다성분 흡수탑에서의 물질,열전달률에 관한 연구

Valeri A. Danilov ,문일
연세대학교 화학공학과

Heat and Mass Transfer Rates Evaluation From Operation Data of a Packed Column on Multicomponent Absorption

Valery A. Danilov and Il Moon†
Department of Chemical Engineering, Yonsei University

Introduction

Design of packed bed columns for gas absorption is complicated by thermal effects associated with heat and mass transfer between phases. Development of new technologies using packed columns set problems which require creation of reliable unit models generalizing the knowledge on heat and mass transfer. A number of correlations have been proposed for heat and mass transfer coefficients calculation in a packed bed derived from pilot plant tests. However, the experimental techniques used did not permit a simultaneous examination of the effect of axial mixing on heat and mass transfer. Methods[1-3] were described of simultaneous evaluation of axial dispersion coefficients and interphase mass transfer coefficients from component concentration profiles. The purpose of this paper is to develop a method of heat and mass transfer rates estimation from column operation data in the case of multicomponent gas absorption taking into account flow patterns.

Parameter Estimation Using Steady State Data

Heat and mass transfer processes in a unit are conventionally described in therms of diffusion model. Unit model is based on the following assumptions: (i) steady state condition; (ii) one - dimensional flow of vapor and liquid; (iii) local phase equilibrium and no resistance to mass transfer at the interface; (iv) liquid and vapor holdup is independent of coordinate.

We need to define objective function and to establish computation consequence of the problem. Required input data for the backward calculation of mass transfer rates are flow rates, temperature and component concentrations in streams entering and leaving the packed bed which are given from experiments or commercial tests. Axial dispersion coefficients $D_{p,L,}$ $D_{p,G}$ are found by minimizing the following objective function:

$$S = \frac{1}{\sigma_L^2}(X_{out,i}^{bal} - X_{out,i}^{calc})^2 + \frac{1}{\sigma_G^2}(Y_{out,i}^{bal} - Y_{out,i}^{calc})^2 + \frac{W_L}{\sigma_{t,L}^2}(T_{L,out}^{bal} - T_{L,out}^{calc})^2 + \frac{W_G}{\sigma_{t,G}^2}(T_{G,out}^{bal} - T_{G,out}^{calc})^2 \quad (1)$$

subject to

$$-L\frac{dX_i}{dz} - \varepsilon_L \rho_{m,L} S_{col} D_{p,L}\frac{d^2X_i}{dz^2} = S_{col}\rho_{m,L}K_{v,L,i}^{\bullet}(X_i - X_i^*) \quad (2)$$

$$G\frac{dY_i}{dz} - \varepsilon_G \rho_{m,G} S_{col} D_{p,G}\frac{d^2Y_i}{dz^2} = -S_{col}\rho_{m,G}K_{v,L,i}^{\bullet}(X_i - X_i^*) \quad (3)$$

$$-C_{p,L}L\frac{dT_L}{dz} - \rho_{m,L}C_{p,L}\varepsilon_L S_{col} D_{p,L}\frac{d^2T_L}{dz^2} = S_{col}K_{v,t}^{\bullet}(T_G - T_L) \quad (4)$$

$$G\frac{dH_G}{dz} - \rho_{m,G}\varepsilon_G C_{p,G} S_{col} D_{p,G}\frac{d^2T_G}{dz^2} = -S_{col}K_{v,t}^{\bullet}(T_G - T_L) \quad (5)$$

$$z = h,\ X_i = X_{0,i} - \frac{\rho_{m,L}\varepsilon_L S_{col} D_{p,L}}{L}\frac{dX_i}{dz},\ T_L = T_{L,0} - \frac{\rho_{m,L}\varepsilon_L S_{col} D_{p,L}}{L}\frac{dT_L}{dz} \quad (6)$$

$$z = 0,\ \frac{dX_i}{dz} = 0,\ \frac{dT_L}{dz} = 0 \quad (7)$$

$$z = 0,\ Y_i = Y_{0,i} + \frac{\rho_{m,G}\varepsilon_G S_{col} D_{p,G}}{G}\frac{dY_i}{dz}, \tag{8}$$

$$z = 0,\ H_{G,i} = H_{G,0} + \frac{C_{p,G}\rho_{m,G}\varepsilon_G S_{col} D_{p,G}}{G}\frac{dT_G}{dz} \tag{9}$$

$$z = h\ ,\ \frac{dY_i}{dz} = 0,\quad \frac{dH_G}{dz} = 0 \tag{10}$$

$$D_{p,L,min} < D_{p,L} < D_{p,L,max},\ D_{p,G,min} < D_{p,G} < D_{p,G,max} \tag{11}$$

where $\sigma_L, \sigma_G, \sigma_{t,L}, \sigma_{t,G}$ - root - mean - square; $Y^{bal}_{out,i}$, $X^{bal}_{out,i}$ - concentrations of i - component in liquid and vapor streams leaving the packed bed according to mass balance equation; $Y^{calc}_{out,i}$, $X^{calc}_{out,i}$ - concentrations of i - component in liquid and vapor streams leaving the packed bed predicted by the unit model; $Y_{0,i}$, $X_{0,i}$ - concentrations of i - component in liquid and vapor streams entering the packed bed; $T^{bal}_{G,out}$, $T^{bal}_{L,out}$ - temperatures of liquid and vapor streams leaving the bed according to heat balance equation; $T^{calc}_{G,out}$, $T^{calc}_{L,out}$ - temperatures of liquid and vapor streams leaving the packed bed predicted by the model; $T_{G,0}$, $T_{L,0}$ - temperatures of liquid and vapor streams entering the packed bed. W - weighting coefficient; D_p - axial dispersion coefficient; K_t - overall heat transfer coefficient; L - liquid flow rate; G - vapor flow rate; H - enthalpy; ρ_m - molar phase density; ε - phase volume fraction in two phase flow; S_{col} - area.

It should be noted that the unit model equations (1) - (11) are strongly nonlinear and coupled. The conventional approach to solve optimization problem (1) - (11) including ordinary differential equations is to directly apply standard discretization techniques to transform ODE constraints into a large set of algebraic constraints.

Mean overall heat and mass transfer driving forces are computed as follows

$$\Delta\overline{X}_i = \frac{1}{h}\int_0^h (X_i - X_i^*)dz,\ \Delta\overline{T} = \frac{1}{h}\int_0^h (T_G - T_L)dz \tag{12}$$

where h - packing height.

Mass transport coefficient by definition is

$$K^{\bullet}_{v,L,i} = \frac{M_{L,i}}{V\,\rho_{m,L}\Delta\overline{X}_i} \tag{13}$$

Molar flow rate of i - component transferred through interphase $M_{L,i}$ is found from component - material balance.

Heat transport coefficient is

$$K^{\bullet}_{v,t} = \frac{Q}{V\,\Delta\overline{T}} \tag{14}$$

Heat flux transferred through interphase Q is calculated from heat balance.

Global iteration by equations (1) - (14) are repeated until successive temperature and concentration profiles converge.

To determine the values of the unknown parameters we need to minimize the deviation of the unit model prediction from column operating data. This is the objective of the parameter estimation problem. As a result of commercial data processing by proposed method we can determine the unit model parameters and corresponding transfer coefficients. The given algorithm was realized by commercial package MATLAB. Unit model test for goodness of fit was carried out by experimental data processing for multicomponent absorption in a packed column given in literature.

Results and Discussion

Bassyoni and McDanlel[4] et al. have presented the results of field tests of packed bed absorption column. Experimental data reported include product flow rates, composition and temperature profiles over the packed height. Field tests were made on a packed absorber at the Zoller Gas Plant at Refugio (Texas). The packed absorber had a diameter of 0.9144 m and it was packed with 2-in Pall rings. Other experimental details may be found in the publication[4].

The results from calculations by our unit model for multicomponent absorption using estimated parameters in the industrial column are presented in Table 1 and Fig. 1.

Table 1 Results of computation of the packed absorber by the model

Quantity	Lean gas		Rich oil		Mass transport coefficient, 1/s
	Experiment[4], mole fraction	Model, mole fraction	Experiment[4], mole fraction	Model, mole fraction	
1 Carbon dioxide	$6.8098\ 10^{-3}$	$6.6131\ 10^{-3}$	$4.7073\ 10^{-3}$	$4.7073\ 10^{-3}$	$3.1845\ 10^{-4}$
2 Nitrogen	$2.8199\ 10^{-3}$	$2.7048\ 10^{-3}$	$1.5934\ 10^{-3}$	$1.5934\ 10^{-3}$	$-4.7081\ 10^{-3}$
3 Methane	$9.3778\ 10^{-1}$	$8.7272\ 10^{-1}$	$2.4525\ 10^{-1}$	$2.4525\ 10^{-1}$	$6.0486\ 10^{-4}$
4 Ethane	$4.6434\ 10^{-2}$	$5.4705\ 10^{-2}$	$1.3291\ 10^{-1}$	$1.3291\ 10^{-1}$	$9.5911\ 10^{-4}$
5 Propane	$5.2298\ 10^{-3}$	$1.8710\ 10^{-2}$	$1.4805\ 10^{-1}$	$1.4805\ 10^{-1}$	$6.9952\ 10^{-4}$
6 Isobutene	$2.2999\ 10^{-4}$	$4.2671\ 10^{-3}$	$4.3007\ 10^{-2}$	$4.3007\ 10^{-2}$	$3.0692\ 10^{-4}$
7 n-Butane	$3.9999\ 10^{-5}$	$2.6163\ 10^{-3}$	$2.7335\ 10^{-2}$	$2.7335\ 10^{-2}$	$1.9891\ 10^{-4}$
8 Isopentane	$9.9996\ 10^{-6}$	$6.7319\ 10^{-4}$	$7.0368\ 10^{-3}$	$7.0368\ 10^{-3}$	$7.3582\ 10^{-5}$
9 n-Pentane	$9.9996\ 10^{-6}$	$3.2205\ 10^{-4}$	$3.3164\ 10^{-3}$	$3.3164\ 10^{-3}$	$5.2459\ 10^{-5}$
10 Hexane	$3.9999\ 10^{-6}$	$1.4516\ 10^{-4}$	$1.4997\ 10^{-3}$	$1.4997\ 10^{-3}$	$6.9640\ 10^{-6}$
11 Heptane	$6.0000\ 10^{-5}$	$2.4609\ 10^{-3}$	$2.5500\ 10^{-2}$	$2.5503\ 10^{-2}$	$-3.2928\ 10^{-5}$
12 Octane	$3.2999\ 10^{-4}$	$1.4461\ 10^{-2}$	$1.5007\ 10^{-1}$	$1.5008\ 10^{-1}$	$-2.0870\ 10^{-4}$
13 Nonane	$1.1000\ 10^{-4}$	$1.2286\ 10^{-2}$	$1.2913\ 10^{-1}$	$1.2915\ 10^{-1}$	$-1.6490\ 10^{-4}$
14 Decane	$1.2771\ 10^{-4}$	$7.3051\ 10^{-3}$	$8.0575\ 10^{-2}$	$8.0539\ 10^{-2}$	$-9.5296\ 10^{-5}$
Total flow rate, kmole/s	0.31873	0.31873	0.05423	0.05423	
Temperature, K	269.11	268.9	264.11	264.0	

Phase equilibrium and mixture properties were computed using IVC - SEP program package[5].

Table 1 suggests that the discrepancy between predicted and measured concentrations for components presented in the range 1 % mol is quite large. This is mainly due to the large discrepancy in the amount of methane transferred from vapor to liquid phase. The direction of mass transfer in the case absorption is from vapor to liquid and hence the composition profiles in Fig.1 are monotonic. Satisfactory fit of computation results with experimental data confirms applicability of diffusion model for heat and mass transfer processes simulation in a packed bed.

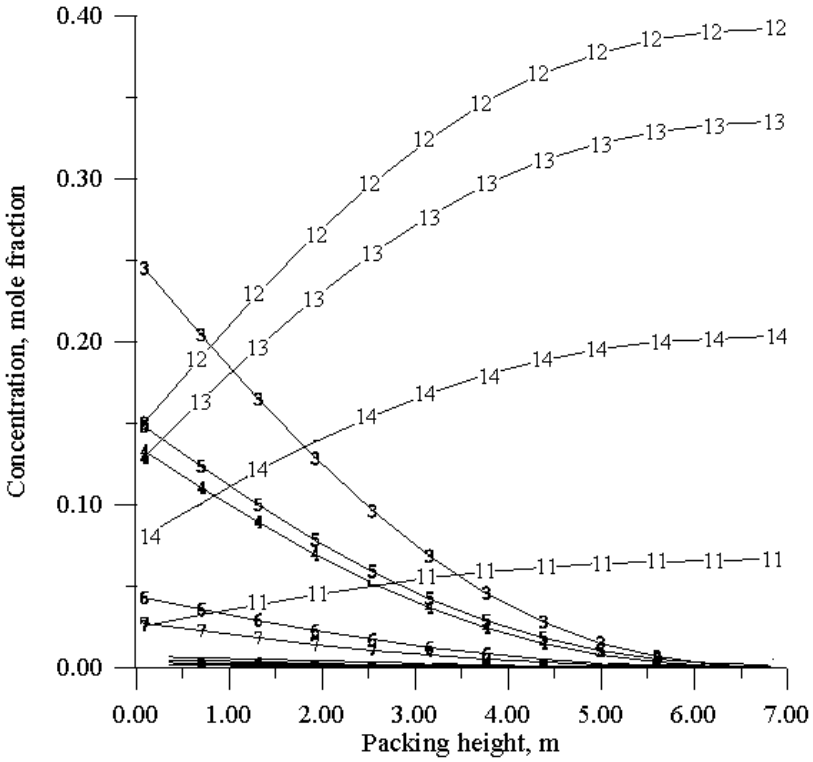

Figure 1. Predicted component concentration profiles for the packed absorber. Axial dispersion coefficient in liquid phase 1.0 10^{-4} m^2/s; Axial dispersion coefficient in vapor phase 1.34 10^{-3} m^2/s; Liquid holdup 3.9 10^{-2}; Heat transport coefficient 4356.93 $W/(m^3 K)$; Column pressure 5.45 MPa; Packing height 7 m.

Conclusion

The proposed model is equally applicable to the simulation of distillation and absorption columns. The developed methodology allows simultaneous evaluation of unit model parameters from commercial data for a packed column of any scale separating any mixture. Application of the proposed method for different packings will allow us to create data bank on heat and mass transfer for columns of different scale. Generalization of commercial data will lead to development of new reliable models and correlations for heat and mass transfer coefficients.

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