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Letters to the Editors

Prediction of multicomponent distillation efficiencies

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Dear Sirs,

Medina *et al.*[1] have recently proposed a method for the prediction of Murphree efficiencies in multicomponent systems from information on the efficiencies of the constituent binary pairs. Briefly, they suggest the following procedure.

(1) Calculate the number of overall gas phase mass transfer units for each binary system $(N_{OG})_{ij}$ $(ij = 12, 13, 23)$ from

$$(N_{OG})_{ij} = -\ln(1 - (E_{OG})_{ij}) \tag{1}$$

(2) Calculate the number of ternary overall gas phase mass transfer units $(\mathbf{N}_{OG})_{ij}$ $(ij = 11, 12, 21, 22)$ from

$$\begin{aligned}
(\mathbf{N}_{OG})_{11} &= (N_{OG})_{13}[y_1(N_{OG})_{23} + (1-y_1)(N_{OG})_{12}]/\omega \\
(\mathbf{N}_{OG})_{12} &= y_1(N_{OG})_{23}[(N_{OG})_{13} - (N_{OG})_{12}]/\omega \\
(\mathbf{N}_{OG})_{21} &= y_2(N_{OG})_{13}[(N_{OG})_{23} - (N_{OG})_{12}]/\omega \\
(\mathbf{N}_{OG})_{22} &= (N_{OG})_{23}[y_2(N_{OG})_{13} + (1-y_2)(N_{OG})_{12}]/\omega
\end{aligned} \tag{2}$$

with

$$\omega = y_1(N_{OG})_{23} + y_2(N_{OG})_{13} + y_3(N_{OG})_{12} \tag{3}$$

(3) The ternary Murphree efficiencies are then to be calculated from knowledge of the matrix of overall gas phase mass transfer units $[\mathbf{N}_{OG}]$ calculated above from eqns (2).

It is important to appreciate here that the relations (2) originate from the Maxwell–Stefan diffusion equations for ideal gas mixtures[2, 3] and are strictly applicable in the manner suggested by Medina *et al.* if the following three conditions are satisfied.

(1) The interphase transfer process is vapour phase diffusion controlled and the vapour phase can be considered to be thermodynamically ideal. If the resistances in both the vapour and liquid phases are important then the procedure suggested elsewhere[2–4] should be used to take both the resistances into account.

(2) A film model can be applied to describe the vapour phase controlled diffusion process, i.e.

$$(N_{OG})_{ij} \propto D_{ij} \tag{4}$$

The linearized theory of multicomponent mass transfer[5] allows the use of the eqns (2) for the generation of the ternary parameters also for the case in which the dependence of the binary number of overall transfer units is described by a correlation of the type

$$(N_{OG})_{ij} \propto D_{ij}^n, \quad 0 < n \le 1 \tag{5}$$

(3) Equimolar counter diffusion prevails and the flux corrections on the composition profiles in the film are ignored[3].

Examination of the diffusion coefficient data[6] for the system cyclohexane (1)-*n*-heptane (2)–toluene (3) shows the binary pair diffusivities to be

$$D_{12} = 0.041\ \mathrm{cm^2/s}, \quad D_{13} = 0.0478\ \mathrm{cm^2/s},$$
$$D_{23} = 0.0424\ \mathrm{cm^2/s}$$

Since the values of the D_{ij} are close to one another one might expect the binary $(N_{OG})_{ij}$ to be also close to one another, as also the binary pair Murphree efficiencies. However the binary efficiency data[6] show significant differences in the binary $(E_{OG})_{ij}$. Also, the binary pair overall gas phase number of transfer units follow the general trend

$$(N_{OG})_{12} < (N_{OG})_{13} < (N_{OG})_{23} \tag{6}$$

leading to the conclusion that a diffusional type model of the type given by eqn (5) is not valid. If a diffusional type model is not valid then the eqns (2) used by Medina *et al.* to generate ternary parameters from binary parameters cannot be applied. Other factors such as surface tension variations are possibly playing a dominant role. Such effects are not covered by the Maxwell–Stefan diffusion equations, the basis of multicomponent transfer models. We would like to remark here that in our earlier publication[2], we used the Maxwell–Stefan diffusion equations for the prediction of ternary efficiencies only after verifying that the diffusional model of the type given by eqn (5) was applicable for the system studied: ethanol–*t*-butanol–water.

The agreement between experimental Murphree efficiencies and the theoretical predictions according to the procedure of Medina *et al.* is not a proof of the validity of their method but underlines the importance of analysing experimental multicomponent mass transfer data with extreme caution.

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Fractional order moments

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Dear Sirs,

Referring to my recent paper concerning negative order moments[1], another type of moments may be considered, which might also avoid the overweighting of certain parts of measured curves $f_{ex}(t)$. The high weighting of the tail end of experimental curves is due to the t^n term in the integral

$$\mu'_n = \frac{1}{\mu_0}\int_0^\infty t^n f(t)\,dt \tag{1}$$