

# Kinetic interpretation on mercury oxidation and transformation in simulated flue gases

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**Abstract** The approach coupled with computation fluid dynamics (CFD) and complex chemical kinetic computation to predict the oxidation of the elemental mercury in flue gas was discussed in this paper. According to the oxidation mechanism of the elemental mercury, the reactions which were in close relationship with mercury oxidation were determined by the sensitivity analysis method. The mercury oxidation process was simulated under the atmospheric pressure condition with different flue-gas compositions. The three-dimensional concentration distribution of mercury within the cylindrical flue duct and the impact of the temperature, concentration of  $\text{Cl}_2$ ,  $\text{HCl}$ ,  $\text{NO}$ , and  $\text{O}_2$  on the mercury oxidation were also obtained. The simulation results were compared with the experimental results of Mamani-Paco and Widmer. The results show that coupling computation solves the problem of the combination of the CFD with the complex kinetic mechanism. The promotion effect of  $\text{Cl}_2$  on the oxidation of elemental mercury is much better than that of  $\text{HCl}$ . The temperature window ranged from 950 to 1,150 K for the higher oxidizing rate of the elemental mercury was determined. The slight enhancement of  $\text{NO}$  on mercury oxidization was observed which was controlled by the competition between two reaction pathways.  $\text{O}_2$  weakly promotes homogeneous  $\text{Hg}$  oxidation, especially under the condition of high temperature. 1.1, 2.6 and 3.1 % of mercury was oxidized in the presence of 0, 4 and 16 %  $\text{O}_2$  at 600 K, respectively. However, 12.5, 22.5 and 26.0 % of  $\text{Hg}$  oxidation has been obtained at 1,200 K.

**Keywords** Mercury transformation · Chemical kinetics · Coupling · Computation fluid dynamics

## Introduction

Trace element mercury in the coal may be emitted into atmosphere during the process of coal combustion, which will pollute the air and do harm for the health of humans. Coal-fired power plants have been considered to be the primary anthropogenic source of mercury into the atmosphere. In consequence, there have been initiatives to regulate the emission of mercury at a lower level and to develop the mercury emission control technologies. Mercury in the flue gas is most commonly classified in three forms: elemental mercury ( $\text{Hg}^0$ ), gaseous oxidized mercury ( $\text{Hg}^{2+}$ ) and particle-bound mercury ( $\text{Hg}_p$ ) (Luo et al. 2006; Chen et al. 2007; Lee et al. 2006a, b). The particulate bound mercury is usually trapped by ash collection devices within power plants, such as electrostatic precipitators (ESP), mechanical hoppers or bag houses. Oxidized forms of mercury (such as  $\text{HgCl}_2$ ) are easier to capture as they are water soluble and can be removed by wet scrubber technologies.  $\text{Hg}^0$  in the vapor phase is difficult to control and is likely to enter the global atmospheric cycle because of its high vapor pressure and low water solubility (Li et al. 2003; Lee et al. 2006a, b; Duan et al. 2008). Hence, there are some trials to convert  $\text{Hg}^0$  into  $\text{Hg}^{2+}$  species such as  $\text{HgO}$ ,  $\text{HgSO}_4$  and  $\text{HgCl}_2$ , in order to increase the removal efficiency of mercury.

In order to control mercury emissions effectively under a wide range of conditions, a predictive models need to be developed and supplied to process engineers to retrofit conventional APCDs or design new mercury abatement processes. A better understanding of mercury chemistry

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reaction mechanism of mercury conversion under different thermal and chemical conditions is needed to build such models. The chlorination of mercury is the most dominant mechanism during and after coal combustion. Several elemental research efforts have investigated the factors that affect homogeneous Hg speciation in flue gas or simulated flue gas. At flame temperatures, thermochemical equilibrium analysis indicates mercury will exist in the elemental state. As temperatures fall, the favored equilibrium product shifts to HgCl. The crossover temperature between the elemental and oxidized forms increases from 530 to 740 °C as the background HCl concentration goes from 50 to 3,000 ppm. Hall et al. (1991, 1995) and Widmer and West (2000) proposed one-step global reaction mechanisms to model the observed depletion of Hg<sup>0</sup> in the presence of Cl<sub>2</sub> or HCl. While such mechanisms can give plausible qualitative results, they are generally not suited for examining the effects of other flue gas constituents on Hg chlorination. Sliger and Kramlich (2000) published a model which was used to predict the data obtained in their experimental work. It was found that the model was able to predict about half of their experimental data accurately. However, several activation energy values used in key reactions were negative. Of those efforts, Edwards et al. (2001) provided the most complete Hg chlorination pathways to date as well as a pathway involving HgO, with model predictions in good accord with experimental data for higher reactor temperatures but a drastic under-prediction of Hg chlorination for lower temperatures. Niksa et al. (2001) published a kinetic model to predict the importance of NO and H<sub>2</sub>O in a gas stream. The predictions seemed to correspond well with the experimental data. However, the authors made use of oxygen radicals for initiating the reaction between elemental Hg and Cl radicals, the results obtained were less realistic. Xu et al. (2003) published a detailed kinetic model consisting of 107 reactions and 30 species to simulate mercury speciation in flue gas. The performance of the model presented in their study was assessed through comparisons with the experimental results of Mamani-Paco and Helble (2000), Widmer and West (2000), and Sliger and Kramlich (2000). The results showed that the model calculations only followed the Sliger et al.'s experimental trends. Although great success has been achieved in understanding the kinetic mechanism during the conversion of the mercury speciation, the present modeling can only solve the transient or steady-state problems in a homogeneous stirred reactor. Typical computation fluid dynamics (CFD) solutions can only handle global (single-step) reactions or a set of severely reduced chemical reaction steps while still producing a stable solution in a time-frame that suits modern design cycles. Low-emission combustion system design depends on the simulation of both chemical and fluid flows.

The coupling of CHEMKIN-CFD is a chemistry module that addresses the problem of CFD's computational stiffness by providing efficient and accurate solution algorithms that assure robust coupling of the chemistry and the flow. CHEMKIN-CFD needs a chemical-kinetics mechanism and thermodynamic data in CHEMKIN format, as well as optional CHEMKIN-based molecular-transport properties. CHEMKIN-CFD solves coupled conservation equations at every grid point, at every iteration and at every time-step within a CFD simulation.

This study focuses on developing an approach to simulate the conversion of mercury through both chemical and fluid flows aspects, which coupled with CFD and complex chemical kinetic computation. The goal of this research is to identify the major factors such as temperature, flue-gas constituents, which affect mercury speciation and conversion in flue gas. The understanding of mercury oxidization may help predict conversion of mercury speciation in flue gases from coal-fired utility boilers, which will be helpful toward the research of mercury control technology. The work was carried out in Nanjing Normal University during 2010.9–2011.5.

## Materials and methods

The simplified assumptions made for the oxidation process of gaseous mercury in this model are as follows:

- 1) Mercury reaction is simplified as homogenous reaction of Hg and Cl;
- 2) Since the shape of flue has certain symmetry, the gas flow in the flue is simplified as one-dimensional plug flow model;
- 3) Only C, H, O, N, Hg and Cl are considered in the model.

### Physical model

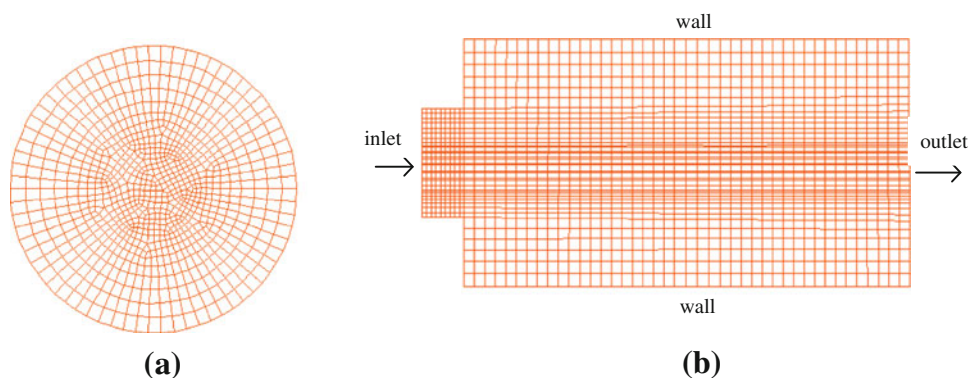
In simulation, similar to the Mamani-Paco and Helble (2000) experiment, a three-dimensional cylinder with a radius of 2.5 and 10.5 m in height was considered. The first step of the CFD simulation was the mesh generation. The quality of grid generation has great significance on computational simulation. Since the shape of flue has certain symmetry, the flue was assumed as a straight pipe. A simple three-dimensional axial symmetry model was created and meshed using Gambit software, as is shown in Fig. 1.

### Mathematic model

Numerical 3D predictions have been carried out with the finite volume code Fluent 6.2.16 using an standard  $k$ - $\epsilon$



**Fig. 1** Grid schematic **a** Plane grid at  $z = 10$  m. **b** Plane grid at  $x = 0$  m



model for turbulence which is the most widely used and validated turbulence model (Patankar 1980). The value of each coefficient in this model is:  $c_\mu = 0.09$ ,  $c_1 = 1.44$ ,  $c_2 = 1.92$ ,  $\sigma_k = 1.0$  and  $\sigma_\epsilon = 1.3$ . For steady, incompressible flow, momentum equations, energy and species conservation equations are taking into account.

In order to reflect the influence of chemical reaction and turbulence in the flue gas on mercury oxidation, based on Eddy Dissipation Concept (EDC) model, 3-D double precision solver is selected for computation (Magnussen 1981; Gran and Magnussen 1996). CHEMKIN-CFD can be more efficient than CFD chemistry solvers in converging to a solution. In this paper, FLUENT is used to calculate the flow field, which was coupled with the CHEMKIN kinetic mechanism to obtain the concentration distribution mercury and other compositions in the flue gas.

#### Chemical reaction model

The reduced chemical reaction mechanism consisting of 22 species and 26 reactions proposed by Widmer and Sliger et al. is adopted, which is widely verified by experiments and applied in coal-fired gas purification simulation. Main reaction mechanism in this model includes eight reactions between mercury and chlorine, which describe the oxidation mechanism of mercury and the 18 elementary reactions involving chlorine are taken from Sliger, which are obtained from NIST database.

#### Boundary conditions

Velocity-inlet boundary condition is defined at the inlets. Velocity at the inlet is 7.5–15 m/s according to the resident time. The pressure at the outlet is defined as normal atmosphere and the exterior walls were modeled as adiabatic. The “no-slip” boundary condition was used for the gas phase at the wall, with only the tangential velocity and then keeping the constant temperature at 400 K.

#### Results and discussion

The  $\text{Hg}^0$  conversion rate is defined as:

$$\text{Hg}^0 \text{ conversion rate} = \frac{[\text{Hg}^0]_{\text{in}} - [\text{Hg}^0]_{\text{out}}}{[\text{Hg}^0]_{\text{in}}} \quad (1)$$

where  $[\text{Hg}^0]_{\text{out}}$  and  $[\text{Hg}^0]_{\text{in}}$  are the concentrations of  $\text{Hg}^0$  measured at the outlet and inlet of the reactor, respectively.

#### Sensitivity analysis of oxidation reaction on $\text{Hg}^0$

Sensitivity analysis is a formal procedure to determine quantitatively how the solution to a model depends on certain parameters in the model formulation. The sensitivity analysis allows to understand how the model will respond to changes in the rate parameters. It also provides insight about how important certain reaction pathways are to the model's predictions.

Table 1 shows the oxidation pathway of  $\text{Hg}^0$ . The rate coefficients are in the modified Arrhenius form,  $k = AT^b \exp(-E/RT)$ . Elemental mercury was chosen as reference species, and sensitivity analysis was carried out for the eight oxidation reactions at 1,195 K, in the presence of 50 ppm HCl. The composition of flue gas is the same as the experiment made by Sliger and Kramlich (2000), as is shown in Table 2. The greater the absolute value of the sensitivity coefficient (S) is, the more effect of this reaction on  $\text{Hg}^0$  will be. The results were shown in Fig. 2.

Sensitivity analysis indicates that mercury oxidation was most sensitive to the coefficients of reactions R1, R7 and R5 listed in Table 1, which is consistent with the simulation result of Xu et al. (2003). When time is approaching 1.4 s, the absolute values of these reactions' sensitivity coefficient all exceed  $3.0\text{E}-7$ . The sensitivity coefficients of other reactions are relatively lower. The sensitivity analyses show that mercury is oxidized by a Cl-atom recycle process, so that the concentrations of both Cl and HOCl, HCl are the important components containing



**Table 1** The reactions rate coefficient data using the modified Arrhenius form  $k = AT^\beta \exp(-E/RT)$  involved in mercury oxidation mechanism

NO.	Reactions	$E/(\text{cal}\cdot\text{mol}^{-1})$	$\beta$	$A/(\text{cm}^3/\text{mol}\cdot\text{sec})$	Source
R1	$\text{Hg} + \text{Cl} + \text{M} = \text{HgCl} + \text{M}$	−14,400	1.4	2.40E8	Widmer
R2	$\text{Hg} + \text{Cl}_2 = \text{HgCl} + \text{Cl}$	34,000	0.0	1.39E14	Widmer
R3	$\text{HgCl} + \text{Cl}_2 = \text{HgCl}_2 + \text{Cl}$	1,000	0.0	1.39E14	Widmer
R4	$\text{HgCl} + \text{Cl} + \text{M} = \text{HgCl}_2 + \text{M}$	3,100	0.0	2.19E18	Widmer
R5	$\text{Hg} + \text{HOCl} = \text{HgCl} + \text{OH}$	19,000	0.0	4.27E13	Widmer
R6	$\text{Hg} + \text{HCl} = \text{HgCl} + \text{H}$	79,300	0.0	4.94E14	Widmer
R7	$\text{HgCl} + \text{HCl} = \text{HgCl}_2 + \text{H}$	21,500	0.0	4.94E14	Widmer
R8	$\text{HgCl} + \text{HOCl} = \text{HgCl}_2 + \text{OH}$	1,000	0.0	4.27E13	Widmer
R9	$\text{Cl} + \text{Cl} + \text{M} = \text{Cl}_2 + \text{M}$	−1,800	0.0	14.400	Sliger
R10	$\text{H} + \text{Cl} + \text{M} = \text{HCl} + \text{M}$	0	0.0	17.000	Sliger
R11	$\text{HCl} + \text{H} = \text{H}_2 + \text{Cl}$	3,500	0.0	13.360	Sliger
R12	$\text{H} + \text{Cl}_2 = \text{HCl} + \text{Cl}$	1,200	0.0	13.930	Sliger
R13	$\text{O} + \text{HCl} = \text{OH} + \text{Cl}$	3,510	2.87	3.530	Sliger
R14	$\text{OH} + \text{HCl} = \text{Cl} + \text{H}_2\text{O}$	−223	1.65	7.430	Sliger
R15	$\text{O} + \text{Cl}_2 = \text{ClO} + \text{Cl}$	3585	0.0	12.790	Sliger
R16	$\text{O} + \text{ClO} = \text{Cl} + \text{O}_2$	−193	0.0	13.200	Sliger
R17	$\text{Cl} + \text{HO}_2 = \text{HCl} + \text{O}_2$	894	0.0	13.030	Sliger
R18	$\text{Cl} + \text{HO}_2 = \text{OH} + \text{ClO}$	−338	0.0	13.390	Sliger
R19	$\text{Cl} + \text{H}_2\text{O}_2 = \text{HCl} + \text{HO}_2$	1951	0.0	12.800	Sliger
R20	$\text{ClO} + \text{H}_2 = \text{HOCl} + \text{H}$	14,100	0.0	11.780	Sliger
R21	$\text{H} + \text{HOCl} = \text{HCl} + \text{OH}$	7,620	0.0	13.980	Sliger
R22	$\text{Cl} + \text{HOCl} = \text{HCl} + \text{ClO}$	258	0.0	12.260	Sliger
R23	$\text{Cl}_2 + \text{OH} = \text{Cl} + \text{HOCl}$	1,810	0.0	12.100	Sliger
R24	$\text{O} + \text{HOCl} = \text{OH} + \text{ClO}$	4,372	0.0	12.780	Sliger
R25	$\text{OH} + \text{HOCl} = \text{H}_2\text{O} + \text{ClO}$	994	0.0	12.255	Sliger
R26	$\text{HOCl} + \text{M} = \text{OH} + \text{Cl} + \text{M}$	56,720	−3.0	10.250	Sliger

**Table 2** Flue gas compositions for the experiments

Species	Composition (mole fraction)		
	Mamani-Paco and Helble (2000)	Widmer and West (2000)	Sliger and Kramlich (2000)
O <sub>2</sub>	0.0	0.10	0.0743
CO <sub>2</sub>	0.13	0.10	0.0615
H <sub>2</sub> O	0.26	0.08	0.123
Hg <sup>0</sup>	50 µg/m <sup>3</sup>	370E−9	53 µg/m <sup>3</sup>
Cl <sub>2</sub>	Varied as indicated	Not defined	Not defined
HCl	Not defined	3,000 E−6	Varied as indicated
N <sub>2</sub>	Balance	Balance	Balance

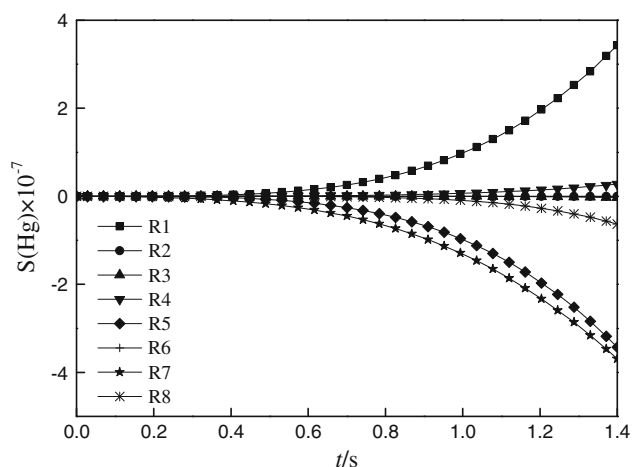
chlorine in the reaction system, which has significant effect on mercury oxidation.

#### Effects of Cl<sub>2</sub> on mercury oxidation

The effects of Cl<sub>2</sub> concentration on Hg conversion were studied in detail by experiments of Mamani-Paco and Helble (2000). For all cases, the residence time is approximately 1.4 s. The reaction temperature and pressure are 1,353 K and 1 atm, respectively. The chlorine concentrations in the

flue gas ranged between 50, 100, and 300 ppm. Initial compositions of the flue gas are shown in Table 2. In order to verify the precision of modeling prediction in this paper, the kinetic simulation results were compared with the experimental data of Mamani-Paco. The results are illustrated in Fig. 3. In Mamani-Paco et al. experiment, with the increasing of Cl<sub>2</sub> from 50, 100 and 300 ppm, 8.5, 38.5 and 65.5 % of the mercury was oxidized in average. In kinetic calculations, 17.5, 32.5 and 55.4 % of the mercury was oxidized in the presence of 50, 100 and 300 ppm

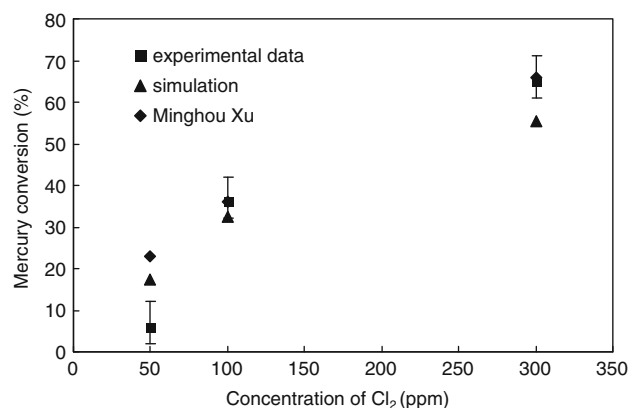




**Fig. 2** Hg sensitivity derivatives versus time for present mechanism

$\text{Cl}_2$ , respectively. It shows that the prediction results in this paper are consistence with Mamani-Paco and Helble (2000) experimental data and Xu et al. (2003) calculation results.

The distributions of elemental mercury concentration in reactor are shown in Fig. 4. It is obviously that  $\text{Hg}^0$  is oxidized quickly after entering the reactor. The concentration of elemental mercury is decreased along the central axes and mercury is also oxidized when spreading toward the pipe wall. When  $\text{Cl}_2$  concentration increased from 50 to 300 ppm, the oxidation of mercury is enhanced to a great extent. The increasing of  $\text{Cl}_2$  concentration promoted the oxidation of elemental mercury. The oxidation process took place in the whole reactor. As mentioned in Mamani-Paco et al.'s experimental work, the mercury concentration was only monitored at exit of the reactor to obtain the oxidation efficiency of elemental mercury through reactor. The previous modeling works also gave the results in a



**Fig. 3** Comparison of the kinetic model predictions with Mamani-Paco and Helble (2000) experimental data and Xu et al. (2003) model predictions

closed, steady-state perfectly stirred reactor. The results in this work presented the transient 3D concentration distribution in a practical reactor which coupled with fluid dynamic in detail. The oxidation efficiency at exit of reactor agreed with the experimental results of Mamani-Paco et al.'s work.

#### Effects of HCl on mercury oxidation

In order to investigate the effect of both HCl and  $\text{Cl}_2$  on the oxidation of mercury in gas, an experiment was also conducted with both HCl and  $\text{Cl}_2$  present simultaneously by Mamani-Paco and Helble (2000). This experiment was conducted in the presence of  $50 \mu\text{g}/\text{m}^3$  mercury, 50 ppm  $\text{Cl}_2$  and 100 ppm HCl. It is observed that when the total concentration of Cl increased, the mercury oxidation rate has only a little difference with that when only 50 ppm  $\text{Cl}_2$  exists. Kinetic modeling was also carried out in this paper to simulate this phenomenon. The simulation results under both conditions are shown in Fig. 5. In the presence of 50 ppm  $\text{Cl}_2$  with and without HCl (100 ppm), the mercury concentration decreases along the axial distance in the reactor. Although both  $\text{Cl}_2$  and HCl introduced atom Cl in reaction zone, similar mercury oxidation efficiency (about 18.2 %) was observed at the exit of reactor, which is consistent with the results obtained for oxidation with  $\text{Cl}_2$  alone. These results are in accord with Mamani-Paco and Helble (2000) experimental data.

#### Prediction of mercury conversion at different temperature

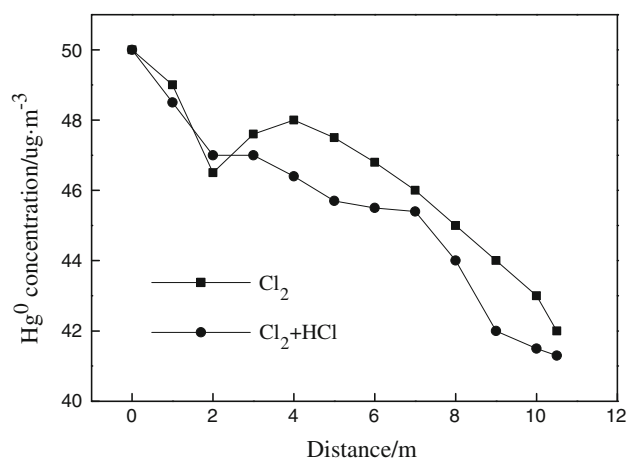
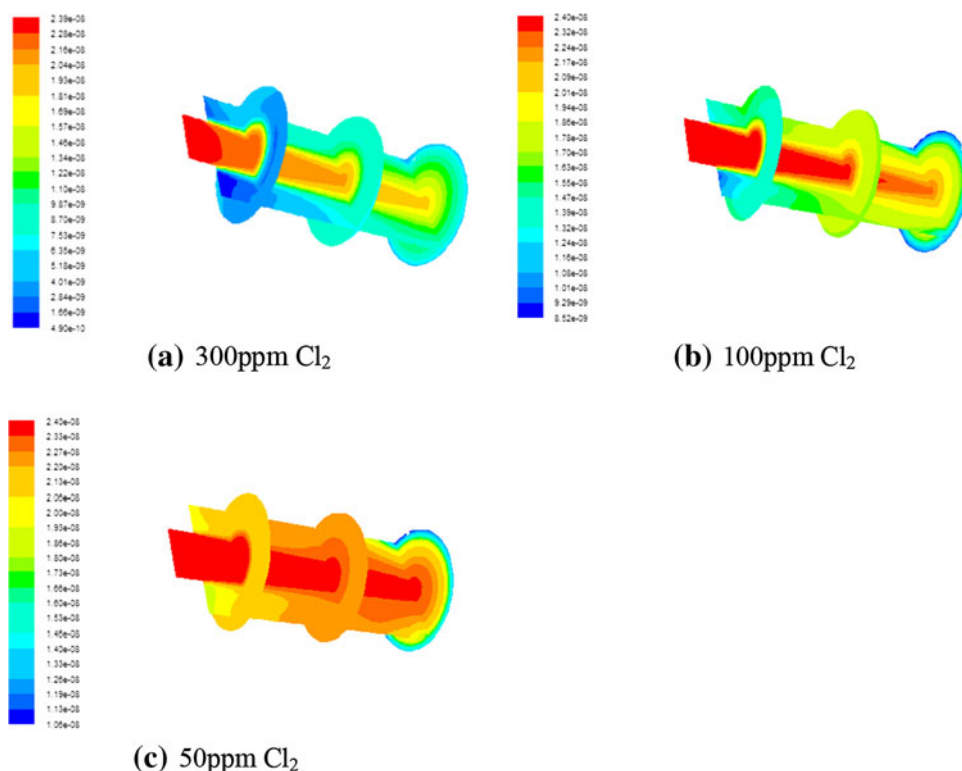
The effects of temperature on Hg concentration were studied, in which the gas compositions was the same as that in Widmer et al. experiment. The pressure is 1 atm. Residence times for each temperature are listed in Table 3.

Figure 6 shows the comparison of predicted Hg conversion with the experimental and modeling data of Widmer and West (2000), Edwards et al. (2001) and Xu et al. (2003)'s model predictions. Widmer and West (2000) kinetic mechanism agreed with the experimental conversion of mercury, but the deviation at high temperature is great where mercury conversion is thermodynamically controlled. There are deviations among other three calculation results, especially at lower temperatures, but they can follow the similar mercury conversion trend. The temperature window for the higher oxidation rate of the elemental mercury is in the range from 950 to 1,150 K range. When the temperature is above 1,100 K, the mercury oxidation rate will decreased. However, the result trends of the four groups are generally the same. The reason for this discrepancy may result from the difference of parameters in oxidation mechanism and kinetics.





**Fig. 4** The mole concentration distribution of elemental mercury for different concentration of  $\text{Cl}_2$  in flue gas



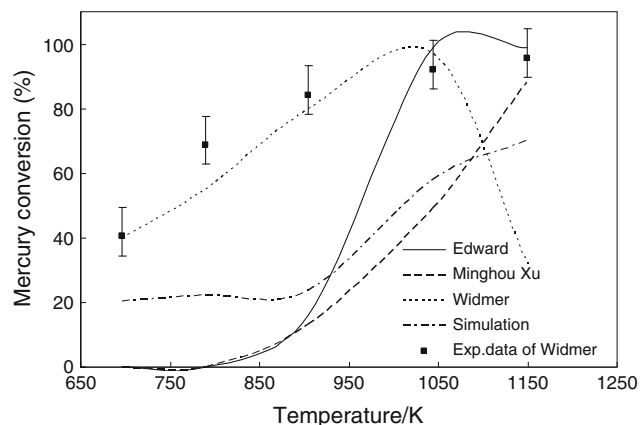
**Fig. 5** The effect of  $\text{Cl}_2$  and HCl on mercury concentration in reactor (Kinetic calculations)

**Table 3** Experimental conditions for Widmer et al. experiment

Gas temperature (K)	HCl concentration (ppm)	Residence time (sec)
696	3,000	1.16
790	3,000	1.02
904	3,000	0.89
1,044	3,000	0.77
1,149	3,000	0.70

#### Effects of NO on mercury oxidation

Nitric oxide is a common constituent in real flue gas. The complex impact of NO on homogeneous mercury oxidation has a potentially important practical implication. The simulation was carried out under the gas composition condition as  $\text{CO}_2$  (13 %),  $\text{O}_2$  (4 %), HCl (60 ppm),  $\text{Hg}^0$  ( $18.75 \mu\text{g}\cdot\text{m}^{-3}$ ), NO (0, 400 and 800 ppm) and  $\text{N}_2$  as balance. The chemical reaction mechanism consisting of 30 species and 107 reactions proposed by Xu et al. (2003)



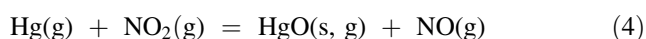
**Fig. 6** Comparison of the kinetic model predictions with the experimental and modeling data of Widmer and West (2000), Edwards et al.'s (2001) and Xu et al. (2003)'s model predictions in the presence of 3,000 ppm HCl



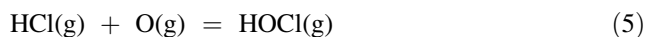
was applied. As shown in the Fig. 7, NO enhances mercury oxidation slightly in the  $\text{CO}_2/\text{O}_2/\text{N}_2/\text{HCl}/\text{Hg}$  system at low temperature zone. The maximum oxidation rate was obtained for 400 ppm of NO at 1,200 K. The oxidation rate dropped to 7.8 % for 800 ppm NO at same condition. Zhou et al. (2007) presented the following possible reaction pathway when NO was added to  $\text{CO}_2/\text{O}_2/\text{N}_2/\text{HCl}/\text{Hg}$  system which supported the oxidation promotion process at low temperature is as follows:



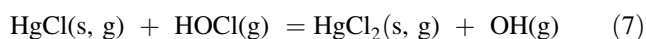
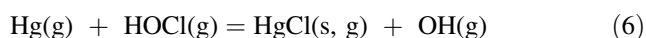
Elemental mercury is hypothesized to react with active O atoms and produced  $\text{HgO}$  (s, g) via the following pathways.



Furthermore, active O atoms reacted with HCl to form  $\text{HOCl}$  (g) via



and then  $\text{HOCl}$  oxidized  $\text{Hg}^0$  vapor to  $\text{HgCl}_2$  via the following pathways:



It has been reported that NO can either promote or inhibit mercury oxidation, depending upon the NO concentration (Niksa et al. 2001a, b). The previous work noted that NO can potentially be an effective inhibitor of mercury oxidation through its effect in reducing the concentration of OH in the flue gas. The formation of  $\text{HOCl}$  from OH and Cl is essential for the oxidation of Hg, which oxidizes  $\text{HgCl}$  into  $\text{HgCl}_2$  and OH. The elimination of OH resulted in following reaction (8):

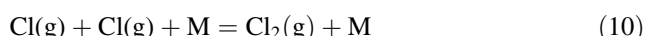
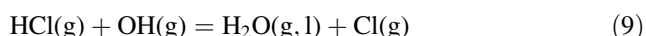


which was believed to inhibit mercury oxidation (Zhou et al. 2007). Therefore, the conversion of NO in the  $\text{CO}_2\text{--O}_2\text{--N}_2\text{--HCl}$  system was dependent on the competition between reactions (2)–(7) and (8).

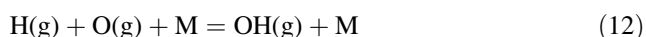
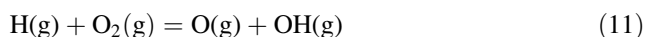
#### Effects of $\text{O}_2$ on mercury oxidation

On the basis of 3.4, the extent of mercury conversion under different  $\text{O}_2$  concentrations, 0, 4 and 16 %, was obtained. For all cases, the residence time is approximately 2.0 s. It can be seen that  $\text{O}_2$  weakly promotes homogeneous Hg oxidation, especially under the condition of high temperature, as illustrated in Fig. 8.

As indicated in sensitivity analysis above, the key pathway of mercury oxidation is reaction associated with Cl and  $\text{Cl}_2$  species. In simulated flue gas, Cl and  $\text{Cl}_2$  come from the following reactions:



The presence of oxygen will promote the generation of the OH through reactions (11) and (12) at high temperature:



Other literatures indicated that the reactions (13) and (14) also play important roles to oxidize elemental mercury.

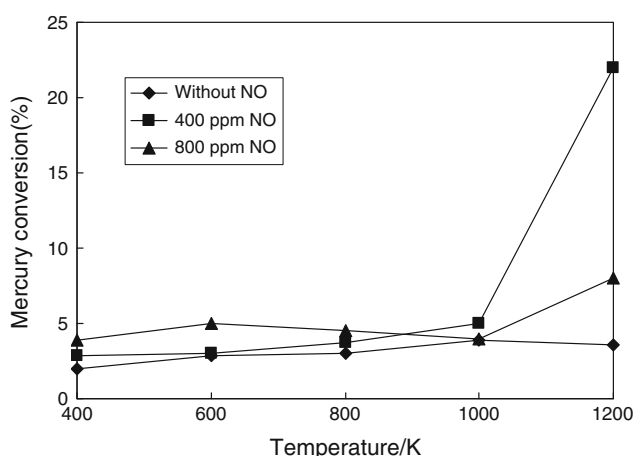
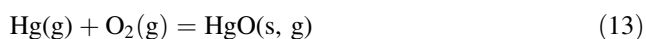


Fig. 7 Effect of NO on Hg transformation

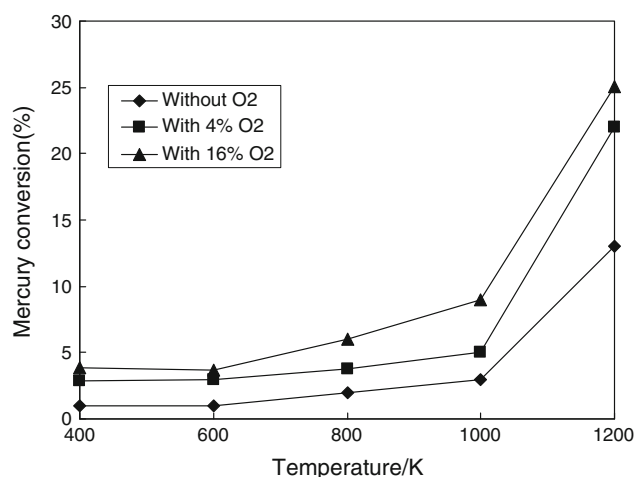


Fig. 8 Effect of  $\text{O}_2$  fraction on Hg transformation



## Conclusion

A method to simulate the oxidation and conversion of the elemental mercury in flue gas which coupled with CFD and complex chemical kinetic computation was presented in this paper. The three-dimensional concentration distribution of mercury within the cylindrical reactor was obtained. The impact of the temperature and compositions of flue gas were also discussed and the simulation results were compared with the experimental results of Mamani-Paco and Widmer. More mercury oxidization occurs with a higher reaction temperature and higher  $\text{Cl}_2$  concentration in the flue gases. In the present work, NO enhances mercury oxidization process which was dependent on the competition between reactions (2)–(7) and (8).  $\text{O}_2$  weakly promotes homogeneous mercury oxidation, especially under the condition of high temperature. The possible pathway of this enhancement related to the direct oxidation of O atom, OH radical and attendant Cl atom which was induced by the presence of oxygen.

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