LETTERS TO THE EDITOR

To the Editor:

In “Influence of Mass Transfer in Distillation: Residue Curves and Total Reflux” (Dec. 2004), Taylor et al.[1] presented some comments on our article entitled “On the dynamics of simple batch distillation processes” published in *Chemical Engineering and Processing*[1]. They agreed with most of our assumptions, but considered the change of the total vapor pressure across the film as rather unusual. They argue that this difference leads to bulk fluid motion across the film, and that it is “standard practice” in mass-transfer modeling to assume the transfer to be isobaric. In our opinion this is misleading for simple batch distillation because there is a bulk fluid motion across the film. The batch distillation process is a differential distillation, where back-diffusion is not allowed to occur. Vapor is formed at the liquid-vapor interface across the film toward the bulk vapor driven by the pressure difference across the film. This difference may be generated by a vacuum system, by a heat exchanger, or by both. The existence of a pressure difference across the film is fundamental for the vapor outflow from the equipment. Taylor et al.[1] use an argument that can be found in the book of Doherty and Malone, where it is stated that “the vapors are removed from contact from the liquid as soon as they are formed”, that is, at infinite velocity, which requires a very high pressure difference across the film to say the least.

The correct question is: would the film theory model apply to films where bulk motion occurs? Most of our group contends with the journal editors and referees that this question is centered on this important point. The answer is yes. To emphasize this point let us consider the simple mathematical exercise that includes the convective term in the film theory

$$D_{ab}\frac{d^2C}{dX^2} + V\frac{dC}{dX} = 0$$

$$X = 0 \quad C_A = C_A^S$$

$$X = \delta \quad C_A = C_A^\infty \qquad (1)$$

The obtained solution is

$$C_A = C_A^S + (C_A^\infty - C_A^S)\frac{\left(\exp\left(-\frac{V\delta}{D_{AB}}\right) - 1\right)}{\left(\exp\left(-\frac{V\delta}{D_{AB}}\right) - 1\right)} \qquad (2)$$

The flux across the film is calculated as usual

$$q_A - x_A(q_A - q_B) = K_c(C_A^S - C_A^\infty) = -D_A\frac{dC_A}{dX}\bigg|_{X=0} = N_A \qquad (3)$$

$$N_A = V\frac{\left(\exp\left(\frac{V\delta}{D_{AB}}\right)\right)(C_A^S - C_A^\infty)}{\left(\exp\left(\frac{V\delta}{D_{AB}}\right) - 1\right)} \qquad (4)$$

So

$$K_{GA} = V\frac{\left(\exp\left(\frac{V\delta}{D_{AB}}\right)\right)}{\left(\exp\left(\frac{V\delta}{D_{AB}}\right) - 1\right)} \qquad (5)$$

If the absence of fluid motion across the film is assumed, the above equation becomes

$$K_{GA} = \frac{D_{AB}}{(\delta)} \qquad (6)$$

As stated by the film theory. The regime of the mass transfer, in the simple batch distillation will depend on the dimensionless number

$$\frac{V\delta}{D_{AB}}$$

The expression of the overall mass-transfer coefficient at the liquid/vapor interface satisfies the fact that there is vapor moving across the gas film with finite velocity in simple batch distillation. On the other hand, this velocity reaches a maximum when the vapor bulk pressure becomes zero. So, for the correct interpretation of the transfer phenomenon, this velocity cannot be neglected, that is, the pressure difference between interface and the bulk of the vapor is different of the zero.

In the simple batch distillation process, the total molar net flux is different from zero, that is, Eq. A10 (see Taylor et al.[1]) may not be applied in this case, although to be largely employed for conventional distillation processes. On the other hand, the “n” mass-transfer coefficients employed by Silva et al. are all interrelated by the Eq. A8 (see Taylor et al. [1]), and their values establish a link between the interface pressure (which is determined by the thermodynamic properties of the liquid) and bulk pressure which is determined by the transport properties, that is, Eq. A8 (see Taylor et al. [1]). So, the mass-transfer coefficients should not satisfy Eq. A10 (see Taylor et al. [1]) for a simple batch distillation, where there would be a net mass flux across the liquid/vapor interface.

On the other hand, the mass-transfer coefficient values were varied in a broad range in order to test all dynamic behaviors foreseen by the model. Probably, in some cases, there are no real physical systems with these values for mass-transfer coefficients. However, this fact does not invalidate the model.

Taylor et al. [1] affirm that the calculations performed in our article are wrong. We suppose that this affirmation refers to the residual curves presented in the figures of our article. These figures were built using a Runge-Kutta-Merson procedure, implemented in Pascal language. To test the correctness of our assumption, we performed again the calculations using Maple software, and we obtained the same results as before. So, there are no errors in our article.

In the simulation performed in our article we considered a small laboratory distiller whose interfacial area was 3185 cm². These data was not mentioned in the original article, and is very important for the reproduction of the figures, as the model is very sensitive of the design equipment, that is, the interfacial area. So, we are very sorry if the lack of this information has led our article readers to erroneous calculations. The simulation of the model showed itself to be very sensitive to interfacial area changes. This may easily be observed by anyone who plays with the model using different values for interfacial area.

In our viewpoint, the work is consistent and it is correct, presenting a more adequate model for the simple batch distillation processes.

Literature Cited

1. Taylor R., Baur R, Krishna R. Influence of mass transfer in distillation: residue curves and total reflux. *AIChE J*. 2004;50:3134-3148.
2. Silva JMF, Knoechelmann A., Meirelles AJA, Wolf-Maciel MR, Lopes CE. On the dynamics of nonequilibrium simple batch distillation processes. *Chem Eng and Processing*. 2003;42:475-485.

J. M. F. Silva*,
A. Knoechelmann, and C. E. Lopes
Chemical Engineering Dept.,
Technology Center,
Federal University of Pernambuco (UFPE),
Recife, PE, Brazil 50670-901

M. R. Wolf-Maciel
Faculty of Chemical Engineering, State University of Campinas (UNICAMP) and Chemical Process Dept.-Laboratory of Development Process Separation, Cidade Universitária Zeferino Vaz-6066-Campinas
São Paulo, Brazil 13081-970

Antonio J. A. Meirelles
State University of Campinas (UNICAMP)-
Food Engineering Dept. (FEA)
Physical Separation Laboratory(LASEFI)
PO.Box 6121, Campinas/SP,
13083-970, Brazil

AIChE Journal, Vol. 52, 1968 (2006)

DOI 10.1002/aic.10766