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Eulerian-Eulerian numerical simulation for a flue gas desulfurization tower with perforated sieve trays

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ABSTRACT

The CFD simulation based on the Eulerian-Eulerian model has been utilized to a small-scale Flue Gas Desulfurization (FGD) tower with perforated sieve trays. Most of the relevant studies have focused on the flow structures without the consideration of the chemical effects. In order to study the interactions between the flow structure and chemical reaction, the species transport equations of the chemical reactions have been implemented in the present study.

The numerical investigation of this study includes the liquid phase distributions, streamlines of the gas phase, chemical source term, and mass fraction of SO_2 gas. The complex vortical structure due to the implement of the sieve trays results in a sufficient large two-phase contact area. It also increases the number of times that the gas phase interacts with the liquid layer above the sieve trays and enhances flow mixing between regions of intense and weak chemical reactions. Correspondingly, the sieve trays can improve the SO_2 removal efficiency. This study can help to carry out the numerical based optimal design of the full-scale tower in the future.

1. Introduction

Besides negative environmental impacts, such as the acidification of the soil and global warming, the sulfur dioxide (SO_2) is harmful to the human body. The SO_2 is the major by-product of the exhaust gas from the fossil-fuel power and steel plant. A facility to desulfurize the exhaust flue gas is necessary before it enters the environments. A spray scrubber tower is the most common set of technology to remove SO_2, which is the so-called Flue Gas Desulfurization (FGD) tower. Inside the facility, the contact between the upward gas and downward alkaline liquid flow from the spray nozzles can trigger a series of chemical reactions to remove the SO_2 component from the gas phase [1–9]. The fundamental chemical reactions and relevant numerical studies have been highlighted in Sections 1.1 and 1.2 respectively. Since a series of sieve trays have been implemented into the FGD tower of the current study, Section 1.3 discusses the industrial applications of the sieve trays and the relevant numerical approach. The goal of this study is to develop a reliable CFD tool that can handle the two-phase flow simulation and its interactions with chemical reactions within a small-scale FGD tower. As a result, the numerical based optimal design of the full-scale tower can be carried out in the future.

1.1. The chemical reactions within the FGD tower

The complex chemical mechanisms, including the absorption, hydrolysis, dissociation, neutralization, dissolution, and oxidation, could occur within the flue desulfurization tower. Within the active region of the spray nozzles, the absorption due to the mass transfer between the SO_2 gas and liquid sulfurous slurry is the key part of the desulfurization process [1]. As the absorption takes place, the sulfur dioxide hydrates to form the sulfurous acid ($SO_2 \cdot H_2O$), and it loses one proton to form bisulfite (HSO_3^-) and a second proton to form sulfite (SO_3^{-2}) during the dissociation process [1–4]. Due to the simplification in the mathematical model, these three sulfurous components are usually modelled as a single variable as the sulfurous slurry [4]. As for the alkaline liquid from the spray nozzles, the dissociation of the magnesium hydroxide solution ($Mg(OH)_2$) can provide additional hydroxide (OH^-) that can neutralize the acidity of the sulfurous slurry [5].

In the bottom tank of the FGD tower, the calcium carbonate ($CaCO_3$) is usually used to neutralize the acidity of the sulfurous slurry before it leaves the facility as the waste water. The dissolution of $CaCO_3$ into the acidic slurry provides the carbon species HCO_3^- and CO_3^{-2}, which can neutralize the acidic slurry and produce the calcium ion (Ca^{+2}) in this process [1,2,4]. Furthermore, the bottom tank provides an adequate residence time for the complete oxidation of HSO_3^- into SO_4^{-2}. Consequently, the precipitation

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between sulfate ions (SO_4^{-2}) and the calcium ions occurs to form the gypsum ($CaSO_4{\cdot}2H_2O$) [2,4].

Sai et al [3] have carried out a series of FGD experiments at different equilibrium pH values to obtain the corresponding molar concentrations of H_2SO_3, HSO_3^-, and SO_3^{2-} respectively. As the pH value increases from 0 to 5, the molar concentration of H_2SO_3 decreases while that of HSO_3^- increases, and the concentration of SO_3^{2-} is extremely small. The further increment of pH value above 5 results in an opposite trend. The H_2SO_3 becomes insignificant as the concentration of HSO_3^- declines. As for that of SO_3^{2-}, it increases significantly and almost dominates after pH > 9 [1,2,4,10]. Please see Sections 3.2–3.4 for further details.

1.2. The previous numerical literatures of FGD tower

Different geometric setup of the facility can result in different preferable routes of the fluid flow within the FGD tower [4,5,6,8,9], which can influence the residence time of the fluid flow, two-phase contact area, gas-slurry slip velocity, and even could generate back flow inside the facility. As a result, the equation sets of Navier-Stokes equations, including the transport phenomenon of the continuity, momentum, species, and turbulence, can describe the detailed two-phase flow structures much better than the ideal simplified mathematical model that assumes uniform flow conditions [3,4,6–9].

The category that uses Navier-Stokes equations is the so-called Computational Fluid Dynamics (CFD) technique because the equation sets are solved numerically instead of analytically due to the highly nonlinearity. Within the CFD framework, the two-phase flow interactions can be treated by Eulerian-Lagrangian or Eulerian-Eulerian model. For both models, the first phrase "Eulerian" indicates that the background major phase, which is the exhaust gas in this study, is considered as the continuous carrier phase by Navier-Stokes equations. The second phrase "Lagrangian" of the Eulerian-Lagrangian model means that the liquid phase has been treated as numerous dispersed droplets and tracked as a large number of particles. The two-phase momentum exchange is usually updated through the two-ways coupling in this kind of study, and the movement of the droplet is dominated by the gravity and empirical two-phase drag forces. The interactions between gas and liquid hydrodynamics inside a spray scrubber or a desulfurization spray tower have already been analyzed by this Eulerian-Lagrangian model in Refs. [1,2,11–13]. Similarly, Ali et al. [14] and Li et al. [15] have also applied this kind of framework to the dust removal process inside a venturi scrubber and an umbrella plate scrubber respectively. When the chemical reactions are taken into considerations, the two-film theory and Henry's Law are usually applied as the SO_2 absorption model [2,11,12,16].

On the contrary, the Eulerian-Eulerian model treats not only the gas but also the liquid phase as continuous phases, and each phase requires its own sets of Navier-Stokes equations due to the two-phase slip velocity (please see Section 3.1). The Eulerian-Lagrangian model in the previous paragraph is built on the assumption that the liquid phase is dilute, which makes it reasonable to treat the droplet as the discrete phase. Therefore, the liquid volume fraction must be smaller than 0.1 [17,18]. For example, the maximum liquid volume fraction is 0.05 as reported in Ref. [2]. However, for the current study of interest, a series of perforated sieve trays have been placed inside a pilot FGD tower. The liquid phase could accumulate above the sieve tray, and hence its volume fraction could be locally much higher than 0.1, which contradicts the assumption of the Eulerian-Lagrangian model. As the consequence, the Eulerian-Eulerian model is more suitable in this study. Similar situations can also be seen from numerical literatures relevant to the industrial application of the sieve tray [5,19–26].

Most of the previous studies by Eulerian-Eulerian model have focused on the flow structures without the consideration of the chemical effects. In order to study the interactions between the flow structure and chemical reaction within a tray-equipped FGD tower, the species transport equations have been implemented for the chemical reactions in the present study. Similar model sets can be referred to Ref. [4]. The source terms of the species transport equations are determined by Henry's law constants, mass transfer coefficients, enhancement factors, molecular weights, and molar concentrations [4,10].

Since there are many species involved in the chemical mechanisms (please see Section 3.2 for further details), it is impractical to solve the transport equations for all of them. In order to reduce the required number of species transport equations of this study, a prepared chemical database that accounts for the detailed chemical mechanisms is coupled with the fluid flow solver of CFD (please see Sections 3.3 and 3.4). Under this framework, it can significantly reduce the numerical difficulties, such as the convergence issue and computational time.

1.3. Industrial applications of sieve trays

Most engineering designs are optimal under a more uniform flow conditions [5,27], which could be achieved with the implement of the sieve trays [5,27–33]. Therefore, the sieve tray, or to say a perforated plate, has widely been used in the industrial applications. For example, the electrostatic precipitator device, which is used to reduce the dust emission, can achieve its best collecting performance if the uniform distribution of the gas flow is expected in the system when the sieve trays are applied [28–31]. Besides, the implement of a perforated plate at the inlet of a wind tunnel can significantly reduce the turbulence intensity and uncertainty of the free stream [5,27,32,33]. The perforated sieve trays are also capable of separating liquid mixtures as a filter, which can be applied in petroleum and petrochemical chemical industries [5,19,20,24–26]. By Eulerian-Eulerian CFD techniques, the two-phase mixing by the sieve tray and its optimal design can be studied through a series of numerical experiments.

In order to reduce the SO_2 emissions, the Open Spray Tower (OST) is the most frequently installed scrubber type for a desulphurization plant, and it covers the major part of the market today [2]. The key design issues for this kind of facility include wide spraying angles, multiple spray layers, and layouts of the nozzle arrays [2,11–13]. In Refs. [2,11,13,16], the diameter of the droplet is reported as the order of millimeter. However, with suitable arrangements of the spray nozzles, a good liquid coverage within the tower still can be achieved even the droplet size is as coarse as millimeter, providing strong chemical reactions between the carrier gas phase and discrete droplets.

Alternatively, the perforated plates can also be applied as the sieve trays within the desulphurization tower, which is the particular interest of this study. Recently, Chen et al. [11] has found out that the SO_2 removal efficiency for a tray-equipped tower is around 7% better than that of an OST. Instead of resolving the complex perforated structures of the sieve tray by a large number of grid points, a source term that approximates the pressure drop across the tray regions has been added into the momentum equations. This is the so-called porous media model [5,11,31]. The value of the source term can be determined based on the fluid velocity, density, and the perforated characteristics, such as the hole diameter, pitch distance, tray thickness, and the hole Reynolds number [5,31]. As for the further details of the porous media model, please see Refs. [5,31].

Since the performance of the porous media model has already been comprehensively evaluated in our previous study [5] based on conditions for the single phase flow fields, this study and its