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Mathematical Modeling of Packed Column for NO_x Gas Removal using Hydrogen Peroxide Solution

C. Maheswari*, R. Vinoth, L. Kanimozhi and B. Meenakshipriya

Abstract: This work mainly focused on the design and modeling of packed column for NO_x gas removal using hydrogen peroxide absorbent. Mathematical modeling was carried out for the column with packing material Intalox ceramic saddles with 6 mm diameter. The de-nitrification process was carried out to make the NO removal process such that various parameters such as packed column sizing, packing material, absorbents used were determined for the NO_x removal process by wet scrubbing technique. This modeling determines of liquid flow rate, diameter, and packing height, which offers enhanced the absorption NO_x of gas, mathematical modelling is based on two film theory of gas liquid absorption.

Keywords: NO_x emission; absorption; two film theory; packed column.

1. INTRODUCTION

Nitric oxide is emitted from the automobile engines, fossil fuel power plants. These emitted gaseous reacts with atmospheric air and causes severe effects in the environmental. The Nitric oxide gas converted in to nitric acid, which was a main cause of the acid rain formation. Furthermore, both NO and NO_2 contribute in ozone layer depletion. There are various types of emission controlling approaches develop by the industrialists and researchers such as selective catalytic reduction (SCR), selective non-catalytic reduction (SNCR), and adsorption and wet scrubbing. Other than this, a new upgrading method for effluent reduction process is wet scrubbing process, which is the most effective method to abate the gas particle through the mass transfer technique. Wet scrubbers have some unique characteristics useful for fine particulate control.

Absorption with chemical reaction involves removing the impurities from gas phase and dissolving them into the liquid phase by making a chemical reaction between them. The absorption process is described by the mathematical model based on a two-film theory of gas-liquid absorption. The two film theory proposed by Whitman (1923) is the simplest theory designed for mass transfer analysis. The most commonly used device for absorption process is a packed column, since packed area in the column is used to develop more interfacial area between gas and liquid which increases the absorption rate [11]. NO_x is more challenging to take away from the wet scrubbers, because most of it is in the form of nitric oxide (NO), which having a very low solubility. The wet scrubbing process is implemented through, the newly designed packed column for NO_x emission control process and the main absorbent used for the wet scrubbing process is hydrogen peroxide which is used as absorbent. To rise the absorption rate of NO_x, oxidizing agents were get together effectively both in the gas phase (ozone, chlorine dioxide, hydrogen peroxide,) [9] & [6] or in the liquid phase (potassium permanganate, sodium chlorite etc.). An oxidizing

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process using hydrogen peroxide in the scrubbing solution appears to be very attractive, as it results in the production of valuable nitric acid without generating any other polluting byproduct [10].

2. ABSORBENT SELECTION PARAMETERS

Based on the literature survey various type of absorbents were used in the packed column are tabulated in table 1. It is clear that various absorbents are used for NO_x emission control process such as $NaClO_2$, aqueous HNO_3, H_2O_2, potassium permanganate, NH_3 etc., Hence H_2O_2 is considered as an optimized absorbent for NO_x removal process which can be used in the modeling of packed column.

Table 1
Absorbent selection

Author	*Absorbents used*	*Mole conc./ feed rate of absorbent*	*Removal efficiency*	*Height of packed column*
H.K LEE et al. [7]	$NaClO_2$	0-50ml/min	67%	ID-0.015m,height-1.0m
Collins et al [1].	H_2O_2	Molar ratio-1.0	>90%	Height 1.5m
Kasper et al[6].	$HNO_3$with added H_2O_2	HNO_3-0-2M, H_2O_2-0.02M	90%	Height 2m

3. MODELING OF THE PACKED COLUMN FOR NO EMISSION CONTROL PROCESS

3.1 Packed Column

Packed bed columns are ultimately utilized in absorption, desorption, and direct heat transfer processes in chemical, environmental protection such as processes in thermal power stations like water purification.

3.2 Design Of Packed Column

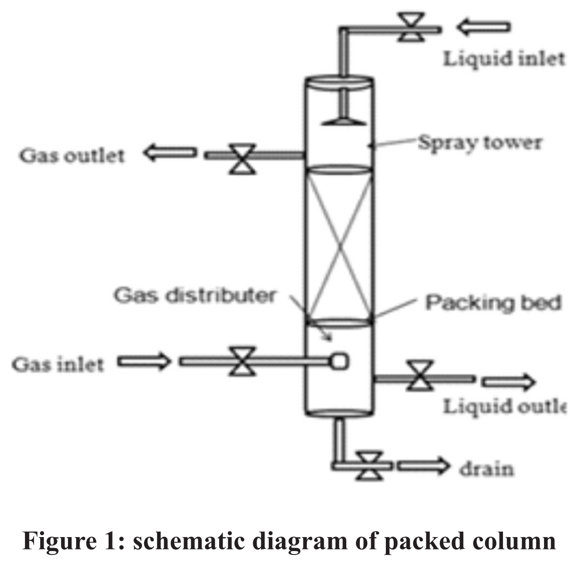

Figure 1: schematic diagram of packed column

Figure 1 shows the schematic representation of packed column, which consists of liquid sprayer, gas and liquid inlet, gas distributor and a packed bed. The liquid solvent is allowed to enter the column at the top through a liquid distributor and then it flows down through the surfaces of the packing materials. The gas phase enters at the bottom of the column, which flows upward through the packing materials, through which mass transfer takes place from the gas to liquid films. Better performance of the column is obtained by properly designing the parameters of the column such as absorbent used, diameter, total height, packing material, type of packing material used, packing height and Liquid/Gas (L/G) ratio. Packed column and its parameters used by the various researchers are shown in the table 2

Table 2
Parameters of packed column

Parameters	*Thomas et al.[10]*	*Vanderschuren et al.[5]*	*Kenig et al.[8]*
Diameter(m)	0.045	0.045	0.025
Height(m)	0.45	0.45	1
Flow rate of liquid(lph)	37.4	30.7	19.6
Flow rate of gas(m^3/s)	2.8*10^-4	2.8*10^-4	49*10^-5
Packing material	10mm glass rasching ring	10mm glass Rasching ring	12.5mm ceramic rasching ring

3.3 Mathematical Modeling of the Packed Column

3.3.1 Determination of L_m/G_m Ratio

The minimum liquid and gas requirement are determine based on solubility of gas (NO) in a liquid (aqueous nitric acid) which determines the amount of pollutant absorbed from the gas phase to liquid phase. The mostly used method for analyzing the solubility data is to use an equilibrium diagram. It is a plot between mole fraction of solute in the liquid phase denoted as 'X' and the mole fraction of solute in the gas phase denoted as 'Y' which is indicated in figure 2

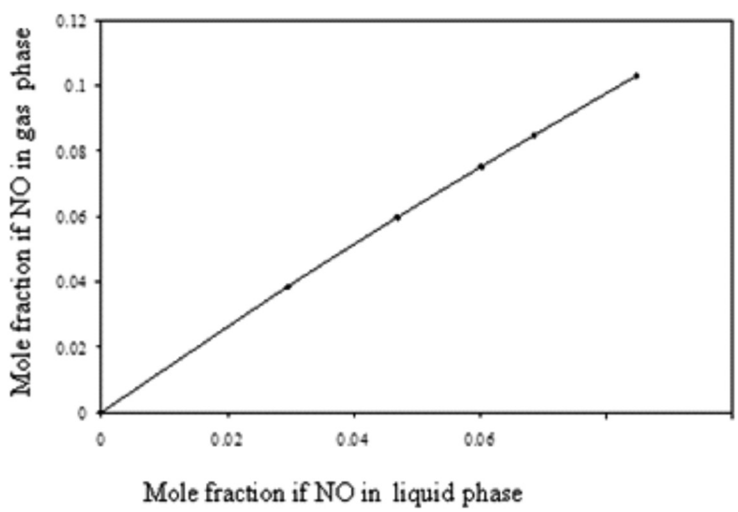

Figure 2: Equilibrium diagram

To remove the required amount of NO the temperature is to be maintained at 20°C. Let us take following assumption,

Inlet concentration $y_1 = 1\%$ of NO by volume

=0.01 mole fraction of NO

Outlet concentration $y_2 = 98\%$ reduction of NO from inlet concentration

$=(2\%)(y_1)$

$=(0.002)*(0.01)$

$=0.0002$ mole fraction of NO

For a constant flow rate of gas, the increase in liquid flow rate causes the liquid to fill completely in the packing and stops the liquid flow into the packed area. Based on the literature review the following parameters used to modeling packed column. Hendry's constant m =0.0014 which is taken from the Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry and from the figure 3, flooding factor $K_4 = 0.7$ then K_4 -Flooding factor (0.6 to 0.8); G_m -Gas mass flow rate (kg/sec); L_m -Liquid mass flow rate (kg/sec) and m - Henry's constant.

Let $G_m = 1 \, m^3/_{hr}$

$G_m = 3.383 * 10^{-4} \, Kg/_{sec}$

$$\frac{L_m}{G_m} = \frac{H}{\text{flooding factor}} \quad (1)$$

Substituting the flooding factor and henry's constant in the equation (1)

$L_m = 0.002285 \, Kg/_{sec}$

Converting into the mass function

$L_m = 4.44 \, l/_{hr}$

Hence, the liquid flow rate to the packed column (L_m) is chosen as 5 lph approximately for experimental analysis.

3.3.2. Determination of Packed Column Diameter

Packed column diameter should be optimized and it is calculated for 70% of the flooding velocity to achieve the economic pressure drop and decent liquid and gas distribution [11]. The flooding velocity is calculated by Sherwood correlation which is shown in Figure 3.

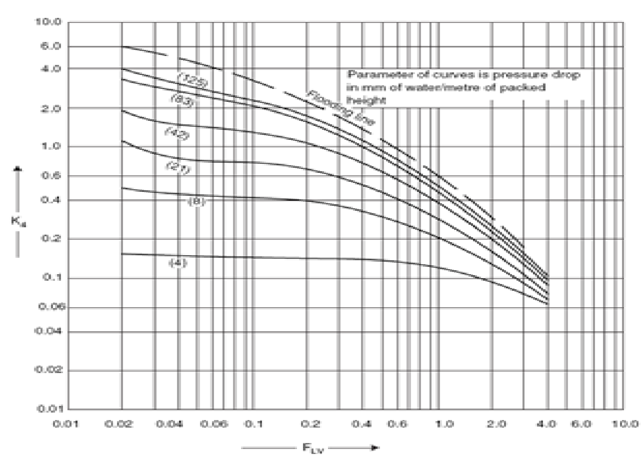

Figure 3: Flooding factor and pressure drop correlation

From the Figure 3, the flooding factor (K_4) is identified for the corresponding pressure drop (F_{LV}) in the packed column and it is used to calculate the column diameter. The pressure drop (F_{LV}) is represented as

$$Abscissa(F_{LV}) = \frac{L_w^*}{V_w^*}\left(\frac{\rho_v}{\rho_L}\right)^{0.5} \quad (2)$$

$$F_{LV} = \frac{L_m}{G_m}\sqrt{\frac{\rho_G}{\rho_L}} \quad (3)$$

where, ρ_G –gas (NO) density (1.21 kg/m^3), ρ_L -liquid (aqueous H_2SO_4) density (1857 kg/m^3), G_m -molar flow rate of gas (0.0003383 kg/sec) and L_m -molar flow rate of liquid (0.002285 kg/sec). By substituting the molar flow rate of liquid and gas and also their corresponding densities in equation (6) then, we get . Thus the calculated pressure drop (F_{LV}) is 0.1724. Another factor to be considered while determining the liquid flow rate into the column is flooding. It is the gas velocity at which the liquid droplets become entrained in the escaping gas stream and it is expressed as

$$K_4 = \frac{mL_m}{G_m} \quad (4)$$

From the flooding factor, the gas mass flow rate / column cross sectional area (V_w^*) is determined and it is expressed as

$$V_w = \left[\frac{K_4\rho_v(\rho_L-\rho_v)}{13.1F_P\left(\frac{\mu_L}{\rho_L}\right)^{0.1}}\right]^{0.5} \quad (5)$$

$$V_w = 2.15\,{}^{Kg}/_{m^2 s}$$

Based on the above parameters, the calculated gas mass flow rate / column cross sectional area (V_w^*) is 2.15 kg/m^{2}s.

The area of the packed column (a) is calculated as

$$A = \frac{G_m}{V_w} \quad (6)$$

$$A = 1.573 * 10^{-3} m^2$$

$$D = 0.0447 \approx 0.045\text{m}$$

Hence the area of the packed column is determined as A=0.001573m^2 and the diameter of the packed column is D= 0.045m

3.3.3. Determination of Packing Height of the Packed Column

The packing height directly refers to the depth of packing material required to do the maximum required removal efficiency. Computation of packed height (Z) of the column is expressed as,

$$Z = H_{OG}\, N^{OG} \quad (7)$$

Where N_{OG} represents the number of transfer units and H_{OG} represents height of transfer units. The number of transfer unit for gas phase is calculated graphically by figure 4 and it is represented as,

$$N_{OG} = \ln \frac{y_1}{y_2} \quad (8)$$

$N_{OG} = 1.6$

Determination of absorption factor (m G_m/L_m)

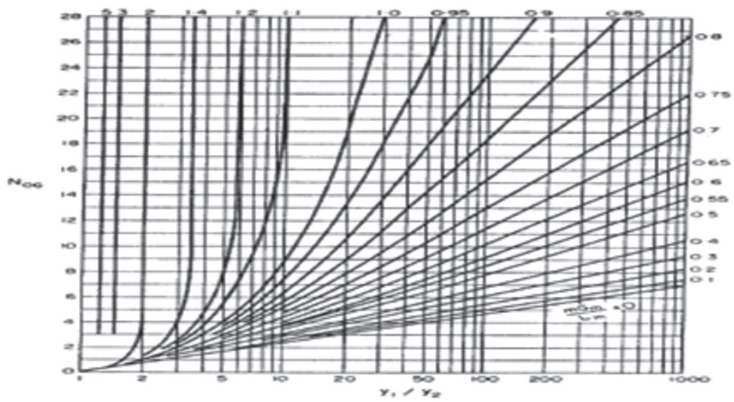

Figure 4: Colburn diagram [11].

Height of the transfer unit is taken between 0.3 to 1.2 m

$$Z = H_{OG} N_{OG} = 1.6 \tag{9}$$

Z = *0.48m*

From these calculated parameters the packed column design has been determined and tabulated in table 3 and its photographic view is shown in figure 5,

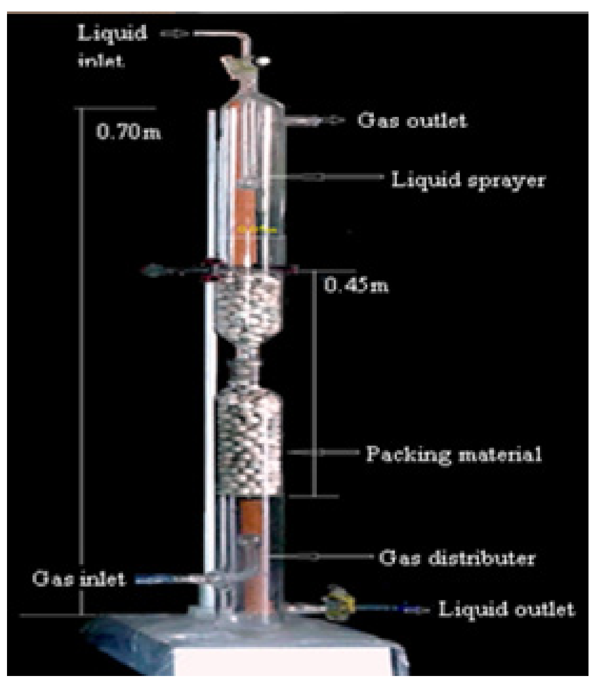

Figure 5: Photographic view of the packed column

Table 3
Calculated parameter of packed column

S. no	*Parameter*	*Calculated value*
1	Liquid flow rate to the packed column	5-10lph
2	Gas flow rate to the packed column	1 m^3/hr
3	Packed column height	0.70m
4	Packed column diameter	0.045m
5	Packed area	0.48m
6	Packing materials	Intalox ceramic saddles with 6 mm diameter
7	Absorbents	$NaClO_2$, H_2O_2, HNO_3, $HNO_3$with added H_2O_2
8	Inlet concentration of NO	100 – 1000 ppm

4. CONCLUSION

The mathematical modeling is carried out to improve the NO_x removal efficiency using the mixed gas analysis. The packed column sizing, packing material, absorbents used were determined for the NO removal process using wet scrubbing process. The mathematical modeling shows that the great removal efficiency was obtained for NO_x removal is by using the hydrogen peroxide as absorbent, which gives more than more efficient removal when externally added to the aqueous HNO_3.

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