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Recent Progress in Heat and Mass Transfer Modeling for Chemical Vapor Deposition Processes

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Abstract: Chemical vapor deposition (CVD) is a vital process for depositing thin films of various materials with precise control over thickness, composition, and properties. Understanding the heat and mass transfer mechanisms during CVD is essential for optimizing process parameters and ensuring high-quality film deposition. This review provides an overview of recent advancements in the heat and mass transfer modeling for chemical vapor deposition processes. It explores innovative modeling techniques, recent research findings, emerging applications, and challenges in the field. Additionally, it discusses future directions and potential areas for further advancement in CVD modeling.

Keywords: CVD; chemical vapor deposition; heat transfer; mass transfer; surface engineering; modeling

1. Introduction

Chemical Vapor Deposition (CVD) is a widely used technique for fabricating high-quality thin films and coatings, crucial in industries like semiconductors, photovoltaics, and advanced materials [1]. It involves the chemical reaction of vapor-phase precursors on a heated substrate, forming a solid thin film [2]. The versatility and precision of CVD make it essential for producing thin films with excellent uniformity, purity, and adhesion.

CVD's importance in thin film deposition is especially pronounced in the semiconductor industry, where it is crucial for manufacturing integrated circuits and other microelectronic devices [3]. Thin films created through CVD are crucial for forming active layers, insulating barriers, and conductive pathways in these components. The precise control of film thickness at the nanometer scale and the ability to achieve excellent step coverage over complex topographies are vital for the miniaturization and performance enhancement of semiconductor devices [4].

Beyond semiconductors, CVD is widely used in the production of photovoltaic cells [5], where thin films of materials like silicon, cadmium telluride, and copper indium gallium selenide are deposited to create efficient solar cells. In optics, CVD is used to deposit antireflective coatings, optical filters, and waveguides [6]. Additionally, the aerospace and defense industries utilize CVD to produce wear-resistant and corrosion-resistant coatings, enhancing the durability and performance of critical components [7].

The widespread use of CVD across various high-tech industries highlights its significance. The ability to precisely control the chemical composition and microstructure of thin films through process parameter adjustments allows for the creation of materials with properties tailored to specific applications. This flexibility makes CVD a valuable tool for technological advancement and innovation [8].

The effectiveness of CVD processes heavily depends on the dynamics of heat and mass transfer. Accurate modeling of these phenomena is crucial for optimizing the deposition process, ensuring uniform film thickness, and achieving desired material properties [9].

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Heat transfer in CVD involves conduction, convection, and radiation of thermal energy to and from the substrate and reactor walls [10]. Maintaining the substrate at an optimal temperature is essential for promoting the desired chemical reactions while avoiding thermal degradation or stress [11]. Inconsistent temperature distribution can lead to non-uniform film growth, defects, and reduced material performance [12]. Therefore, understanding and controlling heat transfer is fundamental to producing high-quality thin films.

Mass transfer involves the transport of gaseous precursors to the substrate surface and the removal of by-products from the reaction zone. Efficient mass transfer ensures uniform delivery of reactants to the substrate, promoting consistent deposition rates and film composition [13]. Factors such as gas flow dynamics, precursor concentration, and reactor design significantly impact mass transfer. Poor mass transfer can result in precursor depletion, incomplete reactions, and non-uniform deposition [14].

This review article provides a thorough examination of recent advancements in heat and mass transfer modeling for CVD processes. The intricate interplay between heat transfer, mass transfer, and chemical reactions within the CVD environment necessitates sophisticated modeling to accurately predict film growth and properties. The review covers a broad range of CVD systems, including thermal CVD, plasma-enhanced CVD (PECVD), and metal-organic CVD (MOCVD). Each system presents unique challenges and opportunities regarding heat and mass transfer, and the review highlights specific modeling techniques and solutions developed for each. In addition to fundamental aspects of heat and mass transfer, the review explores various modeling methodologies, ranging from analytical models and empirical correlations to advanced numerical simulations. It discusses the advantages and limitations of different approach and their applicability to different CVD processes and materials. Computational models incorporating fluid dynamics, thermodynamics, and kinetics can simulate different reactor designs, precursor chemistries, and operating conditions, aiding researchers and engineers in optimizing processes. These models help predict deposition rates, film uniformity, and material properties, reducing the need for extensive experimental trials.

Advances in numerical methods, such as finite element analysis, computational fluid dynamics (CFD), and multi-scale modeling techniques, are highlighted for their role in enhancing model accuracy and efficiency. These models account for gas-phase reactions, surface kinetics, and thermodynamic properties, providing a comprehensive understanding of the deposition process. The review also explores the latest developments in computational tools, focusing on the integration of CFD, multi-physics simulations, and machine learning techniques to improve model accuracy and predictive capabilities. Case studies and recent research examples illustrate the practical implementation of these models and their impact on process optimization.

By synthesizing existing knowledge and identifying gaps in current research, the review aims to provide a roadmap for future studies and innovations in the field. It serves as a valuable resource for researchers and engineers looking to improve the modeling of heat and mass transfer in CVD systems.

2. Fundamentals of CVD

To apply thin ceramic coatings that enhance wear resistance under friction conditions, two entirely different vapor phase deposition processes are typically used [15]: Chemical Vapor Deposition (CVD) and Physical Vapor Deposition (PVD). In the CVD process, a coating of reaction products is generated on the substrate through a chemical reaction occurring in the gas phase, usually carried out at atmospheric pressure. Coatings produced by CVD are uniform, even on the surfaces of complex-shaped products [16]. The substrate temperature is higher in CVD processes compared to PVD [17]. For instance, when producing a TiN layer using chemical deposition, the temperature is approximately 1000°C, whereas in the physical process it is around 500°C. In chemical vapor deposition, layers are formed on the surface of a heated material as a result of a chemical reaction in the gas phase. Therefore, the production of CVD layers is a continuation of thermochemical treatment processes in a gas atmosphere, especially diffusion metallization.

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During the CVD process, reactive gaseous substrates, usually with a carrier gas, flow around the substrate, and the coating is formed by the decomposition of the reactive gas mixture on the treated surface and the incorporation of released metal atoms or chemical compounds into the layer [18]. There are three main stages in the process [19]:

- production of a chemical compound of the applied element with high volatility (easily evaporating),
- transport of gas (vapor) from the forming compound to the place of deposition without its disintegration,
- the chemical reaction necessary to produce a coating on the surface of the product.

Chemically, vapor deposition layers are the of a chemical reaction on the surface of a heated substrate. Therefore, the basic condition of the process is the availability of a chemical compound of the applied element that vaporizes at a reasonably low temperature and decomposes upon contact with the substrate, leading to the formation of the element or chemical compound [20]. Figure 1 shows the transport and reaction processes that take place during CVD.

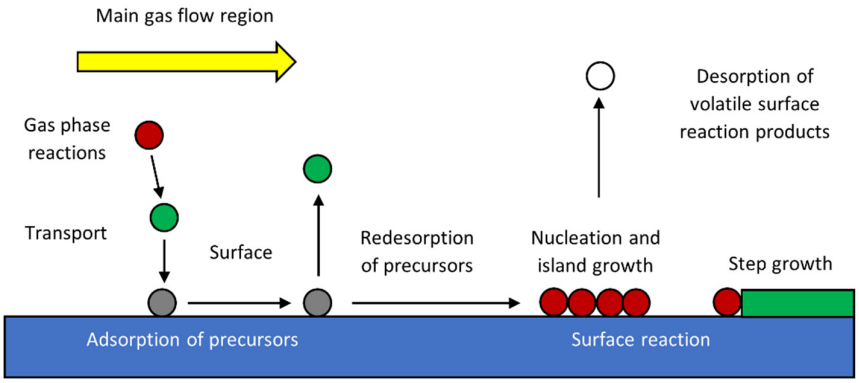

Figure 1. CVD scheme (transport and reaction processes).

The CVD process is used to produce layers from metallic and non-metallic materials as well as their compounds, including carbides, nitrides, borides, and oxides [21,22].

The charge is placed on graphite or nickel trays. The reducing and diluting gas, usually dry hydrogen, is introduced into the reactor simultaneously with the start of heating the charge. After the charge reaches the process temperature, reactive components are supplied to the chamber. During the process, the gaseous components introduced into the reactor react on the surface of the workpiece, forming a coating and gaseous reaction products. In many CVD processes, gases such as HF or HCl are formed during the reactions, which are neutralized by passing them through chemical or cryogenic traps. The CVD coating deposition cycle, including heating and cooling of the products, is long and can take up to 12 hours. Therefore, it is practical to install a separate reactor for each type of coating composition, e.g., one for TiC/TiN and another for TiC/Al2O3. This way, contamination of the chamber with substances other than those used for producing the specific type of layer is avoided.

The reactions occurring in the gaseous substrates that lead to the formation of coatings require an energy source. Different variants of the CVD process differ in the type of energy source used, resulting in variations in the properties of the produced coatings. Typical energy sources include the hot surface of the coated products, direct or alternating current plasma at radio frequency or microwave frequency. Sometimes, the heat of combustion of process gases serves as the energy source, such as the combustion of acetylene during the CVD process for producing diamond-like coatings [23]. The chemical reactions occurring in the thermal CVD process on the surface of the product between gaseous reagents are thermally activated. Therefore, to ensure the process proceeds at a satisfactory rate, a temperature usually higher than 900°C is required. The plasma CVD process allows a significant reduction in temperature to the range of 300-700°C. The use of metal-organic compounds, on the other hand, allows the process temperature to be reduced even further, to around

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500°C. Low-temperature processes enable the production of layers on substrates made of materials with low melting points, as well as materials that undergo phase transformations above the deposition temperature. The low deposition temperature of plasma CVD limits the stresses caused by the large difference in the coefficient of thermal expansion between the substrate and the coating. This primarily limits the tendency for deformation and cracking during the cooling of the product from the coating production temperature to room temperature.

The CVD process can be conducted under atmospheric pressure conditions (100 kPa) [24,25] or reduced pressure conditions (0.1-6.6 kPa) [26]. The process is practically applicable when the chemical reactions occurring ensure obtaining a coating of the required thickness of 5-15 μm within a reasonable time of 5-6 hours. The rate of chemical reactions and the deposition rate in the CVD process increase exponentially with temperature, according to the Arrhenius equation [24]. Therefore, high-temperature processes are preferred from a kinetic standpoint. However, the high temperature adversely affects the substrate, causing changes in its microstructure and mechanical properties.

Since the mechanical properties of the substrate are crucial, significant effort has been made to find chemical reactions that allow the CVD process to be conducted at relatively low temperatures. The temperature to which the substrate is heated during the process usually ranges from 600 to 1100°C. This temperature is sufficient to cause significant and often undesirable changes in the microstructure of the steel. Therefore, heat treatment is necessary after the process to ensure the required microstructure and properties of the substrate. The development of CVD processes is driven by the aim to reduce the deposition temperature. One of the low-temperature processes is plasma-assisted CVD [27].

CVD processes are used to produce coatings made of metals, ceramics, as well as diamond and diamond-like layers. This method can produce coatings from metals that cannot be deposited electrolytically and have high melting points, such as W, Mo, Re, Nb, Ta, Zr, and Hf. Refractory metals are deposited at temperatures significantly below their melting or sintering temperatures. Diamond and diamond-like layers, chemically deposited from a gaseous mixture of hydrogen and hydrocarbons, have properties similar to natural diamond [28]. Currently, CVD processes are primarily used to produce coatings on cutting tools. The coatings produced are usually multilayered, utilizing the best properties of each layer material [29]. For example, a TiN layer provides a low coefficient of friction and resistance to galling, while an Al2O3 layer is characterized by high oxidation resistance and high-temperature stability, which is beneficial when the cutting speed is high [30]. Meanwhile, TiC and Ti(C,N) layers provide high resistance to abrasive wear under friction conditions [31].

The advantage of the CVD process is the ability to deposit coatings on partially obscured surfaces, such as the internal surfaces of small-diameter holes (< 1 mm). As with other processes, a strong bond between the coating and the substrate is only possible if the substrate surface is clean and free from oil and grease residues, oxides, and other contaminants [19].

The high substrate temperature promotes the mutual diffusion of atoms from the substrate into the coating and vice versa. Therefore, the bond between the coating and the substrate produced by a high-temperature process is a strong metallic bond. However, when the atoms of the layer form brittle intermetallic phases with the atoms of the substrate, such mutual diffusion is undesirable as it reduces mechanical properties and leads to delamination of the coating. To avoid this, diffusion barriers are used in the form of interlayers made of materials that do not form brittle phases with either the substrate or the deposited outer coating. In some applications, multilayer CVD coatings are beneficial. They not only provide good adhesion to the substrate and limit mutual diffusion, but also allow for advantageous changes in mechanical, chemical, and physical properties across their cross-section [32]. For example, on carbide tools, three successive layers are deposited in the order from the substrate: titanium carbide, titanium carbonitride, and titanium nitride. Such a coating shows significantly greater durability compared to a single-layer coating. Sometimes, coatings consisting of ten layers are used.

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The microstructure of coatings produced by the CVD process usually consists of columnar grains, although equiaxed grains typically form at the beginning of the process (near the surface of the product) [33,34]. The type of microstructure and grain size depend significantly on the process conditions [35]. Often, the most desirable microstructure does not form at a high deposition rate. Therefore, it is necessary to balance the cost criteria of the process (high deposition efficiency) with the microstructure that ensures good tribological properties.

Coatings formed during the CVD process result from the absorption of deposited atoms on the substrate surface, their migration across the substrate surface, and the formation of atom clusters by the adsorbed atoms. These clusters, upon reaching a critical size by the addition of new atoms, become grain nuclei. A significantly higher growth rate of grains in the direction parallel to the substrate surface than in the perpendicular direction leads to the formation of a thin, dense coating layer with a well-defined structure and surface topography. Grain nucleation on the substrate is heterogeneous, so the cleanliness of the substrate, its roughness, and its crystalline structure greatly influence the nucleation and growth of grains, as well as the microstructure and surface topography of the coating [36].

In general, the microstructure of the coating and the topography of its surface depend on [37,38]:

- the process temperature, which affects the mobility of atoms,
- supersaturation,
- process duration,
- pressure in the chamber,
- gas flow rate (laminar or turbulent),
- spatial position of the substrate in the chamber,
- substrate surface preparation.

Generally, increasing the reaction temperature and process duration increases the volume fraction of the crystalline structure while decreasing the amorphous fraction. Similarly, reducing the gas flow rate and the degree of supersaturation has the same effect. Grains in the immediate vicinity of the substrate are very small, about 1 μm in size. However, at a distance of about 1 μm from the substrate, the grains achieve much larger sizes. Grains with a favorable crystalline orientation grow faster and eliminate grains with less favorable orientations that grow more slowly. Additionally, grain growth is energetically easier compared to the nucleation of new grains on the surface of the growing layer. In the coating zone away from the substrate, a microstructure of equiaxed or columnar grains can be distinguished.

Increasing the deposition temperature changes the topography of the external surface of the coating. A relatively low temperature and short deposition time lead to the formation of a coating with a surface roughness of about 1 μm with characteristic spherical protrusions. Increasing the temperature or the time causes needle-shaped grains to begin dominating the surface of the coating. Further increasing the deposition temperature or prolonging the time promotes the formation of a coarse-grained equiaxed microstructure.

CVD can be classified according to three parameters [39]:

- operating conditions (atmospheric pressure CVD (APCVD), low pressure CVD (LPCVD), and ultrahigh vacuum CVD (UHVCVD)),
- physical characteristics of vapor (aerosol-assisted CVD (AACVD) and direct liquid injection CVD (DLICVD)),
- substrate heating (hot wall CVD, and cold wall CVD).

3. Heat Transfer Modeling

Heat transfer modeling is crucial for optimizing Chemical Vapor Deposition (CVD) processes as it directly impacts the quality and properties of thin films. The primary objective is to ensure uniform temperature distribution across the substrate, which is essential for consistent deposition rates and uniform film thickness. Variations in temperature can lead to defects, stress, and variations in material properties.

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Heat transfer models assist in designing CVD reactors and processes that maintain stable thermal environments, promoting high-quality film deposition. These models help determine optimal process conditions such as substrate temperature, precursor flow rates, and reactor pressure. By simulating various thermal scenarios, researchers can identify conditions that maximize deposition efficiency while minimizing energy consumption and material waste, which is vital for scaling up from laboratory to industrial production.

Thermal gradients within the reactor affect deposition processes, growth rates, and film morphology. Accurate modeling allows for better control of these factors. Proper temperature control prevents premature precursor decomposition and ensures complete chemical reactions, thereby avoiding poor film quality. Additionally, modeling helps design controlled heating and cooling protocols to mitigate thermal stress, cracking, and delamination.

Heat transfer modeling is essential for designing and scaling up CVD reactors by evaluating different configurations for effective thermal management. It often integrates with other multiphysics models, including mass transfer, fluid dynamics, and chemical kinetics, providing a comprehensive understanding of the CVD process. This integration helps optimize gas flow patterns, temperature distribution, and precursor delivery.

Effective heat transfer management enhances energy efficiency, reduces consumption, and improves sustainability by identifying energy-saving opportunities and minimizing the environmental impact of CVD operations.

Heat transfer modeling plays a crucial role in CVD processes by enabling precise control and optimization of temperature distribution, which is essential for achieving uniform thin-film coatings and high-quality material growth. For example, the performance of SiC devices is highly dependent on the material quality of SiC substrates, which is influenced by heat and mass transfer within the CVD reactor [40]. Numerical simulations and modeling help understand the complex interactions of fluid dynamics, thermodynamics, and surface reactions, which are critical for predicting and controlling the deposition process [41]. Modeling has been used to evaluate new reactor concepts for SiC bulk growth, demonstrating the impact of gas flow and temperature distribution on the deposition area [42]. Additionally, reactor geometry, such as a cone top configuration, can significantly affect gas flow patterns and deposition rates, reducing non-uniformity in film thickness [9]. Temperature distribution on the wafer surface is another critical factor, influencing chemical reactions during the CVD process. Models have shown significant temperature drops in narrow gaps between the wafer and heater under low-pressure conditions [43]. In applications like X-ray anodes, heat transfer modeling optimizes the design for better thermal management, reducing maximum temperatures in critical components [44]. Furthermore, in-line CVD processes for coating optical fibers benefit from coupled radiation and convection heat transfer models to predict temperature profiles and improve coating uniformity [45]. Numerical models also ensure the stability and uniformity of substrate heating, which is vital for depositing oxide semiconductor layers containing nanoparticles [46]. Overall, heat transfer modeling integrates thermodynamic, kinetic, and transport data to link film properties to process parameters, highlighting its indispensable role in advancing CVD technology [47].

Recently, there has been increasing interest in using various modeling tools to simulate heat transfer in CVD processes. These approaches include Continuum Models (based on Finite Element Analysis (FEA) and Computational Fluid Dynamics (CFD)), Molecular Dynamics (MD) Simulations, the Lattice Boltzmann Method (LBM), Hybrid Approaches, and Multi-Physics Modeling. The following sections will analyze selected solutions developed over the last decade.

3.1. Continuum-Based Approaches

The study of continuum-based models in heat transfer during Chemical Vapor Deposition (CVD) processes has seen significant advancements over the last decade, with various research papers contributing unique insights and methodologies.

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3.1.1. Finite Element Analysis

The finite element analysis (FEA) has been extensively applied to model heat transfer during Chemical Vapor Deposition (CVD) processes, offering various advantages and facing certain limitations.

Houston and Sime developed a self-consistent model for hydrogen plasma in MPA-CVD reactors, highlighting the practical performance of the discontinuous Galerkin method. However, the complexity of the model posed implementation difficulties [48].

Sime's thesis on MPA-CVD reactors introduced automatic code generation for DG finite element formulations, simplifying the implementation process, though the approach remains prone to human error [49].

Cheimarios et al. reviewed multiscale models for CVD, stressing the need to link different scales to optimize the process, particularly for patterned and flat surfaces [50].

Zhou and Hsieh's work on FDM, a related additive manufacturing process, demonstrates the reliability of numerical modeling in predicting thermal responses and bonding mechanics, which can be analogous to CVD processes [51].

Khanafer et al. further explore FDM by developing a 3-D computational model to analyze transient heat transfer and inter-layer adhesion, validated against experimental data, suggesting potential applications in CVD modeling [52].

Gabrielli et al. reviewed strategies to reduce computational effort in FEA of rolling-element bearings, which can be adapted to optimize CVD reactor simulations by balancing accuracy and computational load [53].

Lisik et al. validated a CVD reactor model in ANSYS CFX, confirming the model's accuracy in simulating heat and mass transfer under various conditions [54].

Kleimanov et al. developed a numerical model using COMSOL Multiphysics to ensure substrate temperature stability and uniform layer deposition in a CVD reactor for oxide semiconductor layers containing gold nanoparticles [46].

Aranganadin et al. discussed the design of a 3-D MPECVD chamber using FEM to achieve accurate simulation results by incorporating multiple physical interfaces [55].

Stupple et al. used FEA to model heat transfer in a water-cooled copper-based X-ray anode with a CVD diamond heat spreader, demonstrating significant temperature reduction [44].

Table 1 presents a summary of various aspects of selected articles in the field of application of the FEM method.

Table 1. Analysis of selected articles in the field of use of finite element method.

Title	Advantages	Disadvantages	Gaps and Limitations
Numerical Modelling of MPA-CVD Reactors with the Discontinuous Galerkin Finite Element Method [48]	High accuracy in solving complex PDEs.	Resource and time-intensive.	The model's focus on axisymmetric scenarios may not account for all plasma distribution perturbations, limiting its applicability to reactors with non-axisymmetric features.
	Integrating multiple physical phenomena (e.g., gas dynamics, electromagnetic fields, plasma chemistry) into a single model offers a holistic view of reactor processes.	Complex implementation requiring numerical modeling expertise.	Although robust in simulations, the model requires further real-world validation to ensure alignment with experimental data.

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	Applying the model to various reactor geometries demonstrates its versatility and potential for optimizing reactor design and operation.	The model's assumptions and simplifications may not fully capture all real-world reactor interactions.	The need for extensive computational resources and specialized expertise may limit the adoption of these simulations in routine industrial processes.
Thermal Analysis of Fused Deposition Modeling Process Using Infrared Thermography Imaging and Finite Element Modeling [51]	Integrating infrared thermography with FEM provides detailed thermal analysis during the FDM process. The authors present a robust framework for coupling different scales. The findings offer valuable insights for optimizing FDM process parameters, such as printing speed and layer thickness, to reduce thermal-induced defects and enhance the mechanical properties of printed parts. Validating FEM simulations with infrared thermography strengthens the model's credibility.	The study primarily focuses on a specific material, typically acrylonitrile butadiene styrene (ABS). Finite element modeling is computationally intensive and resource-demanding, limiting accessibility in some settings. Real-time integration requires specialized equipment and expertise, not always available in all settings.	Including more materials would enhance the study's applicability and relevance. Further investigation is needed to scale the approach to larger, more complex parts and different FDM printers. The study focuses on immediate thermal effects; examining long-term stability and performance under varied conditions would provide a more comprehensive understanding.
Thermal Analysis of Fused Deposition Modeling Process Based Finite Element Method: Simulation and Parametric Study [52]	FEM allows high-resolution simulation of temperature distribution and gradients in FDM. A parametric study shows how print speed, layer thickness, and extrusion temperature affect the thermal profile. The findings provide valuable guidelines to enhance the quality of FDM-produced parts in	FEM simulations are resource-intensive, requiring significant expertise, which may limit their use by small to medium-sized enterprises. The study focuses on a specific thermoplastic commonly used in FDM. Although valuable, the simulations have limited experimental validation.	More comprehensive experimental validation of the simulation results is needed. Incorporating dynamic variables like environmental temperatures and humidity would improve the study. The scalability to larger and more complex prints is not fully addressed.

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	the additive manufacturing industry.		
Verification of Thermo-Fluidic CVD Reactor Model [54]	The article's main strength is verifying the numerical model with experimental data.	ANSYS CFX simulations are computationally intensive and resource-demanding.	The findings are specific to certain reactor configurations and conditions.
	Using ANSYS CFX offers a high-fidelity approach to modeling thermo-fluidic phenomena in CVD reactors.	The study is specific to the modeled CVD reactor's conditions and configurations.	Incorporating dynamic variables like temperature fluctuations and varying gas compositions would improve real-world relevance.
	The study tackles practical challenges in CVD reactor operation, like managing heat and mass transfer under varying conditions.	The study's experimental validation is limited despite its focus on model verification.	More extensive experimental data is needed to validate the model under diverse conditions.
Modelling of Heat Transfer in an Aluminum X-Ray Anode Employing a CVD Diamond Heat Spreader [44]	Using CVD diamond as a heat spreader innovatively manages thermal loads in X-ray anodes.	The numerical simulations are resource-intensive, requiring significant expertise.	Including different anode materials and configurations would enhance the study's relevance.
	Numerical modeling offers detailed insights into thermal behavior, identifying critical heat buildup areas and showing effective mitigation by the CVD diamond heat spreader.	The study focuses on aluminum X-ray anodes with CVD diamond heat spreaders.	Incorporating dynamic conditions like varying power loads and environmental temperatures would improve the study.
	The findings have practical implications for X-ray equipment design and operation.	The experimental validation is somewhat limited in scope.	Investigating long-term performance and durability under continuous operation would provide valuable insights.

3.1.2. Computational Fluid Dynamics (CFD)

The last decade has seen significant advancements in the application of Computational Fluid Dynamics (CFD) to model heat transfer during Chemical Vapor Deposition (CVD) processes, as evidenced by the reviewed papers.

Lee et al. highlighted the importance of considering slip-flow regimes and heterogeneous reactions to accurately simulate heat transfer and hydrogen generation in HFCVD processes, emphasizing the correlation between gas temperature and hydrogen concentration gradients on substrates [56].

Libreros et al. discussed the complementary nature of theoretical, experimental, and CFD methods in optimizing flat fin heat exchangers, which is relevant for CVD reactor design [57].

Tran et al. demonstrated the use of Proper Orthogonal Decomposition (POD) to reduce the complexity of CFD models in CVD processes, making them more computationally efficient [58].

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Passos et al. explored the synthesis of polymeric biomaterials in a vertical CVD reactor, using CFD to optimize heat and mass transfer for uniform material deposition [59].

Silva et al. used CFD steady-state simulations to determine the hydrodynamic and thermal properties of the flow field in a modified CVD process, achieving good agreement with reference studies [60].

Zhou et al. employed the sliding mesh method in CFD to study the real-time dynamics of transport phenomena in MOCVD, finding that susceptor moving speed significantly affects film uniformity [61].

CFD simulations using a three-dimensional hexahedral mesh and finite volume method have been employed by Park et al. to solve momentum, continuity, energy, and chemical species equations, showing good agreement with reference studies [62].

CFD simulation of a tungsten crucible CVD reactor revealed that axial heat convection is more intense than radial convection, and a uniform temperature distribution is achieved with an upper gas inlet, which is beneficial for tungsten deposition [63].

Table 2 presents a summary of various aspects of selected articles in the field of application of the CFD method.

Table 2. Analysis of selected articles in the field of use of CFD.

Title	Advantages	Disadvantages	Gaps and Limitations
Two-Dimensional Computational Fluid Dynamics Modeling of Slip-Flow Heat Transfer in the Hot Filament Chemical Vapor Deposition Process [56]	The use of two-dimensional CFD modeling provides a high-resolution analysis of heat transfer in the HFCVD process.	While two-dimensional modeling provides valuable insights, it simplifies the reactor's real-world three-dimensional nature, potentially overlooking complex interactions and flow characteristics.	Extending the modeling to three dimensions would capture more complex flow and heat transfer phenomena.
	The study's emphasis on slip-flow heat transfer is relevant for HFCVD processes operating under low-pressure conditions where slip-flow effects are significant.	Despite being two-dimensional, CFD simulations are computationally intensive and require significant resources and expertise.	Extensive experimental validation is needed to corroborate the CFD results.
	Insights from the CFD simulations can improve HFCVD reactor design and operation.	The study may have limited experimental validation.	Incorporating dynamic operating conditions, like transient temperature changes and varying gas compositions, would provide a more realistic representation of the HFCVD process.
CFD Study of Chemical Vapor Deposition Reactor for Synthesis of PHEMA [59]	CFD provides detailed insights into fluid dynamics and heat transfer within the CVD reactor.	CFD simulations are computationally intensive, requiring substantial resources and expertise.	Expanding the study to include different polymers and reactor designs would enhance the generalizability of the findings.
	The study's findings can optimize key process parameters like	The study focuses on a specific polymer	Incorporating dynamic operating conditions, like fluctuating temperatures

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	temperature, pressure, and gas flow rates, improving the quality and efficiency of PHEMA synthesis.	(PHEMA) and reactor design.	and varying gas compositions, would better represent the CVD process.
	The research has significant practical implications for the chemical and materials engineering industries.	The extent of experimental validation is limited.	Investigating the long-term performance and stability of synthesized PHEMA under different environmental conditions would provide valuable insights.
Numerical Simulation on Modified Chemical Vapor Deposition (MCVD) Thermal Flow Field [60]	CFD allows high-resolution analysis of thermal and flow fields within the MCVD reactor.	CFD simulations are computationally intensive, requiring significant resources and expertise.	Including different materials and MCVD reactor configurations would enhance the generalizability of the findings.
	The study provides insights into optimizing process parameters like heat flux, gas flow rates, and rotation speed.	The study is specific to the MCVD process used for optical fiber preform manufacturing.	Incorporating dynamic operating conditions, like transient temperature changes and varying gas compositions, would provide a more realistic representation of the MCVD process.
	The findings are applicable to the optical fiber manufacturing industry, where precise control over the deposition process is essential.	The extent of experimental validation is limited.	Investigating the long-term performance and stability of the deposition process under continuous operation would provide valuable insights.
Unsteady Heat and Mass Transfer for Multi-Component Particle Deposition in the Modified Chemical Vapor Deposition [62]	Emphasizing multi-component particle deposition is crucial for real-world applications, where multiple materials are often deposited simultaneously.	The simulations are computationally intensive, requiring significant resources and expertise.	Including different CVD processes and materials would enhance the generalizability of the findings.
	Examining unsteady heat and mass transfer provides insights into transient behaviors during MCVD.	The study is focused on the MCVD process, which may limit the generalizability to other CVD methods.	Incorporating dynamic operating conditions, like varying gas compositions and temperature fluctuations, would better represent the deposition process.
	Computational simulations provide detailed analysis of the deposition process,	The scope of experimental validation is limited.	Investigating the long-term stability and performance of the deposited layers under

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	helping identify optimal conditions and predict parameter effects on deposition quality.		continuous operation would provide valuable insights.
	CFD provides detailed analysis of flow and heat transfer within the tungsten crucible CVD reactor.	CFD simulations are computationally intensive, requiring substantial resources and expertise.	Including different materials and CVD reactor designs would enhance the generalizability of the findings.
Numerical Simulation Study on Flow and Heat Transfer of the Tungsten Crucible CVD Reactor [63]	The study addresses practical challenges in the CVD process, applicable to industrial settings.	The study focuses on a tungsten crucible CVD reactor, which may limit the generalizability to other CVD reactors or materials.	Incorporating dynamic operating conditions, like transient temperature changes and varying gas compositions, would better represent the deposition process.
	The article investigates various process parameters, like gas flow rates, temperature distributions, and reactor geometry.	The scope of experimental validation is limited.	Investigating the long-term stability and performance of the deposition process under continuous operation would provide valuable insights.

3.2. Molecular Dynamics (MD) Simulations

The last decade has seen significant advancements in the application of Molecular Dynamics (MD) simulations to model heat transfer during Chemical Vapor Deposition (CVD) processes. These simulations have been pivotal in understanding and optimizing the multiscale nature of CVD, which involves complex interactions from the macroscopic reactor scale to the atomic scale of the deposited films [50].

For instance, MD simulations have been employed to predict the behavior of supercritical CO2 in heat transfer applications, highlighting the importance of accurate thermal coefficients and the challenges associated with the mutability of supercritical properties [64].

In the context of CVD, MD has been used to simulate the sulfurization of MoO3 by H2S/H2 mixtures, revealing critical reaction pathways and intermediates that enhance the quality of MoS2 layers [65].

Additionally, the development of constant chemical potential molecular dynamics (CμMD) has provided new insights into concentration-driven processes, such as crystallization and surface adsorption, which are fundamental to CVD [66].

Overall, the integration of MD simulations with other computational techniques has significantly improved the design, analysis, and optimization of CVD processes, paving the way for the development of novel materials and more efficient reactors.

Table 3 presents a summary of various aspects of selected articles in the field of application of the MD simulations.

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Table 3. Analysis of selected articles in the field of use of MD simulations.

Title	Advantages	Disadvantages	Gaps and Limitations
Quantum Molecular Dynamics Simulations of Chemical Vapor Deposition Synthesis of MoS2 Crystal Assisted by H2 Partial Pressures [65]	Applying quantum molecular dynamics to study the CVD process is innovative, offering atomic-level insights not easily accessible through experiments, aiding in understanding sulfurization mechanisms.	QMD simulations are resource-intensive, requiring significant expertise.	Including other materials synthesized via CVD would enhance the study's generalizability and provide broader insights into optimizing CVD processes.
	By investigating the role of H2 partial pressures, the study addresses a critical factor in the CVD process. Understanding how H2 influences the sulfurization of MoO3 is essential for optimizing the synthesis of high-quality MoS2 crystals.	The study's focus on MoS2 synthesis may limit its generalizability to other materials or processes.	Incorporating dynamic conditions, such as varying H2 concentrations and temperatures, would offer a more comprehensive understanding of the CVD process.
	The article thoroughly analyzes how different H2 environments affect the sulfurization process, providing valuable insights for optimizing CVD conditions for MoS2 synthesis.	Although insightful, the study offers limited discussion on experimental validation.	Investigating the long-term stability and performance of synthesized MoS2 crystals under various conditions would provide insights into their practical applications.
Non-Equilibrium Modeling of Concentration-Driven Processes with Constant Chemical Potential Molecular Dynamics Simulations [66]	Introducing CμMD simulations marks a significant advancement in molecular dynamics.	CμMD simulations are computationally demanding.	Expanding experimental validation to more conditions and systems would strengthen the findings.
	The study's detailed analysis of concentration-driven processes shows the versatility of CμMD simulations across various systems.	Implementing CμMD simulations requires expertise in molecular dynamics and non-equilibrium thermodynamics.	Including varied dynamic conditions in simulations would offer a more comprehensive understanding of non-equilibrium processes.
	The findings have broad applicability in material science, chemistry, and biology.	Experimental validation is crucial to confirm the simulations' accuracy and applicability.	Investigating long-term stability under constant chemical potential conditions would provide valuable practical insights.

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3.3. Lattice Boltzmann Method (LBM)

The Lattice Boltzmann Method (LBM) has significantly advanced in modeling heat transfer during Chemical Vapor Deposition (CVD) processes, leveraging its mesoscopic approach to handle complex boundaries and parallelization effectively. This method models fluid flow using fictive particles, which simplifies the integration of thermodynamics into transport equations and enhances its flexibility in dealing with multiphase flows, making it highly suitable for CVD applications [67].

Recent studies have demonstrated LBM's efficacy in simulating 3D liquid-vapor phase changes and heat transfer in irregular geometries, which are prevalent in CVD reactors [68,69].

The Immersed Boundary-LBM (IB-LBM) has shown particular effectiveness in modeling radiative heat transfer in 2D irregular geometries, highlighting its potential for handling the complex geometries encountered in CVD processes [70].

Additionally, LBM's capability to simulate natural convection and entropy generation in non-Newtonian fluids under magnetic fields has been explored, providing valuable insights into optimizing heat transfer in CVD reactors [71].

The development of multiple-relaxation-time LBM approaches has further improved the efficiency and accuracy of simulations, making it a promising candidate for 3D liquid-vapor phase change modeling in CVD [72].

Moreover, the method's application in predicting heat transfer and phase change in multi-layer deposition processes has been validated against experimental data, underscoring its reliability [73].

LBM's intrinsic second-order accuracy and efficient interface treatments for conjugate heat transfer make it a robust tool for modeling thin layers in CVD processes [74].

LBM has been successfully applied to model the drying of colloidal suspensions, enhancing heat conduction in nanoparticle deposition, which is analogous to the fine control required in CVD processes [75].

Bibliometric analysis of LBM research indicates a growing focus on multiscale models and hybrid methods, which are crucial for accurately capturing the multiscale nature of CVD processes. Overall, LBM's unique advantages, such as easy handling of complex geometries, parallel simulations, and continuous development, make it a powerful tool for advancing the understanding and optimization of heat transfer in CVD processes.

The paper by Łach et al. introduces a heat flow model based on the lattice Boltzmann method (LBM) for phase transformation, which can be adapted to simulate the heat transfer in CVD processes due to its capability to handle complex boundaries and phase changes [76].

Svyetlichnyy et al. discuss the development of a platform for 3D simulation of additive layer manufacturing, highlighting the importance of accurately modeling the changes in the state of matter. This is crucial for CVD, where precise control of temperature and reactant flow impacts the quality of the deposited layers [77].

The application of cellular automata and LBM in additive layer manufacturing presented by Svyetlichnyy et al. provides a framework that can be leveraged for modeling the deposition and heat distribution in CVD, ensuring uniform layer formation [78].

Finally, Łach and Svyetlichnyy (2024) present a 3D model of carbon diffusion during diffusional phase transformations, which can be directly applied to model mass transfer during CVD, enhancing the understanding of reactant diffusion and product layer growth [79].

Table 4 presents a summary of various aspects of selected articles in the field of application of the LBM method.

Table 4. Analysis of selected articles in the field of use of LBM method.

Title	Advantages	Disadvantages	Gaps and Limitations
Lattice Boltzmann Method and Its Applications [69]	The article provides a comprehensive overview of LBM, covering its theoretical foundations and practical applications.	LBM's computational intensity is a primary challenge, particularly for large-scale simulations. Discussing strategies for	The article lacks extensive coverage of scalability challenges and solutions for very large or complex systems.

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		optimizing efficiency and managing resources would enhance the article.	
	The article lacks extensive coverage of scalability challenges and solutions for very large or complex systems.	Expanding the discussion to include fields like biomedical engineering and material science would broaden the article's scope beyond hydroinformatics.	While LBM excels in steady-state simulations, it faces challenges in dynamic and transient processes.
	The authors clearly explain the LBM methodology, making it accessible to readers of varying expertise levels.	Focusing primarily on theoretical and computational aspects, the article would benefit from more discussions on experimental validations and real-world case studies.	Highlighting more interdisciplinary applications of LBM would increase the article's appeal to a wider audience.
Analysis of Radiative Heat Transfer in Two-Dimensional Irregular Geometries by Developed Immersed Boundary–Lattice Boltzmann Method [70]	Combining the immersed boundary method (IBM) with the lattice Boltzmann method (LBM) enhances the accuracy of radiative heat transfer simulations in irregular geometries.	The hybrid IB-LBM approach is computationally intensive, potentially limiting its practical use for large-scale problems or users with limited resources.	Expanding to three-dimensional geometries would improve the findings' generalizability.
	Addressing two-dimensional irregular geometries, the study tackles a common challenge in heat transfer simulations.	Focusing on two-dimensional geometries may not capture the full complexity of three-dimensional systems.	Evaluating the method under dynamic conditions would provide a more comprehensive assessment of its capabilities.
	The article thoroughly analyzes simulation results, detailing how various parameters affect radiative heat transfer in irregular geometries.	The article relies mainly on numerical simulations, with limited experimental validation.	Discussing strategies to optimize IB-LBM computational efficiency, such as parallel computing or algorithmic improvements, would enhance practical accessibility.
An Efficient Thermal Lattice Boltzmann Method for Simulating Three-Dimensional Liquid–Vapor Phase Change [72]	The article presents an advanced thermal LBM for three-dimensional liquid-vapor phase change simulations.	Despite efficiency improvements, the thermal LBM still demands significant computational resources.	Expanding the study to include different types of phase change phenomena and fluid flow scenarios would enhance the generalizability of the findings.
	A major strength is the focus on computational	Focusing on liquid-vapor phase change may limit	

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	efficiency, making the optimized thermal LBM feasible for large-scale simulations.	the findings' generalizability to other phase change or fluid flow problems.	Investigating the method's performance under dynamic and transient conditions, such as varying heat fluxes and pressure changes, would provide a more comprehensive understanding of its capabilities.
	The article thoroughly analyzes simulation results, including comparisons with existing methods.	More extensive experimental validation would enhance the article.	Further optimizing computational efficiency through parallel computing or algorithmic improvements would make the thermal LBM more practical for large-scale simulations.
Accuracy of Interface Schemes for Conjugate Heat and Mass Transfer in the Lattice Boltzmann Method [74]	The study compares multiple interface schemes, highlighting their accuracy and computational efficiency.	Evaluating multiple interface schemes through extensive simulations is computationally demanding.	Expanding the study to include a wider range of heat and mass transfer problems would enhance the generalizability of the findings.
	Addressing conjugate heat and mass transfer, the article focuses on a crucial aspect of thermal and fluid dynamics simulations, relevant for material and phase interactions.	The study's insights on conjugate heat and mass transfer may not apply to other heat and mass transfer problems.	Testing interface schemes under dynamic conditions, like varying heat fluxes and pressure changes, would offer a more comprehensive understanding.
	Combining theoretical analysis with numerical simulations strengthens the study's conclusions.	More extensive experimental validation would enhance the article.	Optimizing the computational efficiency of interface schemes would improve their accessibility for practical applications.
Lattice Boltzmann Modelling of Colloidal Suspensions Drying in Porous Media Accounting for Local Nanoparticle Effects [75]	The study uses the lattice Boltzmann method to model the complex drying of colloidal suspensions involving multiphase flows and nanoparticle interactions.	Including nanoparticle effects makes LBM simulations computationally intensive.	Including various porous materials and drying conditions would enhance the findings' generalizability.
	Incorporating local nanoparticle effects like viscosity changes, surface tension variations, and drying rate reductions,	The study's insights on colloidal suspensions in porous media may not apply to other drying processes or materials.	Investigating the method's performance under dynamic and transient conditions, such as varying temperatures

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the model offers detailed simulations.		and humidity levels, would provide a more comprehensive understanding of its capabilities.
The article comprehensively analyzes how different parameters affect the drying process.	More extensive experimental validation would enhance the article.	Studying the long-term stability of dried colloidal structures under different environments would offer practical application insights.

4. Mass Transport Modeling

Mass transport modeling is a critical component in the analysis and optimization of Chemical Vapor Deposition (CVD) processes. It involves understanding and predicting the movement and distribution of reactant gases, intermediates, and by-products within the CVD reactor. This modeling is essential for controlling the deposition of thin films on substrates, ensuring uniformity, quality, and efficiency.

Mass transport modeling helps analyze how reactant gases flow through the reactor, including understanding laminar or turbulent flow regimes, flow patterns, and how these affect the distribution of reactants near the substrate surface. The boundary layer, the thin region adjacent to the substrate where the gas velocity changes from zero (at the substrate) to the free stream value, significantly influences mass transport. Modeling the boundary layer helps predict local deposition rates.

The shape and dimensions of the CVD reactor impact gas flow and reactant distribution. Mass transport models assist in designing reactor geometries that promote uniform gas distribution and efficient reactant delivery to the substrate. Proper placement and design of gas inlets and outlets ensure that reactants are evenly distributed and by-products are efficiently removed, minimizing dead zones and enhancing film uniformity.

Mass transport modeling helps determine the concentration profiles of reactants within the reactor, crucial for predicting local deposition rates on the substrate, which depend on the availability of reactants at the surface. Temperature gradients within the reactor affect reaction kinetics and mass transport properties. Models that incorporate thermal effects can predict how temperature variations influence the deposition rate and uniformity.

Achieving uniform film thickness across the substrate is critical for high-quality coatings. Mass transport models identify the conditions that lead to uniform reactant distribution and deposition rates. By manipulating mass transport parameters, it is possible to influence film characteristics such as thickness, composition, grain size, and stress, leading to improved film quality.

When scaling up from laboratory to industrial scale, maintaining process consistency is challenging. Mass transport models help understand how changes in reactor size affect gas flow and deposition rates, enabling effective scale-up. Models can guide the adjustment of process parameters such as flow rates, pressures, and temperatures to maintain optimal conditions during scale-up.

Efficient use of reactants is critical for cost-effective and environmentally friendly CVD processes. Mass transport models optimize reactant flow to maximize utilization and minimize waste. By optimizing heat and mass transfer, models help design processes that require less energy for heating and maintaining the desired reactor conditions.

Mass transport modeling is often integrated with thermal, chemical reaction, and fluid dynamics models to provide a comprehensive understanding of the CVD process. This holistic approach captures the interplay between different physical phenomena. Combining mass transport with chemical kinetics and thermal analysis enhances the accuracy of predictions regarding film properties and process outcomes.

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Mass transport modeling is indispensable in the development, optimization, and scaling of CVD processes. It enables a detailed understanding of reactant distribution, gas flow dynamics, and deposition mechanisms. By providing insights into how reactants and by-products move and interact within the reactor, mass transport models facilitate the design of more efficient reactors, improve film quality, and ensure uniform deposition. This modeling is essential for achieving high-performance CVD processes, reducing waste, and enhancing overall process efficiency.

Mass transport modeling plays a crucial role in CVD processes by providing insights into the complex interactions between fluid dynamics, thermodynamics, and chemical reactions, which are essential for optimizing deposition quality and efficiency. These models help elucidate the basic mechanisms of multi-species transport and their interplay with gas and surface reactions, as seen in the development of 3D CFD models for pyrocarbon deposition [80]. The integration of mass transport with chemical kinetics models, such as those for carbon-coated optical fibers, allows for the optimization of coating quality by validating different reactor models under various conditions [81]. Mass transport modeling also addresses the challenges of uniform precursor concentration and convective mass transport in reactors, as demonstrated in studies on pulsed-pressure CVD systems [82]. Furthermore, these models are essential for predicting growth rates and doping non-homogeneity in SiC epitaxial growth processes, aiding in the development of new CVD processes [83,84]. The application of reduced-order models [58], such as the Proper Orthogonal Decomposition (POD) method [85], significantly reduces the complexity of the governing equations, making it feasible to control transport processes more efficiently. Overall, mass transport modeling is indispensable for advancing CVD technology, enabling precise control over deposition parameters and enhancing the quality and uniformity of the deposited films [86].

4.1. Diffusion-Based Models

Diffusion-based models, particularly those leveraging stochastic differential equations (SDEs), have shown significant promise in various domains, including the modeling of complex processes like chemical vapor deposition (CVD). Fishman et al. introduced novel approaches to diffusion models constrained by inequality metrics, relevant for applications like robotics and protein design, which can potentially be adapted for precise control in CVD environments [87]. Yang et al. provided an extensive survey of diffusion models, categorizing them into efficient sampling, improved likelihood estimation, and data structure handling, highlighting their broad applicability and potential enhancements for CVD processes [88]. These studies collectively illustrate how diffusion-based models can be optimized and adapted to improve the precision and efficiency of CVD processes, leveraging advancements in computational techniques and theoretical frameworks. The following subsections present selected solutions in this area.

4.1.1. Fick's Laws of Diffusion

Fick's laws of diffusion are pivotal in modeling Chemical Vapor Deposition (CVD) processes, as they describe the transport mechanisms essential for material deposition. The first law, which relates the diffusive flux to the concentration gradient, and the second law, which predicts how diffusion causes concentration to change over time, are instrumental in designing and optimizing CVD systems.

Paul et al. introduce Fick's laws, detailing the derivation and solutions of the second law for various conditions, which are crucial for estimating diffusion coefficients in CVD processes [89].

Poirier and Geiger apply Fick's law to the diffusion of chemical species through a phase due to concentration gradients, offering essential insights for modeling diffusion in materials used in CVD processes [90].

Donev et al. explore a mesoscopic model of diffusion in liquids, highlighting the importance of thermal fluctuations and random advection in addition to Fick's law, enhancing our understanding of diffusion in CVD processes at different scales [91].

Cheimarios et al. emphasize the multiscale nature of CVD, illustrating how Fick's laws are applied at different scales to model the diffusion and deposition of thin films. Their work reviews

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various methodologies and the transfer of information between scales, highlighting the complexity of accurately modeling CVD processes [50].

Andreucci et al. extend Fick's laws to inhomogeneous media, relevant for CVD processes involving spatially varying properties. They discuss the geometric interpretation of reversibility and hydrodynamic scaling, providing insights into the macroscopic behavior of diffusion in CVD [92].

Additionally, Gavriil et al. critically assess the application of Fick's law in food packaging, which parallels the challenges in CVD processes by addressing complex transport phenomena and environmental interactions [93].

Philipse discusses Brownian motion and diffusion equations, explaining how particle positions and orientations evolve over time, foundational for understanding diffusion in CVD processes [94].

Sibatov and Sun discusses the generalized Fick law in the context of fractional operators, describing dispersive transport in disordered semiconductors, relevant for advanced CVD process modeling [95].

These studies underscore the significance of Fick's laws in providing a foundational understanding of diffusion in CVD and similar processes.

Table 5 presents a summary of various aspects of selected articles in the field of application of the Fick's Laws of Diffusion.

Table 5. Analysis of selected articles in the field of use the Fick's Laws of Diffusion.

Title	Advantages	Disadvantages	Gaps and Limitations
Fick's Law and Diffusivity of Materials [90]	The chapter thoroughly covers Fick's first and second laws of diffusion.	The chapter focuses on theoretical aspects with limited experimental validation.	Expanding the discussion to cover a wider range of materials, including non-metallic systems, would enhance the applicability of the principles discussed.
	The discussion includes practical applications in materials processing, valuable for engineers and scientists in metallurgy, ceramics, and materials science.	Detailed insights into metallurgical applications are provided, but diffusivity in other materials may not be comprehensively covered.	Exploring interdisciplinary applications, such as in biological systems or environmental engineering, would show Fick's law's broader utility.
	The authors provide clear explanations of complex concepts, accessible to both students and professionals.	The mathematical treatment may be challenging for readers without a strong background in mathematics or transport phenomena.	Incorporating modern diffusivity measurement techniques and recent advancements would provide an up-to-date perspective.
A Reversible Mesoscopic Model of Diffusion in Liquids: From Giant Fluctuations to Fick's Law [91]	The study introduces a reversible mesoscopic model with thermal fluctuations, offering a more accurate view of diffusion in liquids and challenging the traditional irreversible model based solely on Fick's law.	The accurate mesoscopic model is computationally intensive, requiring significant resources and limiting its use for large-scale or real-time simulations.	Extending the model to include diffusion in other states of matter and complex fluids would enhance its generalizability.

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	The authors present a strong theoretical framework linking microscopic fluctuations to macroscopic diffusion behavior.	The model is specifically tailored for diffusion in liquids, which may limit its generalizability to other states of matter such as gases or solids.	Testing under dynamic conditions, like varying temperature and pressure, would clarify the model's capabilities and limitations.
	Using Lagrangian numerical methods, the study captures the stochastic nature of particle movements and thermal fluctuations, essential for accurate mesoscopic diffusion modeling.	The study could benefit from more extensive experimental validation despite strong theoretical and numerical development.	Optimizing computational efficiency would make the model more practical for real-world applications.
Fick and Fokker–Planck Diffusion Law in Inhomogeneous Media [92]	The study thoroughly explores Fick's law and the Fokker–Planck equation in inhomogeneous media.	The study's mathematical models and equations are highly complex.	Expanding the study to include a broader range of applications and different types of diffusion processes would enhance the generalizability of the findings.
	Integrating Fick's law with the Fokker–Planck equation provides a comprehensive diffusion modeling framework for inhomogeneous media.	Despite robust theoretical insights, the article lacks extensive experimental validation.	Testing diffusion models under dynamic conditions, like time-varying gradients and external fields, would provide a more comprehensive understanding.
	The authors use rigorous mathematical methods to derive and validate their models.	Focusing on inhomogeneous media may limit the results' generalizability to other diffusion processes.	Simplifying the complex mathematical models without losing accuracy would make the findings more accessible.
Continuity, Gradients and Fick's Diffusion Laws [94]	The article thoroughly explores continuity, gradients, and Fick's laws.	While the theoretical coverage is extensive, the article could benefit from more practical examples and applications.	The article could broaden its scope to include interdisciplinary applications of Fick's laws.
	The author explains complex concepts clearly and concisely.	The advanced mathematical treatment may be challenging for readers without a strong math or physics background.	The discussion is primarily focused on linear systems. Addressing Fick's laws in dynamic and non-linear systems would enhance the discussion.

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	The article places Fick's laws in historical context, highlighting their evolution and significance in diffusion theory.	The article focuses on theory and lacks discussion on experimental validation.	Including recent advancements in diffusion would complement the historical perspective.
Dispersive Transport Described by the Generalized Fick Law with Different Fractional Operators [95]	Using fractional calculus to generalize Fick's law for dispersive transport is innovative, addressing traditional models' limitations in disordered systems.	The fractional differential equations and their solutions are mathematically complex, which might limit the accessibility of the study to researchers who are not well-versed in advanced mathematical techniques.	Incorporating diverse experimental data would validate and demonstrate the models' robustness across various scenarios.
	The article presents a detailed theoretical framework, linking fractional derivatives to observable ToF experiment phenomena.	Robust theoretical models need more extensive experimental validation to confirm their real-world accuracy and applicability.	Testing fractional models under dynamic conditions, like varying temperature or electric fields, would deepen understanding of their practical applicability.
	The findings have broad implications for studying charge transport in disordered systems like amorphous semiconductors, organic bulk heterojunction cells, and perovskite solar cells, making the study relevant in materials science and electronics.	Focusing on Riemann–Liouville derivatives, the study could explore other fractional operators or hybrid models for a more comprehensive understanding of dispersive transport phenomena.	Simplifying or optimizing fractional models would make them more accessible for industrial use with limited computational resources.

4.1.2. Boundary Layer Approaches

Boundary layer approaches are crucial in the modeling of Chemical Vapor Deposition (CVD) processes, as they help in understanding the transport phenomena near the substrate surface where deposition occurs. These approaches allow for detailed analysis of the kinetics, transport, and reaction mechanisms within the boundary layer.

Zhang et al. investigate the impact of boundary layers on the deposition rates and characteristics of polycrystalline silicon in a CVD process using trichlorosilane and hydrogen, highlighting the importance of controlling boundary layer thickness to enhance deposition uniformity and quality [96].

Aghajani et al. study the deposition of SiC on C/C composites using CVD, exploring the deposition kinetics by varying process parameters such as time, temperature, and precursor composition, and employing boundary layer theory to understand the deposition rates and coating characteristics [97].

Boi et al. examine the growth of Fe-filled carbon nanotubes using boundary layer chemical vapor synthesis, a method that exploits random fluctuations within the viscous boundary layer, discussing how tangential and perpendicular growth modes affect the synthesis process [98].

Lukashov et al. propose an analytical model for the deposition of thermal barrier coatings via Metal-Organic CVD (MO CVD), using the reacting boundary layer model to analyze the diffusion combustion of precursors and evaluate coating growth rates and precursor efficiency [99].

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Kleimanov et al. present a numerical model of a CVD reactor used for producing oxide semiconductor layers, aiming to ensure uniform substrate heating and layer deposition by simulating the induction heating process and analyzing the impact of the boundary layer on deposition uniformity [46].

Sayevand and Machado address singularly perturbed fractional differential equations displaying boundary layer behavior, introducing a novel operational matrix technique to approximate solutions, enhancing the accuracy and stability of boundary layer models, which is vital for predicting deposition rates in CVD processes [100].

Timms and Purvis present a one-dimensional model for the initiation of shear bands in reactive materials, using boundary layer analysis to identify key physical properties controlling the reactive shear banding process, providing insights into localized plastic deformation relevant for understanding stress effects in CVD processes [101].

Table 6 presents a summary of various aspects of selected articles in the field of application of the boundary layer approaches.

Table 6. Analysis of selected articles in the field of use the boundary layer approaches.

Title	Advantages	Disadvantages	Gaps and Limitations
Deposition Kinetics and Boundary Layer Theory in the Chemical Vapor Deposition of β-SiC on the Surface of C/C Composite [97]	The study provides valuable insights into optimizing CVD parameters for β-SiC coatings on C/C composites.	The study primarily focuses on experimental observations. Integrating computational modeling could provide a more comprehensive understanding of the deposition mechanisms and boundary layer dynamics.	Extending the study to include different materials and substrates would enhance the generalizability and applicability of the findings across various industrial applications.
	The use of XRD and FESEM allows for a detailed analysis of the coating's phase composition and microstructure, which is crucial for understanding the deposition process and improving the quality of the coatings.	The research is specific to β-SiC on C/C composites. Expanding the scope to other materials and composites would increase the findings' generalizability.	Investigating dynamic conditions like fluctuating temperatures and precursor flow rates would better represent the CVD process.
	The findings are significant for industries like aerospace and electronics that rely on high-quality β-SiC coatings.	The study does not address the environmental impact of the CVD process, such as the emissions and by-products generated during deposition. Including this analysis would provide a more holistic view of the process's sustainability.	Examining the long-term stability and performance of β-SiC coatings under operational conditions would provide insights into their practical applications and durability.
Possible Interplay of Tangential and Perpendicular Modes in the	The study's exploration of tangential and perpendicular growth modes offers new insights	Replicating the study's precise CVD parameter control may be challenging.	Including other metal-filled CNTs would offer a broader understanding of growth mechanisms.

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Growth of Fe-Filled Carbon Nanotubes [98]	into Fe-CNT formation mechanisms.		
	The article comprehensively analyzes nanotube structures using various characterization techniques.	The detailed insights on Fe-CNTs may not apply to other filled carbon nanotubes or nanomaterials.	Studying Fe-CNT growth under varying temperatures and gas compositions would reveal the process's sensitivity to environmental changes.
	Understanding Fe-CNT growth mechanisms has significant implications for nanotechnology and materials science applications.	Scaling up the synthesis and analysis methods for large-scale Fe-CNT production may be difficult.	Evaluating Fe-CNTs' long-term stability and performance in practical applications would provide insights into their durability and limitations.
Analytical Model of the Process of Thermal Barrier Coating by the MO CVD Method [99]	The article provides a robust analytical framework for understanding the deposition process in MO CVD. By integrating diffusion combustion reactions and convection conditions, the model offers a detailed mechanism for the growth of TBCs.	The model's computational intensity may limit its industrial use without significant resources.	Including different coatings and precursors would enhance the model's generalizability.
	The study's focus on 7YSZ coatings, widely used in aerospace and energy industries, enhances its practical relevance.	The model is tailored specifically for MO CVD processes and 7YSZ coatings.	Testing under dynamic conditions like varying temperatures and flow rates would better assess its capabilities.
	Model predictions validated against experimental data strengthen the proposed approach's credibility and practical applicability.	Although the model is compared with experimental data, the scope of this validation is somewhat limited.	Examining long-term stability and performance under operational conditions would provide insights into practical applications and durability.
Numerical Simulation of CVD Reactor for Oxide Semiconductor Layer Deposition [46]	The use of detailed numerical simulations to model the CVD reactor processes is a significant strength.	The simulations require significant computational resources, limiting accessibility to advanced research facilities.	Expanding the study to include different types of semiconductor materials and reactor configurations would enhance the generalizability of the findings and provide broader insights into the CVD process.
	The study tackles practical CVD challenges	The study focuses on a specific CVD reactor and	

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	like substrate temperature stability and uniform layer deposition.	material system (oxide semiconductors with gold nanoparticles).	Testing under dynamic conditions like varying temperatures and gas flow rates would better reveal the reactor's capabilities and limitations.
	Combining fluid dynamics, heat transfer, and materials science offers a comprehensive approach to CVD reactor design.	While the simulations are thorough, the study would benefit from more extensive experimental validation to confirm the accuracy and applicability of the simulated results under real-world conditions.	Optimizing computational efficiency would make simulations more practical for industrial use.
Accurate Splitting Approach to Characterize the Solution Set of Boundary Layer Problems [100]	Using fractional calculus for boundary layer problems offers a novel perspective on differential equations.	The complex mathematical models may limit accessibility for non-specialists.	Expanding the approach to include a wider range of differential equations and boundary conditions would enhance its generalizability and applicability.
	The modified truncated Chebyshev series and operational matrix technique ensure high accuracy, crucial for practical applications.	Focusing on specific boundary layer problems may limit the approach's generalizability.	Simplifying the mathematical techniques while maintaining accuracy would broaden accessibility.
	Detailed methodology, including stability and error analysis, makes the findings robust and reliable.	More empirical data is needed to enhance the method's practical applicability.	Testing under dynamic and transient conditions would provide a comprehensive understanding of the method's capabilities.

4.2. Kinetic Monte Carlo (KMC) Simulations

Kinetic Monte Carlo (KMC) simulations are a powerful tool for modeling chemical vapor deposition (CVD) processes, offering detailed insights into the physicochemical phenomena occurring at various scales. KMC methods are particularly advantageous for studying deposition processes due to their ability to address larger time and spatial scales compared to molecular dynamics (MD) and provide a more detailed approach than continuum-type models [102].

Pineda and Stamatakis present the basic principles, computational challenges, and successful applications of KMC simulations in heterogeneous catalysis. Their work highlights the integration of first-principles calculations with KMC to accurately model reactions over surfaces, which is critical for designing novel catalysts used in CVD processes [103].

Cheimarios et al. present modern applications of Monte Carlo and KMC models in deposition processes, including physical and chemical vapor deposition, atomic layer deposition, and electrochemical deposition [104].

Chen et al. propose an all-atom KMC model to simulate the growth of graphene on a Cu substrate, including essential atomistic events such as deposition, diffusion, and attachment of carbon species, successfully predicting various graphene morphologies and growth kinetics [105].

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Papanikolaou and Stamatakis discuss the fundamentals and applications of KMC simulations in modeling reactions on catalytic surfaces, reviewing the principles of KMC simulations and their relevance in heterogeneous catalysis and CVD processes [106].

Rodgers et al. present a three-dimensional KMC model to simulate diamond CVD, including adsorption, etching, lattice incorporation, and surface migration events. The model accurately reproduces experimental growth rates and provides insights into growth mechanisms under different conditions [107].

Osman and Mitra simulate the growth of polymer films on two-dimensional surfaces using KMC, modeling the initial growth of iCVD surface reactions, assuming room temperature substrates and specific reactor pressures. The simulation results are compared with experimental data for initial growth, demonstrating the potential of KMC in modeling polymer film deposition [108].

Heiber introduces Excimontec, a Python package for simulating ionic transport properties in crystalline materials using KMC. The tool aids in understanding and optimizing organic semiconductor devices by modeling the behavior of excitons and polarons in semiconductor layers, relevant for CVD processes [109].

Edward and Johnson use an atomistic multi-lattice KMC model to understand defect generation in multi-layered graphene caused by the adsorption and diffusion of epoxy groups. The simulations reveal the temperature and pressure dependencies of defect formation, providing insights into the role of epoxy diffusion in CVD processes [110].

Agarwal et al. introduce the QSD-KMC approach for modeling state-to-state dynamics in complex systems, such as biomolecular dynamics. The method retains time resolution even in highly non-Markovian dynamics, which can be applied to CVD processes to model long timescale reactions and state transitions [111].

Table 7 presents a summary of various aspects of selected articles in the field of application of the Kinetic Monte Carlo (KMC) simulations.

Table 7. Analysis of selected articles in the field of use the Kinetic Monte Carlo (KMC) simulations.

Title	Advantages	Disadvantages	Gaps and Limitations
An All-Atom Kinetic Monte Carlo Model for Chemical Vapor Deposition Growth of Graphene on Cu(111) Substrate [105]	The all-atom kMC model accurately captures atomic interactions and surface dynamics in graphene growth.	The all-atom kMC model is computationally intensive, requiring significant resources and time.	Including substrates like Ni(111) or SiC would broaden the findings' generalizability and deepen understanding of graphene growth.
	The model includes factors like hydrogen partial pressures, surface diffusion, and carbon-copper interactions.	The study focuses on the Cu(111) substrate, though it's not the only one used for graphene growth.	Testing under dynamic conditions, like varying temperature and pressure, would better evaluate the model's capabilities and limitations.
	The findings have significant implications for the optimization of industrial graphene production.	Despite detailed theoretical insights, the study lacks extensive experimental validation.	Increasing the extent of experimental validation through systematic comparison with empirical data would help confirm the model's accuracy and enhance its practical applicability in industrial settings.

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	The article explains KMC simulation principles and their application to surface reactions.	KMC simulations require significant resources and time, limiting accessibility to well-equipped facilities.	Expanding the study to include a wider range of surface reactions and catalytic systems would enhance the generalizability of the findings.
Toward the Accurate Modeling of the Kinetics of Surface Reactions Using the Kinetic Monte Carlo Method [106]	Focusing on heterogeneous catalysis, the study is highly relevant to industrial applications in chemical engineering and materials science.	Complex models demand expertise in computational techniques and physical chemistry, restricting use to specialists.	Testing KMC simulations under dynamic conditions, like varying temperatures and pressures, would provide a fuller understanding of their capabilities.
	Case studies show KMC simulations' practical utility in predicting reactions and optimizing catalytic processes.	While the article provides extensive theoretical insights, more experimental validation would enhance the robustness and applicability of the findings.	Integrating KMC with methods like density functional theory (DFT) could offer a holistic approach to modeling catalytic processes.
	The detailed kMC model comprehensively explains diamond growth at the atomic level in the CVD process.	Three-dimensional kMC simulations require substantial resources, limiting accessibility to well-equipped facilities.	Including various materials and deposition techniques would enhance the model's generalizability.
Three-Dimensional Kinetic Monte Carlo Simulations of Diamond Chemical Vapor Deposition [107]	The use of three-dimensional simulations offers a more realistic representation of the deposition process compared to previous one- or two-dimensional models.	Tailored to diamond CVD, the model may need modifications for other materials or deposition processes.	Testing under different gas compositions and temperatures would better understand the model's capabilities.
	The findings have significant implications for optimizing the CVD process to improve the quality and efficiency of diamond film production, which is crucial for industrial applications.	While the simulations provide detailed theoretical insights, the study could benefit from more extensive experimental validation to confirm the accuracy and practical applicability of the results.	Correlating with experimental data under diverse conditions would strengthen the model's validity and real-world relevance.
A Basic Monte Carlo Model of Initiated Chemical Vapor Deposition Using Kinetic Theory [108]	Using a Monte Carlo model for iCVD simulation offers a new molecular-level perspective on deposition mechanisms.	Monte Carlo simulations are computationally intensive, limiting practicality for real-time or large-scale applications.	Including other CVD processes and materials would enhance the findings' generalizability and understanding of deposition mechanisms.

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	Applying kinetic theory, the model captures particle dynamics, leading to precise predictions and optimization.	Tailored to iCVD, the findings may not generalize to other CVD processes.	Testing the model under varying temperatures and pressures would better evaluate its capabilities.
	The findings improve control and efficiency in the iCVD process, essential for producing high-quality polymeric films.	The article lacks extensive experimental validation of the simulation results. Including more experimental data would enhance the credibility and applicability of the model.	Optimizing Monte Carlo simulations' computational efficiency would make the approach more practical for industrial use.
Atomistic Multi-Lattice Kinetic Monte Carlo (KMC) Modeling of Hyperthermal Oxidation of Multi-Layer Graphene [110]	The multi-lattice KMC model advances understanding of graphene oxidation.	KMC simulations require significant computational resources and expertise.	Including more thermal and environmental conditions would provide a comprehensive understanding of oxidation processes.
	Focusing on the atomic scale reveals specific oxidation mechanisms in multi-layer graphene.	Focusing on hyperthermal oxidation may not cover all real-world oxidation conditions for graphene.	Investigating dynamic thermal conditions would offer a realistic representation of real-world applications.
	The findings have broad implications for the development and optimization of graphene-based materials, which are of significant interest for their exceptional electronic, thermal, and mechanical properties.	The study could benefit from more extensive experimental validation to corroborate the simulation results.	Optimizing KMC simulation efficiency would make the approach more accessible for research and industry.

4.3. Multi-Scale Modeling Techniques

Multiscale modeling of mass transport during chemical vapor deposition (CVD) involves integrating various scales to accurately predict and optimize the deposition process. At the macroscopic level, computational fluid dynamics (CFD) models are employed to simulate the complex reacting flow within the CVD reactor, capturing the transport phenomena and temperature-dependent physical properties to understand the interplay between gas and surface reactions. This is complemented by mesoscale models that link reactor-scale heat and mass transport equations with phase-field equations to predict the morphology and distribution of synthesized materials, such as 2D materials like MoS2. At the microscopic level, models focus on the detailed surface chemistry and the effects of micro-topography on species consumption, as seen in the deposition of silicon from silane on trenched wafers. Multiscale approaches also involve coupling different software packages to handle large-scale transport-reaction models and small-scale reactive precursor gas models, ensuring that fast reaction processes are accurately represented without losing critical information [50]. Momeni et al. developed a multiscale model linking CVD control parameters to the morphology, size, and distribution of synthesized 2D materials. The model couple's reactor-scale heat and mass transport equations with mesoscale phase-field equations to predict and control the growth

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morphology of 2D materials like MoS2. The framework is experimentally validated, demonstrating its capability to optimize growth conditions [112].

Geiser proposed a multiscale model based on two different software packages. The large scales are simulated with CFD software based on the transport-reaction model (or macroscopic model), and the small scales are simulated with ordinary differential equations (ODE) software based on the reactive precursor gas model (or microscopic model) [113].

Table 8 presents a summary of various aspects of selected articles in the field of application of the multi-scale modeling.

Table 8. Analysis of selected articles in the field of use the multi-scale modeling.

Title	Advantages	Disadvantages	Gaps and Limitations
Multiscale Modeling in Chemical Vapor Deposition Processes: Models and Methodologies [50]	The article effectively integrates multiple length scales, from atomic to macroscopic levels, providing a detailed understanding of CVD processes.	Multiscale modeling requires significant computational resources, which can be a limiting factor for its widespread adoption in industrial settings.	The lack of extensive experimental validation at all scales is a significant gap.
	The authors present a robust framework for coupling different scales.	The methodologies presented are complex and require a high level of expertise in both modeling and computational techniques.	The models are often tailored to specific CVD processes or materials, which can limit their generalizability.
	Bridging these scales helps optimize reactor designs and process parameters, improving film quality and efficiency.	While the models are theoretically robust, experimental validation across all scales is challenging.	The scalability of the models to larger industrial processes is not fully addressed.
Multiscale Framework for Simulation-Guided Growth of 2D Materials [112]	The study's strength is its comprehensive multiscale approach.	The multiscale nature of the framework introduces significant computational complexity.	Including more 2D materials would enhance the framework's utility and generalizability.
	Systematic MoS2 growth experiments validate the model, showing its practical applicability.	Findings on MoS2 growth may not directly apply to other 2D materials without model modifications.	Incorporating real-time data and feedback could improve CVD process control accuracy and efficiency.
	The framework optimizes CVD parameters for reproducible, scalable production of high-quality 2D materials.	Assumptions and simplifications for feasible simulations may limit prediction accuracy under varied growth conditions.	Testing the model under varying environmental conditions would provide a more robust understanding of its applicability.
Multiscale Modeling of Chemical Vapor Deposition (CVD) Apparatus: Simulations and Approximations [113]	Using CFD and ODE software for different scales is a major advancement.	Integrating CFD and ODE models requires significant computational resources.	Expanding the study to include a variety of materials and CVD processes would provide a more comprehensive understanding of the multiscale modeling approach and its versatility.
	The study tackles practical CVD challenges like ensuring	The study focuses on specific materials (SiC and TiC), which	

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uniform and stable thin film deposition.	might limit the generalizability of the findings.	Testing under dynamic conditions, like varying temperatures and gas flow rates, would better represent industrial CVD processes.
The article thoroughly explains the models, methods, and upscaling techniques to integrate microscale interactions into the macroscale model.	The study could benefit from more extensive experimental validation to confirm the accuracy of the simulation results.	Optimizing computational efficiency through parallel computing or algorithmic improvements would make the approach more accessible and practical for routine use.

4.4. Machine Learning and Data-Driven Approaches

Machine learning (ML) and data-driven approaches have been increasingly applied to model mass transport in Chemical Vapor Deposition (CVD) processes, offering enhanced predictive capabilities and optimization potential.

Xie and Stearrett studied benchmark data imputing, feature selection, and regression algorithms for ML-based CVD virtual metrology. They found that linear feature selection regression algorithms underfit the data, suggesting that a nonlinear feature selection and regression algorithm combined with nearest data imputing can achieve up to 70% prediction accuracy. This significantly reduces CVD processing variation and improves wafer quality, demonstrating ML's potential in enhancing metrology in mass production [114].

Costine et al. discussed an ML approach that uses data from published growth experiments to predict growth performance in unexplored parameter spaces. By leveraging literature data on MoS2 thin films grown using CVD, the study employs unsupervised and supervised ML methods to uncover design rules that classify monolayers and guide future CVD experiments, optimizing growth conditions for desired microstructures and morphologies [115].

Yoshihara et al. constructed an ML model to design experimental CVD conditions for forming large-area graphene. The model predicts graphene domain size from CVD growth conditions and spectral information of the Cu surface, demonstrating faster graphene growth compared to traditional methods. This approach highlights the efficacy of ML in optimizing CVD conditions for large-scale applications [116].

Zeng et al. integrated ML with computational fluid dynamics (CFD) to identify core factors influencing the phase composition of boron carbide deposits. By combining ML and CFD, the prediction error is significantly reduced, providing accurate predictions of the deposited boron-carbon ratio. This approach highlights the potential of ML in optimizing deposition conditions and understanding mass transport mechanisms [117].

Khosravi and Zeraati modeled the length of CNTs prepared by floating catalyst CVD using hybrid artificial neural networks (ANN) and gene expression programming (GEP). The models consider various CVD parameters, with ANN-MPSO (modified particle swarm optimization) providing accurate predictions for CNT length. The results highlight the effectiveness of ML in predicting outcomes based on CVD process parameters [118].

Dritsas and Trigka, focusing on cardiovascular disease prediction, demonstrated the efficacy of supervised ML techniques in handling complex datasets and improving prediction accuracy. The methodologies and insights can be adapted to optimize mass transport models in CVD processes [119].

Koronaki et al. presented an equation-free, data-driven approach for reduced order modeling of CVD processes, utilizing the Proper Orthogonal Decomposition (POD) method and Artificial Neural Networks (ANN) for model development, with the Support Vector Machine (SVM) classification algorithm used to identify clusters of data corresponding to different process states [120].

Table 9 presents a summary of various aspects of selected articles in the field of application of the machine learning and data-driven.

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Table 9. Analysis of selected articles in the field of use the machine learning and data-driven.

Title	Advantages	Disadvantages	Gaps and Limitations
Machine Learning Based CVD Virtual Metrology in Mass Produced Semiconductor Process [114]	The study performs a cross-benchmark analysis on various data imputing methods, feature selection techniques, and regression algorithms. This thorough evaluation helps in identifying the most effective combinations for accurate VM in CVD processes.	Implementing GB and NN algorithms requires substantial computational resources.	Including diverse datasets from various CVD processes and semiconductor devices would enhance the findings' robustness and applicability.
	Non-linear regression algorithms, especially gradient boosting (GB) and neural networks (NN), significantly improve prediction accuracy over traditional linear models.	Non-linear algorithms showed high accuracy but raised overfitting concerns, especially with GB.	Testing VM models under dynamic conditions would provide a comprehensive understanding of their capabilities and limitations.
	The findings have direct applications in the semiconductor industry, where efficient and accurate VM can lead to reduced processing times, lower costs, and improved wafer quality.	More extensive validation across different CVD processes and conditions is needed.	Optimizing ML algorithms for computational efficiency while maintaining accuracy would make the VM approach more practical for industrial use.
Data-driven Assessment of Chemical Vapor Deposition Grown MoS2 Monolayer Thin Films [115]	Applying ML methods to optimize the CVD process is a significant advancement.	The study relies heavily on data from existing literature, which may introduce biases or inconsistencies due to variations in experimental setups and reporting standards.	Including more experimental conditions and substrate types would enhance understanding of the CVD process.
	The study compiles a comprehensive dataset on MoS2 CVD growth conditions from various sources.	While the study uses ML to draw conclusions, more direct experimental validation of the predicted optimal conditions would strengthen the results.	Combining ML predictions with systematic experimental studies would validate the model's accuracy and optimize the CVD process.
	The findings have practical implications for the synthesis of high-quality MoS2 monolayers, which are crucial for	The ML models used are complex and require significant computational resources.	Real-time monitoring and adjustment of CVD parameters based on ML predictions could improve

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	applications in electronics and optoelectronics.		efficiency and quality control.
Machine Learning Method for Determining Chemical Vapor Deposition Conditions for Large-Area Graphene Growth [116]	Integrating machine learning to optimize CVD processes is a significant advancement.	ML model accuracy relies on the quality and quantity of training data; data limitations or biases can affect predictions.	Applying ML to other materials and CVD processes would broaden its applicability.
	High-quality, large-area graphene is essential for industrial applications like electronics, sensors, and flexible devices.	Optimizing CVD conditions with ML algorithms demands significant computational resources and expertise.	Testing ML models under varying temperatures and pressures would assess their practical utility.
	The use of machine learning enables the analysis of large datasets to discern complex relationships between process parameters and graphene quality.	Promising results need extensive experimental validation across various setups and conditions to ensure robustness and reliability.	Optimizing ML algorithms' computational efficiency would make them more accessible for industrial use.
Predictive modeling of the length of prepared CNT by CVD through ANN-MPSO and GEP [118]	The use of ANN-MPSO and GEP presents an innovative approach to modeling and predicting CNT lengths, leveraging the strengths of both machine learning and evolutionary algorithms.	The hybrid modeling approach is computationally intensive, needing substantial resources and expertise.	Including various nanomaterials and CVD processes would enhance the findings' generalizability and modeling insights.
	By focusing on optimizing the CVD process, the study addresses a critical need in the production of high-quality CNTs, which have numerous applications in nanotechnology and materials science.	Focusing on CNT length prediction may limit applicability to other CNT production aspects or different nanomaterials.	Testing models under dynamic conditions, like varying temperatures and gas flow rates, would better reveal their capabilities.
	The detailed analysis of various process parameters provides valuable insights into the factors that influence CNT growth, aiding in process control and optimization.	The article could benefit from more extensive experimental validation to confirm the accuracy and robustness of the predictive models under various conditions.	Simplifying computational models while maintaining accuracy would make them more accessible for industrial use.
Classification of States and Model Order Reduction of Large Scale	The combination of POD and ANN for MOR in CVD processes is a novel approach.	Integrating POD, ANN, and SVM requires significant machine learning and	Extending the approach to various CVD processes and reactors would enhance its

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		computational modeling expertise.	generalizability and applicability.
Chemical Vapor Deposition Processes with Solution Multiplicity [120]	The study tackles the challenge of simulating large-scale, computationally intensive CVD processes due to nonlinearity and multiple solutions.	While the study presents a robust theoretical framework, the validation of the reduced-order models could be more extensive.	Testing reduced-order models under dynamic conditions, like transient temperature and pressure changes, would improve understanding of their robustness.
	The article provides a detailed methodology, including the classification of states using Support Vector Machine (SVM) algorithms and the subsequent development of reduced-order models.	Focusing on CVD processes with solution multiplicity may limit applicability to other chemical processes.	More extensive experimental validation would strengthen the models' credibility and demonstrate practical relevance.

5. Combined Heat and Mass Transfer Modeling

The complex modeling of heat and mass transfer in the CVD process is essential for optimizing the deposition process, ensuring high-quality film production, and achieving economic and environmental benefits. By leveraging advanced modeling techniques, researchers and engineers can design more efficient and effective CVD systems, leading to advancements in semiconductor technology and other fields that rely on high-quality thin films.

The coupling of heat and mass transfer in CVD processes is crucial because the temperature distribution affects the reaction rates, which in turn influence the concentration fields. Additionally, the exothermic or endothermic nature of the reactions can significantly alter the temperature field. The coupled equations can be solved using numerical methods such as finite difference, finite element, or finite volume methods.

5.1. Coupled Heat and Mass Transfer Equations

Kuvyrkin et al. construct a mathematical model describing the CVD process on a curvilinear plate. The model accounts for convective heat transfer, radiative heat transfer, and mass transfer during substance attachment to the surface. A numerical algorithm is proposed to find the temperature profile over time, with results and analysis provided for different materials. This model helps in understanding and optimizing deposition on complex geometries [121].

Lukashov et al. propose an analytical model for the growth of thermal barrier coatings during Metal-Organic Chemical Vapor Deposition (MOCVD). The model considers the coating deposition process as independent global reactions of diffusion combustion under convection conditions on a permeable surface. The rate of coating growth and precursor efficiency are analytically evaluated, and the model's accuracy is confirmed through comparison with experimental data [99].

An et al. investigate the heat and mass transfer performance in a three-dimensional bell-shaped polysilicon CVD reactor. They analyze the distributions of velocity, temperature, and concentrations of key components, as well as the silicon deposition rate. The study finds that higher inlet velocities lead to more uniform distributions and better deposition performance, providing insights for reactor design optimization [122].

Reznik et al. perform physical and mathematical simulations of SiC deposition in a porous carbon–carbon composite material. The results of parametric calculations of heat and mass transfer at macro- and microlevels are presented, analyzing the compaction of pore space by a SiC matrix depending on reaction medium parameters [123].

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Wejrzanowski et al. study the relationship between heat and mass transfer in a hot wall CVD reactor and the epitaxial growth of SiC. The research focuses on achieving homogeneous film thickness by modeling heat and mass transfer distributions during the epitaxial growth process, providing valuable insights for reactor design and optimization [40].

Raji and Sobhan develop a mathematical model for CNT synthesis through catalytic CVD. They use COMSOL software to solve the governing equations for momentum, energy, and mass transport, providing insights for optimal furnace design [124].

Lisik et al. provide a numerical model of a CVD reactor validated against experimental data, focusing on heat and mass transfer [54].

Table 10 presents a summary of various aspects of selected articles in the field of application of the coupled heat and mass transfer equations.

Table 10. Analysis of selected articles in the field of use the coupled heat and mass transfer equations.

Title	Advantages	Disadvantages	Gaps and Limitations
Analytical Model of the Process of Thermal Barrier Coating by the MO CVD Method [99]	The study provides a detailed analytical model that describes the complex interactions and reactions during the MO CVD process.	The study focuses specifically on 7-8% Yttria-Stabilized Zirconia coatings. While this is a common material for TBCs, the findings may not be directly applicable to other materials or coating systems without further modification and validation.	Including other TBC materials would enhance the model's generalizability.
	The model's predictions of growth rate and precursor efficiency are valuable for industry.	The model assumes independent global reactions, which may not fully capture the complexity of interactions in the CVD process.	Testing under dynamic conditions, like varying temperatures and gas flow rates, would better reveal the model's capabilities and limitations.
	Validation against experimental data enhances the model's credibility and relevance.	Large-scale industrial use may require significant computational resources and expertise, limiting accessibility for smaller manufacturers.	Simplifying the model while maintaining accuracy would make it more practical and accessible for broader industry use.
Mathematical Modeling of Chemical Vapor Deposition of Material on a Curvilinear Surface [121]	The focus on curvilinear surfaces in CVD processes is innovative, addressing a significant gap in existing research which predominantly focuses on flat surfaces.	The model and numerical methods are computationally intensive.	Including various curvilinear geometries would enhance the model's generalizability and insights.
	Incorporating various heat and mass transfer mechanisms enhances the model's robustness.	The study is tailored to specific curvilinear geometries, which might limit the generalizability of the findings to other	Testing under dynamic conditions like varying temperatures and deposition rates would

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		shapes and configurations.	better evaluate the model's capabilities.
	The numerical algorithm validates the theoretical model, ensuring feasible and accurate solutions.	The study provides limited experimental validation.	Simplifying the model while maintaining accuracy would make it more practical for industrial applications.
Heat and Mass Transfer Characteristics of Three-Dimensional Bell-Shaped Polysilicon Chemical Vapor Deposition Reactor [122]	The bell-shaped reactor design represents an innovative approach to addressing non-uniform deposition issues commonly encountered in traditional reactor designs.	Detailed CFD simulations require significant computational resources, limiting practicality for some organizations.	Expanding the study to include other semiconductor materials would enhance the generalizability of the findings and provide a broader understanding of the reactor's capabilities.
	The use of CFD simulations allows for a comprehensive analysis of heat and mass transfer phenomena, providing insights that are difficult to obtain through experimental methods alone.	Focusing on polysilicon deposition may limit the findings' applicability to other materials or processes.	Testing the reactor under varying conditions like fluctuating temperatures and gas flow rates would better assess its practical applicability.
	Findings can optimize reactor parameters, enhancing deposition uniformity and efficiency for high-quality polysilicon production.	The study lacks extensive experimental validation to confirm the simulations' accuracy and reliability.	Exploring scalability for industrial production would ensure practical implementation in large-scale manufacturing.
Heat and Mass Transfer in the Chemical Vapor Deposition of Silicon Carbide in a Porous Carbon–Carbon Composite Material for a Heat Shield [123]	The use of both physical and mathematical simulations provides a thorough analysis of the heat and mass transfer phenomena occurring during the CVD process.	The simulations are resource-intensive, requiring significant expertise.	Including different materials and CVD processes would enhance the findings' generalizability and provide broader insights.
	By focusing on the deposition of SiC into carbon–carbon composites, the study addresses a critical area in the development of high-performance materials for aerospace applications.	Focusing on SiC and carbon-carbon composites may limit the findings' applicability to other materials or processes.	Testing the CVD process under varying temperature and pressure profiles would better assess its capabilities and limitations.
	The article examines parameters like temperature distribution,	The study offers robust theoretical insights but	Studying the long-term stability and performance of the deposited SiC

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	gas flow rates, and deposition rates in detail.	limited experimental validation.	coatings under different environmental conditions would provide valuable insights into their practical applications and durability.
A Computational Model for Predicting the Mass Transport in a CVD Reactor for Carbon Nanotube Synthesis [124]	The study integrates gas flow, diffusion, and reaction kinetics affecting mass transport.	The model's complexity necessitates significant computational resources, which may limit its accessibility for real-time process control or smaller research facilities.	Including different materials and reaction conditions would enhance the model's generalizability and usefulness across CVD processes.
	Incorporating detailed interactions improves prediction accuracy for CNT growth rates and uniformity, crucial for industrial applications.	Applying the model to other materials or CVD processes would need major modifications and further validation.	Testing under varying temperatures and pressure profiles would better evaluate the model's capabilities.
	The findings can optimize CVD processes in the semiconductor industry, enhancing efficiency and cost-effectiveness of CNT production.	The study would benefit from more extensive experimental validation to ensure the model's predictions align with real-world data, enhancing its reliability and practical applicability.	Optimizing computational efficiency would make the model more practical for routine industrial use.

5.2. Phase Change Phenomena

Leone et al. perform kinetic calculations of the chemical phenomena during the epitaxial growth of silicon carbide. The study focuses on the effects of precursor types and growth temperatures on the deposition process, considering gas-phase reactions and phase changes [125].

Geiser and Arab develop a four-phase model for CVD processes, incorporating phase changes and transport phenomena to optimize the deposition of metallic bipolar plates [126].

Jamshidi et al. use thermodynamic equilibrium calculations to model gas-phase species in a thermal plasma CVD reactor, considering ionic species and phase changes during polycrystalline diamond deposition [127].

Vignoles provides a comprehensive review of modeling techniques for chemical vapor infiltration (CVI), including phase change phenomena, for the preparation of fiber-reinforced composites [128].

Fashu et al. use a phase-field (PF) model to investigate the growth morphology of two-dimensional (2D) materials during CVD. The model, based on Burton-Cabrera-Frank (BCF) crystal growth theory, explores the effects of substrate temperature and concentration of absorbed atoms on the substrate. The results demonstrate that the rich morphology of 2D islands in CVD growth can be reproduced, showing transitions from dendritic to compact shapes with increasing substrate temperature [129].

In a review article, Sabzi et al. discuss the factors influencing CVD system design, including substrate geometry, temperature, chemical composition, and deposition processes. The paper highlights the role of phase change phenomena, such as surface reaction kinetics, diffusion, and

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desorption, in determining the deposition rate and microstructure of ceramic coatings during CVD processes [130].

Table 11 presents a summary of various aspects of selected articles related to phase change phenomena.

Table 11. Analysis of selected articles in the field of phase change phenomena.

Title	Advantages	Disadvantages	Gaps and Limitations
Gas-Phase Modeling of Chlorine-Based Chemical Vapor Deposition of Silicon Carbide [125]	The study details gas-phase reactions, crucial for understanding SiC CVD deposition mechanisms.	Detailed gas-phase modeling needs significant computational resources, limiting real-time application.	Including various SiC precursors and deposition conditions would enhance the findings' generalizability and offer broader CVD insights.
	Chlorine-based CVD processes produce high-quality SiC films.	Relevant for chlorine-based CVD, the findings may not directly apply to other precursors or methods without adaptation.	Testing under dynamic conditions like varying temperatures and pressures would better assess the system's capabilities and limitations.
	The insights gained from the gas-phase modeling are directly applicable to industrial CVD processes, aiding in the production of high-quality SiC layers for electronic and optoelectronic applications.	The study heavily relies on computational models.	Optimizing model computational efficiency would make them more practical for industrial use and real-time adjustments.
Simulation of Chemical Vapor Deposition: Four-Phase Model [126]	Incorporating four phases, the model provides detailed and realistic CVD process simulations for accurate predictions and optimizations.	The detailed multiphase model requires significant computational resources, which may limit its practical applicability, especially for real-time process control.	Including various materials and CVD processes would enhance the model's generalizability and industrial applicability.
	Considering gas flow dynamics, plasma interactions, and reaction kinetics, the model offers a holistic CVD process view.	Tailored to specific CVD processes, the model may not generalize well to other deposition processes or materials.	Testing under varying temperatures and pressures would better assess the model's capabilities.
	This detailed framework optimizes process parameters, enhancing efficiency and layer quality for industrial applications.	While the theoretical framework is robust, more extensive experimental validation would enhance the credibility and practical relevance of the findings.	Optimizing computational efficiency without sacrificing accuracy would make the model more practical for industrial use.
Thermodynamics Modeling of Gas	The study offers an in-depth thermodynamic	The complex thermodynamic models	Expanding the study to include different types of

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Phase Processes in Polycrystalline Diamond Deposition During Thermal Plasma Chemical Vapor Deposition [127]	analysis of gas-phase processes in polycrystalline diamond deposition.	may limit accessibility to non-specialists.	materials and CVD processes would enhance the generalizability of the findings.
	The models consider temperature, pressure, and chemical composition.	The study's theoretical models are robust but lack extensive experimental validation.	Testing the models under dynamic conditions like varying gas flows and temperatures would better assess their capabilities.
	The findings significantly improve polycrystalline diamond production quality and efficiency.	The focus is specifically on polycrystalline diamond deposition using thermal plasma CVD.	Optimizing CVD process parameters based on these models could improve deposition quality and efficiency.
Modeling of Chemical Vapor Infiltration Processes [128]	The article offers a comprehensive understanding of CVI processes through various modeling techniques.	The models discussed are often highly complex, requiring significant computational resources and expertise.	Expanding the discussion to include other types of chemical vapor deposition processes would enhance the generalizability of the findings.
	Detailed methodology descriptions make it a useful guide for developing and implementing CVI models.	The article is heavily focused on CVI processes for composite materials.	Testing the models under dynamic conditions like changing temperatures or pressures would better evaluate their capabilities.
	The findings and discussions are highly relevant to the practical aspects of CVI processes in industry.	While the article discusses various modeling techniques, there is less emphasis on the experimental validation of these models.	Simplifying and optimizing the models without losing accuracy would make them more accessible and practical.
Phase-field Modelling of 2D Island Growth Morphology in Chemical Vapor Deposition [129]	The PF model effectively captures the diverse island morphologies observed in 2D materials, such as dendritic, triangular, and hexagonal shapes, under different conditions.	The PF model's detailed simulations are computationally intensive, limiting real-time use and accessibility for some researchers.	Including more 2D materials would enhance the model's generalizability and usefulness in various CVD applications.
	The integration of various growth conditions, such as substrate temperature and atomic interactions at the island edges, allows for a comprehensive study of their effects on island morphology.	While insightful for 2D material growth, findings may not apply to other materials or processes without further research.	Testing under dynamic conditions like fluctuating temperatures and gas compositions would better assess the model's capabilities.

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The findings are significant for optimizing CVD processes to control the shape and size of 2D islands, which is crucial for applications in electronics and nanotechnology.	The study would benefit from more extensive experimental validation to corroborate the model's predictions with real-world data, enhancing its reliability and applicability.	Optimizing to reduce computational demands while maintaining accuracy would make the model more practical for industrial use.

5.3. Surface Reaction Kinetics

Jansen discusses the processes involved in modeling surface reactions in CVD, including the use of lattice models to represent adsorption sites and defects. The study also covers the implementation of processes and the importance of reducing noise in kinetic Monte Carlo simulations [131].

Badran and Shi investigate the decomposition kinetics of 1-methylsilacyclobutane (MSCB) in a hot wire CVD reactor. Using vacuum ultraviolet laser single photon ionization and time-of-flight mass spectrometry, they determine the rate constants and activation energies for different decomposition pathways, highlighting the catalytic role of the tungsten filament in the reactor [132].

Reinke characterizes the surface kinetics of titanium isopropoxide (TTIP) and water in HV-CVD, deriving activation energies for desorption, hydrolysis, and pyrolysis, and demonstrating the deposition of epitaxial barium titanate films at a low temperature of 400°C [133].

Reinke further investigates the surface reaction kinetics of TTIP in high vacuum CVD of titanium dioxide, providing quantitative predictions of precursor impinging rates and examining the activation energies of surface reaction steps [134].

Song et al. propose surface kinetic mechanisms for the epitaxial growth of SiC using methyltrichlorosilane (MTS) in a hydrogen environment, discussing the components of surface species and growth rates under different mechanisms [135].

Sabzi et al. discuss the factors influencing CVD system design, focusing on surface reaction kinetics, diffusion, and desorption reactions [130].

Muneshwar and Cadien present a first-order kinetic model for atomic layer deposition (ALD) reactions, simulating the effects of precursor exposure, post-precursor purge, reactant exposure, and substrate temperature on growth per cycle [136].

Konar and Nessim, in a mini-review, focus on the synthesis of transition metal selenides using ambient-pressure CVD, emphasizing their application in energy storage and the influence of surface morphology on reaction kinetics [137].

Yuesong Xiang et al. investigates the controlled synthesis of 2D magnetite nanosheets using CVD, emphasizing the importance of surface reaction kinetics in their formation [138].

Tomasini details the role of surface energy and activation energy in determining the reaction kinetics in CVD processes, focusing on molecular hydrogen dissociative adsorption and precursor thermal decomposition [139].

Zhao et al. discuss the tuning of crystal dimensions through growth temperature and hydrogen concentration, linked to surface reaction and mass transport mechanisms [140].

Table 11 presents a summary of various aspects of selected articles related to surface reaction kinetics.

Table 12. Analysis of selected articles in the field of surface reaction kinetics.

Title	Advantages	Disadvantages	Gaps and Limitations
Surface Kinetics of Titanium Isopropoxide in High Vacuum Chemical	The authors developed a surface kinetic model for TTIP and water, including first- and second-order reactions.	The kinetic model and simulations are computationally intensive, needing significant resources.	Including different CVD processes and precursors would enhance the findings' generalizability.

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Vapor Deposition [134]	The study uses 363 data points across various deposition parameters, like substrate temperature and precursor rates.	The study focuses specifically on the HV-CVD process using TTIP and water.	Testing under varying precursor concentrations and temperatures would better assess the model's capabilities.
	The findings have significant practical relevance for optimizing HV-CVD processes in the semiconductor and thin-film industries.	Although the model is validated against a substantial dataset, the study could benefit from additional experimental validation under various conditions to further confirm the robustness and accuracy of the model.	Optimizing computational efficiency would make the kinetic model more accessible for industrial use.
Surface Kinetic Mechanisms of Epitaxial Chemical Vapour Deposition of 4H Silicon Carbide Growth by Methyltrichlorosilane-H_2 Gaseous System [135]	The article provides an in-depth analysis of the kinetic mechanisms at play during the CVD process. By dissecting both gas-phase and surface reactions, it offers a granular understanding of the factors influencing SiC growth, which is crucial for optimizing deposition conditions.	The complexity of the reactions and the detailed kinetic modeling may pose challenges for readers who are not well-versed in chemical kinetics and CVD processes.	Including various precursors and carrier gases would broaden understanding of the CVD process for SiC and other materials.
	Focusing on the efficient MTS-H_2 system, it highlights chlorine's role in enhancing deposition rates and film quality.	While the study is thorough in its theoretical analysis, it could benefit from more extensive experimental validation.	Testing dynamic conditions like varying temperatures and gas flow rates would better evaluate kinetic mechanisms and their impact.
	The insights gained from this study can directly impact the semiconductor industry, particularly in the production of high-quality SiC epitaxial layers.	Focusing on the MTS-H_2 system may limit applicability to other precursor systems or deposition processes.	Examining long-term stability and performance of SiC layers under different conditions would provide insights into their practical applications in high-stress environments like power electronics and aerospace.
A Review on Sustainable Manufacturing of Ceramic-Based Thin Films by Chemical	The review comprehensively covers CVD aspects like reaction kinetics, deposition mechanisms, and	The detailed discussion on reaction kinetics and deposition mechanisms might be complex for readers without a strong	Extending the research to include other types of materials and their respective CVD processes would provide a more

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Vapor Deposition (CVD): Reactions Kinetics and the Deposition Mechanisms [130]	parameter effects on ceramic thin film quality and efficiency.	background in chemical engineering or materials science.	holistic view and increase the applicability of the findings across different industries.
	Emphasizing sustainable practices, the article discusses optimizing CVD to reduce waste and energy use.	While the review is comprehensive, it could benefit from more extensive experimental data to validate the theoretical aspects discussed.	Investigating how temperature, pressure, and precursor flow rates affect CVD could optimize the process under various conditions.
	The article provides detailed insights into the methodological aspects of CVD, making it a valuable resource for researchers and practitioners aiming to improve the efficiency and sustainability of their processes.	The focus on ceramic-based thin films may limit the applicability of the findings to other materials.	A lifecycle analysis of the CVD process would offer a complete view of its sustainability.
	The use of CVD for synthesizing high-quality Fe3O4 nanosheets is a significant advancement, offering a controlled and scalable method for producing two-dimensional materials with desirable properties.	The study emphasizes Fe3O4 nanosheet synthesis and initial characterization, less on practical device integration.	Investigating nanosheet stability under various conditions would provide insights into durability and reliability.
Chemical Vapor Deposition of Two-Dimensional Magnetite Nanosheets and Raman Study of Heat-Induced Oxidation Reaction [138]	The combination of Raman spectroscopy, X-ray diffraction, and atomic force microscopy provides a thorough characterization of the nanosheets, ensuring a detailed understanding of their structural and chemical properties.	While the study details the oxidation process, it could benefit from a deeper exploration of the conditions affecting the oxidation rate and the stability of the resulting α-Fe2O3 phase.	Exploring dynamic CVD conditions like varying gas compositions and flow rates would deepen understanding of synthesis parameters.
	The findings have potential applications in spintronic devices and other advanced technologies, where the magnetic properties of these nanosheets could be exploited.	Challenges and optimizations for large-scale CVD nanosheet production are not extensively addressed.	Functional testing in device applications would enhance the study's practical relevance and showcase real-world potential.
Chemical Vapor Deposition of	The study offers a thorough examination of	Focusing on elemental crystallogens may limit	Including a wider range of materials would

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Elemental Crystallogen Thin Films [139]	CVD techniques, providing detailed insights into reaction kinetics, deposition mechanisms, and the influence of various process parameters.	generalizability to other CVD materials.	enhance the findings' generalizability and applicability across CVD processes.
	Focusing on elemental crystallogens, it addresses crucial materials for semiconductor and microelectronics industries.	While the study is detailed, more extensive experimental validation under varying conditions would strengthen the reliability of the results.	Testing under varying temperatures and pressures would provide a comprehensive understanding of the deposition process.
	The article outlines strategies for optimizing CVD conditions to enhance film quality, valuable for manufacturing applications.	Optimization strategies may need sophisticated equipment and precise control, challenging in large-scale production.	Studying long-term stability and performance under operational conditions would offer valuable insights for practical applications.

6. Challenges and Opportunities in CVD Modeling Including Heat and Mass Transfer Aspects

Recently, various articles have discussed the challenges and limitations in chemical vapor deposition (CVD) modeling, as well as future directions and opportunities.

Filho et al. describe the modeling challenges in scaling up AACVD processes, including the prediction of aerosol behavior, heat and mass transfer coefficients, and reaction rate constants under uncertainty [141].

Lee et al. discuss technical challenges in MOCVD growth of 2D materials, emphasizing the need for control over nucleation and growth stages to enable practical applications [142].

Jiang et al. highlight recent advances and challenges in the CVD growth of 2D vertical heterostructures, focusing on controllable synthesis, growth temperature, precursor design, and substrate engineering [143].

Dong et al. present a theoretical framework for 2D material CVD synthesis, discussing challenges and opportunities in exploring CVD mechanisms to better understand 2D material synthesis [144].

Qun Wang et al. focus on challenges in the controllable CVD fabrication of high-quality TMD films, emphasizing the importance of controlling precursor concentration, nucleation density, and oriented growth [145].

Heat and mass transfer modeling for CVD processes presents both challenges and opportunities. Considering the challenges, the following points can be noted:

- Modeling heat and mass transfer for CVD processes requires addressing complex interactions between different phases (gas and solid), necessitating advanced modeling techniques and considerable computational resources.
- Achieving accurate modeling of flow fields is essential but challenging, as it requires accounting for heat transfer contributions from multiple phases.
- The significant computational demands of accurate simulations present a major challenge, requiring the use of advanced hardware and optimization techniques, such as GPU acceleration.
- Ensuring the accuracy and applicability of numerical models is challenging and necessitates extensive validation against experimental data, which can be resource-intensive. Without proper validation, the predictive power of these models is limited.

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- Incorporating advanced techniques such as fuzzy logic and artificial intelligence into CVD modeling can improve predictive capabilities. However, these methods require sophisticated implementation and validation, posing additional challenges.

Considering the opportunities, the following points can be noted:

- Advanced simulation tools such as CFD facilitate the creation and validation of numerical models without requiring physical prototypes, potentially streamlining the design process and lowering costs.
- CFD and other advanced modeling techniques provide significant opportunities for optimizing the design and performance of heat exchangers, which are crucial components in CVD processes.
- Methods such as fuzzy logic-based models can effectively predict heat transfer coefficients, offering valuable tools for optimizing industrial processes and enhancing model accuracy.
- Incorporating AI and machine learning into CVD modeling enhances predictive capabilities and optimizes process parameters by uncovering patterns not evident through traditional methods.
- Real-time monitoring and control in CVD processes ensure optimal conditions, enhancing product quality and reducing material waste.
- Collaboration among material science, engineering, and computer science researchers can create more accurate CVD models, addressing the complex challenges of these processes.
- Using dimpled surfaces can enhance heat transfer and reduce flow resistance, making CVD processes more efficient.

Considering the opportunities, it is worth focusing on parallel programming, which can significantly advance the modeling of CVD processes by providing the computational power necessary to tackle these systems' inherent complexities. By enabling high-resolution, real-time, and scalable simulations, parallel programming enhances our ability to optimize and control CVD processes, paving the way for innovations in materials science and manufacturing. The potential roles and benefits include:

- CVD processes involve multiscale phenomena, and parallel programming efficiently simulates these models by distributing tasks across multiple processors, allowing simultaneous solving of molecular dynamics and continuum mechanics equations.
- CVD processes often involve solving large PDE systems for heat, mass, and momentum transfer. Parallel programming reduces computation time by dividing the domain into sub-domains and solving them concurrently, which is crucial for real-time process optimization and control.
- Parallel programming distributes computational demands, enabling high-resolution simulations to capture detailed CVD process features like intricate temperature gradients and concentration profiles.
- Conducting parametric studies on CVD outcomes is computationally intensive. Parallel programming allows simultaneous simulations with different parameters, drastically reducing time and crucially optimizing process parameters and product quality.
- In advanced manufacturing, real-time control and monitoring of CVD processes are vital. Parallel computing enables real-time simulations and adjustments, ensuring the process stays within desired parameters and reduces defects.
- As CVD models grow in complexity and size, scaling simulations across multiple processors is crucial. Parallel programming provides the scalability to handle larger models without exponentially increasing computation time.
- CVD processes often involve coupled phenomena, like fluid flow and chemical reactions. Parallel programming allows simultaneous solving of these models, ensuring more accurate and realistic simulations.

Parallel programming can model the deposition of advanced materials, requiring detailed simulations of multicomponent systems. High-fidelity simulations optimize reactor design for better uniformity and efficiency in thin-film deposition. Combining parallel computing with machine

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learning enhances predictive modeling, enabling faster convergence to optimal conditions and more robust control strategies.

7. Conclusions

This review has provided an overview of recent advancements in heat and mass transfer modeling for Chemical Vapor Deposition (CVD) processes. Through a comprehensive analysis of literature published over the past decade, several key findings and trends have emerged.

Firstly, significant progress has been made in developing sophisticated computational models that accurately capture the complex interplay of thermal, fluid, and chemical phenomena inherent in CVD processes. These models range from continuum-based approaches such as finite element analysis and computational fluid dynamics to atomistic methods like molecular dynamics and kinetic Monte Carlo simulations. Each approach offers unique insights into different length and time scales, enabling a deeper understanding of the fundamental mechanisms governing heat and mass transport.

Furthermore, advancements in numerical techniques, parallel computing, and high-performance computing have enabled the simulation of increasingly complex CVD systems with greater accuracy and efficiency. Coupled with experimental studies, these models have facilitated the optimization of process parameters, the prediction of deposition rates and film properties, and the exploration of novel materials and processes.

However, several challenges remain. The integration of experimental data with computational models continues to pose difficulties, particularly in reconciling discrepancies in spatial and temporal resolutions and ensuring the quality and consistency of experimental validation data. Additionally, the complexity of multiphysics interactions and the sheer scale of parameter spaces in CVD present ongoing challenges for model development and validation.

Looking ahead, future research directions should focus on addressing these challenges through interdisciplinary collaborations, advanced experimental techniques, and the continued development of computational methodologies. By leveraging emerging technologies such as machine learning, data assimilation, and in-situ monitoring, researchers can enhance the predictive capabilities of CVD models and further accelerate innovation in materials science and engineering.

8. Future Directions

Taking into account future directions of activities, a review article is planned that will provide a comprehensive overview of the current state and future potential of Chemical Vapor Deposition (CVD) modeling. It will include recent advancements in CVD modeling techniques, focusing on advanced computational methods that improve simulation precision and efficiency, the integration of detailed surface chemistry for better prediction accuracy, recent developments in real-time monitoring and control strategies, and high-throughput computational methods for process optimization. The practical applications of advanced CVD modeling will be demonstrated across various fields, including semiconductor device fabrication, thin film coatings for energy applications, advanced materials synthesis, and emerging nanotechnology applications. The paper will also address current challenges and limitations in CVD modeling, such as complex reaction mechanisms, high computational costs, lack of experimental validation, and the need for realistic boundary conditions. Finally, it will outline future directions and opportunities, highlighting the integration of computational models with experimental techniques, the development of predictive models, advancements in multi-scale modeling, and the application of artificial intelligence and machine learning to optimize CVD processes and accelerate material discovery.

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