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# A Numerical Solution Strategy for Dynamic Simulation of Post-combustion $CO_2$ Capture

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**Abstract**

This paper describes in detail the numerical solution of a dynamic process developed for post-combustion absorption based $CO_2$ capture. The method used in this work is sequential modular integration. This means that each process unit is modeled and integrated individually while co-ordination algorithms are developed to synchronize process units in time and provide input between connecting units. A pressure-flow interaction algorithm (p-f network solver) is also developed to provide estimates of downstream pressures for each unit. This is required in order to calculate the outlet flow from the units. The complete process plant model is developed to enable simulation of the post-combustion $CO_2$ capture process at power plant load variations. Two examples of load variations are presented in this paper.



*Keywords*: post-combustion $CO_2$ capture; dynamic modelling; sequential modular integration; pressure flow network solver

## 1. Introduction

We are now moving towards realization of full-scale $CO_2$ removal plants for power generation. However, varying electricity demand caused by seasonal variations in ambient conditions during a year will force a more flexible operation of the fossil fueled power stations. In fact power plants may also change load quite frequently to cope with changing demand on a daily basis. Together with the increasing

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use of renewable sources, this will require an even higher degree of flexibility in fossil-fueled power generation.

It is difficult to predict dynamic behavior of chemical processes, especially for complex processes such as an integrated $CO_2$ capture process downstream a power plant process. Dynamic simulation is a valuable tool to study and identify possible challenges related to daily operation, and identify any negative effects and potential operational bottlenecks for the integrated power- and $CO_2$ capture process at transient conditions.

The purpose of the present work has been to develop and demonstrate a dynamic process model for simulation of a simplified post-combustion absorption based $CO_2$ capture process at varying process conditions.

**Nomenclature**

| | |
|---|---|
| $C_v$ | Valve constant [kg/s √(Pa)] |
| $f(u)$ | Manipulating variable |
| $W$ | Mass flow rate [kg/s] |
| $P$ | Pressure [Pa] |
| $t$ | Time [s] |
| $T_h$ | Global time step [s] |
| $\delta$ | Directionality (+1/-1) |
| $\tau$ | Volume multiplied with density pressure differential [kg/Pa] |

Subscripts

| | |
|---|---|
| $i,j$ | Node index |
| $k$ | Time index |

## 2. Sequential modular integration

The sequential modular based method (modular integration) implies that the process is divided into sub-systems which typically represent process units and all sub-systems are integrated individually. An overall process plant model is used to handle communication between connecting units and synchronizing them in time. The process plant model will treat each process unit as a “black box” that produces output given input.

The total simulation window is divided into time intervals and ccouplings between units occur only at the end of each time interval. The unit’s external variables of entering mass flows and downstream pressures need to be described as functions of time, such as polynomials.

The sequential modular based method offer the possibility of computational speed through parallel processing of the individual process units. An additional advantage is the possibility of tailoring the integration algorithm to each process unit and its dynamic behaviour, which offers desirable convergence and stability properties. Specifying initial conditions that satisfy the system of equations for each process

unit is also easier compared to specifying consistent initial conditions for the simultaneously solved complete process model [1].

### *2.1. Process unit modeling*

In order to demonstrate modular integration and the pressure-flow network solver, a simplified model of the $CO_2$ absorption process (indicated by the grey-shaded units shown in Figure 1) is considered here. This means that the cross heat-exchanger and pumps are treated as black boxes in the simulations implying that the solvent temperatures and pressures at the inlet of both the absorber and the stripper are fixed. The absorber model is based on the column model described by Kvamsdal et al [2]. The regeneration part of the $CO_2$ capture process is here treated as one unit which consists of a packed column, a reboiler and a condenser, and the complete model is described in detail by Enaasen et al (2012) [3]. A simplified flash tank model with fixed temperature and equilibrium constants is used for simulation of reboiler and condenser in the regeneration part.

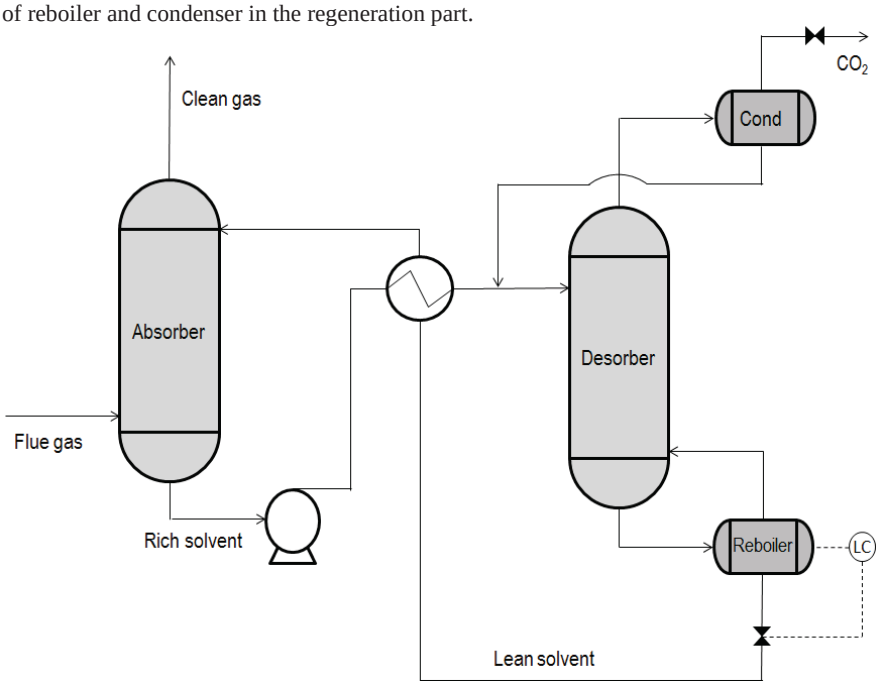


Fig. 1. Flowsheet of the simulated process

### *2.2. Coordination algorithms*

The sequential modular based method requires additional coordination algorithms to handle information flow between units and a pressure-flow network solver, which predicts downstream pressures.

The co-ordination algorithm should also keep the various process units synchronized in time and it should be able to handle recirculation loops. The simulation window is divided into time intervals (with

time step $T_h$), and couplings between units is allowed at the end of each time interval. Thus, input variables to each unit such as flow rate, pressure, temperature and composition are updated at the end of each time step as a function of time based on their respective gradients during the current time interval. Recirculation loops must be iterated, and a direct substitution method is used for this purpose.

### *2.3. Pressure-flow network solver*

Since outlet flow from a process unit is pressure driven, the downstream pressures must also be provided to each unit. Hence, pressure-flow interaction loops exist between the connected process units. These loops may be solved by an iterative procedure on the modular integration level. Alternatively, by decoupling the problem in two levels (one for fast pressure dynamics and one for slow dynamics) the loops can be solved by a pressure-flow interaction algorithm (p-f network solver) on flowsheet level without or with minimum iteration. Pressure predictions will subsequently be used as input to the modular integration level.

The overall process can be described by unidirectional graphs where the vertices are nodes representing the units and the connections represent streams between units in which the pressure can propagate from one unit to another. The $W_{ij}$ represent the mass flow rate from unit *i* to unit *j* (see Figure 2). As the graph is undirected it implies that $W_{ij} = W_{ji}$.

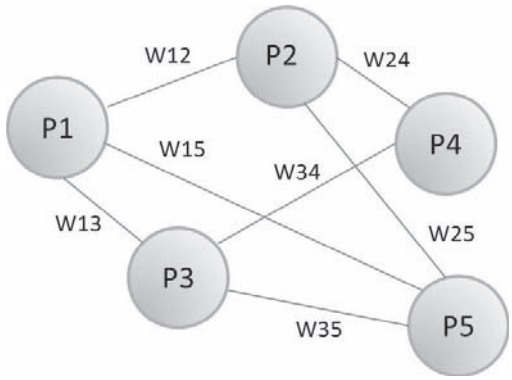


Fig. 2. Illustration of units and connections in the pressure-flow network solver

The flow between nodes *i* and *j* may be given by a model similar to the valve equation:

$$W_{ij} = C_v f(u)\sqrt{P_i - P_j} \tag{1}$$

Also compressors and pumps may be represented by similar equations, where the flow rate is calculated from the work input and the pressures.

The model of pressure change in node *i* is given by

$$\frac{dP_i}{dt} = \frac{1}{\tau_i}\sum_j^n \delta_{ij} W_{ij} \tag{2}$$

where δ takes care of directionality by being +1 when directed to node *i* from node *j*, and -1 when

directed from node *i* to node *j*, or otherwise 0. The parameter τ is given by

$$\tau_i = V_i\left(\frac{\partial \rho_i}{\partial P_i}\right) \tag{3}$$

and can be considered a constant in this context.

Based on the present situation of mass flow rates, it is desired to predict how the pressure will evolve in each unit. A linearization of the pressure model is made by linearizing the valve equation (1) around time $t_k$:

$$\frac{dP_i}{dt} = \frac{1}{\tau_i}\sum_j^n \delta_{ij} W_{ij}^k + \frac{1}{\tau_i}\sum_j^n \delta_{ij}\left(\frac{\partial W_{ij}}{\partial P_i}\right)_{P_j} \frac{dP_i}{dt}(t-t_k) + \frac{1}{\tau_i}\sum_j^n \delta_{ij}\left(\frac{\partial W_{ij}}{\partial P_j}\right)_{P_i} \frac{dP_j}{dt}(t-t_k) \tag{4}$$

Applying the time horizon concept and introducing $T_h$ being the global time step $T_h = t_{k+1}-t_k$ and converting to matrix form:

$$\left[\mathbf{I} - T_h \mathbf{J}_k\right]\frac{d\mathbf{P}}{dt} = \begin{bmatrix} \frac{1}{\tau_1}\sum_j^n \delta_{1j} W_{1j}^k \\ \vdots \\ \frac{1}{\tau_n}\sum_j^n \delta_{nj} W_{nj}^k \end{bmatrix} \tag{5}$$

which by implicit Euler integration yields:

$$\mathbf{P}_{k+1} - \mathbf{P}_k = T_h\left[\mathbf{I} - T_h \mathbf{J}_k\right]^{-1} \begin{bmatrix} \frac{1}{\tau_1}\sum_j^n \delta_{1j} W_{1j}^k \\ \vdots \\ \frac{1}{\tau_n}\sum_j^n \delta_{nj} W_{nj}^k \end{bmatrix} \tag{6}$$

This is solved as a linear system $Ax = b$ without iterations.

For typical process plant simulations the assumption of a fast propagating pressure change is reasonable. As the changes in composition due to chemical reaction, separation and phase separation happen on a large time scale in comparison with the pressure change, the pressure propagation in the process units can be described as a pseudo steady-state process [4]. By removing this fast mode of the model, the stiffness of solving the collection of sub-problems in the network solver is simplified.

## 3. Results

Two examples of load variations are simulated. In the first case, the feed gas flow rate to the absorber column is increased by 10%, while as in the second case, the $CO_2$ composition in the feed gas to the absorber is decreased by 10%. The time interval ($T_h$) used in these simulations is 10 seconds.

### *3.1. Increase in feed gas flow rate*

The feed gas flow rate is increased by 10% in one single step change. Figure 2 and 3, shows the loading in the rich solvent exiting the absorber and the lean solvent exiting the regeneration unit, respectively, both as functions of time. The rich loading is increasing as the gas load to the absorber is increased, and the lean loading is increasing as well when rich loading is increased. The effect on lean

loading is however very small and this is partly caused by the simplified flash tank model used in the model of the reboiler in the regeneration section. However, a time delay in mass transportation from the absorber column to the stripper column is observed, since the loading in the solvent exiting the stripper remains constant for about 200 seconds after the disturbance is introduced. This is an effect of the process unit's capacitance, and it demonstrates the importance of including correct equipment sizing in dynamic modeling.

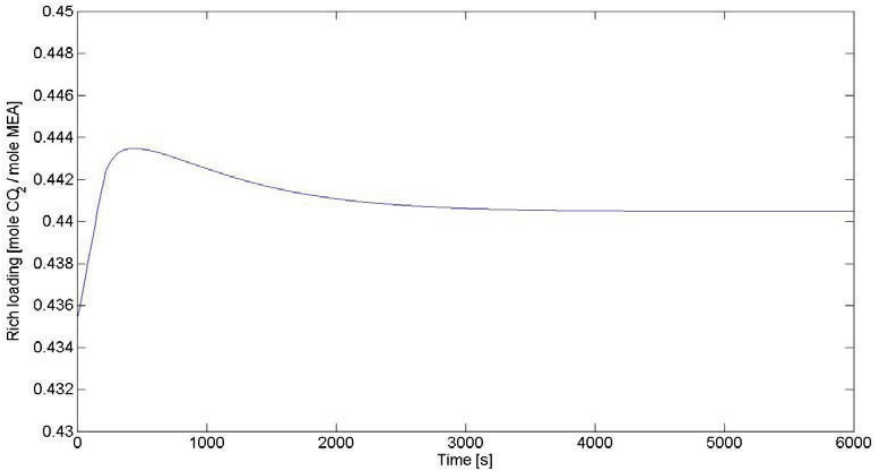


Fig. 3. Loading in rich solvent exiting the absorber as a function of time

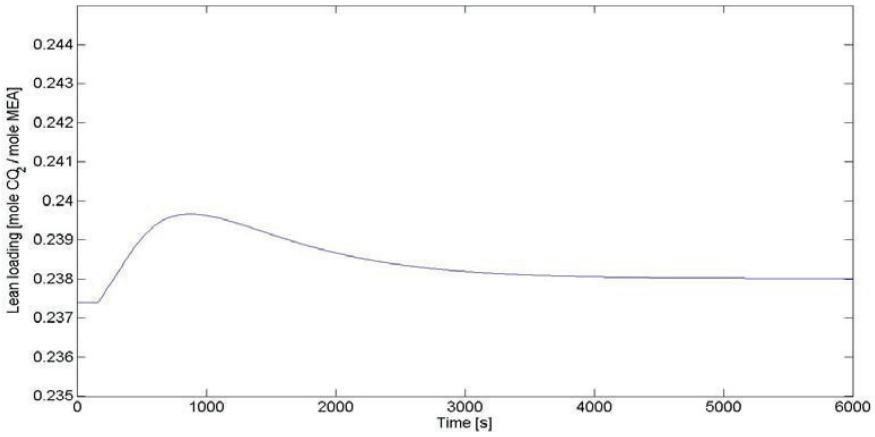


Fig. 4. Loading in lean solvent exiting the stripper as a function of time

### *3.2. Decrease in $CO_2$ load in the feed gas*

In the second case, the $CO_2$ concentration in the feed gas to the absorber is decreased by 10 %. The rich and lean loading in this case is presented as functions of time in Figure 4 and 5. In this case the rich loading is decreasing as $CO_2$ concentration in the feed gas is decreased, and the same effect is observed in the loading of the lean solvent exiting the stripper. The effect on lean loading is however very small also in this case.

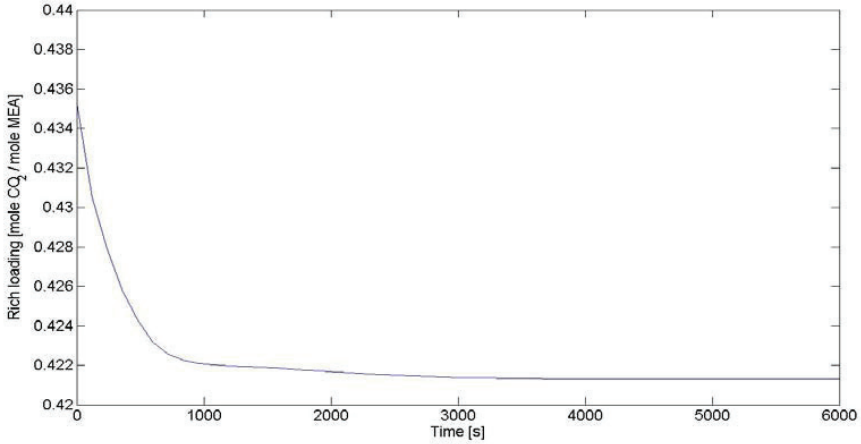


Fig. 5. Loading in rich solvent exiting the absorber as function of time

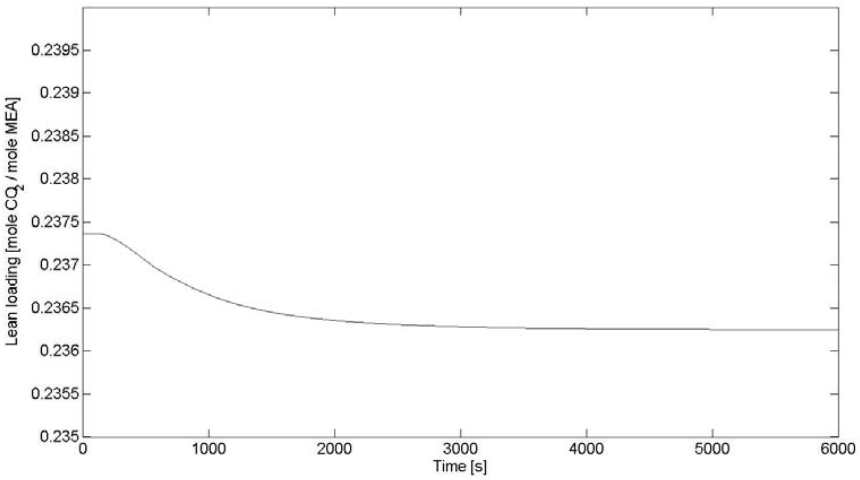


Fig. 6. Loading in lean solvent exiting the stripper as function of time

## 4. Conclusions

Modular integration is investigated as a numerical solution strategy for simulation of post-combustion $CO_2$ capture processes. The method proves to offer desirable convergence and stability properties for a simplified plant model consisting of an absorber model and a regeneration model. In future work, a more accurate dynamic flash tank model will be developed and implemented in the unit model of the regeneration section. This model will include differential equations representing the energy balances which will allow variations in the flash temperature, in addition to an equilibrium model predicting actual equilibrium constants. A cross heat-exchanger will also be included in the overall process model in order to enable studies of transient behaviour in a more realistic manner where also liquid temperatures in the inlet streams to the columns are allowed to vary.

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