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Research Article

Study on Correlation Characteristics of PCDD/Fs Isomers Generation during the Coal-Combustion Process with Sludge Mixing

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Abstract: The 17 toxic polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) isomers as a persistent and refractory organic pollutant are one of the pollutants produced in solid fuel (including pulverized coal and mixed fuel) combustion, and regulating their distribution characteristics is an important aspect of effectively reducing their toxic equivalent. In this study, a correlation model of PCDD/Fs toxic equivalent was proposed to quantitatively analyze the correlation between HCl and SO_2 concentrations in the reaction atmosphere, meanwhile, a pathway-diagnosis method of PCDD/Fs isomers transformation was adopted to analyze the PCDD/Fs distribution characteristics of coal combustion and that mixed with 10% sludge. The results show that the inflection point for the derivative of the relationship between HCl concentration and SO_2 concentration moves towards the direction of lower SO_2 concentration and higher HCl concentration with the increase of PCDD/Fs toxic equivalent. Besides, the functional pathways of mixing sludge on PCDD/Fs generation in coal combustion were obtained by calculating chlorine substitution probability. It has been deduced that five transformation pathways were improved by mixing sludge. Next, the critical pathways of the influence from mixing sludge on the distribution characteristics of PCDD/Fs isomers in coal combustion were analyzed by drawing the percentage content migration diagram of PCDD/Fs isomers and the average toxic equivalent migration diagram that combined with the toxic equivalent of PCDD/Fs isomers. The results showed that the main reasons for mixing sludge to further reduce the average toxic equivalent of PCDD/Fs isomers in coal combustion were the increased chlorine substitution probability at the 4-position of 12378 Pentachlorodibenzo-p-dioxin (12378-PeCDD), the decreased chlorine substitution probability at the 4-position of 2378 Tetrachlorodibenzo-p-furan (2378-TeCDF), and the increased total chlorine substitution probability of 23478 Pentachlorodibenzo-p-furan (23478-PeCDF), 123478-Hexachlorodibenzofuran (123478-HxCDF) and 123678-HxCDF respectively. Finally, the functional pathway diagram of PCDD/Fs isomers generated from coal combustion with sludge mixing was drawn.

***Keywords*:** PCDD/Fs isomers, correlation model, chlorine substitution probability, sludge mixing, function pathway

1. Introduction

The combustion process of solid fuels, which includes pulverized coal[1], municipal solid waste[2] and plastic waste[3],

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has been considered as the main source of PCDDs and PCDFs. PCDD/Fs can participate in the natural circulation and bioaccumulation of humans and animals, and have high toxicity. Therefore, it is closely related to carcinogenicity and teratogenicity, and is classified as persistent organic pollutants.[4] It's called "dioxins" for short, but in fact it consists of 75 types of PCDD and 135 types of PCDF[5], as well as their structures have been shown in Figure 1. It should be pointed out that only 17 toxic PCDD/Fs isomers have attracted much attention, and 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) is the most toxic one.[6]

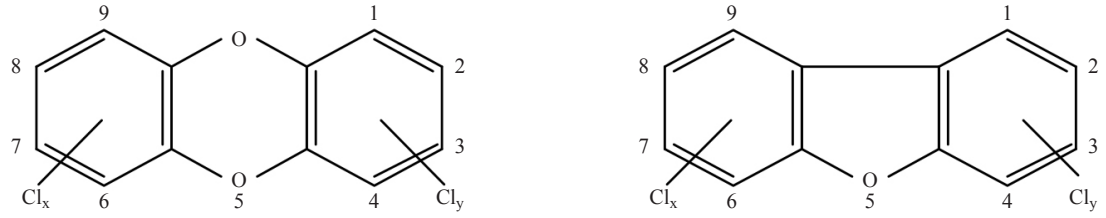

Figure 1. Molecular structure diagram of PCDD/Fs

So far, the mechanisms of its formation and inhibition have been widely studied by scholars. At the same time, some important conclusions have been widely recognized by personages of all circles. For example, PCDD/Fs[7] can be directly generated by chlorination of gaseous components such as hydrocarbons and phenols under the action of chlorine sources, and heterogeneous synthesis of combustion products such as CO and CO_2 under the action of catalytic metals on the fly ash surface with carbon residue, O_2 and chlorine sources.[8] Moreover, studies have shown that solid fuels mainly release chlorine in the form of HCl under high temperature conditions[9], but in the presence of O_2, they can be converted into Cl_2 through the Deacon reaction[10], and the activity of Cl_2 is much higher than that of HCl.[7] Yifan Wang et al.[11] studied the inhibitory effect of urea on PCDD/Fs using a sintered tank and analyzed its possible dechlorination inhibitory mechanism. It was found that the toxic equivalent of urea was greatly reduced by mixing urea particles, indicating that urea has the effect of inhibiting chlorination and enhancing dechlorination. Hence, dechlorination becomes an important step to inhibit their formation by mixing inhibitors. Yen-Chen Hsu et al.[12] have verified that thiourea as an inhibitor can reduce the chlorination degree of PCDD. They hold that the oxidation of organic sulfides or elemental sulfur leads to the formation of SO_X (such as SO_2 and SO_3), which can effectively inhibit the chlorination of Diphenylene dioxide (DD) and Diphenylene oxide (DF) into PCDD/Fs.[13] Distinctly, the high-S product is an important factor to inhibit PCDD/Fs formation, which provides a theoretical basis for inhibiting their formation by the component deployment of solid fuels. Han Zi-xi et al.[14] studied the mixed combustion of municipal solid waste and biomass, and the results showed that baking can reduce the total amount of dioxins by 98.63% and the toxicity equivalent of volatile dioxins by 99.09%. Ri-gang Zhong et al.[15] carried out the co-combustion experiment of sludge and municipal solid waste, and found that PCDD/Fs production has been reduced by 32% when 5% sludge was mixed compared to municipal solid waste combustion alone. In the evaluation of the distribution characteristics of PCDD/Fs, more attention is paid to the ratio of PCDDs to PCDFs, rather than the transformation among PCDD/Fs isomers. For example, Peng Tao Cai et al.[16] believed that when the ratio of PCDDs to PCDFs is greater than 1, it indicated that de novo synthesis the main way of PCDD/Fs generation. Takashi Fujimori et al.[17] considered that de novo synthesis should involve the formation of C-C bonds through oxidation and subsequent chlorination, as well as chlorination. For the distinctions of PCDD/Fs isomers, Qiuju Gao et al.[18] deeply discuss the generation mechanism of PCDDs and PCDFs, respectively. However, the specific generation pathways are still not stated clearly. It has been found from the emission characteristics of PCDD/Fs isomers that there are some significant differences between their actual content distribution characteristics and their toxic equivalent distribution characteristics. For instance, our previous report[19] pointed out that compared with the conventional incineration mode, the PCDD/Fs production was reduced by 42% and the toxic equivalent was reduced by 20% when using Fe-based CLC. Gan Min et al.[20] by utilizing the suppressing functions of sulfur and calcium

compounds from $CaSO_4$ decomposing in the fly ash balls, and some similar conclusions have been obtained by detecting PCDD/Fs content and some similar conclusions have been obtained by detecting PCDD/Fs content. Noteworthily, the degree of reduction of PCDD/Fs produced is different from the degree of reduction of toxic equivalent, which indicates that the distribution characteristics and formation pathways of PCDD/Fs isomers have undergone a fundamental change. We calculated the probability of chlorine substitution by the position substitution (PSTS) prediction method[21], which reflects the intensity of chlorination during the formation of PCDD/Fs, and then we proposed a pathway substitution (PTWS) prediction method[22] to distinguish PCDD/Fs isomers, but it still does not involve a more specific correlation with HCl concentration and SO_2 concentration.

For this purpose, a correlation model of PCDD/Fs toxic equivalent was first proposed to quantitatively analyze the correlation between HCl and SO_2 concentrations and meanwhile a method[22] for diagnosing the transformation pathways among PCDD/Fs isomers was adopted to study the functional pathways of mixing sludge on PCDD/Fs isomers for coal combustion by calculating the probability of chlorine substitution as well as analyzing the percentage of PCDD/Fs isomers and their average toxic equivalent migration. All the selected experimental data are coal combustion and that with 10% sludge. It is expected to lay a theoretical foundation for low PCDD/Fs emissions from subsequent coal combustion and solid fuel blending by obtaining the correlation characteristics of PCDD/Fs isomers generation from coal combustion with sludge mixing.

2. Experimental data

In this work, the experimental data of PCDD/Fs isomers in coal combustion and that mixed with sludge is derived from the existing reports[23], as shown in Table 1. It can be seen that the toxic equivalent distributions of PCDD/Fs isomers are significantly different under the five operation conditions. Meanwhile, Figure 2 shows the toxic equivalent distribution of 17 toxic PCDD/Fs isomers. Notably, the distribution rule of isomers is not clear, even for the highest toxic equivalent under different conditions. Therefore, it is necessary to carry out a systematic study on the correlation of PCDD/Fs generation and the transformation among PCDD/Fs isomers.

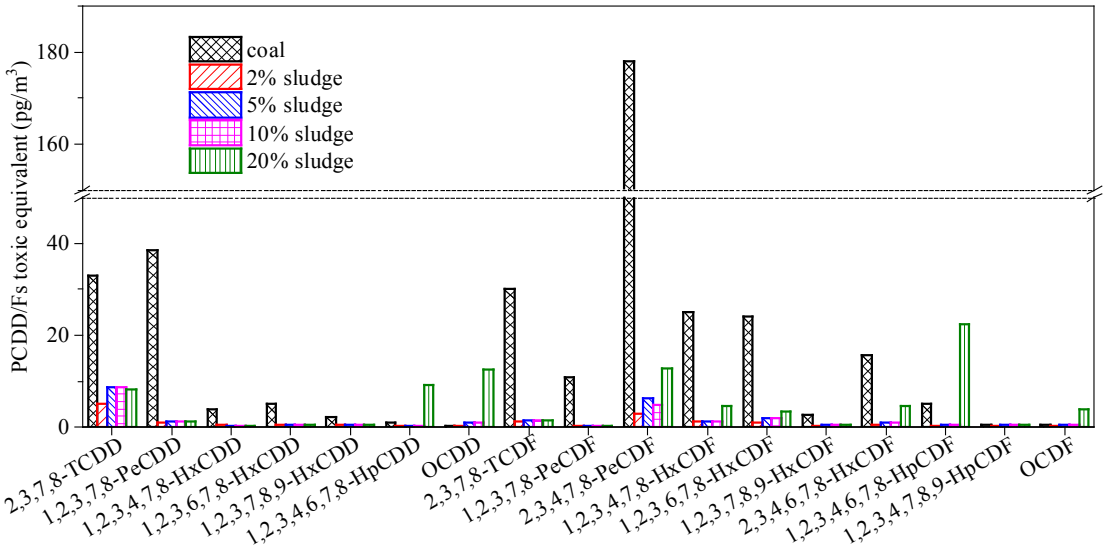

Figure 2. Toxic equivalent distribution of PCDD/Fs isomers

Table 1. Experimental data on Toxic Equivalent Quantity (TEQ) of PCDD/Fs isomers under two operating conditions

Conditions	HCl concentration (mg/m^3)	SO_2 concentration (mg/m^3)	PCDD/Fs toxic equivalent (pg/m^3)
Coal	93	260	152.8
2% sludge	83	296	17.4
5% sludge	89	388	27.1
10% sludge	89	412	25.8
20% sludge	92	436	87.2

3. Modeling approach

3.1 *Theoretical basis*

In the existing literature reports, studies have shown that HCl concentration is positively correlated with PCDD/Fs content[24], in which there is a self-equilibrium relationship between HCl and Cl_2 concentration.[7] However, the existence of SO_2 can react with Cl_2 to form HCl, which greatly reduces its chlorination activity. Meanwhile, it has been reported that SO_2 can react with catalytic metals to destroy their catalytic properties, which is negatively correlated with the production of PCDD/Fs. As shown in Figure 3, HCl concentration was associated with SO_2 by setting a linearly correlated function, and a polynomial correlation was determined by combining them into a new function value and matching it with toxic equivalent. On this basis, the process of chlorine migration among PCDD/Fs isomers was further quantitatively analyzed, and the conversion relationship among PCDD/Fs isomers was determined by calculating the chlorine substitution probability. The specific process can be referred to the existing literature.[25]

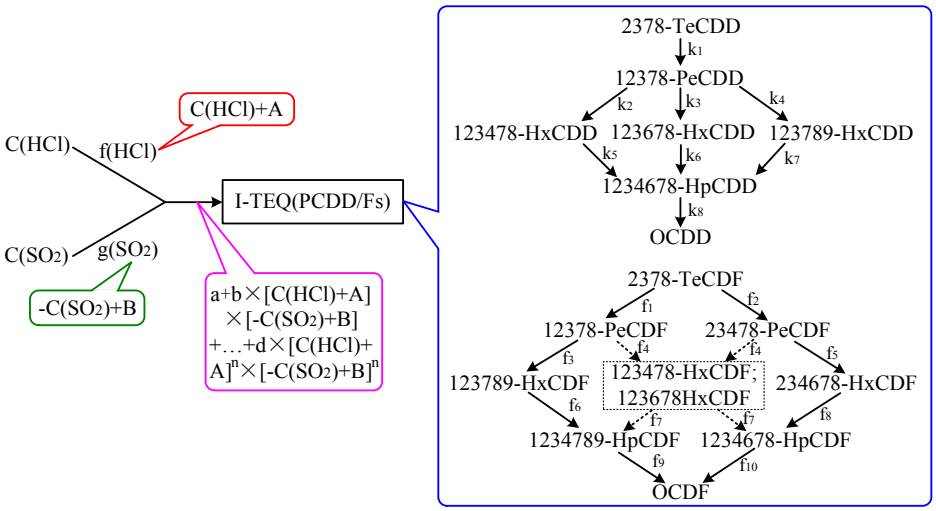

Figure 3. Schematic diagram of the correlation characteristics from PCDD/Fs generation

3.2 *Methodology*

Figure 4 is the logical relationship diagram of the correlation model. Firstly, the experimental data were plotted on a contour line, and the initial output values A and B were performed, while the data points with large deviations were

eliminated. Then, it would be done to select the associated function expression (initially, n = 1), and randomly select the correlation coefficient, calculate the similarity value (S_{total}), which was used for comparing the size determination with the existing value. If it is less than the original value, the number of calculations is directly determined. While the value is greater than the original value, the coefficients would be replaced, and then the number of calculations is determined. In the judgment of calculating number (i), if i is not more than 10000, the correlation coefficient will be randomly selected again for a new round of optimization. While if i is greater than 10000, the correlation coefficients will be output and the function expression will be determined. When the index (n) value is less than or equal to 3, i will be set to zero again, and a new round of calculation will be carried out. When n is greater than 3, the calculation would be terminated.

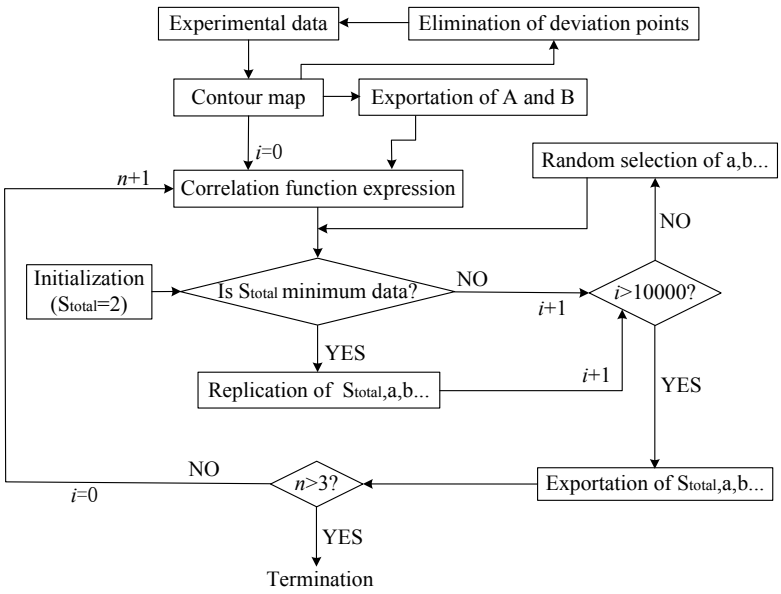

Figure 4. Logical relationship of the correlation model

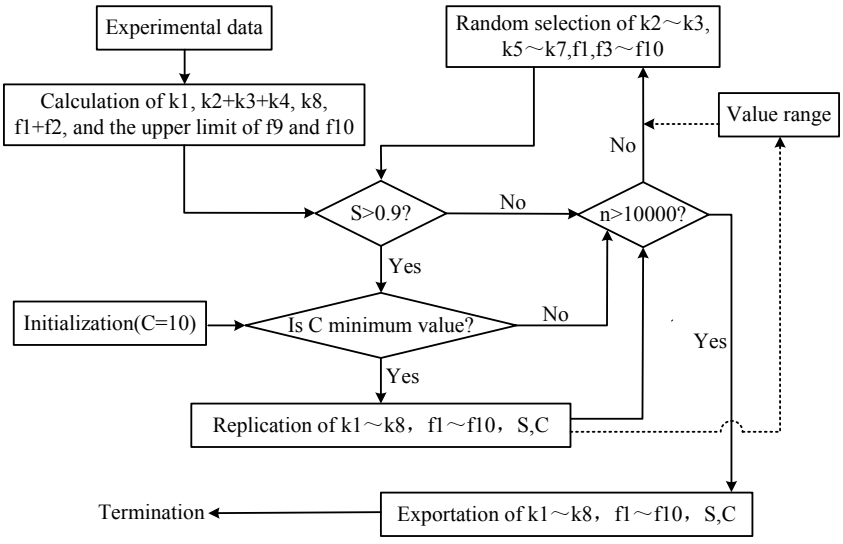

Figure 5. Logical relationship of the pathway-diagnosis method

Figure 5 shows the logical relationship of the pathway-diagnosis method. It mainly analyzes the probability of the formation of isomers according to the experimental values. The k1~k8 value represents the probability of chlorine substitution among 7 toxic PCDD isomers, and the f1~f10 value represents the probability of chlorine substitution between PCDF isomers. The chlorine substitution combinations were optimized by the evaluation indexes (S and C) listed in section 2.3. The random method used is based on the theory of most probable probability. Using the most probable method can predict the actual isomer conversion situations to the best possible extent. By combining multiple measurements of experimental data and multiple optimizations of this method, the error is further avoided. A more detailed theoretical overview is available in the reference[25].

3.3 *Evaluation indicators*

The reliability and accuracy of the prediction model are verified by similarity (S), average percentage content error (C) and average toxicity equivalent (M).[25] S and C can be used to optimize the compositional accuracy of isomers, while M was used to evaluate the changing degree of toxicity during the migration of chlorine element. Thereinto, S represents the difference between the evaluation value and the experimental value. The closer the similarity S is to 1, the more accurate the predictions will be. The circumscription of similarity is shown in equation (1).

$$S = \frac{\sum A_i B_i}{\sqrt{\sum (A_i)^2 \sum (B_i)^2}} \tag{1}$$

Among them, the predicted value and experimental value of each component in the PCDD/Fs isomer are represented by A_i and B_i respectively.

C is used to further evaluate the accuracy of the predicted value from the perspective of PCDD/Fs isomer percentage content. *C* is defined as shown in equation (2).

$$C = \frac{1}{i} \sum |A_i - B_i| \tag{2}$$

Where i represents the PCDDs isomers and PCDFs isomers, respectively.

M is used for analyzing the toxicity equivalent migration laws of PCDD/Fs isomers, and stands for the accumulation of the percentage content of PCDD/Fs isomers and the corresponding toxicity equivalent product.[25] Its definition is shown in equation (3).

$$M = A_i \cdot (\text{I-TEF})_i \tag{3}$$

4. Results and discussion

4.1 *Correlation with HCl and SO_2*

Figure 6 shows the correlation among PCDD/Fs toxic equivalent, HCl concentration and SO_2 concentration. First of all, it can be found that at a specific toxic equivalent, HCl concentration and SO_2 concentration present a hyperbolic trend, which is related to the model set. At the same time, the trend of this correlation curve shows a monotonic trend, and their derivative has a specific inflection point. It can be seen that as the toxic equivalent increases, this inflection point will extend in the direction of lower SO_2 concentration and higher HCl concentration. In addition, it can be determined that at a given concentration of HCl and SO_2, the increase in toxic equivalent caused by changing their concentration values can be regarded as a change in a multi-nomial fitting function, while the specific function relationship is not fixed and it is related to the amount of change. As shown in Figure 7, by comparing the predicted results with the experimental results, it is found that, except for mixing 2% sludge, the other working conditions are in good agreement. This is because the mixing 2% sludge is deleted as individual deviation points during the modeling

process. Thus, in the process of model construction, logarithmic points need to be optimized to further optimize the accuracy of the model. For example, 2% mixing conditions are eliminated in this work.

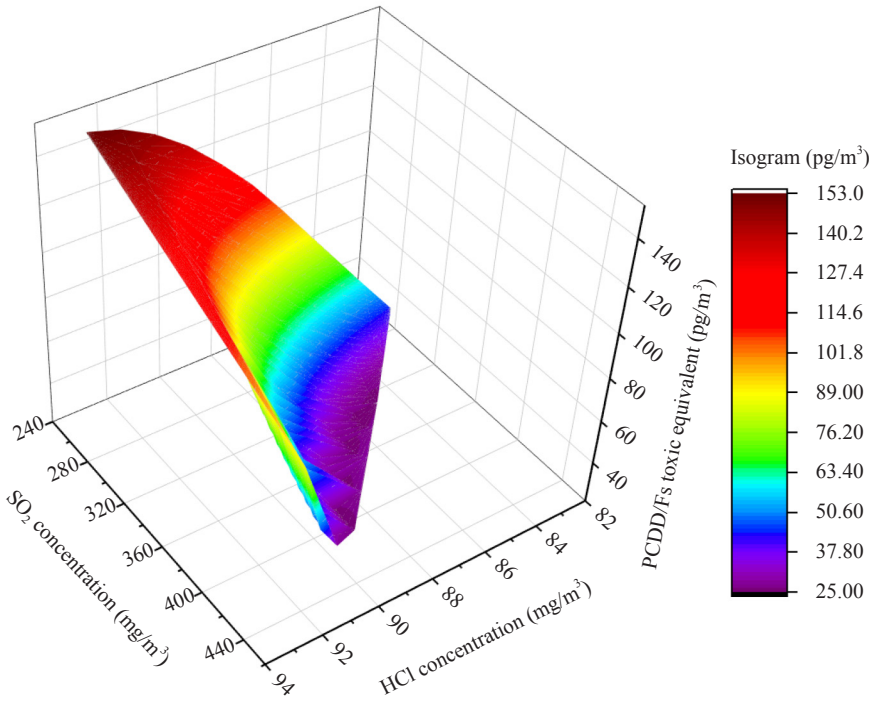

Figure 6. Correlation among PCDD/Fs toxic equivalent, HCl concentration and SO_2 concentration

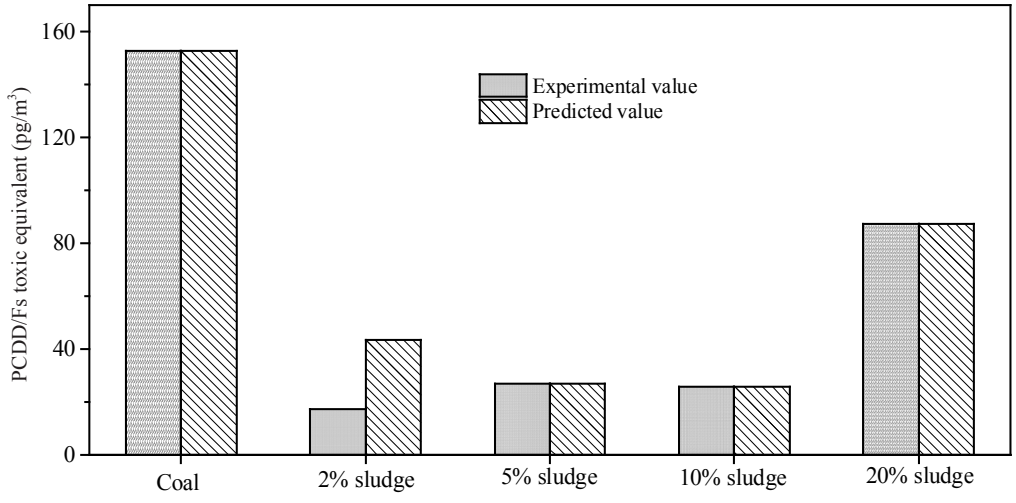

Figure 7. Logical relationship of the pathway-diagnosis method

4.2 *Chlorine substitution probability*

Based on the above analysis, the combustion conditions of mixed 10% sludge and single pulverized coal were

selected as the comparison conditions. To further ascertain the effect of mixing sludge on PCDD/Fs generation in coal combustion, the chlorine substitution probabilities of PCDD/Fs isomers were calculated, and these results are shown in Figure 8. It can be found that there are error ranges in these calculated chlorine substitution probability values, which should be related to the accuracy of the chlorine substitution probability value and the error evolution in the calculation process. For PCDDs isomers, mixing sludge significantly increased the chlorine substitution probability in the transformation process of 123678-HxCDD to 1234678-HpCDD and the transformation process of 1234678-HpCDD to OCDD. For PCDFs isomers, mixing sludge significantly increased the chlorine substitution probability in the transformation process of 123789-HxCDF to 1234789-HpCDF and the transformation processes of 1234789-HpCDF and 1234678-HpCDF to OCDF. In conclusion, sludge blending can change the distribution characteristics of PCDD/Fs isomers by changing the specific conversion pathways between the isomers.

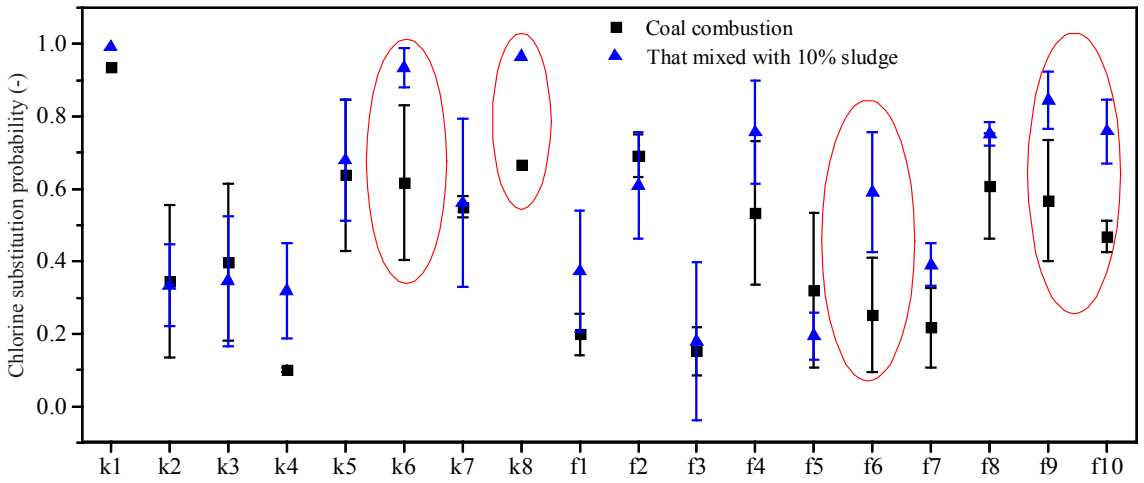

Figure 8. Chlorine substitution probability of PCDD/Fs isomers

4.3 *Chlorine element migration situation*

In order to further explore the influences from mixing sludge on the chlorine migration situation, the migration diagram of PCDD/Fs isomer percentage content (Figure 9) and the average toxic equivalent migration diagram (Figure 10) were drawn respectively. It should be pointed out that the process of increasing the number of chlorine substitutions can also predict the successive advance process brought about by the occurrence of chlorine substitution. For the PCDDs isomers, it can be found from Figure 9(a) that the impacts from mixing sludge are mainly the conversion ratio from 12378-PeCDD to 123478 Hexachlorodibenzo-p-dioxin (123478-HxCDD) and the conversion ratio from 1234678-HpCDD to OCDD. While it can be found from Figure 10(a) that the main reason that the mixing sludge reduces the average toxic equivalent of PCDDs is the increased chlorine substitution probability of 12378-PeCDD at position 4. Similarly, it can be found from Figure 9(b) that the mixing sludge caused many changes in the PCDFs isomers content, mainly including the further chlorine substitution probability of 2378-TeCDF, as well as the generation situation of 1234(6)78 Hexachlorodibenzo-p-furan [1234(6)78-HxCDF], 1234789-HpCDF, and OCDF. However, it can be found from Figure 10(b) that the main reasons for mixing sludge to further reduce the average toxic equivalent of PCDFs isomers in coal combustion are the decrease in the chlorine substitution probability of 2378-TeCDF at position 4, as well as the increase in total probability of further chlorine substitution for 23478-PeCDF, 123478-HxCDF and 123678-HxCDF.

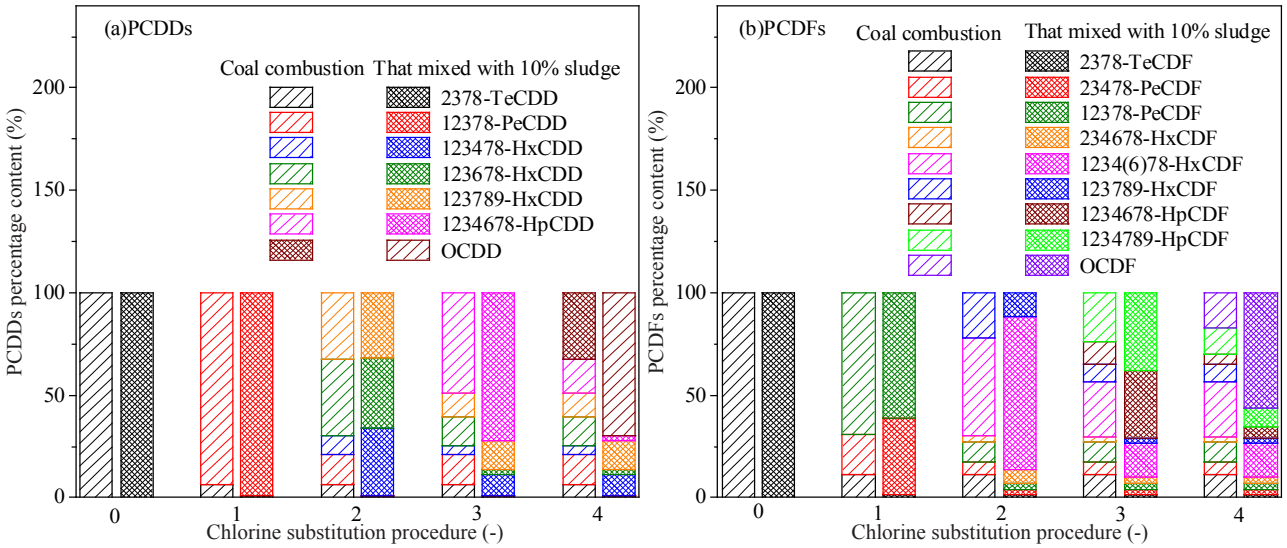

Figure 9. Percentage content of PCDDs(a) and PCDFs(b)

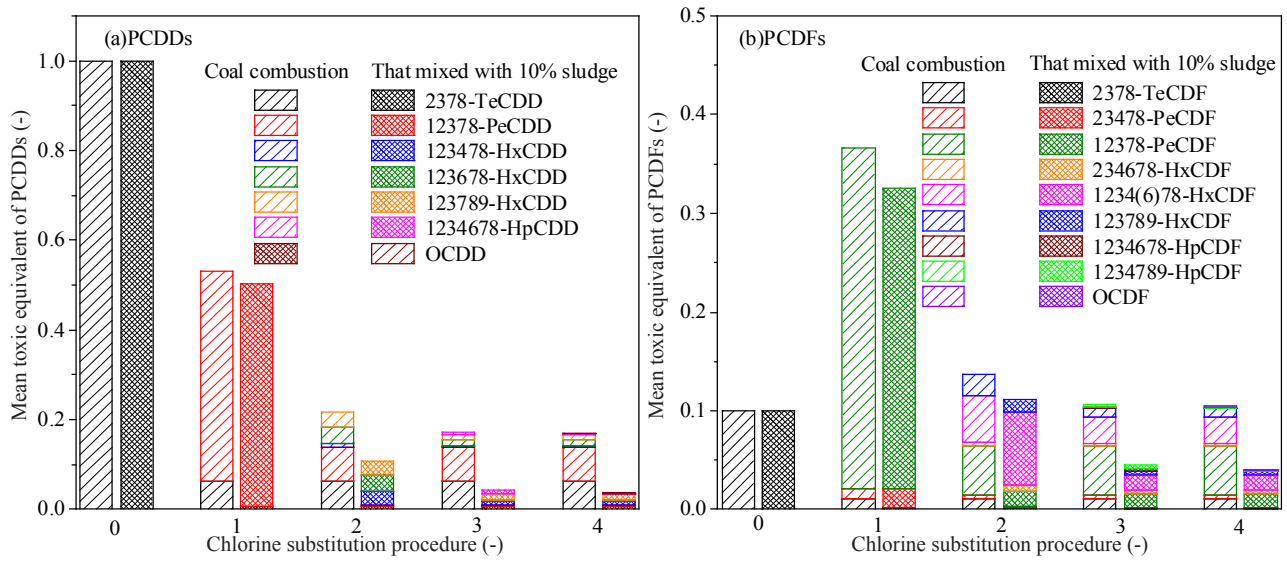

Figure 10. Average toxic equivalent of PCDDs(a) and PCDFs(b)

4.4 *Function pathway of mixing sludge*

To elaborate the functional pathways of sludge mixing on the formation of PCDD/Fs isomers from coal combustion, the main functional pathways and key toxic pathways emerge respectively according to the above results, as shown in Figure 11. Obviously, Figure 11 not only clarifies the effect of sludge mixing on the transformation among PCDD/Fs isomers, but also points out the main reasons for changing the toxic equivalent distributions of PCDD/Fs isomers, which provides a new idea for the follow-up related technology research. What's more, the application of functional pathways diagnosis can distinguish the transformation among PCDD/Fs isomers for the number of substances from the transformations among PCDD/Fs isomers for the toxic equivalent, which is conducive to exploring the inhibition or promotion pathways from the perspective of microscopic mechanism, and is also conducive to the artificial

intervention of specific PCDD/Fs toxic isomers. At the same time, it provides a theoretical basis for adjusting the ratio of solid waste to inhibit the formation of PCDD/Fs.

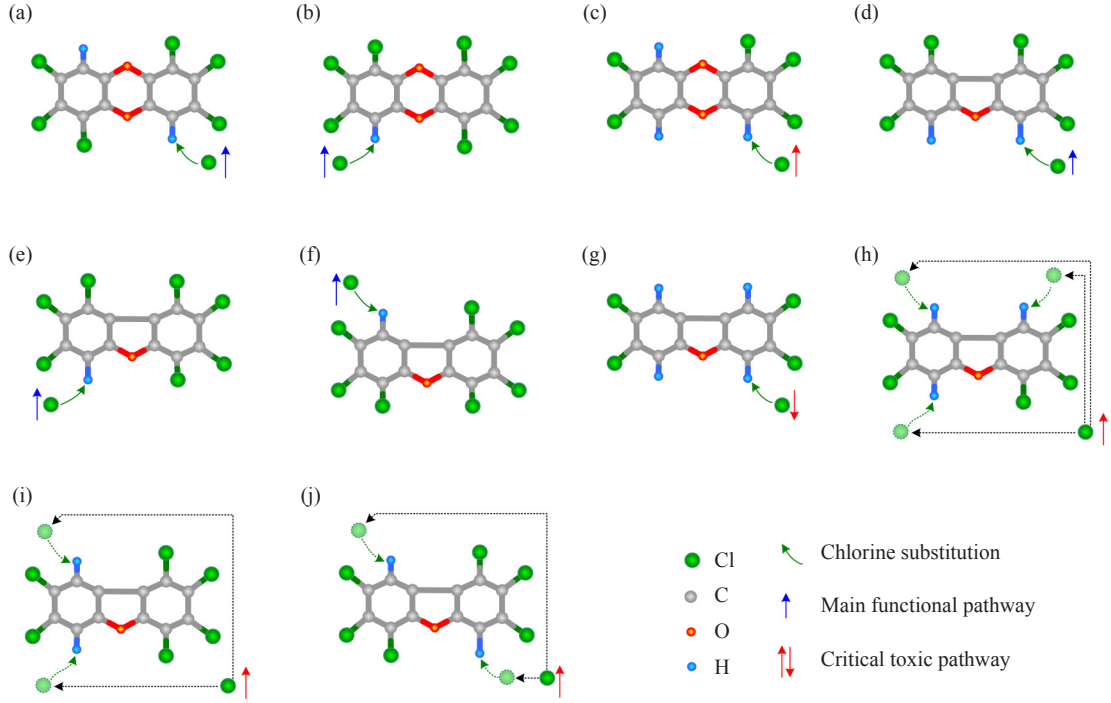

Figure 11. Functional pathways of mixing 10% sludge for PCDD/Fs isomers

5. Conclusion

In view of the effect of sludge mixing on the distribution characteristics of PCDD/Fs isomers in the coal combustion process, a correlation model of PCDD/Fs toxic equivalent was proposed to quantitatively analyze the correlation between HCl and SO_2 concentrations, and meanwhile a method for diagnosing the transformation pathways among PCDD/Fs isomers was used to deeply analyze the PCDD/Fs distribution characteristics of coal combustion and that mixed with 10% sludge, respectively. The specific conclusions are as follows:

(1) There is the trend of this correlation curve with a monotonic trend form at a specific toxic equivalent, and meanwhile their derivative has a specific inflection point. This inflection point will extend in the direction of lower SO_2 concentration and higher HCl concentration with the toxic equivalent increases.

(2) The sludge mixing mainly improved five transformation pathways, including the conversion process from 123678-HxCDD to 1234678-HpCDD, the conversion process from 1234678-HpCDD to OCDD, the conversion process from 123789-HxCDF to 1234789-HpCDF, and the conversion process from 1234789-HpCDF and 1234678-HpCDF to OCDF.

(3) Increasing the chlorine substitution probability of 12378-PeCDD at position 4, decreasing the chlorine substitution probability of 2378-TeCDF at position 4, and increasing the total probability of further chlorine substitution for 23478-PeCDF, 123478HxCDF and 123678-HxCDF, respectively, are the main reasons for further reducing the average toxic equivalent of PCDD/Fs isomers produced in coal combustion with sludge mixing.

Conflict of interest statement

The authors declare no competing financial interest.

Acknowledgments

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