



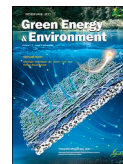
Multiscale simulation of biomass gasification in fluidized bed reactors

Downloaded from: <https://research.chalmers.se>, 2026-10-24 11:34 UTC

Citation for the original published paper (version of record):

Luo, H., Ström, H., Xiong, Q. et al (2026). Multiscale simulation of biomass gasification in fluidized bed reactors. *Green Energy and Environment*, 11(6): 1490-1519.
<http://dx.doi.org/10.1016/j.gee.2026.07.003>

N.B. When citing this work, cite the original published paper.



Review Article

Multiscale simulation of biomass gasification in fluidized bed reactors

Hao Luo ^{a,*}, Henrik Ström ^b, Qingang Xiong ^c, Ruiyan Sun ^d

^a School of Chemistry and Chemical Engineering, Wuhan University of Science and Technology, Wuhan, 430081, China

^b Department of Mechanics and Maritime Sciences, Chalmers University of Technology, Goteborg, 41296, Sweden

^c School of Chemical Engineering and Pharmacy, Wuhan Institute of Technology, Wuhan, 430205, China

^d College of Biotechnology and Pharmaceutical Engineering, Nanjing Tech University, Nanjing, 211816, China

Received 1 April 2026; revised 30 June 2026; accepted 1 July 2026

Available online 4 July 2026

Abstract

Biomass fluidized bed gasifier (BFBG) is core equipment for producing sustainable syngas, which is one of the alternatives to replace fossil fuels in producing green fuels or chemicals. Multiscale simulations provide powerful tools to reveal the biomass gasification behaviors in fluidized bed reactors, thereby supporting the design, optimization, and scaling-up of BFBG. This paper systematically reviews sub-models (molecular-scale, particle-scale, and meso-scale models) and reactor-scale models for the multiscale simulation of the BFBG. First, the advantages and disadvantages of various drying models, pyrolysis kinetics, and char gasification models at the molecular scale are discussed. The particle-scale models (i.e., zero-dimensional, corrected zero-dimensional, interface-based, and two-/three-dimensional models) are analyzed in terms of their accuracy and computational demands. The development of meso-scale models is also addressed. Additionally, machine learning methods used to assist in developing sub-models across different scales are summarized. Then, from the perspective of multiscale coupling between models at various scales, the strengths and limitations of reactor-scale models for multiscale simulation of the BFBG are analyzed. Finally, the conclusions of this review and perspectives for future research, which aim to develop fast, reliable, and efficient models for the multiscale simulation of the BFBG, are presented.

© 2026 Institute of Process Engineering, Chinese Academy of Sciences. Publishing services by Elsevier B.V. on behalf of KeAi Communications Co. Ltd. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

Keywords: Multiscale simulations; Biomass gasification; Sub-models; Reactor-scale models; Fluidized bed gasifier

1. Introduction

As a carbon-neutral and renewable energy source with abundant availability, biomass is considered one of the alternatives to substitute for fossil fuels to reduce CO₂ emissions [1–4]. The main technologies for converting large quantities of biomass into bioenergy are thermochemical conversion processes, such as pyrolysis, gasification, and combustion [5]. Among these, gasification is an important route for converting biomass into high-value-added sustainable syngas, which can

be further used to produce green fuels or chemicals [6–8]. Due to its excellent performance in heat and mass transfer, mixing, fuel flexibility, and scalability, the fluidized bed has become one of the mainstream reactors for biomass gasification [9–11]. However, the biomass fluidized bed gasifier (BFBG) is a multiscale complex system characterized by the coexistence of multiple phases and components, as well as strong nonlinear coupling among hydrodynamics, external heat and mass transport, intra-particle transport, and complex gasification reactions [12,13]. In addition, biomass feedstocks vary significantly in size, density, porosity, and chemical composition, which exert significant effects on the performance of BFBG [14]. Thus, the design, optimization, and scale-up of fluidized bed gasifiers via experimental methods are not only time-consuming but also costly. Therefore, it is essential to

* Corresponding author.

E-mail addresses: luohaohg@hnu.edu.cn, haoluo@wust.edu.cn (H. Luo).

Peer review under the responsibility of Editorial Board of Green Energy & Environment

develop efficient and reliable models for the BFBG to support their design, optimization, and scale-up, thereby achieving high-efficiency utilization of biomass feedstocks [9].

As illustrated in Fig. 1, BFBG involves multiscale physical phenomena that span a broad range of spatial and temporal scales [12]. At the molecular scale, the thermochemical conversion of biomass into syngas entails a series of consecutive or parallel reactions (e.g., primary pyrolysis, secondary pyrolysis, tar oxidation and cracking, and char gasification), which take place at spatial and temporal scales of nanometers and nanoseconds, respectively [15]. At the particle scale, temperature, concentration, and conversion gradients induced by intra-particle heat and mass transfer are observed within the particles [16]. This is because biomass feedstocks are typically millimeter-scale porous particles, whose size is constrained by the energy consumption associated with the crushing process [17]. At the meso-scale, complex interactions between biomass particles, bed materials, and gas lead to the formation of meso-scale structures (such as particle agglomerates and bubbles). These structures significantly affect the external heat and mass transfer processes between biomass particles and their surrounding environment [18], thereby indirectly influencing intra-particle heat and mass transfer as well as reactions at both the particle and molecular scales. At the reactor scale, the boundary conditions of the BFBG are determined by its operating parameters and geometric configurations, and the flow and mixing behaviors of gas, bed materials, and biomass particles can vary substantially within the reactor [11]. Therefore, the overall performance of the BFBG is dominated by the multiscale coupling chain of "flow-external heat and mass transport(meso-scale)-intra-particle transport (particle scale)-reactions (molecular-scale)". Accordingly, a multiscale model is indispensable to efficiently and reliably facilitate the design, optimization, and scale-up of the BFBG.

Given the significant disparities in spatial and temporal scales across different levels, directly integrating these models requires a time-step size and mesh size smaller than those of the smallest resolved scale in the simulation, resulting in

dramatically increased computational demand [15,19,20]. Consequently, some simplifications have been made to improve the efficiency of the model while attempting to maintain its reliability. Fig. 2 lists the mainstream models for the multiscale simulation of the BFBG based on their resolved resolution and computational demands. Both the Eulerian-Lagrangian (E-L) approach and Eulerian multi-fluid model (MFM) solve the governing equations for mass, momentum, heat, and species transport of different phases [13]. The difference lies in that the E-L approach tracks each individual particles or parcels, while the MFM treats solid phases as continuous phases [13]. Thus, the spatial and temporal evolution of each individual particle (such as residence time, particle collisions, and particle shape) can be more easily obtained via the E-L approaches [21], which involves higher computational demand compared to the MFM [13]. Unlike the CFD-DEM and MFM, the computational fluid dynamics-chemical reactor network (CFD-CRN) model does not directly solve the detailed governing equations. Instead, its topological structure and parameters are derived from detailed information obtained from CFD simulations [22–24]. This model is relatively new and is expected to be a promising approach for the multiscale simulation of the BFBG in terms of both accuracy and efficiency [25–27]. In contrast to the CFD-CRN model, the CRN model uses empirical correlations to determine its topological structure and parameters, making it commonly applicable for simulating bubbling BFBG [28–31]. The thermodynamic equilibrium and kinetic (EK) models assume that the biomass gasification process occurs sequentially in the BFBG (i.e., drying, pyrolysis, bio-tar cracking, char gasification, and gas phase oxidation and reduction reactions) [32]. The impact of fluid dynamics is usually ignored, and a series of thermodynamic and kinetic modules in process simulators are employed to describe the biomass gasification process. Due to its simplicity, the EK model has been widely used to obtain global performance [33–35]. Data-driven surrogate (DS) models learn the implicit nonlinear multiple input–output mappings from high-quality experimental datasets [36] or

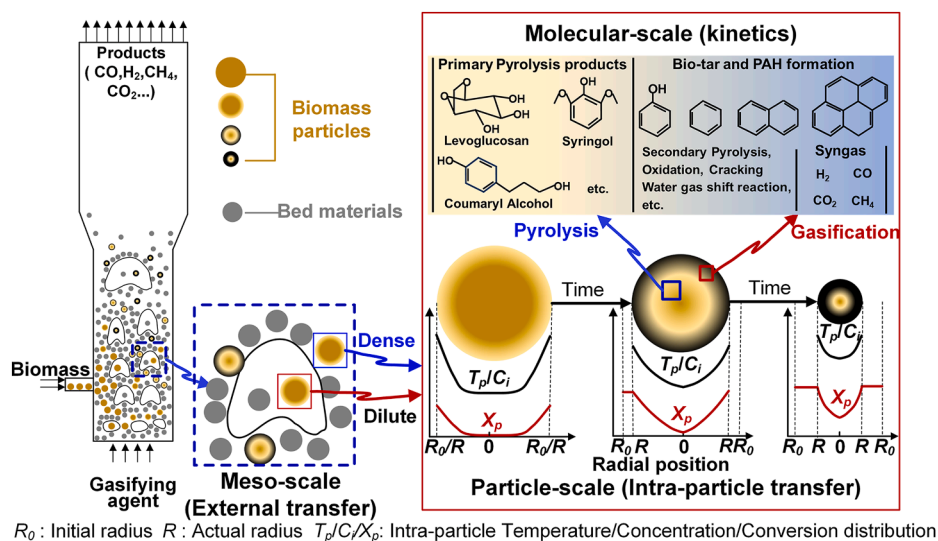


Fig. 1. Multiscale physical-chemical processes inside the BFBG.

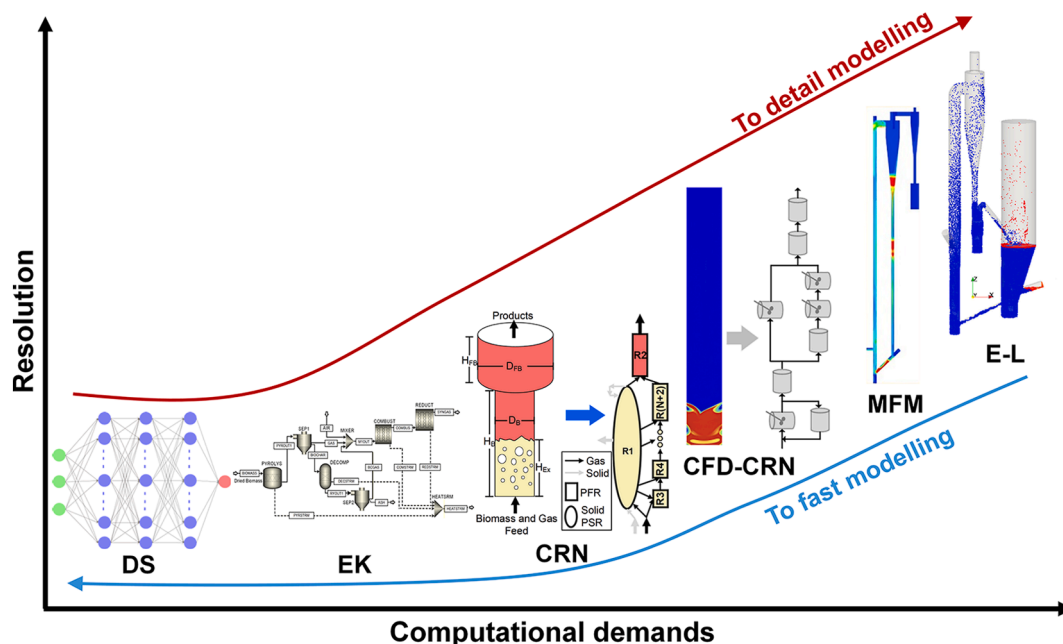


Fig. 2. Mainstream models for multiscale simulation of BFBG. EK: Reprinted with permission from Ref. [40]. Copyright (2023) Elsevier. CRN: Reprinted with permission from Ref. [30]. Copyright (2024) Elsevier. CFD-CRN: Reprinted with permission from Ref. [26]. Copyright (2017) Elsevier. MFM: Reprinted with permission from Ref. [41]. Copyright (2018) Elsevier. E-L: Reprinted with permission from Ref. [42]. Copyright (2022) Elsevier.

precomputed high-fidelity simulations of the BFBG [37]. They predict the key performance of a BFBG (such as syngas species composition, gasification efficiency, and char conversion), thereby attracting considerable attention in recent years [38]. Although numerous models have been extensively employed to investigate the biomass gasification behavior in the BFBG, previous literature reviews usually focus on only one of these models and fail to highlight the importance of multiscale coupling of sub-models at different scales [9,19,32,39]. Therefore, it is essential to review the state-of-the-art research on the multiscale simulation of BFBGs and point out its future directions.

The purpose of this review is to summarize the recent progress in the multiscale simulation of the BFBG. First, the recent developments of sub-models for the multiscale simulation of the BFBG are reviewed. Then, the multiscale coupling of sub-models in reactor-scale simulation of the BFBG is discussed. Finally, conclusions and perspectives on the development of efficient and reliable multiscale simulation models for the BFBG are provided.

2. Sub-models for multiscale simulation of the BFBG

Multiscale simulation of the BFBG requires the implementation of sub-models ranging from the molecular scale to the meso-scale within the reactor-scale model. These sub-models exert significant effects on the modeling results [9,43–45], thus, the recent developments of sub-models for the multiscale simulation of the BFBG are reviewed in this section.

2.1. Molecular-scale model

As shown in Fig. 3, the gasification process of raw biomass to gas products can be divided into the following sequential processes: drying, pyrolysis, char gasification, and homogeneous reactions (i.e., bio-tar cracking, gas-phase oxidation and reduction reactions). Among those reactions, drying, pyrolysis, and char gasification are heterogeneous processes. The net rate depends not only on the operating conditions but also on the physical properties of biomass feedstocks [9], resulting in significantly different models adopted in the literature. Thus, the molecular-scale models for drying, pyrolysis, and gasification are discussed in the following sections.

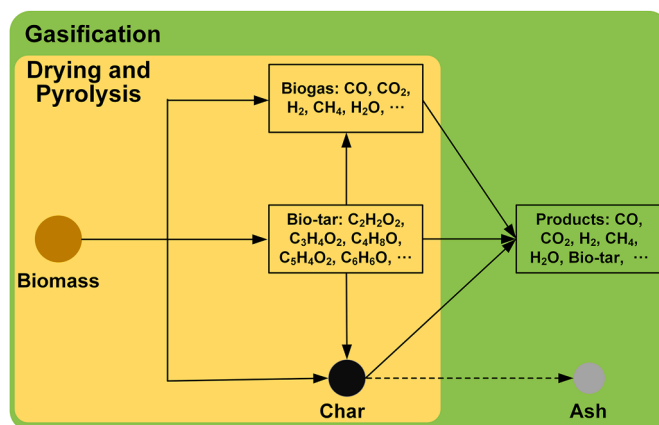


Fig. 3. Gasification process of raw biomass to gas products.

2.1.1. Drying model

Drying is an endothermic process in which bound water or free liquid water within porous biomass is evaporated upon heat supply. The net drying rate is dominated by heat transfer when the temperature exceeds the boiling point, whereas it is limited by external mass transfer under low-temperature conditions [19]. The heat flux model, the equilibrium model, and the kinetic model are the most widely used drying models in multiscale simulations of the BFBG.

The heat flux model assumes that water evaporation occurs only at the boiling temperature, and that the heat transferred to a representative volume equals the evaporation enthalpy of the released moisture. Since this model is independent of the physical properties of biomass particles and can be easily implemented in numerical codes, it has been extensively applied in particle-scale simulations [46–49]. However, a key drawback is that the net moisture evaporation rate is expressed as a step function, which may introduce numerical instabilities [19]. Furthermore, the model typically assumes a constant boiling temperature of 373.15 K, even though rapid moisture release can lead to pressures significantly above atmospheric pressure [47,49,50]. Therefore, the boiling temperature should be modified according to local conditions [48]. In addition, the model presumes a zero drying rate below the boiling point, thereby underestimating moisture removal at low temperatures. Owing to these limitations, the model is seldom used in reactor-scale simulations of BFBG [51,52].

The equilibrium model assumes that thermodynamic equilibrium is established between the liquid moisture inside biomass particles and water vapor in the gas phase [53]. The driving force for drying is the difference between the equilibrium moisture concentration and the vapor-phase concentration [47]. Although the model was initially developed to describe drying under low-temperature conditions [54], it has been widely adopted for both particle-scale and reactor-scale simulations of biomass gasification [55–59].

In contrast to the heat flux and equilibrium models, which are derived from heat- and mass-transfer mechanisms, the kinetic model represents the drying process using a first-order Arrhenius expression [60]. Benefiting from its straightforward implementation and numerical stability [19], this model has been extensively employed in biomass gasification simulations [61–65], particularly in reactor-scale CFD simulations of BFBG [66–68]. Its main limitation is that the pre-exponential factor and activation energy must be adjusted according to the physical properties of biomass particles and operating conditions [47]. Maziarka et al. [49] evaluated various kinetic models for simulating the pyrolysis of thermally thick biomass particles, and found that the kinetic parameters proposed by Gentile et al. [69] yielded the best agreement with the experimental data of Lu et al. [56].

Although all three models have been applied in biomass gasification simulations and can provide reasonable predictions of the drying process [19], the kinetic model remains

the most preferred choice for multiscale simulations of BFBG due to its simplicity [66–68].

2.1.2. Pyrolysis kinetic model

Pyrolysis kinetic model is widely adopted to predict the pyrolysis rate and the yields of gas, tar, and char in multiscale simulations of the BFBG [70–72]. The actual chemistry underlying biomass pyrolysis is believed to involve thousands or even millions of elementary reactions, so a complete mechanistic understanding remains elusive, and no detailed elementary reaction networks have been established in the literature [12,73]. On the other hand, from an engineering perspective, the primary focus is placed on the overall pyrolysis rate and the main distribution of pyrolysis products [9]. For this reason, lumped pyrolysis kinetics remains the dominant approach used in the multiscale simulation of the BFBG. The typical kinetic schemes for describing biomass pyrolysis are summarized in Fig. 4.

2.1.2.1. Scheme A: one-step global kinetics. The one-step global kinetics assumes that biomass undergoes direct conversion to char and gases, as shown in Fig. 4 (a). This is the most simplified scheme adopted by many researchers in both particle-scale and reactor-scale simulations, since its kinetic parameters (i.e., pre-exponential factor, activation energy, and reaction order in the Arrhenius equation) can be easily fitted from experiments and its computational cost is relatively low [19]. However, since the physical properties of biomass and operating conditions exert significant effects on pyrolysis processes, the parameters of Scheme A vary considerably in the literature, as summarized by Luo et al. [75], making it difficult to select appropriate kinetic parameters for the multiscale simulation of the BFBG. To improve the adaptability of kinetic parameters to diverse biomass feedstocks and variable operating conditions, Xing et al. [76] proposed a ML-enhanced one-step global kinetics. Balsora et al. [77] adopted a similar strategy, with model input features derived from elemental analysis, proximate analysis, and macroscopic component quantification (i.e., cellulose, hemicellulose, lignin, and extractives). Xiao et al. [78] systematically evaluated the influences of input feature selection on the predictive accuracy of ML-based kinetic prediction and verified that taking cellulose, hemicellulose, and lignin contents as neural network input variables yields superior prediction performance for the activation energy of biomass pyrolysis. The general workflow for ML-based kinetic parameter calibration of biomass pyrolysis is illustrated in Fig. 5. First, biomass feedstocks are comprehensively characterized via standard analysis methods to determine their macroscopic component contents, as well as the proportions of moisture, volatiles, fixed carbon, and ash, together with elemental composition data. Experiments or detailed modellings are adopted to obtain the mass loss history or reaction rate under various operating conditions with various biomass feedstocks [78–84]. The acquired temporal mass loss and reaction rate data are then

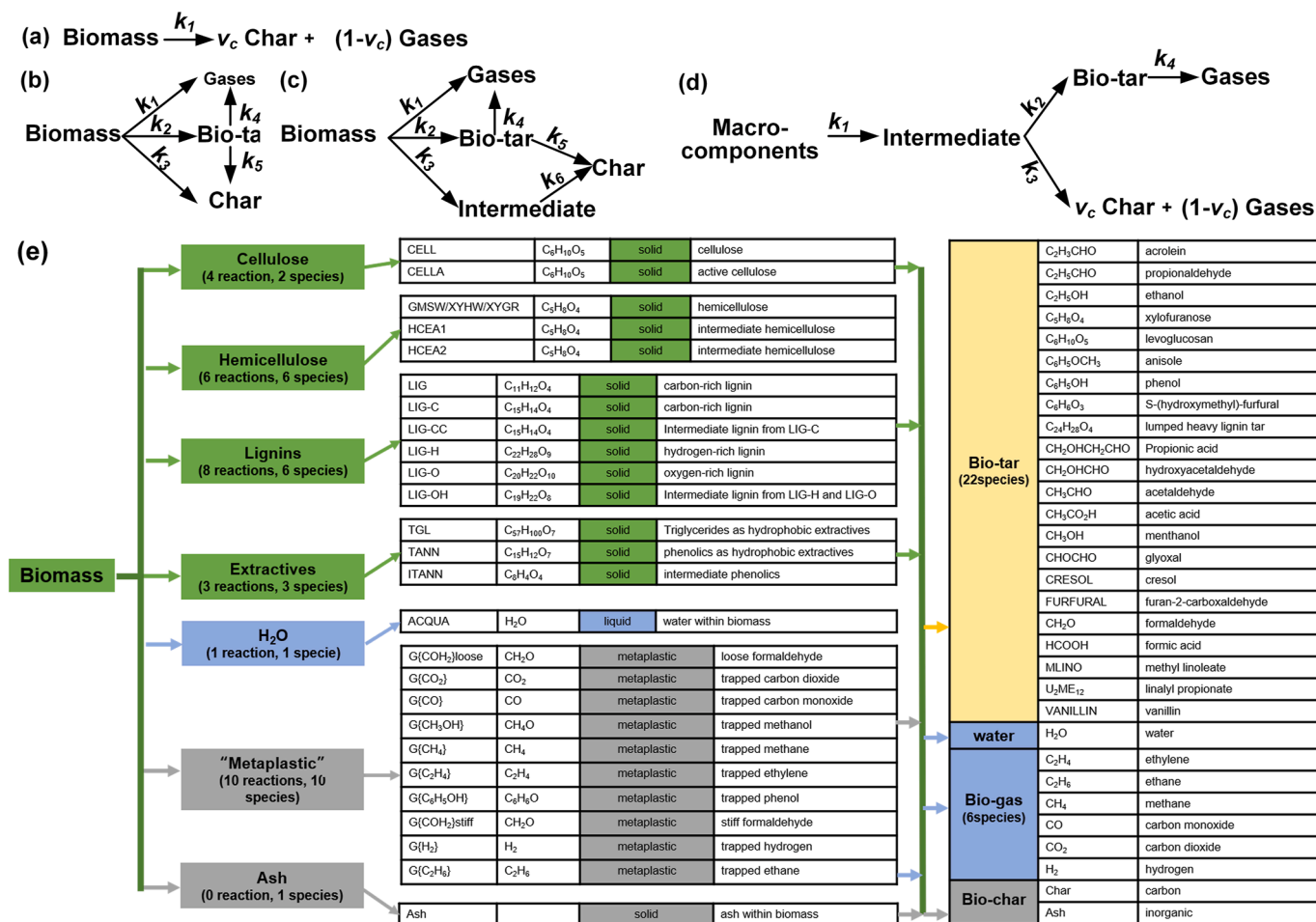


Fig. 4. Typical kinetic schemes for describing biomass pyrolysis processes. (a) Scheme A: one-step global kinetics. (b) Scheme B: two-step semi-global kinetics. (c) Scheme C: two-step semi-global kinetics. (d) Scheme D: lumped chemical structure based kinetics. (e) Scheme E: detailed chemical structure based kinetics. Reprinted with permission from Ref. [74]. Copyright (2022) Elsevier.

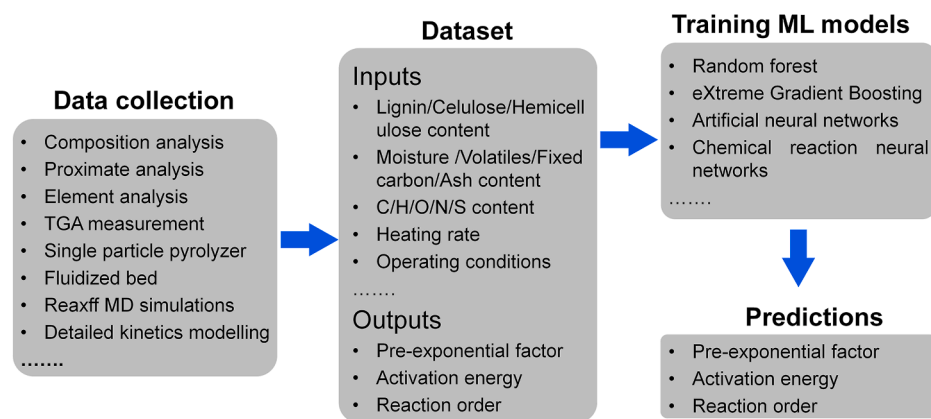


Fig. 5. General workflow to derive kinetic parameters of biomass pyrolysis using machine learning methods.

processed to calculate the corresponding kinetic parameters, which are further compiled into a standardized dataset with clearly defined input–output variable pairs. Third, the constructed dataset is employed to train and optimize a high-performance ML model [83]. The well-trained ML model is

implemented to predict the kinetic parameters for biomass pyrolysis reactions [76]. Despite the merits of ML-assisted one-step global kinetics enabling parameter adaptability to various biomass feedstocks and operating conditions, the Scheme A is still oversimplified in most cases. Not only does

it rely on additional empirical correlations to determine the split ratio of gases to char, but it also fails to provide detailed information regarding the yield distribution of individual gaseous species [70,72].

For product yield prediction of biomass pyrolysis via the one-step global kinetics, the empirical correlations proposed by Neves et al. [72] have been widely employed in the multiscale modelling of the BFBG. These correlations are developed based on extensive experimental datasets that cover broad pyrolysis conditions and diverse biomass feedstocks. As shown in Table 1, they enable the quantification of yields of CO, H₂, and CH₄ as well as bio-char, alongside the elemental (C, H, O) compositions of bio-char and bio-tar. The yield of CO₂, H₂O, and other light hydrocarbons are calculated by element mass balance. Nevertheless, these empirical correlations exhibit limited fitting accuracy because pyrolysis product yields are solely correlated with operating temperature, the coefficient of determination (R-square) for most correlations is lower than 0.9. Consequently, ML methods have gradually replaced the empirical correlations to predict the yield of biomass pyrolysis product. Current ML-based yield prediction frameworks correlate pyrolysis product distribution with readily measurable parameters, including elemental (C/H/O) contents and proximate analysis indices (ash, moisture, volatile matter, and fixed carbon), as well as critical operating parameters such as reaction temperature and heating rate [85–89].

2.1.2.2. Scheme B and C: two-step semi-global kinetics. The two-step semi-global kinetics was first proposed by Shafizadeh and Chin [90] to describe the tar-cracking process, as shown in Fig. 4 (b). The kinetic parameters proposed by Wagenaar et al. [91] have been commonly used in both particle-scale and reactor-scale modeling, and the results indicate that Scheme B can provide reasonable predictions of the overall pyrolysis rate and char yield in most cases [60]. However, Park et al. [92] pointed out that Scheme B fails to accurately capture the peak temperature profile caused by endothermic reactions. Thus, an intermediate component, with subsequent decomposition via endothermic reactions to form char, was added to Scheme B,

resulting in Scheme C as illustrated in Fig. 4 (c). This modification enables the accurate capture of the peak temperature inside biomass particles [92]. Although Schemes B and C do not require an empirical correlation to determine the split ratio of gases to char (in contrast to Scheme A), their kinetic parameters still need to be adjusted according to the biomass feedstocks to improve prediction accuracy [93]. Furthermore, they fail to predict detailed information on the yield of individual gas species without additional empirical correlations.

2.1.2.3. Scheme D: lumped chemical structure based kinetics. Even though the chemical composition of a biomass particle is highly complex as summarized by Johansen [94], the biomass can be represented by several key macro-components, namely cellulose, hemicellulose, and lignin, as shown in Eq. (1). Each macro-component is assumed to be converted into intermediate products, followed by parallel decomposition reactions that generate bio-tar, char, and gas species, respectively [73,95]. Additionally, a tar-cracking process is incorporated into Scheme D, as illustrated in Fig. 4 (d). The parameters of Scheme D proposed by Miller and Bellan [96] are listed in Table 2, it has been widely used in both particle-scale and reactor-scale modelling of biomass pyrolysis process [97–104]. A comparative study by Xiong et al. [98] shows that

Table 2

A commonly used kinetic parameters for Scheme D [96].

Macro-components	Parameters	ν_c for k_3	Pre-exponential factor (s^{-1})	Activation energy (kJ/mol)
Cellulose	k_1	0.35	2.80×10^{19}	242.4
	k_2		3.28×10^{14}	196.5
	k_3		1.30×10^{10}	150.5
Hemicellulose	k_1	0.6	2.10×10^{16}	186.7
	k_2		8.75×10^{15}	202.4
	k_3		2.60×10^{11}	145.7
Lignin	k_1	0.75	9.60×10^8	107.6
	k_2		1.50×10^9	143.8
	k_3		7.70×10^6	111.4
Tar	k_4		4.28×10^6	108.0

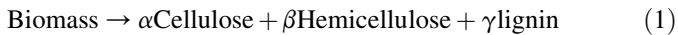
Table 1

The empirical correlations used to determine the yield of pyrolysis product [72].^a

Items	Empirical correlations	R-square
Yield of CO	$Y_{CO,F} = Y_{H_2,F} \left(3 \times 10^{-4} + \frac{0.0429}{1 + (T/623)^{-7.23}} \right)^{-1}$	0.56
Yield of H ₂	$Y_{H_2,F} = 1.145(1 - \exp(-0.0011T))^{9.384}$	0.94
Yield of CH ₄	$Y_{CH_4,F} = -2.18 \times 10^{-4} + 0.146Y_{CO,F}$	0.88
Yield of bio-char	$Y_{ch,F} = 0.106 + 2.43 \exp(-0.0066T)$	0.56
Element of carbon in bio-char	$Y_{C,ch} = 0.93 - 0.92 \exp(-0.0042T)$	0.65
Element of hydrogen in bio-char	$Y_{H,ch} = -0.0041 + 0.10 \exp(-0.0024T)$	0.75
Element of oxygen in bio-char	$Y_{O,ch} = 0.07 + 0.85 \exp(-0.0048T)$	0.56
Element of carbon in bio-tar	$Y_{C,tar} = (1.05 + 1.9 \times 10^{-4}T)Y_{C,F}$	0.07
Element of hydrogen in bio-tar	$Y_{H,tar} = (0.93 + 3.8 \times 10^{-4}T)Y_{O,F}$	
Element of oxygen in bio-tar	$Y_{O,tar} = (0.92 - 2.2 \times 10^{-4}T)Y_{O,F}$	0.07

^a T is the pyrolysis temperature. The subscript F represent dry ash free feedstock based.

the Scheme D can give better prediction of product yield of biomass pyrolysis than Scheme B.



where α , β , γ represent the composition fractions of each component in the biomass, which can be determined through experimental measurements.

The advantage of this scheme is that it can be applied to any biomass feedstock primarily composed of cellulose, hemicellulose, and lignin. Nevertheless, an empirical correlation is still required to determine the content of species in the tar and gas phases. Furthermore, the pyrolysis process involves more parameters and reactions, which results in a significantly higher computational cost compared to Schemes A, B, and C, especially in the multiscale CFD simulation of the BFBG [104].

2.1.2.4. Scheme E: detailed chemical structure based kinetics. The detailed chemical structure-based kinetics was originally proposed by Ranzi [105] from the CRECK group and has since undergone continuous subsequent modifications to the representative macro-components and their kinetic parameters to enhance its predictive performance [106–110]. As shown in Fig. 4 (e), biomass is assumed to be composed of cellulose, hemicellulose, lignin fractions (hydrogen-rich lignin, oxygen-rich lignin, and carbon-rich lignin), and extractives (hydrophobic and hydrophilic extractive components), involving a rather large number of reactions (including drying), gas, and solid species. The composition of these macro-components can be determined via elemental analysis [107]. Thus, Scheme E does not rely on pyrolysis experiments to determine the yield of gas, bio-tar, and bio-char. Furthermore, this scheme can predict not only the yields of gas, bio-tar, and bio-char but also the compositions of pyrolysis products. A comparative study on modeling biomass pyrolysis using schemes C and E indicates that scheme E exhibits better performance in predicting biomass heating rate, pyrolysis rate, and particle shrinkage, whereas Scheme C underestimates the pyrolysis rate under low-temperature conditions [74]. The main drawback of Scheme E is its high complexity, which leads to a dramatic increase in computational cost when incorporated into a multiscale CFD model. Although Scheme E is rarely used in the multiscale CFD simulation of the BFBG [111,112], it has been commonly adopted in CFD-CRN and CRN models for BFBG simulation [113] as well as particle-scale simulations [114–119].

2.1.3. Kinetics of heterogeneous char reactions

Table 3 summarizes the main heterogeneous char reactions during biomass gasification, including char oxidation, and CO_2 and H_2O gasification, and char methanation. For char oxidation, the ratio of CO to CO_2 (η) depends on both operating conditions (e.g., temperature and O_2 concentration) and biomass feedstock type, as discussed by Morin et al. [120]. The commonly used correlations for η are illustrated in Fig. 6. The correlations proposed by Morin et al. [120] and Tognotti et al. [121] yield similar values of η across most temperature

Table 3

The heterogeneous char reaction during biomass gasification.

Reactions	Stoichiometric equation
Oxidation	$\text{C} + \frac{\eta+2}{2\eta+2}\text{O}_2 \rightarrow \frac{\eta}{\eta+1}\text{CO} + \frac{1}{\eta+1}\text{CO}_2$
CO_2 gasification	$\text{C} + \text{CO}_2 \rightarrow 2\text{CO}$
H_2O gasification	$\text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2$
Methanation	$\text{C} + 2\text{H}_2 \rightarrow \text{CH}_4$

ranges, whereas those reported by Arthur [122], and Linjewile and Agarwal [123] produce markedly different profiles. The probable reason for this discrepancy is the use of different char materials: artificial graphite coal char and petroleum coke were employed in the experiments by Arthur [122] and Linjewile and Agarwal [123], whereas biomass char was utilized in the studies by Tognotti et al. [121] and Morin et al. [120]. Although the correlation developed by Tognotti et al. [121] has been validated over a wide temperature range and widely adopted for modeling biomass combustion and gasification in numerous studies [124–126], it should still be noted that biomass feedstock characteristics exert a significant influence on the value of η .

Regarding the kinetics of heterogeneous char reactions, both volume-based and surface-based kinetics have been widely adopted in modeling, with their corresponding expressions given in Eqs. (2) and (3), respectively.

$$\frac{dX}{dt} = k_0 \exp\left(-\frac{Ea}{RT}\right) P^n f(X)^a \quad (2)$$

$$\frac{dX}{dt} = k_0 \exp\left(-\frac{Ea}{RT}\right) P^n S(X) f(X)^a \quad (3)$$

Where k_0 and Ea is the pre-exponential factor and activation energy, respectively. P is the partial pressure of O_2 , H_2O , and CO_2 . $f(X)$ is a function describing the effects of particle conversion on char reactivity, various expressions of $f(X)$ can be found in the reference. $S(X)$ is a function modeling the evolution of specific surface area. To characterize the dynamic

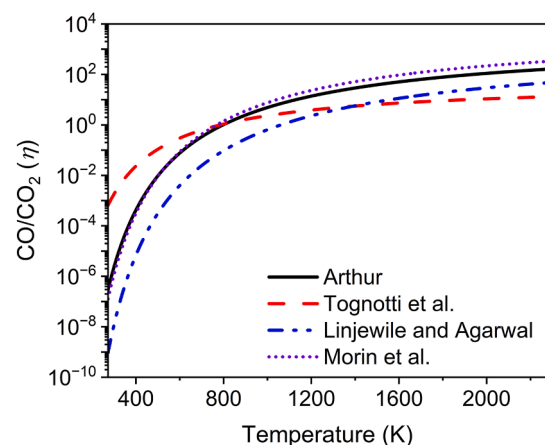


Fig. 6. CO/CO_2 ratio determined from the expression of Morin et al. [120], Tognotti et al. [121], Arthur [122], and Linjewile and Agarwal [123].

evolution of the specific surface area of biomass char during gasification, four classical models have been extensively applied in previous studies, namely the constant specific surface area model, constant reactivity model, random pore model, and classical capillary model [56,124,127–129]. The constant specific surface area model assumes that the specific surface area remains constant during biomass char conversion and can deliver reliable predictions for high-temperature oxidation scenarios where external mass transfer dominates the reaction process. Differently, the constant reactivity model assumes a constant char reaction rate alongside a progressive increase in specific surface area, the char conversion predicted by this model shows good agreement with the few experimental data until the conversion up to 60%. The random pore model, originally established by Bhatia et al. [130], has emerged as a widely adopted model for describing the specific surface area evolution of coal and biomass char particles during combustion and gasification. However, its practical application requires a structural parameter calibrated from experimental measurements or derived from the initial pore size distribution. By contrast, the classical capillary model posits that char particle pores expand as porosity develops, which correspondingly increases the specific surface area [131]. Nevertheless, comparative analysis between model predictions and experimental measurements reveals insufficient valid data to identify the most optimal model for biomass char conversion, leaving no definitive consensus in the existing research [132].

A large variation exists in the reported parameters of both volumetric-based and specific surface area-based kinetics as shown in Fig. 7, thus, it is difficult to find a universal kinetic parameter to model char gasification for various biomass

feedstocks. The reason is that char reactivity highly depends on both feedstocks and operating conditions. For example, the inorganic species and content have significant effects on the char reactivity. Luo et al. [127] found that the overall char reaction rate of pine wood char is much lower than beech wood char, due to the potassium content of pine wood char (150 mg/kg) is much lower than that of beech wood char (1700 mg/kg). Guo et al. [133] investigated the effects of biomass feedstocks on the char reactivity with 40 different wood species, and found that different feedstocks result in different gasification reactivities. Therefore, the selected kinetics of heterogeneous char reactions for multiscale simulation of BFBG should be not only restricted to the same biomass feedstocks but also similar operating conditions. Otherwise, a large deviation may be observed between experimental and modeling results [19].

ML method has been widely applied to quantify the correlations between multi-dimensional input variables and corresponding model outputs [168–170], offering a feasible avenue for the development of universal kinetic models for biomass char gasification. A recent study has demonstrated that deep neural networks can be utilized to construct generalized predictive models for the kinetic parameters governing coal char combustion [171]. Nevertheless, the reactivity of char oxidation, CO₂ gasification, and H₂O gasification is strongly dependent on multiple influencing factors, including feedstock characteristics (e.g., elemental and proximate analysis results, inorganic element content, particle size, and density), operational conditions (e.g., temperature, gaseous component concentration, and pressure), and the pore structure of char particles (e.g., pore size distribution and porosity). Accordingly, a high-quality and comprehensive database of

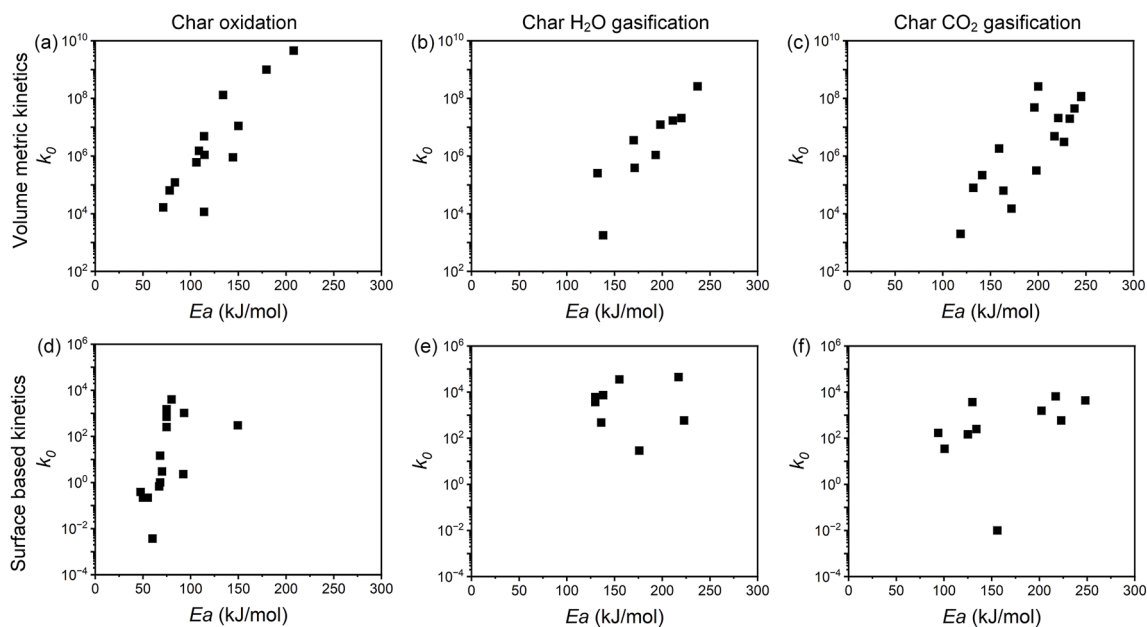


Fig. 7. Parameters for heterogeneous char reaction kinetics. (a), (b), and (c) are the kinetic parameters for the volume-based rate expressions of char oxidation, H₂O gasification, and CO₂ gasification, respectively. (d), (e), and (f) are the kinetic parameters for the surface-based rate expressions of char oxidation, H₂O gasification, and CO₂ gasification, respectively. The corresponding data were obtained from the following references: char oxidation [54,57,120,132,134–148], H₂O gasification [46,139,144,148–157], and CO₂ gasification [132,134,151,152,154,157–167].

kinetic parameters is a prerequisite for establishing a robust, universal ML-based predictive model for biomass char gasification. However, systematic and large-scale datasets of this kind remain scarce in the existing literature, representing a critical research gap and a promising direction for future investigations.

Regarding char methanation kinetic model, both volume-based and surface-based kinetic models have been implemented in multiscale simulation of the BFBG. In contrast to the kinetic parameters for char oxidation, CO_2 and H_2O gasification, the parameters for surface-controlled char methanation exhibit relatively minor variability. The widely adopted surface-based kinetic parameters for char methanation are reported as $k_0 = 3.42 \times 10^{-3} \text{ m/(s} \cdot \text{K)}$ and $E_a = 129.703 \text{ kJ/mol}$ [41,54,111,137,140,172–181]. For volume-based char methanation kinetics, the most commonly used parameter set was originally proposed by Syamlal and Bissett [182] and subsequently modified by Snider et al. [183] and Liu et al. [184] in the CFD modelling of the BFBG using multiphase particle-in-cell (MP-PIC) method. Notably, the reaction rate proposed by Liu et al. [184] is five times of Snider et al. [183]. Both parameter sets from Snider et al. [183] and Liu et al. [184] have been extensively employed in the CFD modelling of the BFBG [42,66,185–190]. However, alternative char methanation kinetic parameter sets have also been adopted in the CFD simulation [144,191–193] and process modelling [194–201] of the BFBG. Therefore, the selection of volume-based kinetic parameters of char methanation should be chosen to match the conditions of the BFBG as closely as possible.

2.2. Particle-scale model

Numerous numerical models have been proposed to simulate the biomass gasification process at the particle scale. Fig.

8 summarizes the typical particle-scale models for biomass gasification regarding their application range, accuracy, and computational cost. More details on the particle-scale model will be discussed as below.

2.2.1. 0D model

The 0D model assumes that sub-particle scale variables (such as temperature, concentration, and particle conversion) are uniformly distributed in the particle, leading to the neglect of intra-particle mass and heat transport, while external mass and heat transfer are considered in the model [202]. Since the spatial distribution at the sub-particle level does not need to be solved, only ordinary differential equations (ODEs) need to be solved in the 0D model, making it the simplest and most easily implemented model in the mainstream multiscale simulation models for BFBG. Therefore, it is the most widely used particle-scale model in the literature [111,175,181,188,203–205]. However, biomass is difficult to comminute primarily due to its robust lignocellulosic framework, in which cellulose, hemicellulose, and lignin form a tightly cross-linked structure with high mechanical strength and toughness. The fibrous nature of cellulose and the binding effect of lignin resist mechanical breakage, while high moisture content also increases material plasticity and reduces grinding efficiency. These characteristics result in high energy consumption and low efficiency in biomass size reduction [206]. Fig. 9 (a) shows a comparison of the typical particle size distributions of coal and biomass; the size of biomass particles is significantly larger than that of coal, resulting in pyrolysis and gasification rates comparable to those of intra-particle heat and mass transfer as shown in Fig. 9 (b). Therefore, neglecting intra-particle heat and mass transfer is unreasonable for most cases of BFBG. A series of particle-scale models for biomass thermochemical conversion processes also proves that the 0D model overestimates the overall heating rate and reaction rate for large

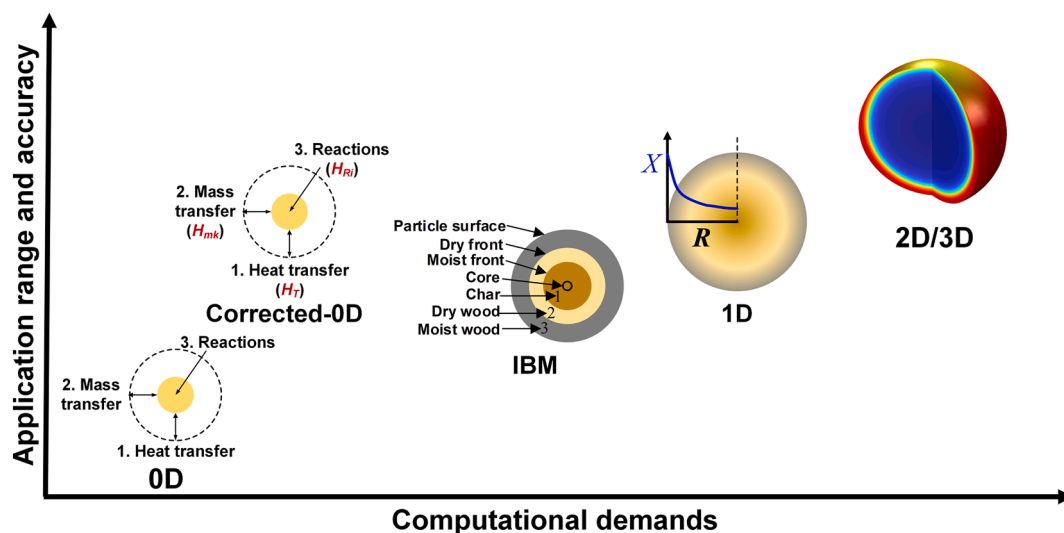


Fig. 8. Typical particle-scale models for biomass gasification. 0D: zero-dimensional model. corrected-0D: 0D model with correction factors to consider the impact of intra-particle heat transfer. IBM: interface-based model. Reprinted with permission from Ref. [43]. Copyright (2013) Elsevier. 1D: one-dimensional model. 2D/3D: two-/three-dimensional model. Reprinted with permission from Ref. [119]. Copyright (2026) Elsevier.

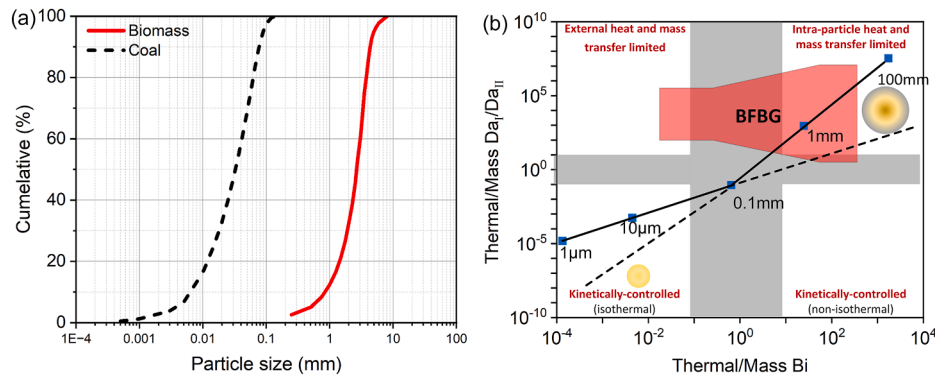


Fig. 9. Typical particle size distributions of coal and biomass particles used in fluidized bed gasifiers (a): the data source of cumulative curve of biomass. Reprinted with permission from Ref. [206]. Copyright (2019) Elsevier. Control regimes of biomass gasification in BFBG are analyzed by thermal and mass Biot numbers (Bi) and Damköhler numbers (b): The Bi is defined as the ratio of the external transfer rate to the intra-particle mass or heat transfer rate. The internal Damköhler number (Da_i) is defined as the ratio of the reaction rate to the intra-particle heat or mass transfer rate. The external Damköhler number (Da_{ii}) is defined as the ratio of the reaction rate to the external heat or mass transfer rate; for more details on their definitions, refer to Gómez-Barea and Leckner [9].

biomass particles [63,116,117,207,208]. Thus, a more advanced particle-scale model is required for the multiscale simulation of the BFBG.

2.2.2. Corrected-0D model

The main disadvantage of the 0D model is that its application range is limited to the kinetically controlled regime, due to the neglect of intra-particle heat and mass transfer. To extend its application scope, corrected-0D models have been proposed, which incorporate intra-particle heat and mass transfer through various correction methods. For example, Dong et al. [209] and Zhong et al. [101] proposed an indirect approach to modify the reaction rate constant by combining intrinsic kinetics with heat penetration rate, aiming to investigate the impact of intra-particle heat transfer on biomass pyrolysis. Compared with the original 0D model, the corrected-0D model predicts a lower yield of bio-tar and a higher yield of char [101], indicating the significant role of intra-particle heat transfer in biomass pyrolysis. However, this indirect method is not suitable for modeling char gasification, as both intra-particle and external mass transfer also exert significant effects on char reactivity. In addition, this method has not been fully validated through detailed particle-scale or reactor-scale experiments, and its reliability and flexibility still need further verification in future research.

An alternative approach to deriving corrected-0D models is to quantitatively analyze the impact of intra-particle heat and mass transfer on biomass gasification by using detailed particle-scale models (e.g., interface-based model, 1D model, and 2D/3D models). Joakim et al. [93] first obtained the spatial and temporal evolution of biomass pyrolysis via a 1D model with apparent kinetics derived from small particles, and then used the particle-resolved data to develop pyrolysis kinetics that account for intra-particle heat transfer effects, significantly improving the prediction accuracy of the 0D model. Espeskvist et al. [210] adopted a similar method, using simulation data from an interface-based model (IBM) to determine the apparent kinetics for large biomass particles, which also

enhanced the predictive performance of the 0D model. It should be noted that intra-particle heat and mass transfer not only affect the reaction rate but also interact with external mass transfer, thus forming a coupling chain of flow-external transport-intra-particle transport-reactions. Therefore, the aforementioned corrected-0D models still overestimate the external heat and mass transfer rates [93], and further optimization is required to better align with actual operating conditions.

To simultaneously account for the influences of intra-particle transport on both external transport and reactions, Luo et al. [202] introduced a corrected-0D model by defining correction coefficients for external heat transfer (H_T), external mass transfer (H_m), and reaction rate (H_r). The correction coefficients are determined through a quantitative comparison of the external heat transfer rate, external mass transfer rate, and reaction rate predicted by the 0D and 1D model, respectively. These correction coefficients can be correlated as a function of particle-scale gasification parameters, such as the dimensionless particle temperature ($\theta = (T_p - T_{p0})/(T_e - T_{p0})$, where T_{p0} , T_p , and T_e represent the initial particle temperature, particle temperature, and environmental temperature, respectively), Biot number, and particle conversion. Fig. 10 (a) and 10 (b) show a comparison of the 0D, corrected-0D, and 1D models used in the particle-scale modeling of biomass pyrolysis for medium-sized (3–5 mm) and large-sized (24.5 mm) particles, respectively. Zheng et al. [211] also demonstrated that the corrected-0D model can be easily implemented in reactor-scale simulations. Fig. 10 (c) presents a comparison of these three models in the particle-scale modeling of the char gasification. The results indicate that the corrected-0D model yields similar results to those of the 1D model, whereas the 0D model overestimates the overall heat transfer rate and reaction rate. This confirms that the correction method effectively extends the application range of the 0D model to regimes controlled by either external or intra-particle heat and mass transfer.

Since determining the correction coefficients requires solving the 1D model, the procedure is rather complex. To efficiently obtain the correction coefficients, a machine

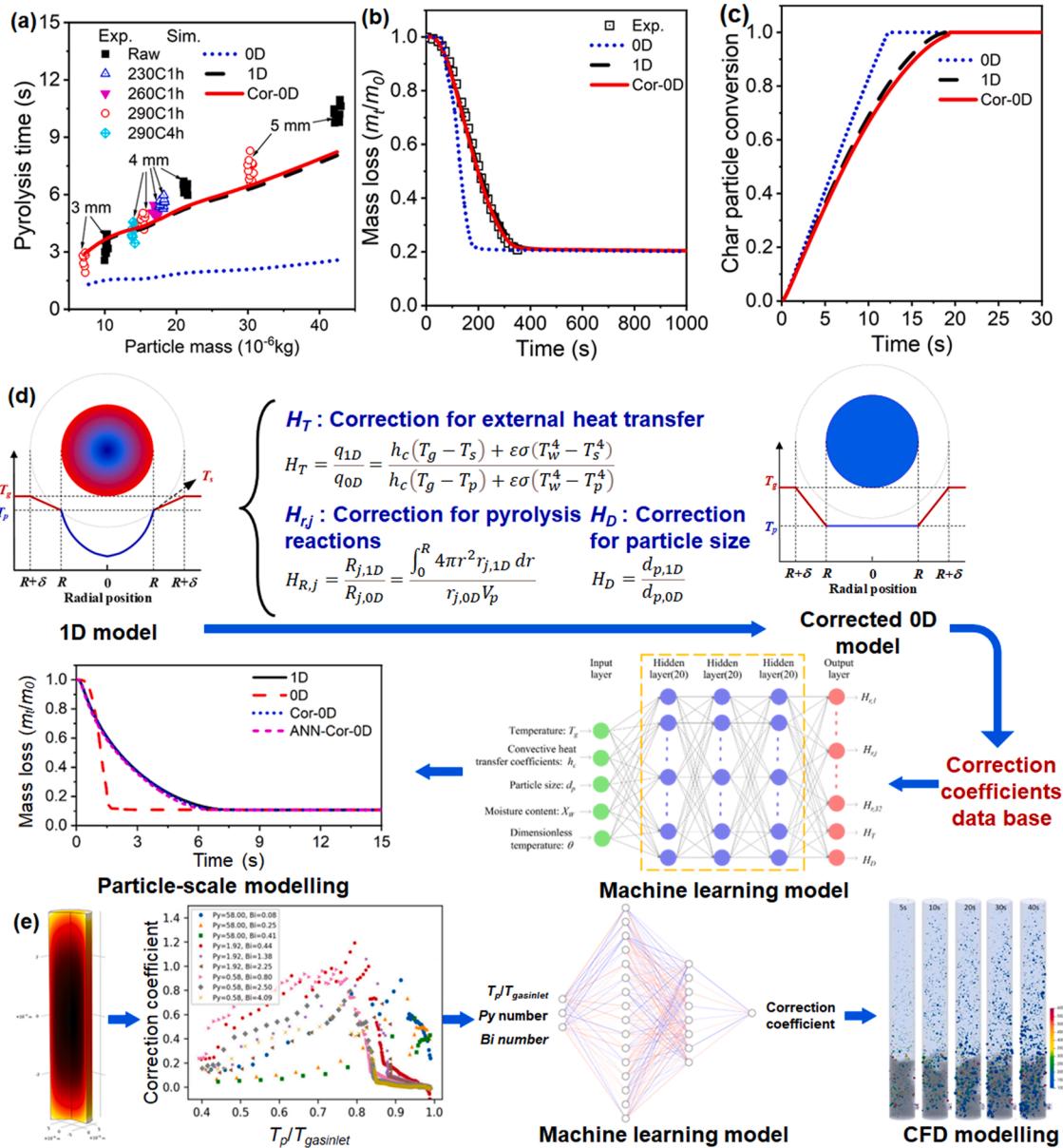


Fig. 10. A comparison of 0D, corrected-0D, and 1D model in predicting particle-scale biomass pyrolysis (a) and (b), and char gasification process (c), and machine learning method employed to determine correction coefficients proposed by Luo et al. [117] (d) and Lu et al. [212] (e). 0D: 0D model, 1D: 1D model, Cor-0D: corrected-0D model. The original data of Fig. 10 (a) is adapted from Luo et al. [202]; Reprinted with permission from Ref. [202]. Copyright (2020) American Chemical Society. The original data of Fig. 10 (b) and (d) are adapted from Luo et al. [117]; Reprinted with permission from Ref. [117]. Copyright (2023) Elsevier. Fig. 10 (e) is reprinted from Lu et al. [212]; Reprinted with permission from Ref. [212]. Copyright (2022) Elsevier.

learning method has been applied to predict them, as illustrated by Luo et al. [117], as shown in Fig. 10 (d). A similar approach was adopted by Lu et al. [212], who used the method to model biomass pyrolysis in a bubbling fluidized bed reactor (see Fig. 10 (e)). Their findings show that coupling a machine learning-derived corrected-0D model into reactor-scale CFD simulations not only improves prediction accuracy compared to the 0D model but also significantly reduces computational costs compared to the 1D model. Therefore, the machine learning-assisted corrected-0D model is expected to serve as a reliable and efficient particle-scale model for the multiscale simulation of the BFBG.

2.2.3. Interface-based model

The interface-based model (IBM) was originally proposed by Thunman et al. [137] for modeling biomass combustion. This model divides a biomass particle into four layers (i.e., moist wood, dry wood, char, and core layers) and assumes that drying, pyrolysis, and char gasification reactions occur exclusively at infinitely thin interfaces: the moist front, dry front, and particle surface, respectively, as shown in Fig. 7. The intra-particle heat transfer within each layer is solved using heat balance equations. It is worth noting that the IBM model can be simplified to the unreacted shrinking core model when drying and pyrolysis processes are neglected. This

simplification is feasible, because char oxidation, CO_2 gasification, and H_2O gasification reactions occur exclusively on the outer surface of the unreacted core [124,178]. Accordingly, the unreacted shrinking core model represents a special case of the IBM model [1].

The primary motivation for developing the IBM model is to reduce the computational cost of reactor-scale CFD simulations for biomass thermochemical conversion processes involving large-sized particles. Mehrabian et al. [54] implemented the IBM into a CFD model to simulate particle-scale experiments and demonstrated that it can provide good predictions of biomass thermal conversion processes. Ström and Thunman [43] discussed the computational efficiency of the IBM model when integrated with a CFD model and concluded that the IBM model is suitable for large-scale simulations. Consequently, the IBM model has been extensively applied in reactor-scale CFD modeling of biomass thermochemical conversion processes [45,177,213].

Since the IBM model assumes that reactions occur at the infinitely thin interfaces between different layers, a prerequisite is that the reaction rate is much faster than the intra-particle heat and mass transfer rates ($\text{Da}_1 \gg 1$). For cases where the reaction rate is comparable to the intra-particle heat and mass transfer rates, a large deviation may be observed between experimental data and modeling results [178,207,214]. Another weakness of the IBM model is that the boundary conditions for each individual particle must be solved; thus, it can only be implemented in CFD-DEM models and is not easily integrated into MFM, CFD-CRN, and CRN models. Moreover, the IBM remains complex when handling the highly varied boundary conditions of biomass particles while maintaining high computational efficiency, and the assumption of an infinitely thin interface reaction zone may reduce the robustness of the CFD solver [19].

2.2.4. 1D model

The 1D model directly and simultaneously solves the external and intra-particle heat and mass transfer, as well as reaction processes. If a momentum balance equation is included, the flow field inside the particle can also be resolved, thus enabling easy acquisition of both spatial and temporal distributions. Therefore, the 1D model has been extensively employed to investigate biomass gasification behavior at the particle scale for simple geometries (i.e., spherical, cylindrical, and flat particles) [56,127,132].

Although numerous particle-scale simulations have shown that the 1D model can provide reasonable predictions of biomass gasification for large particles under various operating conditions, its application in reactor-scale simulations of the BFBG remains rarely reported in the literature [112,208,215]. Von Berg [215] implemented a 1D pyrolysis model in the reactor-scale CFD modeling of biomass gasification in the BFBG. They found that incorporating a 1D model into the CFD simulation significantly improved the simulation performance, but it also led to a significant increase in computational demand. A similar conclusion was drawn from a study by Gao et al. [115]. Thus, one of the main weaknesses of the 1D model is its low computational efficiency, which makes it

unaffordable for the large-scale BFBG simulations. Another shortcoming of the 1D model is the same as that of the IBM model, it also requires tracking each individual particle to obtain its boundary conditions. Consequently, the 1D model is only applicable in the CFD-DEM.

2.2.5. 2D/3D models

Compared with the 1D model, the 2D/3D model not only can directly solve the external and intra-particle heat and mass transfer as well as reaction processes, but also can account for the anisotropic characteristics and complex shapes of biomass particles. These advantages enable the 2D/3D model to investigate biomass gasification behavior with various particle shapes [119]. However, an increase in dimensionality leads to greater complexity in model implementation and higher computational costs. Therefore, the 2D/3D model has only been gradually employed to investigate biomass gasification behavior at the particle scale [65,69,119,216–219]. The application of 2D/3D particle-scale models in multiscale simulations is rarely reported in the literature. Recently, Lu et al. [217] proposed a glued-sphere CFD-DEM method to model the pyrolysis of biomass particles with arbitrary shapes in a fluidized bed reactor. This model has been validated by both particle-scale and reactor-scale experiments. However, the glued-sphere method only solves intra-particle heat transport phenomena and ignores intra-particle mass transfer, making it still far from being applicable in reactor-scale simulations of the BFBG.

2.2.6. Coupling evolution of particle physical morphology in particle-scale models

The morphological evolution of biomass particles during gasification exerts a remarkable influence on intra-particle and external heat and mass transfer. Therefore, incorporating such morphological variations into particle-scale models is essential for accurate reaction prediction. As summarized in a recent review [16], particle morphological evolution during biomass gasification is primarily driven by particle shrinkage and fragmentation. Particle shrinkage is generally governed by mass loss stemming from moisture evaporation, pyrolysis, and char conversion. Accordingly, particle shrinkage is commonly assumed to be a function of particle conversion. Di Blasi proposed a classical model that adopts three parameters (α , β , and γ) to characterize the particle shrinkage process [220]. Specifically, α is used to describe to what extent the volumetric shrinkage is increasing linearly with the char mass, β is used to describe the amount of the solid volume is added to the gas phase volume due to conversion reactions, and γ is used to account the particle shrinkage caused by internal structural changes of biomass particle. This model has been widely implemented in CFD simulations of biomass thermochemical conversion processes [221–224]. However, these three parameters are not related to the common definition of shrinkage factors as described by Hagge and Bryden [225]. Moreover, the selection of α , β , and γ values lacks universal criteria, as these parameters are calibrated to fit experimental data rather than measured directly via experiments [19]. To address this

limitation, a more intuitive and straightforward method assumes a linear correlation between particle shrinkage and biomass solid conversion, enabling shrinkage factors to be easily determined from experimental measurements. This simplified shrinkage model has been widely adopted in numerous studies [56,93,117,226,227]. Since particle shrinkage is defined as a function of particle conversion, the shrinkage model can be conveniently coupled with either the global particle conversion calculated by 0D and corrected-0D models or the localized particle conversion resolved by high-fidelity particle-scale models (e.g., IBM, 1D, and 2D/3D models). The fragmentation of biomass particles occurs when intra-particle stress exceeds the particle's structural strength. As the pressure, porosity, and temperature of particle have significant effects on the intra-particle pressure force, stress limit of the material, and thermal stress, the fragmentation of biomass particles can only be implemented in a detailed particle-scale models (i.e., IBM, 1D, and 2D/3D models), while the 0D and corrected-0D models are not easy to describe the evolution of particle physical morphology caused by the fragmentation.

2.3. Meso-scale model

Meso-scale models are used to describe the momentum (via drag models), heat (via interphase heat transfer models), and mass (via interphase mass transfer models) exchange between fluid and solid phases. The accuracy of meso-scale models has a significant impact on the external heat and mass transfer

between biomass particles and their surroundings, thereby affecting the overall performance of reactor-scale models. Therefore, meso-scale models also play an important role in the multiscale simulation of the BFBG. Since the exchange between fluid and solid phases is explicitly resolved in CFD models, but it is not explicitly resolved in other reactor-scale models, the discussion of meso-scale models focuses mainly on the multiscale CFD simulation of the BFBG. As the grid is the minimum element after the discretization of the governing equations of the CFD model, the commonly employed meso-scale models can be classified into three types (i.e., Homogeneous model [228], Filtered model [229], and EMMS model [230]) based on how the sub-grid structure is solved, as shown in Fig. 11. The expressions of the commonly used meso-scale models are summarized in Table 4.

Homogeneous models assume that field variables within each grid are uniformly distributed, regardless of grid size, as shown in Fig. 11 (a). These models are usually derived from experimental measurements. For drag models describing the momentum exchange between fluid and solid phases, representative models include Gidaspow [228], Wen and Yu [232], Ergun [233], Syamlal–O'Brien [234], and Huilin–Gidaspow [235], which have been widely used in CFD simulations of BFBG. The Wen and Yu [232] and Ergun [233] drag models are widely employed to model dilute and dense fluidized bed reactors, respectively. The Syamlal–O'Brien drag model is proposed as a favorable choice for bubbling and turbulent fluidized bed reactors [234]. The Gidaspow drag model is a combination of the Wen and Yu, and Ergun drag models,

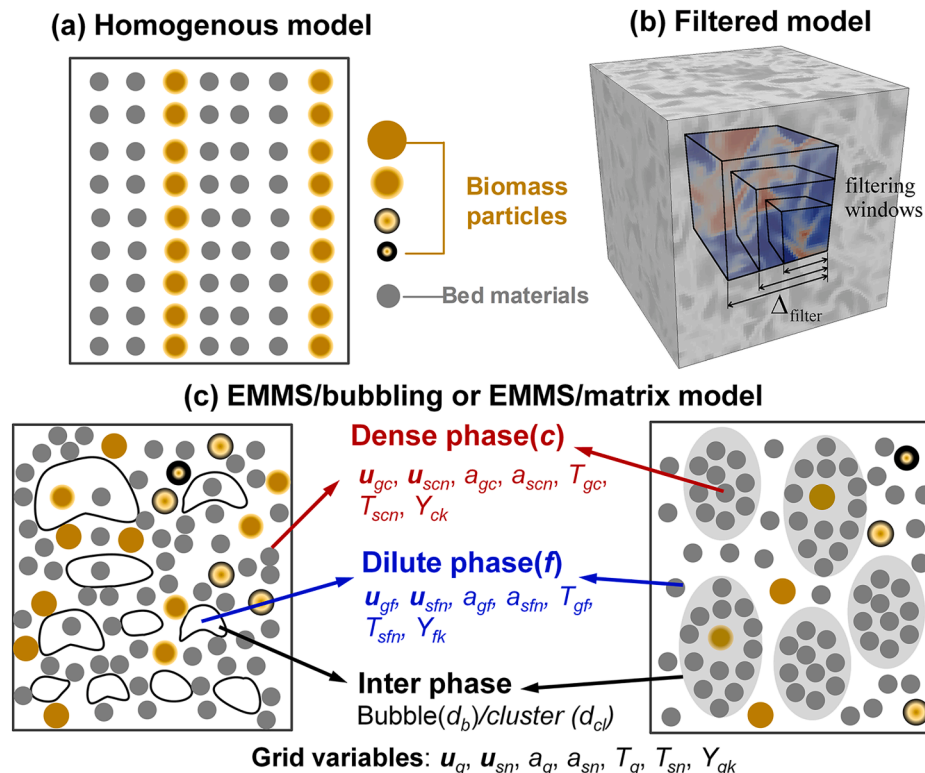


Fig. 11. Commonly employed meso-scale models in the multiscale simulation of BFBG. (a) Homogenous model. (b) Filtered model. Reprinted with permission from Ref. [231]. Copyright (2016) Elsevier. (c) EMMS/bubbling or EMMS/matrix model.

Table 4
Expressions of the commonly used meso-scale models.

Models	References	Expressions
Drag models		
Homogenous	Wen and Yu [232]	$\beta = \frac{3}{4} C_D \frac{\epsilon_s \epsilon_g \rho_g}{d_s} u_g - u_s \epsilon_g^{-2.65}$ $C_D = \begin{cases} \frac{24}{\epsilon_g \text{Re}} \left[1 + 0.15 (\epsilon_g \text{Re})^{0.687} \right] & (\text{Re} < 1000) \\ 0.44 & (\text{Re} \geq 1000) \end{cases}$
	Ergun [233]	$\beta = 150 \frac{\epsilon_s^2 \mu_g}{\epsilon_g d_s^2} + \frac{1.75 \epsilon_s \rho_g}{d_s} u_g - u_s $
	Gidaspow [228]	$\beta = \begin{cases} \frac{3}{4} C_D \frac{\epsilon_s \epsilon_g \rho_g}{d_s} u_g - u_s \epsilon_g^{-2.65} & (\epsilon_g \geq 0.8) \\ 150 \frac{\epsilon_s^2 \mu_g}{\epsilon_g d_s^2} + \frac{1.75 \epsilon_s \rho_g}{d_s} u_g - u_s & (\epsilon_g < 0.8) \end{cases}$
	Syamlal-O'Brien [234]	$\beta = \frac{3 \epsilon_s \epsilon_g \rho_g}{4 \nu_r^2 d_s} C_D u_g - u_s $ $C_D = \left[0.63 + \frac{4.8}{\sqrt{\text{Re}/\nu_r}} \right]^2$ $\nu_r = 0.5 \left[A - 0.06 \text{Re} + \sqrt{(0.06 \text{Re})^2 + 0.12 \text{Re}(2B - A) + A^2} \right]$ $A = \epsilon_g^{4.14}, B = \begin{cases} 0.8 \epsilon_g^{1.28} & (\epsilon_g \leq 0.85) \\ \epsilon_g^{2.68} & (\epsilon_g > 0.85) \end{cases}$
	Huilin-Gidaspow [235]	$\beta = \frac{3}{4} \phi C_D \frac{\epsilon_s \epsilon_g \rho_g}{d_s} u_g - u_s \epsilon_g^{-2.65} + (1 - \phi) \left(150 \frac{\epsilon_s^2 \mu_g}{\epsilon_g d_s^2} + \frac{1.75 \epsilon_s \rho_g}{d_s} u_g - u_s \right)$ $\phi = \frac{\arctan[150 \times 1.75(0.2 - \epsilon_s)]}{\pi} + 0.5$
	Di Felice [236]	$\beta = \frac{3}{4} \left(0.63 + \frac{4.8}{\sqrt{\text{Re}}} \right)^2 \frac{\rho_g \epsilon_g \epsilon_s u_g - u_s }{d_s} \epsilon_g^\chi$ $\chi = 3.7 - 0.65 \exp \left[- \frac{(1.5 - \log \text{Re})^2}{2} \right]$
	Mazzei and Lettieri [237]	$\beta = \frac{3}{4} \left(0.63 + \frac{4.8}{\sqrt{\text{Re}}} \right)^2 \frac{\rho_g \epsilon_g \epsilon_s u_g - u_s }{d_s} \epsilon_g^{2-2n}$ $n = \frac{4.8 + 0.42 \text{Re}^{3/4}}{1 + 0.175 \text{Re}^{3/4}}$
	Filtered	$\beta = \frac{3}{4} C_D \frac{\epsilon_s \epsilon_g \rho_g}{d_s} u_g - u_s \epsilon_g^{-2.65} H_D$ The expression of H_D can be found in the corresponding reference
	EMMS	$\beta = \frac{3}{4} C_D \frac{\epsilon_s \epsilon_g \rho_g}{d_s} u_g - u_s \epsilon_g^{-2.65} H_D$ The value of H_D depends on physical properties of gas and solid phase, and operating conditions of fluidized bed and can be obtained by solving the EMMS model.

(continued on next page)

Table 4 (continued)

Models	References	Expressions
Interphase heat and mass transfer models^a		
Homogenous	Ranz and Marshall [275]	$Nu = 2.0 + 0.6Re^{1/2} Pr^{1/3}$
	Li and Mason [276]	$Nu = \begin{cases} 2.0 + 0.6\epsilon_g^{3.5} Re^{1/2} Pr^{1/3} & (Re < 200) \\ 2.0 + 0.5\epsilon_g^{3.5} Re^{1/2} Pr^{1/3} + 0.02\epsilon_g^{3.5} Re^{0.8} Pr^{1/3} & (200 \leq Re < 1500) \\ 2.0 + 0.00045\epsilon_g^{3.5} Re^{1.8} & (Re > 1500) \end{cases}$
	Gunn [277]	$Nu = (7 - 10\epsilon_g + 5\epsilon_g^2)(1 + 0.7Re^{0.2} Pr^{0.33}) + (1.33 - 2.40\epsilon_g + 1.2\epsilon_g^2)Re^{0.7} Pr^{0.33}$
	Zhu et al. [278]	$Nu = (-0.83 + 16.21\epsilon_g - 14.67\epsilon_g^2)(1 - 0.01Re^{0.2} Pr^{1/3}) + (1.5 - 2.60\epsilon_g + 1.31\epsilon_g^2)Re^{0.7} Pr^{1/3}$
Filtered	Huang et al. [279,280], Li et al. [281,282], Zhu et al. [283], Lei et al. [284], Du et al. [285], Wang et al. [286]	As the expression of the filtered based heat and mass transfer model is rather complex, its detailed expression of can be found in the corresponding references.
EMMS	Dong et al. [287,288], Liu et al. [289], Liu et al. [290], Zhang et al. [291,292]	As the expression of the EMMS based heat and mass transfer model is rather complex, its detailed expression of can be found in the corresponding references.

Note: u is the velocity (m/s), β is drag coefficient for gas and solid phase ($kg/m^3/s$), ϵ is volume fraction, C_D is the drag coefficient for a single particle, d_s is the particle diameter (m), ρ is the density (kg/m^3), the subscript g and s is gas and particle phase, respectively. H_D is the heterogeneous index.

^a The expression of a heat transfer model can be converted to mass transfer model by substituting Prandtl number (Pr) and Nusselt number (Nu) as Schmidt number (Sc) and Sherwood number (Sh). Therefore, only the expression of Nu is listed in the Table 4. The Nu and Sh can be further used determine the interphase heat and mass transfer coefficients.

aiming to extend the application range of drag models [228]. Since the Gidaspow drag model is a discontinuous function, it was further modified by Huilin and Gidaspow with a transition equation to improve numerical stability. Details on the discussion of homogeneous drag models can be found in Wang et al. [44]. For heat and mass transfer models, the correlations of Ranz and Marshall [275], and Gunn [277] have been extensively employed in multiscale simulations of BFBG. The Ranz and Marshall equation is derived from single-particle experiments, while the Gunn model is derived from fixed-bed experiments and has been extended to applications in fluidized bed reactors. Dong et al. [287,288] summarized the commonly employed homogeneous mass transfer models and observed a large variation in the Sherwood number when using these correlations. In addition to deriving correlations from experimental data, high-fidelity discrete numerical simulations have also been gradually employed to develop interphase exchange models [44]. However, numerous studies have found that grid size has a significant effect on modeling results, as the heterogeneous structure at the sub-grid level is not resolved [229,254]. Thus, one weaknesses of homogeneous models is that fine grids are required in CFD simulations [293], which significantly increases computational costs and even makes large-scale simulations unaffordable [208,294]. Another shortcoming of homogeneous drag models is that their correlations are derived from experimental data or high-fidelity simulation data under narrow operating conditions, making the extension of these models to other conditions questionable.

Compared to fine-grid simulations using homogeneous meso-scale models, the computational cost of coarse-grid simulations is much lower [258]. Therefore, numerous studies have been conducted to account for the heterogeneous structure at the sub-grid level to enable coarse-grid simulations [229,291,295]. The filtered method is one of the representative

approaches to account for the impact of heterogeneous structures on modeling results [229,231,243,245,246]. This model derives interphase exchange correlations from highly resolved periodic domain simulations, which are usually a function of filter size, as shown in Fig. 11 (b). The filtered drag model was first introduced by Igcı et al. [238] to simulate the hydrodynamic behaviors of bubbling fluidized beds and circulating fluidized beds using MFM. In this model, the drag coefficient is expressed as a function of filter size and voidage. They found that grid-independent simulation results are achieved when the filtered model is incorporated into the two-fluid model, indicating that the model is applicable to coarse-grid simulations. The filtered method has been used in a series of studies to derive phase exchange correlations for the MFM [246,247,250,279]. Although the filtered drag model has been extensively employed in multiscale simulations of hydrodynamic behaviors in fluidized bed reactors, its application to BFBG is rarely reported in the literature. One reasons is that the heterogeneous structure at the sub-grid level is not explicitly resolved by the filtered method; therefore, it is not easily used to derive heat and mass transfer correlations, as the reacting flow-transport-reaction processes are much more complex than multi-phase flow behaviors alone. In addition, the parameters in the filtered model are obtained from CFD simulations with pre-defined physical properties of gas and solid phases. However, the physical properties of gas and solid phases change significantly during biomass gasification processes; thus, extending the filtered method to multiscale simulations of the BFBG is suggested for future work.

In addition to the filtered method, an alternative approach to account for the impact of heterogeneous structures on flow-transport-reaction behaviors is the energy minimization multi-scale (EMMS) method. Originally proposed by Li [296] to predict the saturation carrying capacity of circulating fluidized

beds at the global scale, the EMMS method was further developed by Yang et al. [252,253], who introduced an acceleration term for both dense and dilute phases to obtain a heterogeneous structure-dependent EMMS drag model (as shown in Fig. 11 (c)), which is the first version of the EMMS model incorporated into the MFM. This model exhibits much better performance than the Gidaspow drag model in predicting hydrodynamic behaviors. Wang and Li [254] further extended the model using a two-step scheme (namely the EMMS/matrix model) and defined a heterogeneity index ($H_D = \beta/\beta_{Wen \text{ and } Yu}$, where β is the effective drag coefficient and $\beta_{Wen \text{ and } Yu}$ is the coefficient given by Wen and Yu) to quantitatively describe the effects of heterogeneous structures on drag force. Lu et al. [258] found that the modeling results of the EMMS/matrix model show weak grid dependence and are applicable to coarse-grid simulations for fast fluidization under various conditions. The EMMS model was further modified by Shi et al. [260] and Hong et al. [261] to enable its application in bubbling fluidized beds (EMMS/bubbling). Similar to the EMMS/matrix model, Luo et al. [266] revised the heterogeneity index as a binary function of slip velocity and voidage, and they found that the model provides good predictions of the

hydrodynamic behaviors of bubbling and turbulent fluidized beds in coarse-grid simulations. Since the heterogeneous structure is explicitly resolved in the EMMS model, it can be easily implemented to account for the effects of heterogeneous structures on heat and mass transfer between gas and solid phases, as demonstrated by Liu et al. [289] and Zhang et al. [291]. Moreover, the EMMS model has been extensively employed in large-scale simulations of fluidized bed reactors [256,297–300]. Therefore, the EMMS model is expected to be one of the most promising meso-scale models for multiscale simulations of the BFBG.

In recent years, ML methods have been extensively used to assist the development of filtered models and EMMS models [243,245,248,271,273]. Lu et al. [245] developed a filtered CFD-DEM drag model using an artificial neural network, as shown in Fig. 12 (a). This model exhibited higher accuracy than the homogeneous Wen and Yu drag model and the filtered drag model derived from the two-fluid model; they also highlighted that conventional nonlinear regression should not be abandoned if it can achieve regression performance similar to that of machine learning models. Zhu et al. [243] employed machine learning methods to analyze the effects of input

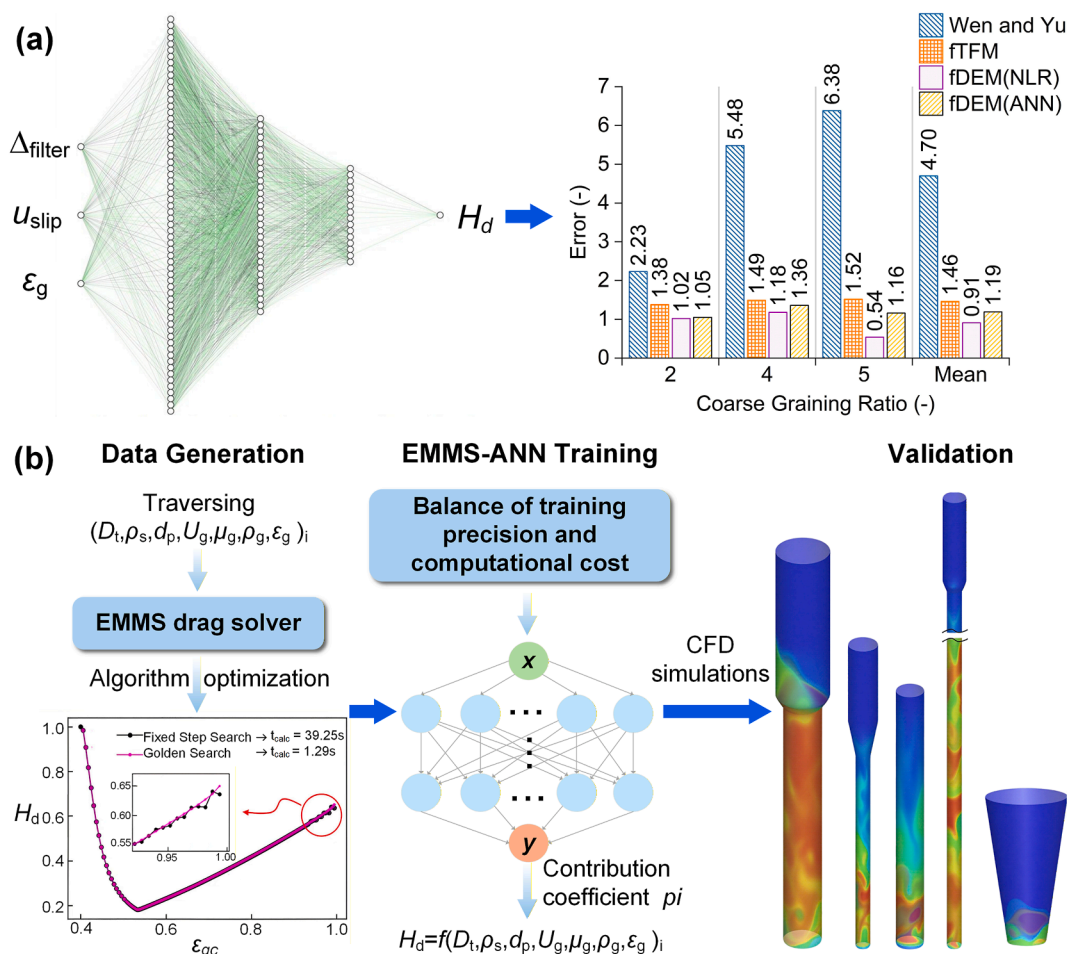


Fig. 12. Application of ML method to assist the development of meso-scale model. (a) ML derived filtered CFD-DEM drag model. Reprinted with permission from Ref. [245]. Copyright (2022) American Chemical Society. (b) ML derived EMMS drag model. Reprinted with permission from Ref. [231]. Copyright (2016) Elsevier.

parameters on the performance of the filtered drag model. The use of ML methods to derive filtered models can also be found in the literature [243,245,248,249,251,283]. Yang et al. [271] developed a generic EMMS drag model for simulating dense fluidized bed reactors using an artificial neural network, which extended the EMMS drag model to various operating conditions and material properties. This is because the heterogeneity index is correlated as a function of multiple parameters, as shown in Fig. 12 (b). A similar method was also adopted by Stamatopoulos et al. [273] to simulate a fluidized bed reactor for chemical loop combustion. Therefore, ML methods are indeed a powerful tool to assist the development of meso-scale models.

3. Multiscale coupling in the simulation of BFBG

3.1. Thermodynamic equilibrium and kinetic model

The thermodynamic equilibrium and kinetic (EK) model assume that drying, biomass pyrolysis, char gasification and oxidation, as well as gas-phase oxidation and gasification, occur separately in the BFBG. In process simulation tools (such as Aspen Plus and AVEVA PRO/II), a series or parallel combination of thermodynamic equilibrium, kinetic, mixing, and separation modules is used to simulate the biomass gasification process [34,198,301,302]. This model is employed to investigate the global heat and mass balance of the BFBG, rather than the detailed flow, heat, and mass transfer processes within it. The particle-scale models and meso-scale models are generally not resolved in the EK model; instead, empirical correlations and molecular-scale models are directly integrated into the modules, as summarized in Fig. 13. Therefore, there is no direct coupling between the EK model and particle- and meso-scale models.

The main advantage of the EK model is that it provides the most efficient way to obtain the global performance of the BFBG, due to its low computational cost. Thus, it has been extensively employed in the process modeling of BFBG, as summarized in recent reviews [32,38]. For example,

Lombardelli et al. [302] assumed that biomass gasification reactions occur sequentially. They adopted the RYield and RStoic modules to simulate biomass pyrolysis and char gasification, respectively, and employed a REquil module to simulate gas-phase oxidation and reduction reactions. The results were used in the techno-economic assessment of process configurations for producing bio-methanol from residual forestry biomass gasification. A similar method was also adopted by Fan et al. [201] to optimize the operating conditions of BFBG. However, the EK model ignores the interaction between bed material and biomass particles, making it difficult to analyze the effect of particle properties on the overall characteristics of the reactor. Kaushal and Tyagi [303] attempted to incorporate empirical hydrodynamic equations for fluidized beds, enabling the model to preliminarily analyze the influence of bed material particle size on gasification efficiency and product yields. Nevertheless, the accuracy and generalizability of these empirical equations have yet to be verified. Moreover, the assumption that reactions occur separately results in a decoupled process of drying, biomass pyrolysis, char gasification, and gas-phase oxidation and reduction. This is inconsistent with the actual situation in fluidized beds, where multiple reactions occur simultaneously and are mutually coupled. More importantly, the EK model mainly focuses on the overall mass and energy balance and global performance of the BFBG; the details of particle- and meso-scale transport processes are not coupled in the model. Thus, it can only reflect the effects of parameters such as temperature, pressure, and feed flow rate on the overall performance, and is unable to conduct in-depth analysis of the influences of factors such as biomass particle properties, particle size, and reactor geometry configurations [32,38].

3.2. Chemical reactor network model

Unlike EK models, which are mainly developed based on the characteristics of the biomass gasification process, chemical reactor network (CRN) model is established based on the hydrodynamic behaviors of BFBG. In this model, the BFBG is first divided into multiple zones according to its

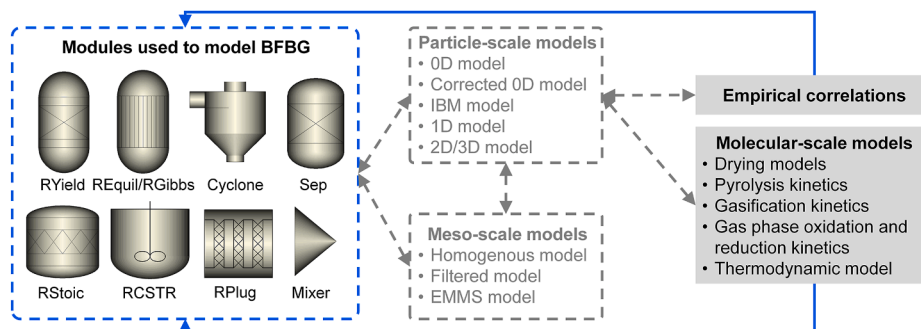


Fig. 13. Multiscale coupling in the thermodynamic equilibrium and kinetic model for modelling BFBG. RYield: a module to predict the yield of reaction product. REquil/RGibbs: thermodynamic equilibrium model to predict reaction product using equilibrium equations or free energy minimization method. Cyclone: a module to separate solid and gas phase. Sep: a module designed for quick separation simulations and preliminary process design without rigorous thermodynamic calculations. RStoic: a module to simulation reactions using strict mass balance principle without requiring kinetics data. RCSTR and RPlug are kinetic based module with assumption of perfect mixing and without radial mixing, respectively. Mixer: a module to mixing inlet streams into a single stream using strict mass and heat balance principles. The grey dash line means that the model is not coupled.

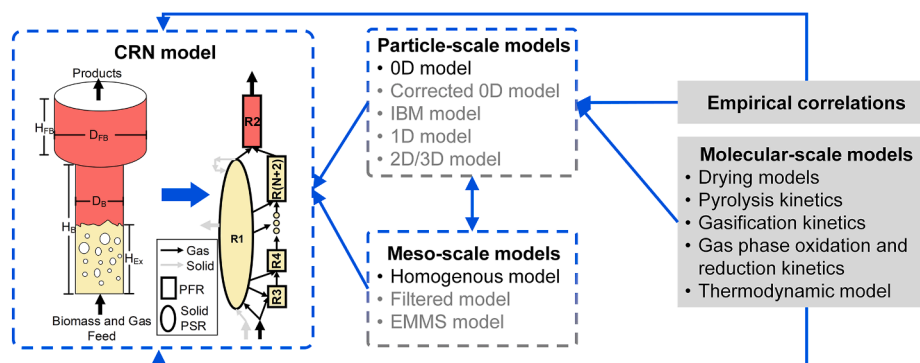


Fig. 14. Multiscale coupling in the chemical reactor network model for modelling the BFBG. The dimensions of the BFBG can be considered in the CRN model (H_{FB} : height of freeboard, D_{FB} : diameter of the freeboard, H_B : height of bubbling bed, D_B : diameter of the bubbling bed, H_{EX} : expanded bed height). The topology structure of CRN model is adapted from Berkel et al. [30]; Reprinted with permission from Ref. [30]. Copyright (2024) Elsevier.

flow field or solid-phase concentration distribution to form the topological structure of the CRN model. Then, ideal reactor modules, either continuous stirred tank reactors (CSTRs) or plug flow reactors (PFRs), are selected for each zone based on its flow regime characteristics, and finally interconnected according to its topological structure [22,28–30,303,304]. As the topological structure of the CRN model is predefined, the coupling method between the CRN model and particle and meso-scale models is more likely one-way coupling. A summary of the multiscale coupling of CRN models is given in Fig. 14.

Kaushal et al. [303] established a CRN model for a BFBG by dividing the dense phase region into multiple bubble phases and an emulsion phase based on the two-phase theory, coupled with empirical correlations from fluidized bed hydrodynamic models. A 0D model was employed to describe the char conversion process. This CRN model can not only predict the outlet composition and product yields, but also obtain the axial distribution of component concentrations. However, this model adopted a lumped reaction kinetic model, which is unable to predict the detailed composition of tar. Stark et al. [28] and Richard et al. [304] divided a bubbling BFBG into a dense phase region and a dilute phase (freeboard) region based on its hydrodynamic structure. They selected an isothermal CSTR module for the dense phase region and an isothermal PFR module for the dilute phase, forming a topological structure of series-connected CSTR and PFR modules. A detailed biomass gasification mechanism was also integrated into the CRN model; thus, more detailed information about the products can be obtained through this model. Berkel et al. [30] refined the CRN configuration for the dense phase region based on the classical two-phase theory [305], dividing the dense phase region at the bottom of the bubbling BFBG into an emulsion phase and a bubble phase. The emulsion phase was described using a CSTR module, while the bubble phase was represented by multiple series-connected PFR modules. The optimal number of PFR modules for the bubble phase was determined by experimental data. In their work, empirical correlations and molecular models were directly integrated into the CRN, in a similar way to EK models.

Since only kinetic-based models are employed in the CRN model, drying, biomass pyrolysis, char gasification, and gas-phase oxidation and reduction reactions can be simulated simultaneously. Additionally, reactor geometry configurations, simplified meso-scale, and particle-scale models can also be integrated together. These features offer several advantages over EK models (e.g., the CRN model can provide a coarse spatial distribution of species concentrations, and its performance is superior to that of the EK model). Therefore, the CRN model has become one of the mainstream methods in the multiscale simulation of the BFBG in recent years. However, the model still lacks the ability to integrate advanced particle- and meso-scale models. The impacts of intra-particle transport processes and meso-scale structures are still rarely accounted for in the model. Moreover, the transport parameters between individual ideal reactors in CRN models rely excessively on empirical correlations, and the artificially established topological structure of the CRN model is usually oversimplified, thereby restricting its application range and generalizability.

3.3. Computational fluid dynamics model

Computational fluid dynamics (CFD) model, including both Euler-Lagrange (E-L) method and Eulerian multi-fluid model (MFM), solves the detailed continuity, momentum, energy, and species transport equations to describe the multi-scale transport-reaction phenomena during the biomass gasification process. The detailed spatial and temporal distributions of various variables (such as velocity, temperature, particle conversion, and species concentration) can be simultaneously obtained from CFD simulations. Therefore, CFD models are applicable to support the design, optimization, and scale-up of the BFBG. Since the detailed coupled flow, transport, and reaction processes are fully resolved, all sub-models reviewed in Section 2 can be implemented in CFD models, as shown in Fig. 15. The empirical correlations used to determine the yield of pyrolysis products and the molecular-scale models used to determine reaction rates are integrated into particle-scale models to derive the source terms for CFD

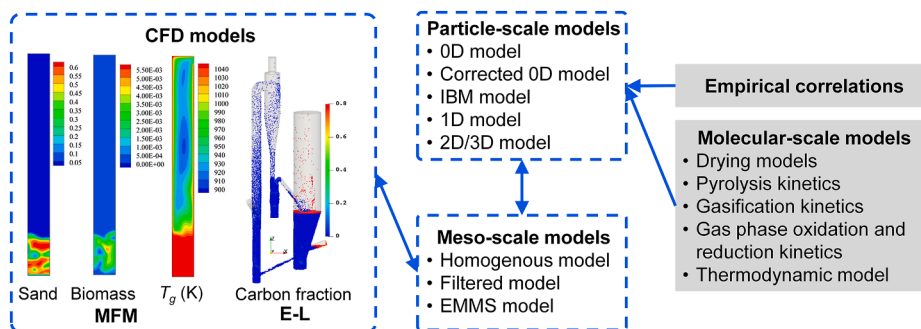


Fig. 15. Multiscale couplings in the CFD model for the modelling of BFBG. MFM: Reprinted with permission from Ref. [111]. Copyright (2018) Elsevier. E-L: Reprinted with permission from Ref. [42]. Copyright (2022) Elsevier.

models. Particle-scale models and meso-scale models are coupled in CFD models using interphase exchange coefficients (i.e., drag coefficient, convective heat and mass transfer coefficients). Moreover, the interactions between particle-scale models, meso-scale models and their impacts can be explicitly presented in the governing equations in a reactor-scale CFD model. Therefore, a two-way coupling method is typically adopted [13]. Additionally, the meso-scale structure is restricted by the operating conditions and reactor geometry configuration of the BFBG.

Table 5 summarizes the sub-models used in reactor-scale CFD simulations of the BFBG employing the MFM and E-L approaches. For the meso-scale drag model, a homogeneous model is commonly used in reactor-scale CFD simulations to describe the interphase exchange between gas and solid phases. Since the heterogeneous structure at the sub-grid level is not resolved in the homogeneous model, a fine grid size is required for reactor-scale simulations, as reported by Li et al. [293]. Fine-grid simulations lead to a significant increase in computational cost, which is unaffordable for large-scale simulations [294].

To improve the accuracy of coarse-grid simulations, the EMMS and filtered drag models have been gradually employed in the reactor-scale modeling of the BFBG [112,175,189,212,217,306–308]. For example, Chen et al. [175] found that the EMMS drag model provides better predictions of the outlet gas species composition of a bubbling BFBG than a homogeneous drag model (Gidaspow drag model). Luo et al. [306,309] demonstrated that the pressure profiles of a BFBG obtained using the EMMS drag model are in better agreement with experimental data compared with the Gidaspow drag model. The filtered drag model also exhibits superior performance in predicting the hydrodynamic behaviors of fluidized bed reactors [245].

Although meso-scale structures have been proven to have significant effects on heat and mass transfer between gas and solid phases [279,291,310,311], they are rarely implemented in reactor-scale CFD simulations of the BFBG. The most widely used correlations to describe interphase heat and mass transfer are still homogeneous models (i.e., Gunn [277], Li and Mason [276], Ranz and Marshall [275]). Therefore, further development of meso-scale interphase heat and mass exchange

models that account for the impacts of heterogeneous structures, as well as their implementation in reactor-scale simulations, will be required in future work.

As shown in Table 5, the most used particle-scale model for reactor-scale CFD simulations of BFBG is the 0D model. This is because the 0D model is the simplest model, as discussed in Section 2, and requires the least computational demand. Recent studies have also demonstrated that using 0D models in CFD simulations is feasible for large-scale reactive simulations [300,312]. However, numerous studies have shown that the 0D model fails to predict the biomass pyrolysis and char gasification processes for large-sized particles [74,116,208,313]. Therefore, more advanced models (corrected-0D, IBM, 1D, 2D/3D) have been gradually employed in reactor-scale CFD simulations of biomass thermochemical conversion in fluidized bed reactors [112,202,208,213,215]. Nevertheless, current advanced models mainly focus on accounting for the intra-particle temperature gradient during the biomass pyrolysis process, and their application in gasification processes is rarely reported [75]. Moreover, integrating a more advanced model (i.e., 1D, 3D, and IBM) into reactor-scale CFD simulations is rather complex and time-consuming. Among various particle-scale models, coupling a corrected-0D model in reactor-scale simulations requires almost the same computational cost as the oversimplified 0D model. Additionally, the corrected-0D model is easily implemented in reactor-scale CFD models and achieves almost the same accuracy as the 1D model. Therefore, the corrected-0D model can be considered a good alternative to replace IBM/1D/2D/3D models in reactor-scale simulations, enabling fast and efficient reactor-scale simulations in future work.

In the reactor-scale CFD modeling of the BFBG, the kinetics of pyrolysis, char gasification, and gas-phase oxidation and reduction are generally included. Regarding computational cost, a simple pyrolysis kinetic scheme is often employed in reactor-scale CFD modeling. However, a simple kinetic scheme requires the use of empirical correlations to predict the yield of pyrolysis products. In recent years, several studies have attempted to implement Scheme E to describe biomass pyrolysis in reactor-scale modeling, which increases the computational demand for solving species transport equations [111,112,179] but avoids the need for

Table 5

A summarize of sub-models used in reactor-scale CFD simulation of BFBG.

References	Meso-scale	Particle-scale	Molecular-scale
Eulerian multi-fluid model (MFM)			
Oevermann et al. [314]	Homogenous drag model.	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Gerber [140]	Homogenous drag model.	0D	Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Liu et al. [191]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Thankachan et al. [315]	Homogenous drag, heat, and mass transfer model	0D	Char gasification, global gas phase oxidation and reduction
Xue and Fox [144]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Couto [316]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Silva and Rouboa [317]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Chen [318]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Chen [175]	EMMS drag model, Homogenous heat, and mass transfer model	0D	Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Stark et al. [25]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Eri et al. [111]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme E Char gasification, global gas phase oxidation and reduction
Li et al. [319]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Luo et al. [306]	EMMS drag model	—	—
Yin et al. [307]	EMMS drag model, Homogenous heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Kang et al. [188]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Manu and Madav [203]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Luo et al. [202] Zheng et al. [211]	Homogenous drag, heat transfer model Homogenous drag model, Homogenous heat, transfer model	Corrected-0D Corrected-0D	Pyrolysis: Scheme A Pyrolysis: Scheme A
Euler-Lagrange model (E-L)			
Oevermann et al. [314]	Homogenous drag model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Tang et al. [192]	Homogenous drag model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Xie et al. [185]	Homogenous drag model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction

(continued on next page)

Table 5 (continued)

References	Meso-scale	Particle-scale	Molecular-scale
Jin [51]	Homogenous drag, heat transfer model	1D	Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Gerber [52]	Homogenous drag model	0D	Drying: Heat flux model Pyrolysis: Scheme B Char gasification, global gas phase oxidation and reduction
Ku et al. [320]	Homogenous drag, heat, and mass transfer model	0D	Drying: Heat flux model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Liu et al. [66]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Ostermeier et al. [321]	Homogenous drag, heat, and mass transfer model	0D	Drying: Equilibrium model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Kong et al. [187,322]	Homogenous drag, heat, and mass transfer model Various drag models	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Wang et al. [67]	Homogenous heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Yang et al. [186]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Zhang et al. [42]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Von Berg et al. [215]	Homogenous drag, heat, and mass transfer model	1D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Yang et al. [58]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Bai et al. [190]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Sun et al. [189]	EMMS drag model, Homogenous heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Wang et al. [179]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme E Char gasification, global gas phase oxidation and reduction
Yang et al. [59]	Homogenous drag, heat, and mass transfer model	0D	Drying: Equilibrium model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Graf et al. [308]	EMMS drag model, Homogenous heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Hashemisohi et al. [204]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme E Char gasification, global gas phase oxidation and reduction

(continued on next page)

Table 5 (continued)

References	Meso-scale	Particle-scale	Molecular-scale
Sun et al. [64,323]	Homogenous drag, heat, and mass transfer model	0D	Drying: Kinetic model Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Vásquez et al. [181]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Huang et al. [205]	Homogenous drag, heat, and mass transfer model	0D	Pyrolysis: Scheme A Char gasification, global gas phase oxidation and reduction
Wang et al. [112]	Filtered drag model, Homogenous heat, and mass transfer model	1D	Drying: Kinetic model Pyrolysis: Scheme E Char gasification, global gas phase oxidation and reduction
Lu et al. [212].	Filtered drag model, Homogenous heat transfer model	Corrected-0D	Drying: Kinetic model Pyrolysis: Scheme E
Lu et al. [217]	Filtered drag model, Homogenous heat transfer model	3D	Drying: Kinetic model Pyrolysis: Scheme B
Ku et al. [213]	Homogenous drag, heat, and mass transfer model	IBM	Pyrolysis: Scheme A

empirical correlations to determine pyrolysis product yields. Since bio-tar species are clearly defined in Scheme E, a comprehensive tar-cracking model can also be implemented in reactor-scale CFD simulations. Various drying models have been used in reactor-scale modeling, but the kinetic model is the most employed.

Although CFD models can characterize the multiscale flow-external transport-intra-particle transport-reaction behaviors in BFBG, it should be noted that the main drawback of CFD models is their high computational cost, especially when a detailed molecular-, advanced particle-, and meso-scale models are incorporated into the model. Therefore, CFD models are still challenging to apply at the process scale to support the design and optimization of the BFBG [22].

3.4. CFD-CRN model

The CFD-CRN model uses detailed multi-field information from CFD simulations to construct the topological structure of

the CRN and determine its linkages and structural parameters, thereby achieving indirect coupling between CFD and process simulations. Fig. 16 summarizes the multiscale coupling in the CFD-CRN model for modeling BFBG. In general, empirical correlations as well as molecular-scale, meso-scale, and particle-scale models can be comprehensively integrated. Furthermore, advanced particle- and meso-scale models can be embedded within each CRN zone of the coupled CFD-CRN framework. Notably, particle- and meso-scale modelling exert considerable influences on the topological structure of the CRN in the CFD-CRN model since the detailed information required for CRN construction is explicitly derived from CFD simulation results. Accordingly, the multi-scale coupling strategy adopted in the CFD-CRN model can be classified as a quasi-two-way coupling method.

Arora et al. [26] artificially constructed a CRN consisting of 4 CSTRs and 5 PFRs based on gas-phase flow patterns and residence time distributions obtained from two-dimensional non-reacting flow simulations using an MFM model, into

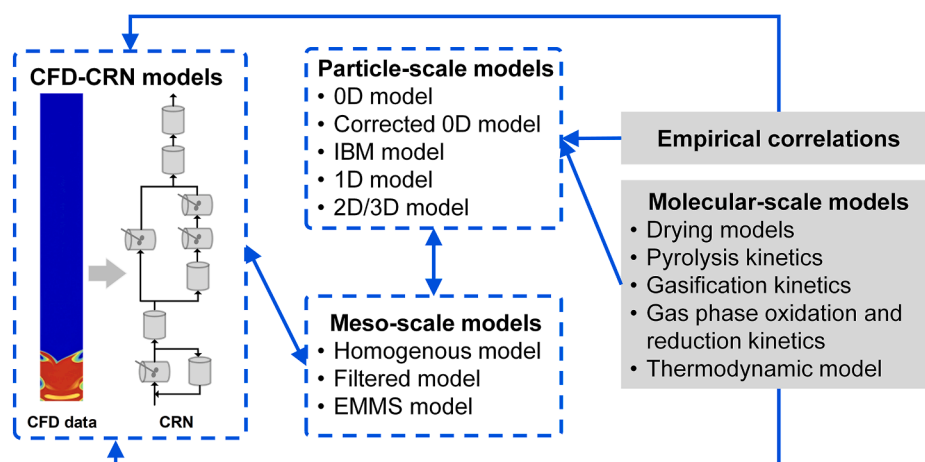


Fig. 16. Multiscale coupling in the CFD-CRN model for modelling BFBG. The contour plot of the CFD data is adapted from Arora et al. [26]; Reprinted with permission from Ref. [26]. Copyright (2017) Elsevier.

which a homogeneous drag model was incorporated. The topological structure, linkages, and structural parameters were optimized by fitting the residence time distribution. Similar methods have been applied to processes including polyethylene gasification [324], circulating fluidized bed reactors [23], and catalytic cracking [325]. Nevertheless, it is not appropriate to construct a CRN solely based on non-reacting flow CFD simulation data for processes such as biomass gasification, which is accompanied by substantial volatile release. Therefore, Stark et al. [25] developed a CFD-CRN model consisting of 2 PFRs and 1 CSTR based on flow field information from two-dimensional reacting-flow simulations using an MFM model. Compared with the CRN model derived from the two-phase theory using empirical correlations [28], this model significantly improved the prediction accuracy of tar species, demonstrating that the CFD-CRN model coupled with multi-field information from reacting-flow CFD simulation data can better reflect the actual biomass gasification processes in the BFBG. Kumar et al. [27] developed a CFD-CRN model for bubbling BFBG based on CFD-DEM simulation data. This model not only reproduced the axial species concentration distribution in excellent agreement with the CFD-DEM simulation results, but also achieved an order-of-magnitude improvement in computational efficiency, with the computation time reduced from 3 days to 20 ms. Therefore, compared with a CFD model, the CFD-CRN model can capture consistent characteristics of the biomass gasification process in BFBG while delivering a remarkable boost in computational efficiency.

CRN topological structure generation methods can be broadly classified into two categories: artificial construction methods and auto-generation method [22]. Owing to its capacity to efficiently utilize multi-physics field data, auto-generation method has gradually superseded artificial construction methods and become the mainstream methodology for single-phase combustion reactors [326–328]. For instance, Gao et al. [326] established quantitative zoning strategies and criteria based on multi-field data (temperature, velocity, species distribution, etc.) from CFD simulations, and developed an automatic CRN generation algorithm tailored for NO_x emission prediction in combustors. The algorithm enables automatic determination of CRN topological structure and parameters, and the CFD-CRN model delivers accurate prediction of NO_x concentration at the reactor outlet. Savarese et al. [327] proposed a fully automatic CRN generation algorithm for combustion reactors based on the K-means unsupervised clustering algorithm, which processes CFD multi-field data without requiring manually predefined zoning strategies or criteria. However, the BFBG features multiscale complexity arising from multiphase flow, multi-component species, and tight coupling among hydrodynamics, extra-particle transport, intra-particle transport, and chemical reactions. Automatic CRN generation algorithms developed for single-phase reactors cannot be readily extended to such systems; as a result, artificial construction methods remain the dominant approaches to determine the topological structure of the CFD-CRN model [113,329]. Nevertheless, artificial construction

methods typically rely exclusively on the analysis of flow fields or solid concentration fields from CFD simulations, yielding CRNs with oversimplified architectures [25–27,30]. Such CRNs fail to faithfully capture the actual multiphase, multi-field, multiscale structures within the reactor, and their application is generally restricted to bubbling fluidized beds for biomass gasification with simple geometries [30]. Therefore, existing CRN construction methods for the BFBG suffer from two major limitations: reliance on expert experience and the absence of standardized automatic generation algorithms and poor understanding of the underlying correlation between the multiphase, multi-field, multiscale reactor structures and the topology as well as parameters of CRNs, which impedes the development of well-structured and physically consistent CRNs. Accordingly, developing a CRN auto-generation algorithms with adaptation to the multiphase, multi-field, multiscale structures in the BFBG should be focused in the future work.

Besides the CRN auto-generation algorithms, another main drawback of existing CFD-CRN models is that they ignore the effects of meso-scale heterogeneous structures (such as particle clusters and bubbles) on interphase transport and intra-particle transport at the sub-particle scale, as the CFD model used to construct the CFD-CRN model incorporates a 0D model and a homogeneous model. Numerous studies have confirmed that intra-particle transport processes and meso-scale structures exert a significant impact on biomass gasification processes [117,124,291,309]. Moreover, a CRN with a fixed topological structure and parameters is usually adopted in the reactor-scale modelling of the BFBG, but it can only achieve satisfactory prediction performance within a narrow range close to the operating conditions of the original CFD simulation [22]. When the operating conditions deviate significantly, the prediction deviation of the model increases markedly [30]. However, the multiscale flow-transport-reaction behaviors in the BFBG are closely related to the physical properties of biomass particles, operating conditions, and geometric configurations [14], resulting in weak adaptive construction capability of the CFD-CRN model. Therefore, developing an adaptive CFD-CRN model with considering the effects of meso-scale heterogeneous structures on interphase transport and intra-particle transport at sub-particle scale is very essential for future work.

3.5. Data-driven surrogate models

With the rapid advancement of artificial intelligence methodologies and the computational capabilities of computer hardware and software, data-driven surrogate (DS) models have been gradually employed to model biomass gasification processes [37,85,86,180,330–343]. Fig. 17 shows the main procedures to derive a DS model and its applications in BFBG. The key to deriving a DS model is the quality of the database. In general, the data is obtained from either BFBG experiments or numerical simulation based on EK, CRN, CFD, and CFD-CRN models. Whether the particle- and meso-scale models considered in the DS models depends on the source of the

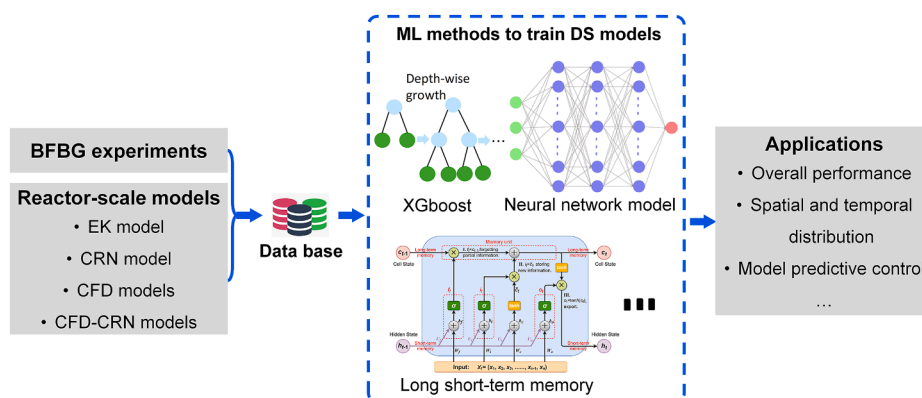


Fig. 17. Multiscale coupling in the DS model for modelling BFBG. Long short-term memory: Reprinted with permission from Ref. [345]. Copyright (2023) Elsevier.

data. Notably, the particle- and meso-scale models are not explicitly coupled in the DS model. For example, Zhao et al. [330] employed machine learning (ML) methods to develop a DS model for predicting the H_2 yield during supercritical water gasification of biomass, and the model also highlighted the influence of variables involved in supercritical water gasification of biomass on hydrogen production. Faridi et al. [333] proposed a DS model for the spatial and temporal prediction of temperature in BFBG using a dynamic recurrent neural network method, and this DS model was applied to the online automatic control of BFBG operating conditions [180,344]. As demonstrated in recent studies [335,340,345,341], the spatial and temporal distributions of multi-field variables in the BFBG can be predicted by a DS model derived from CFD simulation data using ML methods (such as XGBoost, neural network models, and long short-term memory). The recently developed physics-informed neural networks, which reduce data reliance, embed physical laws, and boost simulation accuracy and robustness, have been applied to reconstruct multi-physics fields in fluidized bed reactors [346,347], their application to predict the spatial and temporal distributions of multi-field variables in BFBG is still rarely reported in the literature, due to the inherently complex multiscale transport-reactive phenomena in BFBG.

The DS model offers remarkable advantages in simulating the BFBG over the EK, CRN, CFD, and CFD-CRN models. This model relies on historical experimental or high-fidelity simulation data instead of detailed physical and chemical mechanisms, enabling fast prediction under various operating conditions with significantly reduced computational costs. Additionally, the model is highly adaptive to the complex nonlinear relationships between operating parameters (such as temperature, equivalence ratio, and steam-to-biomass ratio) and gasification performance indicators (syngas composition, carbon conversion efficiency, and tar yield) [39]. Moreover, the DS model supports rapid parametric analysis, multi-objective optimization, and real-time control, making it particularly suitable for the design, optimization, and scale-up of the BFBG where repeated calculations are required. However, the inherent multiscale phenomena of the BFBG are challenging to be explicitly revealed using the DS model. Its

accuracy and generalization ability strongly depend on the quantity, quality, and distribution of training data; insufficient data or biased samples can lead to poor predictions, especially under extreme operating conditions [346]. Discrepancies in data acquisition standards, operating condition definitions, and measurement protocols across datasets introduce systematic biases into model training [348]. For the BFBG, experimental data from different laboratories and numerical data from varied simulation setups commonly differ in spatiotemporal resolution and parameter calibration benchmarks. Direct integration of inconsistent datasets without standardized pre-processing distorts the intrinsic mapping between operating conditions and reactor performance, ultimately impairing the prediction accuracy and physical consistency of trained DS models. The unquantified data uncertainty may amplify the risk of prediction deviations in industrial scenarios. For cross-source data deviations, data from distinct sources (e.g., lab-scale experiments, pilot-scale tests, and full-scale CFD

Table 6

Multiscale couplings and performance of reactor-scale simulation of the BFBG.

Reactor-scale models	EK	CRN	CFD	CFD-CRN	DS
Coupling of molecular-scale models					
Drying model	Y	Y	Y	Y	N
Pyrolysis kinetic model	Y	Y	Y	Y	N
Gasification kinetic model	Y	Y	Y	Y	N
Gas phase oxidation and reduction	Y	Y	Y	Y	N
Coupling of particle-scale models					
0D	N	Y	Y	Y	N
Corrected-0D	N	Y	Y	Y	N
1D	N	N	Y	N	N
IBM	N	N	Y	N	N
2D/3D	N	N	Y	N	N
Coupling of meso-scale models					
Homogenous model	N	Y	Y	Y	N
Filtered model	N	Y	Y	Y	N
EMMS model	N	Y	Y	Y	N
Predictive ability					
Overall characteristics	Y	Y	Y	Y	Y
Spatial and temporal distribution	N	Y	Y	Y	Y
Computational cost					
Accuracy	+	++	+++++	++++	++

simulations) exhibit pronounced distribution shifts arising from differences in reactor geometry and operating conditions. Training DS models directly on unaligned multi-source data reduces model adaptability in the modelling of the BFBG, which multi-scale and multi-phase complexities widen the distribution gap across data sources [349]. Furthermore, the DS model cannot reliably extrapolate beyond the range of the training dataset, and its performance degrades significantly when applied to new feedstocks or reactor structures without additional data. Therefore, the DS model is suggested to be employed when a large set of high-quality data is available.

4. Conclusions and perspectives

This paper systematically reviews the sub-models (molecular-, particle-, and meso-scale models) and reactor-scale models for the multiscale simulation of the BFBG. Table 6 summarizes the multiscale coupling strategies adopted in reactor-scale models for the BFBG simulation. The predictive performance, computational cost, and accuracy of these models generally depend on the multiscale coupling of physical models across different scales. The main conclusions and perspectives for future work are outlined as follows.

- (1) The EK model has been extensively employed in process-scale simulations to obtain the overall characteristics of the BFBG. However, the EK model is usually oversimplified, as it neglects particle- and meso-scale phenomena. Thus, extensive fine-tuning of model parameters is required to fit experimental data. Considering the trade-off between accuracy and computational cost, the EK model is recommended for rough performance evaluation of processes involving a BFBG unit.
- (2) Various molecular-scale models, 0D or corrected-0D models, and homogeneous models can be incorporated into CRN models with an affordable computational cost. These models can provide both the overall characteristics of the BFBG and coarse spatial-temporal distributions of key parameters. Therefore, the CRN model is suggested to replace the EK model in process-scale simulations to deliver more accurate results. Nevertheless, since numerous empirical correlations are used to construct the topological structure of CRNs, the CRN model is currently limited to bubbling BFBGs with simple geometric configurations.
- (3) CFD models are a promising tool to support the design, optimization, and scale-up of the BFBG, as they enable the full resolution of the coupling chain of “flow-external transport-intra-particle transport-reactions”. However, multiscale CFD simulations of the BFBG require massive computational resources. Therefore, future research should focus on developing efficient multiscale coupling methods to reduce the computational costs of CFD models.
- (4) The CFD-CRN model constructs the topological structure of CRN based on multi-field variables obtained from CFD simulations. Once the CRN is established, the computational demand can be significantly reduced, striking a good balance between accuracy and efficiency for multiscale simulation of the BFBG. However, the artificial construction of CRN topological structures is hard to fully utilize multi-field data and has weak adaptive capability. Thus, future research may focus on developing multiscale multi-phase adaptive CFD-CRN models by combining CRN auto-generation algorithms and ML methods [327].
- (5) The DS model offers remarkable advantages in terms of fast simulation of the BFBG. However, it is challenging to explicitly incorporate the underlying physicochemical mechanisms into the DS model. Therefore, future work should prioritize the development of physics-informed DS models. It is also worth noting that the performance of DS models relies heavily on high-quality datasets.
- (6) ML methods have been extensively used to derive sub-models for reactor-scale simulations, which can significantly enhance their adaptability while reducing computational costs. Nevertheless, the cross-scale coupling of ML-derived sub-models still requires further development.
- (7) Although significant efforts have been devoted to developing meso-scale drag models based on heterogeneous structures, the extension of these models to interphase heat and mass transfer remains rarely reported in the multiscale simulation of the BFBG. Therefore, accounting for the impact of meso-scale structures on interphase heat and mass transfer remains a key challenge for future multiscale simulations of the BFBG.
- (8) Since char gasification kinetics exhibit significant variability across different biomass feedstocks and operating conditions, further research should focus on developing a universal kinetic model for char gasification by incorporating inorganic content as a key physical property of biomass particles.
- (9) With regard to accuracy and efficiency, the corrected-0D model is expected to serve as a reliable and efficient particle-scale model for the multiscale simulation of the BFBG. Therefore, the coupling approaches between the corrected-0D model, meso-scale models, and reactor-scale model should be further investigated

CRedit authorship contribution statement

Hao Luo: Writing – review & editing, Writing – original draft, Visualization, Resources, Investigation, Funding acquisition, Formal analysis, Data curation. **Henrik Ström:** Writing – review & editing. **Qingang Xiong:** Writing – review & editing. **Ruiyan Sun:** Writing – review & editing, Writing – original draft, Investigation, Funding acquisition, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

This study was financially supported by the National Natural Science Foundation of China (No. 22208254, 22378197, 22478126).

References

- [1] H. Luo, X. Wang, X. Liu, X. Wu, X. Shi, Q. Xiong, J. Anal. Appl. Pyrolysis 162 (2022) 105433.
- [2] W. Deng, Y. Feng, J. Fu, H. Guo, Y. Guo, B. Han, Z. Jiang, L. Kong, C. Li, H. Liu, P.T.T. Nguyen, P. Ren, F. Wang, S. Wang, Y. Wang, Y. Wang, S.S. Wong, K. Yan, N. Yan, X. Yang, Y. Zhang, Z. Zhang, X. Zeng, H. Zhou, Green Energy Environ. 8 (2023) 10–114.
- [3] J. Zhang, M.S. Webber, Y. Pu, Z. Li, X. Meng, M.L. Stone, B. Wei, X. Wang, S. Yuan, B. Klein, B. Seemala, C.E. Wyman, K.K. Ramasamy, M. Thorson, M.H. Langholtz, J.S. Heyne, A. Koishybay, S. Adhikari, S. Cao, A.D. Sutton, G.A. Tuskan, Y. Román-Leshkov, A.J. Ragauskas, T. Ling, B.H. Davison, Green Energy Environ. 10 (2025) 1210–1234.
- [4] S. Bao, X. Yang, Z. Yu, Y. Shi, Y. Lu, Green Energy Environ. 10 (2025) 452–470.
- [5] D. Lee, H. Nam, M. Won Seo, S. Hoon Lee, D. Tokmurzin, S. Wang, Y.-K. Park, Chem. Eng. J. 447 (2022) 137501.
- [6] H. Sayhan Akci Turgut, I. Dincer, Energy Convers. Manage. 310 (2024) 118474.
- [7] T. Wang, T. Zhou, C. Li, M. Zhang, Q. Song, H. Yang, Energy Convers. Manage. 321 (2024) 119065.
- [8] X. He, Green Energy Environ. 6 (2021) 15–21.
- [9] A. Gómez-Barea, B. Leckner, Prog. Energy Combust. Sci. 36 (2010) 444–509.
- [10] B. Leckner, Powder Technol. 411 (2022) 117935.
- [11] J.R.C. Rey, A. Longo, B. Rijo, C.M. Pedrero, L.a.C. Tarelho, P.S.D. Brito, C. Nobre, Fuel 377 (2024) 132776.
- [12] A. Anca-Couce, Prog. Energy Combust. Sci. 53 (2016) 41–79.
- [13] F. Alobaid, N. Almohammed, M. Massoudi Farid, J. May, P. Rößger, A. Richter, B. Eppe, Prog. Energy Combust. Sci. 91 (2022) 100930.
- [14] V.S. Sikarwar, M. Zhao, P. Clough, J. Yao, X. Zhong, M.Z. Memon, N. Shah, E.J. Anthony, P.S. Fennell, Energy Environ. Sci. 9 (2016) 2939–2977.
- [15] L. Lu, X. Gao, J.-F. Dietiker, M. Shahnam, W.A. Rogers, Chem. Eng. Sci. 248 (2021) 117131.
- [16] Z. Yang, Q. Hu, Y. Chen, H. Yang, C.-H. Wang, X.T. Bi, H. Chen, Chem. Eng. Sci. 302 (2025) 120816.
- [17] M. Masche, M. Puig-Arnavat, J. Wadenbäck, S. Clausen, P.A. Jensen, J. Ahrenfeldt, U.B. Henriksen, Fuel Process. Technol. 173 (2018) 89–102.
- [18] B. Leckner, Int. J. Heat Mass Transfer 168 (2021) 120860.
- [19] I. Haberle, Ø. Skreiberg, J. Łazar, N.E.L. Haugen, Prog. Energy Combust. Sci. 63 (2017) 204–252.
- [20] H. Ström, H. Luo, Q. Xiong, Energ. Fuel. 38 (2024) 17179–17190.
- [21] S. Wang, Y. Shen, Prog. Energy Combust. Sci. 109 (2025) 101221.
- [22] N. Jourdan, T. Neveux, O. Potier, M. Kanniche, J. Wicks, I. Nopens, U. Rehman, Y. Le Moulec, Chem. Eng. Sci. 210 (2019) 115196.
- [23] Y. Du, S. Li, X. Chen, Y. Li, B. Wang, C. Yang, Chem. Eng. Sci. 269 (2023) 118470.
- [24] Y. Du, H. Cheng, S. Li, X. Chen, Y. Li, W. Ren, C. Yang, Chem. Eng. Sci. 287 (2024) 119722.
- [25] A.K. Stark, C. Altantzis, R.B. Bates, A.F. Ghoniem, Chem. Eng. J. 303 (2016) 409–424.
- [26] P. Arora, A.F.A. Hoadley, S.M. Mahajani, A. Ganesh, Chem. Eng. Res. Des. 117 (2017) 274–286.
- [27] R. Varun Kumar, M. Gopinath M, B. Kusum Kumar, H. Goyal, Ind. Eng. Chem. Res. 64 (2025) 999–1010.
- [28] A.K. Stark, R.B. Bates, Z. Zhao, A.F. Ghoniem, Energ. Fuel. 29 (2015) 2437–2452.
- [29] B. Das, A. Bhattacharya, A. Datta, Fuel 280 (2020) 118582.
- [30] L.L. Berkel, P. Debiagi, H. Nicolai, M.A. Amjed, A. Stagni, C. Hasse, T. Faravelli, Fuel 357 (2024) 129731.
- [31] S. Iannello, Z. Bond, A. Sebastiani, M. Errigo, M. Materazzi, Fuel 338 (2023) 127234.
- [32] Ö.Ç. Mutlu, T. Zeng, Chem. Eng. Technol. 43 (2020) 1674–1689.
- [33] H. Wan, F. Feng, B. Yan, J. Liu, G. Chen, J. Yao, Energy Convers. Manage. 318 (2024) 118902.
- [34] H. Shi, Y. Huang, Y. Qiu, J. Zhang, H. Song, T. Tang, H. Liu, S. Sun, J. Zhu, Energy 344 (2026) 139821.
- [35] H. Shi, Y. Huang, Y. Qiu, J. Zhang, Z. Li, H. Song, T. Tang, Y. Xiao, H. Liu, Energy Convers. Manage. 332 (2025) 119695.
- [36] K. Wang, H. Xu, C. Yang, T. Qiu, Green Energy Environ. 6 (2021) 432–443.
- [37] L.C.G. Velandia, S. Garcia-Freites, M. Sanjuan, D. Acosta, A. Aristizabal, M.L. Botero, S. Builes, Biomass Bioenerg. 209 (2026) 108931.
- [38] A. Kushwah, T.R. Reina, M. Short, Sci. Total Environ. 834 (2022) 155243.
- [39] P. Suparmin, N. Purwanti, L.O. Nelwan, S.S. Mardjan, IOP Conf. Ser. Earth Environ. Sci. 1386 (2024) 012018.
- [40] Y. Ayub, Y. Hu, J. Ren, W. Shen, C.K.M. Lee, Eng. Appl. Artif. Intell. 126 (2023) 107018.
- [41] X. Yu, P.H. Blanco, Y. Makkawi, A.V. Bridgwater, Chem. Eng. Process. 130 (2018) 284–295.
- [42] F. Zhang, S. Yang, B. Yang, H. Wang, Energy 238 (2022) 121736.
- [43] H. Ström, H. Thunman, Combust. Flame 160 (2013) 417–431.
- [44] J. Wang, Chem. Eng. Sci. 215 (2020) 115428.
- [45] M.A. Gómez, C. Álvarez-Bermúdez, S. Chapela, A. Anca-Couce, J. Porteiro, Energy 281 (2023) 128243.
- [46] H. Fatehi, X.S. Bai, Combust. Sci. Technol. 186 (2014) 574–593.
- [47] I. Haberle, N.E.L. Haugen, Ø. Skreiberg, Energ. Fuel. 32 (2018) 10668–10682.
- [48] K.S. Kung, A.F. Ghoniem, Energy 187 (2019) 115989.
- [49] P. Maziarka, A. Anca-Couce, W. Prins, F. Ronsse, Chem. Eng. J. 446 (2022) 137088.
- [50] I. Haberle, N.E.L. Haugen, Ø. Skreiberg, Energ. Fuel. 32 (2018) 6847–6862.
- [51] G. Jin, Ind. Eng. Chem. Res. 52 (2013) 11344–11353.
- [52] S. Gerber, M. Oevermann, Fuel 115 (2014) 385–400.
- [53] C. Di Blasi, Chem. Eng. Sci. 53 (1998) 353–366.
- [54] R. Mehrabian, S. Zahirovic, R. Scharler, I. Obernberger, S. Kleditzsch, S. Wirtz, V. Scherer, H. Lu, L.L. Baxter, Fuel Process. Technol. 95 (2012) 96–108.
- [55] S.S. Alves, J.L. Figueiredo, Chem. Eng. Sci. 44 (1989) 2861–2869.
- [56] H. Lu, W. Robert, G. Peirce, B. Ripa, L.L. Baxter, Energ. Fuel. 22 (2008) 2826–2839.
- [57] X. Gao, Y. Zhang, B. Li, X. Yu, Energy Convers. Manage. 108 (2016) 120–131.
- [58] M. Yang, J. Zhang, S. Zhong, T. Li, T. Løvås, H. Fatehi, X.-S. Bai, Combust. Flame 236 (2022) 111744.
- [59] M. Yang, S.M. Mousavi, H. Fatehi, X.-S. Bai, Fuel 337 (2023) 127104.
- [60] H. Luo, Z. Lu, P.A. Jensen, P. Glarborg, W. Lin, K. Dam-Johansen, H. Wu, Fuel 260 (2020) 116410.
- [61] K.M. Bryden, M.J. Hagge, Fuel 82 (2003) 1633–1644.
- [62] C.D. Di Blasi, C. Branca, S. Sparano, B. La Mantia, Biomass Bioenerg. 25 (2003) 45–58.
- [63] H. Lu, E. Ip, J. Scott, P. Foster, M. Vickers, L.L. Baxter, Fuel 89 (2010) 1156–1168.
- [64] H. Sun, S. Yang, G. Bao, H. Wang, AIChE J. 70 (2024) e18407.
- [65] R. Caraccio, E. Cipriano, A. Frassoldati, T. Faravelli, Chem. Eng. J. 531 (2026) 174297.
- [66] H. Liu, R.J. Cattolica, R. Seiser, Int. J. Hydrogen Energy 41 (2016) 11974–11989.
- [67] S. Wang, K. Luo, J. Fan, Chem. Eng. Sci. 217 (2020) 115550.
- [68] S. Yang, J. Liang, S. Wang, H. Wang, Energy 224 (2021) 120093.
- [69] G. Gentile, P.E.A. Debiagi, A. Cuoci, A. Frassoldati, E. Ranzi, T. Faravelli, Chem. Eng. J. 321 (2017) 458–473.

- [70] C. Di Blasi, *Prog. Energy Combust. Sci.* 34 (2008) 47–90.
- [71] C. Di Blasi, *Prog. Energy Combust. Sci.* 35 (2009) 121–140.
- [72] D. Neves, H. Thunman, A. Matos, L. Tarelho, A. Gómez-Barea, *Prog. Energy Combust. Sci.* 37 (2011) 611–630.
- [73] Q. Xiong, Y. Yang, F. Xu, Y. Pan, J. Zhang, K. Hong, G. Lorenzini, S. Wang, *ACS Sustain. Chem. Eng.* 5 (2017) 2783–2798.
- [74] H. Luo, X. Wang, K. Krochmalny, L. Niedzwiecki, K. Czajka, H. Pawlak-Kruczek, X. Wu, X. Liu, Q. Xiong, *Biomass Bioenerg.* 166 (2022) 106619.
- [75] H. Luo, *Modelling of Biomass Combustion and Gasification: from Particle-scale to Reactor-scale*, Technical University of Denmark, 2019.
- [76] J. Xing, H. Wang, K. Luo, S. Wang, Y. Bai, J. Fan, *Renew. Energy* 136 (2019) 104–114.
- [77] H.K. Balsora, K. S. V. Dua, J.B. Joshi, G. Kataria, A. Sharma, A.G. Chakinala, *J. Environ. Chem. Eng.* 10 (2022) 108025.
- [78] K. Xiao, X. Zhu, *ACS Omega* 9 (2024) 48125–48136.
- [79] F. Guo, Y. Dong, Z. Lv, P. Fan, S. Yang, L. Dong, *Energy Convers. Manage.* 93 (2015) 367–376.
- [80] S. Pielsticker, K. Schlögel, T. Kreitzberg, O. Hatzfeld, R. Kneer, *Fuel* 254 (2019) 115589.
- [81] C. Branca, C. Di Blasi, *Thermochim. Acta* 697 (2021) 178878.
- [82] W. Ji, F. Richter, M.J. Gollner, S. Deng, *Combust. Flame* 240 (2022) 111992.
- [83] L. Li, Z. Luo, L. Liu, Y. Wang, W. Zhu, J. Shi, Q. Wei, *Energy* 344 (2026) 140026.
- [84] B. Lv, X. Zhao, Z. Fu, S. Gao, M. Zheng, Z. Hu, X. Gao, Y. Xue, *J. Anal. Appl. Pyrolysis* 195 (2026) 107706.
- [85] V.H. Xavier Bernardes, R. Gedraite, N. Spogis, S. Arvelos Altino, *Int. J. Hydrogen Energy* 215 (2026) 153747.
- [86] Z. Yang, Q. Hu, P. Xue, Q. Chen, Y. Chen, H. Yang, H. Chen, *Int. J. Hydrogen Energy* 100 (2025) 556–565.
- [87] J. Shen, M. Yan, M. Fang, X. Gao, *Bioresour. Technol. Rep.* 20 (2022) 101285.
- [88] K. Yang, K. Wu, H. Zhang, *Energy* 254 (2022) 124320.
- [89] C. Tsekos, S. Tandurella, W. De Jong, *J. Anal. Appl. Pyrolysis* 157 (2021) 105180.
- [90] F. Shafizadeh, P.P.S. Chin, in: I.S. Goldstein (Ed.), *Wood Technology: Chemical Aspects*, American Chemical Society, Washington, 1977, pp. 57–81.
- [91] B. Wagenaar, W. Prins, W.P.M. Van Swaaij, *Fuel Process. Technol.* 36 (1993) 291–298.
- [92] W.C. Park, A. Atreya, H.R. Baum, *Combust. Flame* 157 (2010) 481–494.
- [93] J.M. Johansen, P.A. Jensen, P. Glarborg, M. Mancini, R. Weber, R.E. Mitchell, *Energy* 95 (2016) 279–290.
- [94] J.M. Johansen, *Power Plant Burners for Bio-Dust Combustion*, Technical University of Denmark, 2015.
- [95] Q. Xue, T.J. Heindel, R.O. Fox, *Chem. Eng. Sci.* 66 (2011) 2440–2452.
- [96] R.S. Miller, J. Bellan, *Combust. Sci. Technol.* 126 (2010) 97–137.
- [97] Q. Xiong, S.-C. Kong, A. Passalacqua, *Chem. Eng. Sci.* 99 (2013) 305–313.
- [98] Q. Xiong, S. Aramideh, S.-C. Kong, *Environ. Prog. Sustain. Energy* 33 (2014) 756–761.
- [99] S. Aramideh, Q. Xiong, S.-C. Kong, R.C. Brown, *Fuel* 156 (2015) 234–242.
- [100] Q. Xiong, F. Xu, E. Ramirez, S. Pannala, C.S. Daw, *Fuel* 164 (2016) 11–17.
- [101] H. Zhong, Q. Xiong, Y. Zhu, S. Liang, J. Zhang, B. Niu, X. Zhang, *Renew. Energy* 141 (2019) 236–245.
- [102] H. Zhong, F. Xu, J. Zhang, Y. Zhu, S. Liang, B. Niu, X. Zhang, *Renew. Energy* 135 (2019) 208–217.
- [103] H. Zhong, Q. Xiong, L. Yin, J. Zhang, Y. Zhu, S. Liang, B. Niu, X. Zhang, *Renew. Energy* 152 (2020) 613–626.
- [104] G. Ren, J. Xu, H. Ström, H. Sun, J. Dai, Q. Xiong, *Fuel* 425 (2026) 139414.
- [105] E. Ranzi, A. Cuoci, T. Faravelli, A. Frassoldati, G. Migliavacca, S. Pierucci, S. Sommariva, *Energ. Fuel* 22 (2008) 4292–4300.
- [106] E. Ranzi, M. Corbetta, F. Manenti, S. Pierucci, *Chem. Eng. Sci.* 110 (2014) 2–12.
- [107] P.E.A. Debiagi, C. Pecchi, G. Gentile, A. Frassoldati, A. Cuoci, T. Faravelli, E. Ranzi, *Energ. Fuel* 29 (2015) 6544–6555.
- [108] P.E.A. Debiagi, G. Gentile, M. Pelucchi, A. Frassoldati, A. Cuoci, T. Faravelli, E. Ranzi, *Biomass Bioenerg.* 93 (2016) 60–71.
- [109] P. Debiagi, G. Gentile, A. Cuoci, A. Frassoldati, E. Ranzi, T. Faravelli, *J. Anal. Appl. Pyrolysis* 134 (2018) 326–335.
- [110] L.L. Berkel, P. Debiagi, H. Nicolai, F. Cerciello, M.Y. Suleiman, O. Senneca, C. Hasse, T. Faravelli, *Fuel* 409 (2026) 137793.
- [111] Q. Eri, J. Peng, X. Zhao, *Appl. Therm. Eng.* 129 (2018) 1358–1368.
- [112] B. Wang, Z. Ma, S. Li, J. Dai, M. Patrascu, X. Gao, *Chem. Eng. J.* 501 (2024) 157546.
- [113] S. Döbal, L.L. Berkel, P. Debiagi, H. Nicolai, T. Faravelli, C. Hasse, S. Hartl, *Fuel* 364 (2024) 131096.
- [114] T. Chen, X. Ku, J. Lin, H. Ström, *Energ. Fuel* 34 (2020) 1940–1957.
- [115] X. Gao, L. Lu, M. Shahnam, W.A. Rogers, K. Smith, K. Gaston, D. Robichaud, M. Brennan Pecha, M. Crowley, P.N. Ciesielski, P. Debiagi, T. Faravelli, G. Wiggins, C.E.A. Finney, J.E. Parks, *Chem. Eng. J.* 418 (2021) 129347.
- [116] Z. Lao, Y. Shao, X. Gao, *Ind. Eng. Chem. Res.* 61 (2022) 16843–16856.
- [117] H. Luo, X. Wang, X. Liu, L. Yi, X. Wu, X. Yu, Y. Ouyang, W. Liu, Q. Xiong, *Chem. Eng. Sci.* 280 (2023) 119060.
- [118] F. Li, K. Wu, K. Yang, Z. Ge, J. Feng, H. Zhang, *Fuel* 341 (2023) 127635.
- [119] Z. Zhou, Z. Cai, S. Wang, W. Wang, H. Ström, X. Wu, Q. Xiong, H. Luo, *Fuel* 428 (2026) 140258.
- [120] M. Morin, S. Pécate, M. Hémati, *Chem. Eng. Res. Des.* 131 (2018) 488–505.
- [121] L. Tognotti, J.P. Longwell, A.F. Sarofim, *Symposium on Combustion* 23 (1991) 1207–1213.
- [122] J.R. Arthur, *Trans. Faraday Soc.* 47 (1951) 164–178.
- [123] T.M. Linjewile, P.K. Agarwal, *Fuel* 74 (1995) 5–11.
- [124] H. Luo, X. Liu, L. Niedzwiecki, X. Wu, W. Lin, B. Lu, W. Wang, H. Wu, *Proc. Combust. Inst.* 39 (2023) 3529–3538.
- [125] D. Kim, S. Choi, *J. Mech. Sci. Technol.* 29 (2015) 4951–4961.
- [126] C.R. Shaddix, F. Holzleithner, M. Geier, B.S. Haynes, *Combust. Flame* 160 (2013) 1827–1834.
- [127] H. Luo, Z. Lu, P.A. Jensen, P. Glarborg, W. Lin, K. Dam-Johansen, H. Wu, *Proc. Combust. Inst.* 38 (2021) 3919–3928.
- [128] Y.B. Yang, V.N. Sharifi, J. Swithenbank, L. Ma, L.I. Darvell, J.M. Jones, M. Pourkashanian, A. Williams, *Energ. Fuel* 22 (2008) 306–316.
- [129] F. Mermoud, F. Golfier, S. Salvador, L. Van De Steene, J.L. Dirion, *Combust. Flame* 145 (2006) 59–79.
- [130] S.K. Bhatia, D.D. Perlmutter, *AIChE J.* 26 (1980) 379–386.
- [131] S. Dasappa, P.J. Paul, H.S. Mukunda, U. Shrinivasa, *Chem. Eng. Sci.* 49 (1994) 223–232.
- [132] H. Fatehi, X.-S. Bai, *Appl. Energy* 185 (2017) 998–1006.
- [133] S. Guo, Z. Lu, J. Chen, Z. Bao, J. Cai, S. Yao, *Biomass Convers. Biorefinery* 14 (2023) 18367–18380.
- [134] C.D. Blasi, F. Buonanno, C. Branca, *Carbon* 37 (1999) 1227–1238.
- [135] A. Zolin, A. Jensen, P.A. Jensen, *Energ. Fuel* 15 (2001) 1110–1122.
- [136] J. Adánez, L.F. de Diego, F. García-Labiano, A. Abad, J.C. Abanades, *Ind. Eng. Chem. Res.* 40 (2001) 4317–4323.
- [137] H. Thunman, B. Leckner, F. Niklasson, F. Johnsson, *Combust. Flame* 129 (2002) 30–46.
- [138] J. Porteiro, J.L. Míguez, E. Granada, J.C. Moran, *Fuel Process. Technol.* 87 (2006) 169–175.
- [139] L. Nowicki, A. Antecka, T. Bedyk, P. Stolarek, S. Ledakowicz, *J. Therm. Anal. Calorim.* 104 (2010) 693–700.
- [140] S. Gerber, F. Behrendt, M. Oevermann, *Fuel* 89 (2010) 2903–2917.
- [141] S. Hermansson, H. Thunman, *Combust. Flame* 158 (2011) 988–999.
- [142] Y. Haseli, J.A. Van Oijen, L.P.H. De Goey, *Bioresour. Technol.* 102 (2011) 9772–9782.
- [143] M.A. Gómez, J. Porteiro, D. Patiño, J.L. Míguez, *Fuel* 117 (2014) 716–732.
- [144] Q. Xue, R.O. Fox, *Powder Technol.* 254 (2014) 187–198.
- [145] J. Li, M.C. Paul, P.L. Younger, I. Watson, M. Hossain, S. Welch, *Appl. Energy* 156 (2015) 749–755.

- [146] R.B. Bates, C. Altantzis, A.F. Ghoniem, *Energ. Fuel.* 30 (2016) 360–376.
- [147] A. Anca-Couce, P. Sommersacher, A. Shiehnejadhesar, R. Mehrabian, C. Hochenauer, R. Scharler, *Energy Proc.* 120 (2017) 238–245.
- [148] G.N. Cereijo, P. Curto-Risso, W.A. Bizzo, *Biomass Bioenerg.* 99 (2017) 38–48.
- [149] A. Galgano, C. Di Blasi, A. Horvat, Y. Sinai, *Energ. Fuel.* 20 (2006) 2223–2232.
- [150] M. Barrio, B. Gøbel, H. Rimes, U. Henriksen, J.E. Hustad, L.H. Sørensen, in: A.V. Bridgwater (Ed.), *Progress in Thermochemical Biomass Conversion*, Blackwell Science Ltd., Oxford, 2001.
- [151] K. Matsumoto, K. Takeno, T. Ichinose, T. Ogi, M. Nakanishi, *Fuel* 88 (2009) 519–527.
- [152] K. Umeki, K. Yamamoto, T. Namioka, K. Yoshikawa, *Appl. Energy* 87 (2010) 791–798.
- [153] Q. Xu, S. Pang, T. Levi, *Chem. Eng. Sci.* 66 (2011) 2232–2240.
- [154] L. Van De Steene, J.P. Tagutchou, F.J. Escudero Sanz, S. Salvador, *Chem. Eng. Sci.* 66 (2011) 4499–4509.
- [155] S. Nilsson, A. Gómez-Barea, P. Ollero, *Fuel* 105 (2013) 764–768.
- [156] A. Gómez-Barea, B. Leckner, *Fuel* 107 (2013) 419–431.
- [157] J. Billaud, S. Valin, M. Peyrot, S. Salvador, *Fuel* 166 (2016) 166–178.
- [158] W.F. Degroot, F. Shafizadeh, *Fuel* 63 (1984) 210–216.
- [159] E. Cetin, B. Moghtaderi, R. Gupta, T.F. Wall, *Combust. Sci. Technol.* 177 (2006) 765–791.
- [160] D.K. Seo, S.K. Lee, M.W. Kang, J. Hwang, T.-U. Yu, *Biomass Bioenerg.* 34 (2010) 1946–1953.
- [161] T. Mani, N. Mahinpey, P. Murugan, *Chem. Eng. Sci.* 66 (2011) 36–41.
- [162] L. Wang, J. Sandquist, G. Varhegyi, B. Matas Güell, *Energ. Fuel.* 27 (2013) 6098–6107.
- [163] W. Huo, Z. Zhou, X. Chen, Z. Dai, G. Yu, *Bioresour. Technol.* 159 (2014) 143–149.
- [164] I. Sircar, A. Sane, W. Wang, J.P. Gore, *Fuel* 119 (2014) 38–46.
- [165] H.J. Jeong, S.S. Park, J. Hwang, *Fuel* 116 (2014) 465–470.
- [166] C.C. Sreejith, C. Muraliedharan, P. Arun, *Fuel Process. Technol.* 130 (2015) 197–207.
- [167] J. Salinero, A. Gómez-Barea, D. Fuentes-Cano, B. Leckner, *Combust. Flame* 192 (2018) 190–204.
- [168] Y. Ren, R. Huang, S. Zhao, X. Zhu, Y. Lin, T. Su, C. Wang, N. Ren, *Green Energy Environ.* (2026) <https://doi.org/10.1016/j.gee.2026.03.027>.
- [169] Y. Chu, Y. Li, Y. Lyu, D. Zhang, H. Li, W. Yang, J. Li, L. Zhang, *Green Energy Environ.* 11 (2026) 940–967.
- [170] H. Yin, M. Xu, Z. Luo, X. Bi, J. Li, S. Zhang, X. Wang, *Green Energy Environ.* 9 (2024) 54–70.
- [171] Y. Zhou, A. Peng, H. Wu, *Combust. Flame* 288 (2026) 114967.
- [172] B. Peters, C. Bruch, *J. Anal. Appl. Pyrolysis* 70 (2003) 233–250.
- [173] L.M. Armstrong, S. Gu, K.H. Luo, *Ind. Eng. Chem. Res.* 50 (2011) 5959–5974.
- [174] L.M. Armstrong, S. Gu, K.H. Luo, *Chem. Eng. J.* 168 (2011) 848–860.
- [175] J. Chen, G. Yu, B. Dai, D. Liu, L. Zhao, *Energ. Fuel.* 28 (2014) 6351–6360.
- [176] R. Mehrabian, A. Shiehnejadhesar, R. Scharler, I. Obernberger, *Fuel* 122 (2014) 164–178.
- [177] J. Zhang, T. Li, H. Ström, T. Løvås, *Chem. Eng. J.* 387 (2020) 123964.
- [178] T. Steiner, K. Schulze, R. Scharler, A. Anca-Couce, *Combust. Flame* 256 (2023) 112940.
- [179] J. Wang, X. Ku, *Chem. Eng. Sci.* 272 (2023) 118608.
- [180] I. Khurram Faridi, E. Tsotsas, W. Heineken, M. Koegler, A. Kharaghani, *Chem. Eng. Sci.* 293 (2024) 120000.
- [181] R.D. Gomez Vásquez, J.D. Rhenals-Julio, J.M. Mendoza, J. Acevedo, A.J. Bula Silvera, *Appl. Therm. Eng.* 272 (2025) 126454.
- [182] M. Syamlal, L.A. Bissett, METC Gasifier Advanced Simulation (MGAS) Model, USDOE Morgantown Energy Technology Center, WV (United States), 1992.
- [183] D.M. Snider, S.M. Clark, P.J. O'rourke, *Chem. Eng. Sci.* 66 (2011) 1285–1295.
- [184] H. Liu, R.J. Cattolica, R. Seiser, C.-H. Liao, *Appl. Energy* 160 (2015) 489–501.
- [185] J. Xie, W. Zhong, B. Jin, Y. Shao, H. Liu, *Bioresour. Technol.* 121 (2012) 36–46.
- [186] S. Yang, F. Fan, Y. Wei, J. Hu, H. Wang, S. Wu, *Energy Convers. Manage.* 210 (2020) 112689.
- [187] D. Kong, S. Wang, K. Luo, C. Hu, D. Li, J. Fan, *Renew. Energy* 157 (2020) 466–481.
- [188] P. Kang, G. Zhang, Z. Ge, Z. Zha, H. Zhang, *Appl. Energy* 311 (2022) 118619.
- [189] H. Sun, S. Yang, G. Bao, K. Luo, J. Hu, H. Wang, *Chem. Eng. J.* 457 (2023) 141312.
- [190] Z. Bai, W. Hu, X. Zhu, S. Wang, Y. Gu, *Energy Convers. Manage.* 293 (2023) 117500.
- [191] H. Liu, A. Elkamel, A. Lohi, M. Biglari, *Ind. Eng. Chem. Res.* 53 (2014) 5554–5563.
- [192] Y.-L. Tang, D.-J. Liu, Y.-H. Liu, Q. Luo, *Energ. Fuel.* 24 (2010) 5602–5610.
- [193] C. Hu, K. Luo, S. Wang, L. Sun, J. Fan, *Chem. Eng. Sci.* 195 (2019) 693–706.
- [194] B. Hejazi, J.R. Grace, X. Bi, A. Mahecha-Botero, *Energ. Fuel.* 31 (2017) 1702–1711.
- [195] Q. Dang, X. Zhang, Y. Zhou, X. Jia, *Fuel Process. Technol.* 212 (2021) 106604.
- [196] A. Pitkäjä, J. Ritvanen, S. Hafner, T. Hyppänen, G. Scheffknecht, *Fuel* 289 (2021) 119868.
- [197] Y. Cao, Y. Bai, J. Du, *Clean Technol. Environ. Policy* 26 (2024) 839–848.
- [198] D. Zhu, Q. Wang, Z. Zhang, G. Xie, Z. Luo, *Energy* 318 (2025) 134919.
- [199] H. Rashidi, A. Duffy, W. Doherty, *Biomass Convers. Biorefinery* 15 (2025) 21745–21760.
- [200] E. Nicolucci, O. Palone, M. Colozzi, B. Domenico, *Int. J. Hydrogen Energy* 177 (2025) 151620.
- [201] H. Fan, H. Zhang, G. Li, X. Zhang, Z. Luo, L. Huang, S. Zhang, *Biomass Bioenerg.* 204 (2026) 108403.
- [202] H. Luo, W. Lin, K. Dam-Johansen, H. Wu, *Energ. Fuel.* 34 (2020) 9620–9631.
- [203] J. Manu, V. Madav, *Case Stud. Therm. Eng.* 39 (2022) 102429.
- [204] A. Hashemisohi, L. Wang, A. Shahbazi, *Chem. Eng. Res. Des.* 206 (2024) 1–11.
- [205] M. Huang, J. Luo, J. Chen, B. Chen, L. Yi, *Powder Technol.* 452 (2025) 120553.
- [206] M. Masche, M. Puig-Arnavat, P.A. Jensen, J.K. Holm, S. Clausen, J. Ahrenfeldt, U.B. Henriksen, *Powder Technol.* 350 (2019) 134–145.
- [207] T. Li, H. Thunman, H. Ström, *Combust. Flame* 213 (2020) 117–131.
- [208] L. Von Berg, A. Anca-Couce, C. Hochenauer, R. Scharler, *Energy Convers. Manage.* 286 (2023) 117070.
- [209] N.H. Dong, K.H. Luo, Q. Wang, *Fuel Process. Technol.* 161 (2017) 199–203.
- [210] A. Espeskvist, T. Li, P. Glarborg, P.A. Jensen, *Energies* 14 (2021) 1018.
- [211] Q. Zheng, Y. Tian, W. Wang, F. Li, B. Lu, Q. Zheng, S. Kuang, *Chem. Eng. J.* 521 (2025) 166604.
- [212] L. Lu, M. Brennan Pecha, G.M. Wiggins, Y. Xu, X. Gao, B. Hughes, M. Shahnam, W.A. Rogers, D. Carpenter, J.E. Parks, *Chem. Eng. J.* 431 (2022) 133853.
- [213] X. Ku, F. Shen, H. Jin, J. Lin, H. Li, *Ind. Eng. Chem. Res.* 58 (2019) 1720–1731.
- [214] J. Wang, S. Hu, X. Liu, *Chem. Eng. J.* 450 (2022) 138227.
- [215] L. Von Berg, A. Anca-Couce, C. Hochenauer, R. Scharler, *Fuel* 324 (2022) 124677.
- [216] T. Chen, X. Ku, T. Li, B.S.A. Karlsson, J. Sjöblom, H. Ström, *Chem. Eng. J.* 417 (2021) 127923.
- [217] L. Lu, X. Gao, M. Shahnam, W.A. Rogers, *Chem. Eng. J.* 419 (2021) 129564.
- [218] Y. Cho, S.-C. Kong, *Energ. Fuel.* 37 (2023) 5926–5941.
- [219] Y. Cho, S.-C. Kong, *Powder Technol.* 452 (2025) 120570.
- [220] C. Di Blasi, *Chem. Eng. Sci.* 51 (1996) 1121–1132.
- [221] T. Li, X. Ku, T. Løvås, *Energy Proc.* 105 (2017) 505–510.
- [222] C. Hu, K. Luo, S. Wang, L. Sun, J. Fan, *Ind. Eng. Chem. Res.* 58 (2019) 1404–1416.

- [223] J. Wang, X. Ku, S. Yang, *Energ. Fuel.* 36 (2022) 3665–3679.
- [224] J. Wang, X. Ku, Z. Liu, *Energ. Fuel.* 37 (2023) 4413–4428.
- [225] M.J. Hagge, K.M. Bryden, *Chem. Eng. Sci.* 57 (2002) 2811–2823.
- [226] H. Luo, L. Niedzwiecki, A. Arora, K. Mościcki, H. Pawlak-Kruczek, K. Krochmalny, M. Baranowski, M. Tiwari, A. Sharma, T. Sharma, *Energies* 13 (2020) 3018.
- [227] S.M. Mousavi, H. Fatehi, X.-S. Bai, *Combust. Flame* 237 (2022) 111725.
- [228] D. Gidaspow, R. Bezburuah, J. Ding, *Hydrodynamics of Circulating Fluidized Beds: Kinetic Theory Approach*, 7th Fluidization Conference, 1991.
- [229] Y. Igci, A.T. Andrews, S. Sundaresan, S. Pannala, T. O'Brien, *AIChE J.* 54 (2008) 1431–1448.
- [230] J. Li, C. Cheng, Z. Zhang, J. Yuan, A. Nemet, F.N. Fett, *Chem. Eng. Sci.* 54 (1999) 5409–5425.
- [231] A. Sarkar, F.E. Milioli, S. Ozarkar, T. Li, X. Sun, S. Sundaresan, *Chem. Eng. Sci.* 152 (2016) 443–456.
- [232] C. Wen, Y. Yu, *Chem. Eng. Prog. Symp. Ser.* 62 (1966) 100–111.
- [233] S. Ergun, *Chem. Eng. Prog.* 48 (1952) 89–94.
- [234] M. Syamlal, D. Gidaspow, *AIChE J.* 31 (1985) 127–135.
- [235] L. Huilin, D. Gidaspow, *Chem. Eng. Sci.* 58 (2003) 3777–3792.
- [236] R. Di Felice, *J. Int. Multiphase Flow* 20 (1994) 153–159.
- [237] L. Mazzei, P. Lettieri, *Chem. Eng. Sci.* 62 (2007) 6129–6142.
- [238] Y. Igci, S. Pannala, S. Benyahia, S. Sundaresan, *Ind. Eng. Chem. Res.* 51 (2011) 2094–2103.
- [239] S. Schneiderbauer, S. Puttinger, *AIChE J.* 59 (2013) 4077–4099.
- [240] S. Schneiderbauer, S. Pirker, *AIChE J.* 60 (2014) 839–854.
- [241] S. Rauchenzauner, S. Schneiderbauer, *Int. J. Multiphase Flow* 126 (2020) 103237.
- [242] S. Rauchenzauner, S. Schneiderbauer, *Chem. Eng. Sci.* 247 (2022) 117104.
- [243] L.-T. Zhu, J.-X. Tang, Z.-H. Luo, *AIChE J.* 66 (2020) e16973.
- [244] L.-T. Zhu, Y.-X. Liu, J.-X. Tang, Z.-H. Luo, *Chem. Eng. Sci.* 204 (2019) 228–245.
- [245] L. Lu, X. Gao, J.-F. Dietiker, M. Shahnam, W.A. Rogers, *Ind. Eng. Chem. Res.* 61 (2022) 882–893.
- [246] C.C. Milioli, F.E. Milioli, W. Holloway, K. Agrawal, S. Sundaresan, *AIChE J.* 59 (2013) 3265–3275.
- [247] C.C. Milioli, F.E. Milioli, *Chem. Eng. Sci.* 267 (2023) 118266.
- [248] Y. Jiang, J. Kolehmainen, Y. Gu, Y.G. Kevrekidis, A. Ozel, S. Sundaresan, *Powder Technol.* 346 (2019) 403–413.
- [249] Y. Jiang, X. Chen, J. Kolehmainen, I.G. Kevrekidis, A. Ozel, S. Sundaresan, *Chem. Eng. Sci.* 230 (2021) 116235.
- [250] Y. Zhang, M. Jiang, X. Chen, Y. Yu, Q. Zhou, *Chem. Eng. Sci.* 225 (2020) 115835.
- [251] B. Hardy, S. Rauchenzauner, P. Fede, S. Schneiderbauer, O. Simonin, S. Sundaresan, A. Ozel, *Ind. Eng. Chem. Res.* 63 (2024) 8383–8400.
- [252] N. Yang, W. Wang, W. Ge, J. Li, *Chem. Eng. J.* 96 (2003) 71–80.
- [253] N. Yang, W. Wang, W. Ge, L. Wang, J. Li, *Ind. Eng. Chem. Res.* 43 (2004) 5548–5561.
- [254] W. Wang, J. Li, *Chem. Eng. Sci.* 62 (2007) 208–231.
- [255] J. Wang, W. Ge, J. Li, *Chem. Eng. Sci.* 63 (2008) 1553–1571.
- [256] A. Nikolopoulos, D. Papafotiou, N. Nikolopoulos, P. Grammelis, E. Kakaras, *Chem. Eng. Sci.* 65 (2010) 4080–4088.
- [257] A. Nikolopoulos, C. Samlis, M. Zeneli, N. Nikolopoulos, S. Karellas, P. Grammelis, *Chem. Eng. Sci.* 229 (2021) 116013.
- [258] B. Lu, W. Wang, J. Li, *Chem. Eng. Sci.* 64 (2009) 3437–3447.
- [259] B. Lu, W. Wang, J. Li, *Chem. Eng. Sci.* 66 (2011) 4624–4635.
- [260] Z. Shi, W. Wang, J. Li, *Chem. Eng. Sci.* 66 (2011) 5541–5555.
- [261] K. Hong, Z. Shi, W. Wang, J. Li, *Chem. Eng. Sci.* 99 (2013) 191–202.
- [262] A. Ullah, K. Hong, S. Chilton, W. Nimmo, *Powder Technol.* 281 (2015) 129–137.
- [263] Q. Zhou, J. Wang, *Chem. Eng. Sci.* 122 (2015) 637–651.
- [264] E. Ghadirian, H. Arastoopour, *Powder Technol.* 288 (2016) 35–44.
- [265] L. Lu, J. Xu, W. Ge, G. Gao, Y. Jiang, M. Zhao, X. Liu, J. Li, *Chem. Eng. Sci.* 155 (2016) 314–337.
- [266] H. Luo, B. Lu, J. Zhang, H. Wu, W. Wang, *Chem. Eng. J.* 326 (2017) 47–57.
- [267] N. Ahmad, Y. Tong, B. Lu, W. Wang, *Chem. Eng. Sci.* 200 (2019) 257–267.
- [268] S. Hu, X. Liu, *Chem. Eng. Sci.* 205 (2019) 14–24.
- [269] Z. Qin, Q. Zhou, J. Wang, *Chem. Eng. Sci.* 207 (2019) 358–378.
- [270] H. Wang, Y. Lu, *Ind. Eng. Chem. Res.* 60 (2021) 18136–18153.
- [271] Z. Yang, B. Lu, W. Wang, *Chem. Eng. Sci.* 246 (2021) 117003.
- [272] C. Du, C. Han, Z. Yang, H. Wu, H. Luo, L. Niedzwiecki, B. Lu, W. Wang, *Ind. Eng. Chem. Res.* 61 (2022) 8566–8580.
- [273] P. Stamatopoulos, D. Stefanitsis, M. Zeneli, N. Nikolopoulos, *Chem. Eng. Sci.* 282 (2023) 119286.
- [274] H. Sun, H. Zhang, N. Zhang, L. Wang, *Chem. Eng. Sci.* 336 (2026) 124472.
- [275] W.E. Ranz, W.R. Marshall, *Chem. Eng. Prog.* 48 (1952) 141–148.
- [276] J. Li, D.J. Mason, *Powder Technol.* 112 (2000) 273–282.
- [277] D. Gunn, *Int. J. Heat Mass Transfer* 21 (1978) 467–476.
- [278] L.-T. Zhu, Y.-X. Liu, Z.-H. Luo, *Chem. Eng. J.* 374 (2019) 531–544.
- [279] Z. Huang, L. Wang, Q. Zhou, *AIChE J.* 67 (2021) e17185.
- [280] Z. Huang, Z. Zhang, L. Wang, Q. Zhou, *AIChE J.* 70 (2024) e18521.
- [281] Y. Li, Y. Yu, C. Zhang, Z. Huang, Q. Zhou, *Particuology* 57 (2021) 176–186.
- [282] Y. Li, S. Han, Y. Yu, X. He, Z. Huang, Q. Zhou, *AIChE J.* 69 (2023) e17917.
- [283] L.-T. Zhu, B. Ouyang, H. Lei, Z.-H. Luo, *AIChE J.* 67 (2021) e17299.
- [284] H. Lei, L.-T. Zhu, Z.-H. Luo, *AIChE J.* 67 (2021) e17121.
- [285] S. Du, Z. Zhang, J. Ma, Z. Huang, B. Yang, Q. Zhou, *AIChE J.* 72 (2026) e70108.
- [286] L. Wang, Y. Zhang, Y. Yu, Z. Huang, Q. Zhou, *Phys. Fluids* 36 (2024) 123363.
- [287] W. Dong, W. Wang, J. Li, *Chem. Eng. Sci.* 63 (2008) 2798–2810.
- [288] W. Dong, W. Wang, J. Li, *Chem. Eng. Sci.* 63 (2008) 2811–2823.
- [289] C. Liu, W. Wang, N. Zhang, J. Li, *Chem. Eng. Sci.* 122 (2015) 114–129.
- [290] S. Liu, B. Lu, S. Zhong, X. Zhang, W. Wang, Z. Liu, *Chem. Eng. Sci.* (2025) 121248.
- [291] X. Zhang, Y. Tian, B. Lu, Y. Xu, W. Wang, *Chem. Eng. Sci.* 323 (2026) 123223.
- [292] X. Zhang, Y. Tian, B. Lu, W. Wang, *Chem. Eng. Sci.* 298 (2024) 120408.
- [293] T. Li, A. Gel, S. Pannala, M. Shahnam, M. Syamlal, *Powder Technol.* 254 (2014) 170–180.
- [294] H. Neau, R. Ansart, C. Baudry, Y. Fournier, N. Méricoux, C. Koren, J. Laviéville, N. Renon, O. Simonin, *Powder Technol.* 444 (2024) 120018.
- [295] H. Lin, Y. Si, J. Dai, Z. Li, Y. Liu, L. Wang, X. Gao, Y. Cheng, *Chem. Eng. J.* 496 (2024) 153907.
- [296] J. Li, *Powder Technol.* 111 (2000) 50–59.
- [297] B. Lu, N. Zhang, W. Wang, J. Li, J.H. Chiu, S.G. Kang, *AIChE J.* 59 (2013) 1108–1117.
- [298] B. Lu, J. Zhang, H. Luo, W. Wang, H. Li, M. Ye, Z. Liu, J. Li, *Chem. Eng. Sci.* 171 (2017) 244–255.
- [299] C. Zhang, B. Lu, W. Wang, M. Liu, C. Lu, M. Ye, *Chem. Eng. J.* 446 (2022) 136849.
- [300] Y. Wu, S. Zhong, B. Lu, S. Liu, Y. Xu, W. Wang, *AIChE J.* 71 (2025) e18845.
- [301] D.K. Singh, J.V. Tirkey, *Biomass Bioenerg.* 158 (2022) 106370.
- [302] G. Lombardelli, R. Scaccabarozzi, A. Conversano, M. Gatti, *Biomass Bioenerg.* 188 (2024) 107315.
- [303] P. Kaushal, J. Abedi, N. Mahinpey, *Fuel* 89 (2010) 3650–3661.
- [304] R.B. Bates, A.F. Ghoniem, W.S. Jablonski, D.L. Carpenter, C. Altantzis, A. Garg, J.L. Barton, R. Chen, R.P. Field, *AIChE J.* 63 (2017) 1543–1565.
- [305] J.F. Davidson, D. Harrison, *Chem. Eng. Sci.* 21 (1966) 731–738.
- [306] H. Luo, W. Lin, W. Song, S. Li, K. Dam-Johansen, H. Wu, *Fuel Process. Technol.* 195 (2019) 106146.
- [307] W. Yin, S. Wang, K. Zhang, Y. He, *Renew. Energy* 151 (2020) 216–225.
- [308] C. Graf, F. Coors, F. Marx, P. Dieringer, M. Zeneli, P. Stamatopoulos, K. Atsonios, F. Alobaid, J. Ströhle, B. Eppele, *Energ. Fuel.* 38 (2024) 18660–18673.

- [309] X. Wang, X. Li, L. Yi, A. Lyngfelt, T. Mattisson, X. Wu, H. Luo, Q. Xiong, *Chem. Eng. Sci.* 295 (2024) 120211.
- [310] S. Wang, T. Zhang, G. Liu, H. Lu, L. Sun, *Fuel* 139 (2015) 646–651.
- [311] Z. Huang, L. Wang, Y. Li, Q. Zhou, *Chem. Eng. Sci.* 239 (2021) 116645.
- [312] Y. Cui, C. Yu, D. Shi, X. Wang, *Appl. Therm. Eng.* 235 (2023) 121299.
- [313] H. Luo, X. Wang, X. Wu, L. Niedzwiecki, H. Pawlak-Kruczek, X. Liu, Q. Xiong, *Chem. Eng. J.* 460 (2023) 141813.
- [314] M. Oevermann, S. Gerber, F. Behrendt, *Particuology* 7 (2009) 307–316.
- [315] I. Thankachan, S. Rupesh, C. Muraleedharan, *Appl. Mech. Mater.* 592–594 (2014) 1903–1908.
- [316] N. Couto, V. Silva, E. Monteiro, P. Brito, A. Rouboa, *Renew. Energy* 77 (2015) 174–181.
- [317] V. Silva, A. Rouboa, *Energy Convers. Manage.* 99 (2015) 28–40.
- [318] J. Chen, W. Yin, S. Wang, C. Meng, G. Yu, T. Hu, F. Lin, *J. Renew. Sustain. Ener.* 8 (2016) 063105.
- [319] Z. Li, H. Xu, W. Yang, M. Xu, F. Zhao, *Fuel* 246 (2019) 466–475.
- [320] X. Ku, T. Li, T. Løvås, *Chem. Eng. Sci.* 122 (2015) 270–283.
- [321] P. Ostermeier, F. Fischer, S. Fendt, S. Deyoung, H. Spliethoff, *Fuel* 255 (2019) 115790.
- [322] D. Kong, K. Luo, S. Wang, J. Yu, J. Fan, *Chem. Eng. J.* 428 (2022) 131847.
- [323] H. Sun, G. Bao, H. Liu, J. Hu, H. Wang, *Renew. Energy* 220 (2024) 119682.
- [324] Y. Du, Q. Yang, A.S. Berrouk, C. Yang, A.S. Al Shoaibi, *Energ. Fuel* 28 (2014) 6830–6840.
- [325] Y. Du, H. Zhao, A. Ma, C. Yang, *Ind. Eng. Chem. Res.* 54 (2015) 8732–8742.
- [326] Q. Gao, F. Lei, Z. Zhang, *J. Tsinghua, Univ. (Sci. & Technol.)* 63 (2023) 612–622.
- [327] M. Savarese, A. Cuoci, W. De Paepe, A. Parente, *Fuel* 343 (2023) 127945.
- [328] J. Geng, J. Shuai, F. Lei, H. Qi, *J. Tsinghua, Univ. (Sci. & Technol.)* 65 (2025) 1887–1896.
- [329] A. Sebastiani, F. Parrillo, F. Ardolino, U. Arena, S. Iannello, M. Materazzi, *Chem. Eng. J.* 506 (2025) 159763.
- [330] S. Zhao, J. Li, C. Chen, B. Yan, J. Tao, G. Chen, *J. Clean. Prod.* 316 (2021) 128244.
- [331] S. Ascher, X. Wang, I. Watson, W. Sloan, S. You, *Bioresour. Technol.* 364 (2022) 128062.
- [332] J. Kang, L. Zhao, W. Li, Y. Song, *Renew. Energy* 194 (2022) 359–365.
- [333] I.K. Faridi, E. Tsotsas, W. Heineken, M. Koegler, A. Kharaghani, *Appl. Therm. Eng.* 219 (2023) 119334.
- [334] P. Xue, T. Chen, X. Huang, Q. Hu, J. Hu, H. Zhang, H. Yang, H. Chen, *Int. J. Hydrogen Energy* 49 (2024) 356–370.
- [335] H. Zhong, X. Yu, J. Zhang, L. Jiao, B. Niu, R. Tang, X. Shi, V.S. Vladimirovich, Q. Xiong, *Ind. Eng. Chem. Res.* 63 (2024) 3744–3754.
- [336] U.K. Jadoon, I. Díaz, M. Rodríguez, *Fuel Process. Technol.* 278 (2025) 108340.
- [337] J. Moreno, M. Cobo, F. Buendia, N. Sánchez, *Renew. Sustain. Energy Rev.* 210 (2025) 115151.
- [338] S. Ren, Y. Zhang, Q. Weng, S. Wu, C. Fu, Q. Zhu, B. Zhu, F. Si, *Int. J. Hydrogen Energy* 215 (2026) 153826.
- [339] Y. Guo, H. Liu, R. Mei, S. Wang, Z. Yan, *Bioresour. Technol.* 443 (2026) 133863.
- [340] Y. Ban, X. Li, S. Wang, K. Luo, J. Fan, *Chem. Eng. Sci.* 324 (2026) 123307.
- [341] B. Wang, H. Jin, H. Su, L. Guo, *Particuology* 108 (2026) 168–182.
- [342] M. Cakar, M.A. Insel, H. Sadikoglu, O. Yucel, *Energy* 342 (2026) 139709.
- [343] P. Cihan, F. Alfara, H.K. Ozcan, M.N. Ciner, A. Ongen, *Int. J. Hydrogen Energy* 204 (2026) 153232.
- [344] I.K. Faridi, E. Tsotsas, A. Kharaghani, *Processes* 12 (2024) 254.
- [345] H. Zhong, Z. Wei, Y. Man, S. Pan, J. Zhang, B. Niu, X. Yu, Y. Ouyang, Q. Xiong, *J. Clean. Prod.* 391 (2023) 136192.
- [346] H. Hoorijani, Y. Ouyang, G.J. Heynderickx, K.M. Van Geem, *Curr. Opin. Chem. Eng.* 50 (2025) 101193.
- [347] B. Zhang, Y. Xie, W. Fan, F. Song, *Chem. Eng. Sci.* 324 (2026) 123352.
- [348] J. Fan, Z. Dai, J. Cao, L. Mu, X. Ji, X. Lu, *Green Energy Environ.* 9 (2024) 1878–1890.
- [349] L.-T. Zhu, X.-Z. Chen, B. Ouyang, W.-C. Yan, H. Lei, Z. Chen, Z.-H. Luo, *Ind. Eng. Chem. Res.* 61 (2022) 9901–9949.