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Numerical Simulation of Fluidized Bed Gasifier Coupled with Solid Oxide Fuel Cell Fed with Solid Carbon

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Abstract: A model of a fluidized bed coupled with direct carbon solid oxide fuel cell (SOFC) is developed to explore the effect of coupling between fluidized bed and solid oxide fuel cell. Three gas–solid flow regimes are involved including fixed bed, delayed bubbling bed and bubbling bed. The anode reaction of SOFC is treated as the coupling processes of Boudouard gasification of carbon and electrochemical oxidation of CO. The effects of inlet velocity of the fluidizing agent CO₂, carbon activity, channel width and coupling extent on the system performance are investigated. The results show that the inlet velocity of CO₂ can promote the gasification rate in the anode, but too high velocities may lower CO molar fraction. The gasification rate generally increases with the increase of the channel width and carbon activity. The overlapping area between the anode surface and the initial carbon bed, gas–solid regime and carbon activity have a significant influence on the gasification rate and the maximum current density the system can support. Overall, the mass transport in the anode is dramatically enhanced by the expansion of the carbon bed, back-mixing, solid mixing and gas mixing, especially for the delayed bubbling bed and bubbling bed. This indicates that the adopted coupling method is feasible to improve the anode performance of direct carbon solid oxide fuel cell.

Keywords: solid oxide fuel cell; two-fluid model; fluidized beds; current density; Boudouard gasification

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1. Introduction

Direct carbon solid oxide fuel cell (DC-SOFC) is an electrochemical device that converts the chemical energy in solid carbon into electrical energy at an elevated temperature with high efficiency, fuel flexibility and low pollution [1–4]. The total reaction occurring in DC-SOFCs is $C(s) + O_2(g) \rightarrow CO_2(g)$, which is the same as the combustion of carbon, while the difference is that the solid carbon in DC-SOFC is electrochemically oxidized in the anode chamber by O^{2-} ion transporting through the electrolyte and CO₂ and electrons are produced in the anode without touching with oxygen or air. The electrons transport through external circuit generating electricity. The high concentration of CO₂ produced in the anode is cost-effective for capture and storage, and minimizing NO_x is produced [5–8]. The theoretical thermodynamic efficiency of DC-SOFC is close to 100%, much higher than that of a traditional coal-fired power station, which is limited by the Carnot cycle.

Compared with other fuel cells fed with gaseous fuel (such as H₂, natural gas, CH₄), the exclusive characteristic of DC-SOFC is the solid fuel, which has a higher volumetric energy density. The solid fuel is convenient and safe to transport and can be obtained widely from coal [9–15] and biomass [3,16] (such as almond shells [17], wheat straw [18], corn cob char [19], pepper straw [20], and pomelo peel [21]). The concentration of solid fuel will not decrease due to the co-existence with gaseous products during the operation of the fuel cell, and thus the theoretical potential will not reduce. However, the solid fuel is too stable to be

oxidized, and thus the DC-SOFCs need to work at elevated temperatures (600~1000 °C) and the direct electrochemical reaction of solid fuel can only occur at the solid–solid interface between fuel and electrolyte, which limits the performance of DC-SOFCs.

Although the solid–solid interface is limited and the direct electrochemical oxidation of solid carbon is ignorable, CO produced by Boudouard gasification ($C(s) + CO_2(g) \rightarrow 2CO(g)$) can act as a shuttle between solid carbon and the TPBs (triple phase boundaries, TPBs) in anodes of SOFC [22–24]. CO is electrochemically oxidized into CO_2 ($CO(g) + O^{2-} \rightarrow CO_2(g)$) at TPBs and CO_2 can transfer back to solid carbon and produce CO according to Boudouard gasification. Based on this mechanism, the performance of DC-SOFC will be affected by the electrochemical oxidation of CO at TPBs in anodes, the Boudouard gasification and mass transport between anode and solid carbon fuel [25–27]. Besides development of new anode material and microstructure [19,28–30], which can improve catalytical activity, mass transport, ionic or electronic conductivities of anode, plenty of experimental evidence demonstrates that carbon activity and transport properties in the anode can significantly influence the DC-SOFC performance [3,13,17,21,25,31–34]. Liu et al. [31] operated a tubular SOFC fed with the activated carbon and the results indicated that the fuel gas in the anode was insufficient and the mass transport in the anode was poor. Cai et al. analyzed [25] the qualitative coupling relationship between the gasification of a fixed carbon bed and SOFC, and found that when the gasification rate (R_{tot}) was larger than the electrochemical oxidation rate of CO (R_e) and smaller than $2R_e$, DC-SOFC could continuously maintain the composition of exhaust gas varied with the R_{tot}/R_e . Bai et al. [32] added 5wt.% Fe in the form of Fe_2O_3 into the activated carbon and the peak power density (PPD) reached 465 mW/cm² at 850 °C, but the stability of DC-SOFC was limited due to degradation of the Boudouard gasification rate. Jiao et al. [33] compared the effect of desulfurization of the low-rank coal on the performance of DC-SOFC with nickel-yttrium stabilized zirconia (Ni-YSZ) anode and the PPD increased from 115 to 221 mW/cm² at 900 °C after desulfurization. An et al. [21] operated DC-SOFC with a Ni-YSZ anode utilizing pomelo peel char as fuel; the PPD was as high as 518 mW/cm² and the limiting current density was higher than 16,500 A/m². Zhou et al. [34] found that the open circuit voltage (OCV), PPD, and fuel utilization reduced with increasing distance between the fixed carbon bed and anode. When there was no gas flowing into the anode chamber, the cell performance including OCV, PPD, and limiting current density would reduce with increasing anode chamber size. They also found that a smaller anode chamber results in a lower overall resistance and a higher PPD and OCV. According to the above experimental studies, it is deduced that the activity of carbon fuel and mass transport in the anode chamber has a remarkable influence on cell performance. However, all of the above studies are based on a fixed carbon bed in which the major mass transport mechanism in the anode chamber is diffusion and natural convection. In such systems, the mass transport and Boudouard gasification rate of the carbon bed reduced significantly as the operation went on, causing a poor cell durability.

To enhance the Boudouard gasification and the mass transport in the anode chamber and further improve cell durability, Gür et al. [11,17,23] proposed a fluidized bed coupled with DC-SOFC. As a preliminary study, they chose helium as the fluidizing gas to establish the relationship between oxygen atom flux in anode exhaust and the oxygen ion flux through electrolyte [35]. Simultaneously, Lee et al. [17] tested different carbonaceous fuels, such as synthetic carbon, coal, and biomass, in a fluidized anode of DC-SOFC, and the results showed that the type of carbon fuel had a significant influence on cell performance. Thereafter, Gür et al. [11] developed a fluidized bed gasifier integrated with SOFC, in which the gasifier and SOFC could operate separately at different temperatures, while the effluent gas from a gasifier was able to directly flow into the tubular SOFC. They tested the effect of inlet velocity on the concentration of effluent gas to ensure that the equilibrium concentration of CO is obtained in the outlet of gasifier and the PPD of SOFC achieved as high as 0.45 W/cm² at 0.64 V with fuel utilization of 55%. Lee et al. [36] modeled the Boudouard gasification integrated with SOFC and emphasize was put on the gasification of carbon. They obtained the kinetic parameters for the Boudouard gasification

experimentally and operated a fluidized carbon bed under different carbon bed heights, temperatures, and inlet flow velocities. However, in these studies, the carbon bed was described as a porous media and the moving of solid carbon particles was ignored.

Although an excellent contribution to the technology of gasifiers coupled with SOFC was made by researchers, most of the studies focused on the fixed bed. The bed with buoyancy and suspensions of solid particles was not considered [17,23,35–38]. As mentioned above, mass transport in the fixed carbon bed is the limiting factor for the performance and stability of DC-SOFCs [31,34] and can be enhanced with increasing gas velocities, especially when the solid particles are fluidized. The aim of this study is to numerically explore the influence of the coupling between SOFC and fluidized bed gasifiers on the system performance. Firstly, the gas–solid flow regimes (including fixed bed, delayed bubbling bed and bubbling bed) changing with inlet velocities are calculated; secondly, the fluidized bed gasifiers with different active carbon fuels, CO_2 inlet velocities and channel width are investigated; thirdly, the fluidized bed gasifier coupled with SOFCs under different current densities are explored. The benefits of gas–solid flows and coupling between gasifiers and SOFC are illustrated and a feasible method to improve the cell performance of DC-SOFC is suggested.

2. Physicochemical Model

Figure 1 shows the model of the fluidized bed gasifier coupled with DC-SOFC. There are several advantages to coupling SOFC with a fluidized bed gasifier. Firstly, compared with direct electrochemical oxidation of solid carbon where the solid–solid contact between solid carbon fuel and active sites in anodes is requisite; SOFC coupled with a fluidized bed gasifier can dramatically promote the cell performance by increasing the contact area between active sites and fuel. Secondly, compared with operating SOFC and fluidized bed gasifier separately, SOFC coupled fluidized bed gasifier can provide a more uniform concentration of fuel gas by in situ gasification in the anode chamber, as shown in the next section. Thirdly, Boudouard gasification is endothermic, while SOFC will release heat unavoidably. When combining SOFC and gasifier in the same chamber, the efficiency of system can be improved further by thermal coupling. Lastly, the balance of plant for DC-SOFC can be simplified. In this study, the simulations are conducted to explore the coupling effect on mass transport in the anode chamber. The heat transfer between SOFC and gasifier will be considered in the further work and is neglected here.

Figure 1. Model of fluidized bed gasifier coupled with DC-SOFC.

In fluidized bed gasifiers coupled with SOFC, as shown in Figure 1, there are several coupled physicochemical processes, namely, the gas–solid flow, Boudouard gasification of solid carbon, electrochemical oxidation of CO occurring at TPBs in the anode and the mass transport in the chamber. These physicochemical models are introduced below.

2.1. Boudouard Gasification of Carbon

The thermodynamic mechanism proposed by Ma et al. [39] was used to describe Boudouard gasification of solid carbon particles. In this model, Boudouard gasification can be divided into five steps: (1) a reversible CO₂ adsorption reaction on the free carbon site producing CO gas and oxygenated carbon site; (2) the escape of surface oxygenated carbon from the bondage of surrounding atoms in the bulk; (3) the interaction of CO₂ and a chemisorbed oxygen, which is a rate-limiting step; (4) the reversible CO adsorption on the active sites; and (5) the formation of CO₂ by interacting between CO gas and adsorbed CO, as shown follows.

where C_f represents the free carbon site on the solid surface, C(O) is oxygenated carbon, C_b is the carbon atom in the solid particle, C(CO) is adsorbed CO on the free carbon site, k_i is the reaction rate constant of the *i*th reaction and the subscripts ‘f’ and ‘b’ mean the forward and backward of the reversible reactions, respectively. The reaction rate constant k_i of the *i*th reaction can be calculated according to Arrhenius equation,

$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right) \quad (6)$$

where A_i is pre-exponent constant, E_i is activation energy (J/mol), R is ideal gas constant and R = 8.314 J/(mol·K), and T is operation temperature (K). The values of A_i and E_i measured using pressurized thermogravimetric analyzer were used (shown in Table 1) [36,37]. The more details of measurements procedure are introduced elsewhere [36,39]. In the steady condition, the concentrations of C_f, C(O), C(CO) on the solid surface are in equilibrium and the sum of their concentration fraction is unit,

$$\frac{d[\text{C}(\text{O})]}{dt} = k_{1f}[\text{CO}_{2(g)}][\text{C}_f] - k_{1b}[\text{CO}_{(g)}][\text{C}(\text{O})] - k_2[\text{C}(\text{O})] = 0 \quad (7)$$

$$\frac{d[\text{C}(\text{CO})]}{dt} = k_{4f}[\text{CO}_{2(g)}][\text{C}_f] - k_{4b}[\text{C}(\text{CO})] - k_5[\text{C}(\text{CO})][\text{CO}_{(g)}] = 0 \quad (8)$$

where [] denotes the concentration in unit of mol/m² for C_f, C(O), C(CO) on the solid surface and mol/m³ for CO_(g) and CO_{2(g)} in the chamber. The Boudouard gasification rate, R_C (mol/(m²·s)), of solid carbon can be calculated,

$$R_C = M_C A_s \{k_2[\text{C}(\text{O})] + k_3[\text{CO}_{2(g)}][\text{C}(\text{O})] - k_{4f}[\text{CO}_{2(g)}][\text{C}_f] + k_{4b}[\text{C}(\text{CO})]\} \quad (9)$$

where M_C is the molar mass of carbon (g/mol) and A_s is the active site density (mol/m²). The production rate R_{CO} (mol/s) of CO can be obtained by,

$$R_{CO} = 2R_C S_C m_p \quad (10)$$

where S_C denotes the specific area of carbon particle (m²/g) and m_p denotes the mass of the particle (g). According to this thermodynamic mechanism, R_C varies with operating temperature and CO₂ concentrations.

Table 1. Parameters in Boudouard gasification model.

Pre-Exponent Constant	Value	Activation Energy (J/mol)	Value
A_{1f}	5.00×10^3	E_{1f}	1.85×10^5
A_{1r}	1.08×10^2	E_{1r}	8.97×10^5
A_2	1.00×10^{13}	E_2	3.75×10^5
A_3	1.00×10^{-4}	E_3	5.80×10^4
A_{4f}	0.877	E_{4f}	1.48×10^5
A_{4r}	1.00×10^{13}	E_{4r}	4.55×10^5
A_5	1.01×10^7	E_5	2.62×10^5

2.2. Momentum and Mass Transport in Gas–Solid Flows

Reactive gas–solid flows are described based on two-fluid model (TFM). In TFM, the governing equations for gas–solid flows with chemical reaction are briefly introduced as follows. The continuum equations for the solid carbon and gas are,

$$\frac{\partial(\varepsilon_g \rho_g)}{\partial t} + \frac{\partial(\varepsilon_g \rho_g U_{gi})}{\partial x_i} = N_p \Delta m_p \quad (11)$$

$$\frac{\partial(\varepsilon_C \rho_C)}{\partial t} + \frac{\partial(\varepsilon_C \rho_C U_{Ci})}{\partial x_i} = -N_p \Delta m_p \quad (12)$$

where ε_g , ε_C are volume fractions of gas and carbon particle (vol.%); ρ_g , ρ_C are densities of gas and carbon particle (g/m³); U_{gi} , U_{Ci} are velocities of gas and carbon particle along i direction (m/s); t is time (s); N_p is the number of carbon particles per volume (1/m³); Δm_p is the consumption rate of carbon particle (g/s). The first term on the left is the accumulation term of the total mass, the second term denotes the convection term, and the term on the right-hand side is the interphase mass transfer due to Boudouard gasification. The species conversion equations of CO and CO₂ are,

$$\frac{\partial(\varepsilon_g \rho_g X_{CO})}{\partial t} + \frac{\partial(\varepsilon_g \rho_g U_{gi} X_{CO})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(D_{CO} \frac{\partial X_{CO}}{\partial x_i} \right) + 2 \frac{M_{CO}}{M_C} N_p \Delta m_p \quad (13)$$

$$\frac{\partial(\varepsilon_g \rho_g X_{CO_2})}{\partial t} + \frac{\partial(\varepsilon_g \rho_g U_{gi} X_{CO_2})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(D_{CO_2} \frac{\partial X_{CO_2}}{\partial x_i} \right) - \frac{M_{CO_2}}{M_C} N_p \Delta m_p \quad (14)$$

where X_{CO} , X_{CO_2} denote mass fractions of CO and CO₂ (wt.%); D_{CO} , D_{CO_2} represent diffusivities of CO and CO₂ (g/(m·s)); M_C , M_{CO} and M_{CO_2} are molar mass of carbon, CO and CO₂, and $M_C = 12$ g/mol, $M_{CO} = 28$ g/mol, $M_{CO_2} = 44$ g/mol. The terms on the left hand are the mass accumulation and convective species mass flux, respectively. Those on the right-hand side are the diffusive species mass flux and source term due to Boudouard gasification. The momentum conversion equations for gas and solid phases are,

$$\frac{\partial(\varepsilon_g \rho_g U_{gi})}{\partial t} + \frac{\partial(\varepsilon_g \rho_g U_{gj} U_{gi})}{\partial x_j} = -\varepsilon_g \frac{\partial \sigma_{gij}}{\partial x_j} - F_{gCi} + \varepsilon_g \rho_g g_i + S_{gC} \quad (15)$$

$$\frac{\partial(\varepsilon_C \rho_C U_{Ci})}{\partial t} + \frac{\partial(\varepsilon_C \rho_C U_{Cj} U_{Ci})}{\partial x_j} = -\varepsilon_C \frac{\partial \sigma_{cij}}{\partial x_j} + \frac{\partial \sigma_{Cij}}{\partial x_j} + F_{gCi} + \varepsilon_C \rho_C g_i - S_{gC} \quad (16)$$

U_{gi} , U_{Ci} are the velocities of gas and solid carbon along direction i (m/s); σ_{gij} , σ_{Cij} are the gas and solid carbon stress tensors (Pa); F_{gCi} is gas/carbon momentum interface transfer caused by physical interaction between gas and solid carbon (N/m³); g_i is acceleration due to gravity (m²/s); S_{gC} is the momentum transfer caused by Boudouard gasification (N/m³). F_{gCi} is calculated using the model correlated by Gidaspow et al. [40]. The detailed description of the governing equations for gas–solid flows can be obtained in references [41,42].

2.3. Electrochemical Reaction of CO

SOFC consists of a porous anode and cathode, as well as compact electrolytes in between. In the anode, there are electronic conductors (such as Ni, Ag, Pt), ionic conductors (such as YSZ, GDA), and pores. CO is treated as the only fuel of SOFC and the direct electrochemical oxidation of solid carbon in SOFC is ignorable due to the ignorable contact between solid carbon and TPBs. During operation, the electrochemical reaction occurs at the triple-phase boundaries (TPBs) in the anode where oxygen ions and CO are consumed, producing CO₂ gas and electrons as follows,

The produced CO₂ diffuses away from the porous anode and reacts with solid carbon particles in the anode chamber or flows away from the chamber. Electrons travel along the current collector and external circuit and then into the cathode of SOFC. In the cathode, electrons and O₂ combine with each other and the reaction is,

The produced oxygen ion O^{2−} passes the electrolyte and reacts with CO in the anode. The relationship between current density, I , and CO consumption rate, J_{CO} (CO₂ production rate, J_{CO_2}) on the anode surface can be described by,

$$J_{\text{CO}_2} = -J_{\text{CO}} = \frac{I}{nF} \quad (19)$$

where F is the Faraday constant and $F = 96,485.3$ C/mol, n is the number of electrons transferred per CO oxidized and $n = 2$. The theoretical potential $E_{\text{DC-SOFC}}$ of DC-SOFC can be calculated according to the Nernst equation,

$$E_{\text{DC-SOFC}} = -\frac{\Delta G^0}{nF} + \frac{RT}{nF} \ln \left(\frac{P_{\text{CO},a} P_{\text{O}_2,c}^{0.5}}{P_{\text{CO}_2,a}} \right) = -\frac{\Delta G^0}{nF} + \frac{RT}{nF} \ln \left(\frac{C_{\text{CO},a} C_{\text{O}_2,c}^{0.5}}{C_{\text{CO}_2,a}} \right) \quad (20)$$

where ΔG^0 represents the Gibbs free energy of reaction $\text{CO}_{(g)} + 1/2\text{O}_{2(g)} = \text{CO}_{2(g)}$ (J/mol); $P_{\text{CO},a}$, $P_{\text{CO}_2,a}$, $P_{\text{O}_2,c}$ are partial pressures of CO, CO₂ in the anode and O₂ in the cathode, respectively, and $P_{\text{O}_2,c} = 0.21$ atm when air is used as oxidant; $C_{\text{CO},a}$, $C_{\text{CO}_2,a}$, $C_{\text{O}_2,c}$ are the molar fraction of CO, CO₂ in the anode and O₂ in the cathode, respectively, and $C_{\text{O}_2,c} = 21.0$ mol.%.

2.4. Model Assumption

The main assumptions adopted in this simulation are shown as below:

1. The carbon particle is treated as a porous sphere with 155 μm diameter whose specific area is 750 m²/g [36]. The mass transport rate inside the particle is sufficiently large to keep the Boudouard gasification in a kinetically limited regime. In other words, the reaction rate of the gasification is uniquely determined by the kinetic rate. Since the material parameter in present study is same as that in [36], the reasonability of this assumption has been tested using the Thiele modulus in that literature.

2. The mass change of carbon particles is ignored. Compared with the total mass of carbon particles, the consumed carbon estimated using the maximum kinetic rate in the present study is less than 1.2% after 30 s when the simulation reaches the statistically quasi-steady state; thus, the mass change of carbon particles is ignorable and the particle density could be regarded as invariant during simulation.
3. Temperature is uniform, and heat transfer in the system is not considered.
4. CO₂ and CO are only gases in the anode chamber and are treated as ideal gases.
5. SOFC is working under fixed current density mode and SOFC is simplified as reactive boundary with different fixed species fluxes.

3. Simulation Method

The simulation is conducted in MFiX 19.2.2 (Multiphase Flow with Interphase eX-change, MFiX), a free open-source multiphase flow resolver, which is a powerful tool to simulate the gasification of solid fuel and allows users to develop model conveniently [43]. TFM is the most mature model in MFiX and can calculate dense, reactive multiphase flow by treating both solids and gases as interpenetrating continua. TFM is adopted to describe the gas–solid flow and the governing equations are solved using finite volume method. The implicit Euler scheme with the first-order accurate is employed for temporal discretization and Superbee, a second-order accurate scheme, is used for spatial discretization. The automatic time-step adjustment is utilized to accelerate calculation. A grid size smaller than $8d_p$ (d_p stands for the diameter of solid particle) is thought to be fine enough [42,44]; about $4d_p$ is adopted here to achieve a satisfied accuracy and grid independency. The electrochemical reactions occur in SOFC are treated as reactive boundary conditions in MFiX and the SOFCs are operating under fixed current densities.

The fluidized bed gasifier coupled with DC-SOFC is simplified as a 2D rectangle domain with the size of $W \times H_R$, where W is the width and H_R is the height. The initial still carbon bed is H_C high with 45.0% porosity, as shown in Figure 1. The fluidizing agent CO₂ flow into the channel from the bottom with different velocities, and the carbon particles react with CO₂ producing CO according to Boudouard gasification as described in Section 2.1. CO is electrochemically oxidized on the SOFC boundaries and CO₂ is produced at the same time. The parameters adopted in this simulation are listed in Table 2.

Table 2. Parameters adopted in TFM simulations.

Parameter	Value
Reactor height, H_R (m)	0.200
Initial bed height, H_0 (m)	0.100
Temperature, T (K)	1173
Particle diameter, d_p (μm)	155
Particle density, ρ_p ($\text{kg}\cdot\text{m}^{-3}$)	1000
Bed voidage, ε_0	0.450
CO ₂ dynamic viscosity, μ_{CO_2} (Pa·s)	4.446×10^{-5}
CO dynamic viscosity, μ_{CO} (Pa·s)	4.443×10^{-5}
Specific surface area of the char, S_C ($\text{m}^2\cdot\text{g}^{-1}$)	750
Gravitational acceleration, g ($\text{m}\cdot\text{s}^{-2}$)	9.807
Faraday constant, F ($\text{C}\cdot\text{mol}^{-1}$)	96,485.3
Gas constant, R ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)	8.314
Inlet gas composition, x_{CO_2}	100%
Grid resolution, Δx (μm)	$4.3 d_p$
Gibbs free energy, G_0 ($\text{kJ}\cdot\text{mol}^{-1}$)	180.549
Time step, Δt (s)	$10^{-8}\sim 10^{-3}$

The boundary conditions are set as below. The bottom of the channel is the inlet and a constant velocity with 100.0 mol.% CO₂ is set; the upper part of the channel is the outlet and an atmospheric pressure is applied; the side walls of the channel are non-flux

boundaries when no SOFCs are placed and are reactive boundaries with fixed species fluxes when SOFCs are applied. It should be noted that even though the SOFC is coupled with a fluidized gasifier, not all of side walls are SOFCs. That is to say, only part of the side walls are reactive boundaries and other parts are still non-flux boundaries. Additionally, in typical fluidized beds, the gas inflow exhibits a fluctuating behavior owing to the limited pressure drop in the distributor. This feature indeed has a considerable effect on the bubble evolution and mass transfer [45]. In this study, the continuous gas inflow is set, and the effect of the pulsed inlet condition is left for the future.

4. Results and Discussion

In this section, the model of fluidized bed gasifier is tested by comparing with experimental study first, and then the effects of CO_2 inlet velocity, $v_{\text{CO}_2, \text{in}}$, activity of carbon fuel and channel width, W , on the performance of gasifier are discussed. Finally, fluidized bed gasifiers coupled with SOFC are explored and the influences of coupling between SOFC and three typical gas–solid flows, namely fixed bed, delayed bubbling bed and bubbling bed, are explored.

4.1. Model Validation

To validate the model of a fluidized bed coupled with Boudouard gasification, a fluidized bed gasifier with different carbon bed height was simulated and compared with the experimental result obtained by Lee et al. [36]. As shown in Figure 2, the gasifiers with three different carbon bed heights (2.5 cm, 5.1 cm and 7.6 cm) operating at 1173 K, 1223 K and 1273 K have been simulated and the CO molar fraction along the height were obtained, which are in good agreement with the experimental tests, verifying the reliability of the model.

Figure 2. Fluidized bed gasifier with different carbon bed.

When the SOFC and gasifier are combined in one chamber, they need to operate at the same temperature, so the operating temperature is a critical factor for this system. Boudouard gasification accelerates with the increasing temperature. That means a relatively high temperature benefits the gasification while SOFC needs a relatively low temperature to achieve a good durability. In this study, 1173 K is set, at which the Boudouard gasification rate is not too low and SOFC with Ni-YSZ still has a good performance [17,33].

4.2. Fluidized Bed Gasifiers

4.2.1. Effects of CO₂ Inlet Velocity

Before simulation of the fluidized bed gasifier, the gas–solid flow without Boudouard gasification was calculated first to explore the effect of CO₂ inlet velocity, $v_{\text{CO}_2, \text{in}}$, on the gas–solid flow. Utilizing the correlation reviewed in the book by J.R. Grace et al. [46], the minimum fluidized velocity and the minimum bubbling velocity are estimated as 0.585 cm/s and 1.407 cm/s, respectively. Six different CO₂ inlet velocities ranging from a value less than the minimum fluidized velocity to a value greater than the minimum bubbling velocity were chosen. As shown in Figure 3, the gas–solid flow regimes change with the CO₂ inlet velocity ($v_{\text{CO}_2, \text{in}}$). At $v_{\text{CO}_2, \text{in}} = 0.2$ and 0.5 cm/s, the carbon particles are stagnant (Figure 3a,b); at $v_{\text{CO}_2, \text{in}} = 0.9$ cm/s, the carbon particles are fully suspended by the gas and the carbon bed sets up to homogeneously fluidize and expand (Figure 3c); as $v_{\text{CO}_2, \text{in}}$ increases to 1.5 or 3.0 cm/s, bubbles appear in the carbon bed (Figure 3d,e); as $v_{\text{CO}_2, \text{in}}$ raises further, the bubbles in the carbon bed may coalesce into larger bubbles called gas slugs (Figure 3f). The above flow regimes are the fixed bed, delayed bubbling bed, bubbling bed and slugging bed, respectively. In this study, $v_{\text{CO}_2, \text{in}}$ is controlled to avoid flowing away of carbon particle from outlet and only the fixed bed, delayed bubbling bed and bubbling bed have been considered.

Figure 3. Gas–solid flows with different CO₂ inlet velocities, $v_{\text{CO}_2, \text{in}}$. (a) 0.2 cm/s, (b) 0.5 cm/s, (c) 0.9 cm/s, (d) 1.5 cm/s, (e) 3.0 cm/s, (f) 11.0 cm/s.

4.2.2. Effects of Activity of Carbon Fuel and CO₂ Inlet Velocity

Activities of different types of carbon fuel vary in a wide range and an abundance of experimental studies are focused on developing activity catalyst to enhance the fuel activity; therefore, it is practically meaningful to explore the effects of carbon activity and CO₂ inlet velocity, $v_{\text{CO}_2, \text{in}}$. According to Section 2.1, the activity of carbon fuel can be enhanced by increasing active site density, raising the temperature, reducing activation energy, and so on. Here, activity is changed by varying the active site density, A_s . A_s of carbon particles utilized by Lee et al. [36] is determined to be 7.2×10^{-6} mol/m² by fitting the experimental data and A_s changing from 7.2×10^{-6} mol/m² to 3.6×10^{-4} mol/m² is

considered. The effects of A_s on CO molar fraction distribution in fluidized bed gasifiers are shown in Figure 4.

Figure 4. CO molar fraction distribution in fluidized bed gasifiers with different active site densities A_s , $7.2 \times 10^{-6} \text{ mol/m}^2$, $3.6 \times 10^{-5} \text{ mol/m}^2$, $7.2 \times 10^{-5} \text{ mol/m}^2$, $1.44 \times 10^{-4} \text{ mol/m}^2$, $3.6 \times 10^{-4} \text{ mol/m}^2$. (a) Fixed bed with $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$, (b) Delayed bubbling bed with $v_{\text{CO}_2,\text{in}} = 0.5 \text{ cm/s}$, (c) Bubbling bed with $v_{\text{CO}_2,\text{in}} = 1.5 \text{ cm/s}$, (d) Bubbling bed with $v_{\text{CO}_2,\text{in}} = 3.0 \text{ cm/s}$.

Figure 4a shows the CO molar fraction distribution in a fixed bed gasifier with $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$. It can be seen that for all of the active site densities (A_s) considered here, CO molar fraction at the outlet is close to the equilibrium molar fraction (97.4 mol.%), and with increasing of A_s the distance in the carbon bed to reach CO equilibrium concentration reduces. In the fixed bed, convection is weak, carbon particles are stagnant, the carbon bed can be thought of as porous media, mass transport in the carbon bed are

diffusion and convection, and there is ignorable concentration gradient in the transversal the transversal direction.

Figure 4b shows the CO molar fraction distribution in a delayed bubbling bed with CO_2 inlet velocity $v_{\text{CO}_2,\text{in}} = 0.5 \text{ cm/s}$. It is shown that, when $A_s = 7.2 \times 10^{-6} \text{ mol/m}^2$, CO concentration reduced significantly with the increase of $v_{\text{CO}_2,\text{in}}$ and CO molar fraction in the chamber is much lower than its equilibrium value. It is because the gasification rate of carbon is too slow for a delayed bubbling bed and the period for CO_2 to pass the carbon bed is not long enough to reach the equilibrium. It should be mentioned that when $v_{\text{CO}_2,\text{in}} = 0.5 \text{ cm/s}$, the carbon bed in the channel converts from a fixed bed into a delayed bubbling bed after adding Boudouard gasification and the bed expansion can be observed in Figure 5. In the delayed bubbling bed, the carbon particles are fully suspended by the gas phase, the carbon bed is expanding uniformly, and the porosity of the carbon bed reduces. All of these changes benefit mass transport in the carbon bed. Figure 4c, d is CO molar fraction distribution in bubbling beds with $v_{\text{CO}_2,\text{in}} = 1.5$ and 3.0 cm/s , respectively. It is observed that, at $v_{\text{CO}_2,\text{in}} = 1.5 \text{ cm/s}$, CO concentration reduces further for $A_s = 7.2 \times 10^{-6} \text{ mol/m}^2$ and CO concentration at the outlet cannot reach the equilibrium for $A_s = 3.6 \times 10^{-5} \text{ mol/m}^2$ either. As $v_{\text{CO}_2,\text{in}}$ is as high as 3.0 cm/s , only for $A_s = 1.44 \times 10^{-4} \text{ mol/m}^2$, the CO molar fraction at the outlet can be close to the equilibrium. In the bubbling beds, the bubbles form in the carbon bed, the carbon bed is expanding significantly with moving bubbles in it, the mass transport is dramatically increased due to the fluid-like solid particle, which cannot be described by mass transport in porous media anymore. Due to the significant convection and the motion of solid particles along the channel, there is considerable concentration gradient in the transversal direction.

Figure 5. Effect of active site densities A_s and inlet velocity $v_{\text{CO}_2,\text{in}}$ on (a) carbon bed height, H_C , (b) total gasification rate, R_{tot} .

Figure 5a gives the effect of A_s and $v_{\text{CO}_2,\text{in}}$ on the carbon bed height, H_C , and total gasification rate, R_{tot} , in the channel. The carbon bed height, H_C , is defined as the lowest height where the time-averaged gauge pressure is zero. H_C can describe the conversion of gas–solid flows to some extension. For the fixed bed, H_C is equal to initial bed height, while for the delayed bubbling bed and bubbling bed, H_C is larger than the initial bed height due to the suspending of solid carbon particles. R_{tot} is the sum of gasification rate of whole system in unit of mol/s, which should match with the output current to maintain a steady operation. As shown in Figure 5a, H_C increases with $v_{\text{CO}_2,\text{in}}$ due to the interaction between the particles and gas flow while the influence of A_s on H_C is complicated. When H_C is equal to the initial bed height, which means a fixed bed, there is an ignorable influence of A_s on

H_C , while as the carbon bed begins expanding, H_C raises with A_s . This phenomenon is caused by the coupling effects between gas–solid flows and gasification, which will increase the volume of gases. As shown in Figure 5b, R_{tot} is affected by active site density A_s and CO_2 inlet velocity $v_{CO_2,in}$. As CO concentration at the outlet is lower than the equilibrium concentration, like $v_{CO_2,in} = 0.5$ cm/s and $A_s = 7.2 \times 10^{-6}$ mol/m², shown in Figure 4b, R_{tot} increases with the increase of A_s and $v_{CO_2,in}$. Conversely, as CO concentration at the outlet reaches equilibrium concentration, R_{tot} is linear with v_{CO_2} and does not increase with increase of A_s anymore. Thus, for a given carbon fuel and geometrical structure of anode chamber, there is critical $v_{CO_2,in}$, to achieve the largest R_{tot} and a near equilibrium concentration of CO at the outlet. This conclusion is also very useful to design DC-SOFC with a separated fluidized bed gasifier.

In the validation part, the fluidized bed gasifier with $A_s = 7.2 \times 10^{-6}$ mol/m² have a good agreement with Lee's experimental test for activated carbon particles [36]. That is to say, for activated carbon tested by Lee et al., critical $v_{CO_2,in}$ to maximize gasification rate should be lower than 0.5 cm/s to reach an equilibrium CO concentration. However, for other more active carbon fuel, increasing $v_{CO_2,in}$ is suggested to achieve an enhanced mass transport in the anode chamber and a higher gasification rate.

4.2.3. Effects of Channel Width

According to Cai's study [25], to maintain the steady and continuous operation of DC-SOFC, the gasification rate and the current density should match each other; the consumption of CO by SOFC should be equal to the production rate of CO by Boudouard gasification. In order to provide enough CO to SOFC under high current densities, it is critically important to raise the production rate of CO. When the activity of carbon is fixed, widening the channel can raise the production rate of CO conveniently. Figure 6 shows the effects of channel width on the bed height H_C , and total gasification rate, R_{tot} . In this section, the active site density, A_s , is 7.2×10^{-5} mol/m², and the fixed bed with $v_{CO_2,in} = 0.2$ cm/s, the delayed bubbling bed with $v_{CO_2,in} = 0.5$ cm/s, and the bubbling bed with $v_{CO_2,in} = 1.5$ cm/s are considered. The width of channel is set as 1 cm, 2 cm, 4 cm and 6 cm, respectively.

Figure 6. Effect of channel width, W , and inlet velocity $v_{CO_2,in}$ on (a) carbon bed height, H_C , (b) total gasification rate, R_{tot} .

As shown in Figure 6, R_{tot} increases with channel width linearly, while the effects on bed height, H_C , varies with the gas–solid flow regime. For the fixed bed with $v_{CO_2,in} = 0.2$ cm/s, H_C keeps the initial bed height; for the delayed bubbling bed with $v_{CO_2,in} = 0.5$ cm/s, H_C decreases with increasing channel width slightly, indicating that the

expansion of the carbon bed is weakened; for the bubbling bed with $v_{\text{CO}_2,\text{in}} = 1.5 \text{ cm/s}$, H_C reduces significantly when the channel width varies from 1 cm to 2 cm and then reduces slightly with increasing of the channel width. Combined with Figure 4b, it can be concluded that for given A_s and $v_{\text{CO}_2,\text{in}}$, widening the channel can increase the total gasification rate, R_{tot} , linearly.

4.3. Fluidized Bed Gasifiers Coupled with SOFC

Fluidized bed gasifiers coupled with SOFC operating under different constant current densities are simulated and the effects of coupling extent between fluidized bed gasifiers and SOFC on system performance are discussed. Two different active site densities, $7.2 \times 10^{-6} \text{ mol/m}^2$ and $7.2 \times 10^{-5} \text{ mol/m}^2$, of carbon particles are considered. Carbon particles with $A_s = 7.2 \times 10^{-6} \text{ mol/m}^2$ tested by Lee et al. [36] are referred to as low activity carbon fuel and those particles with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$ are referred to as high activity carbon fuel. Two SOFCs are placed on both side walls symmetrically with the anodes inside and the current density is set as 1000, 2000, 5000, 8000, 10,000, 15,000 A/m^2 , respectively. The coupling extent is measured by the overlapping area between the anode surface and the carbon bed, as shown in Figure 1, where d_{SOFC} is the distance between inlet and SOFCs. The channel length H_R is 20 cm and the width, W , is 4 cm. The initial carbon bed is 10 cm high and the size of SOFC is set as 10 cm long, which is available for most of SOFC producers [47–49]. Four different positions of SOFC including $d_{\text{SOFC}} = 0.0, 2.5, 5.0$ and 7.5 cm are involved to investigate the influence of coupling extent. Three gas–solid flow regimes, namely, fixed bed, delayed bubbling bed and bubbling bed are explored.

4.3.1. Low Activity Carbon fuel with $A_s = 7.2 \times 10^{-6} \text{ mol/m}^2$

Fluidized bed gasifier coupled with SOFCs utilizing low activity carbon fuel is simulated and two inlet CO_2 velocities, $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$ and 0.5 cm/s , are considered. The CO molar fraction along the channel for different conditions is shown in Figure 7. Figure 7a,c,e are the average CO molar fraction and Figure 7b,d,f are the CO molar fraction near the side walls where SOFCs are placed. It can be seen from Figure 7 that CO molar fraction at the outlet reduces as SOFCs are moved upwards. With the moving up of the SOFCs, the coupling extent reduces and more and more of the anode surface operates beyond the carbon bed, where no gasification happens to produce CO and only the electrochemical oxidation of CO occurs. This indicates that larger d_{SOFC} results in lower CO concentration in exhaust gas and more of carbon is oxidized into CO_2 , instead of CO, accounting for a higher fuel efficiency. As the current density increases from 1000 to 2000 A/m^2 (Figure 7c,d), CO concentration near the outlet is close to zero for $d_{\text{SOFC}} = 5.0, 7.5 \text{ cm}$, which means these systems cannot support 2000 A/m^2 . For $d_{\text{SOFC}} = 0.0, 2.5 \text{ cm}$, the CO concentration is much higher than zero, indicating that the system can support 2000 A/m^2 . This result demonstrates that the coupling extent can change the limiting current density in the anode chamber and a higher coupling extent leads to a higher limiting current density.

When the SOFC and gasifier are operated separately, an equilibrium CO molar fraction benefits the cell performance because a higher CO concentration accounts for a higher cell performance according to Equation (20). This is not the case when the SOFC and fluidized bed are coupled together, as shown in Figure 7b–f. When $v_{\text{CO}_2,\text{in}}$ increases from 0.2 to 0.5 cm/s , CO molar fraction reduces and equilibrium concentration cannot be reached as shown in Figure 4b, but increasing $v_{\text{CO}_2,\text{in}}$ benefits the cell performance at 2000 A/m^2 (Figure 7b–f). When $v_{\text{CO}_2,\text{in}}$ raises from 0.2 to 0.5 cm/s , all of the systems can operate steadily under 2000 A/m^2 . The positive impacts of coupling extent and $v_{\text{CO}_2,\text{in}}$ can be explained according to Figure 8, where the effects of coupling extent and $v_{\text{CO}_2,\text{in}}$ are shown.

Figure 7. Averaged CO molar fractions (a,c,e) and CO molar fractions near side walls (b,d,f) along channel for fixed bed gasifiers coupled with SOFCs with $A_s = 7.2 \times 10^{-6} \text{ mol/m}^2$. (a,b) 1000 A/m^2 , $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$; (c,d) 2000 A/m^2 , $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$; (e,f) 2000 A/m^2 , $v_{\text{CO}_2,\text{in}} = 0.5 \text{ cm/s}$.

Figure 8. (a) Carbon bed height, H_C , and (b) total gasification rate, R_{tot} of fluidized bed coupled with SOFC with $A_s = 7.2 \times 10^{-6}$ mol/m².

As shown in Figure 8a, there is no change in H_C at $v_{CO_2,in} = 0.2$ cm/s. This is because the flows are in the fixed bed regime. However, at $v_{CO_2,in} = 0.5$ cm/s, it is noticeable that H_C decreases slightly especially when d_{SOFC} attains lower values. This is not surprising since the flows at such condition are in the delayed bubbling bed regime. The radial mixing of the bed is not sufficiently strong and the increased gases due to gasification form low solid volume fraction structures near the bed boundaries. These structures then find pathways to go upwards along the bed boundaries. Figure 8b shows that the total gasification rate is promoted with the increase of the coupling extent. In summary, for activated carbon particle with $A_s = 7.2 \times 10^{-6}$ mol/m² utilized by Lee et al. [36], the coupling extent and $v_{CO_2,in}$ are two critical parameters to improve the cell performance. Although increasing inlet velocity reduces CO molar fraction in anode chamber, the total gasification rate goes up and thus the maximum current density is enhanced.

4.3.2. High Activity Carbon Fuel with $A_s = 7.2 \times 10^{-5}$ mol/m²

Fluidized bed gasifiers coupled with SOFCs fed with high activity carbon fuel have been investigated and three different inlet CO₂ velocities, 0.2 cm/s (fixed bed), 0.5 cm/s (delayed bubbling bed) and 1.5 cm/s (bubbling bed), have been considered. The CO molar fraction along the channel under 5000, 8000, 10,000 A/m² is shown in Figure 9.

Similar to that observed in Figure 7 the CO molar fractions in exhaust gas reduce with the increasing of d_{SOFC} and the coupling extent has positive effects on cell performance. One of the important differences is that the concentration gradient increases in transversal direction, which can be observed by comparing the averaged CO molar fraction in Figure 9a,c,d with CO molar fraction near the side walls in Figure 9b,e,f. Although the averaged CO molar fraction at a given height is larger than zero, the CO molar fraction near the side walls is close or equal to zero for several cases. The current density of 5000 A/m² cannot be supported at $d_{SOFC} = 7.5$ cm and 10,000 A/m² can only be maintained at $d_{SOFC} = 0.0$ cm. This illustrates that the CO concentration gradient cannot be ignored when the current density is 5000 A/m² or higher, and the mass transport is a considerable factor for system performance.

Figure 9. Averaged CO molar fractions (a,c,e) and CO molar fraction near side walls (b,d,f) along channel for fixed bed gasifiers coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{\text{CO}_2,\text{in}} = 0.2 \text{ cm/s}$. (a,b) 5000 A/m^2 , (c,d) 8000 A/m^2 , (e,f) $10,000 \text{ A/m}^2$.

The influence of coupling extent and inlet velocity on gas–solid flows and total gasification rate can be observed in Figure 10. The bed height, H_C , keeps the initial height except

at $d_{\text{SOFC}} = 0.0$ cm under $10,000 \text{ A/m}^2$. The carbon bed expands slightly at $d_{\text{SOFC}} = 0.0$ cm under $10,000 \text{ A/m}^2$. The total gasification rate, R_{tot} , increases with increasing current density and coupling extent, as shown in Figure 10b. This is a critical difference between DC-SOFCs and fuel cells utilizing gaseous fuel. As gaseous fuel is utilized, raising the gaseous fuel flux is the only way to support an increasing current density, while as solid carbon is fed, the in situ gasification of carbon accelerates with the increasing current density, which can provide more CO.

Figure 10. (a) Carbon bed height, H_C and (b) total gasification rate, R_{tot} of fluidized bed coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{\text{CO}_2, \text{in}} = 0.2 \text{ cm/s}$.

When $v_{\text{CO}_2, \text{in}}$ increases to 0.5 cm/s , the gas–solid flows are delayed bubbling beds, in which the carbon particles are suspending but no observable bubbles forms in the carbon bed. The increasing porosity and enhanced convection in the delayed bubbling bed benefits mass transport and further promotes the gasification reaction of carbon. CO molar fraction along the channel for delayed bubbling bed gasifiers coupled with SOFC is illustrated in Figure 11. As shown in Figure 11, 5000 A/m^2 can be maintained by all systems due to the enhanced mass transport and $10,000 \text{ A/m}^2$ can be operated at $d_{\text{SOFC}} = 0.0$ and 2.5 cm indicating improvement of system performance.

Figure 11. Cont.

Figure 11. Averaged CO molar fractions (a,c,e) and CO molar fraction near side walls (b,d,f) along channel for delayed bubbling bed gasifiers coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{\text{CO}_2,\text{in}} = 0.5 \text{ cm/s}$. (a,b) 5000 A/m^2 , (c,d) 8000 A/m^2 , (e,f) $10,000 \text{ A/m}^2$.

An ideal CO concentration profile appears in Figure 11a,b at $d_{\text{SOFC}} = 2.5 \text{ cm}$ under 5000 A/m^2 . As shown in Figure 11b, the CO concentration on the anode surface keeps a relatively high CO molar fraction for most of the anode surface with no observable concentration reduction along the channel. In this domain, a balance between the electrochemical oxidation of CO and gasification of carbon is reached. On the anode surface above carbon bed where there are no carbon particles, only electrochemical oxidation occurs and CO is consumed rapidly, reducing CO concentration in exhaust gas and raising fuel efficiency. To achieve a lower CO concentration at the outlet of the channel and increase fuel utilization further, the length of SOFC can be elongated properly. This is another critical benefit of DC-SOFC. Geometrical optimization of DC-SOFC can improve the cell performance further, but this is beyond the scope of this study.

The impacts of the coupling extent and current density on carbon bed height and total gasification rate can be seen in Figure 12. Both the H_C and R_{tot} increase with the increase of coupling extent gradually and the effects of current density weaken with the increase of d_{SOFC} . There is only a slight difference of carbon bed height under varying current densities while the total gasification rate increases significantly with increasing current density. It can be found that the total gasification rate increases as high as six times after combining with SOFCs, which can explain the improvement of cell performance shown in

Figure 11. A significant improvement of system performance is obtained, and the benefits of coupling between fluidized bed gasifiers and SOFCs are observed again.

Figure 12. (a) Carbon bed height, H_C and (b) total gasification rate, R_{tot} of fluidized bed coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{CO_2,in} = 0.5 \text{ cm/s}$.

More interesting phenomena appear when the inlet CO_2 velocity, $v_{CO_2,in}$, increases to 1.5 cm/s. At such a condition, many bubbles form in the carbon bed. First, carbon particles move in axial and radial directions in the bubbling beds, causing both axial and radial solids mixing and gas mixing. The gas mixing and solid mixing are related and affected by each other. For example, back-mixing caused by the downward motion of carbon particles and horizontal gas mixing resulted from lateral solids mixing are two important mass transport mechanisms in bubbling beds. Particularly, the horizontal gas mixing is a feasible way to enhance mass transport in the radial direction. This is the second new phenomenon in the bubbling bed gasifier. Figure 13 gives CO molar fractions in bubbling bed gasifiers with $v_{CO_2,in} = 1.5 \text{ cm/s}$ under 5000, 10,000, 15,000 A/m². Due to the enhanced horizontal mass transport, the radial concentration gradient weakens for all the cases and four systems with different coupling extents can support a current density as high as 10,000 A/m². Only the system with $d_{SOFC} = 7.5 \text{ cm}$ cannot operate under 15,000 A/m² continuously. The improvement of cell performance caused by enhanced horizontal mass transport is the third new phenomenon.

The carbon bed height, H_C , and total gasification rate, R_{tot} , of the bubbling bed gasifier coupled with SOFCs are shown in Figure 14. The effects of the current density on H_C are much more significant than those in the fixed and delayed bubbling bed and the expansion of the bed becomes a considerable factor to optimize the system performance at $d_{SOFC} = 0$ and 2.5 cm, wherein the CO molar fraction of exhaust gas is close to higher than that in the carbon bed where SOFCs are placed. This is because the carbon bed is higher than the upper boundaries of SOFCs and only gasification of carbon occurs in this domain. The highest total gasification rate is $1.17 \times 10^{-2} \text{ mol/s}$ in all the cases simulated in this study, which is about 28 times higher than that of fixed bed gasifiers with the same active site density ($7.2 \times 10^{-5} \text{ mol/m}^2$) ($4.09 \times 10^{-4} \text{ mol/s}$ shown in Figure 5).

Figure 13. Averaged CO molar fractions (a,c,e) and CO molar fractions near side walls (b,d,f) along channel for bubbling bed gasifiers coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{CO_2,in} = 1.5 \text{ cm/s}$. (a,b) 5000 A/m^2 , (c,d) $10,000 \text{ A/m}^2$, (e,f) $15,000 \text{ A/m}^2$.

Figure 14. (a) Carbon bed height, H_C and (b) total gasification rate, R_{tot} of bubbling bed gasifiers coupled with SOFC with $A_s = 7.2 \times 10^{-5} \text{ mol/m}^2$, $v_{\text{CO}_2, \text{in}} = 1.5 \text{ cm/s}$.

This dramatic promotion of gasification rate is ascribed to the improved mass transport in gas–solid flows. Therefore, the coupling between gasifiers and SOFCs is a feasible way to improve the cell performance of DC-SOFC.

5. Conclusions

The numerical simulation of fluidized bed gasifiers coupled with DC-SOFC have been conducted based on TFM. Three flow regimes including fixed bed, delayed bubbling bed and bubbling bed were involved. A five-step Boudouard gasification model was adopted and the anode reactions of DC-SOFC were treated as the coupling processes between Boudouard gasification of solid carbon particles and electrochemical oxidation of CO in the anode. A model of the fluidized bed gasifiers was tested by comparing with the experimental results in the literature. The effects of inlet velocity of the fluidizing agent CO_2 , carbon activity and channel width on the performance of fluidized bed gasifiers have been explored. The overlapping area between the initial carbon bed and anode surface of SOFC was utilized to explore the effect of the coupling extent on the performance of fluidized bed gasifiers coupled with SOFC. Fixed current densities varying from 1000 to 15,000 A/m² were simulated to test the effect of the coupling extent, inlet velocity of CO_2 on total gasification rate and the maximum current density the system can maintain. The main conclusions include:

- (1) results calculated based on the fluidized bed gasifiers model agree well with the experimental tests, validating its reliability;
- (2) the total gasification rate rises with the increase of inlet velocity, carbon activity and channel width, while too high an inlet velocity reduces CO concentration in the channel;
- (3) in the range this study involved, a higher coupling extent and inlet velocity of CO_2 result in a larger total gasification rate and maximum current density, because of enhanced mass transport by expansion of the carbon bed, back-mixing, solid mixing and gas mixing. The gasification rate rises as high as 28 times that of the fixed bed gasifiers with the same activity of carbon and the maximum current density increases from <5000 A/m² to >15,000 A/m² due to the coupling between fluidized bed gasifiers and SOFC.

In summary, coupling between fluidized bed gasifiers and DC-SOFC is a feasible way to promote the anode performance of DC-SOFCs, and to our best knowledge, it is the first simulation to couple fluidized gas–solid flows with SOFC. Future works will focus on exploring the effect of particle size and temperature distribution in the fuel cell.

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