MATHEMATICAL MODELING OF A COLUMN PURIFICATION OF WASTE INCINERATION EXHAUST GASES

Wellington Balmant, wbalmant@gmail.com[1]
Ericson Dilay, ericson_dilay@yahoo.com.br[1]
DhyogoMiléo Taher, dhyogomt@gmail.com[1]
Daniela Yumi Sugai, dani_sugai@hotmail.com[1]
André Bellin Mariano, andrebmariano@gmail.com[1]
José Viriato Coelho Vargas, vargasjvcv2@gmail.com[1]

Universidade Federal do Paraná, Caixa Postal 19011, Curitiba, PR, Brasil, CEP:81531-980

Abstract. *Municipal solid waste is a source of various environmental problems such as contamination of soil and underground water sources. Today, in Brazil the alternative most used for disposal of this waste is still using "garbage dumps"(50%), which cause a lot of environmental damage. The other half of the waste is disposed of in landfill (27.7%) or controlled landfill (22.5%). The problem with these waste disposal methods is that contaminated soil area which is unable to be used for other purposes. An alternative to this is the incineration of such waste. But this technique generates a large amount of gaseous chemicals such as sulfur and nitrogen oxides. Thus, a purification of incineration of exhaust gases is necessary. This step is critical in the process optimization and is needed for the process be environmentally and economically viable. The aim of this study is to optimize the purification of the gas output from the incineration of municipal solid waste through mathematical modeling. For this the model depicts a gas purification column counterflow where the gas enters at the bottom of the column and liquid (water or water with addition of sodium hydroxide) at the top. The spine plates have cut in half and arranged alternately causing the liquid and gas move zigzag in the system. The model assumes that the system has two phases: liquid and gas phase. It describes the mass transfer between the liquid and gas phase and chemical reactions occurring in liquid phase where the oxides are transformed into acids. From the model it is possible to find the optimum height of the column and flow of liquid necessary for gas purification according to the flow of the incinerator exhaust gases*.

Keywords*: mass transfer, reaction kinetics,*

1. INTRODUCTION

Conama Resolution No. 316,(MMA, 2002), in which Article 27 states that: “Any and all heat treatment system must have receiver units, storage, supply, gases and particulate emissions treatment, wastewater, ashes and slag treatment.”

Incineration is a thermal treatment that receives lots of criticism due to the potential emissions to the atmosphere. According to Jangsawang,et al., (2005), the optimized conditions for the complete decomposition ensures operation of volatile organic compounds into carbon dioxide, water, oxygen and nitrogen. However, it is needed to point out the potential of carbon dioxide (CO2) as a global climate problem aggravating.

An incineration process cannot exist without being interconnected to a technologically advanced system of gas purification, treatment and recirculation of liquids in the process. The incinerator flue gas carry large amounts of substances in concentrations way above the legally permitted emission limits, (ABNT NBR 11175, 1990), and require physical and chemical treatment to remove and neutralize pollutants from the thermal process.

At this level, carbon sequestration mechanisms can be coupled to the waste incinerator projects as an attempt to obtain a clean design aiming to reduced or even zero emissions. However, as the process is developed, new steps may be investigated and inserted into the complex. Mathematical approaches have significant value, since the mathematical model is a powerful theoretical tool to investigate and reveal opportunities for improvements to optimize hydrogen production. Therefore, a mathematical model of the system should be investigated taking into account the essential system parameters. The objective of this study is to develop and introduce a mathematical model of a treatment and purification column of exhaust gas from the waste burn for energy production.

3. MATHEMATICAL MODEL

The modeled system consists of two phases: gas phase and liquid phase. The gas phase consists of the combustion gases from the incinerator. The components considered relevant in the gas phase are carbon dioxide, nitrogen dioxide and sulfur dioxide. All other components of the gas phase were considered inert. The choice of these compounds is due to their environmental importance, as they can cause environmental problems. In liquid phase components considered in the mass balance were carbon dioxide, nitrogen dioxide, sulfur dioxide, bicarbonate ion, nitrate ion, sulfate ion and proton concentration in the liquid phase.

As can be seen in Figure 1, the gas inlet is at the bottom of the system and fluid inlet is at the top. Thus, the flows are countercurrent where the gas goes up by contacting the liquid that goes down. Thus there is a mass transfer across the non-inert components of the gas phase to the liquid phase. It is precisely this transfer that will reduce the concentration of pollutants in the gas phase purifying the gas exhaust. In this model mass transfer between the phases was modeled as obeying Henry's law.

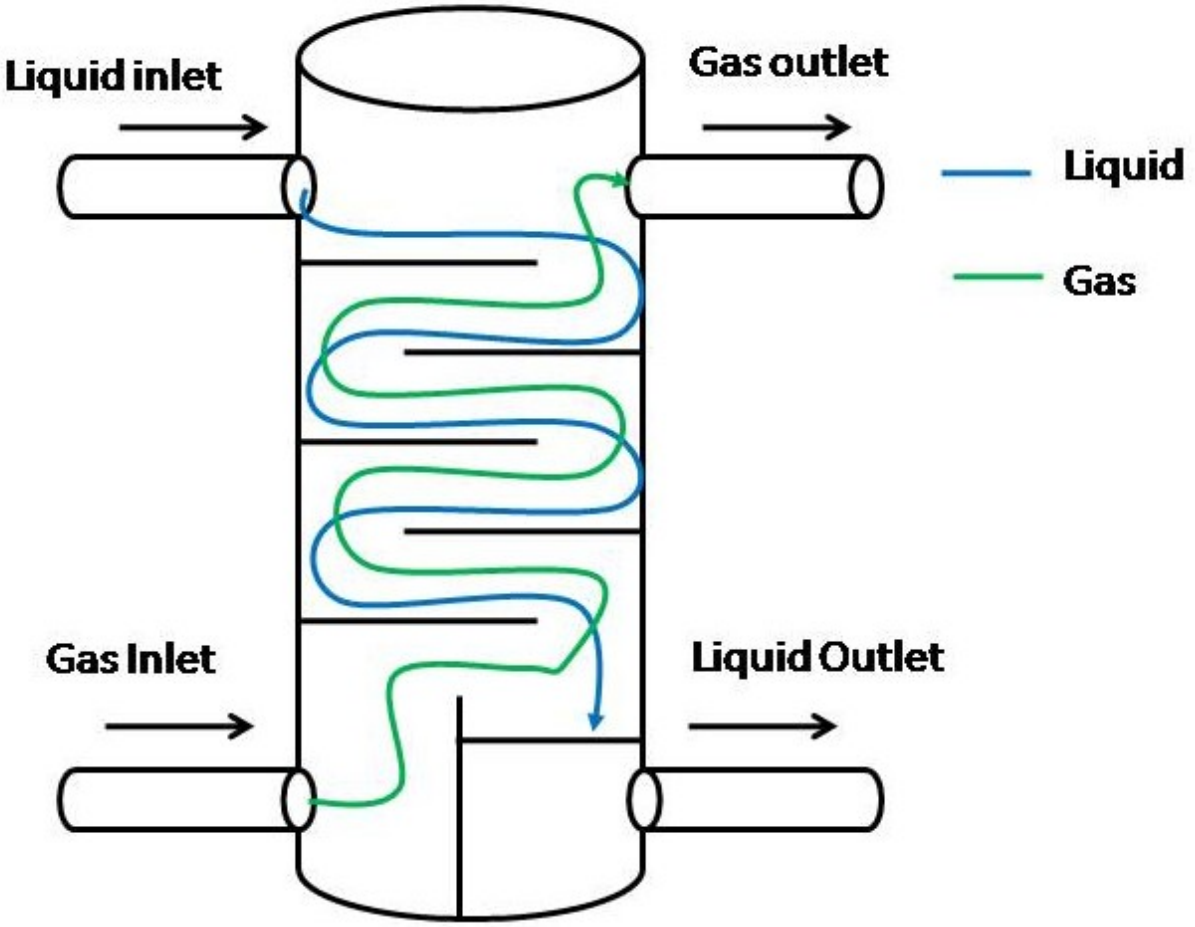

Figure 1. Diagram of modeled system.

Furthermore, there is in the liquid phase chemical reactions that convert the oxides absorbed in the liquid phase acids which release protons. These reactions can be described on Eq.(1), Eq.(2) and Eq.(3) as:

$$CO_2 + H_2O \xrightarrow{k_{co2}} HCO_3^- + H^+ \tag{1}$$

$$NO_3 + H_2O \xrightarrow{k_{no2}} NO_3^- + H^+ \tag{2}$$

$$SO_2 + H_2O \xrightarrow{k_{so2}} SO_3^{-2} + 2H^+ \tag{3}$$

The system has a total of 10 components, $[CO_2]_{aq}$, $[CO_3]_{aq}$, $[NO_2]_{aq}$, $[NO_3]_{aq}$, $[SO_2]_{aq}$, $[SO_3]_{aq}$, $[H^+]_{aq}$, $[CO_2]_{gas}$, $[NO_2]_{gas}$, $[SO_2]_{gas}$. The mass balance for this components on volume control 1 (VC1) is described on Eq.(4), Eq.(5), Eq.(6), Eq.(7), Eq.(8), Eq.(9), Eq.(10), Eq.(11), Eq.(12) and Eq.(13) as :

$$\frac{d[CO_2]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[CO_2]_{aq1}\right) + kla_{CO2} \times \left([CO_2]_{gas,1} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,1}\right) - k_{CO2} \times [CO_2]_{aq,1} \tag{4}$$

$$\frac{d[HCO_3^-]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[HCO_3^-]_{aq1}\right) + k_{CO2} \times [CO_2]_{aq,1} \tag{5}$$

$$\frac{d[NO_2]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[NO_2]_{aq1}\right) + kla_{NO2} \times \left([NO_2]_{gas,1} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,1}\right) - k_{NO2} \times [NO_2]_{aq,1} \tag{6}$$

$$\frac{d[NO_3^-]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[NO_3^-]_{aq1}\right) + k_{NO2} \times [NO_2]_{aq,1} \tag{7}$$

$$\frac{d[SO_2]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[SO_2]_{aq1}\right) + kla_{SO2} \times \left([SO_2]_{gas,1} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,1}\right) - k_{SO2} \times [SO_2]_{aq,1} \tag{8}$$

$$\frac{d[SO_3^-]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left(-[SO_3^-]_{aq,1}\right) + k_{SO2} \times [SO_2]_{aq,1} \tag{9}$$

$$\frac{d[H^+]_{aq,1}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([H^+]_{ini} - [H^+]_{aq,1}\right) + k_{CO2} \times [CO_2]_{aq,1} + k_{NO2} \times [NO_2]_{aq,1} + k_{CO2} \times [CO_2]_{aq,1} + k_{SO2} \times [SO_2]_{aq,1} \tag{10}$$

$$\frac{d[CO_2]_{gas,1}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([CO_2]_{gas,2} - [CO_2]_{gas,1}\right) - kla_{CO2} \times \left([CO_2]_{gas,1} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,1}\right) \tag{11}$$

$$\frac{d[NO_2]_{gas,1}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([NO_2]_{gas,2} - [NO_2]_{gas,1}\right) - kla_{NO2} \times \left([NO_2]_{gas,1} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,1}\right) \tag{12}$$

$$\frac{d[SO_2]_{gas,1}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([SO_2]_{gas,2} - [SO_2]_{gas,1}\right) - kla_{SO2} \times \left([SO_2]_{gas,1} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,1}\right) \tag{13}$$

As can be seen in figure 2 in VC1 the water enters on column without any trace of contaminant oxides and in pH 7. In the gas phase (VC1) the gases are directed out of the column through a chimney. The percentage of treatment of oxide in flue gases can be calculated as:

$$\%CO_2 = \left(1 - \frac{[CO_2]_{aq,1}}{[CO_2]_{ent}}\right) \times 100 \tag{14}$$

$$\%NO_2 = \left(1 - \frac{[NO_2]_{aq,1}}{[NO_2]_{ent}}\right) \times 100 \tag{15}$$

$$\%SO_2 = \left(1 - \frac{[SO_2]_{aq,1}}{[SO_2]_{ent}}\right) \times 100 \tag{16}$$

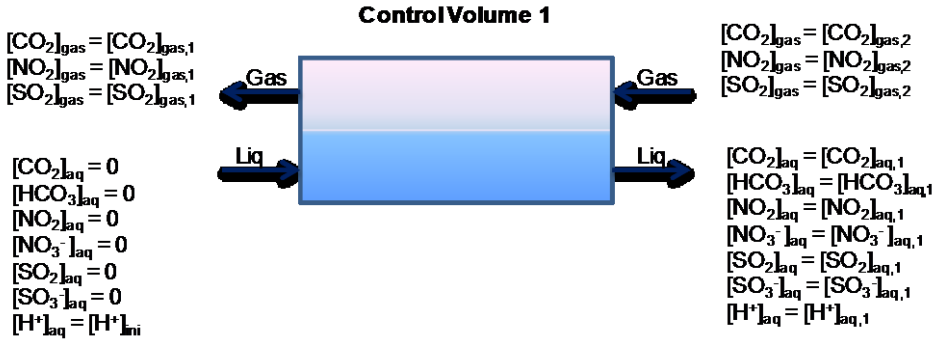

Figure 2. Diagram of control volume 1.

The mass balance for this components on intermediary volume controls i (VCi) is described on Eq.(17), Eq.(18), Eq.(19), Eq.(20), Eq.(21), Eq.(22), Eq.(23), Eq.(24), Eq.(25) and Eq.(26) as

$$\frac{d[CO_2]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([CO_2]_{aq,i-1} - [CO_2]_{aq,i} \right) +$$

$$kla_{CO2} \times \left([CO_2]_{gas,i} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,i} \right) - k_{CO2} \times [CO_2]_{aq,i} \quad (17)$$

$$\frac{d[HCO_3^-]_i}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([HCO_3^-]_{aq,i-1} - [HCO_3^-]_{aq,i} \right) + k_{CO2} \times [CO_2]_{aq,i} \quad (18)$$

$$\frac{d[NO_2]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([NO_2]_{aq,i-1} - [NO_2]_{aq,i} \right)$$

$$+kla_{NO2} \times \left([NO_2]_{gas,i} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,i} \right) - k_{NO2} \times [NO_2]_{aq,i} \quad (19)$$

$$\frac{d[NO_3^-]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([NO_3^-]_{aq,i-1} - [NO_3^-]_{aq,i} \right) + k_{NO2} \times [NO_2]_{aq,i} \quad (20)$$

$$\frac{d[SO_2]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([SO_2]_{aq,i-1} - [SO_2]_{aq,i} \right)$$

$$+kla_{SO2} \times \left([SO_2]_{gas,i} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,i} \right) - k_{SO2} \times [SO_2]_{aq,i} \quad (21)$$

$$\frac{d[SO_3^-]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([SO_3^-]_{aq,i-1} - [SO_3^-]_{aq,i} \right) + k_{SO2} \times [SO_2]_{aq,i} \quad (22)$$

$$\frac{d[H^+]_{aq,i}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([H^+]_{aq,i-1} - [H^+]_{aq,i} \right) + k_{CO2} \times [CO_2]_{aq,i} + k_{NO2} \times [NO_2]_{aq,i} + k_{CO2} \times [CO_2]_{aq,i} + k_{SO2} \times [SO_2]_{aq,i} \quad (23)$$

$$\frac{d[CO_2]_{gas,i}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([CO_2]_{gas,i+1} - [CO_2]_{gas,i} \right) - kla_{CO2} \times \left([CO_2]_{gas,i} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,i} \right) \quad (24)$$

$$\frac{d[NO_2]_{gas,i}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([NO_2]_{gas,i+1} - [NO_2]_{gas,i} \right) - kla_{NO2} \times \left([NO_2]_{gas,i} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,i} \right) \quad (25)$$

$$\frac{d[SO_2]_{gas,i}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([SO_2]_{gas,i+1} - [SO_2]_{gas,i} \right) - kla_{SO2} \times \left([SO_2]_{gas,i} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,i} \right) \quad (26)$$

As can be seen on Fig. 3 on intermediate volume controls (VCi), there is a inlet and a outlet flux. The flux of liquids and gas are counter-current. All intermediate volume controls follow the same pattern.

The mass balance for this components on intermediary on the last volume controls (VCn) is described on Eq.(27), Eq.(28), Eq.(29), Eq.(30), Eq.(31), Eq.(32), Eq.(33), Eq.(34), Eq.(35) and Eq.(36) as

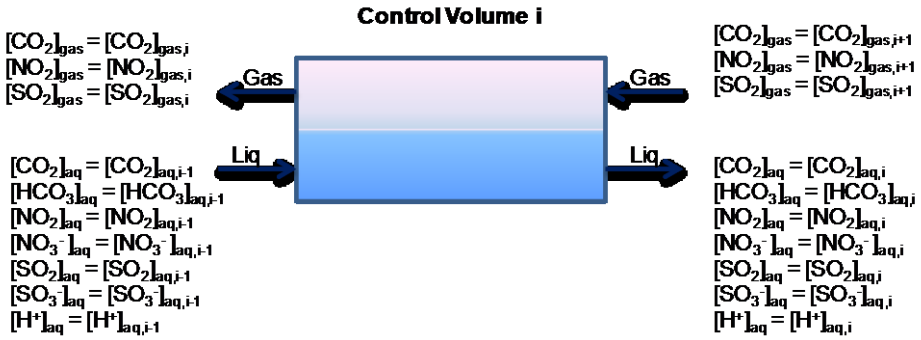

Figure 3. Diagram of control volume i.

$$\frac{d[CO_2]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([CO_2]_{aq,n-1} - [CO_2]_{aq,n} \right) +$$

$$kla_{CO2} \times \left([CO_2]_{gas,n} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,n} \right) - k_{CO2} \times [CO_2]_{aq,n} \quad (27)$$

$$\frac{d[HCO_3^-]_n}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([HCO_3^-]_{aq,n-1} - [HCO_3^-]_{aq,n} \right) + k_{CO2} \times [CO_2]_{aq,n} \quad (28)$$

$$\frac{d[NO_2]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([NO_2]_{aq,n-1} - [NO_2]_{aq,n} \right) +$$

$$kla_{NO2} \times \left([NO_2]_{gas,n} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,n} \right) - k_{NO2} \times [NO_2]_{aq,n} \quad (29)$$

$$\frac{d[NO_3^-]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([NO_3^-]_{aq,n-1} - [NO_3^-]_{aq,n} \right) + k_{NO2} \times [NO_2]_{aq,n} \quad (30)$$

$$\frac{d[SO_2]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([SO_2]_{aq,n-1} - [SO_2]_{aq,n} \right) + kla_{SO2} \times \left([SO_2]_{gas,n} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,n} \right) - k_{SO2} \times [SO_2]_{aq,n} \quad (31)$$

$$\frac{d[SO_3^-]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([SO_3^-]_{aq,n-1} - [SO_3^-]_{aq,n} \right) + k_{SO2} \times [SO_2]_{aq,n} \quad (32)$$

$$\frac{d[H^+]_{aq,n}}{dt} = \frac{Q_{liq}}{V_{liq}} \times \left([H^+]_{aq,n-1} - [H^+]_{aq,n} \right) + k_{CO2} \times [CO_2]_{aq,n} + k_{NO2} \times [NO_2]_{aq,n} + k_{CO2} \times [CO_2]_{aq,n} + k_{SO2} \times [SO_2]_{aq,n} \quad (33)$$

$$\frac{d[CO_2]_{gas,n}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([CO_2]_{ent} - [CO_2]_{gas,n} \right) - kla_{CO2} \times \left([CO_2]_{gas,n} \times R \times Temp \times H_{CO2} - [CO_2]_{aq,n} \right) \quad (34)$$

$$\frac{d[NO_2]_{gas,n}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([NO_2]_{ent} - [NO_2]_{gas,n} \right) - kla_{NO2} \times \left([NO_2]_{gas,n} \times R \times Temp \times H_{NO2} - [NO_2]_{aq,n} \right) \quad (35)$$

$$\frac{d[SO_2]_{gas,n}}{dt} = \frac{Q_{gas}}{V_{liq}} \times \left([SO_2]_{ent} - [SO_2]_{gas,n} \right) - kla_{SO2} \times \left([SO_2]_{gas,n} \times R \times Temp \times H_{SO2} - [SO_2]_{aq,n} \right) \quad (36)$$

As can be seen on Fig. 4 on the last volume control (VCn), there is a entrance of flue gases and the exit o liquid flow.

In the model simulations the parameters were variable within a range, thus seeking to make a parametric evaluation of the model. The evaluated parameters were the mass transfer coefficients, the number of control volumes and the reaction constant. The values of the parameters fixed and varied are shown in Table 1. The model was implemented in FORTRAN, using the Runge-Kutta method of 4th order with integration step 10^{-6} hours. The results are shown when the system reaches the steady state.

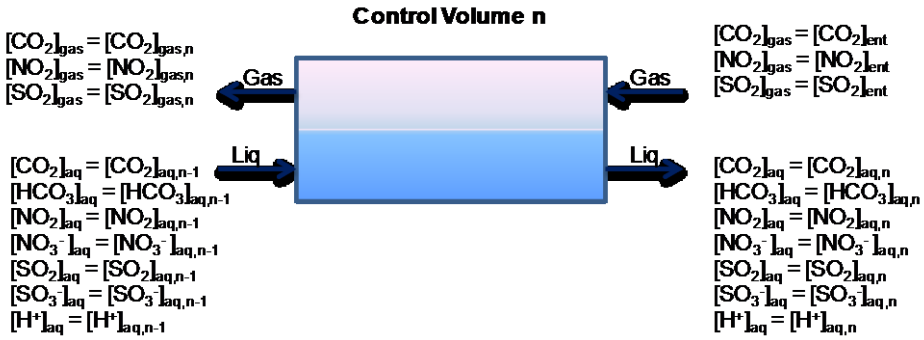

Figure 4. Diagram of control volume n.

Table 1. Parameters utilized on modelsimulation.

Parameters	Description	Value
Q_{gas}	Volumetricflow rate ofgas	175000 [$L.h^{-1}$]
Q_{liq}	Volumetricflow rate ofliquid	5000 [$L.h^{-1}$]
V_{liq}	Gas volume in volume control	40 [L]
$V_{gás}$	Liquid volume in the volume control	10 [L]
kla_{CO2}	CO_2masstransfercoefficient	10 - 10000 [h^{-1}]
kla_{NO2}	NO_2masstransfercoefficient	10 - 10000[h^{-1}]
kla_{SO2}	SO_2masstransfercoefficient	10 - 10000 [h^{-1}]
H_{CO2}	Henry Constant (CO_2)	3.4×10^{-2}[h^{-1}]
H_{NO2}	Henry Constant (NO_2)	2.4×10^{-2}[h^{-1}]
H_{SO2}	Henry Constant (SO_2)	1.2 [h^{-1}]
R	Gas constant	8.205×10^{-2}[h^{-1}]
Temp	System temperature	300 [K]
k_{CO2}	Constant reaction (CO_2)	0.01 - 10 [h^{-1}]
k_{NO2}	Constant reaction (NO_2)	0.01 - 10[h^{-1}]
k_{SO2}	Constant reaction (SO_2)	0.01 - 10[h^{-1}]
$[CO_2]_{ent}$	Molar concentration of CO_2 in the inlet gas	5×10^{-3} [mol.L^{-1}]
$[NO_2]_{ent}$	Molar concentration of NO_2 in the inlet gas	8×10^{-6} [mol.L^{-1}]
$[SO_2]_{ent}$	Molar concentration of SO_2 in the inlet gas	4×10^{-6}[mol.L^{-1}]
$[H^+]_{ent}$	Concentration of protons	1×10^{-7}[mol.L^{-1}]
N	Number of control volume	5 - 20

3. RESULTS

The main results of simulations are presented in Figs. 5, 6 and 7. As can been seen the percentage of treatment is strongly dependent of the value of mass transfer coefficient. Particularly with respect to nitrogen dioxide which is treated only effectively when the mass transfer coefficient is close to 10000 (h^{-1}). To achieve a high values to mass transfer coefficient is necessary to have a great area, because kla depends on area. So in the project of a column of flue gases purification the area of column is a parameter of extreme importance. Other factor that influence the performance of purification is the number of volume control. With more volume control, more taller the column and more efficient in treatment. For example, with N=5 the efficiency of treatment to NO2 is 69% with a kla of 10000 (h^{-1}), while with N=20 the efficiency is 99% with a kla of 10,000 (h^{-1}). These are the two most influent parameters in this study. Another thing important to note is that CO2 is unfeasible in this type of system. In best case scenario the percentage of treatment is just 3,5%. Another thing that has a little effect is the pH of the system that change a little under the treatment. The value of pH was 3,38 in worst case scenario. The difficulty here is to treat this water with some type of basic compound to possibility the recirculation of water. The model proposed in this work must be experimental validated to calibrate the

parameters with precision. The reaction kinetic (k_{NO2}, k_{CO2} e k_{SO2}) has no effect on purification, at least in the range tested in this work.

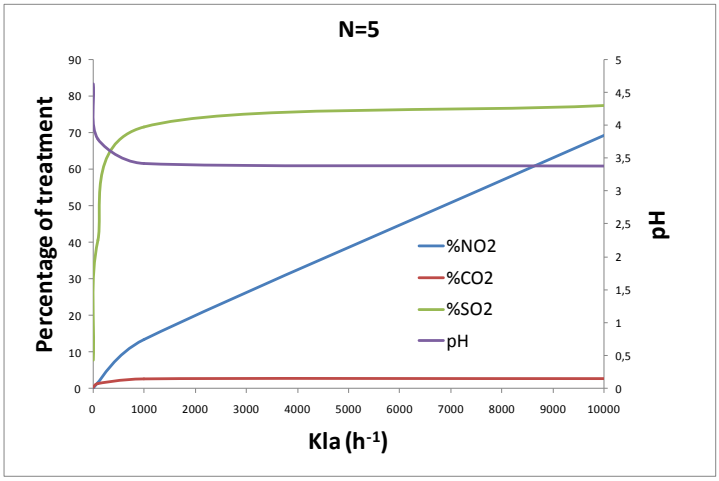

Figure 5. Percentage of treatment in function of mass transfer coefficients for 5 volume control (N=5)

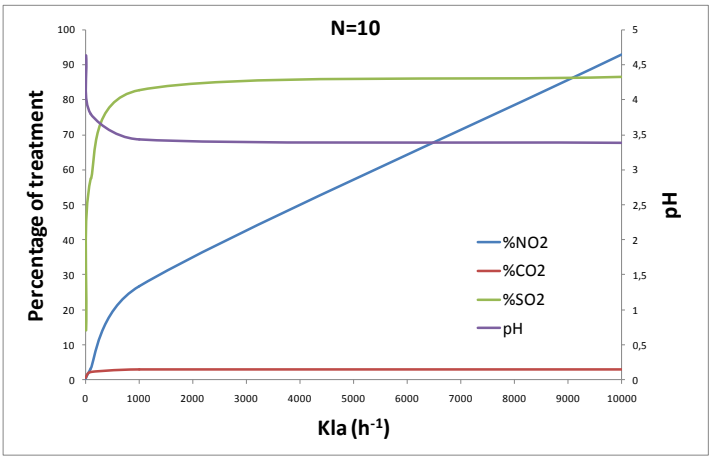

Figure 6. Percentage of treatment in function of mass transfer coefficients for 10 volume control (N=10)

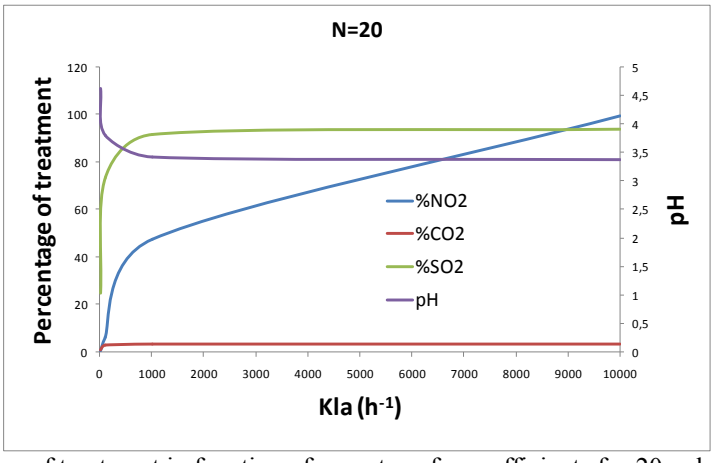

Figure 7. Percentage of treatment in function of mass transfer coefficients for 20 volume control (N=20)

4. CONCLUSION

The model is capable to predict the effect of various parameters on the performance of purification column. The effect of mass transfer coefficient is the most important parameter on design of the column. The must be experimental valited.

5. REFERENCES

ABNT, 1990. ABNT-NBR-11175 regulation. 01 July 2016.
http://www.ambientall.com.br/ambientall_trata/downloads/Norma-ABNT-NBR-11175.pdf

Jangsawang, W., Fungtammasan, B., Kerdsuwan, S., 2015. "Effects of operating parameters on the combustion of the medical waste in a controlled air incinerator". Energy Conversion and Management Vol. 46, p. 3137.

MMA, 2002. “Conama Resolution No 316”. 29 May
2015.http://www.mma.gov.br/port/conama/legiabre.cfm?codlegi=338

6. RESPONSIBILITY NOTICE

The following text, properly adapted to the number of authors, must be included in the last section of the paper: The authors are the only responsible for the printed material included in this paper.