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Dynamic modeling and simulation of CO_2 chemical absorption process for coal-fired power plants

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Abstract

Post combustion capture via chemical absorption is viewed as the most mature CO_2 capture technique. The effects of the addition of CO_2 chemical absorption process on power plant performance have been studied using various steady-state models. However, there are several gaps in the understanding of the impact of post combustion capture on the operability of the power plant. These questions could be addressed by studying the dynamic behavior of such plants. In this study, dynamic models of the CO_2 chemical absorption process were developed and validated. Dynamic analyses of the process reveal that absorber performance is sensitive to L/G ratio and that changes in reboiler duty significantly affect the regenerator performance.

Keywords: Post combustion, CO_2 capture, Chemical absorption, dynamic modeling.

1. Introduction

Power generation from fossil fuel-fired power plants is the largest single source of CO_2 emissions [1]. With growing concerns about the environmental impact of such plants, effective CO_2 emission abatement strategies such as Carbon Capture and Storage (CCS) are required for their continued use. One approach to CCS is post combustion capture which involves the separation of CO_2 from the flue gas stream after combustion occurs. Chemical absorption is well suited for separating CO_2 from streams with low concentration of CO_2.

Chemical absorption involves the reaction of CO_2 with a chemical solvent to form a weakly bonded intermediate compound which may be regenerated with the application of heat [2]. Figure 1 describes one of the most popular technologies proposed for post combustion capture. The facility consists of two main units – the absorber and regenerator. Several studies have shown that the energy requirement for solvent regeneration would have adverse effects on power plant efficiency [3]. However, there are several gaps in the understanding of the impact of post combustion capture on the operability of the power plant. For instance, would such power plants be able to effectively operate at varying loads or what modifications are required during start-up [4]? These questions can be addressed by studying the dynamic behaviour of such plants. To achieve this, accurate dynamic models of the power plant and the CO_2 capture facility are required.

2. Developments in modeling chemical absorption of CO_2

Post combustion capture with MEA is a reactive absorption process. Two main phenomena are involved: mass transfer of CO_2 from the bulk vapour to the liquid

solvent and the chemical reaction between CO_2 and the solvent. A number of studies have employed steady state models of the chemical (or reactive) absorption process at different levels of complexity. Kenig et al describes the different levels of complexity of these models [5]. The equilibrium-based approach assumes theoretical stages in which liquid and vapour phases attain equilibrium while the rate-based approach estimates actual mass transfer rates. These models may assume the reactions are at equilibrium or may consider the reaction kinetics. Reaction kinetics could be considered by including an enhancement factor to estimate actual absorption rates (with chemical reactions) from known physical absorption rates. Otherwise, reaction kinetics could be modelled directly [5].

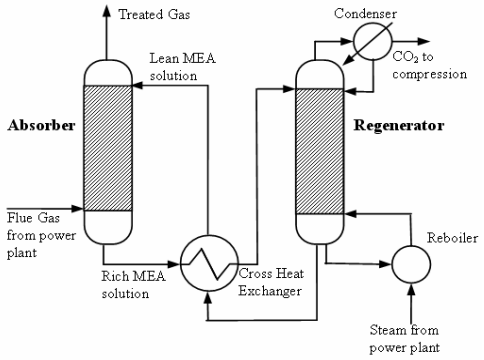


Figure 1 Chemical absorption process for post combustion capture from [4]

The dynamic behavior of the CO_2 absorption process for post combustion capture using MEA has not been extensively studied. Kvamsdal et al considered the dynamic simulation of only the absorber of the process using dynamic models of reduced complexity and also assumed a constant value for the heat of absorption of CO_2 and vaporization of water [4]. Lawal et al considered the dynamic simulation of only the absorber. Mass transfer was based on Maxwell-Stefan formulation and expressions were developed for the heat of absorption of CO_2 [6]. This paper extends the study to the simulation and analysis of both absorber and regenerator columns.

3. Model Development

This section describes the model development of the absorber and regenerator using the rate-based approach for mass transfer. The physical property method used for both approaches is the Electrolyte Non-random-two-liquid (NRTL) model. MEA electrolyte solution chemistry is used to predict the equilibrium mass fractions in the liquid and vapour phases [7]. Mass transfer is described using the two-film theory (Figure 2) using the Maxwell-Stefan formulation. Heat and mass transfer resistances are modelled in the liquid and vapour films. The rate-based model was developed from the Gas-Liquid Contactor model in Process Systems Enterprise's[1] Advanced Model Library using their process modelling tool, gPROMS. Modifications made include the diffusivity (χ) of CO_2 in the liquid phase which was based on expressions provided by Vaidya et al [8]. The diffusivity (χ) of CO_2 and other components in the vapour phase was estimated using the Fuller's equation [9]. Mass transfer coefficients in the liquid and vapour films were determined by correlations given by Onda et al [10]. Expressions for the heat of absorption and the heat lost to the surrounding were obtained from literature [11,12].

[1] Process Systems Enterprise (PSE) Ltd.

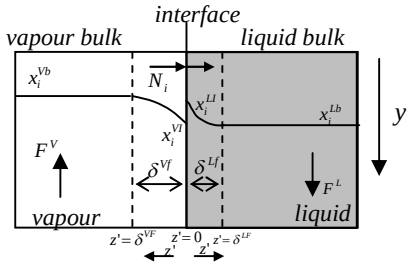


Figure 2 Liquid and vapour bulks, films and interface

3.1. Model Assumptions

The following assumptions were used in developing this dynamic model:

- Plug flow regime and linear pressure drop along the column
- Phase equilibrium at interface between liquid and vapour films
- Negligible solvent degradation

3.2. Model Equations

Mass Balance: $$\frac{dM_i}{dt} = \frac{-1}{L \cdot A}\frac{\partial F_i^L}{\partial y} + N_i \cdot Sp \cdot MW_i \cdot \omega \quad (1)$$

Energy Balance: $$\frac{dU}{dt} = \frac{-1}{L \cdot A}\frac{\partial F_H^L}{\partial y} + Sp \cdot \omega\left(H_{liq}^{cond} + H_{liq}^{conv} + H_{abs}\right) + HL \quad (2)$$

Heat of absorption (or desorption): $$H_{abs} = N_{CO_2} \times h_{abs} \quad (3)$$

Maxwell-Stefan formulation: $$\frac{1}{\delta}\frac{\partial x_i^M}{\partial z'} = \frac{1}{c_t}\sum_{k=1}^{n}\left(\frac{x_i^M N_k - x_k^M N_i}{\chi_{i,k}}\frac{\mu^R}{\mu}\frac{T}{298.15}\right) \quad (4)$$

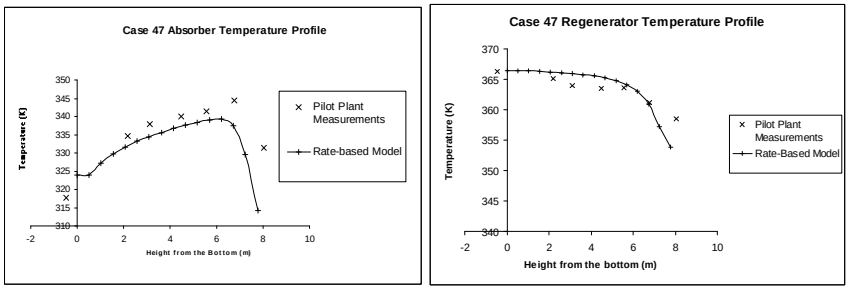
The physical property estimation models were set up in Aspen Properties through the CAPE-OPEN Thermo interface.

4. Model Validation

The models developed were validated using data from a pilot plant study [12]. Both absorber and regenerator columns of the pilot plant are packed columns with diameters of 0.427m and total packing heights of 6.1m [12]. Out of the 48 experimental cases carried out in the study, two cases (Cases 32 and 47) were selected for steady state validation purposes. These two cases were selected because of their relatively high and low liquid to gas (L/G) ratios respectively. Simulation results were validated using the temperature profile of both columns measured in the pilot plant [12]. Both columns were simulated separately for validation. In addition the measured CO_2 loading of the amine solvent taken at different positions was compared with values obtained from simulation.

4.1. Case 47

This case involved a relatively low liquid to gas (L/G) ratio in the absorber thus a lower CO_2 capture level. Because of the reported inaccuracy in the flue gas flow measurement [4,12], its value was adjusted to match reported capture levels (Table 1). The temperature profiles in the absorber and regenerator were used to validate the two models as shown in Figure 3(a) and (b). The rate-based model gives fairly good predictions of temperature profiles.

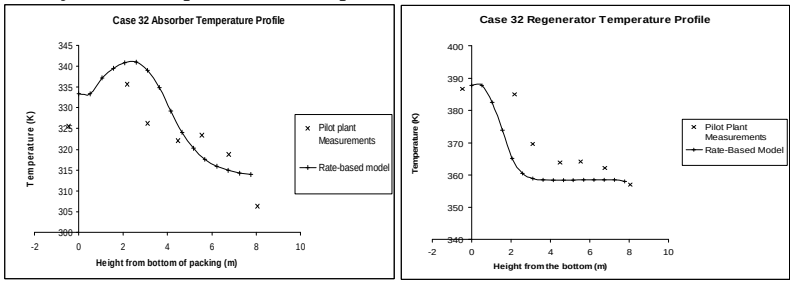


(a) (b)

Figure 3 (a) Absorber and (b) Regenerator temperature profile for Case 47

4.2. Case 32

This case involved a relatively high liquid to gas (L/G) ratio thus a high CO_2 capture level. The inlet flue gas flow rate to the absorber was reduced by about 15% to give better predictions of the temperature profile (Figure 4a). However, this change implies higher CO_2 capture levels than what was measured in the pilot plant (Table 1). This discrepancy may be due to the assumption that the reactions between CO_2 and MEA are at equilibrium as calculated by the electrolyte solution chemistry. Kinetically controlled reactions may therefore provide better predictions of the trend.



(a) (b)

Figure 4(a) Absorber and (b) Regenerator temperature profile for Case 32

Table 1 Comparing CO_2 loading at various locations measured in pilot plant and predicted by rate-based model

	Case 32		Case 47	
	Pilot Plant	Rate Model	Pilot Plant	Rate Model
Absorber Capture Level (%)	95	99.5	69	69.2
Absorber rich MEA loading (mol CO_2/mol MEA)	0.428	0.456	0.539	0.487
Regenerator lean MEA loading (mol CO_2/mol MEA)	0.272	0.260	0.286	0.262

5. Dynamic Analysis

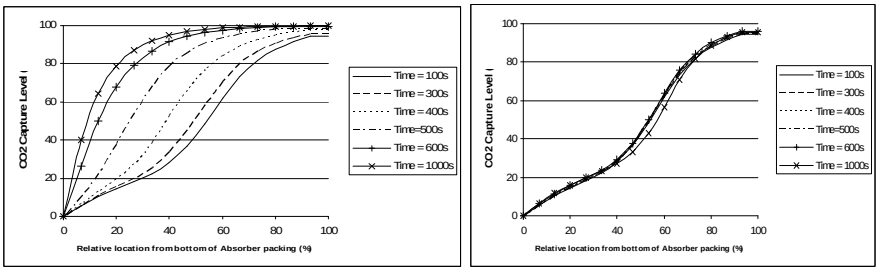
These analyses consider the effect of disturbances on the performance of the columns.

5.1. Reducing Power Plant Load

A 50% reduction in power plant load occurs. Two cases were considered:

- Case-A: Change of flue gas flow rate without changing liquid (solvent) flow rate
- Case-B: Change of flue gas flow rate with corresponding decrease in liquid solvent rate to maintain CO_2 capture level

In Case A, the process was simulated with the base-load conditions (Case 32) for three minutes after which the above changes were implemented in ten minutes. Finally conditions were maintained for eight minutes. From Figure 5a, the 100s curve represents the profile before dropping load. The other curves show a trend of increasing absorption levels with time. Since the flue gas flow rate is ramped down with time while the solvent flow rate is constant, an increase in L/G ratio occurs. In Case B, by reducing the lean solvent feed rate correspondingly (by 50%), roughly the same capture level (Figure 5b) could be maintained through the period of change. This suggests that the absorption process is more sensitive to the L/G (liquid solvent to flue gas) ratio than their actual flow rates. Since the amount of steam required for regeneration corresponds to the amount of lean MEA circulated, the energy requirement of the regenerator could be correspondingly reduced.



(a) Case A (b) Case B

Figure 5(a) and (b) Reducing Power Plant Load

5.2. Reducing Regenerator Reboiler Duty

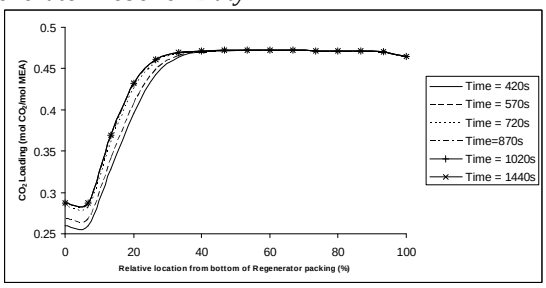


Figure 6 Changes in CO_2 loading profile in regenerator with reducing reboiler duty

The regenerator was simulated with the base-load conditions (Case 32) for seven minutes. A 10% reduction in reboiler duty was implemented over five minutes. Conditions were maintained for 12 minutes. Significant changes in the CO_2 loading profile are observed from the start of the disturbance (time = 420s) onwards especially towards the bottom of the column where CO_2 loading increases (Figure 6). The lean MEA solvent to the absorber would therefore have reduced absorption capacity.

6. Conclusions

This paper presents a study of CO_2 capture using chemical absorption based on the dynamic modelling of the process. Validation results show that the model predicts the absorber and regenerator temperature profiles and CO_2 loadings fairly well. Dynamic analyses show that the absorber performance is more sensitive to the L/G ratio than the actual flow rates of the solvent and flue gas. The performance of the regenerator is significantly affected by the reboiler duty.

Nomenclature

A	Cross sectional area (m^2)	μ	Viscosity (Pa.s)
c_t	Total molar concentration (mol/m^3)	ω	Wetted area ratio
F_i	Component mass flow rate (kg/s)	χ	Diffusivity (m^2/s)
F_H	Enthalpy flow rate (J/s)	*Subscripts*	
H	Heat flux (J/m^2)	*abs*	Absorption
h	Specific Enthalpy (J/kg)	*H*	Enthalpy
HL	Heat loss to surroundings (J/m^2)	*i*	Component number
L	Length of column section (m)	*Liq*	Liquid
L/G	Liquid to gas	*Vap*	Vapour
M	Mass Holdup (kg/m^3)	*Superscripts*	
MW	Molecular weight (kg/mol)	*Cond*	Conduction
N	Molar flux ($mol/m^2.s$)	*Conv*	Convection
n	Number of components	*I*	Interface
Sp	Specific area (m^2/m^3)	*L*	Liquid
U	Energy Holdup (J/m^3)	*Lb*	Liquid bulk
x	Mass fraction	*Lf*	Liquid film
x_i^M	Molar fraction	*R*	Reference
y	Axial position	*V*	Vapour
z'	Film position	*Vb*	Vapour bulk
Greek Symbols		*Vf*	Vapour film
δ	Film thickness (m)		

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