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Review

Pioneering the Future: A Trailblazing Review of the Fusion of Computational Fluid Dynamics and Machine Learning Revolutionizing Plasma Catalysis and Non-Thermal Plasma Reactor Design

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Abstract: The advancement of plasma technology is intricately linked with the utilization of computational fluid dynamics (CFD) models, which play a pivotal role in the design and optimization of industrial-scale plasma reactors. This comprehensive compilation encapsulates the evolving landscape of plasma reactor design, encompassing fluid dynamics, chemical kinetics, heat transfer, and radiation energy. By employing diverse tools such as FLUENT, Python, MATLAB, and Abaqus, CFD techniques unravel the complexities of turbulence, multiphase flow, and species transport. The spectrum of plasma behavior equations, including ion and electron densities, electric fields, and recombination reactions, is presented in a holistic manner. The modeling of non-thermal plasma reactors, underpinned by precise mathematical formulations and computational strategies, is further empowered by the integration of machine learning algorithms for predictive modeling and optimization. From biomass gasification to intricate chemical reactions, this work underscores the versatile potential of plasma hybrid modeling in reshaping various industrial processes. Within the sphere of plasma catalysis, modeling and simulation methodologies have paved the way for transformative progress. Encompassing reactor configurations, kinetic pathways, hydrogen production, waste valorization, and beyond, this compilation offers a panoramic view of the multifaceted dimensions of plasma catalysis. Microkinetic modeling and catalyst design emerge as focal points for optimizing CO_2 conversion, while the intricate interplay between plasma and catalysts illuminates insights into ammonia synthesis, methane reforming, and hydrocarbon conversion. Leveraging neural networks and advanced modeling techniques enables predictive prowess in the optimization of plasma-catalytic processes. The integration of plasma and catalysts for diverse applications, from waste valorization to syngas production and direct CO_2/CH_4 conversion, exemplifies the wide-reaching potential of plasma catalysis in sustainable practices. Ultimately, this anthology underscores the transformative influence of modeling and simulation in shaping the forefront of plasma-catalytic processes, fostering innovation and sustainable applications.

Keywords: plasma; non-thermal plasma reactors; plasma catalysis

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1. Introduction

Recent developments in terms of building sustainable energy systems have led to a significant increase in the installed power of intermittent renewable energy sources (solar and wind). This has led to a mismatch between supply and demand. Therefore, notable effort has recently been directed to improving the flexibility of power systems, which includes both increasing the flexibility of controllable power sources [1,2] and demand-side management. Capacity markets have been created in recent years in many countries, including the Scandinavian countries [3,4], Great Britain [5,6], and Poland [7]. The flexibility of power units can be increased through the use of plasma to support combustion in power plant boilers [8–10]. However, an equally good measure to improve the flexibility and uptake of energy systems is increasing demand relative to supply from intermittent sources, which is called demand-side management. Within demand-side management, technologies called power-to-X are of particular interest [11,12] since they are capable of utilizing excess electricity during low-demand periods and converting it to marketable products. The X in power-to-X stands for a product, and it could indicate hydrogen (PtH) [12], methanol (PtM) [12], or ammonia (PtA) [12]. The advantage of this approach is not only that it results in a new product produced by using electricity purchased at a marginal price but also that it avoids the curtailment of intermittent renewable energy sources at a time of high supply and low demand. In the long-term, changing the energy grid in this direction will result in higher shares of renewable energy in the power mix. In recent years, increased interest has been shown in the application of plasma for hydrogen production [13,14], the catalytic synthesis of ammonia [15–18], the methanation of CO_2 to synthetic natural gas [19,20], the conversion of CO_2 to alcohols [21], and the production of nanomaterials [22], to name but a few applications. Since plasma is typically characterized by its fast startup [23–26], plasma-based technologies are of particular interest with respect to their increased use in the demand-side management of power systems. Achieving this requires industrial-scale power-to-X plasma solutions [11].

Non-thermal plasma (NTP), which is in a non-equilibrium state with different temperatures of electrons, ions, and neutrons [27], has been proven effective in many different applications. Clothiaux, Koropchak, and Moore demonstrated the possibility of the decomposition of the vapor of phosphonofluoridic acid methyl-l,2,2-trimethylpropyl ester using a silent discharge plasma [28]. Dobslaw et al. [29] confirmed the feasibility of using non-thermal plasma for the removal of volatile organic compounds and odor abatement in organic waste treatment plants. In another work, Dobslaw et al. [30] showed a synergy between a non-thermal plasma (dielectric barrier discharge) and the subsequent biotrickling filter. Andersen et al. [31] proved that NTP systems could be effectively used for the abatement of odor nuisances. NTP could also be applied for water purification [32] as well as for disinfection and sterilization purposes [32,33]. Apart from decontamination, NTP can also be effectively used in wastewater treatment plants [34], providing a feasible means of dealing with hazardous chemicals [35]. Moreover, Kvam et al. [36] reported that NTP is capable of inducing damage to the cell surface, which is critical in terms of medical applications, such as disinfection of air to remove multidrug-resistant microbes. Dobslaw and Glocker [37] reported the 100% degradation of CF_4-contaminated air at an industrial scale using NTP. Helbich et al. [38] demonstrated the successful use of NTP for the treatment of emissions of styrene and secondary emissions of germs formed through biological processes, with the efficiencies of removal of volatile organic compounds, germs, and styrene ranging between 96 and 98%. Byeon et al. [39] investigated the removal of gaseous toluene and submicron aerosol particles using a dielectric barrier discharge reactor and reported toluene removal efficiencies ranging between 29% and 46%, depending on the applied voltage, frequency, upstream toluene concentration, and residence time. Nonetheless, caution is needed in such applications since the conversion of toluene in NTP could generate heavy aromatic byproducts, such as phenylethyne, indene, naphthalene, and acenaphthylene, as shown by Wnukowski and Moroń for microwave plasma [40]. NTP plasma has been used for various applications related to gasification technologies,

especially concerning gasification of waste [41] and removal of tars from producer gas [42], which is critical from the point of view of the maintenance and uninterrupted operation of gasifiers [43,44]. Wnukowski et al. [45] reported tar conversion efficiencies ranging between 19 and 100% for atmospheric microwave plasma processing of producer gas from gasification of sewage sludge. Kwon and Im [46] investigated the feasibility of non-thermal plasma gasification for a waste-to-energy power plant with an integrated plasma gasification combined cycle. Performed exergy analysis has shown that in such systems, the plasma gasification unit is the one that contributes the most to the total exergy loss [46]. Since plasma reactors exert such a profound effect on the overall systemic energetic and exergetic efficiency, it is crucial to have the right toolset for efficient design of such reactors.

The march of industrial-scale plasma reactors into new frontiers hinges upon the seamless integration of intricate computational fluid dynamics (CFD) models, which have emerged as indispensable tools for augmenting reactor design and optimization [47,48]. Within the multifaceted arena of plasma generation and its manifold applications, a confluence of variables forms, encapsulating the intricacies of fluid dynamics, chemical kinetics, heat transfer, and radiation energy [49,50]. This introduction serves as a beacon, illuminating the profound significance of computational simulations in decoding the labyrinthine physical and chemical orchestration within plasma reactors. Esteemed software frameworks, including FLUENT, Python, MATLAB, and Abaqus, serve as the very scaffold upon which intricate numerical fluid models are woven, facilitating meticulous scrutiny of phenomena as diverse as turbulence, multiphase flow, and the intricate migration of species. Researchers, through relentless inquiry, unveil the pivotal role of microkinetic modeling and the optimization of catalysts in propelling the engines of efficient CO_2 conversion [51,52].

Against this backdrop, modeling methodologies, such as the intricate weave of neural networks, emerge as indispensable allies, forecasting and refining the efficacy of plasma-catalytic endeavors. The fusion of plasma and catalysts to birth novel valorization pathways, orchestrate syngas symphonies, and affect the metamorphosis of CO_2 and CH_4 stands as a testament to the diverse potential of plasma catalysis within the annals of sustainable practices.

The aim of this review is to summarize the works on modeling plasma and its various chemical engineering applications, thus providing an overview of the approaches used for modeling catalytic plasma processes.

2. Modeling and Simulation in Plasma Catalysis: Insights, Strategies, and Applications

Recent investigations underscore the pivotal significance of modeling and simulation in propelling the frontier of plasma catalysis research. Numerous scholarly articles delve into the application of fluid models within the realm of plasma catalysis, meticulously emphasizing their indispensable role in elucidating phenomena such as streamer propagation, plasma dynamics, and the intricate interplay between plasma and catalyst [53–55]. Strategically optimizing plasma parameters and adeptly managing the fluxes of reactive species stand out as pivotal facets in the realm of plasma catalysis. Research endeavors leverage sophisticated modeling techniques to scrutinize and proffer strategic approaches for fine-tuning reactive species within plasma catalytic systems [56,57].

Innovatively navigating the landscape of modeling approaches, this review meticulously unveils a transformative realm within the artificial neural network (ANN) models and microfluidic chip-based plasma flow chemistry techniques. Beyond conventional bounds, it delves into cutting-edge investigations on surface-induced effects and plasma-catalytic methane reforming. Employing sophisticated fluid modeling techniques, these dedicated inquiries yield profound insights into the intricate dynamics of gas-phase redistribution effects and the nuanced influence exerted by catalyst surfaces. Cumulatively, this scholarly synthesis accentuates the novel contributions that transcend traditional boundaries, underscoring the paramount significance of modeling and simulation. Specifically harnessed through fluid models, this research not only unravels the intricacies of plasma

behavior but also steers the precise control of reactive species, presenting a pioneering blueprint for fine-tuning plasma-catalytic reactors across diverse applications within the expansive domain of plasma catalysis [58–61].

2.1. Exploring Modeling and Simulation in Plasma Catalysis for Ammonia Synthesis: Insights and Innovations

Research in plasma catalysis for ammonia synthesis has been heavily influenced by various modeling and simulation techniques, which have played a vital role in gaining insights and optimizing the process. A significant portion of the literature focuses on microkinetic modeling and fluid dynamics, seeking to explore the contributions of Eley–Rideal reactions in ammonia synthesis under plasma conditions [62–64]. Moreover, researchers have combined kinetic modeling with experimental studies in dielectric barrier discharge reactors to better understand the intricate reaction mechanisms [64,65].

Another key area of research in plasma-catalytic ammonia synthesis is the investigation of plasma effects and reaction mechanisms. Studies have delved into the influence of the material dielectric constant on plasma generation within catalyst pores, revealing important considerations for plasma–catalyst interactions [55]. Additionally, the enhancement of reaction rates beyond the thermodynamic equilibrium in plasma-catalyzed ammonia synthesis has been studied, opening up new possibilities for more efficient ammonia production [66].

Furthermore, researchers have explored the direct conversion of CO_2 and CH_4 into liquid chemicals using plasma catalysis. Experimental studies and simulations have shown promising results in converting CO_2 and CH_4 into valuable products [67]. Meanwhile, other works have emphasized the importance of modeling plasma chemistry and reactor design to optimize the efficiency of CO_2 conversion through plasma catalysis [68].

In the realm of modeling techniques, artificial neural networks (ANNs) and deep learning have been harnessed to enhance plasma catalysis. ANNs have proven useful in predicting the performance of ammonia synthesis in plasma catalysis, enabling better control and optimization of the processing [69]. Similarly, deep learning techniques have been explored in modeling pulsed discharge plasma catalysis, offering novel perspectives for understanding and improving plasma-catalytic reactions [70].

The collective body of work presented in these articles showcases the indispensable significance of modeling and simulation techniques, encompassing microkinetic modeling, fluid dynamics, and artificial neural networks, in advancing plasma catalysis for ammonia synthesis. The studies shed light on plasma effects, reaction mechanisms, and the conversion of CO_2 and CH_4, offering valuable insights into the behavior of plasma-catalytic systems and their potential applications in sustainable ammonia production. As the field of plasma catalysis continues to evolve, these modeling approaches will undoubtedly play a central role in unlocking new horizons for efficient and environmentally friendly ammonia synthesis processes.

2.2. Advancing Ammonia Synthesis through Plasma Catalysis: Unveiling Insights and Innovations via Modeling and Simulation

Research in plasma catalysis has made remarkable progress in comprehending catalyst surfaces, microkinetic modeling, and reaction mechanisms. The first group of articles places emphasis on the significance of catalyst surfaces and microkinetic modeling in plasma catalysis. Wang et al. [71] investigate the role of a Ni/Al_2O_3 catalyst surface in ammonia synthesis using plasma-enhanced catalysis at near-room temperature. Their utilization of density functional theory (DFT) microkinetic modeling yields valuable insights into reaction mechanisms, highlighting the catalyst surface's importance in achieving efficient ammonia synthesis. Sun et al. [72] explore plasma-catalytic nitrogen fixation and its correlation with catalyst microanalysis. Through chemical kinetics modeling, they gain valuable insights into reaction mechanisms and performance, focusing on the role of a TiO2@5% GO catalyst.

The second group of articles delves into the complexities of plasma-catalytic reactions, with a particular focus on plasma characteristics and their influence on reaction mechanisms.

Rouwenhorst et al. [73] discuss the use of plasma-driven catalysis for green ammonia synthesis using intermittent electricity. The study explores the intricate nature of plasma-catalytic reactions, their effects on plasma characteristics, and flow patterns, contributing to the development of sustainable ammonia synthesis methods. Loenders et al. [74] present a microkinetic model for the partial oxidation of methane on Pt (111) surfaces under plasma catalysis. By investigating the influence of different plasma species on reaction kinetics and mechanisms, this study deepens our understanding of plasma-catalytic processes.

Collectively, these articles underscore the importance of catalyst surfaces, microkinetic modeling, and the complexities of plasma-catalytic reactions in advancing the field of plasma catalysis. The application of DFT microkinetic modeling provides valuable insights into reaction mechanisms and catalyst performance, while investigations into plasma characteristics shed light on the intricacies of plasma-catalytic processes. Such research plays a critical role in optimizing plasma catalysis and expanding its applications in sustainable synthesis and chemical transformations.

2.3. Unraveling Complexities: Modeling Approaches in Advancing Plasma Catalysis Understanding and Efficiency

The advancements in plasma catalysis have been fueled by the use of modeling approaches to unravel the intricate interactions between plasma and catalysts. Zhang et al. [75] employ a 2D implicit PIC/MCC model to study plasma streamer propagation within catalyst pores, emphasizing the significance of surface charging during this process. By comparing their results with fluid modeling predictions, the study sheds light on the complexities of plasma–catalyst interactions. Similarly, Michielsen et al. [76] use model calculations to enhance our understanding of plasma catalysis, specifically CO_2 dissociation in a packed-bed DBD reactor. Their investigation of the influence of operating parameters, particularly in helium plasma, offers us a better grasp of the underlying mechanisms. Pan et al. [77] conduct numerical simulations and calculations based on global and fluid models, as well as density functional theory (DFT), to investigate nanosecond-pulsed DBD plasma-catalytic CH_4 dry reforming. Their study highlights the synergistic effects between plasma and catalysts, providing valuable insights into the reaction dynamics and efficiency of this reforming process. On the other hand, Dou et al. [78] delve into the synergistic plasma-catalytic conversion of CO_2 and CH_4 into oxygenates. By investigating the role of metallic cobalt sites and oxygen vacancies in this process and demonstrating the production of CH_3COOH through recombination in a plasma simulation, the study uncovers potential pathways for sustainable oxygenate production.

Collectively, these articles demonstrate the significance of modeling approaches in understanding plasma–catalyst interactions and specific plasma-catalytic processes. The studies shed light on the intricate mechanisms and synergistic effects that occur during plasma catalysis, paving the way for its more efficient and sustainable applications.

2.4. Exploring Mechanisms, Modeling, and Applications in the Realm of Plasma Catalysis

The field of plasma catalysis is a realm of exploration encompassing mechanisms, modeling approaches, and diverse applications. Researchers have made significant contributions to uncovering the mechanisms and developing modeling aspects of plasma catalysis. Mei et al. [79] delve into the reforming of CH_4 with CO_2 using a nanosecond-pulsed DBD plasma, shedding light on the role of the CH_4/CO_2 ratio and total flow in product distribution and the intricate interaction between reactive plasma species and catalysts. Chawdhury et al. [80] investigate a promising plasma-catalytic approach for single-step methane conversion to oxygenates at room temperature, utilizing plasma chemical kinetic modeling to highlight the catalytic facilitation of the conversion process.

Specific applications and advancements in plasma catalysis are also subjects of focused research. Van't Veer et al. [81] explore spatially and temporally non-uniform plasmas, particularly micro-discharges in a packed bed plasma reactor, to gain insights into plasma-catalytic ammonia synthesis. The study incorporates flow simulations and plasma kinetics

modeling, deepening our understanding of micro-discharges' behavior and their role in ammonia synthesis. Ong et al. [82] discuss the application of microwave plasma technology for converting CO_2 into high-value products, emphasizing fluid models and kinetic models to understand plasma behavior and highlighting the potential of microwave plasma catalysis in value-added chemical production.

Collectively, these articles contribute to the advancement of our understanding of plasma catalysis. By providing valuable insights into the underlying mechanisms, modeling techniques, and potential applications of plasma-catalytic reactions, these studies pave the way for optimizing and progressing plasma catalysis for various purposes. The investigation of specific reactions, operating parameters, and spatial–temporal characteristics adds to our knowledge base of plasma catalysis, enabling its potential implementation in sustainable and innovative chemical processes.

2.5. Exploring the Landscape of Plasma Catalysis: Models, Applications, and Challenges

The field of plasma catalysis is enriched by diverse research, encompassing models, applications, and challenges. In the realm of modeling and simulation, researchers have made significant contributions. Cheng et al. [83] present a model for nanosecond-pulsed plasma dry reforming of natural gas, incorporating flow and mixing effects. Their work sheds light on the complexities of plasma-catalytic reactions in this context. Cheng et al. [84] introduce a novel plasma synergistic catalysis model based on computational fluid dynamics (CFD), to examine CO production pathways and the influence of vibrationally excited species, providing valuable insights into reaction mechanisms under plasma conditions. Oskooei et al. [85] utilize a CFD model to simulate the plasma-assisted catalytic reduction of NOx, CO, and HC in diesel engine exhaust, contributing to our understanding of emission control technologies.

Specific applications and challenges in plasma catalysis have also been a focal point of research. Li et al. [57] investigate methane-to-methanol conversion using both heterogeneous catalysis and plasma catalysis, emphasizing continuous flow reactors and advanced simulation techniques, offering potential routes for efficient methanol production. Zhang et al. [86] delve into the formation of micro-discharges inside a mesoporous catalyst in dielectric barrier discharge (DBD) plasmas using a 2D fluid model, uncovering intricate plasma–catalyst interactions in confined spaces. Fu et al. [87] critically review viral disinfection using non-thermal plasma and discuss the potential of the plasma catalysis system, showcasing the diverse applications of plasma catalysis in different domains.

Another crucial aspect of research involves catalyst characterization and process optimization in plasma catalysis. Zhang et al. [88] explore plasma-enhanced catalytic activation of CO_2 in a modified gliding arc reactor, emphasizing the gas flow field and the need for further plasma modeling studies to optimize the process. Kaliyappan et al. [89] investigate the impact of material properties on the plasma-catalytic dissociation of CO_2 using a packed-bed DBD plasma reactor, contributing to the development of efficient catalysts for CO_2 conversion. Zhu et al. [90] study the hybrid plasma-catalytic removal of acetone over CuO/γ-Al_2O_3 catalysts using a response surface method, offering insights into optimizing the process conditions for efficient pollutant removal.

Addressing challenges in catalytic modeling within plasma environments is also a key focus. Viladegut et al. [91] discuss the characterization of catalytic processes in plasma wind tunnels and highlight discrepancies between current catalytic models used in computational fluid dynamics (CFD) and actual catalytic processes. Their work sheds light on the complexities of catalytic processes in plasma environments and highlights the need for improved modeling techniques.

Together, these articles contribute significantly to our understanding and advancement of plasma catalysis. They explore diverse modeling approaches, specific applications in different domains, and the challenges faced in catalytic modeling within plasma environments. This comprehensive research offers valuable insights that can pave the way for future advancements in the field of plasma catalysis.

2.6. Unveiling the Multifaceted Landscape of Advancements in Plasma Catalysis for Sustainable Processes

Research in the field of advancements in plasma catalysis for sustainable processes covers a wide range of topics, including modeling, insights into reactions, system advancements, and kinetic pathways. Researchers have emphasized the significance of modeling and designing plasma-catalytic systems, with a focus on microkinetic modeling and catalyst design for efficient CO_2 conversion [92]. Another area of interest is exploring energy-efficient pathways for pulsed-plasma-activated ammonia synthesis, taking into account reactor structure, plasma dynamics, and mass flow control [93]. Additionally, studies have presented microkinetic models to investigate the non-oxidative coupling of methane over specific catalysts in non-thermal plasma reactors, providing valuable insights into catalyst design for efficient plasma-catalytic processes [94].

Insights into specific plasma-catalytic reactions have been a focus of research, as well. Some articles combine experimental measurements and plasma kinetic modeling to enhance our understanding of ammonia decomposition in specific plasma environments [95]. Other studies explore the effects of specific promoters on plasma-assisted dry reforming of methane over specific catalysts [96].

Advancements in plasma-catalytic systems have been discussed in various articles. These include exploring the application of dielectric barrier discharge non-thermal plasma in the abatement of volatile organic compounds (VOCs), considering catalysts, plasma–catalyst synergy, and fluid modeling [97]. Characterizing the plasma catalytic decomposition of methane, focusing on the role of atomic oxygen, and proposing conceptual models for thermal catalysis and plasma-induced reactions have also been key areas of interest [98]. Moreover, some studies have reviewed the removal of specific pollutants from exhaust gases using non-thermal plasma combined with catalysts, highlighting different plasma–catalyst systems and the use of numerical modeling [99]. Modeling and kinetic pathways in plasma-catalytic reactions have been thoroughly explored, as well. Some articles discuss the modeling of excited species and their role in the kinetic pathways of specific reactions using zero-dimensional flow reactor models [100]. The optimization of plasma catalysts is a critical endeavor in enhancing the efficiency of chemical processes, involving a nuanced adjustment of key parameters to maximize desired outcomes. For instance, the modulation of plasma power and frequency is meticulously calibrated to influence the energy levels and reactive species generated during reactions, directly impacting catalytic activity. Similarly, careful control over gas composition and flow rate is essential, as these factors dictate reaction pathways and selectivity. The surface characteristics of the catalyst, including composition and morphology, significantly influence its catalytic performance. For example, tailoring the morphology of a catalyst to enhance its surface area can lead to increased active sites and improved catalytic activity. Additionally, temperature control, facilitated by effective cooling systems, is crucial in preventing undesired side reactions and maintaining an environment conducive to optimal catalytic performance [93,94,97].

Collectively, these articles contribute to the advancement of plasma catalysis for sustainable processes by providing valuable insights into modeling approaches, reaction mechanisms, catalyst design, and the optimization of plasma-catalytic systems. The diverse range of research highlights the multifaceted nature of plasma catalysis and its potential for various applications in sustainable processes.

2.7. Exploring Modeling, Reactions, Systems, and Kinetics in Plasma Catalysis for Sustainable Processes

Research in the field of advancements in plasma catalysis for sustainable processes covers a diverse range of topics, including modeling, insights into reactions, system advancements, and kinetic pathways. The first group of articles emphasizes the significance of modeling and design in plasma-catalytic systems. Bogaerts and Centi [92] underscore the importance of microkinetic modeling and catalyst design for efficient CO_2 conversion. Pourali et al. [94] contribute with their microkinetic model by studying the non-

oxidative coupling of methane over a Cu catalyst in a non-thermal plasma reactor, providing valuable insights into optimal modeling approaches and catalyst design for efficient plasma-catalytic processes.

Andersen et al. [64] combine experimental measurements with plasma kinetic modeling to elucidate ammonia decomposition in a dielectric barrier discharge plasma. Tu and Whitehead [101] investigate the synergistic effect between plasma and catalysts in atmospheric dielectric barrier discharge dry reforming of methane. Diao et al. [96] explore the effects of a β-Mo_2C promoter on plasma-assisted dry reforming of methane over Mo_2C-Ni/Al_2O_3 catalysts, further contributing to our understanding of reaction mechanisms and the pivotal role of catalysts in plasma-catalytic reactions.

Li et al. [97] explore the application of dielectric barrier discharge non-thermal plasma in VOC abatement, considering catalysts, plasma–catalyst synergy, and fluid modeling. Li et al. [98] provide insights by characterizing the plasma catalytic decomposition of methane, focusing on the role of atomic oxygen and proposing a conceptual model for thermal catalysis and plasma-induced reactions. Zhu et al. [102] review the removal of CH_4 and NOx from marine LNG engine exhaust using non-thermal plasma combined with catalyst, highlighting different plasma–catalyst systems and the use of numerical modeling, showcasing advancements in plasma-catalytic systems for diverse applications.

Maitre et al. [100] discuss the modeling of excited species and their role in the kinetic pathways of non-oxidative coupling of methane by dielectric barrier discharge, presenting a zero-dimensional flow reactor model, providing deeper insights into reaction mechanisms, and outlining the influence of excited species on plasma-catalytic processes.

2.8. Advancing Plasma-Assisted Catalysis: Exploring Reactors, Kinetics, Hydrogen Production, and Computational Analyses

Research in the field of plasma-assisted catalysis has witnessed remarkable advancements in various aspects, spanning reactor configurations, kinetics modeling, hydrogen production, comparative studies, unknowns, and computational analyses with model validation. Scholars have explored different plasma reactor configurations to achieve the selective generation of oxygenates from CO_2 and CH_4, utilizing theoretical modeling to comprehend the underlying processes. Additionally, researchers have investigated the influence of process parameters and packing materials on chemical equilibrium and kinetics in plasma-based CO_2 conversion, shedding light on factors affecting reaction efficiency. Moreover, they have employed modeling techniques to unveil the reaction mechanisms of different plasma sources in CH_4 conversion while also analyzing the impact of flow rates.

The focus then shifted to plasma-catalytic technologies for hydrogen production. Comprehensive models have been developed to understand hydrogen production from alcohol reforming using plasma and plasma-catalytic technologies, investigating the effects of various process parameters on efficiency. Non-thermal atmospheric plasma reactors for hydrogen production from low-density polyethylene have been studied, emphasizing thermal–fluid models to understand the fluid flow and thermal behavior within the system.

Furthermore, comparative studies and exploration of unknown factors in plasma catalysis have been carried out. Scholars have conducted comparative studies of non-thermal plasma-assisted reforming technologies, simulating the catalytic effects of plasma, thus contributing to our understanding of the advantages and limitations of different plasma-assisted processes. Moreover, they have analyzed known knowns, known unknowns, and unknown unknowns in plasma catalysis, utilizing simplified kinetic models and generalized models for specific catalysts, underlining the importance of further research in these areas.

In the realm of computational studies and model validation in plasma-assisted catalysis, researchers have investigated plasma-based dry reforming across different time scales, validating their models by comparing simulation results with experimental data, ensuring accuracy and reliability. In addition, studies on enzyme-catalyzed processes of drug extrac-

tion have utilized plasma-limited flow models to calculate critical parameters, providing insights into drug metabolism and extraction kinetics.

The field of plasma-assisted catalysis has seen substantial growth across multiple dimensions. The comprehensive research on reactor configurations, kinetics modeling, hydrogen production, comparative studies, unknowns, and computational analyses has significantly enriched our understanding of plasma-catalytic processes, paving the way for their optimization and application in various industries and sustainable technologies.

2.9. Advancing the Frontiers of Plasma-Catalytic Processes: Insights across Syngas Production, Reforming, Waste Valorization, and Beyond

This section critically engages with a discernible gap in the existing literature pertaining to the deficiency in methane degradation via NTP, offering a meticulous examination of this underexplored aspect. Positioned within the broader context of plasma-catalytic processes, the research extends its focus across an array of domains, encompassing syngas production, methane reforming, tar evolution, waste valorization, hydrocarbon reforming, carbon dioxide dissociation, plasma-catalytic NOx production, neural network modeling, ammonia synthesis, and CO_2/CH_4 conversion.

Examining syngas production from methane oxidation using non-thermal plasma reactors, this review critically appraises the catalytic role of surfaces and uniform packings in augmenting the efficiency of plasma-based reforming processes. Furthermore, our review encompasses scrutiny of tar evolution in plasma gasification processes, placing emphasis on the catalytic potential of thermal plasma for waste valorization.

Integral to the manuscript's critical examination is the role of modeling and simulation as imperative tools for understanding plasma-assisted reactions, particularly in catalytic partial oxidation and NOx production. This review assesses various influencing factors, including plasma characteristics, flow patterns, and catalyst interactions. Expanding its scope, this review delves into plasma catalysis in hydrocarbon reforming, carbon dioxide dissociation, and the direct conversion of CO_2 and CH_4 into valuable products.

The integration of neural network modeling emerges as a promising yet scrutinized avenue, providing predictive insights into the performance of plasma-catalytic processes. The manuscript also critically evaluates investigations into ammonia synthesis using gliding arc plasma and the strategic use of K-promoters in CO_2/CH_4 conversion.

By critically addressing the deficiency in methane degradation by NTP and subjecting various facets of plasma catalysis to rigorous scrutiny, this manuscript serves as a specialized and pioneering contribution. Its critical analysis not only contributes to our comprehensive understanding of plasma-catalytic processes but also challenges and refines prevailing perspectives, paving the way for more nuanced and impactful advancements in sustainable and efficient chemical transformations within this dynamic field.

3. Development and Application of Computational Fluid Dynamics Models for Optimization of Plasma Reactors on an Industrial Scale

Computational fluid dynamics studies are important for advancing reactor design and optimization at the industrial scale. Plasma generation and utilization consist of physical and chemical phenomena extensively involving transport phenomena for fluids inside the plasma reactors. Turbulence, heat transfer, radiation energy, multiphase flow, fluid interactions, and homogenous and heterogeneous phase reactions are of significant importance in the domain of CFD studies. Based on the key experimental results, a numerical fluid model is usually developed for CFD studies. Often, software like FLUENT, Python, MATLAB, and Abaqus are used for CFD coding and simulation. In steady states, the Navier–Stokes equation is applied in incompressible fluid conditions and physical sub-models. Eddy dissipation for species transport is also studied in colloquium with kinetic models for gas-phase reaction studies. Sometimes, in the CFD models, we utilize built-in functions, while in erroneous design, and evaluate models for user-defined functions [65,103].

3.1. Development and Optimization of CFD Models for Advanced Reactor Design

In fluid models, continuity equations and boundary conditions provide a saturation of onset ions and electrons for recombination reactions' coefficient [104]. Applicable models in CFD modeling of plasma reactors are shown in Figure 1.

$$\frac{\partial n_e}{\partial t} - b_e\left[E\nabla.n_e + \frac{T_e}{e}\nabla^2{\cdot}n_e\right] = n_e v_{ion} - \propto_{reci} \cdot n_e n_i + \sum_i k_j{\cdot}n_q n_r \quad (1)$$

$$\frac{\partial n_i}{\partial t} - b_i\left[-E\nabla.n_i + \frac{T_i}{e}\nabla^2{\cdot}n_i\right] = n_i v_{ion} - \propto_{reci} \cdot n_e n_i + \sum_j k_j{\cdot}n_q n_r \quad (2)$$

n_i and n_i are the electron density and ion density

T_e is the kinetic temperature of reaction ions

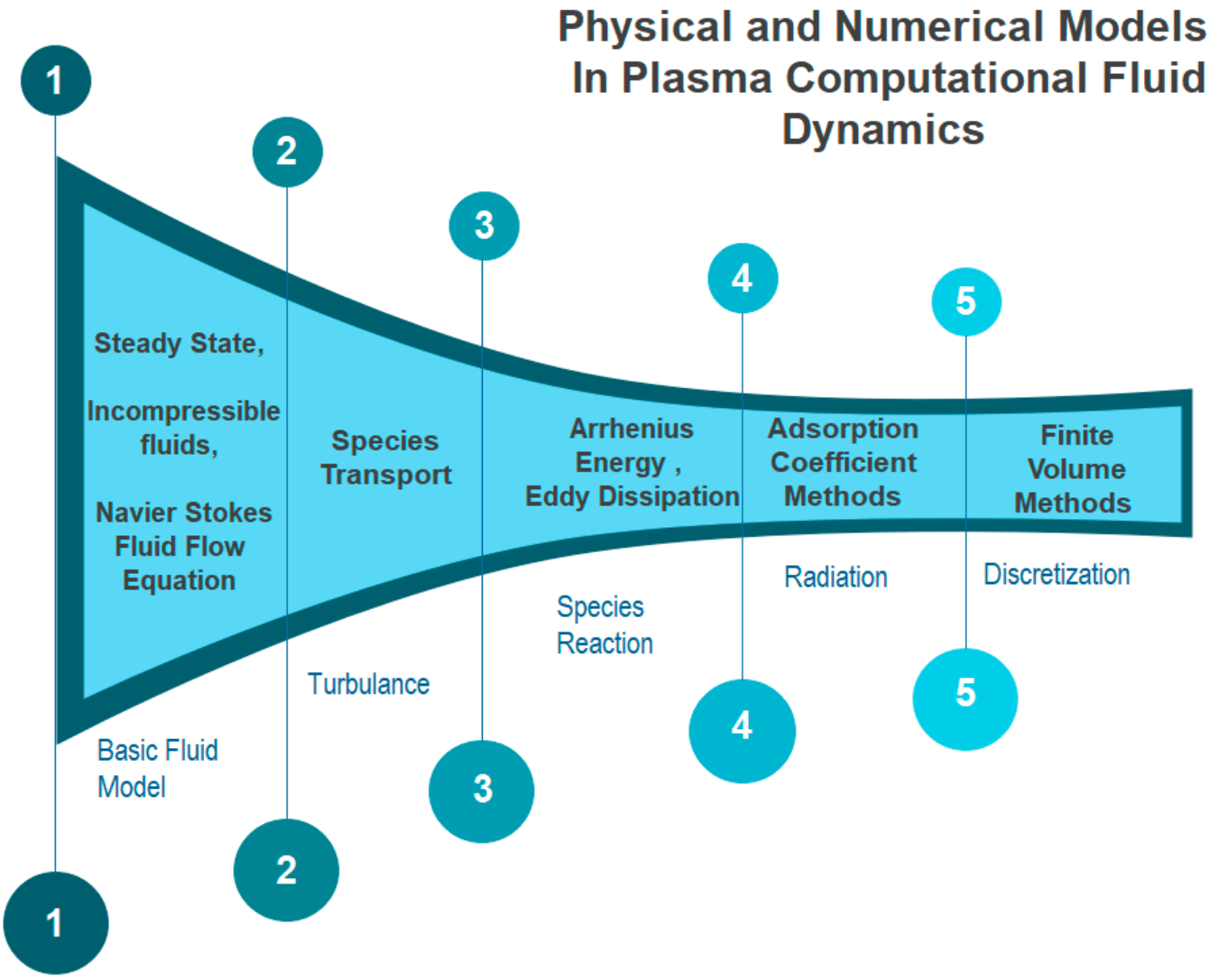

Figure 1. Models applicable to plasma reactor CFD modeling (based on [103]).

Electrons involved E is the electric field, V_{ion} is the frequency, k_i is the rate constant, $\propto_{reci}$ is the recombination coefficient, while q is the charge. B_e, T_e, and T_i are calculated, but the electron distribution is usually determined using the Bolsig + or Boltzmann equation solver.

$$\frac{d\sigma_e}{dt} = n_e v_e - \sigma_e v_e - \sigma_{rw}\sigma_+\sigma_e \quad (3)$$

$$\frac{d\sigma_+}{dt} = (1+\gamma)\cdot n_i v_i - \sigma_{rw}\sigma_+\sigma_e \quad (4)$$

σ_e is for the elctron surface density

σ_+ is the surfacae reaction for the positive coated electrode

Non-equilibrium modeling of species based on the space and time conditions for mass and energy balance in the plasma is achieved with the use of a Poisson equation. The model theoretical equation is decided for studying the electrode behavior in the non-thermal plasma reactor, either symmetrical or asymmetrical. COMSOL software is usually used for micro-fluidic studies in the plasma reactor and utilizes the finite element method. It computes the net velocity terms, current–voltage lead–lag conditions, and phase shifts depending on the alternating current supply conditions. The Poisson Boltzmann equation implicates the linearization limits in the electro-osmotic AC mathematical model in layer distribution structure during geometry and parametric studies. The developed mathematical model can be useful for the analysis of electro-transport phenomena in AC electroosmotic systems, and its predictions are more realistic than those given by the simple capacitor–resistor approaches. A mathematical model that describes the electro-transport behavior in an AC electro-osmosis circuit produces a greater representative for a capacitor resistor approach [105]. Boltzmann equation solvers are required for rigorous mathematical and physical standards for electron transport in swarm experiments within a cross-data set. The condition of the LTE gas mixture for a given composition at a certain pressure and temperature is according to the Law of Mass Action in the ratio of particle densities. Generically, the equation is given as a mixture of N with species Xs for a chemical reaction, with a_s and b_s the required species coefficients.

$$\sum_{s=1}^{N} a_s X_s \leftrightarrow \sum_{s=1}^{N} b_s X_s \quad (5)$$

Law of Mass Action

$$\prod_{s=1}^{N} n_{s\ (a_s - b_s)} = f(T) \quad (6)$$

Transport coefficients are required for the equilibrium plasma. In elemental diffusion, a reasonable amount of pressure fraction is considered from a set of elements in plasma. A constituent inlet composition at a reactor geometry is considered and can be deduced for the saturation of atoms at the coldest temperature spot condition along with the vessel wall. In lieu of the aforementioned, the composition can be obtained from the Law of Mass Action within the segregated mixture. These cases are exemplary in metal halides and consider an interplay between radial plasma diffusion and segregated convection. A low-temperature plasm reactor sliding arc destroys the available solid waste, and a CFD model for the reactor has been proposed in connection to a kinetic model at first. CFD considers electric discharge as a unique heat source and cannot be comprehensible in kinetic modeling. Arrhenius and kinetic calculations are mainly performed in discharge zones. Lab results and proposed models are not available for further development of plasma reactors for specific problems. Decomposition has a basis in carrier gas for required synthesis that is considered as a heat source in the physical effect and chemical source in energetic particle zones, so a non-inert gas is required for decomposition. Mainly, decomposition is on the grounds of partial or sometimes complete oxidation due to oxidizing agents present in the discharge zone. Reaction kinetics are defined by the residence time for the appropriate reaction, and heat source spark discharge is approximated. The flow of electrons through the ionized zone is referred to as a discharge [105,106] (Figure 2).

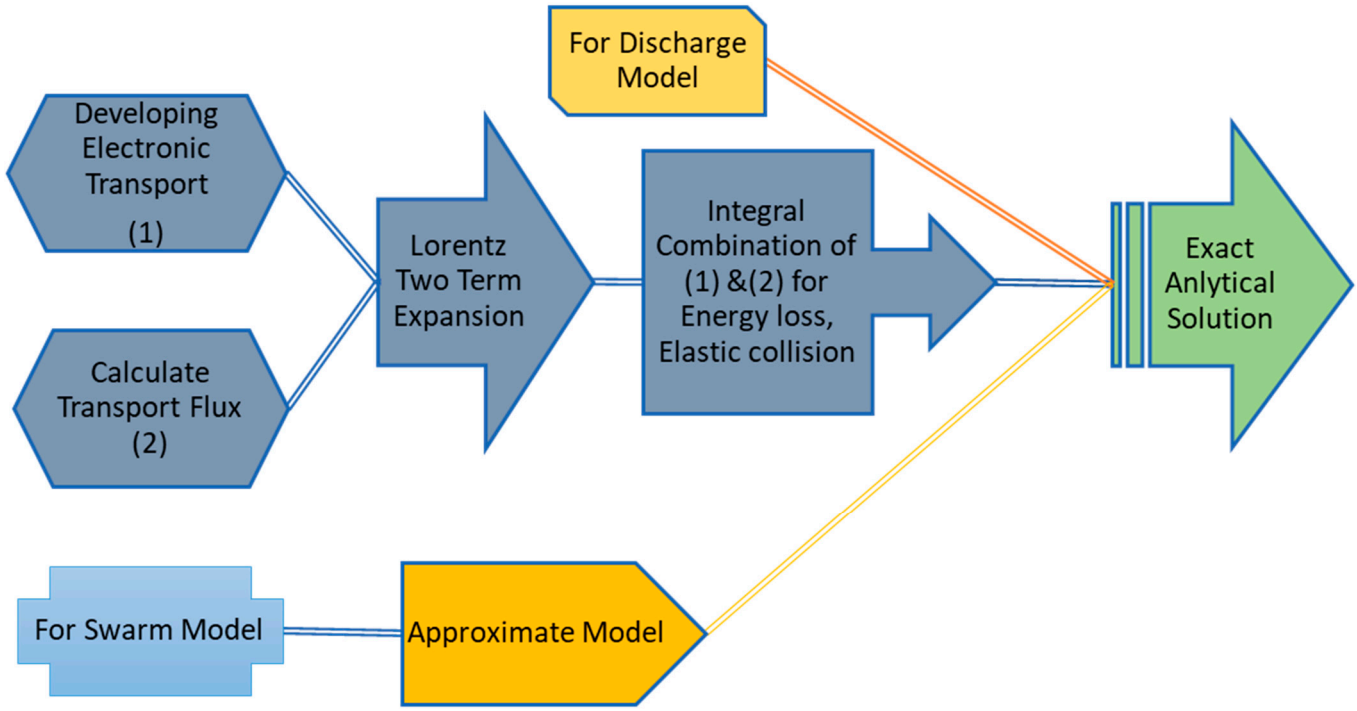

Figure 2. Modeling the flow of electrons (based on [107]).

3.2. Effect of Combining Gas Flow, Electric Potential, and Air Quenching Effects in a Nanosecond Pulse Plasma Reactor Using a Plasma Kinetic Model and Numerical Simulations

For a plasma aerodynamic mechanism in a nanosecond time frame, a DBD pulse reactor for a unique combination of seven species and a course of nine plasma process kinetic models is investigated. All the seven species are integrated for the resultant conservation equation and form a set of governing equations. Following the mechanism, gas flow and electric potential are given by the Poisson equation and Navier Stokes flow equation. A numerical simulation is deduced for the plasma discharge and simultaneously occurring flow actuation. Air-quenching effects are integrated into the experimentation and numerical simulation. The proposed plasma kinetic model includes excited and dominated species for the relevant reaction in order to allow calculation of the actuation in hydrodynamics, usually complicated in nature. Two models, one planar 1D and the second 2D symmetric sheath forming, are proposed for charge accumulation and subsequent emission due to grounded material. Species density and induced electric field occur at the sheath edge. At 460 K, there is a signal pulse of voltage rating 12 kV, the gas temperature increases to 56 K, and in the next 10 ns, the temperature decreases to 460 K. A comparison of H/l for the Poggies model and proposed numerical simulation in N_2 and N_2^+ has a wide range of difference in the mole fraction uniquely dependent on the time frame. N_2^+ has a greater time frame for similar mole fraction degradation, while N_2 has a shorter time frame requirement for similar product destruction [107–109].

The current reduced active model may be used to fully investigate the internal effect of plasma discharge on the surrounding air, as well as to reduce computing costs and focus on the practicality and accuracy of reproductions for multi-faceted scenarios requiring more complex calculations. In 340 K barometrical strain air, plasma discharge copies of the one-layered planar NS-DBD show that charge gathering triggers sheath separation. The mid-gap electric field and outright stream thickness are numerically reproduced, and comparison of the test and numerical outcomes shows that the results are reliable. Exclusively, the mid-gap electric field is 2×10^6 V/m, and the stream thickness is 6×10^4 A/m^2, for the two-dimensional NS-DBD with a symmetrical configuration at 310.3 K and low pressure of 4740 Pa, and the sheath boundary is identified as the location where the space charge density gradient peaks. The increase in rapid electron and ion density occurs at the

edge of the plasma sheath. The power density produces strong spikes (with the order of about 1010 W/m^3) near the edge of the sheath at the peak of the input waveform. The numerical density of electrons and ions at the peak voltage is in the magnitude of about 1018 m^3. Consequently, pulse energy increases rapidly after breakdown, and the resulting heat release leads to the formation of weak shock waves originating near the sheath edge [110,111].

Tar generation is a huge drawback of bio-originated stock gasification [112], which is an impediment to gaining ground in efforts to move toward clean energy. Steam improving [113] is a promising strategy for discarding tar in the biomass gasification process, as has been shown in the published pilot tests. In the cited paper, the steam improving of tar is investigated in a lab-scale level chamber reactor with Chemkin reenactment and in a pilot-scale tar reformer with CFD generation. A lot of enhanced reaction modes and modeling data are produced from experiment-scale work, which is applied in the CFD portfolio to predict the detailed cooperation in a pilot-scale tar reformer. The conjecture concerning CFD application is in alignment with the data from the pilot test. The results uncover that the tar in the reformer is generally suppressed by the steam, not the oxygen implanted in the reformer, and the reaction occurs inside the underlying 1 m of the length of the reformer, where the intermediates of the reaction are broken down quickly. CFD proliferation shows that the arrangement of the reformer can be improved by using a much shorter length, saving additional energy. The existing work displays an absolute cycle from the examination of some aspects in modeling-scale work to their subsequent assessment at the pilot scale [114,115].

The first outcomes of researchers' sustained energy put into demonstrating biomass gasification in the plasma reactor are introduced. A mathematical model was originally created for methane as (I) it is a notable synthetic and commonplace gas, and (II) the energy system associated with biomass gasification is generally complex. In addition, as opposed to bio-oil, methane enjoys the benefit of being infused in the reactor as a gas. Thus, the discontinuity of the fluid stream and dissipation need not be considered. The response of methane steam-based reforming was additionally tentatively considered and contrasted with the mathematical expectations obtained through familiar CFD (computational fluid dynamics) [116]. In the literature, the primary exploratory after-effects of steam changing of methane have been introduced, spanning cycle yields and expulsion of tars, which have been used to substantiate the worldwide dynamic model. Mathematical recreations have then been utilized to decide the essential boundaries in the development of novel syngas [117].

3.3. Mathematical Modeling for Non-Synergistic Transformation in Low-Temperature Plasma of Biomass

Non-synergist steam-based transforming of methane has been tentatively concentrated on utilizing low-temperature plasma. An initial phase has been begun in the investigation of an enhancing thermal interaction of biomass gasification. Notwithstanding non-ideal working conditions, methane is changed by up to 70% in carbon monoxide and hydrogen, in a low-volume response. Based on these investigations, a mathematical model suggesting an improved active plan was created. The forecasts of the model were in somewhat decent concurrence with tests and affirmed the significance of plasma enthalpy in the creation of excellent syngas. The rate of reaction deduced by the model is as follows:

$$r_i\left(\text{kmol}\cdot\text{m}^{-3}\text{s}^{-1}\right) = f_c \exp\left(-125520.\frac{10^5}{RT}\right) C_{CH_4} C_{H20} \quad (7)$$

A comparison of experimental and modeling results shows that flow rates of 19.6 Nl min^{-1} and 39.4 Nl min^{-1} for a N_2 inert plasma length correspond to 1.84, 1.71, 1.10, and 1.03 Nl min^{-1}, respectively, for tar and methane conversion to carbon monoxide at a temperature of about 700 K [117,118].

3.4. Investigating the Complexities of Plasma Modeling through Hybrid Simulation Strategies and Mathematical Models: Coupling Electrodynamics, Non-Thermal Plasma Dynamics, and Flow Field Modeling

Researchers have put forwarded several assumptions for model simplification. Usually, there is an assumption of no background gas heating for a low-pressure plasma discharge model, and thermodynamic equilibrium deviation is not accounted for in high-pressure plasma zones. The researchers demonstrate that under the conditions that they have studied, the plasma gas is locally heated, which gives rise to shock waves that are microscopic in size. Here, we see another example of a simulation in which various plasma-physical modeling types (for the electrodynamics, the non-thermal plasma dynamics and the flow field and background gas temperature) are coupled. This provides a great example of the application of hybrid strategies to contemporary problems in plasma technology. Particle hybrid modeling reflects the continuum and fluid models. Space coordinates are used in the Boltzmann method for the low-thermal-equilibrium plasma phase. These are usually defined in statistical properties of plasma particles and consider variables like species densities, velocities, mean energies, and temperature. Sturdy nonconformity is not allowed due to evenness conditions, i.e., the Monte Carlo technique. Plasma modeling is either for weak species or lower in concentration. The MC method is usually a group of elements in a given time and space. Stochastic scheming for each elastic and inelastic collision is conducted at random times. There are molecular dynamics revisions to particle performance and plasma wall behavior, whose arrangements are at the molecular level. The matter is in the condensed state for stream film, etching, and sputter processes at industrial scales. The combination of particle and MC model is a hybrid [106,107,119–126].

In the approximation of ultra-cold plasma expansion simulation, an interplay of atomic and electronic plasma processes is widely studied. The ionization of cold atomic gas is driven by electrons, which are controlled and tuned by laser frequency. The body recombination process reports lower temperature collision for Rydberg electrons and atoms. Simulation reproduces the experimentation results, as well as time-dependent results that describe the unique population conversion of Rydberg gas due to collision and sintering. These simulation results are best in a time span of 10 ms to 100 ms, due to the toco-relation of binding energies and radial velocity, and for initial carrier electron and gas atoms [96]. Three-body recombination due to electrons' ion combinations usually occurs in the vicinity of positive ions, and energy is generally carried by any of two electrons not connected for extra energy. The recombination rate increases mainly due to the decrease in electron temperature. The recombination process is usually favorable at the ground and lower temperatures; however, calculations are complicated in comparison with MC simulations [127].

Due to the complexities of plasma, numerical simulation codes are used in parts for different discharges and regimes. They are usually referred to as toolkit designs. The sub-model can be assembled in a compiler and implemented as needed for physical self-consistent models. Examples of these are the consistent Plasimo and Hybrid Plasma Equipment Model. Some commercial Multiphysics software tools for simulating the equilibrium and non-equilibrium in lieu of self-consistent conditions are applicable with guided parameters. Physics and mathematical models have an atomic and quantum physical model for the structure of electrons and atomic species in the radiations and their consecutive interactions [123,128].

Previous researchers have taken an interdisciplinary approach to plasma modeling in which electromagnetic and fluid flow conditions are incorporated for plasma physical features. Open-source code has a surface for modeling studies and can be simplified according to their concern conditions. Reduced models are a complete plasma system for engineering applications that essentially represent analytical model features and trends. Refinement of the aforementioned self-consistent numerical simulation has a good level of accuracy and sophistication in CAD tools for plasma-induced engineering [119–121,129].

3.5. Development and Simulation of a Fluid Model for Recombination Reactions in Non-Thermal Plasma Reactors with a Focus on Charged Species Dynamics through Computational Fluid Dynamics

Based on a bench-scale experiment, a detailed chemical mechanism and computational fluid model have been proposed. Chemkin software has been used for the kinetics from the experimental bench and further for reformer design and length standardization. CFD studies using ANSYS R.21 highlight that a smaller length is enough for tar removal and reforming. According to a detailed mechanism study, steam is a more key ingredient in comparison to available oxygen. The reaction proceeds in the first 10% of the total length of the reformer due to greater intermediates in the initial length [114]. In order to commercialize and advance a plasma reactor, methane-to-ethylene conversion via plasma catalytic oxidation has been modeled and simulated based on data from experimental lab results. Aspen Hysys V-10 compares the simulation results for process simulation with single-route methane to ethylene and a hypothetical process for the plasma catalytic conversion of ethylene to methane in a two-step procedure. Plasma hybrid catalytic transformation requires less than 21% of direct electricity. Due to the advent of this option and the vast renewable energy share, it seems possible to electrify the fossil fuel chain with optimum engineering economies and process intensification, with a processing cost of two-thirds of the original cost, whilst catalytic deactivation remains an issue in the commercialization of the project [121].

In NTP reactors under atmospheric conditions (Figure 3), a fluid model is proposed for unconsidered reactions, usually at the recombination stage for charged species and their coefficients. The impact of charged species in recombination steps is mainly due to the densities involved. The kinetic equation is a predefined step for the computer simulations for calculating coefficients of charged species based on the electron and neutral ion temperatures. At 10 kHz of AC input voltage, results show that the charged species that have evolved are mainly dependent on the temperature, dielectric material, ion density, and plasma discharge, which saturate the recombination steps quickly. The recombination reaction is basically due to the surface reactions. Charged species predicted by the fluid model are also a result of the continuity equation for the excited and charged species including all atmospheric reactions formerly neglected, and due to using the Poisson equation for the diffusion coefficient, ionization rate, and discharge volume. Usually, a uni-electrode dielectric coating, mainly thermionic emissions, increases the electron temperatures in comparison to uncoated electrodes [104].

Graph results show the simulated behavior of NTP DBD systems for unconsidered atmospheric gas using kinetic theory with multiple reactions involving mainly important charged species for the evolution of charged species in COMSOL and BOLTZMAN Solver. The temperature for ion-kinetic reactions mostly depends on the autoionization process. Spatial–temporal variation in the plasma volume for recombinative air kinetic reactions leads to more autoionization for saturation of ion-kinetic temperature. In one-dimensional conditions, radiation and heat transfers can be neglected, but a greater-dimensional model incorporates the respective species densities based on the aforementioned.

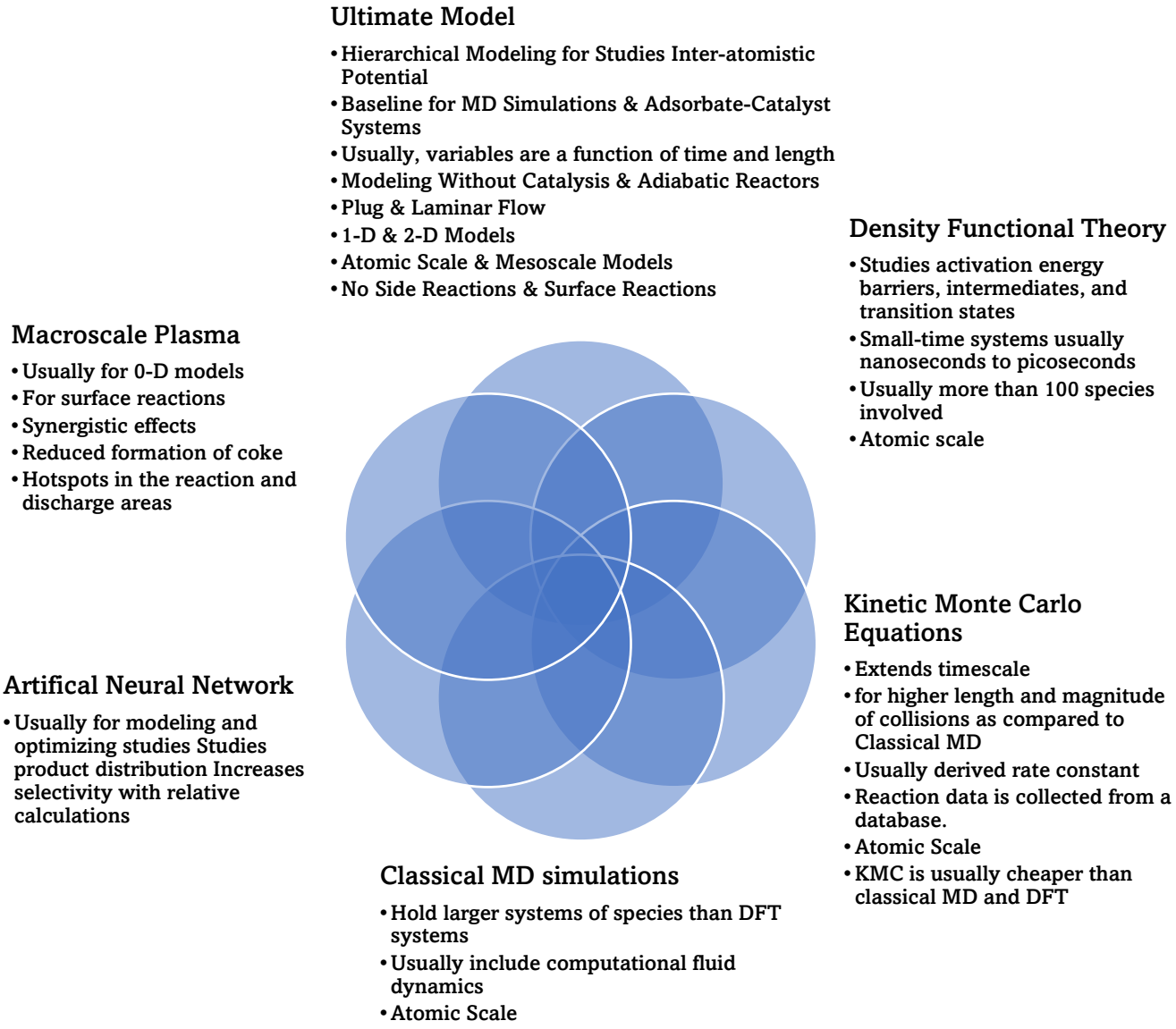

Figure 3. Different modeling approaches for modeling of plasma reactors (based on [130]).

A hybrid multi-model approach has been used in the literature for chemical kinetics, which studies the degradation rates using a process intensification strategy of rotation with conversion (in COMSOL), the geometry of the electrode, electric field strength, electrostatic conditions, electrode surface area, and velocity calculations in a plasma reactor. The T&T reactor utilizes Gibbs energy with variable parameters such as temperature and pressure. The Navier Stokes equation and mass conservation equation can be used for multiple species and the generation of a 3D model in COMSOL. The software uses a built-in comprehensive nominal residual method for iteration and convergence of the model and validation with experimental results. The degradation rate of gasifier product gas highlights a strong relationship between the decomposition rate with the electrode tip and the electric field intensity in rotational intensified plasma reactors [131,132].

3.6. Hybrid Modeling of Plasma Transport and Chemical Kinetics: Combining PIC and Monte Carlo Approaches with Density Functional Theory and Mechanistic Modeling

Combining Monte Carlo and particle in cell (PIC) for transport and chemical kinetics offers a hybrid method for modeling. The 1D model is easy to compute due to the low computational effort required and limited species, and since the reaction under study has a uniform composition with no consideration of transport phenomena. In fluid modeling,

mass, energy, and momentum balance are combined in the Boltzmann transport equation, yet more computational time is required than in kinetic modeling. If pressure conditions are taken into consideration, i.e., low-pressure conditions, the Monte Carlo equation with fluid models is utilized to study the detailed electron behavior in the plasma region, bringing forth a hybrid fluid model, and boundary conditions, a sticking coefficient, and wall reaction probabilities must be considered for surface reactions in dielectric plasma reactors. A new concept of the qualitative approach, mechanistic modeling, considers activation energies and a reaction rate coefficient based on first principal modeling using ab initio methods or MD simulations. In addition to considering multi-phase physical and chemistry calculations, density functional theory is proposed. Due to the complex nature of plasma and multiple by-products, this incorporates different body energy calculations and configurations to find appropriate and probable reaction mechanisms [120,133,134]. Tar components (naphthalene and phenol) are subjected to degradation similar to the degradation of double carbon bonds and aromatic ring compounds. Double bonds are destroyed by ozone mainly at 1,2 positions as the ethyl and hydroxyl activate further destruction. Naphthalene breakdown at 2,3 positions as the middle deployment increases the destruction rate. Package QCISSTD(T)/63-11 G (d, p) determines the activation energy for toluene, phenol, and naphthalene as 49 kJ/mol, 48.84 kJ/mol, and 28.06 kJ/ mol, while the same package gives the required Arrhenius activation energy expression levels as k = 4.17 $\times$ 10^{10} exp (−5476.4/T), 1.22 $\times$ 10^{12} exp (−5634.7/T), and finally 2.24 $\times$ 10^{12} exp (−3742.8/T) ($cm^3 \cdot mole^{-1} \cdot s^{-1}$) in succession. The ozone degradation rate constants of biomass compounds, in sequence, are the naphthalene molecule > phenol molecule > toluene molecule [135].

3.7. Use of Machine Learning Algorithms for Optimization and Prediction of Plasma Reactor Performance in Plasma Hybrid Modeling

Just like traditional plasma hybrid modeling, machine learning algorithms are used in combination for optimization and prediction studies of reactor performance. Naphthalene is subjected to reforming in a gliding arc plasma reactor. The results of reforming are analyzed in the a three-combination model comprising SVM, DT, and AAN for a complex procedural understanding and hyper-parameter tuning mainly with genetic algorithms. The results show great symmetry between experimental and modeling work. Steam-to-carbon S/C and discharge power are the most influential factors for conversion and energy efficiency, respectively. Variables are coupled for performance calculations. Machine learning modeling shows an optimized tar conversion of 67.2% for an energy efficiency of 7.8 g/kWh [135–137].

Predictions are sometimes not feasible for large carbon and are currently not available in the literature for plasma technologies' advancement. Chang's ANN model was developed a four-experimental-parameter study, underscoring the effect on toluene removal. The parameters are the discharge power, initial concentration, flow rate, and relative humidity. ML algorithms are widely available for prediction studies in the chemical plasma process, with limitations and drawbacks. The most appropriate ML algorithms are supervised learning algorithms for regression classification and prediction problems. ANN methods are self-adapted, autonomously configured, and continuously learning. The only drawback is the large data set requirement for the ANN method's executions and a challenge is avoiding overfitting. Usually, in plasma, chemical process data sets are small and confined. This eventually leads to uncertainty in the anticipated results. SVR is designated for non-linear and higher-order regressions [138]. It has a rare chance of overfitting and so consumes greater training time. In the originated data set, usually containing noise, DT algorithm transformation represents a tree visualization for robust calculations and decisions. Data set confirmation and properties do not affect DT calculations, and no preprocessing is required. Only normalized distribution and standardization are conducted. The results are usually overfitted due to generalization. The only advantage is the processing of large data sets.

Kinetic studies are not feasible for a multi-length-scale complex plasma process, so a powerful machine learning tool is required [138]. ML is required for the prediction and optimization of large chemical processes. In experimentation, there are usually long cycles, complicated procedures, and susceptibility to environmental interference, all of which cost us time and resources in seeking to obtain reliable results. In addition, experimental complexity scales exponentially with the number of variables, restricting the number of experiments and narrowing the range of process parameters. Plasma modeling is a helpful method for understanding the plasma process and building a chemical kinetic model for predicting key reaction data, i.e., rate constant, conversion, and cross-section. The genetic algorithm finds the optimal hyperparameter for each ML algorithm involved, to enhance adaptability and predictive accuracy. KPI-based understanding has been developed for energy efficiency and the conversion of naphthalene [110,139,140].

Determining the reaction key performance (P) for tar plasma involves a casual combination of three algorithms, where the equation is given as

$$P = P_{ANN}X\ W_1\ \ + W_2XP_{SVR} + W_3X\ P_{DT}\ (0 \leq W_1, \leq W_2 \leq W_3 \leq 1) \quad (8)$$

The algorithm's weighted parameters are W_1, W_2, and W_3 for *DT*, SVM, and *ANN*, while *P* is the predicted value's results. The mean square error evaluation formula is used to evaluate the performance of the ML model in terms of optimization for the relative weights using a predefined exhaustion method [136,141]

$$MSE = \sum_{i=1}^{n} (P_i - R_I)^{\ 2} \quad (9)$$

At four total inlet concentration sets of 1.1 g/Nm^3, 1.4 g/Nm^3, 1.7 g/Nm^3, and 2.0 g/Nm^3, model predicted and experimental values are calculated for the conversion (%). The conversion rate varies at 87%, 72%, and 70% at the four designated rates. At lower initial concentrations, models and prediction values are greatly related, while an increase in the concentration creates a significant deviation between the two values. In the case of discharge power (W) values from 32 W to 77 W, the conversion increases from 64% to 73% at 1.7 g/Nm^3 concentration. A great coherence exists between predicted and experimental values for S/C = 0 [114,136,141].

4. Conclusions

In conclusion, the synthesis of these observations underscores the substantial advancements in plasma reactor design and catalytic processes. The integration of modeling and simulation has played a pivotal role in unraveling the intricacies of these domains. The intricate interplay between plasma and catalysts has been meticulously examined, providing profound insights into critical reactions such as ammonia synthesis, methane reforming, and hydrocarbon conversion. Microkinetic modeling and catalyst optimization have emerged as instrumental components, highlighting their pivotal role in driving efficient CO_2 conversion and fostering sustainable chemical processes. The ongoing evolution introduces innovative modeling techniques, including neural networks, with predictive capabilities that significantly enhance the precision of plasma-catalytic processes. The convergence of plasma and catalysts is expanding in its application scope to encompass areas such as waste utilization and syngas production. In this context, plasma catalysis stands out as a promising approach, spearheading environmentally conscious solutions and transformative industrial applications. As this trajectory unfolds, modeling and simulation will persist as invaluable tools, guiding us toward the development of efficient, sustainable, and innovative plasma-catalytic processes, thereby contributing to a more environmentally friendly future grounded in scientific rigor and technological innovation.

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and J.M.; resources, M.Y.A. and A.S.A.; writing—original draft preparation, M.Y.A., A.S.A., J.M. and L.N.; writing—review and editing, M.Y.A., A.S.A., M.J., A.M., L.N. and H.P.-K.; visualization, M.Y.A., A.S.A. and A.M.; supervision, M.Y.A., J.M. and H.P.-K. All authors have read and agreed to the published version of the manuscript.

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