

## Research of Fluent Numerical Simulation on fluidized SO<sub>2</sub> Photocatalytic Reactors

Shuqin WANG<sup>1, a</sup>, Bo BI<sup>2, b</sup> and Chao LI<sup>3, c</sup>

<sup>1,2,3</sup>School of Environmental Science and Engineering,

North China Electric Power University,

Baoding 071003, China

<sup>a</sup>wsqhg@163.com, <sup>b</sup>1289171707@qq.com, <sup>c</sup>1561709773@qq.com

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**Abstract:** The fluidization condition in the SO<sub>2</sub> photocatalytic reactor was optimized by simulating the aspects of raw materials' physical properties (particle size, density) and operating conditions (packing height, inlet gas velocity). The results indicated that particle size and inlet gas velocity had a remarkable influence on the fluidization in the reactor, while 5×10<sup>-4</sup>cm was the optimal particle size and 2.6m/s was the gas velocity. The density, filler height had a little effect on fluidization. The reaction mechanism of SO<sub>2</sub> was imported the Fluent software to simulate the chemical reaction. The calculating models was suited and agreement with the experimental results.

### Introduction

Fluent is a common CFD software which can optimize the structure of reactor and derive the mechanism of the reaction by simulating the flow distribution, temperature field and chemical reaction[1]. The variation of fluidized photocatalysis condition is difficult to observe by original research due to the complex of physiochemical process such as photoelectric transition, adsorption and chemical degradation. The application of Fluent can reduce the workload of experiment and definite the mechanism of photocatalysis reaction[2].

In recent years, many researchers create varieties of reaction model to simulate photocatalytic reactors [3-5]. The theoretical conditions of photocatalytic reactors are researched by mathematics models from indoor pollution control [6-7,9]. Although Fluent can be introduced into the reaction mechanism to simulate the chemical reactions, most scholars just used the mature theory to simulate combustion reaction and scrubber[8-9]. However, it is difficult to produce a satisfactory simulate effect due to the complex of SO<sub>2</sub> photocatalytic process and the fluidized reactors. In this paper the fluidization condition in the SO<sub>2</sub> photocatalytic reactor was optimized. This can provide some references for the control of the harmful gases and performance of photocatalytic reactor.

### The mathematical model and simulation conditions

The selfmade stainless steel reactor was a 81.6-metre-high cylinder, whose radius was 5.5cm. In the middle of the reactor there were two 75.5-centimeter-high lamps, the radius and spacing of which were 1cm and 3cm.

Fluent 6.3 was used the numerical computing software. GAMBIT pre-processing software was used to solve the reactor area and its mesh; k- ε RNG model, P-1 radiation model, simplified model of a porous medium (Porous-jump) and Euler - Eulerian multiphase flow model were used to simulate the internal three-dimensional flow field in the main part of the reactor. The total number of meshes were 143,378.

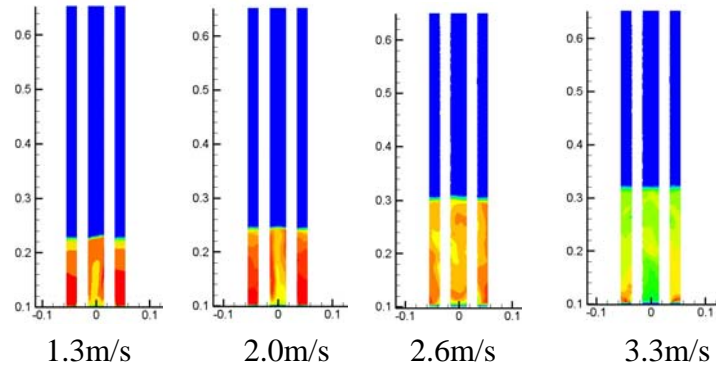
The inlet gas flow of each experiment was 1L/min. Inlet air velocity was 1.3m/s. Solid phase material was clay-based powder with density of 848kg / m<sup>3</sup>, activated carbon with density of 450kg/m<sup>3</sup> and resin with density of 1050kg/m<sup>3</sup>.

## Results and Discussion

### Effect of different inlet velocities on fluidized state

The simulated temperature and velocities in the main part of the reactor were agreement with the experimental results. This showed that the models were suited and the simulation results were credible.

Effects of different inlet velocities on fluidized state were shown in Fig.1, while the packing height was 10cm, the packing density was  $848 \text{ kg/m}^3$  and particle size was  $5 \times 10^{-3} \text{ cm}$ .

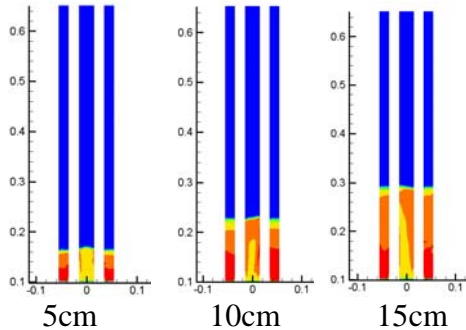


**Fig.1.** Effects of different inlet velocities on fluidized state

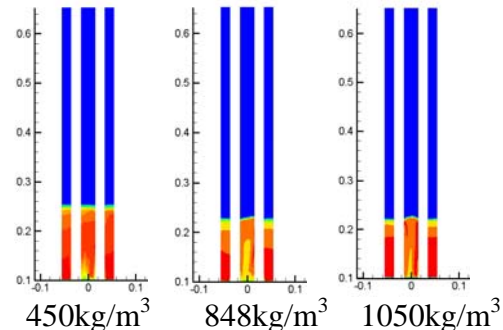
As shown in Fig.1 when the inlet velocity was more than  $2.6 \text{ m/s}$ , the fluidized height increased slowly and the fluidization became extremely disordered. Therefore the  $2.6 \text{ m/s}$  was chosen the optimal inlet velocity.

### Effect of different material properties on fluidized state

Effects of the different filler height and density on the simulating fluidized state were shown in Fig.2, while the inlet velocity was  $1.3 \text{ m/s}$  and particle size was  $5 \times 10^{-3} \text{ cm}$ .



**Fig.2a**

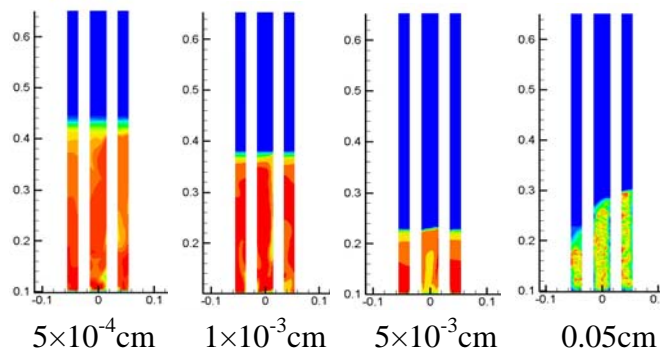


**Fig.2b**

**Fig.2.** Effects of the filler height(2a) and density(2b) on the fluidized state

The Fig.2a shows that the height only effected the length of the stabilization time of the fluidization. And Fig.2b shows that the density has little effect on the fluidized height. Considering the experimental cost, we chose  $10 \text{ cm}$  and  $848 \text{ kg/m}^3$  as the optimal filler height and packing density.

Effects of the particle size on the fluidized state were shown in Fig.3.



**Fig.3.** Effects of the particle size on the fluidized state

Fig.3 shows that when the material particle size exceeds  $5 \times 10^{-3}$  cm, the material inside the reactor was disordered. When the material particle size is  $5 \times 10^{-4}$  cm, the height of fluidization was over two-thirds of the reactor, and reverse dust phenomenon was not obvious, therefore it can be determined as the optimal material particle diameter.

### Simulation of chemical reaction process in reactor

#### Parameter of the chemical reaction model

Chemical reaction models only simulated the main part of the reactor; The k-  $\epsilon$  RNG model, P-1 radiation model, the energy equation and chemical species transport model were used to simulate the chemical reaction in the reactor. Chemical reaction mechanisms were written through CHEMKIN. Reaction mechanisms and equations were imported according the experiment and reaction temperature through Import option. The reaction mechanism and parameters were shown in Table 1, which are obtained from the National Institute of Standards and Technology (NIST) database.

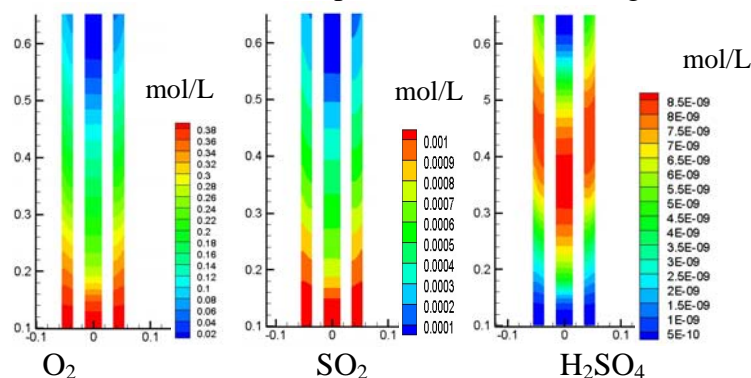
**Table 1.** The reaction mechanism and parameters

	equation	A(cm <sup>3</sup> /(mol.s <sup>-1</sup> ))	Ea(KJ/mol)	Resource
1	O <sub>2</sub> +TiO <sub>2</sub> =TiO <sub>2</sub> +2O	1.20E-17	3.77	NIST
2	O <sub>2</sub> +O=O <sub>3</sub>	8.99E-33	3.67	NIST
3	SO <sub>2</sub> +O <sub>3</sub> =SO <sub>3</sub> +O <sub>2</sub>	3.01E-12	58.2	NIST
4	TiO <sub>2</sub> +O+SO <sub>2</sub> =TiO <sub>2</sub> +SO <sub>3</sub>	4.00E-32	8.31	NIST
5	SO <sub>2</sub> +O=SO <sub>3</sub>	4.00E-32	8.310	NIST
6	SO <sub>3</sub> +O=SO <sub>2</sub> +O <sub>2</sub>	2.32E-16	4.05	NIST
7	H <sub>2</sub> O+SO <sub>3</sub> =H <sub>2</sub> SO <sub>4</sub>	1.81E12	0.99	Reference 10

\*A: Reaction-rate constant

#### The simulation results of chemical reactions reactor

The SO<sub>2</sub> removal efficiency was observed over 90% while the SO<sub>2</sub> was 1000mg/m<sup>3</sup>, O<sub>2</sub> was 300mL/min, N<sub>2</sub> was 0.12m<sup>3</sup>/h, water was 5mL and modifiedTiO<sub>2</sub> was 3g. Simulation specific molar concentration distribution of each component is shown in Fig.4 .



**Fig.4.** Simulation specific molar concentration distribution of each component

Fig.4 shows that the variation concentrations of reactants and products consisted with the experimental results. At the same time, because of the high light intensity between the two lamps, the change of reactant and product concentrations first occurred here, which is also consistent with the reaction mechanisms. The photocatalytic oxidation of SO<sub>2</sub> is obvious .

### Conclusions

1. The results of simulation showed that the packing height (5cm-15cm) had rare influence on fluidized situation; The filler density had a little effect on fluidization; Particle size and inlet gas velocity had greater impact on the fluidization in the reactor. Reducing the particle size was beneficial to the material flow. The optimum particle size was  $5 \times 10^{-4}$  cm, and the inlet gas velocity was 2.6m / s during our experimental conditions.

2. The results of chemical reactions simulation inside the reactor showed that the change of reactant and product concentrations first occurred between the two lamps and the change and concentration distribution trend of reactants and products are consistent with the reaction

mechanisms and empirical data. This suggested that the simulation results were credible.

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