



Simulation of mercury capture by sorbent injection using a simplified model

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ABSTRACT

Mercury pollution by fossil fuel combustion or solid waste incineration is becoming the worldwide environmental concern. As an effective control technology, powdered sorbent injection (PSI) has been successfully used for mercury capture from flue gas with advantages of low cost and easy operation. In order to predict the mercury capture efficiency for PSI more conveniently, a simplified model, which is based on the theory of mass transfer, isothermal adsorption and mass balance, is developed in this paper. The comparisons between theoretical results of this model and experimental results by Meserole et al. [F.B. Meserole, R. Chang, T.R. Carrey, J. Machac, C.F.J. Richardson, Modeling mercury removal by sorbent injection, *J. Air Waste Manage. Assoc.* 49 (1999) 694–704] demonstrate that the simplified model is able to provide good predictive accuracy. Moreover, the effects of key parameters including the mass transfer coefficient, sorbent concentration, sorbent physical property and sorbent adsorption capacity on mercury adsorption efficiency are compared and evaluated. Finally, the sensitive analysis of impact factor indicates that the injected sorbent concentration plays most important role for mercury capture efficiency.

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1. Introduction

Due to the characteristics of volatility, persistence, bioaccumulation and toxicity in the ambient air, mercury pollution can directly give rise to enormous hazardous on neurological health [1–6]. In 2005, US EPA issued the Clean Air Mercury Rule (CAMR) [7,8] to permanently cap and reduce mercury emissions from coal-fired power plant for the first time ever. At present, mercury emissions from flue gas by coal combustion and waste incineration have been the global environmental problem.

Usually, there are three basic species of Hg form in the flue gas: elemental Hg (Hg^0), oxidized Hg (Hg^{2+}) and particle-bound Hg (Hg^p) [9]. Compared with Hg^{2+} which can be removed by wet FGD, and Hg^p which can be removed by dust collector, Hg^0 is more difficult to remove from flue gas because of insoluble property and non-integration with fly ash particles. In the past decade, a number of techniques for the control of mercury emissions from flue gas have been proposed and evaluated from bench to pilot scales [10–13]. The dominant technologies for mercury pollution control can be classified as particulate adsorption methods, oxidation-reduction methods and chemical sedimentation methods. In particulate adsorption methods, the powdered sorbent injection (PSI), as an effective technique especially for Hg^0 , has received a great deal of attention from the EPA, utilities and technol-

ogy developers. For a typical PSI technology, the powdered sorbents such as activated carbon, zeolite and improved fly ash are injected into duct which located between downstream of the plant's air heater and upstream of the existing particulate control device, an electrostatic precipitator (ESP) or a fabric filter (FF). Subsequently, the sorbent adsorbs the mercury from the flue gas and then is captured along with the fly ash in the ESP or FF.

In order to determine the mercury removal capacity by PSI, some efforts have been devoted to the modeling of mercury adsorption mechanism and processes. As early as in 1996, Chen et al. [14] developed a simplest model to describe mercury removal by powdered sorbent injected into the flue gas duct. This model assumed that all mercury molecules that diffuse across the external film are completely captured by the sorbent particle but neglected the effect of concentration of mercury on the external surface. Flora et al. [15] also developed a model that accounted for both external mass transfer resistance and intraparticle transport. The kinetic and adsorption parameters used in this model were obtained from experimental data with pure nitrogen as a carrier gas. Meserole et al. [16] extended the previous work and established a theoretical model by combination of the adsorption characteristics measured in the laboratory with mass transfer considerations, to predict mercury removal by the PSI process in actual flue gas streams. In this model, the Freundlich isotherm equation was employed to determine the surface equilibrium. The parameters obtained by fitting experimental data of fixed bed in bench scale were used for evaluating the impact of mercury concentration and particle size on the removal efficiency in both ESP and FF. Afterward, Serre et al. [17]

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Nomenclature

a_p	sorbent surface area per unit volume (m^2/m^3)
C	mercury concentration in flue gas (kg/m^3)
C_{in}	mercury concentration in flue gas at inlet (kg/m^3)
C_s	sorbent concentration in flue gas (kg/m^3)
d	sorbent particle diameter (m)
D_E	pore effective diffusion coefficient (m/s)
D_K	Knudsen diffusion coefficient (m/s)
D_M	molecular diffusion coefficient (m/s)
k_g	individual mass transfer coefficient for gas phase (m/s)
k_s	individual mass transfer coefficient for particle phase (m/s)
K_g	overall mass transfer coefficient based on gas phase (m/s)
K_s	overall mass transfer coefficient based on particle phase (m/s)
m	reciprocal of coefficient in Freundlich equation
n	reciprocal of exponent in Freundlich equation
q	mercury concentration in sorbent (kg/kg)
Re	Reynolds number
S_{ij}	sensitivity coefficient for i to j
Sc	Schmidt numbers
Sh	Sherwood number
t	time (s)
T	temperature (K)
v	velocity (m/s)
X	independent variable
Y	dependent variable

Greek symbols

ρ_p	sorbent particle density (kg/m^3)
μ	gas dynamic viscosity (Pa s)
η	mercury capture efficiency (%)

Subscript

g	gas
i	gas–particle interface
in	at inlet
p	particle
s	sorbent

Superscript

*	at equilibrium status
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used the similar external mass transfer model to assess the effect of external mass transfer resistance on mercury capture, and concluded that the particle size with 14 μm or less would be sufficient to decrease external mass transfer effects. Recently, Ho et al. [18] presented a process model to simulate elemental mercury sorption by active carbon in confined, semi-fluidized and fluidized bed, respectively. This model coupled the mechanisms of surface equilibrium, external mass transfer and material balance and also used experimental data to fit the adsorption isotherm equation. Malerius and Werther [19] proposed a mercury capture model in dust laden flue gas upstream of an ESP which is used to calculate the influence of the governing parameters on the adsorption process and the efficiency of mercury capture in a sewage sludge incineration plant. Moreover, Flora et al. [20] and Scala and Clack [21] developed a model describing mercury removal in the duct associated with existing dust collector such as ESP and FF. Their models compared the effects of complicated boundary of collector on enhancing mercury removal efficiency. However, in all mercury capture models

mentioned above, some consider the external diffusion rate only, some another need to solve differential equation group with numerical methods which relatively increase computational complexity and difficulty.

The objective of this work is to develop a simplified model that describes mercury removal efficiency in flue gas. This model is based on the combination of theories of mass balance, mass transfer and isothermal adsorption. Subsequently, the comparisons of theoretical with experimental results are performed. The effects of key parameters including the mass transfer coefficient, sorbent concentration, sorbent physical property and sorbent adsorption capacity on mercury adsorption efficiency are evaluated. Further, the sensitive analysis of impact factor for mercury capture efficiency is also involved in this paper.

2. Theory

The control volume of duct between downstream of the air heater and upstream of the particulate collector is shown in Fig. 1. To derive the mathematical model, the following conditions are assumed: the velocity of sorbent particle is approximately equal to the flue gas velocity neglecting the radial velocity, the concentration of sorbent particle is very dilute in flue gas, the sorbent particle is spherical and can be replaced by air dynamic diameter, the same temperatures are taken on the internal sorbent particles, and the effects of other pollutants on adsorption performance of sorbents are neglected.

2.1. Mass transfer rate

Usually, the adsorption process of adsorbate by adsorbent is divided into three steps: external diffusion, internal diffusion and adsorption. Main resistances to adsorption occur in process of external and internal diffusion. The diffusive rate equation in detail will be described below.

2.1.1. External diffusion rate

For external diffusion process, adsorbate from main body of fluid diffuse to the external surface of adsorbent by means of molecular and convective diffusion. In this process, an interphase film between main body of fluid and external surface of adsorbent is generated. Correspondingly, the mass transfer rate in external diffusion is decided by the concentration of adsorbate between outboard and inboard interphase film. It can be expressed as

$$\rho_p \frac{dq}{dt} = k_g a_p (C - C_i) \quad (1)$$

where k_g can be determined from the Sherwood number according to the correlation with the Reynolds and Schmidt numbers which is given by

$$Sh = 2.0 + 0.6Sc^{1/3}Re^{1/2} \quad (2)$$

$$Sh = \frac{k_g d_p}{D_M} \quad (3)$$

$$Sc = \frac{\mu}{\rho_g D_M} \quad (4)$$

$$Re = \frac{v \rho_g d_p}{\mu} \quad (5)$$

The molecular diffusion coefficient, D_M , can be estimated according to Chapman–Enskog correlation for A and B two component mixture systems as follow

$$D_M = \frac{0.001858 T^{3/2} (1/M_A + 1/M_B)^{1/2}}{P \sigma_{AB}^2 \Omega_{AB}} \quad (6)$$

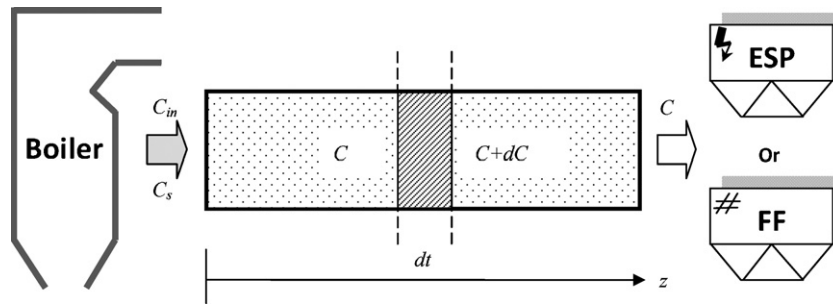


Fig. 1. Schematic diagram of control volume of the flue gas duct.

In Eq. (1), a_p is external surface area per unit volume of adsorbent particle and can be calculated by

$$a_p = \frac{6}{d_p} \quad (7)$$

Combine Eq. (3) with Eq. (7), we have

$$k_g a_p = \frac{6ShD_M}{d_p^2} \quad (8)$$

2.1.2. Internal diffusion rate

For internal diffusion process, adsorbate from the external surface diffuse to the internal surface through the micro-pore on the adsorbent particles. Its diffusive mechanisms are more complicate than external diffusion. To analyze more conveniently, the internal diffusion process is usually treated as the mass transfer process from external to internal surface on adsorbent particles. Correspondingly, the mass transfer rate in internal diffusion is modeled as

$$\rho_p \frac{dq}{dt} = k_s a_p (q_i - q) \quad (9)$$

where k_s can be determined according to the assumption in which the concentration of adsorbate in adsorbent particle obeys a second order parabola distribution.

$$k_s = \frac{10D_E}{d_p} \quad (10)$$

where the pore effective diffusion coefficient, D_E , can be calculated by

$$D_E = \frac{\varepsilon_p}{\tau_p} \left(\frac{1}{D_M} + \frac{1}{D_K} \right)^{-1} \quad (11)$$

where the Knudsen diffusion coefficient is calculated using

$$D_K = 9700 \frac{d_{pore}}{2} \left(\frac{T}{M_A} \right)^{1/2} \quad (12)$$

Combine Eq. (7) with Eq. (10), we obtain

$$k_s a_p = \frac{60D_E}{d_p^2} \quad (13)$$

2.1.3. Total transfer rate

According to what has been described above, once the dynamic adsorption equilibrium status are attained, the total mass transfer rate can be written as

$$\begin{aligned} \rho_p \frac{dq}{dt} &= K_g a_p (C - C^*) = K_s a_p (q^* - q) \\ &= k_g a_p (C - C_i) = k_s a_p (q_i - q) \end{aligned} \quad (14)$$

2.2. Equilibrium equation

2.2.1. Equilibrium isotherm equation

Historically, several classical equilibrium isotherm equations are proposed to model equilibrium adsorption process. They are Langmuir equation, BET equation, Freundlich equation and Koble–Corrigan equation, respectively. Due to better applicability and convenience for description of both physical and chemical adsorption process, the Freundlich isotherm equation is selected here for the calculation. In Freundlich isotherm equation, the equilibrium adsorbent capacity is related to the gas-phase concentration. It can be expressed as

$$q^* = \left(\frac{1}{m} \right) (C^*)^{1/n} \quad (15)$$

Especially, for $n = 1$ Eq. (15) is degraded as a linear correlation.

2.2.2. Total mass transfer coefficient

From Eqs. (14) and (15), we get

$$K_g = \left(\frac{1}{k_g} + \frac{m}{k_s} \right)^{-1} \quad (16)$$

or

$$K_s = \left(\frac{1}{k_g} + \frac{1}{k_s} \right)^{-1} \quad (17)$$

For the emphasized concern of the mercury emission from flue gas, Eq. (16) is selected for prediction of mercury adsorption efficiency in this paper.

2.3. Mass balance equation

In the control volume, the mass balance law is employed. This means that the decrease of mercury in flue gas should be equal to the increase of mercury in adsorbent particles. Therefore, it can be expressed by

$$C_s dq = -dC \quad (18)$$

Re-arrange and integrate Eq. (18) with the boundary conditions: $C = C_{in}$ for $q = 0$ and $C = C$ for $q = q$, we have

$$\int_0^q dq = -\frac{1}{C_s} \int_{C_{in}}^C dC \quad (19)$$

$$q = -\frac{1}{C_s} (C - C_{in}) \quad (20)$$

In the status of adsorption equilibrium, Eq. (20) becomes

$$q^* = -\frac{1}{C_s} (C - C_{in}) \quad (21)$$

Combine Eqs. (15) and (21) with rearrangement, we get

$$C^* = \left[-\frac{m}{C_s} (C - C_{in}) \right]^n \quad (22)$$

2.4. Mercury adsorption efficiency

According to the description of Eq. (14), the total mass transfer rate for gas phase is now used to describe the mercury adsorption

$$\frac{dq}{dt} = \frac{K_g a_p}{\rho_p} (C - C^*) \quad (23)$$

Replace the corresponding parameters in Eq. (23) with Eqs. (18) and (22)

$$\frac{dC}{dt} = -\frac{C_s K_g a_p}{\rho_p} \left[C - \left(-\frac{m}{C_s} (C - C_{in}) \right)^n \right] \quad (24)$$

When the mercury concentration in flue gas is very low, Ho [18] suggested that it is applicable to describe the mercury adsorption process as that the Freundlich exponent is equal to 1. So Eq. (24) is simplified as

$$\frac{dC}{dt} = -\frac{C_s K_g a_p}{\rho_p} \left[C - \left(-\frac{m}{C_s} (C - C_{in}) \right) \right] \quad (25)$$

Integrate Eq. (25) with considering the boundary conditions: $C = C_{in}$ for $t = 0$ and $C = C$ for $t = t$, we have

$$\frac{C}{C_{in}} = \frac{(m/C_s) + \exp \left[-(1 + m/C_s) (C_s K_g a_p / \rho_p) t \right]}{1 + m/C_s} \quad (26)$$

Generally, the mercury capture efficiency in flue gas is defined as

$$\eta = 1 - \frac{C}{C_{in}} \quad (27)$$

Substitute Eq. (26) into Eq. (27), the final correlation will be obtained for determining the mercury adsorption efficiency within t of residence time. After arrangement, it can be written as

$$\eta = 1 - \frac{(m/C_s) + \exp \left[-(1 + m/C_s) (C_s K_g a_p / \rho_p) t \right]}{1 + m/C_s} \quad (28)$$

3. Results and discussion

3.1. Model verification

In order to evaluate the availability and accuracy of present model, the comparison between calculational and experimental results for PSI mercury capture are performed in Fig. 2. All experimental data for mercury removal efficiency were measured by Meserole et al. [16] in pilot-scale conditions, and obtained by using the total mercury concentration between upstream and downstream of the dust collector. An active carbon was used as sorbent with capacity of 0.05×10^{-3} and effective particle diameter of $15 \mu\text{m}$.

Fig. 2(a) shows the comparison between the present model, Meserole's model and experimental value in flue gas duct with ESP in residence time $t = 2$ s and 5 s, respectively. The mercury capture efficiency is an increasing function of the sorbent concentration, as expected. The present model prediction presents the same general trends with Meserole's model and experimental data. Moreover, it is can be seen that the present model result for $t = 2$ s provides the overestimate prediction than Meserole model for $t = 2$ s, even approximately equal to Meserole's model prediction for $t = 5$ s. However, considering the integrated effects of outer and inner diffusion processes on total mass transfer coefficient, the reasonable agreement is obtained between present model and experimental results for both $t = 2$ s and 5 s. Moreover, for both theoretical models, the

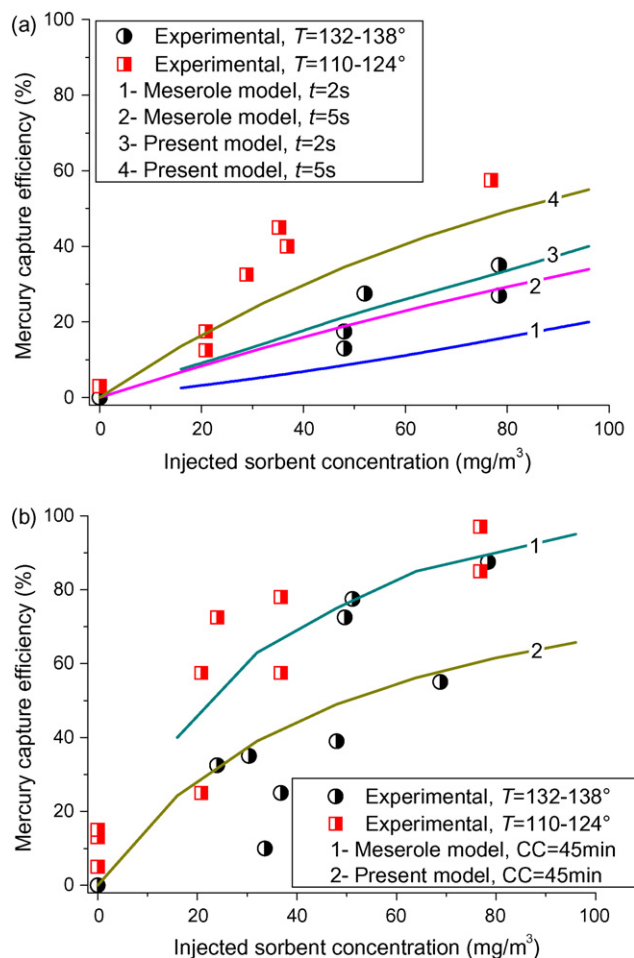


Fig. 2. Comparison of present model with Meserole et al. model and experimental results.

mercury captures efficiency based on a residence time of 2 s is lower than 5 s. This means that longer residence time in duct and ESP can help to enhance mercury adsorption. In addition, although the theoretical result for 5 s residence time by new model presents a similar prediction compared with experimental data at 110–124 °C, this is mainly attributed to the effect of temperature which gives rise to the change of adsorption balance. Further investigation (not shown in this figure) indicates that the present model predictions for mercury capture efficiency are not sensitive to temperature variation within a narrow range.

Fig. 2(b) describes the comparison between the present model and Meserole's model as well as experimental value in flue gas duct with FF operated by air: cloth = 3.048 m/min and cleaning cycle (CC) = 45 min. The present model predictions also take on the similar trends related to Meserole's model and experimental results. However, within a cleaning cycle the present model underestimates the mercury adsorption capability, especially for higher injected sorbent concentration, even up to maximum difference of 30%. This usually results from the accumulation effect of injected sorbent deposited on the filter media which can be regarded as a fixed adsorption bed and improve the mercury adsorption process, as reported by Scala and Clack [21]. In addition, decreasing temperature also can leads to increasing mercury capture efficiency but both models are not sensitive to temperature in a narrow range.

It should be noted that although the present model is essentially predicting mercury adsorption efficiency by PSI which do not includes the effect of particle control devices, it is still able to pro-

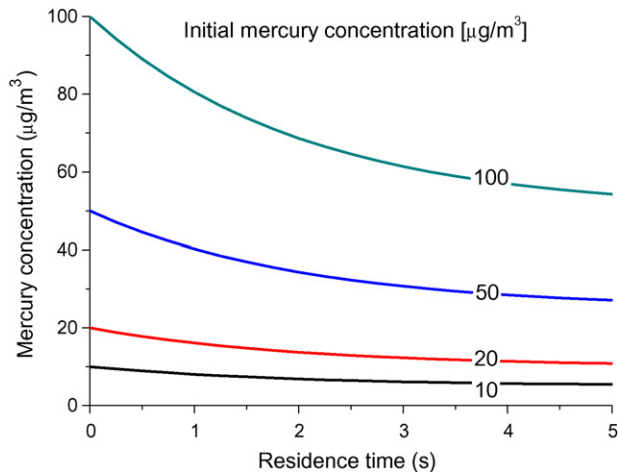


Fig. 3. Effect of initial mercury concentration on adsorption capability ($T = 120^\circ\text{C}$, $d_p = 10\ \mu\text{m}$, $C_s = 50 \times 10^{-6}\ \text{kg/m}^3$, $n = 1$, and $m = 50 \times 10^{-6}$).

vide the reference for further modification when considering the delay-time effect for ESP and the filter cake effect for FF.

3.2. Effect of parameters

3.2.1. Effect of initial mercury concentration

Fig. 3 summarizes the initial mercury concentration as function of mercury residence time in adsorption process by PSI. It is seen that with the increase of initial mercury concentration in flue gas the outlet mercury concentration also increases, e.g., at the inertial mercury concentration of 20 and $100\ \mu\text{g/m}^3$ the outlet mercury concentration through the process of adsorption is 11 and $54\ \mu\text{g/m}^3$, respectively. However, according to the simplified model described by Eq. (26), c/c_{in} for these cases is approximately equal to 0.5, which means that the mercury adsorption is able to capture about 50% of the mercury out of the flue gas, and that the mercury adsorption efficiency is approximately a constant under these operation conditions. This indicates that the mercury adsorption efficiency is independent of the initial mercury concentration when the adsorbate concentration is in low levels.

3.2.2. Effect of adsorbent concentration

Fig. 4 illustrates the effect of adsorbent injection concentration on mercury removal for adsorbent with $T = 120^\circ\text{C}$, $d_p = 10\ \mu\text{m}$,

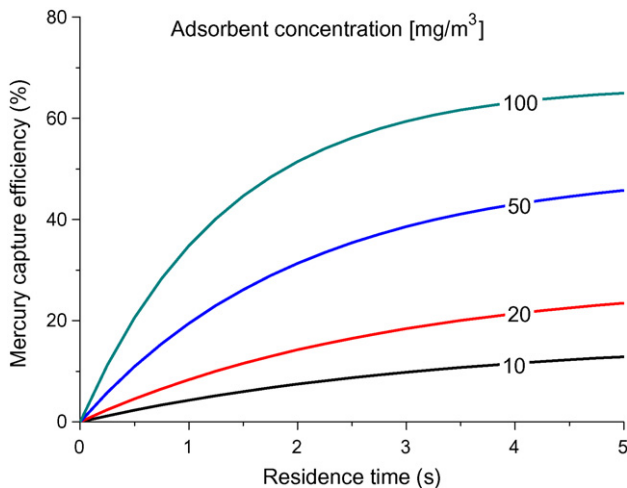


Fig. 4. Effect of adsorbent concentration on mercury capture efficiency ($T = 120^\circ\text{C}$, $d_p = 10\ \mu\text{m}$, $C_{in} = 50 \times 10^{-9}\ \text{kg/m}^3$, $n = 1$ and $m = 50 \times 10^{-6}$).

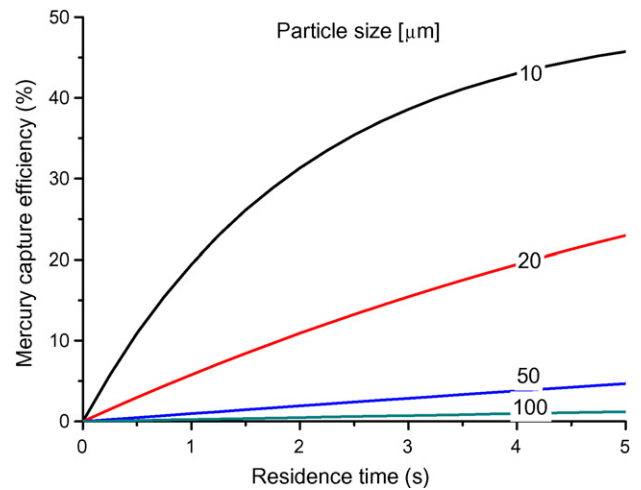


Fig. 5. Effect of adsorbent particle size on mercury capture efficiency ($T = 120^\circ\text{C}$, $C_s = 50 \times 10^{-6}\ \text{kg/m}^3$, $C_{in} = 50 \times 10^{-9}\ \text{kg/m}^3$, $n = 1$ and $m = 50 \times 10^{-6}$).

$C_s = 50 \times 10^{-6}\ \text{kg/m}^3$, $n = 1$ and $m = 50 \times 10^{-6}$. In this case, while the adsorbent concentration varies between 10 and $100\ \text{mg/m}^3$, the mercury removal efficiency of the flue gas varies from 13% to 65% for 5 s of residence time, respectively. Obviously, mercury removal is significantly affected by the adsorbent concentration injected into the flue gas as increase of active adsorption points.

3.2.3. Effect of adsorbent surface area

Fig. 5 compares the effect of adsorbent particle size which relates to external area on mercury removal under conditions of $T = 120^\circ\text{C}$, $C_s = 50 \times 10^{-6}\ \text{kg/m}^3$, $C_{in} = 50 \times 10^{-9}\ \text{kg/m}^3$, $n = 1$ and $m = 50 \times 10^{-6}$. According to the figure, it is found that with the decrease of the particle size from 100 to $10\ \mu\text{m}$ the mercury capture efficiency in flue gas for 5 s increases from 1.2% to 45%. Moreover, the influence extent of particle size on mercury capture efficiency is different. For larger particles such as 100 or $50\ \mu\text{m}$, the mercury capture is not significantly affected. However, for smaller particle such as 20 or $10\ \mu\text{m}$, the mercury capture is significantly improved. Because the smaller particle size provides the more external area which is inverse proportion with square of the particle diameter and allow adsorption equilibrium to be approached more easily and rapidly. These results are also consistent with those of other reports [19].

Note that the specific surface area of particles usually includes both the external surface area of the particles and the internal surface of the pores in particles. Due to insensitiveness of internal surface area on mass transfer coefficient, this effect is not considered in Fig. 5.

3.2.4. Effect of adsorbent capacity

Fig. 6 presents the effect of the adsorbent capacity on the mercury capture efficiency with $n = 1$. It is observed that the tendencies are similar in all cases. With the higher adsorbent capacity, as refer to $1/m$, the mercury capture efficiency based on residence time of 5 s becomes higher. It increases from 20% at 200×10^{-6} capacity to 56% at 25×10^{-6} capacity.

3.3. Sensitivity analysis

In order to theoretically reveal the effects of operation parameters on mercury removal more deeply, the sensitivity analysis is performed in this work. Generally, the sensitivity for a variable X to objective function Y can be expressed by a dimensionless sensitiv-

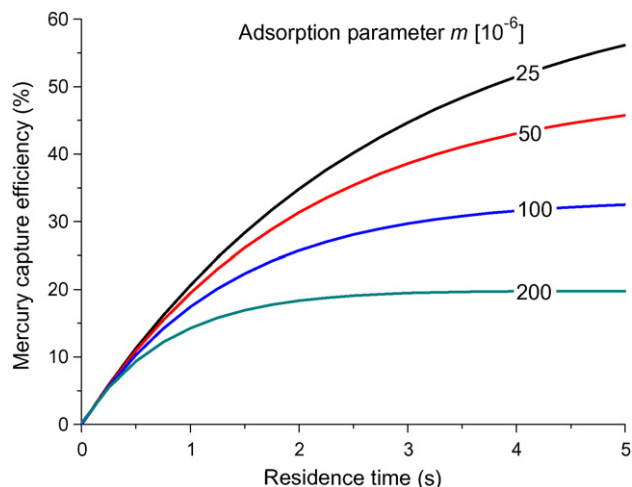


Fig. 6. Effect of adsorbent capacity on mercury capture efficiency ($T=120^{\circ}\text{C}$, $d_p=10\text{ }\mu\text{m}$, $C_s=50\times 10^{-6}\text{ kg/m}^3$, $C_{in}=50\times 10^{-9}\text{ kg/m}^3$ and $n=1$).

ity coefficient which is defined as

$$S_{ij} = \frac{\partial \ln Y_i}{\partial \ln X_j} = \frac{\partial Y_i/Y_i}{\partial X_j/X_j} \quad (29)$$

Correspondingly, the sensitivity analysis results based on Eqs. (28) and (29) are indicated in Fig. 7. In this process, the sensitivity coefficients to mercury capture efficiency are described as functions of residence time. According to the figure, it is observed that the sensitivity coefficients of the adsorbent concentration C_s , overall mass transfer coefficients $K_g a_p / \rho_p$ and time t are greater than 0, indicating that they have positive correlation to mercury capture efficiency which is helpful to mercury adsorption. Moreover, these sensitivity coefficients decrease as the increase of residence time due to the decreasing adsorbent performance. Nevertheless, compared with other impact factors, the adsorbent concentration is still most important to the mercury capture efficiency. In addition, the parameter m in Freundlich isothermal equation gives the negative sensitivity coefficient which indicates that m is unfavorable for mercury adsorption because it has an adverse effect on mercury adsorption. These results can provide a theoretical support for mercury pollution control by PSI technology.

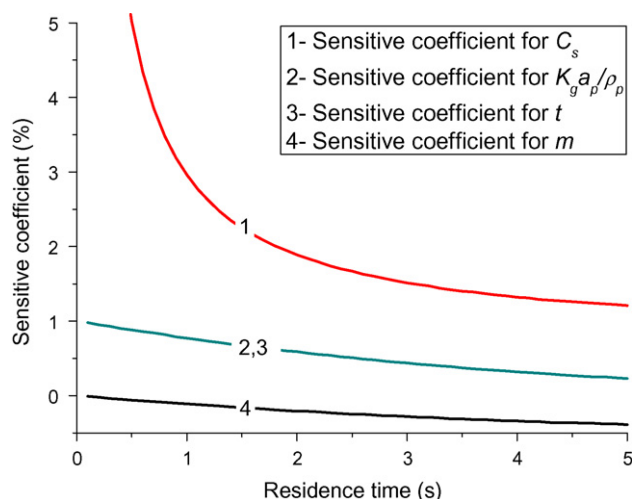


Fig. 7. Sensitivity analysis for operation parameters ($T=120^{\circ}\text{C}$, $d_p=10\text{ }\mu\text{m}$, $C_s=50\times 10^{-6}\text{ kg/m}^3$, $C_{in}=50\times 10^{-9}\text{ kg/m}^3$, $n=1$ and $m=50\times 10^{-6}$).

4. Conclusions

In this work, a mathematical model to predict the mercury capture efficiency by powdered sorbent injection is developed based on the combination of mass transfer theory, adsorption equilibrium equation and mass balance theory. For relatively low level of mercury concentration, this model is the simplified expression when Freundlich exponent is equal to 1. The comparison with experimental results indicates that the present model is able to provide availability and accuracy to a certain extent. Based on the simulated results by simplified model, it is obvious that initial mercury concentration, adsorbent concentration, adsorbent surface area and adsorbent capacity can yield effect on mercury capture efficiency using PSI. Further, the sensitivity analysis indicates that adsorbent concentration is the most important impact factor for mercury capture from flue gases.

With Freundlich exponent being equal to 1, the present simplified model is actually an explicit function as a result of integral to the differential equation. With Freundlich exponent being unequal to 1, or the adsorption equilibrium equation is described as Langmuir or other formula, the present model Eq. (28) is no longer directly used to calculate the mercury capture efficiency. However, the numerical solution for mercury capture efficiency still can be obtained by solving the differential Eq. (23).

Superficially, the present model does not take into account the enhancing impacts of the existing particulate control devices. However, if using the ESP as a following collector, the relatively accurate efficiency for mercury removal still can be achieved by revision of residence time in present model. If using FF as a following collector, the final mercury capture efficiency will be higher than predicted result by present model because of the combined effects of both increasing residence time and dust cake on the filter.

It is indicated that PSI technology has the greatly potential to reduce the mercury emission from the combustion flue gases. Mercury adsorption in PSI technology has been demonstrated to involve both physical and chemical adsorption. Further investigations showed that the capture efficiency of oxidized mercury (HgCl_2) is higher than that of elemental mercury under certain conditions due to the chemical adsorption, which is strongly affected by flue gas composition and sorbent physical properties as well as surface functional groups [22–24]. By considering the effect of physical and chemical adsorption characteristic, the present model can be more effective to predict the capture efficiency for both elemental and oxidized mercury from the combustion flue gases.

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