



Influence of HCl on CO and NO emissions in combustion

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ABSTRACT

The influence of HCl on CO and NO emissions was experimentally investigated in an entrained flow reactor (EFR) and an internally circulating fluidized bed (ICFB). The results in EFR show the addition of HCl inhibits CO oxidation and NO formation at 1073 K and 1123 K. At the lower temperature (1073 K) the inhibition of HCl becomes more obvious. In ICFB, chlorine-containing plastic (PVC) was added to increase the concentration of HCl during the combustion of coal or coke. Results show that HCl is likely to enhance the reduction of NO and N₂O. HCl greatly increases CO and CH₄ emission in the flue gas. A detailed mechanism of CO/NO/HCl/SO₂ system was used to model the effect of HCl in combustion. The results indicate that HCl not only promotes the recombination of radicals O, H, and OH, but also accelerates the chemical equilibration of radicals. The influence of HCl on the radicals mainly occurs at 800–1200 K.

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1. Introduction

Besides sulfur and nitrogen, chlorine is also a harmful element in several fuels used in industrial furnaces, such as coal, biomass and waste, etc. Cl enrichment in coal or biomass is normally associated with organic or inorganic matters, influenced by soil or rock conditions (e.g. chloride brines) and growing process of plants. Organic-associated Cl seems to predominate in coal [1]. The major organic Cl is represented by “semi-organic” Cl, as anion Cl⁻, sorbed on the coal organic surface in pores and being surrounded by pore moisture. Inorganic-associated Cl is salt-like Na and other chlorides, as well as the Cl-bearing silicates, carbonates, sulfides. The origin of chlorine in waste is due to the chlorine-containing constituents, such as polyvinyl chloride (PVC), waste paper, and sodium chloride, etc. During combustion or gasification, the chlorine is released as HCl and Cl₂, which are known to act as inhibitor by catalyzing the recombination of radicals O, H, OH, and HO₂ in the flame. Therefore, HCl is likely to affect the oxidation of CO [2–5] and the formation of NO [6,7] in combustion.

The interactions of CO, NO_x, and H₂O have been previously investigated [8–11]. Results show that the concentration of H₂O has a strong effect on the post-combustion CO oxidation. Furthermore, the interactions occurring between CO, NO_x, and HCl show that the inhibitory effect of HCl is sensitive to the concentration of H₂O and NO and NO plays a catalytic role in the oxidation of CO in post-combustion gases [12,13].

The effect of chlorine on the formation of nitrogen oxides is found mostly in fluidized bed combustion. Under FBC or CFBC conditions, numerous studies have reported that adding HCl or other halides leads to an increase in CO [14–18] and C_xH_y [6,18,19] emissions. However, there is no universal agreement about the effect of chlorine on the formation of nitrogen oxides during combustion [6,15–23]. Julien et al. [17], Winter et al. [21], and Gokulakrishnan and Lawrence [6,22] reported that the formation of NO_x was decreased by the addition of halogens, whereas Liang et al. [15] and Anthony et al. [16,18] found that the halogens enhanced the formation of NO_x.

Up to now, the effect of HCl on NO_x formation is still not well understood because the reaction mechanisms are found very sensitive to the air/fuel ratio, temperature, and concentrations of gaseous components, even the solid (char/bed materials) catalysis during volatiles and char combustion. Wei et al. [7] found that the HCl addition decreased NO emission in pulverized coal flames and explained it by the competition between the reactions of NO formation and reduction. In the present paper, in order to study the effect of HCl on NO formation in gaseous volatile combustion, the experiments are conducted in an entrained flow reactor (EFR), for the first time. In EFR, the factors of fluid flow and gas reaction might be simply and controlled easily. Then the influence of HCl on CO and NO_x is investigated experimentally during coal and coke combustion in an internally circulating fluidized bed (ICFB). Finally, a detailed mechanism is used to analyze and explain the experimental data. The results are useful to analysis the effect of HCl during actual waste and biomass combustion.

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2. Experimental section

The entrained flow reactor (EFR) structure is similar to those used in DTU (Technical University of Denmark), described elsewhere in detail [24]. EFR is applied to investigate the effect of HCl on CO and NO emission during gas reaction. As a precursor for NO_x formation, NH₃ is an important nitrogen-containing component released from coal or char, and thus NH₃ is chosen as nitrogen source in the experiments. The main gas (N₂/O₂) flows through a quartz tube (φ14 mm). Reactants (CO, NH₃, and HCl, etc.) flow through an internal tube (φ4 mm). Heat losses are minimized with electric resistance heater that maintains the reactor tube at the initial reaction temperature. At the entrance of the reaction section, the spherical end of the internal tube has four small drilled orifices. Through the orifices the reactants flow out vertically with the tube axis and are quickly mixed with the main gas flow. The length of reaction zone is 600 mm.

The concentration of N₂, O₂, CO, NH₃, and HCl are controlled separately by mass flow controllers within 1% error, and the moisture content is controlled by a water injector pump within 3% error. In the tests, water is vaporized steadily through a pre-heater and then the moisture flows into the reactor. The total initial gas flow rate is kept on 4 l/min at 293 K and 0.1 MPa. The mixture gases consist of 3% O₂, 3% CO, 1% H₂O, varied NH₃ and HCl, and N₂ as balanced gas. The reacted gases are de-acidified by sodium hydroxide solution and then dehydrated by silica gel, finally taken out to the gas analyzers. NO is determined with an on-line chemiluminescent NO_x analysis (SHIMADZU, Model NOA-305) with an uncertainty of 1%. O₂ and CO are measured continuously with a portable gas analysis (LANDCOM, Model 3500) within errors of 1% and 4% separately.

The schematic of the internally circulating fluidized bed (ICFB) incinerator has been illustrated elsewhere [25]. The fluidizing air enters the bed via bubbling caps (0.6% orifice coefficient). Under the inclined air distributor, the plenum is separated into two equal parts. And then the primary air separately enters the bed from air boxes with high or low air velocity. Unevenly distributed fluidizing air induces a large-size internal circulating flow of solid particle in the dense bed, which may improve the properties of lateral diffusion [26]. Particles under the action of high air velocity move upward sharply and form the fluidized bed, whereas particles in the low air velocity zone move downward slowly and form the moving bed. The cross-section of the dense phase zone is 500 × 240 mm and the height is 1000 mm. In the furnace, the dense phase zone changes gradually into the freeboard with the cross-section of 800 × 280 mm and the height of 3500 mm. Sand is used as bed material and particle diameter is 0.5–1.0 mm. The air velocity is

8.0 u_{mf} in the fluidized zone with high air velocity (u_{mf} is minimum fluidizing velocity) and 2.5 u_{mf} in the moving zone with low air velocity.

ICFB has the advantages to burn the chlorine-containing waste, biomass, and some coals. In order to simplify the experimental factors, coal/char combustion with polyvinyl chloride (PVC-C₂H₃Cl) addition is conducted to investigate the effect of HCl on CO and NO emission in ICFB. Table 1 shows the fuel properties, including a bituminous coal and a commercial coke. Particle diameter of two fuels is in the range of 0.5–15 mm. The feeding rate of fuel was 7.5 kg/h. Pure pulverized PVC particles were added to artificially increase the chlorine content in fuels. The PVC addition ratio was 0–3% of feeding fuel mass, corresponding to 0–1.65% chlorine content in fuels. Temperature was 1123–1223 K in the dense phase zone and decreased in the freeboard. The temperature was 523–573 K at the exit.

A sampling probe was installed at the flue gas exit near the top of the furnace. The temperature of sampling tube lines was heated to 453 K. Concentrations of pollutants in the flue gas were measured by Fourier Transform Infrared (FTIR) spectrometry (Gasmet DX-3000). In the tests, the concentrations of species H₂O, CO, CO₂, NO, NO₂, N₂O, HCl, SO₂, and CH₄ were measured online within 2% error. The concentration of oxygen was measured by oxygen analyzer (TEMET 19) within 0.2% error.

Table 1
Properties of the fuels.

Chemical analysis	Bituminous coal	Coke
Moisture (raw) ^a	7.82	1.06
Proximate analysis (wt%, dry basis)		
Volatile	29.23	1.94
Fixed carbon	58.58	84.19
Ash	12.19	13.87
Volatile (wt%, daf basis)	33.29	2.25
Ultimate analysis (wt%, dry basis)		
Carbon	71.41	83.63
Hydrogen	4.03	0.36
Nitrogen	0.90	0.74
Sulfur	0.27	0.61
Chlorine	0.007	0.067
Oxygen	11.20	0.80
LHV (MJ/kg dry basis)	28.20	28.48

^a "Raw" analysis stands for "as fed to the bed".

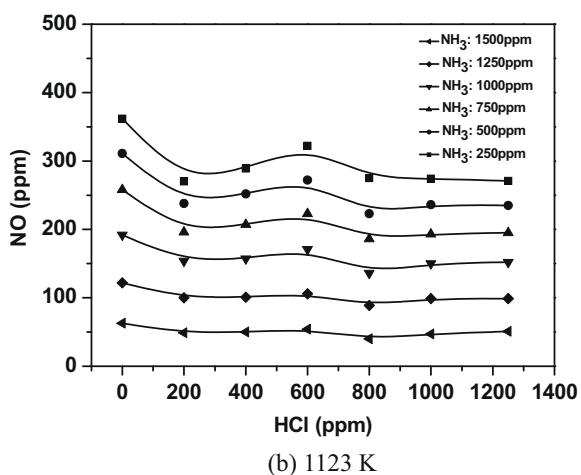
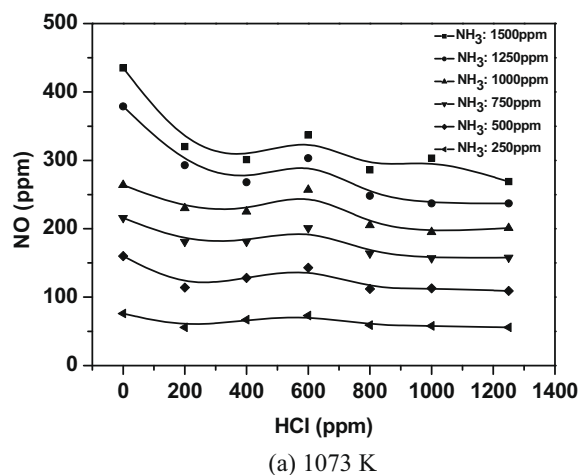


Fig. 1. Concentrations of NO emission from gas reaction in EFR. (0.1 MPa, 3% O₂, 3% CO, 1% H₂O, and N₂ as balanced gas).

3. Experimental results

3.1. Gas reaction experiments in EFR

In Fig. 1, emissions of NO are shown during gas combustion with various NH_3 and HCl concentrations. Although the effect of HCl on NO formation is complicated, it still can be concluded that the NO formation is generally reduced with increasing HCl concentration. When HCl is firstly added to 200 ppm, NO emission decreases obviously. With continuing increase of HCl, the effect of HCl on NO emission becomes weaker, and HCl even slightly leads to increase NO formation at 600 ppm of HCl concentration. Below 200 ppm of HCl, the effect of HCl is significant, then the effect of HCl becomes weak. It is hard to explain the local maximum NO emission at 600 ppm of HCl. With increasing the inlet NH_3 content, the NO reduction by HCl becomes more obvious. In Fig. 1a (at 1073 K), for the initial NH_3 concentration of 1500 ppm, the total reduction rate of NO reaches above 38% (reducing from 435 ppm to 269 ppm) with increasing HCl concentration from 0 to 1250 ppm, while the total reduction ratio is only about 26% for the NH_3 concentration of 250 ppm. Comparing Fig. 1b with Fig. 1a, it seems that the inhibition of HCl on NO formation at 1123 K is weaker than at 1073 K. It seems that the higher temperature may suppress the effect of HCl on NO formation (see the kinetic results in Section 4). The final concentration of NO is determined by the synergistic effect of HCl concentration and temperature. Obviously, the temperature level plays an important role

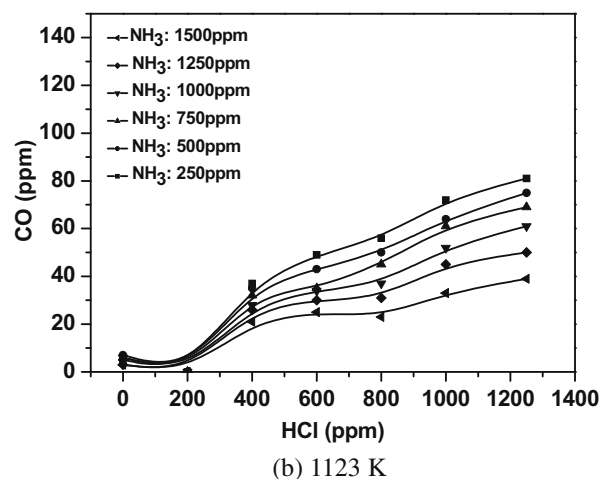
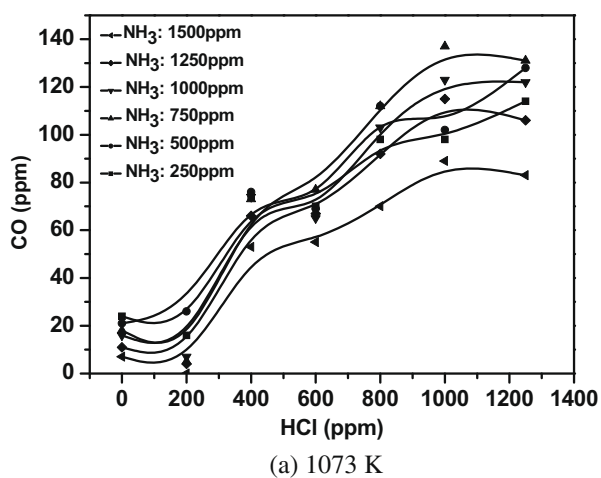


Fig. 2. Concentrations of CO emission from gas reaction in EFR. (0.1 MPa, 3% O_2 , 3% CO, 1% H_2O , and N_2 as balanced gas).

on the effect of HCl on NO formation, which will be an important factor for analyzing the disputed results in the references. Further extensive experiments are in progress in our laboratory.

Emissions of CO are shown in Fig. 2 during gas combustion with various NH_3 and HCl addition. The experimental results indicate that the emissions of CO increase quickly with adding HCl, which means that HCl inhibits the CO oxidation intensively. In Fig. 2b (at 1123 K), although the initial CO concentration keeps constant, the CO emission increases with increasing NH_3 addition. With HCl concentration of 1250 ppm, the maximal CO emission (with the initial 1500 ppm NH_3) is twice the minimum (with the initial 250 ppm NH_3). It seems that the existence of NH_3 also might inhibit the CO oxidation.

3.2. Coal/char combustion experiments in ICFB

Measured concentrations of released SO_2 and HCl from combustion with PVC addition are shown in Fig. 3. Due to the higher sulfur content in coke than coal, the concentration of released SO_2 during coke combustion is higher than during coal combustion. SO_2 emission is approximately 350 mg/ Nm^3 for coke and 250 mg/ Nm^3 for coal. SO_2 also may affect the oxidation of CO and the formation of NO_x [24,27–28]. However, Fig. 3 indicates the PVC addition has little influence on the concentration of released SO_2 . Therefore, the effect of SO_2 on the concentrations of CO and NO_x in combustion may be assumed as constant for various PVC addition ratios.

In Fig. 3, the concentration of HCl increases obviously above a certain chlorine content level (0.3% in coal and 0.5% in coke) with increasing PVC ratio in coal or coke combustion. However, the value of released HCl is lower than that expected if all of the chlorine in PVC is released as HCl. This may be explained by the absorption of chlorine by sodium and calcium in ash [29,30]. In addition, some chlorine in PVC will release as Cl_2 . The equilibrium calculation is used to predict the distribution of chlorine from PVC ($\text{C}_2\text{H}_3\text{Cl}$) in combustion (see Fig. 4). The main species of chlorine are HCl and Cl_2 , and Cl may be released at high temperatures. In Fig. 4, it is found that orders of magnitude of the species of Cl are very different. The concentration magnitude of radicals HCl, Cl_2 , and Cl is about 10^{-2} – 10^{-4} , meanwhile that of radicals HOCl, ClO, and NOCl is about 10^{-6} – 10^{-7} .

Emissions of NO and N_2O are shown in Fig. 5 in combustion with various PVC addition ratios. The baseline of NO emission is 267 mg/ Nm^3 for coal and 215 mg/ Nm^3 for coke. The emission of N_2O is less significant, about 10 mg/ Nm^3 . In Fig. 5, increasing the chlorine content in fuels reduces the emissions of NO and N_2O . In the range of the experiments, the maximum NO emission change rate reaches 16% in coal combustion and 27% in coke com-

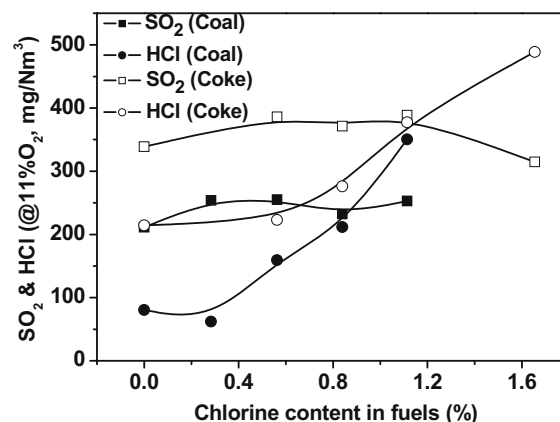
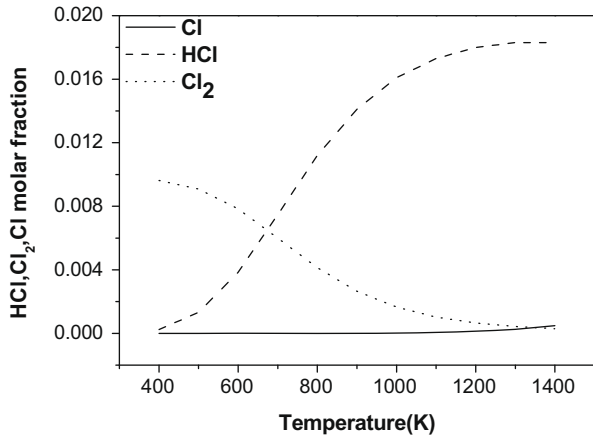
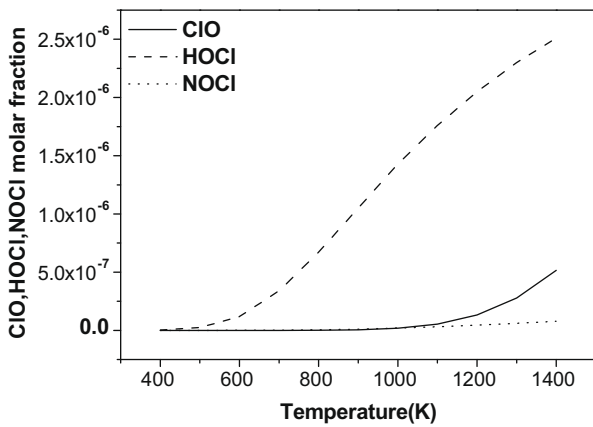


Fig. 3. Concentrations of released SO_2 and HCl from coal/char combustion with PVC addition in ICFB.



(a) HCl, Cl₂, Cl



(b) ClO, HOCl, NOCl

Fig. 4. Distribution of chlorine released from PVC (C₂H₃Cl) by equilibrium calculation.

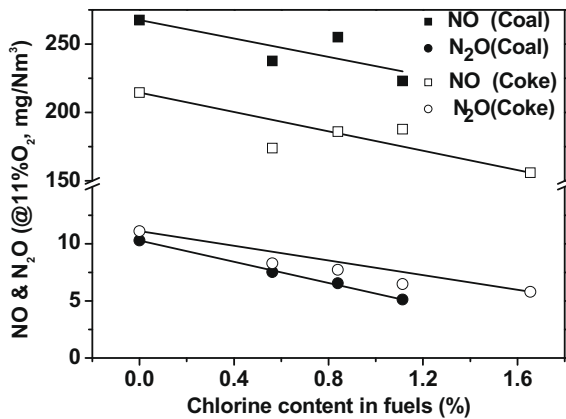


Fig. 5. Concentrations of NO and N₂O from coal/char combustion with PVC addition in ICFB.

bustion. In addition, the maximum N₂O emission change rate reaches about 50% for two fuels.

Fig. 6 shows the emissions of CO and CH₄ in combustion with various PVC addition ratios. Because of the higher content of volatile in coal than in coke, CO and CH₄ emissions are higher during coal combustion. Increasing the chlorine content in fuels inhibits the oxidation of CO, so the CO emission increases significantly. The effect of HCl on CO and CH₄ oxidation in coal combustion is

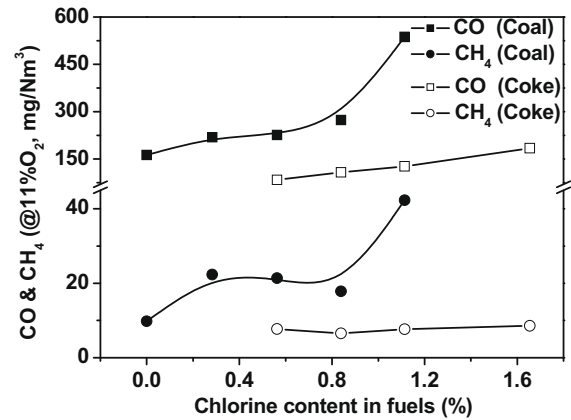


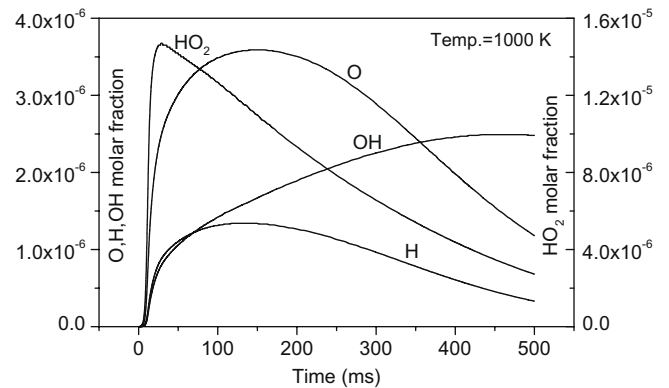
Fig. 6. Emissions of CO and CH₄ from coal/char combustion with PVC addition in ICFB.

more significant than in coke combustion because the inhibition of HCl might occur mainly during the volatile combustion.

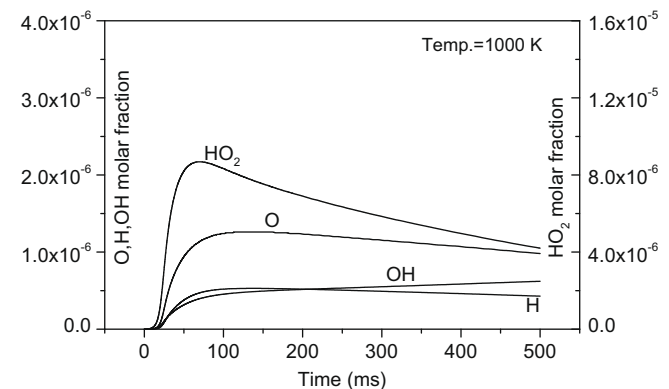
4. Kinetic modeling and discussion

The homogeneous reactions about the influence of HCl on CO oxidation and NO formation are directly connected with the released volatiles, the stoichiometric ratio, and the temperature. In the following, the detailed mechanism of CO/NO/HCl/SO₂ reactions is modeled to explain the experimental results.

The GRI 3.0-mechanism with 325 elementary reactions between 53 species [31] was used as the base reaction mechanism for the C/H/O/N system. Sulfur chemistry mechanism consists of



(a) Without HCl addition



(b) With 0.1% HCl addition

Fig. 7. Concentrations of radicals with varied time in gas combustion.

67 elementary reactions involving 14 sulfur-containing species [24]. Chlorine chemistry mechanism consists of 36 elementary reactions involving 7 chlorine-containing species [12]. Thermodynamic data were taken from the database of Burcat [32] or elsewhere [24,33]. The SENKIN code was used to model the reactions involving interaction of N, Cl, and S species [34]. During the experiments, the reaction temperature range was 1000–1200 K. And the temperature was even below 1000 K in the postcombustion. Therefore, 1000 K was selected as a typical calculating temperature.

Fig. 7 shows the effect of HCl addition on the radicals O, H, OH, and HO₂ under fuel-lean conditions ($\lambda = 2.0$). The calculations are performed for the mixture with initial 4% CO, 12% CO₂, 4% H₂O, 4.35% O₂, 0.1% HCN, 0.1% SO₂, 0.01% Ar, 0 or 0.1% HCl, and a balance of N₂ at 0.1 MPa in a reactor. The concentrations of O and H rapidly reach the peak at about 150 ms for Fig. 7a without HCl addition. The O concentration is 3 times of H concentration because of the reaction $H + O_2 = O + OH$. Then OH concentration increases with the time and reaches a constant. The initial concentration of radical HO₂ sharply increases and reaches the peak at about 25 ms, four times of the peak of radical O. Then the HO₂ concentration rapidly decreases and finally approximates the OH concentration. In the post-combustion zone, firstly O and HO₂ are the privileged radicals in the flame and then the radical OH becomes more and more important. In Fig. 7b, the concentrations of radicals are significantly suppressed by the HCl addition. The peak value of O or H is only one-third of the value in Fig. 7a. This is due to the effect of HCl on inducing the recombination of radicals. Firstly, the concentrations of radicals O, H, and OH rapidly increase and reach the peaks at about 100 ms. Then the concentration curves of radicals O, H, and OH become smoothly. Therefore, the HCl addition not only promotes the recombination of radicals O, H, and OH, but also accelerates the chemical equilibration of radicals.

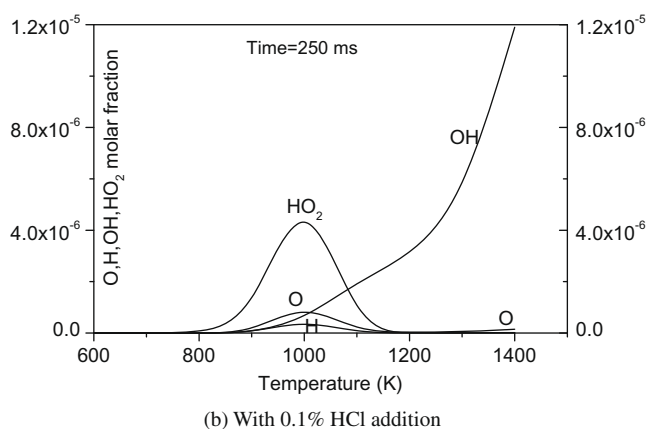
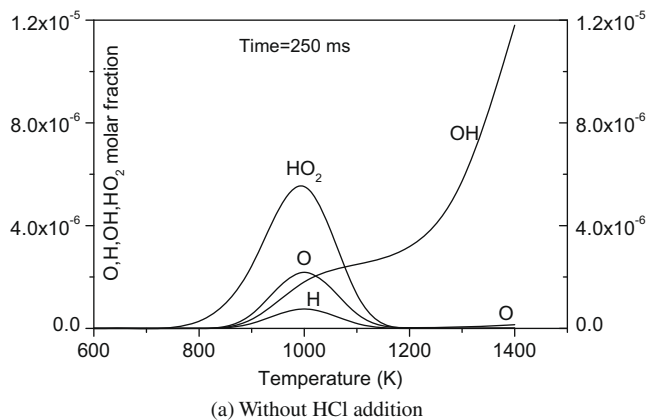


Fig. 8. Concentrations of radicals with varied temperature in gas combustion.

The effect of HCl addition on the radicals with varied temperature is shown in Fig. 8. The calculations are performed at 0.1 MPa and 250 ms for the same mixtures as Fig. 7. In Fig. 8a, the concentrations of radicals O, H, and HO₂ reach the peak values at 1000 K and the bell-like curves occur at 800–1200 K. From 850 to 1200 K, the concentration of radical OH gradually increases. Then the OH concentration sharply increases with the temperature. In Fig. 8, the concentration magnitude of OH radicals in the flame is about 10^{-6} – 10^{-7} , compared with 10^{-9} of [OH] equilibrium value. Such superequilibrium concentrations of free radicals are quite normal in combustion chemistry, and are sustained by the free energy liberated by the combustion process [35]. At 800–1200 K, CO is mainly consumed by the reaction $CO + OH \Rightarrow CO_2 + H$ [12]. Because HCl may act as inhibitors by catalyzing the recombination of radicals (e.g. $OH + HCl \Rightarrow H_2O + Cl$ etc.) in the flame, the oxidation of CO and formation of NO might be influenced by HCl. With HCl addition in Fig. 8b, the peak values of radicals O and H are reduced to about half of the values in Fig. 8a. It can be seen that the influence of HCl on the concentrations of radicals O, H, OH, and HO₂ mainly occurs at 800–1200 K. For example, the OH concentration only decreases in 900–1200 K and when the temperature is higher than 1200 K, OH concentration is less significantly influenced by HCl addition. This may be the reason that the higher temperature suppresses the effect of HCl on NO formation.

5. Conclusions

During the combustion of moist CO and NH₃ in an EFR, HCl was added to study its influence on CO and NO emissions. The experimental results show the addition of HCl inhibits CO oxidation and NO formation, leading to the increase of CO emission and the reduction of NO emission. The higher reaction temperature suppresses the reduction effect of HCl on NO formation.

In an ICFB during coal or coke combustion, pure pulverized PVC particles were added to artificially increase the chlorine content in fuels. The results show that increasing the chlorine content in fuels reduces the emissions of NO and N₂O. The effect of HCl on CO and CH₄ oxidation in coal combustion is more significant than in coke combustion because the inhibition of HCl might occur mainly during the volatile combustion.

A detailed reaction mechanism was modeled to explain the effect of HCl on pollutants from combustion. Results indicate that the concentrations of radicals are significantly suppressed by the HCl addition. The influence of HCl on the radicals mainly occurs at 800–1200 K.

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