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# MODELLING AND PARAMETER ESTIMATION OF A PLATE HEAT EXCHANGER AS PART OF A SOLVENT-BASED POST-COMBUSTION $CO_2$ CAPTURE SYSTEM

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*Abstract*

A mathematical model of a plate heat exchanger (PHE) as part of an amine scrubbing process for post-combustion $CO_2$ capture has been developed and implemented in the Institute for the Design of Advanced Energy Systems (IDAES) process system engineering (PSE) framework. The thermal model is based on the effectiveness-Number of Transfer Units (ε-NTU) approach where the non-smooth min-max capacitance rates are replaced by smooth functions to improve convergence characteristics of the optimization problem. Parameters for the convective heat transfer coefficient correlations are estimated using the data from National Carbon Capture Center (NCCC). The simulation results are found to be in good agreement with the pilot plant data. The model can be utilized for optimizing PHE designs to maximize energy efficiency.

*Keywords*

Plate heat exchanger, parameter estimation, energy efficiency, $CO_2$ capture.

## Introduction

Amine scrubbing is the baseline technology for $CO_2$ capture having wide application in various process industries such as natural gas sweetening, and $CO_2$ capture from coal-fired power plants. One of the major issues of the amine scrubbing processes is high operating cost due to the energy demand for solvent regeneration. To reduce the energy requirements, heat from the lean solvent leaving the stripper bottom is recovered for heating the rich solvent going to the stripper. Efficient recovery of this heat is essential for reducing the energy requirements of amine scrubbing processes. The industry standard for achieving this heat recovery is to use plate heat exchangers (PHEs) that offer high heat transfer coefficient, variable heat transfer area easily accomplished by adding/removing plates, and ease of cleaning.

In the existing literature on post-combustion $CO_2$ capture, the lean/rich solvent heat exchanger is commonly modeled as a counter-current shell and tube heat exchanger. Harun et al. (2012) developed the model of a lean/rich solvent heat exchanger using the counter-current shell and tube heat exchanger model in gPROMS' Process Model Library. The model assumed no phase change, and constant pressure. Flø et al (2015) modeled the heat exchanger as a distributed shell and tube heat exchanger and validated the model with data from an in-house pilot plant. Nittaya et al. (2014) developed the model of a

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countercurrent shell and tube heat exchanger with one tube pass, but they did not present any validation studies.

Several models of PHEs have been developed for non-amine scrubbing applications. Georgiadis and Machietto developed a model of a PHE for milk pasteurization by incorporating a protein fouling model with a dynamic thermal model (Georgiadis and Macchietto, 2000). The model was solved using gPROMS with the finite difference approach. Dardour et al (2009) developed a linear system of first order differential equations representing the number of channels in a PHE which was solved using the shooting method. Gut and Pinto (2003) developed an algorithm to study the impact of PHE configuration on its performance. For amine scrubbing processes, Lin and Rochelle (2017) developed a simple model of a PHE, which was used for minimizing the cost of the exchanger by considering the velocity and log mean temperature difference (LMTD) as the decision variables. To the best of our knowledge, no detailed model of the PHE for amine scrubbing applications is currently available in the open literature. In this work, a one-dimensional mathematical model of a PHE is developed. The model is validated using pilot plant data. A parameter estimation framework is used to estimate the optimal values of the model parameters.

**Mathematical Model of PHE**

An algebraic model of a PHE with plate dividers is developed by applying the ε-NTU method. The ε-NTU method is computationally superior to the LMTD approach to predict unknown temperature of a fluid (Nellis and Klein, 2009).

*Equipment configuration*

PHE is a common type of heat exchanger which consists of many plates stacked together in a frame as shown in Figure 1a. The plates are corrugated with gaskets at the corners and pressed together to form a series of channels where the fluids flow alternatively and exchange heat through the thin plates. A PHE configuration is determined by the number of plates, their perforations and the inlet and outlet connections which define the flow distribution (Gut and Pinto, 2003). For a given number of passes, $P$ , and the number of channels in a pass, $NC$ ,a multi-pass flow configuration of a PHE can be simplified into a series of sub-heat exchangers. Figure 1b is an example of a 4-pass-4-pass PHE configuration, where the series of sub-heat exchangers are formed from adjacent channels in a pass (see Figure 1c). For a PHE with plate dividers, the sub-heat exchangers are in parallel or counter-current flow configuration depending on if P is odd or even, respectively. For a large number of plates (greater than 35 plates), the effect of end plates can be ignored. Hence, the outlet temperature of a pass can be predicted from an energy balance of only one sub-heat exchanger in that pass. The ε-NTU method can be used to estimate the outlet temperature of each sub heat exchangers where assumption of constant thermal properties inherent in the derivation of the ε-NTU method is valid. The boundary conditions are written to make them consistent with the modeling domain that comprises sub-heat exchangers between passes.

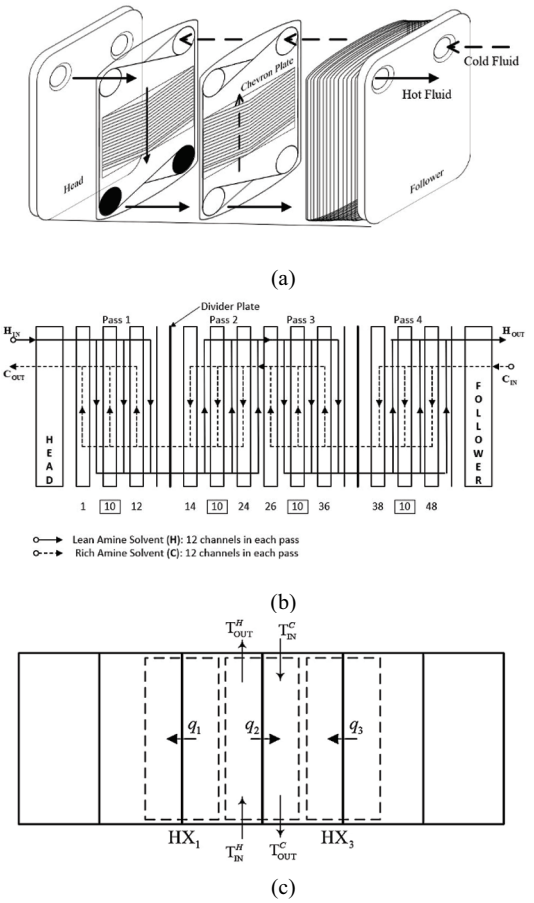



*Figure 1: (a) Typical PHE layout (b) 4-pass-4-pass PHE with 12 channels for each pass and (c) sub-heat exchangers in a pass*

*Thermal model*

The ε-NTU method applied to each sub heat exchanger consists of the following assumptions:

- Steady state and adiabatic operation.
- Constant physical properties in each sub-heat exchanger
- No phase changes and fouling.
- No leakage of fluids

For a generic PHE with $P$ number of passes and $NC_i$ number of channels for pass $i\left(\forall i \in I = \{1,2,...,P\}\right)$,

the governing equations for this approach are developed by applying the energy balance to each sub-heat exchanger as shown in Eqs. (1-2),

$$T^i_{c,out} = T^i_{c,in} + \frac{\varepsilon_i \dot{C}^i_{\min}\left(T^i_{h,in} - T^i_{c,in}\right)}{\dot{C}^i_c}, \qquad \forall i \in I \tag{1}$$

$$T^i_{h,out} = T^i_{h,in} - \frac{\varepsilon_i \dot{C}^i_{\min}\left(T^i_{h,in} - T^i_{c,in}\right)}{\dot{C}^i_h}, \qquad \forall i \in I \tag{2}$$

where $\dot{C}^i_c$ and $\dot{C}^i_h$ are capacitance rates for the cold and hot sides, respectively and are calculated using Eq. (3),

$$\dot{C}^i_c = \frac{\dot{m}_c C_{p,c}}{NC_i}\ ; \quad \dot{C}^i_h = \frac{\dot{m}_h C_{p,h}}{NC_i}; \qquad \forall i \in I \tag{3}$$

The minimum and maximum capacitance rates are defined in Eqs. (4-5) where they are replaced with smooth and continuous operators,

$$\dot{C}^i_{\min} = \min\left(\dot{C}^i_c, \dot{C}^i_h\right) \approx 0.5\left(\dot{C}^i_c + \dot{C}^i_h - \sqrt{\left(\dot{C}^i_c - \dot{C}^i_h\right)^2 + \delta_1}\right) \tag{4}$$

$$\dot{C}^i_{\max} = \max\left(\dot{C}^i_c, \dot{C}^i_h\right) \approx 0.5\left(\dot{C}^i_c + \dot{C}^i_h + \sqrt{\left(\dot{C}^i_c - \dot{C}^i_h\right)^2 + \delta_2}\right) \tag{5}$$

where $\delta_2 > \delta_1$ and are small positive numbers that avoid singularities. The capacitance ratio is therefore defined by Eq. (6),

$$C_{R,i} = \frac{\dot{C}^i_{\min}}{\dot{C}^i_{\max}}, \qquad \forall i \in I \tag{6}$$

The effectiveness, $\varepsilon_i$ of each sub heat exchanger is defined as $\varepsilon_{c,i}$ for counter current flow (Eq. 7) when P is even and as $\varepsilon_{p,i}$ for co-current flow (Eq. 8) when P is odd,

$$\varepsilon_{c,i} = \begin{cases} \dfrac{1-\exp\left[-NTU_i\left(1-C_{R,i}\right)\right]}{1-C_{R,i}\exp\left[-NTU_i\left(1-C_{R,i}\right)\right]}, & C_{R_i} < 1 \\ \dfrac{NTU_i}{NTU_i+1}, \qquad C_{R,i} = 1, \end{cases}, \quad \forall i \in I \tag{7}$$

$$\varepsilon_{p,i} = \frac{1-\exp\left[-NTU_i\left(1+C_{R,i}\right)\right]}{1+C_{R,i}}, \quad \forall i \in I \tag{8}$$

The number of transfer units $(NTU)$ is determined using Eq. (9) for each sub-heat exchanger in each pass.

$$NTU_i = \frac{U_i A}{\dot{C}^i_{\min}}, \qquad \forall i \in I \tag{9}$$

Eq. 10 represents the connectivity between adjacent sub-heat exchangers.

$$T^i_{h,out} = T^{i+1}_{h,in}\ ; \qquad T^i_{c,in} = T^{i+1}_{c,out}\ ; \qquad i = 1,...,P-1 \tag{10}$$

The inlet boundary conditions are also specified as given by Eq. (11).

$$i = \begin{cases} 1, & T^i_{h,in} = T_{h,IN} \\ P, & T^i_{c,in} = T_{c,IN} \end{cases}\ ; \qquad T_{avg} = \frac{T_{h,IN} + T_{c,IN}}{2} \tag{11}$$

$T_{avg}$ is the average temperature used for evaluating the fluid and flow properties.

*Fluid and flow properties*

The fluid properties for loaded amine solvent (specific heat capacity, viscosity and thermal conductivity) are computed from appropriate correlations in the literature (Weiland et al., 1998, Hilliard, 2008, Agbonghae et al., 2014, Morgan et al., 2017). The viscosity, thermal conductivity and specific heat capacity of the liquid mixture were evaluated within the temperature range of 300-400 K. It is reasonable to assume that the physical properties calculated using the average of cold and hot inlet temperatures are constant within the expected range of operation of the PHE for post-combustion $CO_2$ capture applications.

The geometry-dependent flow properties are evaluated using Eqs. (12-16). In Eq. (12), the mass flow velocities in each channel ($G^h_{c,i}, G^c_{c,i}$) are computed for calculating the Reynold number, while the mass flow velocity through the ports ($G^h_p, G^c_p$) are computed using Eq. (13) for the pressure drop calculation given by Eq. (14). $f$ is the fanning friction factor, $D_p$ is the port diameter and $d_e$ is the equivalent channel diameter, where $b$ is the gap between the plates, $w$ is the plate width and $\phi$ account for corrugation.

$$G^h_{c,i} = \frac{\dot{m}_h}{bwNC_i}, \quad G^c_{c,i} = \frac{\dot{m}_c}{bwNC_i}, \quad d_e = \frac{2b}{\phi}, \qquad i \forall P \tag{12}$$

$$G^h_p = \frac{4\dot{m}_h}{\pi D_p^2}, \quad G^c_p = \frac{4\dot{m}_c}{\pi D_p^2}, \quad f = \frac{a_5}{\mathrm{Re}^{a_6}} \tag{13}$$

$$\Delta P = \left(\frac{2f\left(L+D_p\right)PG_c^2}{\rho d_e}\right) + 1.4\left(P\frac{G_p^2}{2\rho}\right) + \rho g\left(L+D_p\right) \tag{14}$$

The heat transfer coefficients of the hot and cold side are computed using Eq. (15) and the overall heat transfer coefficient is calculated using Eq. (16).

$$h_i^H = \left(\frac{\lambda_i^H}{d_e}\right) a_1 \left(\mathrm{Re}_i^H\right)^{a_2} \left(\mathrm{Pr}_i^H\right)^{a_3}, \quad \forall i \in I \tag{15}$$
$$h_i^C = \left(\frac{\lambda_i^C}{d_e}\right) a_1 \left(\mathrm{Re}_i^C\right)^{a_2} \left(\mathrm{Pr}_i^C\right)^{a_3},$$

$$\frac{1}{U_i} = \frac{1}{h_i^H} + \frac{\delta_p}{k_p} + \frac{1}{h_i^C}, \quad \forall i \in I \tag{16}$$

**Model Development and Parameter Estimation**

The model is developed using the modeling and optimization framework being developed by the U.S. Department of Energy's Institute for Design of Advanced Energy Systems (IDAES) (Miller et al., 2018). The IDAES framework is being built on Pyomo, an algebraic modeling language (Hart et al., 2017). For model validation, the parameters $(a_1, a_2, a_3)$ corresponding to the convective heat transfer coefficient (Eq. 15) need to be estimated since the optimal values of these parameters depend on the fluid properties as well as the specifics of the PHE (e.g. configuration, geometry and material of construction). Parameters (see Table 1) in the correlations for the convective heat transfer coefficient (i.e. for Nusselt number) have been primarily obtained for water as the fluid (Saunders, 1988, Gut et al., 2004, Khan et al., 2010). These parameters are not necessarily optimal for the amine system and the specific PHE. For optimal parameter estimation, the IDAES framework is used to estimate parameters and uncertainties where the sIpopt solver generates the covariance matrix for parameter estimates via the reduced Hessian matrix (Pirnay et al., 2012). Data from the NCCC as shown in Table 2 were used for parameter estimation (odd numbered cases) and model validation (even numbered cases). The parameter estimation problem formulation is given by Eq. (17), where *n* is the number of experiments, $\mathbf{h}(\mathbf{x};\boldsymbol{\theta})$ and $\mathbf{g}(\mathbf{x};\boldsymbol{\theta})$ are equality and inequality constraints in the model, respectively. Parameter $a_3$ is fixed to its typical value of 1/3 (Khan et al., 2010).

$$\min_{\theta \in \{a_1, a_2\}} f_{obj} = \sum_{i=1}^{n} \left(Q_{h,i}^{\exp} - Q_{h,i}^{cal}\right)^2$$
$$s.t: \ \mathbf{h}(\mathbf{x};\boldsymbol{\theta}) = 0 \tag{17}$$
$$\mathbf{g}(\mathbf{x};\boldsymbol{\theta}) \le 0$$

*Table 1: Model parameters (Saunders, 1988)*

| Parameter | Value |
|---|---|
| $a_1$ | 0.300 |
| $a_2$ | 0.663 |
| $a_3$ | 0.333 |
| $a_5$ | 1.441 |
| $a_6$ | 0.206 |

*Table 2 : Plant data (NCCC)*

| Case | $\dot{m}_h$ (kg/s) | $\dot{m}_c$ (kg/s) | $T_{h,IN}$ (K) | $T_{h,OUT}$ (K) | $Q_{h,i}^{\exp}$ (kW) |
|---|---|---|---|---|---|
| K01 | 1.892 | 2.013 | 392.4 | 330.6 | 423.524 |
| K02 | 3.279 | 3.415 | 389.7 | 336.9 | 669.439 |
| K03 | 0.883 | 0.927 | 394.1 | 321.7 | 236.316 |
| K04 | 0.833 | 0.929 | 394.4 | 322.5 | 234.116 |
| K05 | 1.892 | 2.005 | 393.9 | 331.6 | 431.931 |
| K06 | 1.892 | 1.964 | 382.6 | 323.6 | 373.310 |
| K07 | 3.278 | 3.362 | 376.5 | 324.7 | 567.498 |
| K08 | 3.237 | 3.348 | 392.8 | 334.8 | 682.963 |
| K09 | 0.883 | 0.928 | 389.8 | 325.0 | 198.385 |
| K10 | 0.883 | 0.934 | 396.0 | 319.1 | 253.653 |
| K11 | 1.892 | 2.103 | 392.3 | 331.4 | 415.363 |
| K12 | 1.892 | 1.994 | 392.5 | 331.2 | 418.457 |
| K13 | 1.892 | 1.968 | 392.5 | 330.6 | 419.694 |
| K14 | 2.459 | 2.611 | 391.3 | 333.1 | 501.607 |
| K15 | 2.459 | 2.599 | 391.1 | 330.1 | 522.263 |
| K16 | 1.148 | 1.209 | 394.2 | 325.1 | 285.436 |
| K17 | 1.892 | 1.960 | 392.4 | 329.9 | 422.490 |

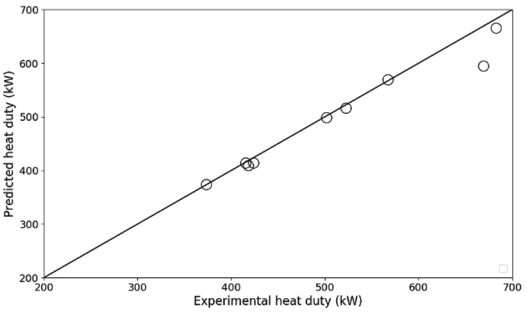
**Results**

The optimal parameters are presented in Table 3. The comparison of calculated vs plant heat load is presented in Figure 2a. The calculated heat loads are found to have ±4% error. Figure 2b compares the calculated and actual plant exit temperatures for both the rich and lean solvents. It can be observed that the model is in excellent agreement with the experimental data. Figure 2c shows the profile of the hot and cold streams along the channels for a specific case. It is observed that the hot end temperature approach is about 3°C, which points to the high heat transfer efficiency of this PHE in the NCCC pilot plant. This is further reflected by the high thermal effectiveness for all cases presented in Table 4.

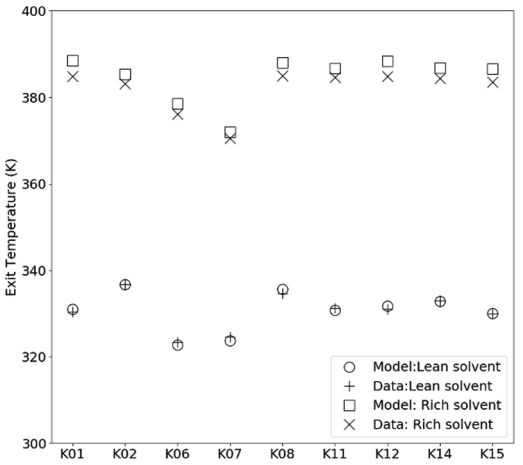
*Table 3 : Optimization results*

| Parameter | Estimate | $\sigma_{SE}$ |
|---|---|---|
| $a_1$ | 0.4000 | 0.0094 |
| $a_2$ | 0.5746 | 0.3724 |

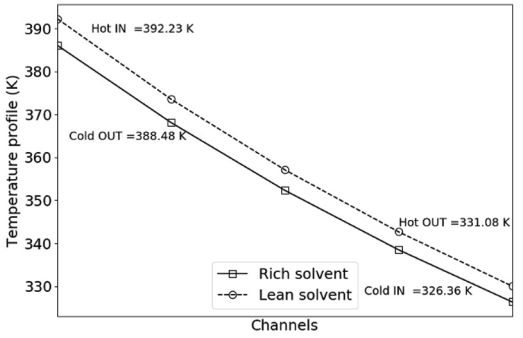
The corresponding capacitance ratios are also included in Table 4. One important consideration of the PHE design is the pressure drop. There can be high pressure drop in PHEs due to the turbulence caused by the narrow flow channels and plate geometry.




(a)




(b)




(c)

*Figure 2: (a) Parity plot for the PHE heat transferred,(b) Exit temperature with plant data,(c) Temperature profile across the channels for case K01*

While high turbulence may be beneficial for increasing the heat transfer coefficient, the tradeoff with the pressure drop must be considered while designing the PHE. The calculated pressure drops for both the cold and hot streams are shown in Table 4. It can be observed that the pressure drop for both streams is around 0.2 bar irrespective of the variations in the flowrates as shown in the corresponding cases in Table 2.

*Table 4 : Performance of PHE showing effectiveness and pressure drop for cases in Figure 2b*

| Case | $\varepsilon$ | $CR$ | $\Delta P_c$ (kPa) | $\Delta P_h$ (kPa) |
|---|---|---|---|---|
| K01 | 0.7842 | 0.9874 | 21.654 | 20.187 |
| K02 | 0.7482 | 0.9893 | 22.705 | 21.370 |
| K06 | 0.7889 | 0.9889 | 22.291 | 21.491 |
| K07 | 0.7509 | 0.9895 | 23.204 | 22.304 |
| K08 | 0.7437 | 0.9923 | 21.965 | 20.774 |
| K11 | 0.8009 | 0.9401 | 21.632 | 20.259 |
| K12 | 0.7849 | 0.9845 | 21.366 | 20.253 |
| K14 | 0.7713 | 0.9795 | 22.228 | 20.867 |
| K15 | 0.7704 | 0.9843 | 22.255 | 20.918 |

## Conclusion

A mathematical model of a PHE as part of an amine-scrubbing process for post combustion $CO_2$ capture has been developed and implemented in the IDAES PSE platform. The thermal model is based on the ε-NTU approach where the non-smooth min-max capacitance rates are replaced by smooth functions to improve the convergence properties of the optimization problem. Parameters corresponding to the convective heat transfer coefficients are estimated with quantified uncertainty using the data from the NCCC pilot plant. An optimal PHE design needs to maximize heat recovery without an unacceptably high pressure drop. The model developed in this work not only provides accurate estimates of the heat transfer in the PHE for a wide operating regime but also provides estimate of the pressure drop as the hardware designs such as the number of passes and/or plate specifications are changed. Therefore the model presented here can be leveraged for optimal design of PHEs for solvent-based post-combustion $CO_2$ capture applications.

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## References


Agbonghae, E. O., K. J. Hughes, D. B. Ingham, L. Ma and M. Pourkashanian (2014). "A semi-empirical model for estimating the heat capacity of aqueous solutions of alkanolamines for $CO_2$ capture." Industrial & Engineering Chemistry Research 53(19): 8291-8301.

Dardour, H., S. Mazouz and A. Bellagi (2009). "Numerical Analysis of Plate Heat Exchanger Performance in Co-Current Fluid Flow Configuration." World Academy of Science, Engineering and Technology 3: 2278-0181.

Flø, N. E., H. Knuutila, H. M. Kvamsdal and M. Hillestad (2015). "Dynamic model validation of the post-combustion $CO_2$ absorption process." International Journal of Greenhouse Gas Control 41: 127-141.

Georgiadis, M. C. and S. Macchietto (2000). "Dynamic modelling and simulation of plate heat exchangers under milk fouling." Chemical Engineering Science 55(9): 1605-1619.

Gut, J. A. W., R. Fernandes, J. M. Pinto and C. C. Tadini (2004). "Thermal model validation of plate heat exchangers with generalized configurations." Chemical Engineering Science 59(21): 4591-4600.

Gut, J. A. W. and J. M. Pinto (2003). "Modeling of plate heat exchangers with generalized configurations." International Journal of Heat and Mass Transfer 46(14): 2571-2585.

Hart, W. E., C. D. Laird, J.-P. Watson, D. L. Woodruff, G. A. Hackebeil, B. L. Nicholson and J. D. Siirola (2017). Pyomo—Optimization Modeling in Python, Springer.

Harun, N., T. Nittaya, P. L. Douglas, E. Croiset and L. A. Ricardez-Sandoval (2012). "Dynamic simulation of MEA absorption process for $CO_2$ capture from power plants." International Journal of Greenhouse Gas Control 10: 295-309.

Hilliard, M. D. (2008). A predictive thermodynamic model for an aqueous blend of potassium carbonate, piperazine, and monoethanolamine for carbon dioxide capture from flue gas PhD Thesis., The University of Texas at Austin.

Khan, T., M. Khan, M.-C. Chyu and Z. Ayub (2010). "Experimental investigation of single phase convective heat transfer coefficient in a corrugated plate heat exchanger for multiple plate configurations." Applied Thermal Engineering 30(8-9): 1058-1065.

Lin, Y.-J. and G. T. Rochelle (2017). "Heat Transfer Enhancement and Optimization of Lean/Rich Solvent Cross Exchanger for Amine Scrubbing." Energy Procedia 114: 1890-1903.

Miller, D. C., J. D. Siirola, D. Agarwal, A. P. Burgard, A. Lee, J. C. Eslick, B. Nicholson, C. Laird, L. T. Biegler and D. Bhattacharyya (2018). Next Generation Multi-Scale Process Systems Engineering Framework. Computer Aided Chemical Engineering, Elsevier. 44: 2209-2214.

Morgan, J. C., A. S. Chinen, B. Omell, D. Bhattacharyya, C. Tong and D. C. Miller (2017). "Thermodynamic modeling and uncertainty quantification of $CO_2$-loaded aqueous MEA solutions." Chemical Engineering Science 168: 309-324.

Nellis, G. and S. Klein (2009). Heat Transfer. New York, USA, Cambridge University Press.

Nittaya, T., P. L. Douglas, E. Croiset and L. A. Ricardez-Sandoval (2014). "Dynamic modeling and evaluation of an industrial-scale $CO_2$ capture plant using monoethanolamine absorption processes." Industrial & Engineering Chemistry Research 53(28): 11411-11426.

Pirnay, H., R. López-Negrete and L. T. Biegler (2012). "Optimal sensitivity based on IPOPT." Mathematical Programming Computation 4(4): 307-331.

Saunders, E. A. D. (1988). Heat exchangers: selection, design & construction, Longman.

Weiland, R. H., J. C. Dingman, D. B. Cronin and G. J. Browning (1998). "Density and viscosity of some partially carbonated aqueous alkanolamine solutions and their blends." Journal of Chemical & Engineering Data 43(3): 378-382.