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Dynamic Modeling of the Solvent Regeneration Part of a CO_2 Capture Plant

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Abstract

In this work, a system of unit operations is modeled and implemented in MATLAB for dynamic simulation of the regeneration part of the CO_2 capture process. The system consists of a stripper, a reboiler and a condenser, and it is solved by a simultaneous equation based method. The method proves to be suitable for solving the regeneration part of the CO_2 capture process and it shows numerically stable behavior in general. Further, two dynamic simulation cases are carried out and compared to steady state simulation results from CO2SIM. The dynamic simulation results show reasonably good agreement with steady state simulations, even though a very simplified flash tank model is used for simulation of reboiler and condenser and a simplified thermodynamic model is applied compared to the more robust CO2SIM model. Due to lack of dynamic pilot data, validation of the dynamic regeneration model has been difficult at this point. However, this is necessary for a thorough validation of the model for transient conditions.

Keywords: Post combustion CO_2 capture; solvent regeneration; dynamic modelling

1. Introduction

It is difficult to foresee dynamic behavior of complex chemical processes, especially integrated processes such as that of a CO_2 capture process located downstream a power plant process. Steady state modeling and simulation has been widely applied for various studies of capture processes for several

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years, but recently there has also been a growing interest for dynamic modeling and simulation. Dynamic modeling and simulation will help us to understand the transient behavior and the interactions of complex chemical processes in a much more efficiently manner.

However, dynamic modeling is more challenging compared to steady state modeling, both with respect to numerics and determining the model parameters. While steady-state models are described by a set of algebraic equations (considered that any spatial domain is discretized), the dynamic models will consist of a set of differential and algebraic equations. Furthermore, compared to steady state simulations, additional properties and parameters are necessary to describe the transient behavior of a system. These additional properties describe the gas and liquid hold-up, in addition to the capacitance of the process equipment. The mass transfer rate equations are described as empirical correlations of the process states. Some of the model parameters used in steady state simulators can often be regarded as constant and independent of any state. This is a reasonable assumption when the states do not change much throughout the process or process unit. However, these states can vary considerably during a course of dynamic simulation. Another difference from steady state modeling and a possible benefit is that the dynamic effects we are studying may not require the same level of model complexity. However, yet this remains to be explored in detail for post-combustion type of CO_2 capture using amine solvents.

A dynamic column model has previously been developed at NTNU and SINTEF. The column model was validated for absorber mode using the corresponding steady state column unit in CO2SIM (an in-house simulator developed at SINTEF and NTNU), and it was verified that the dynamic model at steady state gives similar results to the rigorous steady state model. This ensures that the model is implemented correctly, based on the given assumptions. The dynamic column model was further compared transient performance data obtained in the absorber of the VOCC pilot rig at NTNU and SINTEF. Some results are shown in Tobiesen et al. (2011) [1].

For the present paper a simulation study has been performed to test the dynamic performance of the CO_2 regeneration process. The same column model validated for the absorber is extended with simplified models for the condenser and the reboiler to simulate the regeneration process. Two test cases with variations in the inlet stream to the stripper are simulated, and steady state simulations in CO2SIM have been carried out to validate the dynamic model in steady state mode. However, dynamic pilot data from the regeneration part of the process is very limited and not available in the literature. Thus dynamic model validation is very difficult at the moment.

Nomenclature

a	Hydraulic interfacial area of wetted packing [m^2/m^3]
C	Molar concentration [$kmol/m^3$]
C_p	Specific heat capacity [kJ/kmol K]
F	Molar flow rate [kmol/s]
h	Heat transfer coefficient [W/m^2 K]
ΔH	Heat of reaction [kJ/kmol]
k'	Interfacial mass transfer coefficient [$kmol/m^2$ kPa s]
K	Phase equilibrium constant

L	Height of packing [m]
N	Interfacial molar flux [kmol/m^2 s]
nc	Number of components
n	Total molar hold-up [kmol/h]
P	Pressure [kPa]
R	Universal gas constant [kJ/kmol K]
T	Temperature [K]
t	Time [s]
u	Velocity [m/s]
x	Mole fraction in liquid phase [-]
y	Mole fraction in gas phase [-]
z	Axial distance for packing [m]
ε	Gas or liquid hold-up [-]
Φ	Molar flux [kmol/m^2 s]
Subscripts	
eq	Equilibrium
i	Component number
in	Inlet
L,G	Liquid or gas phase
n	Normalized
ref	Reference

2. Implementation

2.1. Dynamic model equations

The regeneration section modeled here consists of a packed column, a reboiler and a condenser as illustrated in Figure 1.

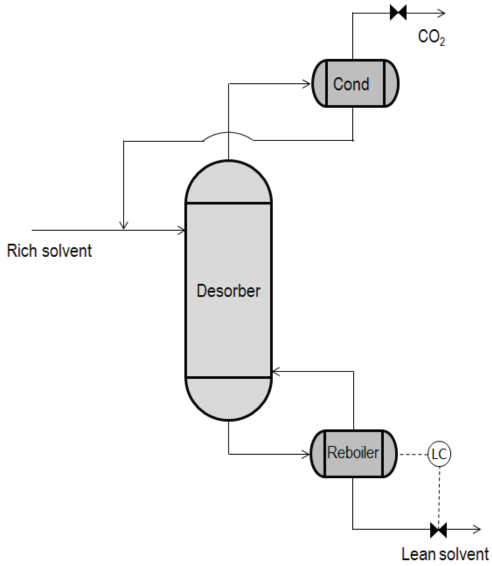

Fig. 1. Flow sheet of the simulated regeneration part of the CO_2 capture plant.

The model for the dynamic packed column is based on the following model equations:

Gas phase equations — *Boundary conditions at $z_n=0$*

$$\varepsilon_G C_G \frac{\partial y_i}{\partial t} = -\Phi_G \frac{1}{L}\frac{\partial y_i}{\partial z_n} - \left(N_i a - y_i \sum_j N_j a\right) \quad (1) \qquad y_i(z_n=0) = y_{i,\text{feed}}$$

$$\frac{\mathrm{d}\Phi_G}{\mathrm{dz}} = -\sum_j N_j a + \frac{\mathrm{d}(\varepsilon_G C_G)}{\mathrm{d}t} \quad (2) \qquad \Phi_G(z_n=0) = \Phi_{G,\text{feed}}$$

$$\varepsilon_G \frac{\mathrm{d}T_G}{\mathrm{d}t} = -u_G \frac{1}{L}\frac{\partial T_G}{\partial z_n} - \frac{a}{\sum_i (C_i C_{p,i})_G}\cdot h_{G/L}(T_L - T_G) \quad (3) \qquad T_G(z_n=0) = T_{G,\text{feed}}$$

Liquid phase equations — *Boundary conditions at $z_n=1$*

$$\varepsilon_L C_L \frac{\partial x_i}{\partial t} = \Phi_L \frac{1}{L}\frac{\partial x_i}{\partial z_n} + \left(N_i a - x_i \sum_j N_j a\right) \quad (4) \qquad x_i(z_n=1) = x_{i,\text{feed}}$$

$$\frac{\mathrm{d}\Phi_L}{\mathrm{dz}} = -\sum_j N_j a \quad (5) \qquad \Phi_L(z_n=1) = \Phi_{L,\text{feed}}$$

$$\varepsilon_L \frac{\mathrm{d}T_L}{\mathrm{d}t} = -u_L \frac{1}{L}\frac{\partial T_L}{\partial z_n} - \frac{a}{\sum_i (C_i C_{p,i})_L}\cdot\left(h_{L/G}(T_L - T_G) - \sum_j \Delta H_j N_j\right) \quad (6) \qquad T_L(z_n=1) = T_{L,\text{feed}}$$

$$C_G = P/(RT_G) \quad (7)$$

$$N_i = k_g^{'}\left(P_i - P_i^{eq}\right) \quad (8)$$

$$z_n = z/L \quad (9)$$

The details on the development of the dynamic packed column model are described by Tobiesen et al. (2011) [1] and Kvamsdal et al (2009) [2].

Both the reboiler and the condenser are simulated as dynamic flash tanks and the flash tank model is based on the differential algebraic equations presented below.

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = F_{in}x_{in,i} - F_G y_i - F_L x_i \quad (10)$$

$$0 = n_i - n_G y_i - n_L x_i \quad (11)$$

$$y_i = K_i x_i \quad (12)$$

$$0 = 1 - \sum_{j=1} y_j \quad (13)$$

Phase equilibrium is assumed in this model, and the equilibrium constants are constant for simplification. The first equation (10) gives *nc* number of equations from which the total component hold-up in both liquid and gas (n_i) is calculated. Equation 11 and 12 gives the molar fractions in the liquid (x_i) and vapor phase (y_i), respectively. The last equation (13) gives the thermodynamic pressure in the flash tank. Included in the flash tank model is also a valve on the vapor side as well as a level controller at the liquid side. The level controller is modeled as a P-controller. The temperature in the flash tank is assumed to be constant.

All independent variables are normalized to increase robustness, both in the packed column model and the flash tank model.

2.2. Numerical solution

The column model contains partial differential equations (PDEs). This requires discretization with regard to the axial direction (column height), and the method of orthogonal collocation is used for this purpose. The discretized PDEs are in this way transformed into a system of ordinary differential equations and algebraic equation (DAE) with time as the independent variable. The flash tank model does not contain any spatial variables, thus this model is already described by a system of DAEs and does not need any similar pre-treatment.

The numerical method for solving the model equations is a simultaneous equation based method. Here, this means that the model equations for all three process units (stripper, condenser, and reboiler) are solved simultaneously by the same integration routine in MATLAB (ode15s).

3. Simulation results and steady state model verification

Two test cases are simulated by the dynamic regeneration model in order to study the dynamic behavior of the regeneration process when two different types of disturbances are introduced. In case 1, the effect of changes in inlet liquid flow rate is studied, while as in case 2, the CO_2 loading in the rich solvent entering the stripper was varied. In both cases the dynamic simulations were performed until a new steady state conditions was reached and the results are compared to steady state simulation results from CO2SIM.

3.1. Case 1

In the first case the flow rate of rich solvent entering the stripper column is increased by 10 % during 60s. Results from the dynamic MATLAB model together with steady state CO2SIM results are presented in the following figures. The superficial liquid velocity profile through the column for some points in time is shown in Figure 2 (a), while the corresponding steady state CO2SIM results (for the base case liquid flow rate and for 10% increase in liquid flow rate) are shown in Figure 2 (b). The effect of increasing liquid flow rate on the liquid temperature and CO_2 loading profiles for some points in time are shown in Figures 3 (a) and (b), respectively. There is only a slight effect observed on temperatures and CO_2 loading profiles when liquid flow rate is increased by 10 %. Similar results were observed with the steady state CO2SIM model and this is in accordance with the equilibrium profile, which is likely very flat for the specific flow rates.

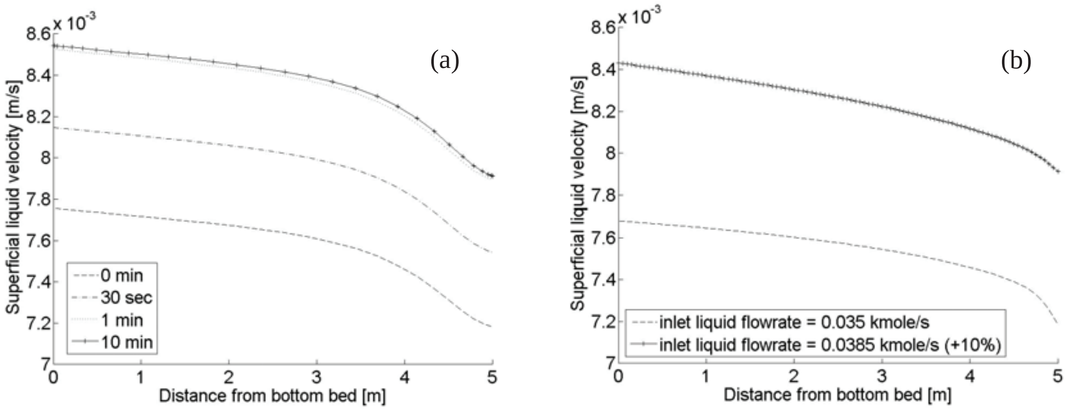

Fig. 2. (a) Superficial liquid velocity in dynamic MATLAB model and (b) superficial liquid velocity in steady state CO2SIM model

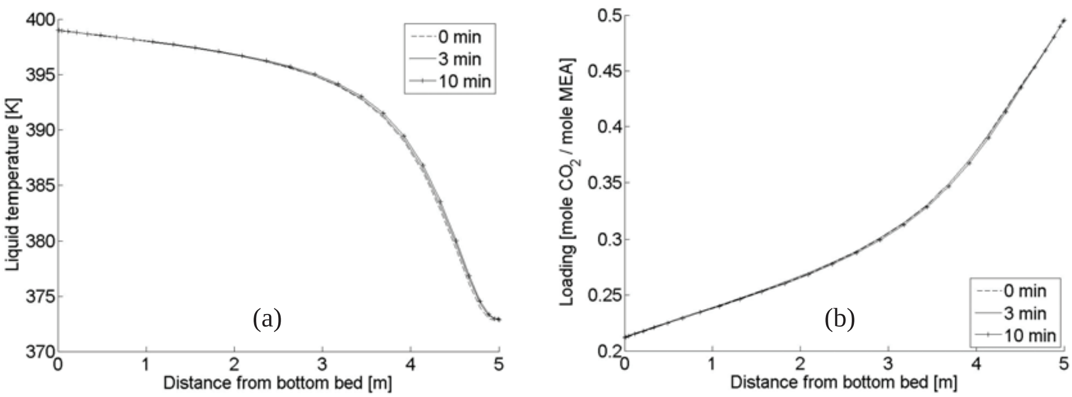

Fig. 3. (a) Liquid temperature profile and (b) CO_2 loading profile in dynamic MATLAB model.

3.2. Case 2

In the second case, the loading of the rich solvent entering the stripper is decreased by 10% during 60s. Results from the dynamic MATLAB model together with steady state CO2SIM results are presented in the following figures. The effects of the loading decrease of the entering solvent on the superficial liquid velocity and the liquid temperature profiles are shown for some points in time in Figures 4 (a) and (b), respectively. The new steady state condition is reached after about 10 minutes. Figure 5 (a) shows the CO_2 loading profile through the stripper column for some points in time as the loading of entering solvent is decreased, while Figure 5 (a) shows the corresponding steady state CO2SIM results (for the base case solvent loading and for 10% decrease in loading of entering solvent). The profile predicted by the dynamic MATLAB model seems slightly more non-linear than the profile predicted by the CO2SIM model, and the observed difference is caused by a slight difference in the packed column model and thermodynamic model. However, the dynamic and steady state results show good agreement.

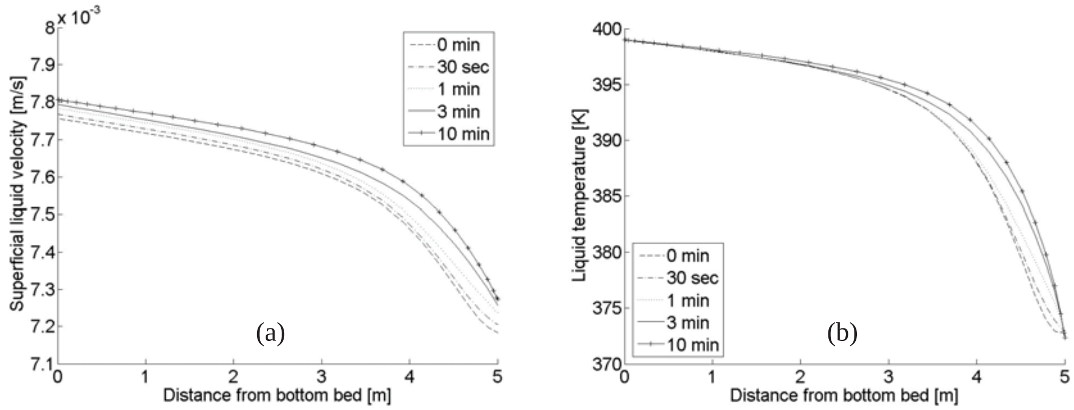

Fig. 4. (a) Superficial liquid velocity profile and (b) liquid temperature profile in dynamic MATLAB model

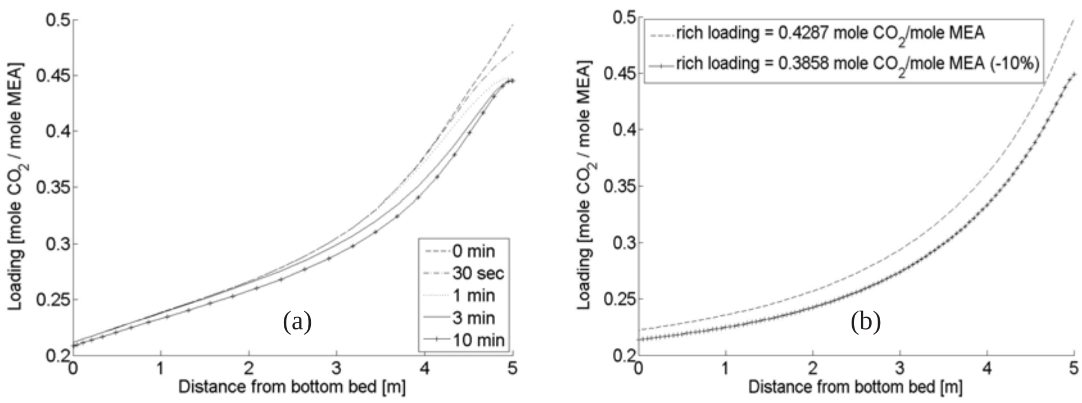

Fig. 5. (a) CO_2 loading profile in dynamic MATLAB model and (b) CO_2 loading profile in steady state CO2SIM model

4. Conclusion

In this work, a dynamic model of the regeneration part of the CO_2 capture process is developed in MATLAB for transient modeling of CO_2 desorption. The model consists of a packed column, a reboiler and a condenser, and the complete system of equations is solved by a simultaneous equation based method. Steady state model verification towards CO2SIM steady state simulations has been presented with two examples of usage. The simultaneous equation based method shows numerically stable behavior for the regeneration section of the CO_2 capture process, and the dynamic simulations at steady state gives similar results to the steady state simulations in CO2SIM. In future work a more accurate dynamic flash tank model will be developed for the reboiler and condenser in the regeneration process. The improved flash tank model will include an equilibrium model predicting phase equilibrium constants as well as differential model equations representing the energy balances to allow calculation of actual flash temperature. A thorough validation towards dynamic pilot data will also be presented.

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