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Prediction of product distributions in coal devolatilization by an artificial neural network model

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ABSTRACT

Currently most coal combustion simulations treat the devolatilization products as a mixture of light gases with a given proportion or a postulate substance, which is obviously different from the reality. To obtain a more accurate treatment on the product distribution from coal devolatilization, an artificial neural network (ANN) model is innovatively developed based on a training database constructed from diverse experimental data for a wide range of coal types under a wide range of heating conditions. The accuracy and applicability of the developed ANN model are validated and compared with that of the chemical percolation devolatilization coupled with the functional group (FG-CPD) model for the validation database, and the relative impact of each input parameter on the evolution of each devolatilization product is evaluated. The results show that the detailed product distributions of coal devolatilization predicted by the proposed ANN model are in good agreement with the experimental data for both the training and validation database, and the ANN model can give a more accurate prediction on both the yield of each component and its evolution compared with the FG-CPD model. The coal composition accounts for the most impact (above 60%) on the product distribution, and the relative impact of C_{daf}, H_{daf}, O_{daf}, coal particle diameter, instantaneous heating rates, particle residence time and particle temperature decrease successively. This ANN model has great potential to be coupled into coal combustion simulations to improve efficiency and accuracy, which will be studied in the future.

1. Introduction

As one of the primary processes in coal combustion, coal devolatilization has a significant influence on the ignition behavior [1], pollutant emissions [2] and the flame stability [3]. Thus, more attention should be paid on the predictions of coal devolatilization rates and the volatiles components in numerical simulations of coal combustion by the Computational Fluid Dynamics (CFD). Currently, most of the coal combustion simulations have only considered the devolatilization rates by using different devolatilization models, such as the one-step model [4], two-step model [5] and Chemical percolation devolatilization (CPD) model [6]. For the volatiles components, it is common to assume a mixture of simple light gases [7–10], such as CH_4, CO_2 and CO, with a given proportion or a postulate substance $C_\alpha H_\beta O_\gamma$ [11,12]. However, in real coal devolatilization process, the released volatiles are a complex mixture of tar and light gases, and the evolution of each component is different [13], thus the assumptions in coal combustion simulations are obviously unreasonable.

To take the detailed product distributions into account in coal devolatilization process, the first traditional method is to develop correlations based on limited experimental data. For instance, Goyal et al. [14] correlated the instantaneous yield of each devolatilization product with the coal temperature. Holstein et al. [15] modeled the evolution of each product with an Arrhenius equation based on the experimental results of selected coal under certain heating condition. However, those developed correlations are only valid for the selected coal types and heating conditions, and are not universal for a wide range of coals and heating conditions. As a result, Genetti et al. [16] proposed a double interpolation method to predict the distribution of devolatilization products from the experimental results of 12 coals in the early version of the CPD model.

Another kind of traditional method to predict the detailed distribution of devolatilization products is based on the coal chemical structures and the related functional group (FG) reactions. Serio et al. [17] proposed the Functional-Group, Depolymerization, Vaporization, Crosslinking (FG-DVC) model to predict the evolution of each devolatilization product based on the functional group of the

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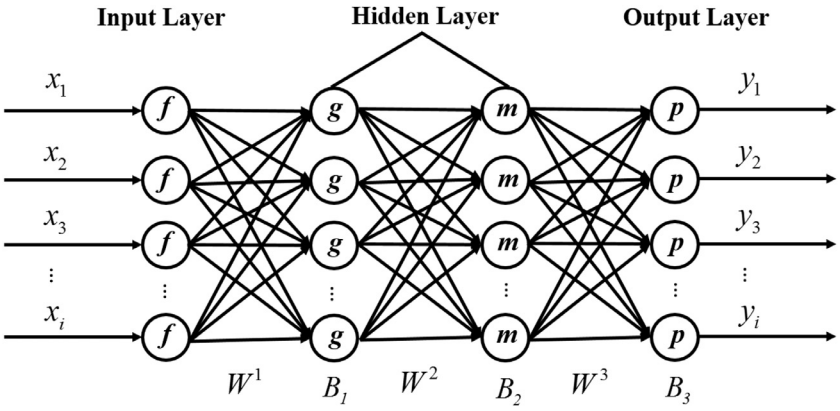

Fig. 1. The simplified topological structure of the ANN.

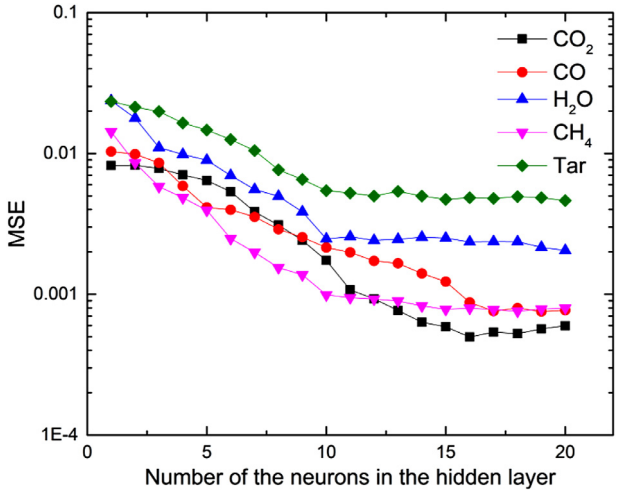

Fig. 2. Plots of the MSE of three-layer ANNs with different neurons in each hidden layer for each devolatilization product.

parent coal. By coupling the functional group compositions of the library coals in the FG-DVC model into the CPD model (referred as the FG-CPD model) [18], the prediction of volatile components of the CPD model can be further improved. However, the developed FG-DVC and FG-CPD models, based on the traditional methods, are found to make large deviations for some coals and heating conditions [19], and are expensive and difficult to be coupled into coal combustion CFD [20].

With the development of the artificial intelligence, an innovative method, the artificial neural networks (ANN), has shown great potential to be an effective tool to handle complex non-linear problems. The ANN method is a biologically inspired computational technique that imitates the behavior and learning process of human brain with cross-linked neurons instead of specific equations [21]. It can update itself through learning from training samples. Recently, the ANN method has been applied to coal thermal science, such as the predictions of coal global pyrolysis [22] and the calorific value of coal [23]. Compared with traditional methods, much less computational resources are required when coupling the ANN models into the CFD [22]. Thus, the ANN method could be an efficient approach for predicting the distribution of coal devolatilization products and improving the treatment on the devolatilization process in coal combustion CFD.

In the previous study [24], a universal-devolatilization-process (UDP) model, considering the effects of coal types and heating rates, has been developed to accurately predict the yield of the total volatiles in coal devolatilization. However, the detailed distribution of devolatilization products is not considered. The purpose of the present study is to develop an ANN model to accurately predict the detailed volatiles components during coal devolatilization using the training database constructed from diverse experimental data. This is different from a previous ANN study on global coal devolatilization [22], in which only particle temperature is considered to characterize the effect of heating conditions. However, it is obvious that the effect of heating conditions cannot be characterized by only temperature. In the present work, both accurate predictions on the product distributions and the effects of heating rates and coal particle diameters are taken into account. The detailed distribution of devolatilization products, including CO, H_2O, CO_2, CH_4 and tar, are predicted, and the accuracy and advantage of the proposed ANN model are thoroughly evaluated by predicting devolatilization products from a wide range of coals and heating conditions. The ANN predictions are compared with the experimental data as well as those predicted by the FG-CPD model, and the relative importance of each input factor on each component is evaluated and discussed.

The remainder of the paper is organized as follows. The detailed introduction about the methods and samples used to develop and validate the ANN model are presented in Section 2. Results of the training of the ANN model, validation of the developed ANN model, and relative importance of each input factor are presented in Section 3. Summary and conclusions are made in Section 4.

2. Methods and samples

2.1. Methods

Figure 1 shows the schematic diagram of the topological structure of the ANN model in the present study. The ANN is composed of three kinds of layer, including input layer, hidden layer and output layer. The input data always flow from the input layer, and then are transferred to the output layer to obtain predictions with the help of activation functions, weight and bias vectors between neurons in the hidden layer. The final output for the ANN with two hidden layers can be expressed as:

$$y = p\left\{m\left[g(f(x)W^1 + B_1)W^2 + B_2\right]W^3 + B_3\right\} \quad (1)$$

where x and y are the scaled input variables and output target vector respectively. W^i and B_i are the ith weight and biases vector for the ith neuron layer, respectively. All the activation functions (f, g,