

Heat and mass transfer model in EDA-CO₂-H₂O system

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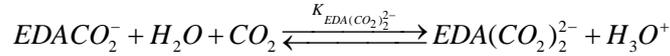
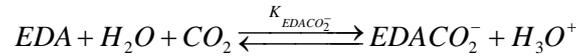
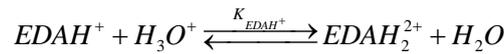
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Abstract:

In CO₂ absorption processes large mass and heat transfer driving forces occur several places, absorber bottom, water wash section and in the desorber. Good fundamental models for the combined heat and mass transfer including chemical reaction and convective mechanisms are still lacking. A proper description of the transfer processes is very important for improved absorption process simulation and optimization.

In this study, implementation of a penetration type model for heat and mass transfer for CO₂ absorption for the EDA-CO₂-H₂O system was done in MATLAB and validated with experimental data from a String of Discs Contactor (SDC). The coupling between chemical equilibrium, mass transfer, heat transfer and chemical kinetics are taken into account and the experimental kinetic data are obtained from the SDC experiments^[1].

The overall chemical reaction taking place in the liquid phase can be written as:



The mass flux in liquid phase can be expressed by using the penetration model:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D(\alpha, T) \frac{\partial C}{\partial x} + R$$

The reaction rate can be defined as:

$$R_1 = k_{2,1} C_{CO_2} C_{EDA} - k_{-2,1} C_{EDACOO^-}$$

$$R_2 = k_{2,2} C_{CO_2} C_{EDACOO^-} - k_{-2,2} C_{EDA(COO^-)_2}$$

By taking into account the reaction heat, the overall heat flux equation in the liquid film can be expressed as following:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\alpha \frac{\partial T}{\partial x} \right) - \left(\frac{-\Delta H_R}{\rho c_p} \right) R$$

In the equation above $-\Delta H_R$ is the heat of reaction in the liquid phase, including all liquid phase reactions, but excluding the heat of physical solution of CO₂. The heat of solution of CO₂, the vaporization heat of volatile species (H₂O and EDA), and the sensible heat transfer of CO₂ are then included in the interface boundary conditions and given as:

$$t > 0, \quad x = 0,$$

$$k_\lambda \frac{\partial T}{\partial x} = h_g (T_i - T_g) - (-\Delta H_s) \left(D_{CO_2} \frac{\partial C_{CO_2}}{\partial x} \right) + c_p M_{CO_2} (T_i - T_g) N_{CO_2} - (-\Delta H_{vap}^{H_2O}) N_{H_2O} - (-\Delta H_{vap}^{EDA}) N_{EDA}$$

The initial conditions of the mass transfer model are crucial for the predictions, but since the speciation data and the reaction equilibrium constant are still lacking, the initial conditions are simplified and assumed as following:

$$C_{CO_2_0} = 0, C_{EDA_0} = 5(1 - \alpha), C_{EDACOO_0^-} = 5\alpha(1 - \alpha), C_{EDA(COO^-)_0^2} = 5\alpha^2$$

The orthogonal collocation method is used for the model calculation^[2]. The prediction results are showed in the following two figures:

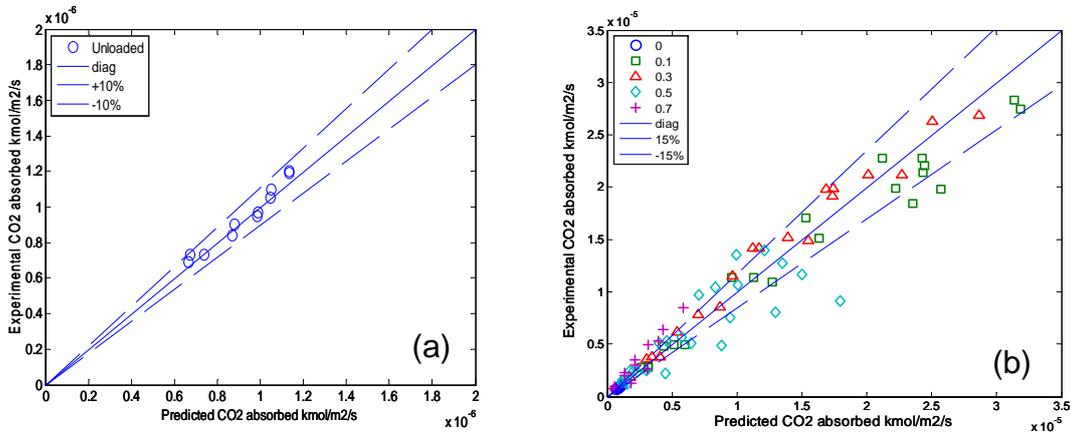


Figure1. The comparison of CO₂ flux between experimental data and model prediction (a) for unloaded solution (b) for loaded solution

Figure 1.a. shows that the model predicts very well the experimental data within 10% uncertainty. In this case the initial condition assumption correct as the free amine concentration is readily known at zero loading, and the first protonation constant and carbamate reaction equilibrium are determined from the mono-carbamate formation. At very low loading or unloaded solution it is just calculated from the initial concentration of EDA.

Figure 1.b. shows the results for loaded solutions, and as can be seen, that the uncertainty increases to more than 15%. The contribution of the dicarbamate reaction will be significant under these conditions and this renders the initial condition assumption less valid. This can be improved only by implementing a rigorous thermodynamic model for the EDA system. In the final work, improvement of the initial conditions will be developed from the speciation data (e.g. from NMR result) and the reaction equilibrium constant could be fitted from thermodynamic work.

Reference

- [1] Hartono, A., and Svendsen, H.F., 2011, Kinetic model of loaded diamine system, under submission to the Chem. Eng. Sci. Journal
- [2] Xiao Luo, Ardi Hartono, Magne Hillestad, Hallvard F. Svendsen, "The study of numerical methods and validation of a heat and mass transfer model in CO₂-MEA system", GHGT10, Amsterdam September 2010