A NEQ rate based model for a post combustion CO_2 capture plant

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Abstract

A dynamic rate based model is developed for simulating a post combustion CO_2 capture plant. The flow sheet used for the model development consists of an absorption column and a de-absorption column as the main components while two heat exchangers and two pumps are included as additional equipment. A reboiler and a condenser are included in the de-absorption column but those are modeled separately.

The absorption column and the de-absorption column are considered to be packed towers with Montz B 200 metal structured packing. A Monoethanolamine (MEA) solvent system is used due to the substantial availability of data in the literature.

The development of the model is done with paying more attention to the distributed models of the absorber and the de-absorber as they are considered to be the main components. The non-equilibrium stage, rate based modeling is used for the absorption and the de-absorption columns. The absorber/de-absorber are discretized into a number of slices. Each slice (controlvolume) in the discretization consist of a bulk liquid phase, a bulk vapour phase and an interface with a liquid and a vapour film and the bulk phases are considered as continuous stirred tank reactors (CSTR). Specie and energy conservation equations are applied for each of the bulk phases.

Reactions which take place in the vapour phase are considered to be negligible. The set of liquid phase reactions and reaction kinetics are taken from the literature. Velocities inside the absorption and de-absorption tower are taken as constant, while the pressure drop is distributed linearly among each control volume along the towers.

Model equations for the bulk phases of the towers are given by

$$
\begin{aligned}
\frac{dn_i^\ell}{dt} &= \dot{n}_{i,\mathrm{in}}^\ell - \dot{n}_{i,\mathrm{out}}^\ell + \dot{N}_{i,\mathrm{trans}} + \dot{N}_{i,\mathrm{gen}} && (1)\\
\frac{dn_i^v}{dt} &= \dot{n}_{i,\mathrm{in}}^v - \dot{n}_{i,\mathrm{out}}^v - \dot{N}_{i,\mathrm{trans}} && (2)\\
\frac{dE^\ell}{dt} &= \sum_{i=1}^{n} \dot{n}_{i,\mathrm{in}}^\ell \tilde{H}_{i,\mathrm{in}}^\ell - \sum_{i=1}^{n} \dot{n}_{i,\mathrm{out}}^\ell \tilde{H}_{i,\mathrm{out}}^\ell + \dot{E}_{\mathrm{trans}} && (3)\\
\frac{dE^v}{dt} &= \sum_{i=1}^{n} \dot{n}_{i,\mathrm{in}}^v \tilde{H}_{i,\mathrm{in}}^v - \sum_{i=1}^{n} \dot{n}_{i,\mathrm{out}}^v \tilde{H}_{i,\mathrm{out}}^v - \dot{E}_{\mathrm{trans}} && (4)
\end{aligned}
$$

where the terms $\dot{N}_{i,\mathrm{gen}}, \dot{N}_{i,\mathrm{trans}}$ and $\dot{E}_{\mathrm{trans}}$ represent the specie generation inside the control volume, interfacial specie transfer and the interfacial energy transfer. The term $\tilde{H}$ represents the molar enthalpy of the different species accordingly. Figure 1 shows an overview of a control volume considered for modelling.

The interface is modelled assuming equilibrium at the interface. Mass and energy conservation at the interface is considered assuming that CO_2 is the only specie which transfers across the interface. The mass transfer across the interface is modelled as

$$
\begin{aligned}
\dot{N}_{\mathrm{CO_2},\mathrm{trans}} &= E K_{\ell,\mathrm{CO_2}} a \left(c_{\mathrm{CO_2}}^{\ell *} - c_{\mathrm{CO_2}}^{\ell} \right) = K_{v,\mathrm{CO_2}} a \left(c_{\mathrm{CO_2}}^{v} - c_{\mathrm{CO_2}}^{v *} \right) && (5)\\
&= \frac{1}{\frac{H_{\mathrm{CO_2}}}{E K_{\ell,\mathrm{CO_2}} a T^*} + \frac{R}{K_{v,\mathrm{CO_2}} a}} \left(\frac{p_{\mathrm{CO_2}}^{v}}{T^v} - c_{\mathrm{CO_2}}^{\ell} \right). && (6)
\end{aligned}
$$

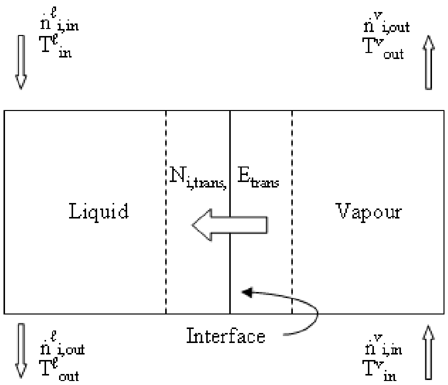

Figure 1: A descretization slice of the absorption / de-absorption tower.

Here $K_{\ell,\mathrm{CO_2}}$, $K_{v,\mathrm{CO_2}}$ and a stand for the liquid phase mass transfer coefficient, gas phase mass transfer coefficient and the mass and heat transfer area available. The '$*$' symbol indicates the interfacial values while c, p and T are used for concentration, pressure and temperature. Henry's law coefficient and the universal gas constant are given with H and R. An enhancement factor (E) is used to introduce the influence of the reactions on the CO_2 transfer. According to Hoff (2003) , the enhancement factor is considered as the same as Hatta number and given by

$$E = \frac{\sqrt{D^{\ell}_{\mathrm{CO_2}}\left(k_{1\mathrm{f}}c^{\ell}_{\mathrm{MEA}} + k_{3\mathrm{f}}c^{\ell}_{\mathrm{CO_2}}\right)}}{K_{\ell,\mathrm{CO_2}}}. \tag{7}$$

Here D and k are the diffusion coefficient and the reaction coefficients of the two reactions where CO_2 is being reacted with MEA. Use of Eq. (6) has forced the model to satisfy the condition introduced by the Eq. (5) .

The interfacial energy transfer relation is developed following the relations presented by Katariya et. al (2007). The convection heat transfer contribution and the contribution due to the mass transfer have considered. The energy transfer across the interface is given by

$$\dot{E}_{\mathrm{trans}} = h^{\ell}a\Delta T^{\ell} + \dot{N}_{\mathrm{CO_2,trans}}\tilde{H}^{\ell}_{\mathrm{CO_2}} = h^{v}a\Delta T^{v} + \dot{N}_{\mathrm{CO_2,trans}}\tilde{H}^{v}_{\mathrm{CO_2}}. \tag{8}$$

The temperature differences ΔT^{ℓ} and ΔT^{v}, are defined as $\left(T^{*} - T^{\ell}\right)$ and $\left(T^{v} - T^{*}\right)$ while the convective heat transfer coefficients are given as h. Involvement of T^{*} in the model equations have forced the model to satisfy the condition introduced by eq. (8).

The two heat exchangers are a process-process heat exchanger and a process-utility heat exchanger, which are modelled with ordinary differential equations. A constant pressure head is considered to include the effect of pumps during the model development.

The model is implemented in MATLAB, and the method of lines (MOL) is used for solving the model equations. The simulated results will be compared with the general information found in literature in terms of CO_2 removal efficiency of the absorption column and the MEA regeneration efficiency in the de-absorption column in the capture plant. Design and operational data perturbations will be used to analyze the sensitivity of the model.

References

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