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Intelligent Intercommunicating Multiscale Engineering: The Engineering of the Future

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1. Introduction

Despite being widely known and investigated as a computer science discipline, artificial intelligence (AI) has attracted incomparable interest from researchers in diversified areas [1]. In 1950, Alan Turing raised the classic question that has inspired numerous researchers to date: "Can machines think?" [2]. The ultimate benchmark of AI was set by Turing's revised "imitation game," also known as the Turing test, in which the intelligence of a model is tested linguistically through the interrogator's evaluation of its similarity to human responses. Turing's work prompted the public to relate AI to computer capabilities, which led to the official identification of the field of AI at the Dartmouth Conference in 1956, organized by the mathematics professor John McCarthy. In his proposal of this historical event, McCarthy set a bold vision of AI, "... on the basis of the conjecture that every aspect of learning or any other feature of intelligence can in principle be so precisely described that a machine can be made to simulate it" [3].

Since its birth, the field of AI has experienced several periods of growth and stagnation. Unrealistically high expectations from many early pioneers caused the first winter of AI to occur roughly between 1974 and 1980, as most attention and funding were suddenly shifted away. Researchers had forecasted that all human tasks could be accomplished by supercomputers within 20 years of the birth of AI. However, the most used AI system by that time, the "expert-rule-based system," could not proceed with sophisticated tasks due to the difficulties of assembling expert-based knowledge that was updated in a timely fashion and extracting the major rules behind those tasks. Later, the development of the ground-breaking concepts of neural networks and back-propagation brought the end of the first winter and drew significant attention—coupled with financial support—back to AI investigations. This boom, however, was terminated due to the limitations of computational resources in the early 1990s. Fortunately, these limitations have gradually been alleviated since the mid-1990s, due to the scaling power of Moore's law [4], as publicly revealed through the news that the supercomputer Deep Blue defeated the famous chess champion, Kasparov, in 1997. Since then, both the development of AI methods (e.g., the invention of convolutional neural networks (CNNs)) and the development of computer devices (e.g., graphical processing units (GPUs)) have triggered a tremendous boost in AI studies in all possible fields.

Andrew Ng is a world-famous leading thinker in AI with numerous titles; he is the founder and chief executive officer (CEO) of Landing AI, the co-founder and chairman of Coursera, a former AI guru of both Google and Baidu, and an adjunct professor of computer science at Stanford University. Ng has referred to AI as the "new electricity," commenting: "Just as electricity transformed almost everything 100 years ago, today I actually have a hard time thinking of an industry that I don't think AI will transform in the next several years." This "new electricity" is now transforming how the world operates and creating enormous economic value. It is expected that there will be a 13 trillion USD increase in the global economy caused by developments related to AI technologies by 2030, according to the McKinsey Global Institute report [5]. These expected economic benefits indicate a new era—the AI transformation era—in which AI technologies and strategies are expected to become transformative industrial practices.

The transition to this new era is reflected in the shift of academic focus in AI investigations toward AI applications within the engineering domain. An analysis of the Web of Science regarding AI-related studies (Fig. 1) shows that the total number of publications on AI investigations has generally increased over time. Until 2018, the changing tendency in the total number of AI-related publications was almost exactly the same as the changing tendency in the number of AI-related publications in the field of computer science. However, within the past four years, the number of AI-related publications in computer science does not show as dramatic an increase as the total number of AI-related publications. On the other hand, the number of AI-related studies in engineering has displayed a significant increase over the last four years. In particular, AI-related publications in chemical engineering (CE), despite being relatively few in comparison with those in other areas, have increased over the last four years, as shown in the inset in Fig. 1. This difference in the tendencies of the number of publications indicates that the focus of development in AI is gradually shifting from methodology improvements, which are primarily conducted in computer science, to transformative

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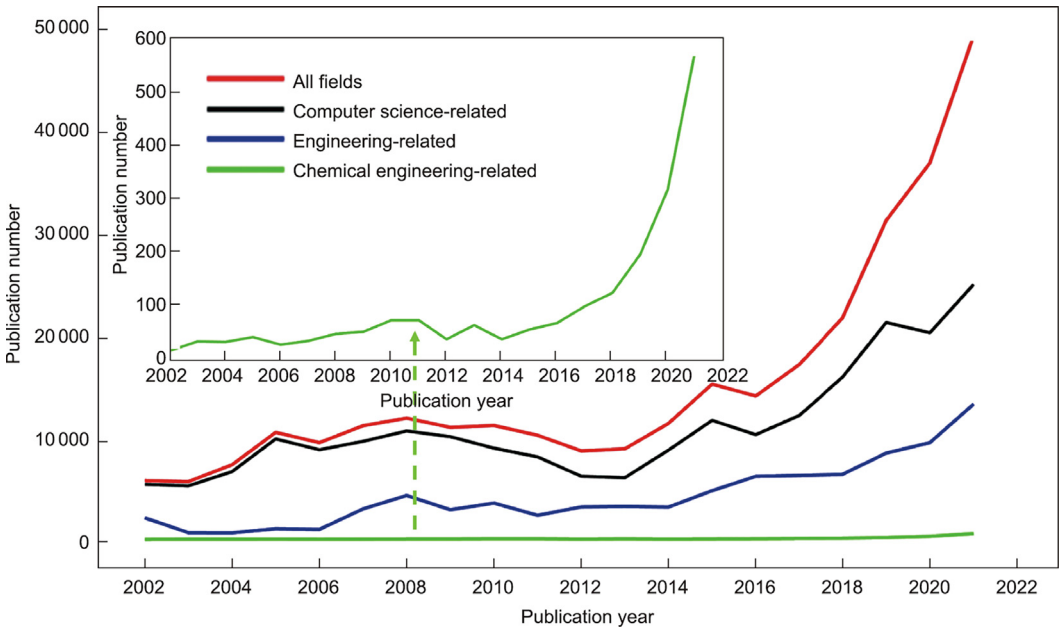

Fig. 1. A Web of Science analysis of the number of publications of AI-related studies over the past two decades with corresponding categories/keywords of "computer science," "engineering," "artificial intelligence," and "chemical engineering."

industrial utilizations, which are practiced in engineering. Nevertheless, solely considering the number of publications, investigations in computer science still currently account for the major contribution to AI development. A new era of AI transformation is being loudly announced by both industry and academia, and this change is analogous to a call to arms for engineers in all fields to turn their attention and efforts to accelerating this transformation for maximal benefits.

Engineers—especially chemical engineers—have certainly acknowledged this call, and AI seems to have quickly become the "apple of our eyes," attracting significant attention from engineers in recent years. In fact, AI development has a history of over 70 years, since Turing proposed the ultimate criterion of AI, and transformative utilization of AI has already achieved a certain level of success in many domains, such as robotics, speech recognition, and natural language processing [6]. However, AI applications in CE did not make a significant impact until after 2005 [6]. This stagnation predominately came from the inherent characteristics of CE itself, which ultimately presented difficulties in the development of transformative AI applications within CE. Despite these difficulties, the tremendous developments in AI methodologies and computer devices still brought a remarkable boost of interest in AI utilization in CE after 2005. The currently popular deep learning method makes it possible to establish a structure with multiple hidden layers, enabling the system to extract system features hierarchically [6,7]. Such modern AI methodologies have also made exceptional progress in areas such as medical practice. The possible dramatic improvements brought by AI to many application areas are urgently needed and expected in CE, an area in the very front lines of critical needs such as heavy-duty manufacturing and energy supplies. Optimized AI utilization in CE is expected to bring about revolutionary improvements in everyday human lives, especially in our global environment. This article highlights the features of and gaps in the transformative utilization of AI in CE and proposes a potential scenario, denoted as intelligent intercommunicating multiscale engineering (IIMSE), for optimal AI utilization in CE with the possibility of maximizing the benefits from the AI transformation. This proposed IIMSE scenario holds the potential to lead the anticipated AI transformation in CE. For readers' reference, this article also discusses the early trials and advancements of the transformative utilization of AI and hybrid modeling applications, which are positioned along the path toward IIMSE. In addition, a specific framework under the IIMSE scenario and additional prospects are proposed as possible future research focuses. This article provides a glimpse of the inevitable transformation in CE brought about by the "new electricity," AI, to inspire more chemical engineers to join this battle for revolutionary development.

2. AI transformation in CE

2.1. Major challenges of AI transformation in CE

In order to build transformative applications of AI in CE, it is necessary to know where the challenges lie. Historically, CE problems suffer from overly sophisticated controlling rules that have led to difficulty in the implementation of earlier AI technologies. This has hindered the development of rule-based expert systems for CE processes, which rely heavily upon such rules. Moreover, a simple structured AI method, such as those developed in the early 1990s, which have only one hidden layer, cannot recognize the complex patterns necessary to satisfy CE requirements. Furthermore, CE processes are generally governed by physical and/or chemical laws, which must be revealed for the development of CE processes. However, empirical AI methodologies cannot provide theoretical interpretations to fulfill this requirement [8]. In addition, CE is not a typical big data domain such as pharmaceutical or language-related fields [6], which limits the data-driven utilization of AI in CE. Due to these aspects of CE, AI transformation is not easy in this field.

2.2. IIMSE: A possible optimal AI utilization scenario in CE

Considering all these challenges, how should chemical engineers battle for AI transformation in our field? An optimal scenario, IIMSE, is introduced here as a new weapon that can potentially exceed the limitations of traditional approaches for the optimized

utilization of AI within CE applications. IIMSE is a hybrid modeling strategy that combines empirical AI methods and multiscale theoretical methodologies with direct information exchange between different scales, connecting microscopic insights to macroscopic observations. More specifically, the "intelligent" in IIMSE refers to exploiting the intelligent capacities of AI algorithms on the basis of a theoretical multiscale modeling scenario (i.e., AI-assisted multiscale modeling), while "intercommunicating" refers to direct information transformation between scales, which would ideally be bidirectional between all investigated scales. At present, however, due to the limits of current models and computing resources, only partial intercommunication can be achieved. Further discussions of AI assistance and the intercommunication mechanism are provided below. The following paragraphs will deliberate on the motivations for the development of IIMSE and reasons why this scenario can play a leading role in the development of AI within CE.

Although some of the main barriers to AI implementation—such as computing capacity and implementation difficulties—are removed or reduced by the increase in accessible computing resources and related methodologies such as deep learning or reinforcement learning, AI utilization is still challenged by its heavy reliance on having sufficient and representative input data samples to learn from. Moreover, empirical AI cannot comprehensively explain a system that is dominated by physical and chemical laws. In order to overcome the issues mentioned above, we suggest combining data-driven AI with theoretical models. In IIMSE, well-known theoretical models can predict and screen the appropriate input samples required for AI training and can also partially interpret the underlying physical and chemical laws. Furthermore, the AI algorithm corrects the errors introduced by the theoretical model predictions, solidifies the unclear aspects of the studied process, and—most importantly—significantly improves the phenomenological models' computational efficiency.

CE systems consist of intrinsic phenomena that evolve over multiple lengths and timescales. For example, a typical CE process can be analyzed using quantum chemistry simulations through the electron distribution information [9]; it can also be investigated by means of computational fluid dynamics (CFD) based on the system hydrodynamics. It should be noted that both of these investigations are conducted to interpret the same system. However, the conclusions obtained cannot be easily connected: It is difficult to relate the energetic outcome at the atomic scale to the two-phase distribution information within an operating unit. This disconnection leads to gaps in understanding between the different scales of the system. In particular, in such cases, the microscopic outcomes such as the elementary reaction mechanisms and favored reaction sites cannot be validated by experimental observations due to the limits caused by spatial and temporal differences. Similarly, few microscopic insights can be provided to support macroscopic observations. The mentioned gaps between the different scales of understanding within CE studies emphasize the necessity of building multiscale investigations for a comprehensive understanding of the studied systems, whose phenomena range from the electronic scale (e.g., density functional theory (DFT)) to the macroscopic scale (e.g., CFD). In this multiscale scenario, the microscopic outcomes lay a foundation for establishing macroscopic models and provide microscopic insights into the macroscopic performance. Conversely, the macroscopic outputs can be directly validated by the experimental results, which can subsequently prove the accuracy of the coupled microscale insights. Multiscale simulations are powerful tools that connect the finest scale behavior to the continuum properties of the studied systems. Without multiscale interpretations, investigations of system behavior are akin to the Chinese idiom of "looking at a leopard through a tube," which refers to how only a "spot" of information can be retrieved for a unilateral understanding of a phenomenon. Accordingly, in order to maximize the benefits of AI transformative utilization in CE, the theoretical model portion of the proposed AI-assisted hybrid scenario should utilize multiscale modeling.

However, multiscale modeling investigations often require intensive computational resources, especially for electron-population-based microscopic simulation techniques, which prevent these theoretical studies from providing efficient computational analysis within practical applications. The expectations of connecting microscopic behavior to macroscopic properties also require a near-impossible amount of computing resources, since more than four scales of theoretical calculations [10,11] are required for the complete understanding of just a single particle. Fortunately, AI has emerged as a handy and efficient tool with the potential to improve the efficiencies of multiscale predictions. Furthermore, the multiscale models within the hybrid scenario, IIMSE, are expected to be capable of direct information transformation. This means that the quantitative results from other simulation scales are interpreted into the information to implement each model scale. For example, between quantum chemistry and molecular simulations, the reaction or adsorption rates together with the surface events required in the molecular simulations are directly computed from the energetic results of the quantum chemistry analyses, where the necessary intercommunication mechanism is established between the two models (e.g., the quantum chemistry and molecular simulation models). Moreover, between the molecular simulation and the continuum equations, the statistical dynamics properties calculated from the molecular simulations are applied as the boundary conditions of the continuum equations, while the results from these equations are fed back to impact the surface revolution of the molecular models. It should be noted that, in these simulations, the key information is transferred between the models, while the core calculation at each scale remains independent to ensure the individual prediction quality of the system properties.

The discussed intercommunication mechanism is imperative in order to expand beyond simplified paralleled multiscale studies in which the results from different scales cannot be directly connected or compared. A simplified paralleled multiscale analysis can be related to a metaphor of multiple investigators studying the same system, each speaking a different language and therefore being unable to communicate without translators. Like the investigators, a multiscale model needs intercommunication mechanism "translators," which can be accomplished using AI and analytical models to foster an appropriate exchange of information between the different scales. In addition, AI algorithms and theoretical models inherently intercommunicate within a serial structure. In particular, AI algorithms can serve as a bridge connecting microscopic information to macroscopic metrics through data mapping, even with unknown parameters or models in between the microscopic and macroscopic models.

In summary, IIMSE—an AI-assisted intercommunicating multiscale modeling scenario that couples data-driven AI methods with comprehensive theoretical multiscale modeling schemes containing intercommunicating features to connect microscopic insights to macroscopic observations—provides the best opportunity to satisfy the requirements of CE development so as to theoretically optimize AI utilization in CE.

2.3. Advantages of IIMSE

By integrating AI with theoretical models, IIMSE opens up the possibility of effectively generating a comprehensive understanding of practical systems at multiple scales and efficiently predicting system performance for specific applications. In addition, the AI algorithms in IIMSE provide tools to correct the errors in the predictions caused by hard-to-access system-oriented parameters in the theoretical models. Moreover, AI paradigms provide solutions

to implement sophisticated processes involving models with unknown mathematical representations. Furthermore, the intercommunicating multiscale models in IIMSE—that is, the theoretical models—address the issue that an empirical AI approach cannot reveal the underlying mechanisms required in CE studies. The theoretical models can also provide adequate data for AI training to lower the cost of data generation in CE processes. With these improvements, IIMSE features potentially revolutionary improvements in computational efficiency, making it possible to operate the computationally intensive interpretations and predictions of a convoluted CE process. The proposed IIMSE scenario is also expected to form an intercommunicating system that connects microscopic insights to macroscopic observations. The connections built by IIMSE will lead to a comprehensive understanding of the studied systems and will enable CE technologies to be directly developed, from microscopic design to process intensification and/or optimization. Therefore, IIMSE can satisfy the requirements of CE development by providing comprehensive interpretations and efficient predictions based on CE features. This method aims to maximize the benefits of AI applications in CE and can potentially accelerate the transformation imparted by AI.

2.4. Early attempts towards IIMSE: From data-driven AI to hybrid modeling

At present, the proposed IIMSE scenario is still in its infancy, leaving almost all avenues open for exploration. Along the path of transformative applications of AI in CE toward the possible future world-leading scenario of IIMSE, early attempts have primarily consisted of purely data-driven AI utilization and simplified hybrid modeling strategies; in other words, AI-assisted single-scale simulations. A few studies have conducted reduced AI-assisted multiscale simulations, in which AI is mostly used to relate mesoscale parameters to macroscopic simulations such as CFD [12,13]. However, either the intercommunicating mechanism was not presented within the theoretical scenario established in these studies, or a connection was not built between the microscopic insights and macroscopic predictions, both of which achievements are expected in IIMSE. Despite these inadequacies, these early attempts in AI transformative utilization illustrate some of the advantages of AI-assisted multiscale models in interpretation and prediction capacities in material development and process intensification.

Among the CE studies that can be thought of as leading towards IIMSE, a comprehensive hybrid modeling scenario combining data-driven AI methods with theoretical intercommunicating multiscale methods, this section presents early attempts ranging from data-driven AI utilization to simplified/reduced hybrid modeling scenarios in both materials development and process intensification. In material functionality development, the assistance of AI has been observed to significantly accelerate the screening process of an extensive pool of candidates for specific applications by relating the critical figures of merit within the materials (e.g., stability, sustainability, or activity) to inexpensive descriptors as the surrogates. For example, in the field of catalyst development in heterogeneous systems, the stability of the catalyst can be related to the prediction of the Gibbs energies. Bartel et al. [14] developed the sure independence screening and sparsifying operator (SISSO) algorithm to accurately forecast Gibbs energies for inorganic crystalline solids, providing an efficient method for the study of material stability. Some studies within this area have focused on a crystal graph CNN technique proposed by Xie and Grossman [15], which presents the possibility for catalyst development based on local chemical environments. The catalyst screening process is significantly enhanced computationally via the application of AI. A favorable adsorption energy prediction is another significant consideration for a heterogeneous catalyst system. With the adoption of AI, large quantities of adsorption configuration data can be efficiently screened by adopting AI to eliminate unnecessary and expensive electronic structure calculations for DFT analysis. Accordingly, AI studies have also focused on developing both hybrid [16,17] and purely data-driven models [18,19] for predicting adsorption energies and conducting automated structure generation [20]. It should be noted that, in microscopic multiscale modeling, algorithms involving quantum chemistry analysis are usually extremely computationally intensive, due to the intense calculations required to analyze the electronic distribution of a system. Accordingly, replacing quantum chemistry analysis with AI algorithms to connect quantum mechanics to molecular simulations is prevalent in studies on this topic. For example, Misawa et al. [21] exploited an artificial neural network (ANN) to correlate atomic configurations and system potential energy functions, which were then passed on to molecular dynamics (MD) simulations to proceed with large spatial and temporal domain MD predictions while maintaining first-principles accuracy. The far-from-equilibrium shock phenomenon was successfully described through their proposed model, with 5000 times higher efficiency than the traditional method. Extensive applications have demonstrated that substituting first-principles potentials with ANN potentials leads to dramatic efficiency improvement in *ab initio* molecular simulations [22,23].

In addition to the fast screening of materials, the mechanism revelation of a chemical reaction is usually computationally intensive due to the need to conduct a first-principles analysis of the electron distributions [24]. Furthermore, surface reaction network establishment necessitates greater computational requirements due to its high complexity. In order to overcome these issues, AI-assisted hybrid models combining AI with *ab initio* calculations can be constructed to speed up the predictions of energetic results by simplifying the electronic structure simulations. The surface reaction network complexity can be addressed by adopting AI to identify the path of minimum energy. Working along these lines, Ulissi et al. [25] adopted trained surrogate AI models to predict the most important reaction step, thereby avoiding the enormous complexity of surface reaction networks caused by hydrocarbons. The surrogate model taught the Gaussian process the adsorption energies based on group additivity fingerprints. Transition-state scaling relations and a simple classifier were furthermore used to determine the rate-limiting step.

In terms of reaction mechanism studies, AI combined with *ab initio* analysis has provided more efficient ways to locate transition states (i.e., saddle points) on the potential energy surface (PES) between the reactants and products. Considering the fact that significant computational resources are spent on conducting accurate calculations of unimportant electronic state structures in traditional *ab initio* calculations, Peterson [26] adopted AI to locate the saddle points on the PES and to reduce the number of intermediate *ab initio* calculations for finding transition states. The located saddle points were subsequently verified using *ab initio* calculations. This work demonstrated that AI can greatly accelerate searches of transition states by significantly reducing the number of *ab initio* force calculations required in case studies.

In addition to materials development, studies in process intensification—mostly CFD coupled with AI—have demonstrated great potential to relate multiple impact factors to system behavior, such as the two-phase distributions of the system. In this approach, the drag force can be correlated to multidimensional features of the system for adequate predictions using AI models. Working along these lines, Jiang et al. [27] adopted ANNs for a drift velocity correlation to the filtered solid volume fraction, the slip velocity, and the pressure gradient. Later on, Zhang et al. [28] and Jiang et al. [29] discovered the effects of neighboring coarse grids and the particle Reynolds number, respectively, through AI analyses. AI coupling

has also been demonstrated to improve process intensification through the usage of AI-assisted system clustering or prediction models based on CFD outcomes [30,31].

In conclusion, AI-assisted hybrid modeling has been demonstrated to be beneficial for CE process intensifications for multidimensional correlations and simulation efficiency improvements in both system predictions and their interpretations. Hybrid modeling combining theoretical models and data-driven AI satisfies the requirements of incorporating and extracting first-principles knowledge. Data-driven AI can be coupled beyond first-principles models or mechanistic models when taking into account a broader concept of hybridization. Both phenomenological models that offer physical explanations of systems built based on empirical relations and incomplete comprehensions that can be interpreted as nonlinear partial differential equations (PDEs) can be integrated into hybrid modeling [32–35]. The flexible and accessible implementations of hybrid models facilitate their widespread utilization and currently remarkable position in AI transformations in CE. Due to the focus of the present article, the wide-ranging applications of hybrid models are not fully elaborated upon here; instead, interested readers are directed to these comprehensive studies for consideration [8,32,36–38].

Unlike the abovementioned pure AI analysis of CE systems and the simplified hybrid models that primarily couple AI with single-scale theoretical analysis, IIMSE emphasizes the effects of AI-assisted multiscale modeling with intercommunicating features that connect microscopic insights to macroscopic observations. However, this comprehensive AI-assisted multiscale simulation is still a mostly hypothetical and ambiguous concept that is currently in a preliminary trial period, even though its advantages of both data-driven AI and comprehensive multiscale modeling have respectively been emphasized in previous CE studies [39–41]. These studies, which are one step closer to IIMSE beyond simplified hybrid models, are known as the reduced hybrid models. Although reduced hybrid models provide a superior process description, they either do not contain comprehensive theoretical models at each scale or do not completely connect microscopic insights to macroscopic observations. Nikolopoulos et al. [12] established an ANN–energy minimization multiscale (ANN–EMMS) drag scheme that adopted ANNs to map the heterogeneity index based on the EMMS model for a wide range of gas–particle mixture properties, which was directly delivered to a CFD model. On the basis of this study, Yang et al. [13] developed a generic EMMS drag model for dense fluidization through the adoption of ANNs. This work furthermore balanced the prediction quality and computational cost of the studied system through ANNs. Despite these contributions, if we solely evaluate their prediction accuracy, these ANN–EMMS models have not yet outperformed traditional models. However, their great potential still stands out due to the advantage of correlating the high-dimensional features, taking into account local/temporal variations and particle size distribution, and making straightforward extensions to other systems without intensive computational requirements. Accordingly, additional investigations are required to contribute to improving this scenario.

Although these reduced models have presented great improvements in process intensification, macroscopic process-intensification phenomena still cannot be related to microscopic insights in these studies. The first reduced hybrid model that provides this connection was created by Chaffart and Ricardez-Sandoval [42], who explored the development of more complex intercommunicating hybrid multiscale models with applications to thin-film deposition. Their model coupled together macroscopic continuum models, which capture reactor operating conditions such as the system temperature, with AI models being used to determine the necessary parameters required to establish a microscale stochastic PDE growth model of the thin-film surface. In their work, the interaction between the gas-phase reactor conditions (i.e., the temperature and partial pressure of the precursor gas species) and the key properties of the thin-film surface (i.e., its roughness and growth rate) were explored. Furthermore, the AI algorithm played a vital role in supplementing the missing empirical microscale properties of the surface and relating the microscale thin-film growth to the macroscopic system behavior. However, theoretical models do not present multiscale features on their own; thus, no intercommunication can be conducted within theoretical simulations. This limits the contribution of this discussed work to the comprehensive understanding of the system. Similarly, on the basis of the same thin-film growth system, Kimaev and Ricardez-Sandoval [43,44] adopted ANNs as a substitute for a multiscale thin-film model in order to perform efficient nonlinear model predictive control.

As mentioned above, these studies are still primitive, and none of them have adopted comprehensive intercommunicating theoretical models that correlate microscopic and macroscopic mechanisms. Consequently, there is an urgent need to develop IIMSE models that can correlate the behavior of microscopic systems, which are dominated by their intrinsic kinetics, with the behavior of bulk-phase fluid interactions, which are dominated by macroscopic hydrodynamics. By combining the advantages of AI and multiscale models, this proposed scenario is expected to be capable of comprehensively explaining and efficiently predicting a wide range of phenomena in CE applications with minimal computational cost.

3. Future perspectives

Among the inevitable changes caused by AI technologies, the proposed IIMSE scenario holds the potential to play a leading role in accelerating the AI-driven transformation within traditional CE applications. Accordingly, Fig. 2 presents a possible example framework under the proposed IIMSE scenario and introduces our future research interest. In this framework, an intercommunicating multiscale model in IIMSE within a particle at the microscopic scale is established using DFT, kinetic Monte Carlo (kMC) simulation, and continuum mass transportation equations in the channel of a particle. Within this model, the DFT analysis provides the elementary reaction mechanisms and the related energetic properties, which are interpreted into surface events and reaction rates to establish a kMC surface model. Subsequently, the statistical dynamics properties from the kMC simulation can be delivered directly to the continuum equations as the boundary conditions in the particle channel. The solutions of the continuum equations, such as the coverages, can be transferred back to the kMC model to affect the evolution of the surface. At the macroscopic scale, a CFD analysis is established to contribute to an understanding of the system hydrodynamics. This CFD analysis achieves process intensification by providing heterogeneous phase distribution and material conversion information.

The system's mechanisms can be revealed by the aforementioned theoretical models. However, they cannot be related from the microscopic to the macroscopic scale, due to the limits of computational capacity and the current partial comprehension of the multiscale phenomenon. With the assistance of ANNs, communication can be built between the comprehensive microscopic multiscale model and the macroscopic CFD model to avoid the complexity caused by the highly empirical mesoscale models that are otherwise required. In the scenario presented in Fig. 2, intercommunication between the microscopic multiscale model and the CFD model is established by the data-driven ANN in a serial structure, which maps macroscopic metrics such as the productivity to microscopic insights such as the reaction rates under

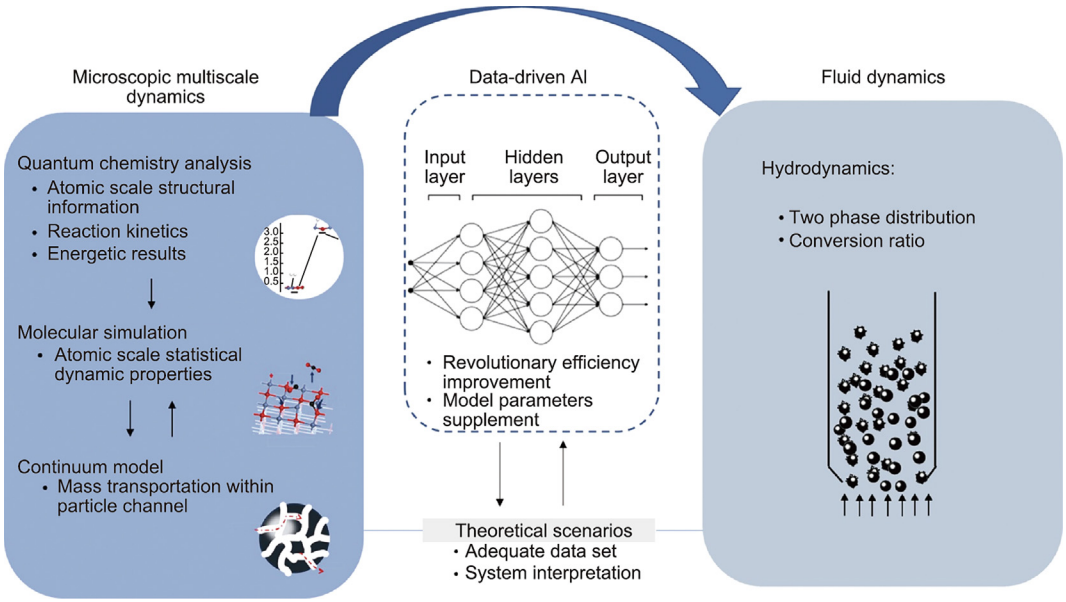

Fig. 2. An example framework of intelligent intercommunicating multiscale modeling.

different combinations of operating conditions, such as temperatures and pressures. Accordingly, this framework relates the microscopic mechanisms dominated by elementary reactions to the macroscopic hydrodynamics, raising the possibility of efficiently predicting the complete system information on the multiple scales on which it occurs by breaking the limit of computing resources with the assistance of AI. Furthermore, this framework has the potential to implement a multiscale modeling strategy directly into CE manufacturing, in order to incorporate the full range of system behavior from microscopic design to process intensification.

In addition to this framework, extensive scenarios encompassed within IIMSE can be further developed using other AI paradigms, such as support-vector machines or random forests, for a wide range of CE applications. Notably, there are numerous hybridization methods for exploiting the features of AI to implement simulations with a partial comprehension of systems or to improve the modeling performance in IIMSE according to the research objectives. The most simplified structures—whether serial or parallel structures—that allow data-driven AI to combine with theoretical models are respectively highlighted when unknown mathematical representations or process parameters in convoluted environments exist and when the available phenomenological mathematical expressions are constrained by their prediction power [32]. A mismatch of theoretical methods can be corrected by combining the outcomes of data-driven models and mechanistic models through weighted or unweighted addition, Kalman filtering, multiplication, and so forth [45]. On the basis of simplified serial and parallel structures, a myriad of mixed algorithms can be further established in IIMSE to fulfill the requirements of extended investigations.

In addition to contributing to the proposed IIMSE, the features of AI open up numerous other possibilities for improving various CE applications in future investigations. For example, another critical topic in CE, that of real-time control, can benefit substantially from AI through the general and flexible intelligent capabilities of AI methods. The real-time control systems required in modern production processes often require high adaptability in order to manage all possible uncertainties within the process. However, the simple mode-switching adaptability used in conventional methods cannot meet this requirement, especially in highly dynamic and sophisticated domains [46]. Therefore, AI technologies provide a potential solution to modern real-time control systems, where even system modes that are difficult to observe can be "detected" and scheduled, thereby ensuring their implementation, by relying on the generality of well-trained AI models. This high adaptability of AI models can also be capitalized upon within the scaleup processes of new technologies from the lab to industrial scale. Furthermore, assistance from AI can be used to address common issues such as unexpected features that may be present at the industrial scale that cannot be observed or predicted from a lab-scale system. As a result, the high adaptability of well-trained AI systems holds the potential to provide economically and computationally efficient scale-ups of new technology by eliminating expensive pilot-scale demonstrations.

4. Concluding remarks

AI, as the "new electricity," is radically transforming operating modes throughout the world. Consequently, it is imperative for chemical engineers to respond to the call of this new AI transformation era and exceed the limitations of current technologies by using this powerful revolutionary innovation to its fullest extent. Rooted in the features and challenges of the CE domain, such as its complexity, the lack of big-data domains, and the necessity of understanding the underlying laws governing chemical systems, the IIMSE scenario is proposed to intellectualize the intercommunication of multiscale phenomenological models in order to provide fast predictions and comprehensive system understandings. The proposed framework under the IIMSE scenario efficiently provides complete process information on each of the relevant scales and relates microscopic reaction mechanisms to macroscopic system hydrodynamics. This scenario aims to bring revolutionary improvements in efficiency and to exceed the limitations of traditional methods in CE investigations, toward the possibility of a direct CE manufactory strategy from microscopic material design to macroscopic process intensification. This IIMSE scenario has the potential to occupy a leading role in the AI transformation within CE, and the potential models under the umbrella of IIMSE scenario can be readily extended to a variety of different studies.

In the current day and age, chemical engineers carry the heavy duties of the world on their shoulders. Due to the inevitable technological change of AI transformation, chemical engineers

are urgently encouraged to embrace and master AI utilization in order to not only efficiently fulfill our duty to society but also win a position in this global competition of technologies.

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