Supercritical CO2 Flow Dynamics: A Survey

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Abstract

This survey paper investigates the complex dynamics of supercritical carbon dioxide (sCO2), focusing on its thermodynamic properties and flow behavior, particularly during phase transitions in transcritical flows. Utilizing Computational Fluid Dynamics (CFD), the study explores the intricate interplay of sCO2's liquid-like density and gas-like transport properties, critical for applications in industrial, technological, and environmental spheres. The paper emphasizes the challenges in modeling sCO2 due to its non-ideal behavior under supercritical conditions, highlighting the limitations of traditional equations of state and the necessity for advanced modeling techniques. Recent advancements in CFD, including the integration of machine learning and high-performance computing, are discussed as transformative tools that enhance simulation accuracy and efficiency. These developments facilitate the exploration of complex phenomena such as impinging jets and multi-phase interactions, crucial for optimizing systems that leverage sCO2's unique properties. The survey underscores the importance of continued research in refining computational methods and experimental frameworks to improve the understanding and application of sCO2 in various engineering contexts. Ultimately, this work aims to drive innovation and optimization in energy production, environmental protection, and industrial processes, addressing contemporary challenges through the enhanced modeling of supercritical CO2 dynamics.

1 Introduction

1.1 Significance of Supercritical CO2

Supercritical carbon dioxide (sCO2) is crucial in industrial and environmental contexts due to its unique properties as a supercritical fluid. Near its critical point, sCO2 exhibits liquid-like densities and gas-like transport characteristics, making it particularly valuable in aerospace propulsion applications [1]. In the chemical industry, sCO2 serves as an efficient solvent, enhancing chemical reactions and processes, especially for poorly soluble compounds in pharmaceuticals [2].

In energy production, sCO2 enhances the flexibility of thermal power plants through advanced control systems [3]. Its use in Brayton cycles within concentrated solar power (CSP) systems illustrates its potential for efficient energy generation while minimizing emissions. Moreover, sCO2's role in heat exchangers is vital for improving thermal performance, essential for various industrial applications [4]. The determination of heat transfer coefficient distributions is critical for the design and operation of industrial devices [5].

From an environmental perspective, sCO2 is integral to CO2 capture and storage (CCS) technologies, which are vital in combating climate change. The efficiency of CO2 capture in solvent-based systems hinges on maximizing the gas-solvent interfacial area, presenting a foundational challenge in CCS design [6]. Additionally, the importance of liquid holdup and mass transfer area in packed columns is essential for enhancing CO2 capture efficiency [7].

The diverse applications of sCO2 underscore its versatility as an efficient medium, facilitating advanced power cycles that enable carbon capture with minimal efficiency loss while serving as a

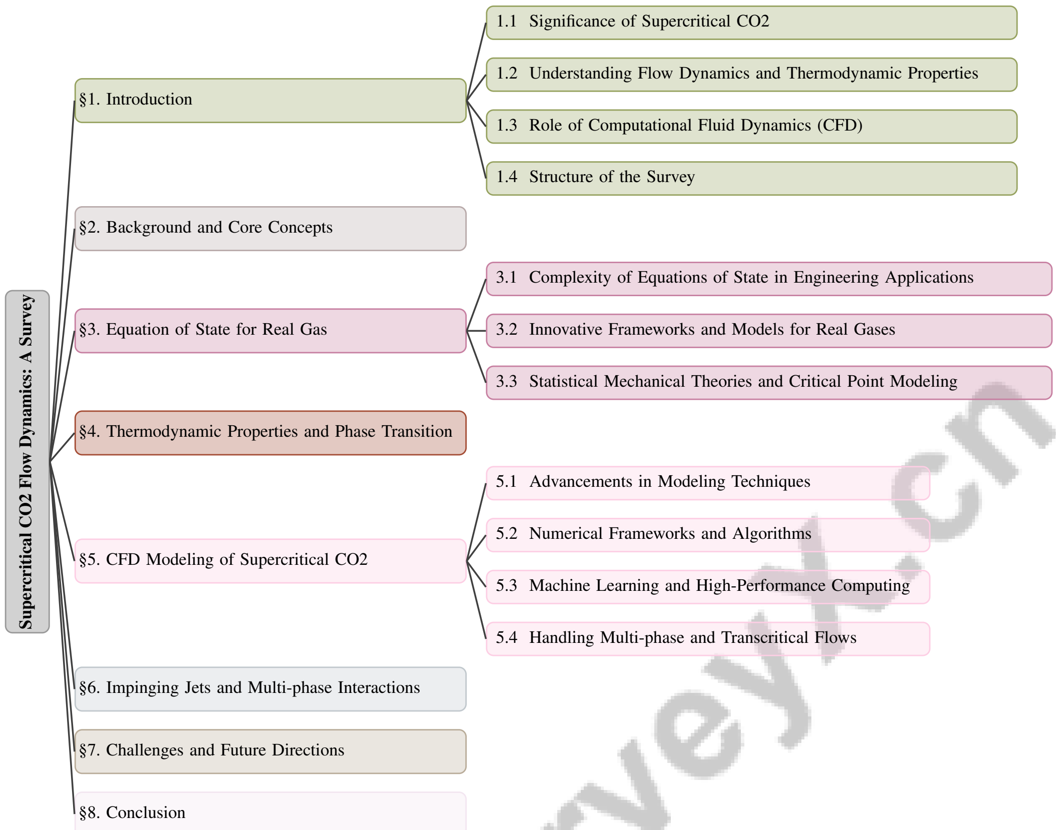


Figure 1: chapter structure

non-toxic solvent in green chemistry. Its properties can be finely tuned through pressure variations, providing tailored solutions for contemporary challenges in energy production, environmental protection, and industrial innovation. Recent advancements in modeling and control methodologies further optimize sCO2 system performance, paving the way for sustainable technological applications [8, 9, 3, 2, 10].

1.2 Understanding Flow Dynamics and Thermodynamic Properties

Understanding the flow dynamics and thermodynamic properties of supercritical carbon dioxide (sCO2) is essential for optimizing engineering systems that utilize this fluid, given its complex behavior under critical conditions. This complexity is particularly pronounced in concentrated solar power (CSP) plants, where cooling system performance is closely linked to flow dynamics control [11]. The non-ideal behavior of sCO2 necessitates a comprehensive understanding of its flow characteristics to ensure efficient operation in supercritical cycles [3].

Accurate modeling of flow behavior near thermodynamic critical points is vital for system performance enhancement. The challenges in predicting droplet behavior under these conditions, as highlighted by Schulte et al. [12], reflect the difficulties in simulating sCO2 dynamics. Additionally, current models often inadequately capture compressible flow characteristics at high pressures, complicating the distinction between real-gas and ideal-gas behaviors [13].

The thermodynamic state significantly influences flow dynamics, as emphasized by Lychagin et al. [14], who underscore the importance of stationary adiabatic flows of real gases. This understanding is critical for designing and operating CCS systems, where precise modeling of CO2 jet behavior resulting from decompression is required [15]. The challenges in directly measuring heat transfer coefficients further highlight the necessity for a thorough grasp of flow dynamics [5].

Limitations in molecular dynamics for capturing large-scale phenomena, alongside the assumptions in computational fluid dynamics (CFD) methods, present significant challenges in simulating fluid dynamics across various scales [16]. Furthermore, uncertainties related to turbulence models in CFD simulations impact prediction reliability in engineering applications, emphasizing the need for improved comprehension of sCO2 dynamics [17].

Local inhomogeneities that alter traditional solubility and activity concepts add further complexity to understanding the flow dynamics and thermodynamic properties of sCO2 [2]. These complexities necessitate the development of advanced models and the acquisition of precise data to enhance the design and operation of sCO2-utilizing systems, ensuring efficiency and reliability across diverse industrial and environmental applications.

1.3 Role of Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is essential for modeling and analyzing sCO2 flow dynamics, offering a sophisticated framework for simulating complex fluid behaviors under varying thermodynamic conditions. The application of CFD is particularly critical for sCO2 due to its non-ideal thermodynamic behavior and the need for precise modeling of phase transitions and thermodynamic properties. Advanced simulation techniques, including machine learning surrogates, significantly enhance the efficiency and accuracy of CFD simulations, facilitating the design optimization of carbon capture systems (CCSs). For example, neural network-based surrogates can drastically reduce computational costs while maintaining low errors in interfacial area estimations, crucial for effective CCS design [18, 6].

The integration of advanced computational methods, such as Model Predictive Control (MPC), with CFD is exemplified by Bone et al. [3], demonstrating how these techniques can effectively manage the dynamics of sCO2 cycles. This integration highlights the necessity of employing advanced modeling approaches to predict sCO2 behavior in various engineering applications.

However, traditional CFD methods face limitations, particularly with compressible two-phase flows, as noted by Bezgin et al. [19]. These methods often struggle with efficiently simulating complex fluid interactions, necessitating the development of more robust computational frameworks. The coupling of system codes like RELAP5-MOD3.3 with reduced-order models of CFD solvers, as proposed by Star et al. [20], represents a significant advancement in enhancing thermal-hydraulic simulation efficiency, improving CFD analysis accuracy and reliability.

In optimizing cooling performance in energy systems, CFD models have been employed to simulate interactions between components, such as axial flow fans and air-cooled heat exchangers, as shown by Boshoff et al. [11]. This application underscores the critical role of CFD in providing detailed insights into fluid dynamics and heat transfer processes.

The importance of CFD in determining heat transfer coefficients is further emphasized by Duda et al. [5], highlighting its role in modeling and optimizing thermal systems. Despite its capabilities, the high computational costs associated with traditional CFD methods pose challenges in evaluating numerous configurations, particularly in CCS systems, as discussed by Bartoldson et al. [6]. This challenge necessitates the pursuit of more cost-effective and efficient computational approaches.

Recent advancements in machine learning (ML) present promising opportunities for enhancing CFD tasks, as explored by Wang et al. [21]. The integration of ML techniques into CFD simulations has the potential to significantly improve modeling accuracy and efficiency, paving the way for more sophisticated analyses of sCO2 flow dynamics. This evolving role of ML in CFD highlights ongoing advancements in computational methodologies, driving the field toward more accurate and efficient simulations.

1.4 Structure of the Survey

This survey is structured to comprehensively explore the flow dynamics and thermodynamic properties of supercritical CO2, emphasizing the role of Computational Fluid Dynamics (CFD) in modeling these phenomena. The paper is organized into several key sections, each addressing critical aspects of the topic.

The introduction emphasizes the significance of supercritical CO2 in various industrial and environmental applications, particularly in enhancing power cycle efficiency for carbon capture during combustion processes. It underscores the urgent need to comprehend the flow dynamics and thermodynamic properties of supercritical CO2, especially given the challenges posed by combustion mechanisms at high pressures and the complex turbulent mixing behaviors in slightly supercritical fluids. This understanding is essential for optimizing processes like natural product extraction and aerospace propulsion, where supercritical CO2 is increasingly utilized [8, 1]. It also outlines the pivotal role of CFD in analyzing these aspects.

The subsequent section delves into background and core concepts, offering definitions and discussions on the unique properties of supercritical CO2 as a real gas. It explores the equation of state and its application in modeling supercritical CO2, alongside an introduction to phase transition and transcritical flow, particularly in the context of impinging jets and multi-phase interactions.

The survey examines various equations of state utilized for modeling real gases, emphasizing their specific applications in supercritical CO2. It highlights the importance of understanding molecular interactions at high pressures, as described by cubic equations of state, and discusses their influence on key thermodynamic properties such as density, enthalpy, and sound speed. Additionally, it explores the implications of real-gas modifications on compressible flow phenomena, including choked-nozzle flow and shock wave behavior in high-pressure scenarios. The survey also evaluates the effectiveness of different chemical kinetic mechanisms for combustion in supercritical CO2, identifying critical reactions that enhance performance under varying conditions [8, 22, 14, 13]. It discusses the complexity of these equations in engineering applications and highlights innovative frameworks and models developed to enhance accuracy and efficiency.

The section on thermodynamic properties and phase transition scrutinizes the challenges in accurately modeling these properties and the impact of phase transitions on flow dynamics. It also addresses the limitations of traditional thermodynamic models and explores the development of unified thermodynamic models for supercritical CO2.

The survey then shifts focus to CFD modeling of supercritical CO2, reviewing advancements in modeling techniques, numerical frameworks, and algorithms. It investigates the synergistic integration of machine learning (ML) techniques and high-performance computing (HPC) to improve CFD simulations, particularly focusing on advanced methodologies for managing complex scenarios such as multi-phase flows and transcritical flow conditions. The study systematically reviews recent advancements in ML applications within CFD, highlights the importance of uncertainty quantification in turbulent flow modeling, and discusses the potential of novel ML algorithms to enhance simulation accuracy and reduce computational time, facilitating intricate analyses of fluid dynamics [23, 17, 21, 24, 25].

A dedicated section analyzes the specific case of impinging jets and their interaction with multi-phase flows, reviewing both experimental and computational studies conducted in this area.

The survey highlights significant challenges in accurately modeling and simulating sCO2 flows, particularly regarding combustion mechanisms and the limitations of current CFD methods. While neural network surrogates have shown potential to enhance simulation speed and accuracy for carbon capture systems, their transferability to new configurations remains a concern. Moreover, the understanding of combustion processes in high-pressure sCO2 environments is still evolving, with recent research identifying critical reaction pathways that could inform future modeling efforts. These findings suggest promising avenues for further research and technological advancements aimed at improving the efficiency and reliability of sCO2 flow simulations [8, 6]. It concludes by summarizing the key findings and reinforcing the importance of continued research in this field.The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Definition and Properties of Supercritical CO2

Supercritical carbon dioxide (sCO2) exists beyond its critical temperature and pressure, exhibiting a unique combination of liquid-like density and gas-like viscosity and diffusivity. These properties arise from intermolecular interactions that differentiate sCO2 from ideal gases [26], crucial for precise solvation control in industrial applications [9]. This distinct behavior is pivotal in processes involving turbulent mixing at slightly supercritical conditions, optimizing various industrial applications [1]. The reactivity of CO2 under these conditions significantly impacts CO2 management technologies [2]. Moreover, predicting the gas-solvent interfacial area in carbon capture and storage (CCS) systems highlights the complexity of sCO2 behavior, essential for enhancing CO2 capture efficiency [6]. The role of sCO2 in CO2 capture processes necessitates precise predictions of liquid holdup and mass transfer area, crucial for optimizing random packed columns [7]. These challenges underscore the need for advanced modeling approaches to capture the intricate interactions and phase transitions characteristic of supercritical states.

2.2 Equation of State and Real Gas Behavior

Modeling supercritical carbon dioxide (sCO2) as a real gas requires sophisticated equations of state (EoS) to account for its non-ideal behavior, especially when traditional ideal gas assumptions fall short. The properties of sCO2, including its liquid-like density and gas-like viscosity, necessitate an EoS that accommodates complex intermolecular forces and phase transitions typical of supercritical fluids [27]. A significant challenge in modeling sCO2 is predicting non-classical non-linear wave behavior in dense gases, which classical models fail to address [28]. This requires models incorporating pressure-dependent compressibility and solubility for accurate sCO2 behavior forecasting [27]. Theoretical approaches like integral equations and fluctuation theory elucidate critical phenomena in fluids, providing insights into sCO2 behavior near its critical point [29]. These approaches are crucial for developing EoS that effectively model the thermodynamic properties of sCO2, especially in scenarios involving complex thermodynamic processes and multi-phase interactions [30]. Integrating chemical kinetic mechanisms, such as the UoS sCO2 mechanism, addresses previous models' limitations by incorporating new findings from sensitivity analyses, crucial for accurately modeling combustion processes in supercritical CO2 environments [8]. The advancement of low-Mach number expansions for real gases, tailored for analyzing turbulent mixing of slightly supercritical fluids, further enhances EoS capabilities to model sCO2 behavior [1]. These developments reflect ongoing efforts to refine EoS for real gases, ensuring accurate predictions of complex interactions and phase transitions in supercritical CO2 systems.

2.3 Phase Transition and Transcritical Flow

Phase transition and transcritical flow are crucial for understanding supercritical carbon dioxide (sCO2), especially in high-pressure and high-temperature applications. At transcritical pressures, the distinction between liquid and gas phases blurs, leading to unique fluid dynamics essential in engineering applications like fuel injection systems and propulsion technologies [31]. The phase transition of sCO2 is characterized by the complex interplay of intermolecular forces influencing solubility and reactivity [2]. This complexity is amplified by thermal fluctuations and non-equilibrium conditions near the critical point, posing significant challenges for accurately modeling multiphase flows [32]. Transcritical flow involves dynamic behaviors of fluids transitioning between subcritical and supercritical states, marked by nonlinear phenomena such as shock wave dynamics and pressure oscillations. These are challenging to simulate due to inherent instability and rapid changes in fluid properties [33]. Capturing these dynamics is crucial for optimizing systems operating under transcritical conditions, including rocket engines and high-speed propulsion systems. A notable area of interest is the behavior of underexpanded jets at engine-relevant conditions, where real-gas effects and mixture-induced phase separation are pronounced. These jets exhibit complex flow patterns and phase transitions inadequately described by classical models, necessitating advanced simulation techniques to account for real-gas effects [34].

In recent years, the study of real gases has gained considerable attention due to its implications in various scientific and industrial applications. A comprehensive understanding of the equation of state for real gases is essential, particularly when addressing the complexities associated with supercritical CO2. This complexity is well captured in Figure 2, which illustrates the hierarchical structure of the complexities, innovations, and statistical theories involved in modeling the equation of state. The figure highlights not only the challenges posed by supercritical CO2 but also the advancements in modeling frameworks and the integration of statistical mechanical theories for critical point modeling. Such visual representation serves to enhance our understanding of the intricate relationships and developments within this field, thereby providing a clearer context for the subsequent discussions in this review.

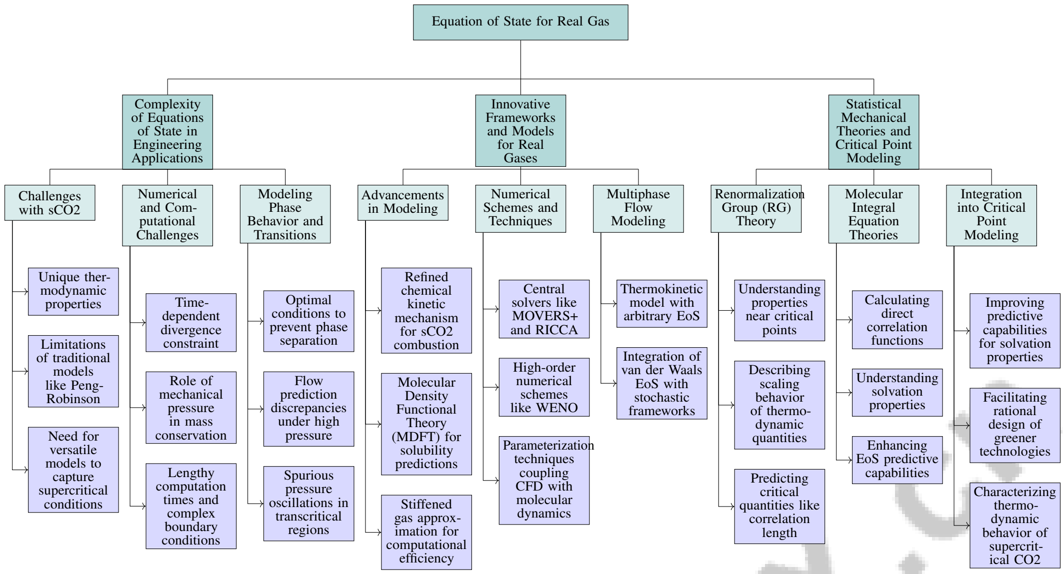


Figure 2: This figure illustrates the hierarchical structure of the complexities, innovations, and statistical theories involved in modeling the equation of state for real gases, highlighting challenges with supercritical CO2, advancements in modeling frameworks, and the integration of statistical mechanical theories for critical point modeling.

3 Equation of State for Real Gas

3.1 Complexity of Equations of State in Engineering Applications

The application of equations of state (EoS) for supercritical CO2 (sCO2) in engineering is complex due to its unique thermodynamic properties, challenging traditional models like Peng-Robinson and Soave-Redlich-Kwong, which are limited to fluids with similar critical compressibility factors [22]. This necessitates developing versatile models to accurately capture sCO2's behavior under supercritical conditions. Accurately representing intermolecular interactions in sCO2 flows is crucial for understanding fluid behavior in combustion and high-temperature processes [26]. Advanced modeling techniques, such as Molecular Density Functional Theory (MDFT), enhance predictions of solvation properties in supercritical fluids [9].

In engineering contexts, particularly low-Mach-number flows, the time-dependent divergence constraint on momentum and mechanical pressure's role in mass conservation complicate numerical solutions, necessitating sophisticated computational methods [35]. Additionally, lengthy computation times and complex boundary conditions in CFD methods highlight the need for more efficient computational frameworks [5]. The intricate nature of sCO2 also complicates modeling phase behavior and transitions, essential for applications like cooling systems. Maintaining optimal conditions to prevent phase separation is critical, as traditional EoS often fail to capture intermolecular forces, leading to flow prediction discrepancies under high pressure [13]. Spurious pressure oscillations and inaccuracies in shock wave representation using standard conservative numerical methods pose challenges in the highly nonlinear transcritical region [33].

As illustrated in Figure 3, this figure encapsulates the complexity of equations of state in engineering applications, highlighting the thermodynamic models, advanced modeling techniques, and numerical challenges faced in computational fluid dynamics. The first image depicts shock wave behavior in a one-dimensional space, emphasizing the non-linear nature of such interactions. The second image visualizes flow in a two-dimensional channel, capturing vortex formation and variations in flow properties. The third image compares density, pressure, velocity, and the fundamental derivative across different simulation methods—Reference, MOVERS+, and RICCA—highlighting the importance of model selection for accurate representation of real gas behaviors. These examples collectively underscore the multifaceted challenges engineers face when addressing EoS in practical applications, where precision and adaptability are essential for effective problem-solving [36, 37, 28].

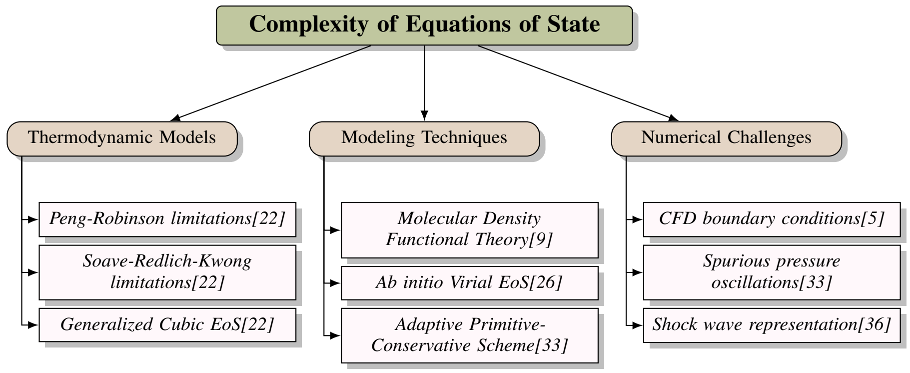


Figure 3: This figure illustrates the complexity of equations of state in engineering applications, highlighting thermodynamic models, advanced modeling techniques, and numerical challenges faced in computational fluid dynamics.

3.2 Innovative Frameworks and Models for Real Gases

Innovative frameworks and models have emerged to simulate the complex behaviors of supercritical carbon dioxide (sCO2) and other real gases in engineering applications. These advancements address challenges such as combustion mechanisms at high pressures, solvation properties under varying conditions, and convective dissolution dynamics. A refined chemical kinetic mechanism for sCO2 combustion enhances ignition delay time predictions, while MDFT improves solubility predictions and supports green chemical process design [8, 9, 10, 27]. Such advancements are crucial for enhancing the accuracy and efficiency of Computational Fluid Dynamics (CFD) simulations.

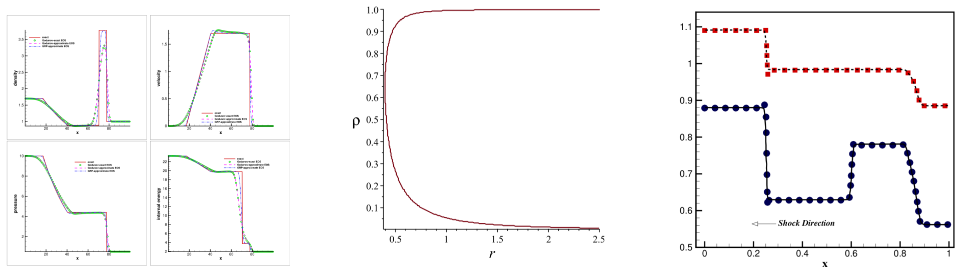
The stiffened gas approximation simplifies the EoS at computational interfaces to facilitate efficient Riemann solvers, improving computational efficiency [36]. Central solvers like MOVERS+ and RICCA accurately capture non-classical wave phenomena in dense gases without requiring complex modifications, enhancing simulation fidelity in shock wave scenarios [28]. High-order numerical schemes, such as the Weighted Essentially Non-Oscillatory (WENO) scheme, with general EoS achieve precise simulations of CO2 flows, particularly in multiphase systems [15]. A linearized cubic EoS describes real-gas behavior in compressible flow scenarios more accurately, providing a nuanced understanding of thermodynamic properties under high pressure [13].

Parameterization techniques coupling CFD with molecular dynamics refine continuum models by embedding molecular-level details, enhancing simulation accuracy through localized molecular insights within larger-scale frameworks [16]. A generalized cubic EoS allows modularized implementation of various EoS, improving flexibility and accuracy in thermodynamic modeling for CFD simulations [22]. In multiphase flow modeling, a thermokinetic model introduces arbitrary EoS, enabling accurate simulation of complex multiphase flows beyond traditional methods' capabilities [30]. Integrating a van der Waals EoS with a stochastic numerical framework effectively captures multiphase flow dynamics, providing a robust tool for simulating interactions between different phases under supercritical conditions [32].

As depicted in Figure 4, the study of real gases under various conditions is complex yet essential in thermodynamics and fluid dynamics. The figures illustrate key aspects of innovative models and frameworks. The first subfigure compares exact and approximate EoS for a gas flow problem, highlighting differences in density, velocity, pressure, and internal energy. The second graph illustrates the relationship between density () and radial distance (r), revealing spatial distribution of gas properties. Lastly, the "Shock Direction" graph employs a logarithmic scale to map shock wave progression in a gas medium, emphasizing the dynamic nature of gas flows. Together, these visualizations underscore the complexity and innovation in modeling real gases, providing a comprehensive framework for understanding their behavior in diverse scenarios [36, 14, 30].

3.3 Statistical Mechanical Theories and Critical Point Modeling

Modeling critical points in supercritical carbon dioxide (sCO2) is significantly enhanced by statistical mechanical theories, particularly renormalization group (RG) theory. RG theory offers a robust



(a) Comparison of Exact and Approximate EOS for a Gas Flow Problem[36]

(b) vs r[14]

(c) Shock Direction[30]

Figure 4: Examples of Innovative Frameworks and Models for Real Gases

framework for understanding properties near critical points, providing insights into critical behavior that classical approaches cannot access [29]. This theoretical approach is crucial for accurately capturing the phase behavior and critical phenomena associated with sCO2, essential for its industrial applications.

RG theory's capacity to describe scaling behavior of thermodynamic quantities near critical points refines EoS for real gases like sCO2. By integrating fluctuations and correlations significant near critical points, RG theory improves our understanding of phase transitions and critical phenomena in supercritical fluids. It accounts for non-Gaussian fluctuations of the order parameter and aids in deriving the EoS for supercritical fluids, as demonstrated in grand partition function analyses. Additionally, RG theory predicts critical quantities such as correlation length critical exponents and isothermal compressibility behavior as a function of density, providing a comprehensive framework for exploring supercritical fluid properties and applications [29, 9, 10, 1]. This insight is invaluable in developing models that predict sCO2 behavior under conditions where traditional models may falter.

In addition to RG theory, various statistical mechanical approaches—including molecular integral equation theories and fluctuation theory—play significant roles in modeling critical points in sCO2. Molecular integral equation theories facilitate calculating direct correlation functions critical for understanding solvation properties under varying conditions, while fluctuation theory provides insights into non-Gaussian fluctuations of the order parameter near critical points, enhancing EoS predictive capabilities for fluids in the supercritical region [29, 9]. These methodologies collectively advance our understanding of sCO2 thermodynamic behavior, crucial for developing efficient and environmentally friendly processes in the chemical industry.

The integration of statistical mechanical theories, particularly MDFT and molecular integral equations, into critical point modeling in sCO2 marks a significant advancement in our understanding of its behavior under critical conditions. This approach enhances predictive capabilities for solvation properties of supercritical CO2 and facilitates the rational design of greener technologies by providing insights into molecular dynamics and structural characteristics of this versatile solvent. By leveraging accurate direct correlation functions derived from molecular dynamics simulations and comparing them with simpler integral equations, researchers can better characterize the thermodynamic behavior of supercritical CO2, thereby opening avenues for its application in various industrial processes, including extraction and combustion [38, 8, 9, 29, 10]. These theoretical frameworks improve prediction accuracy and facilitate the development of innovative applications that exploit the unique characteristics of supercritical fluids.

4 Thermodynamic Properties and Phase Transition

The thermodynamic properties of supercritical carbon dioxide (sCO2) play a pivotal role in understanding phase transitions, necessitating innovative modeling approaches to overcome the limitations of conventional methods. This section delves into the complexities of modeling sCO2, highlighting the need for advanced solutions to accurately depict its behavior under diverse conditions.

4.1 Challenges in Modeling Thermodynamic Properties

Modeling sCO2's thermodynamic properties is complicated by its intricate behavior and the shortcomings of traditional models, especially the universal critical compressibility factor, which inadequately represents diverse fluids, leading to inaccuracies near critical points where fluctuations are significant [22]. Multiphase fluid dynamics under extreme conditions further exacerbate these challenges, as conventional models often ignore essential thermal fluctuations [32]. In thermal systems like heat exchangers, traditional methods lack precision and efficiency, but low-order dynamic models offer promising improvements [4].

To enhance modeling accuracy, integrating advanced theoretical frameworks such as Molecular Density Functional Theory (MDFT) and subsystem density functional theory (DFT) with improved computational techniques is crucial. While Kohn-Sham DFT is computationally demanding, MDFT facilitates rapid calculations of chemical potentials and direct correlation functions, enabling new applications in green technology and energy systems [38, 8, 9, 3, 10].

4.2 Impact of Thermodynamic Properties on Phase Transitions

sCO2's thermodynamic properties critically influence phase transitions, particularly in transcritical flow regimes where the fluid shifts from subcritical to supercritical states. Its unique attributes, such as liquid-like density and gas-like diffusivity, significantly affect these transitions [1]. Near the critical point, substantial fluctuations in density and thermodynamic variables complicate phase behavior predictions [29].

Accurate phase transition predictions are essential in engineering applications for optimizing system performance during rapid pressure and temperature changes. Advanced equations of state that capture subtle variations in thermodynamic properties are necessary to understand phase transitions [22]. These transitions impact fluid properties like compressibility and heat capacity, affecting system efficiency and stability under transcritical conditions [27].

In multiphase flow systems, thermodynamic properties govern phase interactions, where thermal fluctuations and non-equilibrium conditions near the critical point lead to complex phenomena like shock waves and pressure oscillations, crucial for advanced propulsion and fuel injection systems [33]. A comprehensive understanding of sCO2's thermodynamic properties and their impact on phase behavior is vital for accurate modeling [32].

4.3 Limitations of Traditional Thermodynamic Models

Traditional thermodynamic models often inadequately represent sCO2 and other real gases, particularly under non-ideal conditions. The reliance on ideal gas laws fails to capture the thermodynamic behaviors of real-gas mixtures, especially in phase separation and transcritical flows [34]. This inadequacy necessitates advanced models that consider real gas properties and interactions.

As illustrated in Figure 5, the limitations of traditional thermodynamic models are evident, particularly in their inadequate representation of real gases and the computational complexities they entail. The figure highlights not only the challenges associated with traditional approaches but also the advancements in computational fluid dynamics (CFD) simulations that aim to address these issues. Traditional models struggle with the computational complexities of real gas flows. Equations of state (EoS) often fail to capture the intricate dynamics of gas flows under varying conditions, highlighting the need for sophisticated approaches to account for non-ideal gas behaviors [14]. In engineering applications, although some models have been refined for sCO2's properties, challenges persist under extreme conditions or with atypical fluids [22].

In computational fluid dynamics (CFD) simulations, advancements like finite-volume approaches combined with low-dissipative high-order shock capturing schemes exemplify overcoming traditional model limitations [19]. Methods that bypass computational difficulties of exact Riemann solvers for complex EoS, such as the stiffened gas approximation, enhance numerical scheme efficiency and reliability for real gases [36].

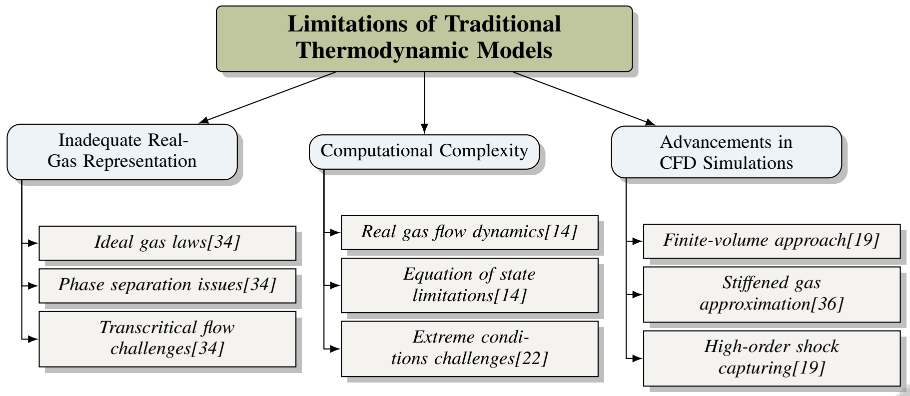


Figure 5: This figure illustrates the limitations of traditional thermodynamic models, highlighting inadequate real-gas representation, computational complexities, and advancements in CFD simulations that address these challenges.

4.4 Unified Thermodynamic Models

Unified thermodynamic models for sCO2 are crucial for overcoming traditional model limitations, particularly in high-pressure combustion and solvation processes. These models enhance simulation accuracy by providing insights into complex chemical kinetics and offering predictive tools for solvation properties under varying conditions, facilitating greener technologies in the chemical industry [8, 9]. Unified models aim to integrate various thermodynamic properties and phase behaviors, enhancing our understanding of sCO2 dynamics under critical conditions.

Integrating molecular-level insights into continuum models allows for accurate representation of complex interactions and phase transitions in supercritical fluids. Molecular Density Functional Theory (MDFT) exemplifies this approach by combining classical density functional theory with molecular interactions to predict solvation properties in supercritical fluids [9]. This integration is vital for accurately modeling sCO2 in industrial processes, where precise thermodynamic property control is crucial.

Advanced statistical mechanical theories, such as renormalization group (RG) theory, provide a robust framework for understanding sCO2's critical behavior near its critical point [29]. These insights refine equations of state for real gases, enabling accurate predictions of phase transitions and critical phenomena in supercritical fluids.

In CFD, parameterization techniques coupling CFD with molecular dynamics enhance simulation accuracy by incorporating molecular-level details into continuum models, offering a comprehensive understanding of sCO2's thermodynamic properties and phase behaviors [16]. Generalized cubic equations of state facilitate modularized EoS implementation, enhancing flexibility and accuracy in thermodynamic modeling for CFD simulations [22]. This approach efficiently handles complex multiphase flows and predicts thermodynamic properties across various conditions.

Unified thermodynamic models for sCO2 represent a significant advancement by integrating insights from studies on combustion mechanisms and solvation properties. A new chemical kinetic mechanism for high-pressure sCO2 combustion improves ignition delay time predictions, while MDFT accurately models solvation properties under varying conditions. This cohesive framework facilitates the design of efficient supercritical CO2 power cycles with intrinsic carbon capture and supports greener chemical processes using supercritical CO2 as a solvent [8, 9]. These models optimize systems relying on sCO2's unique properties, enhancing simulation accuracy and efficiency in industrial and environmental applications.

5 CFD Modeling of Supercritical CO2

To effectively understand the complexities involved in the modeling of supercritical carbon dioxide (sCO2), it is essential to explore the advancements in Computational Fluid Dynamics (CFD) techniques that have emerged in recent years. These advancements not only address the unique

Category	Feature	Method
Advancements in Modeling Techniques	Numerical Methods Enhancement Machine Learning in Simulation Dynamic System Estimation	SMOLD[32] DF-S[6] LODM[4]
Numerical Frameworks and Algorithms	Flow Dynamics Precision Parallel and Quantum Computing Spacetime and Data Correlation	CFVPBA[39], APCS[33], HOCGKS[40] TPU-CFD[41], HQCF[42] SCFVM[43], CFD-LH[7]
Machine Learning and High-Performance Computing	Efficiency and Scalability	JF[18], DRAF[10], JF2[19]
Handling Multi-phase and Transcritical Flows	Advanced Simulation Techniques Phase Interaction Modeling	HWENO[15], GCEoS[22] HPS-VLE[34]

Table 1: The table provides a comprehensive overview of recent advancements in Computational Fluid Dynamics (CFD) modeling techniques for supercritical carbon dioxide (sCO2) systems. It categorizes various features and methods, highlighting innovations in modeling techniques, numerical frameworks, machine learning integration, and the handling of multi-phase and transcritical flows. These developments are crucial for enhancing the accuracy and efficiency of CFD simulations, addressing the complex thermodynamic behaviors of sCO2.

challenges posed by the thermodynamic behavior of sCO2 but also enhance the predictive capabilities of simulations across various applications. Table 1 presents a detailed summary of recent advancements in CFD modeling techniques for supercritical CO2, illustrating key features and methods that enhance simulation accuracy and efficiency. Additionally, Table 5 presents a comprehensive comparison of these advancements, detailing key features and methods that contribute to improved simulation accuracy and efficiency. The following subsection will delve into recent innovations in modeling techniques, highlighting their significance in improving the accuracy and efficiency of CFD simulations for sCO2 systems.

5.1 Advancements in Modeling Techniques

Method Name	**Modeling Techniques**	**Computational Efficiency**	**Application Domains**
HQCF[42]	Quantum Linear Solvers	Quantum-classical Frameworks	Power Generation
SMOLD[32]	Stochastic Numerical Framework	Low Mach Number	Power Generation
DF-S[6]	Deep Fluids-inspired	4000x Speedups	Ccs Design Optimization
LODM[4]	Low-Order Dynamic	Reduced Computational Complexity	Industrial Applications
CFD-LH[7]	Cfd Simulations	High-performance Computing	Co2 Capture
JF[18]	Machine Learning Integration	Automatic Differentiation Optimization	Power Generation
SCFVM[43]	Finite Volume Methods	Computational Intensity	Power Generation

Table 2: Summary of recent advancements in computational fluid dynamics (CFD) modeling techniques for supercritical carbon dioxide (sCO2) systems. The table highlights various methods, their modeling techniques, computational efficiencies, and application domains, illustrating the integration of quantum computing, stochastic methods, and machine learning to enhance simulation capabilities.

Recent advancements in Computational Fluid Dynamics (CFD) modeling techniques have significantly improved the simulation capabilities for supercritical carbon dioxide (sCO2) systems, effectively addressing the complexities of its thermodynamic behavior and phase transitions. Notably, new chemical kinetic mechanisms have been developed to better understand combustion processes in sCO2 environments, particularly at high pressures, enhancing ignition delay time predictions. Additionally, innovative approaches such as neural network surrogates have accelerated the estimation of gas-solvent interfacial areas in carbon capture systems, achieving remarkable speedups while maintaining accuracy. Furthermore, the integration of high-performance computing into differentiable CFD solvers has expanded the modeling capabilities for compressible two-phase flows, facilitating more robust simulations of sCO2 applications. These advancements collectively contribute to more efficient and effective modeling of sCO2, paving the way for improved design and operational strategies in power generation and carbon capture technologies. [8, 6, 19, 3, 10]. The integration of novel computational methods and frameworks has improved both the accuracy and efficiency of these simulations. Table 2 provides a comprehensive overview of the latest advancements in CFD modeling techniques, showcasing the innovative approaches that have been developed to improve the simulation of supercritical CO2 systems.

One notable advancement is the development of a hybrid quantum-classical CFD framework, as proposed by Ye et al., which integrates quantum linear solvers with traditional CFD methods to enhance computational efficiency [42]. This approach leverages the strengths of quantum computing to solve linear systems more efficiently, thereby reducing the computational burden associated with complex CFD simulations.

The Stochastic Method of Lines Discretization (SMOLD) introduced by Chaudhri et al. employs a finite volume approach combined with a three-stage Runge-Kutta scheme for temporal integration, enabling the simulation of thermal fluctuations in multiphase flows [32]. This method is particularly effective in capturing the intricate dynamics of sCO2 under multiphase conditions.

Advancements in surrogate modeling, as demonstrated by Bartoldson et al., have shown significant potential for carbon capture and storage (CCS) design optimization. The developed DF-inspired surrogates achieve rapid and accurate predictions, facilitating the optimization of CCS systems [6].

The use of low-order dynamic models combined with nonlinear Kalman-Filters, as described by Gentsch et al., has improved parameter estimation efficiency in modeling supercritical CO2 [4]. This approach enhances the ability to track and predict system behavior under varying operating conditions.

Fu et al. have proposed methods that utilize local CFD data to enhance the understanding of flow characteristics in packed columns, enabling the development of more accurate correlations for liquid holdup [7]. This advancement is crucial for optimizing the design and operation of systems utilizing sCO2.

The fully-differentiable nature of JAX-FLUIDS, as highlighted by Bezgin et al., allows for seamless integration of machine learning models with high-performance numerical methods, optimizing simulations through automatic differentiation [18]. This capability is instrumental in improving the efficiency and accuracy of CFD simulations.

Li et al. have proposed a new framework for finite volume methods that explicitly incorporates spacetime coupling, aligning numerical methods more closely with the physical principles of fluid dynamics [43]. This approach enhances the fidelity of simulations, particularly in capturing the complex dynamics of sCO2.

Recent advancements in computational fluid dynamics (CFD) models, particularly through the integration of machine learning techniques, significantly enhance the accuracy and efficiency of simulating the intricate behaviors of supercritical CO2. These innovations, such as the development of neural network surrogates that can dramatically speed up simulations while maintaining low error rates, provide essential tools for optimizing engineering systems that utilize supercritical CO2. Moreover, methodologies like model predictive control (MPC) effectively manage the complex dynamics of power cycles involving supercritical CO2, further improving system performance. As a result, these advancements not only facilitate more precise modeling of fluid dynamics but also enable rapid design iterations and optimization in carbon capture and other engineering applications. [18, 21, 6, 3]

5.2 Numerical Frameworks and Algorithms

Method Name	Numerical Techniques	Computational Integration	Application Scenarios
CFVPBA[39]	Finite-volume Framework	Not Mentioned	Shock Wave Dynamics
TPU-CFD[41]	Finite-difference Scheme	Tensor Processing Units	Turbulent Planar Jet
APCS[33]	Adaptive Schemes	Shock Sensor	Shock Tube Problems
HOCGKS[40]	Nonlinear Limiters	-	Shock Wave Interactions
HQCF[42]	Quantum Linear Solvers	Quantum Computing Integration	Fluid Dynamics Simulations
SCFVM[43]	Finite Volume Schemes	-	Compressible Flows
CFD-LH[7]	Finite-volume	High-performance Computing	Carbon Capture Systems

Table 3: This table provides a comprehensive overview of various numerical methods and their applications in Computational Fluid Dynamics (CFD) simulations, specifically focusing on supercritical carbon dioxide (sCO2) systems. The table details the numerical techniques employed, the computational integration methods used, and the specific application scenarios for each method, highlighting the diversity and specialization of approaches in this field.

The development of advanced numerical frameworks and algorithms is crucial for enhancing the accuracy and efficiency of Computational Fluid Dynamics (CFD) simulations involving supercritical carbon dioxide (sCO2). These frameworks are specifically developed to tackle the intricate thermodynamic behavior and flow dynamics of supercritical carbon dioxide (sCO2), which present substantial challenges in the modeling and simulation of combustion processes and carbon capture systems. For instance, the combustion mechanisms in high-pressure sCO2 environments are not well understood, necessitating advanced chemical kinetic models to accurately predict ignition delay times. Additionally, the efficiency of solvent-based carbon capture systems heavily relies on optimizing the gas-solvent interfacial area, a task that can be significantly enhanced through the use of neural network surrogates to replace traditional computational fluid dynamics simulations. Furthermore, the integration of axial flow fans in air-cooled heat exchangers for sCO2 Brayton cycles demonstrates the need for precise modeling to improve cooling efficiency and overall system performance. [11, 8, 6]

A notable contribution to this area is the Conservative Finite-Volume Pressure-Based Algorithm (CFVPBA) developed by Denner et al., which employs a unified thermodynamic closure model and momentum-weighted interpolation for flux definitions. This approach enables accurate predictions for both incompressible and compressible fluids, making it particularly suitable for simulating the complex behaviors of sCO2 [39].

Wang et al. introduced a method that employs a low-Mach number approximation of the Navier-Stokes equations, implemented through a finite-difference scheme on a collocated structured mesh. This framework is instrumental in capturing the subtle flow dynamics of sCO2, especially in scenarios where traditional high-Mach number assumptions may lead to inaccuracies [41].

The Adaptive Primitive-Conservative Scheme (APCS) developed by Xu et al. is another significant advancement, employing a shock sensor to adaptively switch between primitive and conservative forms in smooth and shock-affected regions, respectively. This approach enhances the ability to accurately simulate the complex flow regimes encountered in sCO2 systems [33].

Zhao et al. introduced a direct modeling approach that updates cell-averaged flow variables and their gradients using nonlinear limiters for both spatial and temporal flux functions. This method provides a robust framework for capturing the intricate dynamics of sCO2 flows, ensuring accurate representation of flow variables and gradients [40].

Ye et al. proposed a hybrid quantum-classical framework that utilizes quantum algorithms to solve linear systems derived from the governing equations of fluid dynamics. This integration of quantum computing enhances computational capabilities, offering a promising avenue for tackling the high computational demands of sCO2 simulations [42].

The SCFVM method developed by Li et al. emphasizes the integration of spacetime correlation in fluid dynamics through a unified framework that combines physical modeling and numerical discretization. This approach provides a comprehensive understanding of the temporal and spatial dynamics of sCO2, facilitating more accurate simulations [43].

Fu et al. conducted high-resolution local CFD simulations of a random packed column to extract local flow data, including liquid holdup and superficial liquid velocity. This methodology enhances the understanding of local flow characteristics, contributing to the development of more accurate correlations for sCO2 systems [7].

Recent advancements in numerical frameworks and algorithms, particularly through the integration of machine learning techniques, have significantly enhanced the capabilities of Computational Fluid Dynamics (CFD) models in simulating the intricate behaviors of supercritical CO2. These improvements not only allow for more accurate and efficient simulations but also serve as valuable tools for optimizing engineering systems that utilize this unique fluid. For instance, innovative approaches such as JAX-FLUIDS enable seamless integration of machine learning with traditional CFD methods, facilitating end-to-end optimization and providing gradient information essential for refining models. Furthermore, the development of high-order numerical methods enhances the precision of simulations, thereby contributing to a deeper understanding of complex fluid dynamics phenomena, which is critical for applications in various scientific and engineering disciplines. [18, 21, 44]

As shown in **??**, the study of computational fluid dynamics (CFD) modeling of supercritical CO2 is a complex field that requires sophisticated numerical frameworks and algorithms to accurately simulate and predict fluid behaviors under supercritical conditions. This example delves into the intricate methodologies employed in CFD modeling, highlighting three pivotal components: the architecture of TPU chips, ensemble-based Bayesian filtering procedures, and Bayesian Ensemble Kalman Filters for turbulent flows. The TPU Chip Architecture is crucial for handling the computationally intensive tasks involved in CFD simulations, offering a high-performance setup with its Tensor Processing Unit cores and high-bandwidth memory. Meanwhile, the ensemble-based Bayesian filtering procedure provides a systematic approach to turbulence modeling by integrating augmented states through a Reynolds-Averaged Navier-Stokes (RANS) solver, allowing for a more precise representation of turbulence dynamics. Complementing this, the Bayesian Ensemble Kalman Filter (BEKF) is employed to enhance the simulation of turbulent flows by refining the forward model with parameterized turbulent stress discrepancies, thus improving the accuracy and reliability of the CFD models. Together, these components form a robust framework for advancing the understanding and application of CFD in supercritical CO2 systems. Table 3 presents a detailed comparison of advanced numerical frameworks and algorithms used in CFD simulations, emphasizing their role in enhancing the modeling of supercritical carbon dioxide (sCO2) systems. [**?**]wang2022tensorflowsimulationframeworkscientific,chu2024uncertaintyquantificationcomputationalfluid,chu2024physicsbasedm

5.3 Machine Learning and High-Performance Computing

The integration of machine learning (ML) and high-performance computing (HPC) into Computational Fluid Dynamics (CFD) simulations has ushered in a new era of enhanced modeling and simulation capabilities for supercritical carbon dioxide (sCO2) systems. By integrating the capabilities of machine learning (ML) and high-performance computing (HPC), researchers can effectively tackle the computational challenges inherent in simulating the intricate behaviors of supercritical carbon dioxide (sCO2). This synergistic approach not only enhances the accuracy and efficiency of computational fluid dynamics (CFD) simulations but also facilitates the development of advanced surrogate models and optimization strategies, ultimately paving the way for more complex analyses and real-world applications in various scientific and engineering domains. [21, 37, 24]

One significant advancement in this area is the development of JAX-Fluids, which incorporates advanced parallelization strategies and improved modeling capabilities for two-phase flows [19]. This new version of JAX-Fluids exemplifies how HPC can be utilized to enhance the efficiency and scalability of CFD simulations, enabling the handling of large-scale, complex fluid dynamics problems.

The Dynamic Resource Allocation Framework (DRAF) proposed by Mi et al. showcases the potential of distributed processing frameworks to optimize data processing in CFD simulations. By dynamically allocating computational resources based on real-time workload analysis, DRAF enhances the efficiency of data processing, reducing computational overhead and improving simulation performance [10].

The combination of ML with CFD is further explored by Vinuesa et al., who highlight the potential benefits and challenges of this integration. ML techniques can significantly enhance modeling and simulation capabilities by providing data-driven insights and improving the accuracy of predictions [24]. The use of ML in turbulence modeling, as discussed by Chu et al., offers a promising alternative to traditional methods, with the potential to improve uncertainty quantification and prediction accuracy [17].

Bezgin et al. propose leveraging the capabilities of automatic differentiation in ML to optimize CFD simulations directly. This approach enables a more efficient and accurate representation of fluid dynamics by allowing for the seamless integration of ML techniques into CFD frameworks [18]. The classification of ML methods in CFD, introduced by Wang et al., categorizes these methods into Data-driven Surrogates, Physics-Informed Surrogates, and ML-assisted Numerical Solutions, providing a comprehensive framework for understanding the various applications of ML in CFD [21].

5.4 Handling Multi-phase and Transcritical Flows

Method Name	Simulation Techniques	Phase Interaction Dynamics	Thermodynamic Modeling
HWENO[15]	Weno Scheme	Phase Equilibrium Modeling	Equation OF State
HPS-VLE[34]	Hybrid Solver	Phase Separation Effects	Cubic Equation State
GCEoS[22]	Computational Framework Simulations	-	Generalized Cubic Eos

Table 4: Comparison of methods for simulating multi-phase and transcritical flows, focusing on simulation techniques, phase interaction dynamics, and thermodynamic modeling. The table includes HWENO, HPS-VLE, and GCEoS methods, detailing their unique approaches to phase equilibrium, separation effects, and the use of equations of state.

The accurate simulation of multi-phase and transcritical flow scenarios in Computational Fluid Dynamics (CFD) is crucial for understanding the complex interactions and dynamics of supercritical carbon dioxide (sCO2) systems. Revised Sentence: "The modeling of scenarios involving supercritical carbon dioxide (sCO2) is particularly complex due to the intricate phase transitions and the unique interactions between various phases, which are influenced by factors such as pressure adjustments, intermolecular interactions, and the distinct mechanisms of chemical reactivity, including the formation of carbonic acid and combustion processes under high pressure." [26, 8, 9, 2, 10]

Table 4 provides a comprehensive comparison of various methods used for simulating multi-phase and transcritical flows, highlighting their simulation techniques, phase interaction dynamics, and thermodynamic modeling approaches.

One effective approach to capturing the dynamics of three-phase interactions during depressurization from supercritical states is highlighted by Gjennestad et al. Their method effectively simulates the complex behavior of multi-phase systems, providing valuable insights into the phase interactions that occur during depressurization [15]. This capability is essential for optimizing the design and operation of systems that utilize sCO2, where precise control over phase transitions is critical.

The Hybrid Pressure-Based Solver with VLE Model (HPS-VLE) proposed by Traxinger et al. is another significant advancement in this area. This method effectively simulates underexpanded jets under real-gas conditions, highlighting the importance of accurately capturing the phase separation phenomena that occur in such scenarios [34]. The ability to model these interactions is crucial for applications involving high-speed propulsion systems and fuel injection technologies, where transcritical flow dynamics play a pivotal role.

Moreover, the implementation of a generalized equation of state (EoS) in OpenFOAM, as discussed by Trummler et al., enables the integration of advanced thermodynamic models into existing CFD frameworks without the need for code duplication [22]. This development facilitates the accurate simulation of multi-phase and transcritical flows by allowing for the seamless incorporation of complex EoS into CFD simulations, enhancing the ability to predict and analyze the behavior of sCO2 under various conditions.

Feature	Hybrid Quantum-Classical CFD	Stochastic Method of Lines Discretization	Surrogate Modeling
Computational Efficiency	Enhanced BY Quantum	Moderate	Rapid Predictions
Modeling Approach	Quantum-classical Integration	Finite Volume, Runge-Kutta	Df-inspired Surrogates
Application Focus	Complex Cfd Simulations	Thermal Fluctuations	Ccs Optimization

Table 5: This table provides a comparative analysis of three advanced Computational Fluid Dynamics (CFD) modeling techniques for supercritical carbon dioxide (sCO2) systems. It highlights the computational efficiency, modeling approach, and application focus of each method, including hybrid quantum-classical CFD, stochastic method of lines discretization, and surrogate modeling. These methods are evaluated based on their ability to enhance simulation accuracy and efficiency in complex CFD simulations.

6 Impinging Jets and Multi-phase Interactions

6.1 Overview of Impinging Jet Dynamics

Impinging jets utilizing supercritical carbon dioxide (sCO2) exhibit complex interactions between fluid properties and flow behaviors, heavily influenced by sCO2's thermophysical characteristics. These jets, crucial in cooling systems and propulsion technologies, involve high-velocity fluid impacting surfaces, resulting in intricate flow patterns and heat transfer phenomena [31]. The supercritical state of sCO2, which blurs traditional phase distinctions, complicates flow dynamics due to sensitivity to pressure and temperature variations [34]. Its high density and low viscosity enhance heat transfer and mass transport, making it ideal for efficient thermal management applications.

Interactions between sCO2 and surfaces can induce significant thermal and fluid dynamic effects, such as shock wave formation and boundary layer development, crucial for optimizing systems like advanced cooling technologies and propulsion systems [33]. Accurate simulation of these dynamics is essential for improving efficiency and reliability in engineering applications leveraging sCO2's unique properties.

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Understanding impinging jet dynamics with sCO2 is vital for high-pressure, high-temperature environments. Advancements in modeling techniques and experimental investigations are necessary to comprehend complex interactions within sCO2 systems and improve operational efficiency, especially in high-pressure combustion processes where traditional chemical kinetic mechanisms are limited. Developments like the University of Sheffield's sCO2 mechanism improve predictive capabilities for ignition delay times in methane combustion under elevated pressures, indicating progress in combustion performance optimization. Data-driven surrogate modeling and benchmarking in chemical process engineering facilitate effective domain exploration and sensitivity analysis, optimizing design parameters in sCO2 applications. Advanced CFD simulations and regression techniques aid in understanding system behaviors and refining operational strategies, contributing to the efficient utilization of sCO2's advantageous properties in power generation [8, 37].

6.2 Phase Separation in Underexpanded Jets

Understanding phase separation in underexpanded jets of sCO2 is crucial for high-pressure fuel injection system dynamics. These jets occur when fluid discharges from a nozzle at pressures significantly higher than ambient, leading to rapid expansion and complex flow patterns. The supercritical properties of sCO2 complicate this process, as traditional phase distinctions blur, resulting in unique fluid behaviors [34]. Rapid pressure and temperature changes during sCO2 expansion can induce phase separation, characterized by distinct phases within the jet affecting dynamics and injection efficiency [34]. Accurate prediction and modeling of these transitions are essential for optimizing fuel injection systems, ensuring efficient combustion and energy conversion.

Classical models inadequately describe real-gas effects and mixture-induced phase separation in underexpanded jets, necessitating advanced simulation techniques to capture complex interactions and phase behaviors under supercritical conditions [34]. These simulations provide valuable insights into fluid dynamics and phase separation processes, enabling the development of more efficient and reliable systems utilizing sCO2 for high-pressure applications.

6.3 Experimental Studies on Impinging Jets

Experimental investigations into impinging jets with sCO2 are essential for understanding fluid behaviors and phase interactions under high-pressure and high-temperature conditions. These studies provide insights into combustion mechanisms, particularly in direct-fired sCO2 power cycles where sCO2's properties facilitate efficient gaseous fuel combustion under oxyfuel conditions with minimal carbon capture penalties. Research highlights turbulent mixing characteristics of slightly supercritical fluids, such as ligament formation in shear layers influenced by density contrasts, contributing to a deeper understanding of real-gas behaviors and compressible flow dynamics across applications like aerospace propulsion and energy generation [8, 13, 1].

A key focus of experimental research is on the heat transfer characteristics of sCO2 impinging jets, emphasizing quantifying heat transfer coefficients and analyzing flow patterns to assess cooling performance. Methodologies, including CFD simulations and experimental validations, optimize the design and efficiency of systems like air-cooled heat exchangers in sCO2 Brayton cycle power plants, where accurate modeling of thermal and flow characteristics directly impacts operational effectiveness [11, 8, 5, 2, 37]. The high thermal conductivity and low viscosity of sCO2 enhance heat transfer performance, making it promising for efficient thermal management applications.

Experimental studies on sCO2 systems also examine phase behavior in impinging jets, impacting combustion mechanisms under high-pressure conditions and optimizing systems involving droplets and sprays. This investigation is vital for improving predictive models of combustion efficiency and dynamics in sCO2 power cycles, especially given the challenges posed by extreme ambient conditions. Researchers use advanced diagnostic techniques, such as high-speed imaging and laser-based methods, to capture transient phase changes and flow dynamics during jet impingement, providing valuable data on phase separation onset and shock wave formation, essential for optimizing sCO2 system performance.

Additionally, experimental studies explore the effects of varying operating conditions—pressure, temperature, and nozzle geometry—on sCO2 impinging jets. Such investigations yield critical insights into how parameters like heat transfer coefficients influence flow stability, heat transfer efficiency, and phase transition dynamics. By employing various calculation methods, including Newton's law of cooling, CFD, and inverse methods, researchers enhance understanding and prediction of engineering system behaviors across fields from microelectronics to chemical process engineering. This comprehensive understanding is vital for the effective design and optimization of these systems, ensuring improved performance and reliability in practical applications [37, 5].

Experimental studies on impinging jets involving sCO2 are crucial for advancing knowledge of complex fluid dynamics and phase interactions. Findings from these studies enhance the design of more efficient and reliable systems exploiting sCO2's unique properties, improving performance across various industrial applications, including power generation with reduced carbon capture penalties, optimized combustion mechanisms for high-pressure environments, innovative simulation techniques for carbon capture systems, and effective solvation property prediction tools in chemical processes. Leveraging insights from chemical kinetics, molecular dynamics, and data-driven modeling positions these systems for greater operational efficiency and reduced environmental impact [8, 9, 6, 2, 37].

6.4 Computational Modeling of Multi-phase Interactions

Computational modeling of multi-phase interactions in impinging jets involving sCO2 is crucial for elucidating the intricate dynamics and phase transitions in these systems, particularly in high-pressure environments where combustion mechanisms are poorly understood, and supercritical fluid behavior significantly influences energy production and green technologies [8, 9, 1, 31, 10]. The unique properties of sCO2, exhibiting both liquid-like and gas-like characteristics, present challenges in accurately simulating phase interactions under high-pressure and high-temperature conditions.

Advanced CFD techniques that incorporate real-gas effects and phase transition dynamics are employed to model these interactions. Lychagin et al. provide insights into real gas behavior, essential for developing accurate models that capture intricate phase transition dynamics and flow behaviors in multi-phase systems [14]. Such models are critical for optimizing sCO2-utilizing systems, particularly those involving complex flow regimes and rapid phase changes.

Moreover, computational models must account for interactions between impinging jets and system components, such as heat exchangers. Boshoff et al. emphasize simulating axial flow fan and heat exchanger interactions to optimize cooling efficiency [11]. This is particularly relevant for sCO2 systems, where efficient thermal management is vital for optimal performance.

Developing robust computational models for multi-phase interactions in impinging jets is essential for enhancing our understanding of sCO2 dynamics, especially in high-pressure combustion processes. Recent research underscores the need for improved chemical kinetic mechanisms to accurately model combustion in sCO2 environments, where traditional models often fall short. The University of Sheffield's sCO2 mechanism, for example, has shown superior performance in predicting ignition delay times compared to established models, highlighting the importance of advanced computational approaches. Furthermore, integrating data-driven surrogate modeling techniques with CFD simulations facilitates optimization and sensitivity analysis of these complex systems, contributing to more efficient sCO2 power cycle designs [8, 37]. These models provide valuable tools for optimizing design and operation in engineering systems leveraging supercritical fluid properties, enhancing efficiency and reliability across various industrial applications.

7 Challenges and Future Directions

7.1 Computational Challenges and Algorithmic Inefficiencies

Modeling supercritical carbon dioxide (sCO2) presents substantial computational challenges due to its complex thermodynamic and flow characteristics under varying conditions. Current high-order compact schemes inadequately capture compressible flows, especially near discontinuities like shock waves [40]. Additionally, turbulence models often fail to accurately represent turbulent flows, complicating uncertainty quantification [17]. High-resolution computational fluid dynamics (CFD) simulations are computationally expensive, and limited spatial resolution in experimental methods constrains data reliability for accurate correlations [7]. The explicit nature of some numerical schemes restricts time step sizes, slowing simulation speeds [32]. Methods based on ideal gas assumptions inadequately account for the complex behaviors of real-gas mixtures at supercritical pressures, leading to inaccuracies in jet behavior predictions [34]. Local inhomogeneities in sCO2 further complicate prediction and analysis of reaction mechanisms [2]. The lack of user-friendly, modular, high-performance Python packages for CFD simulations limits educational and research efforts in fluid dynamics [23]. However, hybrid quantum-classical frameworks offer promising solutions by efficiently resolving larger linear systems and achieving high-precision results beyond classical methods' capabilities [42]. Latent space simulations for carbon capture and storage (CCS) design have shown significant reductions in computational time and low prediction errors, facilitating thorough exploration of CCS designs [6].

7.2 Integration of Machine Learning and Advanced Modeling Techniques

Integrating machine learning (ML) with advanced modeling techniques in computational fluid dynamics (CFD) has transformative potential for simulating sCO2 systems. This integration enhances model generalization, reduces computational costs, and improves simulation efficiency. Frameworks like JAX-Fluids facilitate seamless integration of ML models with robust numerical methods, enabling effective handling of complex flow phenomena [18]. Future research should enhance JAX-FLUIDS' robustness, explore more complex flow scenarios, and develop user-friendly interfaces for custom ML model integration. Hybrid models combining data-driven techniques with traditional physics-based simulations show promise in addressing multi-scale dynamics and enhancing CFD simulation generalization [21]. These models significantly improve the accuracy and reliability of CFD simulations in complex fluid dynamics scenarios. Moreover, ML integration into CFD simulations enhances uncertainty quantification, allowing researchers to address aleatory and epistemic uncertainties inherent in turbulence modeling, thereby improving reliability and accuracy [45, 25, 17]. This approach is vital for optimizing sCO2-utilizing systems, providing tools for navigating the complexities of simulating this unique fluid.

7.3 Uncertainty Quantification and Model Validation

Benchmark	Size	Domain	Task Format	Metric
CFD-SM[37]	5,000	Fluid Dynamics	Regression	Mean Absolute Error, R-squared

Table 6: This table presents a representative benchmark used for evaluating computational fluid dynamics (CFD) models, particularly focusing on fluid dynamics. The benchmark includes details on the dataset size, domain, task format, and the metrics used for performance evaluation, specifically Mean Absolute Error and R-squared.

Quantifying uncertainties and validating models are crucial for advancing CFD simulations, particularly for sCO2 systems. The complexities of turbulent flows in high-fidelity simulations challenge interpretability and accuracy, necessitating robust uncertainty quantification methods [17]. Table 6 provides a detailed overview of a benchmark employed in the context of uncertainty quantification and model validation for CFD simulations. The Multi-fidelity Uncertainty Propagation Method (MUPM) employs Gaussian processes to model discrepancies between low- and high-fidelity outputs, enhancing output uncertainty estimation and improving CFD prediction reliability [45]. Model validation is essential for ensuring CFD simulation accuracy and reliability. Integrating physics-informed machine learning techniques provides a framework incorporating physical laws into data-driven models, enhancing interpretability and addressing traditional turbulence model limitations [17]. By improving alignment between simulated and observed data, model validation efforts significantly enhance CFD predictive capabilities.

7.4 Enhancements in Experimental and Computational Frameworks

Advancements in experimental and computational frameworks are vital for overcoming limitations in modeling sCO2 dynamics and enhancing simulation accuracy. Future research should prioritize integrating monitoring methods into complex systems with additional uncertainties, as suggested by Gentsch et al., to improve experimental frameworks [4]. This integration will yield insights into thermal performance and operational efficiency of sCO2-utilizing systems. In the computational realm, enhancing the scalability and applicability of methods like the SCFVM is crucial. Future research should optimize SCFVM for efficiency and explore its applicability across a broader range of fluid dynamics problems [43]. Developing hybrid methods leveraging spacetime coupling and decoupling strategies will further enhance computational model flexibility and accuracy. Expanding datasets through additional CFD simulations with varying packing configurations and liquid loads, as proposed by Fu et al., is necessary for validating and refining liquid holdup correlations [7]. This effort will improve computational models' predictive capabilities, particularly in capturing sCO2 interactions under diverse operational conditions. Refining measurement techniques and developing models for unsteady heat transfer coefficient distributions, as suggested by Duda et al., is critical for enhancing experimental frameworks [5]. These advancements will facilitate a more accurate understanding of heat transfer dynamics in sCO2-utilizing systems, contributing to more efficient thermal management strategies. On the computational side, refining sampling strategies and exploring sophisticated kernel functions for Gaussian processes, as indicated by Wang et al., will enhance uncertainty quantification model capabilities [45]. This refinement is essential for improving prediction accuracy and reliability in CFD simulations involving sCO2. Advancements in experimental and computational frameworks for sCO2 systems, including refined chemical kinetic mechanisms for high-pressure combustion, molecular density functional theory (MDFT) for solvation property prediction, and model predictive control (MPC) methodologies, will significantly enhance understanding and utilization of sCO2 across various industrial and environmental applications. These innovations promise improved efficiency and reliability in power generation and chemical processing by enabling better combustion dynamics modeling, facilitating greener process designs, and optimizing control strategies for power cycles, ultimately leading to more sustainable and effective system performance [8, 3, 9, 10].

8 Conclusion

This survey delves into the intricate flow dynamics and thermodynamic properties of supercritical carbon dioxide (sCO2), underscoring the pivotal role of Computational Fluid Dynamics (CFD) in capturing these complexities. The accurate modeling of sCO2's intermolecular interactions emerges as a cornerstone for enhancing predictive capabilities in supercritical fluid dynamics, which is essential for optimizing engineering systems that utilize sCO2, particularly in scenarios characterized by complex phase transitions and nuanced flow behaviors.

The integration of machine learning (ML) techniques with CFD represents a transformative development, significantly boosting simulation accuracy and efficiency while enabling sophisticated analyses of fluid dynamics. These advancements address the challenges inherent in simulating sCO2's unique properties, equipping researchers and engineers with powerful tools to optimize system performance across various industrial and environmental applications.

Furthermore, the survey highlights the substantial progress made in advanced computational methodologies, which demonstrate robust performance and high-order convergence in capturing the intricate dynamics of multi-phase interactions within CO2 flows. This progress underscores the necessity for continued research efforts aimed at developing innovative computational and experimental approaches. Such endeavors will deepen the understanding of sCO2 flow dynamics and expand its application potential, driving forward technological advancements in this critical field.

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