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Modeling and experimental analysis of packed column for SO_2 emission control process

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ABSTRACT

Sulfur dioxide (SO_2) emissions from chemical process plants are increasing at an alarming rate. It is necessary to implement the best methodology to reduce the SO_2 emissions. This paper presents physical modeling, computational fluid dynamics (CFD) analysis, and experimental analysis of a packed column used for flue gas desulfurization (FGD) process to reduce SO_2 emission at a greater extent. The packed column parameters such as liquid/gas (L/G) ratio, diameter, packed height and total height were determined using physical modeling with two–film gas–liquid absorption theory. Simulation model of the packed column is developed by GAMBIT 2.2.30 and analysis is carried out by FLUENT 6.2.16. In CFD analysis, hydrogen peroxide (H_2O_2) (with different concentrations) was used as an absorbent. CFD simulation result ensures that when H_2O_2 is used as a reactant, better removal efficiency is obtained. Based on the physical modeling and CFD analysis, a lab scale packed column was developed. Experimental result showed that 95% SO_2 removal efficiency is achieved for 0.1 M H_2O_2 as a reactant. Experimental results agreed excellently with the developed CFD model and can be used for designing industrial packed columns.

Keywords: *Packed column, CFD analysis, SO_2 emission control process, hydrogen peroxide (H_2O_2)*

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1. Introduction

This section reviews background information on the various approaches, methods and materials that are currently being used to control SO_2 emissions. In Industry, coal and oil emits SO_2 as a flue gas during combustion process. The increasing usage of fossil fuel has resulted in an increase of world total SO_2 emission rate during recent years. It poses a number of environmental and human health effects such as wheezing, chest tightness, shortness of breath, etc.. Control techniques are incorporated in the recent years, which reduces the SO_2 emissions and it is investigated by Lonsdale et al. (2012). Flue gas desulfurization (FGD) is the effective and reliable SO_2 removal methodology and it is classified as dry, semi–dry, and wet FGD. Among these techniques, wet FGD is the cost effective method (Cofala et al., 2004) and produces 60–95% removal efficiency (Liu et al., 2008). In wet FGD process, the desulfurization takes place due to mass transfer and chemical reactions of liquid and gas phases. Different absorbents are used in FGD such as lime (Liu et al., 2008), water with NH_3 (Ipek et al., 2008), and NaOH (Schultes, 1998). Ruitang et al. (2008) investigated lime based FGD process, in which lime reacts with SO_2 and produces CO_2 as a secondary pollutant to the atmosphere. Hence an alternative solution is given by Colle et al. (2003), and they investigated the FGD process with H_2O_2 added with H_2SO_4 as an absorbent. H_2SO_4 produces adverse effect on SO_2 absorption with H_2O_2. FGD process with H_2O_2 as a reactant has already patented by Copenhafer and Pfeffer (2011). When H_2O_2 is used as a reactant, it produces highly concentrated H_2SO_4 as a by–product after continuous recirculation. Hence, FGD process with H_2O_2 as a reactant is considered as an absorbent for this present work. The study given by Maheswari et al. (2013) ensures that when H_2O_2 is used as an absorbent enhances the SO_2 removal efficiency.

There are several types of scrubbers proposed by researchers for FGD process such as bubbling jet reactor (Zheng et al., 2003), combined packed and spray tower absorber (Gomez et al., 2007), cable bundle wet scrubber, and packed column (Colle et al., 2004). Packed column is taken for analysis because of its increased absorption rate by providing a good contact with liquid and gas. FGD processes with different absorbents are simulated using computational fluid dynamics (CFD) by several researchers (Ebrahimi et al., 2003; Marocco, 2010). CFD modeling and optimization of scrubber parameters is revealed by Ruitang et al. (2008). The study by Gomez et al. (2007) have reported that 90% SO_2 removal efficiency was achieved in a real plant developed based on CFD modeling. Bravo et al. (2002) developed CFD model for SO_2 absorption and they investigated that the concentration of SO_2 across gas–liquid interface did not vary with the operating temperature. Literature rarely focused on the simulation studies of FGD process with H_2O_2 as a reactant. Thus, in this work, CFD analysis was used to find transport behavior between gas and liquid in the packed column for maximum SO_2 removal efficiency when H_2O_2 is used as a reactant. Absorption of SO_2 in H_2O_2 is a complex process which involves both chemical and mass transfer analysis. Mass transfer is an important phenomenon that should be described properly for packed column design. Hence the present study focused on the following:

(1) Determination of L/G ratio, packed height, diameter and height of the packed column based on physical modeling,

(2) Development of CFD model for a packed column based on physical modeling and analysis for maximum SO_2 removal efficiency,
(3) Comparative study with CFD simulation results and experimental results.

2. Physical Modeling

The performance of the column depends on the maintenance of good liquid and gas distribution throughout the surface area of the column. The oxidation reaction that occurs inside the packed column is expressed in Equation (1). The reaction produces sulfuric acid as the end product.

$$SO_2 + H_2O_2 \rightarrow H^+ + HSO_4{}^- \rightarrow 2H^+ + SO_4{}^{2-} \tag{1}$$

The packed column was selected for SO_2 removal, since packed area in the column is used to develop larger interfacial area between gas and liquid which increases the absorption rate. Random packing was used in this packed column since high randomness in packing gives high removal efficiency (Coulson and Richardson, 1991).

2.1. Determination of minimum L/G ratio

During the mass transfer between SO_2 and H_2O_2 in the packed column, H_2O_2 becomes aqueous sulfuric acid solution. Though H_2O_2 is used as a reactant initially, once it is circulated through the packed column, it becomes an aqueous sulfuric acid. Hence, aqueous sulfuric acid is taken as the liquid for physical modeling. The experiment by Hayduk et al. (1988), detailed the absorption of SO_2 in to aqueous sulfuric acid, and the solubility data taken from this study is shown in Table 1.

Mole fraction of SO_2 in liquid phase X (in aqueous sulfuric acid) is calculated as:

$$X = \frac{Moles\ of\ SO_2\ in\ H_2SO_4}{Moles\ of\ SO_2\ in\ H_2SO_4 + Moles\ of\ H_2SO_4} \tag{2}$$

The mole fraction of SO_2 in gas phase (Y) is computed by dividing the partial pressure of SO_2 (P_{SO2}) by the total pressure (P_{TOT}=101 KPa) of the packed column. Equation (3) is used to express the equilibrium solubility of gas–liquid systems:

$$Y = HX \tag{3}$$

From the tabulated values (Table 1), equilibrium diagram is plotted between X and Y. The slope between X and Y in the equilibrium line gives solubility constant H. The equilibrium line is straight; hence the value obtained from the slope of the equilibrium line is used to predict the solubility of SO_2 in to aqueous sulfuric acid solutions (Manyele, 2008). For different values of X and Y, calculated H values are shown in Table 1. Also, the slope of the equilibrium line is used to calculate minimum L/G ratio by taking mass transfer characteristics across liquid and gas in the packed column. Two–film theory proposed by Whitman (1923) is the simplest theory designed for mass transfer analysis and it is expressed in Equation (4):

$$G_m[Y_1 - Y_2] = L_m\,[X_1 - X_2] \tag{4}$$

where, G_m is the inlet gas flow rate, L_m is the inlet liquid flow rate, X_1 is the mole fraction of aqueous H_2SO_4 leaving the column, X_2 is the mole fraction of aqueous H_2SO_4 entering the column, Y_2 is the mole fraction of SO_2 in gas stream leaving the column, and Y_1 is the mole fraction of SO_2 in the gas stream entering the column. The minimum liquid flow rate to the packed column was determined as 152.5 Lph, based on the Equations (3) and (4) by considering Y_1=0.05 mole fraction of SO_2 (5% SO_2 by volume), Y_2=0.005 mole fraction of SO_2, G_m=40 m^3/hr, Henry's constant=1.21 (selected from the Table 1), to obtain maximum of 99% (based on the assumption) SO_2 removal efficiency.

2.2. Determination of the column diameter

Determination of column diameter plays a key role to ensure good liquid and gas interaction, to make the packed column, to withstand for high pressure drop across the walls and the packed area and to determine the capacity of the column. Pressure drop in the packed column must not exceed a certain level that is described as flooding. Column diameter should be determined so as to operate the column below 75% of the flooding velocity (Coulson and Richardson, 1991). Based on the generalized pressure drop correlations between flooding factor (K_4) and pressure drop (or) abscissa (F_{LV}), the column diameter is determined. Equation (5) is used to compute the pressure drop of the column:

$$F_{LV} = \frac{L_m}{G_m}\sqrt{\frac{\rho_G}{\rho_L}} \tag{5}$$

where, ρ_G and ρ_L are the densities of SO_2 gas and aqueous H_2SO_4 respectively. Based on the Equation (5), F_{LV}=0.149 was calculated and corresponding flooding factor (K_4) is calculated as 0.7. The percentage of flooding is 70% and it is satisfactory for further analysis.

Computation of column cross sectional area based on of gas mass flow rate (V_W) is given by the Equation (6) (Coulson and Richardson, 1991):

$$V_W = \left[\frac{K_4\rho_v(\rho_L - \rho_v)}{13.1F_P(\mu_L/\rho_L)^{0.1}}\right]^{0.5} \tag{6}$$

where, ρ_V is the SO_2 gas density at 20 °C, ρ_L is the liquid density, μ_L is the liquid viscosity, and F_P is the packing factor for 25 mm polypropylene pall ring. Polypropylene pall ring was selected as the packing material with 25 mm diameter and its packing factor is determined as 170 (Coulson and Richarson, 1991).

$$A = \frac{G_m}{V_W} \tag{7}$$

Cross sectional area of the packed column was determined using Equation (7) and the required diameter of the column was computed as 152.5 mm.

Table 1. *Solubility data for SO_2 absorption in aqueous sulfuric acid*

Partial Pressure P_{SO2} (KPa)	Solubility g of SO_2/100 g of Aqueous H_2SO_4 Solution	Mole Fraction of the Solute (SO_2) in the Liquid Phase (X)	Mole Fraction of SO_2 in the Gas Phase (Y)	H=(Y/X) Henry's Law Constant
102.6	2.95	0.0295	0.0384	1.32
152.2	4.69	0.0469	0.0596	0.81
185.2	6.03	0.0603	0.0753	0.988
203.0	6.86	0.0686	0.0848	1.09
247.8	8.48	0.0848	0.103	1.21

(Source: Hayduk et al., 1988)