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ANALYSIS OF PACKED DISTILLATION COLUMNS WITH A RATE-BASED MODEL

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Abstract – Multicomponent packed column distillation is simulated using a rate-based model and the simulation results are compared with the experimental results obtained from a 0.2 m diameter pilot-scale packed column. The simulation algorithm used is previously proposed by the authors, which based on an equation-tearing method for (6c+7) equations of one packing segment and the whole column is solved by an iterative segmentwise calculation with the overall normalized θ method for acceleration. The performance of two packings is examined by simulating the pilot-scale column experiments using the published correlations for estimating liquid and vapor phase mass transfer coefficients and an effective interfacial area.

Key words: Distillation, Simulation, Rate-based Model, Heat and Mass Transfer Coefficient, Effective Interfacial Area

INTRODUCTION

Recent development of structured packings for distillation columns are attracting more engineers' attention in retrofitting or improving the existing stage columns. After a new class of simulation method, rate-based or nonequilibrium method, was introduced by Krishnamurthy and Taylor [1985, 1987], it enables us to evaluate more precisely the separation performance of the packed columns. The correlations for hydraulics and other characteristics of commercial packings have been published continuously [Billet and Schlutes, 1993; Bravo et al., 1985; Henriques de Brito et al., 1992, 1994; Fair and Bravo, 1987; Brunazzi et al., 1985; Weiland et al., 1993]. Their applicability to practical distillation is not justified clearly. Successful application of the rate-based method to the packed column distillation simulation depends on the appropriate choice of prediction methods for transport properties and the effective interfacial area for heat and mass transfer.

We have developed a simulation method for packed column distillation based on the rate-based model in which the so-called MERQ (Material balance, Energy balance, Rate, Equilibrium) equations in any segment of the packing are solved with an equation-tearing technique [Mori et al., 1996]. In the following we will compare the experimental results with the simulation results obtained using the published correlations to evaluate their applicability.

ASSUMPTIONS AND BASIC EQUATION

Fig. 1 gives a schematic illustration of a small segment in a packed column.

The model consists of bulk liquid flowing down on a packing surface, bulk vapor flowing up through the space between packings, and vapor-liquid interface. Heat and mass transfer occurs only through this interface. The vapor from the adjacent segment V_{j+1} with the composition $y^V_{j+1,i}$, temperature T^V_{j+1} and enthalpy H^V_{j+1} enters the j-th segment, and after the heat and mass transfers, E^V_j and $N^V_{j,i}$, through the interface the vapor V_j leaves the segment with $y^V_{j,i}$, T^V_j, H^V_j. The corresponding phenomena are assumed to occur in the liquid phase. The column is assumed to be adiabatic. Feed and sidecuts are made between the segments using a collector-distributor device, where the vapor and liquid phase are mixed individually and completely before entering the next segment or sidecuts. The whole column is represented by the stack of the segments, and each segment is numbered from the top to the bottom. According to Fig. 1 the balance equations for the bulk liquid, bulk vapor and interface are given as follows:

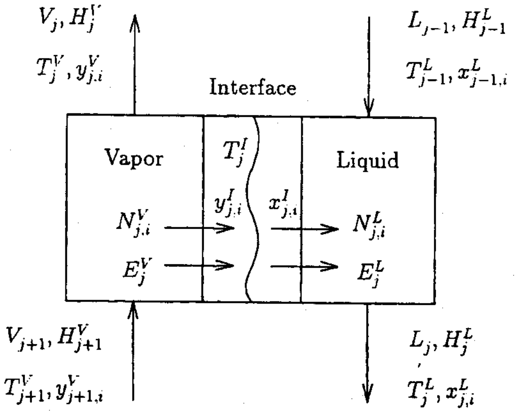

Fig. 1. Rate based model of the j-th segment of packing.

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Total material balance equations

$$L_{j-1}-L_j=-N^L_{j,t}\ a_j \tag{1}$$

$$-V_j+V_{j+1}=N^V_{j,t}\ a_j \tag{2}$$

$$N^L_{j,t}=N^V_{j,t} \tag{3}$$

Component material balance equations

$$L_{j-1}x^L_{j-1,i}-L_jx^L_{j,i}=-N^L_{j,i}\ a_j \qquad (i=1,\cdots,c-1) \tag{4}$$

$$-V_jy_{j,i}+V_{j+1}y^V_{j+1,i}=-N^V_{j,i}\ a_j \qquad (i=1,\cdots,c-1) \tag{5}$$

$$N^L_{j,i}=N^V_{j,i} \qquad (i=1,\cdots,c-1) \tag{6}$$

Energy balance equations

$$L_{j-1}H^L_{j-1}-L_jH^L_j=-E^L_j\ a_j \tag{7}$$

$$-V_jH^V_j+V_{j+1}H^V_{j+1}=E^V_j\ a_j \tag{8}$$

$$E^L_j=E^V_j \tag{9}$$

where N is the mass flux and E_j is the heat flux in the liquid and vapor side films. a is the interfacial area for heat and mass transfer. H is the molar enthalpy of the bulk liquid and vapor.

The mass transfer rates considering bulk flow terms are employed.

Rate equation for mass transfer

$$N^L_{j,i}=\sum_{k=1}^{C-1}k^L_{i,k}(x^I_{j,k}-\overline{x^L_{j,k}})+\overline{x^L_{j,i}}\ N^L_{j,t} \qquad (i=1,\cdots,c-1) \tag{10}$$

$$N^V_{j,i}=\sum_{k=1}^{C-1}k^V_{i,k}(\overline{y^V_{j,k}}-y^I_{j,k})+\overline{y^V_{j,i}}\ N^V_{j,t} \qquad (i=1,\cdots,c-1) \tag{11}$$

In the same way as above, the heat transfer rates are expressed as follows.

Rate equation for heat transfer

$$E^L_j=h^L_j(T^I_j-\overline{T^L_j})+\sum_{i=1}^{C}N^L_{j,i}\ \overline{H^L_{j,i}} \tag{12}$$

$$E^V_j=h^V_j\frac{\varepsilon^V}{e^{\varepsilon^V}-1}(\overline{T^V_j}-T^I_j)+\sum_{i=1}^{C}N^V_{j,i}\ \overline{H^V_{j,i}} \tag{13}$$

ε^V is defined as follow

$$\varepsilon^V=\sum_{i=1}^{C}N^V_{j,i}\ C^V_{p,i}/h^V_j \tag{14}$$

where k is multicomponent mass transfer coefficient, and $\overline{H}$ is partial molar enthalpy of liquid and vapor. h is heat transfer coefficient in the liquid and vapor. Superscripts (-) to the composition and temperature means averaged values considering flow regimes. Phase equilibrium is assumed to hold at the interface.

Equilibrium equation at the interface

$$y^I_{j,i}=\gamma_{j,i}\ p^s_{j,i}\ x^I_{j,i}/P_j \qquad (j=1,\cdots,c) \tag{15}$$

Stoichiometric relation gives the following equations for the compositions of the bulk phase and the interface.

Summation equations

$$\sum_{i=1}^{C}x^L_{j,i}=1 \tag{16}$$

$$\sum_{i=1}^{C}y^V_{j,i}=1 \tag{17}$$

$$\sum_{i=1}^{C}x^I_{j,i}=1 \tag{18}$$

$$\sum_{i=1}^{C}y^I_{j,i}=1 \tag{19}$$

EXPERIMENTAL

A schematic drawing of the packed column distillation plant is shown in Fig. 2.

The dimensions of the packed column and the geometry of the packings, MC-250T and 250S, are listed in Table 1. The feed is introduced at the middle of the column using a collector-distributor device which is considered not to work as a separation element. The enriching and stripping sections consist of six packing elements. The structure of both packings is similar to that of other commercial corrugate sheet-type packings, except that MC-250T is constructed with a metal sheet sandwiched by gauze and MC-250S with a single metal sheet embossed with wave patterns. Thus, the wetting characteristic of MC-250T is close to that of gauze-type packings. The operating conditions and product compositions for the experiment with MC-250T are shown in Table 2. The experiment using MC-250S is conducted with a lower ethanol composition feed under a smaller reflux ratio.

SIMULATION RESULTS AND DISCUSSION

The experiment described above is simulated using a pre-

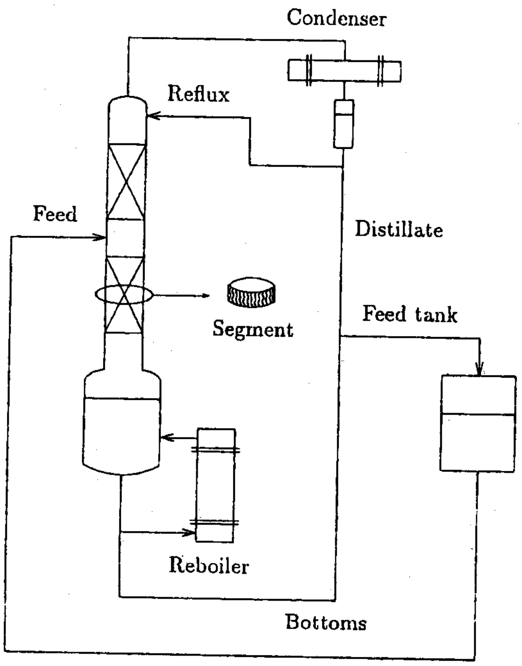

Fig. 2. Packed distillation column.

Table 1. Dimensions of packed column and packing element

Column		
Column height		3.00 m
Packed height		2.20 m
Diameter		0.21 m
Capacity of still		0.30 m^3
Heat transfer area of reboiler		7.80 m^2
Heat transfer area of condenser		12.30 m^2
Packing	**(MC-250T*)**	**(MC-250S*)**
Element diameter	0.199 m	0.199 m
Element height	0.183 m	0.183 m
Height of triangle	9.9×10^{-3} m	9.9×10^{-3} m
Base of triangle	25.4×10^{-3} m	25.4×10^{-3} m
Corrugation spacing	15.6×10^{-3} m	15.6×10^{-3} m
Specific surface area	250 m^2/m^3	250 m^2/m^3
Void fraction	0.98	0.98
Channel flow angle	45°	45°

*MC Pack Co.

Table 2. Experimental conditions

System	Methanol (1)/Ethanol (2)/Water (3)
Pressure	101.4 kPa
Feed	1.11 mol/s T^F=333.15 K (center feed)
	(1) 0.185 (2) 0.045 (3) 0.770
Distillate	0.19 mol/s
Bottoms	0.92 mol/s
Reflux	R_D=6.42, T_1^L=312.55 K

viously proposed method [Mori et al., 1996] with the assumption described in Table 3. The physical properties of pure substance are estimated as in Daubert and Danner [1989]. The correlations for binary mass transfer coefficients, k^{bL} and k^{bV}, and effective interfacial area are listed in Table 4 for two commercial structured packings. The same correlation of the vapor phase mass transfer coefficient as Sulzer BX's is used for Mellapak.

The simulated liquid composition profiles are shown in Fig. 3 and 4 with the observed data including four additional liquid composition taken along the length of the column. Solid lines and dashed lines are obtained using the correlations for "Sulzer BX" and "Mellapak", respectively. The examination of the detail shows that the correlation of "Mellapak" predicts the value of k^{bL} which is about 1/10 of Sulzer BX. This results in the lower separation performance in the simulation.

Table 3. Estimation of properties of mixture

Vapor diffusivity	Brokaw [Reid et al., 1987]
Liquid diffusivity	
(at infinite dilution)	Reddy and Doraisway [Reid et al., 1987]
(at finite dilution)	Vignes [Reid et al., 1987]
Vapor viscosity	Brokaw [Reid et al., 1987]
Vapor thermal conductivity	Lindsay-Bromley [Reid et al., 1987]
Liquid thermal conductivity	Li [Reid et al., 1987]
Others	molar average
Activity coefficient model	ASOG [Tochigi et al., 1990]
Mass transfer coefficient	see Table 4
Heat transfer coefficient	Chilton-Colburn [Brid et al., 1963]

Table 4. Correlations of mass transfer coefficients for structured packings

Packings	Correlation
Sulzer BX	Bravo et al. [1985]
(Sulzer Bros.)	$k^{bL}/\rho_m^{LM}=2\ [D^L u_{Le}/(\pi S)]^{0.5}$
	$Shv=0.0338\ Re_v^{0.8}\ Sc_v^{0.333}$
	$a_e=a_p$
Mellapak	Henriques de Brito et al. [1992]
(Sulzer Bros.)	(250 Y) $k^{bL}/\rho_m^{LM}=3.34\times10^{-5}\ B^{0.302}$
	(500 Y) $k^{bL}/\rho_M^{LM}=1.97\times10^{-5}\ B^{0.302}$
	where B is specific liquid load [$m^3/m^2\cdot h$]
	Henriques de Brito et al. [1994]
	$a_e/a_p=0.465Re_L^{0.30}$

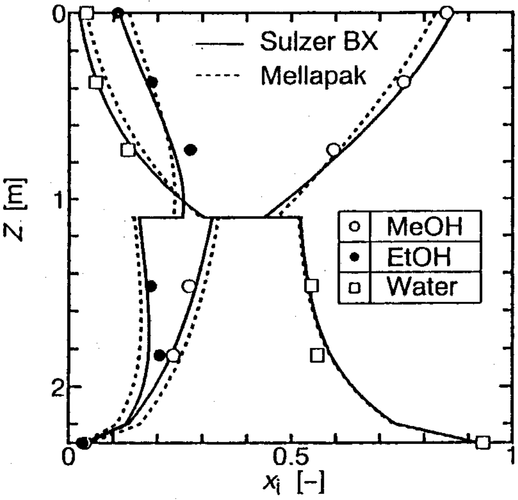

Fig. 3. Simulated composition profiles (MC 250T).

CONCLUSION

The ternary distillation experiments using a 0.2 m packed column are simulated with a rate-based model. The use of the correlations of liquid-phase mass transfer coefficients for

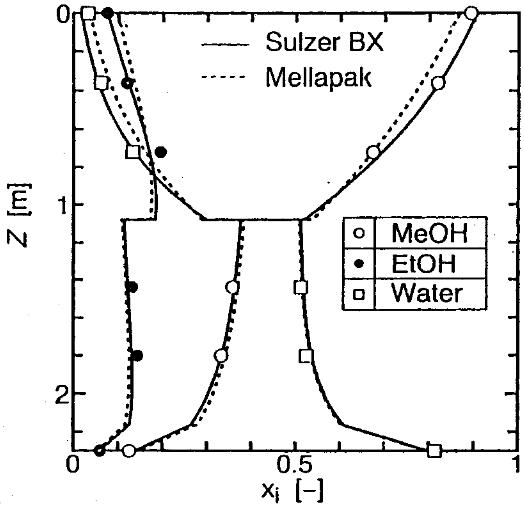

Fig. 4. Simulated composition profiles (MC 250S).

different packings shows a small but definite influence on the simulation results.

The both packings used prove to have the performance close to Sulzer BX predicted using the published correlations.

NOMENCLATURE

a : interfacial area of liquld and vapor $[m^2]$
a_e : effective interfacial area per unit volume $[m^2/m^3]$
a_p : specific surface area of packing $[m^2/m^3]$
c : component number [-]
C_p : heat capacity $[J/kmol \cdot k]$
D : Fick diffusivity $[m^2/s]$
E : heat transfer rate $[W/m^2]$
H : molar enthalpy [J/kmol]
h : heat transfer coefficient $[W/m^2 \cdot k]$
k : multicomponent mass transfer coefficient $[kmol/m^2 \cdot s]$
k^b : zero flux binary mass transfer coefficient $[kmol/m^2 \cdot s]$
L : mole flow rate of the liquld [kmol/s]
N : mass transfer rate $[kmol/m^2 \cdot s]$
P : pressure $[P_a]$
P^S : saturated vapor pressure $[P_a]$
T : temperature [K]
V : molar flow rate of the vapor [kmol/s]
χ : mole fraction in liquid phase [-]
y : mole fraction in vapor phase [-]
Z : position in distillation column [m]

Greek Letters

γ : activity coefficient [-]
ε^V : defined in Eq. (14) [-]
ρ_m : molar density $[kmol/m^3]$

Superscripts

I : referring to interface
L : referring to liquid phase
V : referring to vapor phase
- : average or partial molar value

Subscripts

i : component number
j : segment number
m : mean value
t : referring to mixture total

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