Numerical Simulation of Regeneration Process of Oxygen Carriers in Fluidized Bed

Xu Yao
School of Energy Science and Engineering
Harbin Institute of Technology
Harbin, China
xuyao_sure@126.com

Zhai Ming*
School of Energy Science and Engineering
Harbin Institute of Technology
Harbin, China
zhaiming@hit.edu.cn

Ge Tiezhu
School of Energy Science and Engineering
Harbin Institute of Technology
Harbin, China
370873506@qq.com

Dong Peng
School of Energy Science and Engineering
Harbin Institute of Technology
Harbin, China
dongp@hit.edu.cn

*Corresponding author

Abstract— In recent years, fluidized bed reactors are applied to the regeneration process of oxygen carriers. The regeneration performance of oxygen carriers will have a direct influence on the fuel conversion and the ability of oxygen transfer of oxygen carriers. For this reason, considering the effects of non-uniform structures in fluidized bed reactors, the regeneration process of oxygen carriers in fluidized bed is investigated by means of simulation. Gas-solid flow behavior and temperature field in fluidized bed are obtained. The impact of air to fuel ratio on the oxygen conversion rate is evaluated. The results indicate that a high air to fuel ratio will reduce oxygen conversion efficiency. By comparison with experimental data, the model with consideration of multi-scale structures can obtain a better prediction.

Keywords- Computational fluid dynamics; Fluidized bed; Oxygen carriers; Numerical simulation;reactor

I. INTRODUCTION

Chemical-looping combustion(CLC) technology has attracted more and more attention due to its being low NOX emission with inherent CO2 separation[1-3].Hossain et al. [4] applied the nuclear model and the shrinking nuclear model to the chemical looping combustion. The results indicated that the nuclear model can describe the change of particles reasonably. Kruggel-Emden et al. [5] simulated the CLC process by means of computational fluid dynamics(CFD) method. The buffer system was introduced to eliminate the pulsation of mass flow between reactors. The influence of different mass flow rate was analyzed. It was pointed out that the reactor height should be increased owing to that there was not enough oxygen carriers to regenerate.

Due to the interaction between the particles and gas-solid interaction, the non-uniform spatial distribution of particles is formed. With no consideration of the effects of the non-uniform structures, it will lead to large errors for numerical simulation. In recent years, there is a great amount of development on the solution of gas-solid interaction .Among them, the Energy Minimization Multi-Scale (EMMS) method is widely used to solve the gas-solid interaction[6,7]. Based on this, a two-fluid model coupling with chemical reaction is established considering the impact of non-uniform structures in the reactor. The regeneration process of oxygen carriers in the fluidized bed reactor is simulated. The effect of air-fuel ratio of oxygen conversion rate is also analyzed.

II. MATHEMATICAL MODEL

The governing equations of multiphase flow system consist of mass, momentum and energy conservation for each phase. The solid phase is modeled as a continuum fluid with the kinetic theory of granular flows for closure [8].

A.Continuity equations

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \boldsymbol{u}_g) = \dot{m}_g \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s \boldsymbol{u}_s) = \dot{m}_s \quad (2)$$

Where $\dot{m}_g$ 和 $\dot{m}_s$ represent the mass source term.

B. Momentum balance equations

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \boldsymbol{u}_g) + \nabla \cdot (\alpha_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g) = \nabla \cdot \boldsymbol{\tau}_g + \alpha_g \rho_g \boldsymbol{g} - \alpha_g \nabla p - \beta(\boldsymbol{u}_g - \boldsymbol{u}_s) + \dot{m}_g \boldsymbol{u}_g \quad (3)$$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \boldsymbol{u}_s) + \nabla \cdot (\alpha_s \rho_s \boldsymbol{u}_s \boldsymbol{u}_s) = \nabla \cdot \boldsymbol{\tau}_s + \alpha_s \rho_s \boldsymbol{g} - \alpha_s \nabla p - \nabla p_s + \beta(\boldsymbol{u}_g - \boldsymbol{u}_s) + \dot{m}_s \boldsymbol{u}_s \quad (4)$$

Where β is gas-solid drag coefficient.

C. Energy balance equations

$$\frac{\partial}{\partial t}(\alpha_g \rho_g c_g T_g) + \nabla \cdot (\alpha_g \rho_g c_g T_g \boldsymbol{u}_g) = \nabla(\lambda_g \nabla T_g) + \varphi_{gs}(T_g - T_s) + \dot{m}_g H_g \quad (5)$$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s c_s T_s) + \nabla \cdot (\alpha_s \rho_s c_s T_s \boldsymbol{u}_s) = \nabla(\lambda_s \nabla T_s) + \varphi_{sg}(T_s - T_g) + \dot{m}_s H_s \quad (6)$$

Where H and λ are the enthalpy and thermal conductivity of mixture, respectively.

D. Gas species transport equation

$$\frac{\partial}{\partial t}(\rho_g Y_{g,i}) + \nabla \cdot (\rho_g Y_{g,i} \boldsymbol{u}_g) = -\nabla \cdot J_{g,i} + \dot{m}_{g,i} \quad (7)$$

Where J is the species diffusion flux.

E. Gas-solid drag model

In the momentum balance equation, the momentum exchange plays an important role. Here, a revised gas-solid inter-phase drag model proposed by Wang et al. [9] is used to account for the impact of multi-scale structures. The model is established by using the relationship between acceleration and fluctuating cluster concentration, which avoids the dependence on empirical formula of cluster diameter and expand the application of EMMS model[6].

III. SYSTEM DESCRIPTION

In this work, the regeneration process of oxygen carriers in the fluidized bed reactor is selected as the reference case. The corresponding reaction rate is employed according to the expression proposed by Kruggel-Emden et al. [10].The air reactor component of Kolbitsch et al. [11] is simulated, which has a 4.1m height and 0.15m inner diameter. The gas enters the bottom of reactor at the velocity of 2.38m/s,and the solid circulation flux is specified from the bottom of side wall. The pressure outlet is located at the top of the reactor. The solid density and diameter is 3446 kg/m3 and 0.2 mm,respectively. The simulation time is 40s and the variables are time-averaged for the last 20 s period when the quasi-steady-state has been reached.

IV. RESULTS AND DISCUSSION

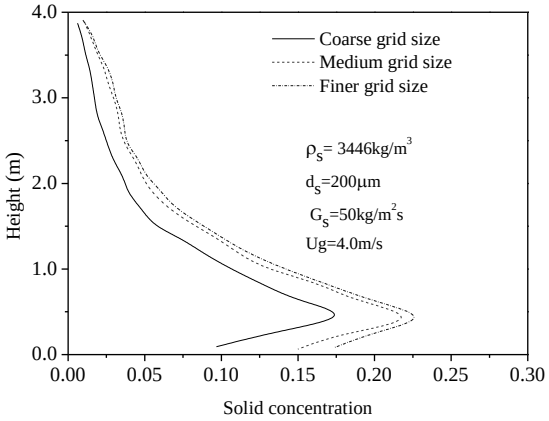

Figure 1. Time-averaged profiles of solid concentration with different grids

Considering the impact of the grid on numerical simulation, the grid-independence investigation is carried out. Three grids of (0.25cm × 0.5cm), (0.5cm × 1cm) and (0.75cm × 2cm) are employed respectively. Fig.2 shows the distribution of particle concentration in the axial direction using different grid scale. For different grids, solid concentration increases and then decreases with the height increased. At the bottom of the reactor, the solid particles enter the reactor from the side wall of the reactor, particle concentration reaches a maximum value. However, the difference is very obvious. It can be found that the particle concentration is underestimated in the axial distribution using coarse grids. The latter two grids predicted a similar the profile of particle concentration. Taking into account the accuracy and computation time, the mid-grid size (0.5cm × 1cm) is selected as the final simulation grid.

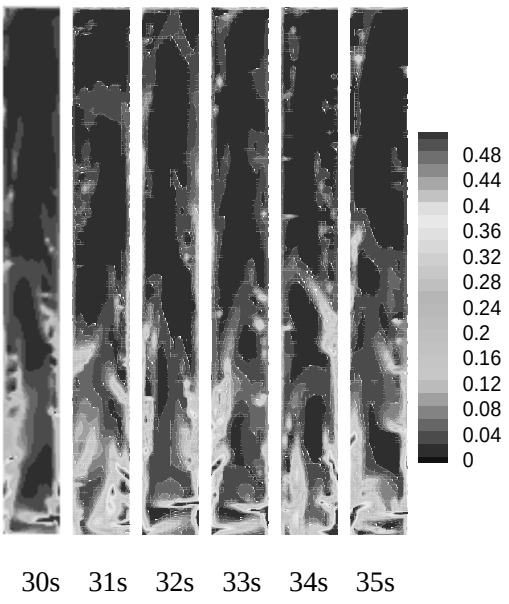

Figure 2. Instantaneous solid concentration in the reactor

Fig.2 shows the instantaneous distribution of the particle concentration in the reactor .It can be seen that solid concentration show a dense zone at the bottom and dilute region at the top. There is a large number of particle clustering near the wall. The interaction between the particles and gas leads to the non-uniform distribution of particles in the space and the formation of clusters. Hence, the gas-solid inter-phase force model used in this paper can capture the dense phase and dilute phase of reactor very well.

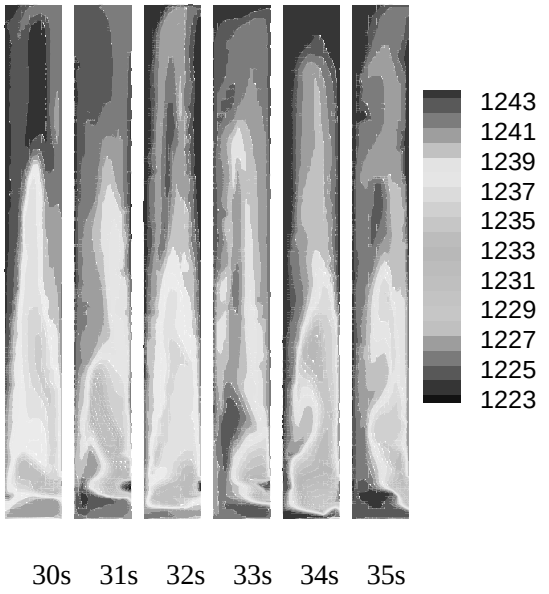

Figure 3. Instantaneous solid temperature in the reactor

Fig.3 shows the instantaneous distribution of solid temperature in the reactor. It can be found that with the reaction in progress, the heat is accumulated along the height of the reactor, which makes temperature increased. The temperature difference between the inlet and outlet reaches about 20 degrees. Owing to an exothermic reaction and a high particle concentration near the wall from Fig.2, there is a greater degree of reaction, and an obvious increase of the temperature. At the upper section of the reactor, the change of the temperature is not as clear as that at the bottom due to a low particle concentration at the top. Near the solid inlet, the inlet temperature of the solid phase is specified, which leads to a local low solid temperature.

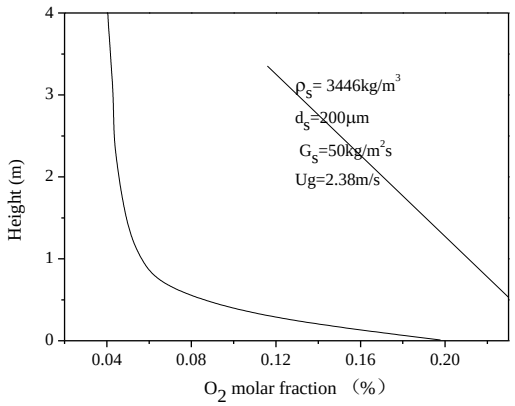

Figure 4. Time-averaged profiles of O2 molar fraction along the axial direction

Fig.4 displays the time- averaged O2 mole fraction along the height of reactor. With the increase in height, the O2 mole fraction is gradually reduced, which implies that the oxygen carriers transfer gaseous oxygen into solid oxygen. A larger degree of the oxygen variation at the bottom is related to the particle concentration. Above the height of 1.0m, the change of oxygen concentration is not significant, which is consistent with the temperature profile as Fig.3. The distribution of oxygen can indirectly reflects the oxidized degree of oxygen carriers. The operation of velocity and the circulation rate of particles will directly affect the rate of oxygen conversion. At the exit, we can find that oxygen is not completely absorbed by the oxygen carriers.

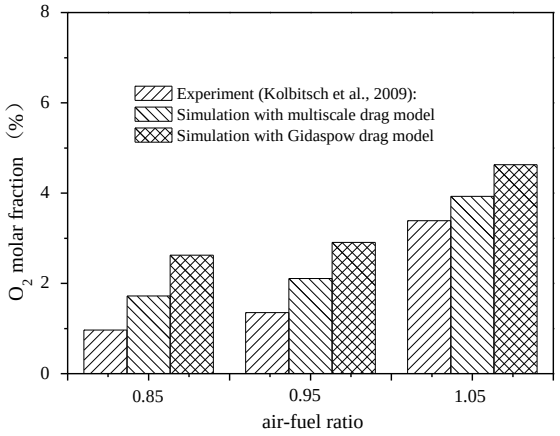

Figure 5. Effects of drag models on the predicted O2 molar fraction

Fig.5 shows the variance the outlet O2 molar fraction with air-fuel ratio. It can be seen that with the air-fuel ratio increased, the mole fraction of oxygen gradually increases, which is due to that the higher air-fuel ratio results in the amount of oxygen increased. Because the solid mass flow rate is constant, the amount of unreacted oxygen is increased and the fraction of oxygen at the outlet is improved. We can find that both the predictions by different drag model reproduce such a trend. However, there are differences between them. The multi-scale drag model can obtain a better prediction on non-uniform structures in the reactor and the simulated result is more consistent with experimental data. While, to some extent, the experimental values are overestimated by the Gidaspow drag model [9], which is attributed to that the effects of clusters are neglected and the non-uniformity of particle distribution can not be predicted very well.

V. CONCLUSION

Considering multi-scale structures in the reactor, the regeneration process of the oxygen carrier in a fluidized bed is studied by means of numerical simulation. The particle concentration, the gas composition and the temperature field are obtained. The effect of multi-scale model on the predicted results is also evaluated. The

results indicate that the prediction by multi-scale drag model is closer to the experimental data. This implies that it is necessary to consider the effect of heterogeneous structures in the simulation of fast fluidized bed.

REFERENCES

[1] Richter H, Knoche K. Reversibility of combustion processes[J]. ACS Symposium Series, 1983 , 235(1): 71–86

[2] Ishida M, Jin H. A new advanced power-generation system using chemical-Looping combustion[J]. Energy, 1994, 9(4): 415–422

[3] Lyngfelt A, Leckner B, Mattisson T. A fluidized-bed combustion process with inherent CO2 separation ; application of chemical-looping combustion[J]. Chemical Engineering Science, 2001, 56: 3101–31133

[4] Hossain M M, Lasa H I. Reduction and oxidation kinetics of Co–Ni/Al2O3 oxygen carrier involved in a chemical-looping combustion cycles[J].Chemical Engineering Science, 2010, 65: 98–106

[5] Kruggel-Emden H, Rickelt S, Stepanek F, et al. Development and testing of an interconnected multiphase CFD-model for chemical looping combustion[J]. Chemical Engineering Science,2010, 65: 4732–4745

[6] Yang N, Wang W, Ge W, et al. Simulation of Heterogeneous Structure in a Circulating Fluidized-Bed Riser by Combining the Two-Fluid Model with the EMMS Approach[J]. Ind. Eng. Chem. Res. 2004, 43:5548-5561

[7] Wang W, Li J H. Simulation of gas–solid two-phase flow by a multi-scale CFD approach-Extension of the EMMS model to the sub-grid level[J].Chemical Engineering Science.2007,62:208-231

[8] Gidaspow D. Multiphase Flow and Fluidization: Continuum and Kinetic Theory Descriptions[M]. San Diego: Academic Press, 1994

[9] Wang J W, Ge W, Li J H. Eulerian simulation of heterogeneous gas-solid flows in CFB risers: EMMS-based sub-grid scale model with a revised cluster description [J]. Chemical Engineering Science.2008,63:1553- 1571

[10] Kruggel-Emden H, Stepanek F, Munjiza A.A comparative study of reaction models applied for chemical looping combustion [J]. Chemical Engineering Research and Design, 2011, 89: 2714–2727

[11] Kolbitsch P, Proll T, Hofbauer H. Modeling of a 120kW chemical looping combustion reactor system using a Ni-based oxygen carrier [J]. Chemical Engineering Science, 2009, 64: 99–108