Dynamic Modelling and Validation of Post Combustion CO_2 Capture Plant

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Introduction

Carbon capture and sequestration has been identified as an important technology by the International Energy Agency that can be used to meet greenhouse gas emission reduction targets. Post-combustion CO_2 capture process, which is the most technologically mature approach, would increase the cost of electricity by 80%, reduce power plant efficiency by 30%, increase water consumption and introduce operability challenges, when it is integrated to a coal-fired power plant. The cost of deploying a demonstration plant to investigate these challenges is estimated to reach $1 Billion, which makes modelling and simulation a viable alternative.

Figure 1: Pilot plant, University of Texas at Austin

Approach To Problem

The complexity of modelling packed columns in a capture plant depends on the extent to which the phenomena of mass transfer and chemical reaction are handled. With MEA solvent, the rate of chemical reactions is very fast, compared to rate of mass transfer. Therefore, a rate-based dynamic model using the two-film theory is developed in gPROMS® advanced modelling environment, with chemical reactions assumed to be in equilibrium. The model is validated dynamically with pilot plant data.

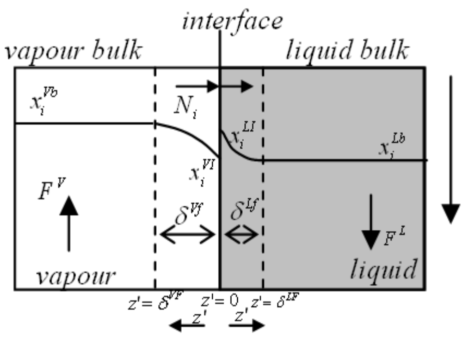

Figure 2: Schematics of Two-Film Theory

CO_2 capture plant models have previously been validated at steady-state, predicting process performance at various operating points. Yet, it is not clear how fast/slow the process will move from one steady-state to another. This is the first successful attempt at a dynamic validation of a capture plant model. The primary benefit such is that it can provide an accurate real-time representation of the process, which can form the basis of an operability study.

Model Development

The following continuity equations are imposed upon the bulk liquid and bulk vapour phases:

Material Balance: $$\frac{dM_i}{dt} = \frac{-1}{A}\frac{\partial F_i}{\partial y} + N_i \cdot MW_i \cdot Sp \cdot \omega$$

Energy Balance: $$\frac{dU}{dt} = \frac{-1}{A}\frac{\partial F_H}{\partial y} + Sp \cdot \omega \cdot \left(H^{cond} + H^{conv}\right)$$

The Maxwell-Stefan formulation is used to describe diffusion of components across the vapour and liquid films:

$$\frac{1}{\delta}\frac{\partial x_i^M}{\partial z} = \frac{1}{c_t}\sum_{k=1}^{n}\left(\frac{x_i^M N_k - x_k^M N_i}{\chi_{i,k}}\frac{\mu^R}{\mu}\frac{T}{298.15}\right)$$

Film material continuity: $$\frac{1}{\delta}\frac{\partial N_i}{\partial z} = 0$$

Notable model assumptions and descriptions:

- Phase equilibrium at interface between liquid and vapour films.
- Reactions are assumed to attain chemical equilibrium at the interface.
- The chemical equilibrium is defined by ElecNRTL Activity Coefficient Model in Aspen Properties.
- No material accumulation in the liquid film, the vapour film and the bulk vapour.
- Film mass transfer coefficients and packing wetted area are described by Onda correlations.
- Heat of Absorption is determined via equations derived from tests at the University of Texas.

Dynamic Validation of Model

Case 1 – Conventional Process

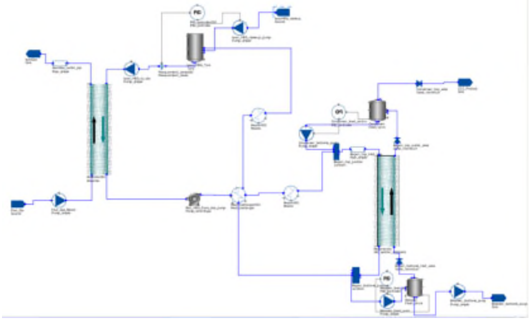

Figure 3: Case 1 Model Topography

Process Inputs and disturbances tracked include:

- Slow decrease in absorber lean solvent flow rate.
- Fluctuating CO_2 Composition of inlet flue gas.
- Increase in the temperature of inlet flue gas.

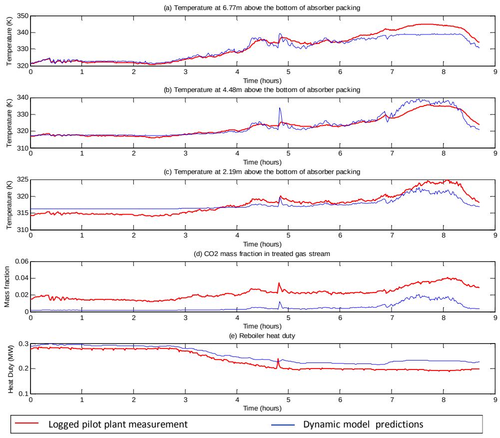

Figure 4: Case 1 Plant and Model Response Comparison

Case 2 – Intercooled Absorber

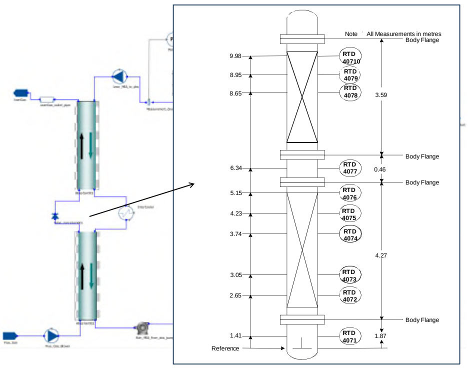

Figure 5: Case 2 Absorber Sensor Location

Process Inputs and disturbances tracked include:

- Step decrease in the intercooled solvent return temperature
- Fluctuating CO_2 composition in the flue gas
- Falling lean amine inlet temperature
- Falling flue gas inlet temperature

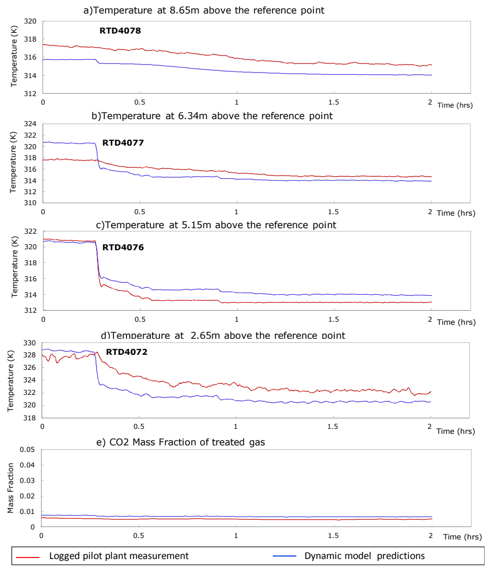

Figure 6: Case 2 Plant and Model Response Comparison

Conclusions

- Model prediction for the absorber temperature profile tracks with pilot plant measurements.
- Model effectively handles a number of process inputs and disturbances at the same time.
- For conventional process, model consistently underestimates treated gas CO_2 concentration and overestimates reboiler duty.
- For intercooled process, model prediction is very close but slightly overestimates treated gas CO_2 concentration.
- Onda wetted area estimate and chemical equilibrium assumption are the likely causes of model discrepancy.

Notation

M	Mass hold up	F	Mass flow rate	N	Molar flux
δ	Film thickness	ω	Wetted area	Sp	Specific Area
U	Energy Hold up	F_H	Enthalpy flow rate	H	Heat flux
C	Molar concentration	x	Molar fraction	χ	Diffusivity

Further Information

Biliyok, C., Lawal, A., Wang, M. and Seibert, F. (2012), "Dynamic modelling, validation and analysis of post-combustion chemical absorption CO_2 capture plant", International Journal of Greenhouse Gas Control, vol. 9, pp. 428-445.