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Experimental and DFT studies of $PM_{2.5}$ removal by chemical agglomeration

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ABSTRACT

Fine particles are significantly harmful to the human body and the atmospheric environment. However, the electrostatic precipitator (ESP) removal efficiency for $PM_{2.5}$ is low, therefore chemical agglomeration technology, which uses various chemical agents to induce particle agglomeration, improving the efficiency of ESP seems to be a promising pretreatment technology. In the present contribution a combination of experimental and DFT calculations has been used to study this technique. We used water, pectin and sodium alginate solutions as agglomeration agents. Experimental results showed that sodium alginate solutions is most effective, the particle diameter increased from 0.1 µm to 1 µm and the ESP removal efficiency of number concentration increased above 20% with chemical agglomeration technology. In theoretical studies we simulated various molecular clusters consisting of water, pectin and sodium alginate in combination with simple model silica particles (TOS) by using DFT calculations to explore the internal interactions in ESP system at molecular level. In our results, water, pectin and sodium alginate interacted with TOS by hydrogen bond, with interaction energy of 4.0 kcal/mol, 6.7 kcal/mol and 7.4 kcal/mol, respectively. Finally, according to the experimental and theoretical results, the chemical agglomeration models were put forward.

1. Introduction

Coal is used mainly to generate electricity in China. However, the combustion of coal results in production of large amounts of ash, which contains submicron fine particles, capable to be suspended in the air persistently and penetrated into the human respiratory system [1–3]. Northern China experienced a long-term and frequent haze and fog cover, which has caused the attention in Chinese society. Therefore, research on fine particle emission properties and control technologies has drawn growing attention.

ESP is a technique which employs the application of an electric field to separate out the suspended particles from the flue gas. ESP removal particles efficiency can reach 99.5% or even higher. However, the removal efficiency of $PM_{2.5}$ is only about 92–95%, especially for 0.1–1 µm particles, which the efficiency is even lower [4–6]. Particle agglomeration technologies are able to increase the mean particle size, which could effectively improve the particles removal efficiency. The adhesive forces being at here include Van der Waals force, attractive electrostatic forces and surface tension of the liquid layer. Common agglomeration methods are based on the exploration of increasing adhesive forces between the components during condensation-induced agglomeration, electric agglomeration, turbulent agglomeration, acoustic agglomeration and chemical-induced agglomeration [4,5,7,8].

Among the above mentioned methods, chemical-induced agglomeration uses chemical agglomeration agents sprayed into the flue before the ESP unit to accelerate the agglomeration between submicron particles. The chemical agglomeration technology is cheaper than other techniques, it can control the emissions of submicron particles and remove toxic trace elements without changing the operation parameters of the ESP [7,9]. The effect of this technology has been studied and proved. This particle agglomeration technique is a useful and promising method to control the emission of submicron particles from coal combustion. Ye et al. injected adsorbents into the flue gas to prevent the formation of ultrafine particles in coal combustion, and it has been found that the concentration of ultrafine particles has decreased significantly [10]. Linak et al. used adsorbents for removal of ultrafine particles and heavy metal trace elements [11]. Zhang et al. had built a dedicated experimental plant and analyzed the influence of various parameters including pH value or flow rate for the efficiency of the experimental process [9]. Yang et al. designed a closed-loop lab ESP with an evaporation chamber yielding the ESP removal $PM_{2.5}$ efficiency which increased by 45%, and simultaneously the SO_3 removal efficiency was raised from 66% to 86% [7,12]. The above mentioned research results indicate that chemical agglomeration is the effective

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method of enhancing the submicron particle removal.

Although many works were carried out based on various experiments, such researches and investigations lacked deep insights into the mechanism of interactions between submicron particles and the agglomeration agent. Density functional theory (DFT) is a method to successfully describe the behavior of atomic and molecular systems and is used for instance for structural prediction of chemical compounds and simulation of chemical reactions [13–15]. In this study, the experiment and DFT calculations were used to study chemical agglomeration technology and internal mechanism. An experimental device was designed to study an ESP removal efficiency improvement by using chemical agglomeration technology. Additionally, the DFT calculations were used to investigate the interactions between reunion agent and silica crystals representing the submicron particles. The results of both theoretical and experimental investigations were thoroughly discussed, compared and summarized.

2. Experimental and modelling

2.1. Experimental setup

An agglomerating test was designed and set up in order to simulate full scale flue gas flow, as shown in Fig. 1. The installation was mainly made up of a coal-fired boiler, a buffer vessel, wastewater evaporation system, an ESP, a WFGD, and analysis-detecting system. The flue gas with volume flux 350 Nm^3/h was generated by the boiler, which burned anthracite. A stirrer was installed in the buffer vessel to ensure the constant particle concentration and size distribution. The flue gas and atomized droplets of agglomeration agent were mixed in the evaporation chamber, and forwarded to the ESP unit by a booster fan. Coarse particles were removed when the flue gas passed through the ESP unit, which was a barb-plate tube type ESP with −40 kV applied voltage. The flue gas desulfurization occurred in the desulfurization tower, and it was discharged from the chimney by the induced draft fan. This operation is conducted under different conditions in the experiment and the specific parameters are shown in Table 1.

Table 1
The experimental operation parameters.

Parameter	Range
Flue gas flow rate (m^3/h)	350
The voltage (kV)	−40
Space between collection electrodes (mm)	300
Operation temperature (°C)	90–150
Agglomeration solution flow (L/h)	15

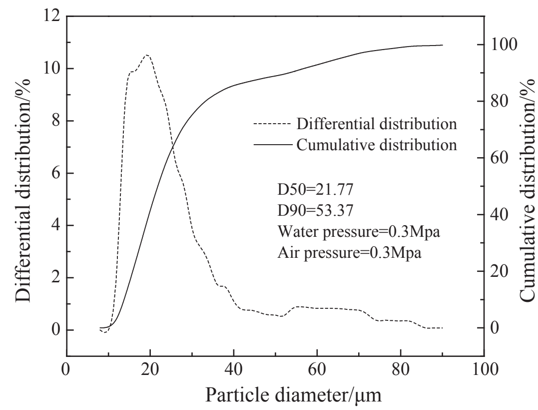
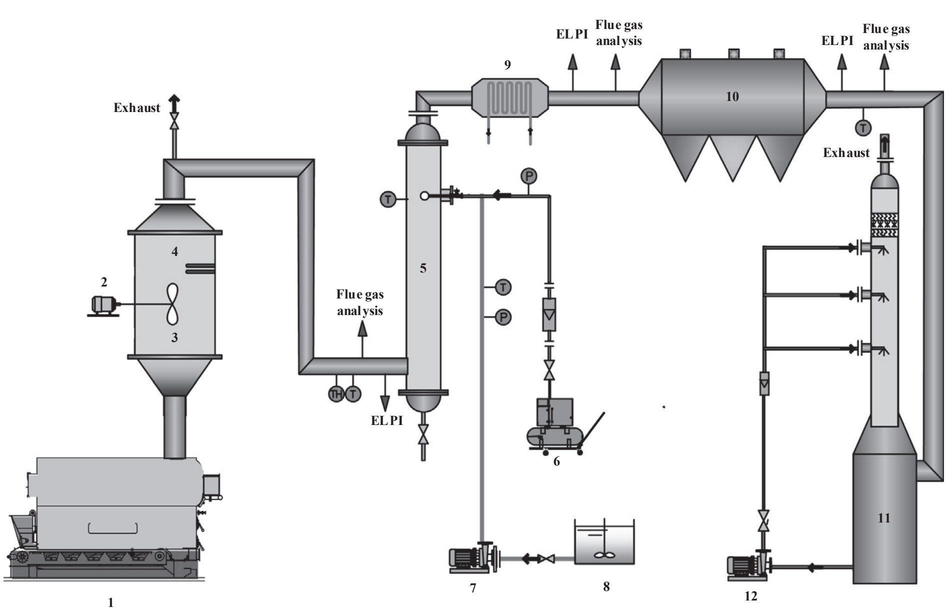


Fig. 2. Differential and Cumulative distribution of water droplets.

2.2. Experimental procedure

In the experimental installation, particles were generated by coal combustion in the boiler and the particle concentration was adjusted by aerosol generator (SAG 410/U). A two-fluid atomization nozzle was designed to generate droplets in the evaporation chamber. The droplets differential and cumulative distributions are shown in Fig. 2. The water droplets were polydisperse with the median diameter (D_{50}) of 21.77 μm and D_{90} of 53.37 μm under the test conditions. The voltage-current characteristics of the ESP is presented in the Fig. 3, the characteristics of ESP discharge was different because of different relative humidity, the



1- coal-fired boiler; 2-stirer; 3- buffer vessel; 4-heat tube; 5-evaporation chamber; 6-booster fan; 7-metering pump; 8- water tank; 9- heat exchanger; 10- ESP; 11-desulfurization tower; 12- metering pump;

Fig. 1. Schematic diagram of experimental system.