan S, Tang J. Recent advances in uncertainty quantification in structural response characterization and system identification. *Probab Eng Mech* 2023;74:103507. <https://doi.org/10.1016/j.probengmech.2023.103507>.
- [244] Farrag A, Yang Y, Cao N, Won D, Jin Y. Physics-informed machine learning for metal additive manufacturing. *Progress in Additive Manufacturing* 2025;10: 171–85. <https://doi.org/10.1007/s40964-024-00612-1>.
- [245] vom Lehn F, Cai L, Pitsch H. Sensitivity analysis, uncertainty quantification, and optimization for thermochemical properties in chemical kinetic combustion models. *Proc Combust Inst* 2019;37:771–9. <https://doi.org/10.1016/j.proci.2018.06.188>.
- [246] Wang S, Shen Y. CFD-DEM modelling of dense gas-solid reacting flow: recent advances and challenges. *Prog Energy Combust Sci* 2025;109:101221. <https://doi.org/10.1016/j.pecs.2025.101221>.
- [247] Azizzadenesheli K, Kovachki N, Li Z, Liu-Schiaffini M, Kossaifi J, Anandkumar A. Neural operators for accelerating scientific simulations and design. *Nature Reviews Physics* 2024;6:320–8. <https://doi.org/10.48550/arXiv.2309.15325>.
- [248] Li Z, Kovachki N, Azizzadenesheli K, Liu B, Bhattacharya K, Stuart A, et al. Fourier neural operator for parametric partial differential equations. arXiv preprint arXiv: 201008895 2020. <https://doi.org/10.48550/arXiv.2010.08895>.
- [249] Pathak J, Subramanian S, Harrington P, Raja S, Chattopadhyay A, Mardani M, et al. Fourcastnet: a global data-driven high-resolution weather model using adaptive fourier neural operators. arXiv preprint arXiv:220211214 2022. <https://doi.org/10.48550/arXiv.2202.11214>.
- [250] Wen G, Li Z, Long Q, Azizzadenesheli K, Anandkumar A, Benson SM. Real-time high-resolution CO 2 geological storage prediction using nested fourier neural operators. *Energy Environ Sci* 2023;16:1732–41. <https://doi.org/10.1039/D2EE04204E>.
- [251] Lu L, Jin P, Pang G, Zhang Z, Karniadakis GE. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. *Nat Mach Intell* 2021;3:218–29. <https://doi.org/10.1038/s42256-021-00302-5>.
- [252] Wang S, Wang H, Perdikaris P. Learning the solution operator of parametric partial differential equations with physics-informed DeepONets. *Sci Adv* 2021;7: eabi8605. <https://doi.org/10.1126/sciadv.abi8605>.
- [253] Li Z, Kovachki N, Azizzadenesheli K, Liu B, Bhattacharya K, Stuart A, et al. Neural operator: graph kernel network for partial differential equations. arXiv preprint arXiv:200303485 2020. <https://doi.org/10.48550/arXiv.2003.03485>.
- [254] Li Z, Kovachki N, Azizzadenesheli K, Liu B, Stuart A, Bhattacharya K, et al. Multipole graph neural operator for parametric partial differential equations. *Adv Neural Inf Process Syst* 2020;33:6755–66. <https://doi.org/10.48550/arXiv.2006.09535>.
- [255] Li Z, Zheng H, Kovachki N, Jin D, Chen H, Liu B, et al. Physics-informed neural operator for learning partial differential equations. *ACM/JMS Journal of Data Science*. 2024;1:1–27. <https://doi.org/10.1145/3648506>.
- [256] Li Z, Meidani K, Farimani AB. Transformer for partial differential equations' operator learning. arXiv preprint arXiv:220513671 2022. <https://doi.org/10.48550/arXiv.2205.13671>.
- [257] Hao Z, Wang Z, Su H, Ying C, Dong Y, Liu S, et al. GNOT: a general neural operator transformer for operator learning. arXiv preprint arXiv:230214376 2023. <https://doi.org/10.48550/arXiv.2302.14376>.
- [258] Rahman MA, Florez MA, Anandkumar A, Ross ZE, Azizzadenesheli K. Generative adversarial neural operators. arXiv preprint arXiv:220503017 2022. <https://doi.org/10.48550/arXiv.2205.03017>.
- [259] Lim JH, Kovachki NB, Baptista R, Beckham C, Azizzadenesheli K, Kossaifi J, et al. Score-based diffusion models in function space. arXiv preprint arXiv:230207400. 2023. <https://doi.org/10.48550/arXiv.2302.07400>.
- [260] Lu L, Meng X, Cai S, Mao Z, Goswami S, Zhang Z, et al. A comprehensive and fair comparison of two neural operators (with practical extensions) based on FAIR data. *Comput Methods Appl Mech Eng* 2022;393:114778. <https://doi.org/10.1016/j.cma.2022.114778>.
- [261] Zhu H, Xie G, Berrouk AS, Liatsis P. Fourier neural Operator-driven transient analysis and control for supercritical CO2 cycles. *Energy (Calg)* 2025;323: 135828. <https://doi.org/10.1016/j.energy.2025.135828>.
- [262] Peyvan A, Kumar V. Fusion DeepONet: a data-efficient neural operator for geometry-dependent hypersonic flows on arbitrary grids. arXiv preprint arXiv: 250101934 2025. <https://doi.org/10.48550/arXiv.2501.01934>.
- [263] Benitez JAL, Furuya T, Faucher F, Kratsios A, Tricoche X, de Hoop MV. Out-of-distribution risk bounds for neural operators with applications to the helmholtz equation. *J Comput Phys* 2024;513:113168. <https://doi.org/10.48550/arXiv.2301.11509>.
- [264] Zhao C, Zhang F, Lou W, Wang X, Yang J. A comprehensive review of advances in physics-informed neural networks and their applications in complex fluid dynamics. *Phys Fluids* 2024;36. <https://doi.org/10.1063/5.0226562>.
- [265] Jagtap AD, Kharazmi E, Karniadakis GE. Conservative physics-informed neural networks on discrete domains for conservation laws: applications to forward and inverse problems. *Comput Methods Appl Mech Eng* 2020;365:113028. <https://doi.org/10.1016/j.cma.2020.113028>.
- [266] Xu J, Wei H, Bao H. Physics-informed neural networks for studying heat transfer in porous media. *Int J Heat Mass Tran* 2023;217:124671. <https://doi.org/10.1016/j.ijheatmasstransfer.2023.124671>.
- [267] Jalili D, Mahmoudi Y. Physics-informed neural networks for two-phase film boiling heat transfer. *Int J Heat Mass Tran* 2025;241:126680. <https://doi.org/10.1016/j.ijheatmasstransfer.2025.126680>.
- [268] Darlik F, Peters B. Reconstruct the biomass particles fields in the particle-fluid problem using continuum methods by applying the physics-informed neural network. *Results Eng* 2023;17:100917. <https://doi.org/10.1016/j.rineng.2023.100917>.
- [269] Niu P, Guo J, Chen Y, Zhou Y, Feng M, Shi Y. Improved physics-informed neural network in mitigating gradient-related failures. *Neurocomputing* 2025;130167. <https://doi.org/10.1016/j.ijheatmasstransfer.2023.124671>.
- [270] Xiang Z, Peng W, Liu X, Yao W. Self-adaptive loss balanced physics-informed neural networks. *Neurocomputing* 2022;496:11–34. <https://doi.org/10.1016/j.neucom.2022.05.015>.

- [271] Maddu S, Sturm D, Müller CL, Sbalzarini IF. Inverse dirichlet weighting enables reliable training of physics informed neural networks. *Mach Learn: Sci Technol* 2022;3:015026. <https://doi.org/10.1088/2632-2153/ac3712>.
- [272] Klawonn A, Langer M, Weber J. Machine learning and domain decomposition methods - a survey. *Computational Science and Engineering* 2024;1:2. <https://doi.org/10.1007/s44207-024-00003-y>.
- [273] Dolean V, Heinlein A, Mishra S, Moseley B. Multilevel domain decomposition-based architectures for physics-informed neural networks. *Comput Methods Appl Mech Eng* 2024;429:117116. <https://doi.org/10.1016/j.cma.2024.117116>.
- [274] Jagtap AD, Karniadakis GE. Extended physics-informed neural networks (XPINNs): a generalized space-time domain decomposition based deep learning framework for nonlinear partial differential equations. *Commun Comput Phys* 2020;28:2002–41. <https://doi.org/10.4208/cicp.oa-2020-0164>. Medium: ED; Size.