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Comment

The correct mathematical description and a suggested solution method for a model in packed columns A note on "A new technique for the determination of mass transfer coefficients in packed columns for physical gas absorption systems" [Chem. Eng. J., 57 (1995) 67]

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1. Introduction

The paper mentioned in the title [1] put forward a very simple but practical mathematical model, with which the mass transfer coefficients in packed columns for physical gas absorption systems can be determined. Based on the fitting of experimental data to model predictions the authors determined the k_La values for a certain packed columns with the Raschig ring under different liquid mass flow rates per unit cross-section area. However, their mathematical solution to the model is not correct, and some mathematical concepts are confused.

2. False aspects in [1]

Applying the separation-of-variables method, the authors got the general solution

$$C=B\exp(-\lambda^2 x)\exp\left[\left(\lambda^2\nu-\frac{kLa}{\varepsilon}\right)t\right] \tag{1}$$

for the governing Eq. (2) (Eq. (9) in [1])

$$\nu\frac{\partial C}{\partial x}+\frac{\partial C}{\partial t}+\frac{k_La}{\varepsilon}C=0 \tag{2}$$

where B is B_1B_2 in [1].

The condition to obtain this general solution is that λ^2 is constant, which does not depend on both x and t. With the wrong boundary condition the authors got λ^2 that is function of t. It is obviously in contradiction with the used separation-of-variables method. If Eq. (16) in [1] is substituted into Eq. (14), Eq. (14) does not satisfy with Eq. (7) in [1].

In fact, with this method the special solution that satisfies with the initial and boundary conditions can not be obtained.

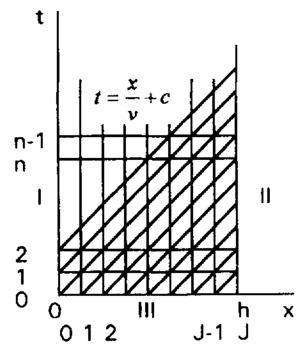

Fig. 1. Diagram of characteristic lines in the solution domain.

According to the differential equation theory, only one boundary condition should be specified in this problem.

3. The correct mathematical description and the suggested solution method

Eq. (2) is a hyperbolic equation. In the solution domain in Fig. 1 only one characteristic line goes from boundary I and boundary III (here we consider the initial line as a boundary also) and not from boundary II. This means we should specify the condition on boundaries I and III. The condition specified on III is called the initial condition. So in the present problem only one initial condition and one boundary condition should specified. The correct mathematical description of the present problem should be stated as follows.

$$\left.\begin{aligned} &\nu\frac{\partial A^0}{\partial x}+\frac{\partial A^0}{\partial t}-\frac{k_La}{\epsilon}\left[\frac{1}{He}\left(p_1+\frac{P_2-P_1}{h}x\right)-A^0\right]=0\\ &A^0|_{t=0}=0\\ &\left.\frac{\partial A^0}{\partial t}\right|_{x=0}=\frac{1}{\tau_R}\left(A^0|_{x=h}-A^0|_{x=0}\right)\end{aligned}\right\} \tag{3}$$

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or

$$\left.\begin{aligned} &v\frac{\partial C}{\partial x}+\frac{\partial C}{\partial t}+\frac{k_La}{\varepsilon}C=0\\ &C|_{t=0}=\frac{k_La}{\varepsilon He}\left(P_1+\frac{P_2-P_1}{h}x\right)-\frac{1}{He}\frac{P_2-P_1}{h}v\\ &\left.\frac{\partial C}{\partial t}\right|_{x=0}=\frac{1}{\tau_R}(C|_{x=h}-C|_{x=0})-\frac{k_La}{\varepsilon}\frac{P_2-P_1}{He}\frac{1}{\tau_R} \end{aligned}\right\} \quad (4)$$

We suggest that this problem be numerically solved with the characteristic line method, shown in Fig. 1. The equation of characteristic line and the corresponding equation are

$$\left.\begin{aligned} &\mathrm{d}t=\frac{1}{v}\,\mathrm{d}x\\ &\mathrm{d}C=-\frac{k_La}{\varepsilon}C\,\mathrm{d}t \end{aligned}\right\} \quad (5)$$

Take $\Delta t=\Delta x/y$ $(\Delta x=h/J)$, where Δx is the step length and J is the number of grids in the x direction. Because $v=$constant, Δ_t will not be varied with time. Except at the point of boundary $x=0$ the values at other points can readily be determined, as shown in Fig. 1. For the point of boundary $x=0$, we have

$$\frac{C_0^{n+1}-C_0^n}{\Delta t}=\frac{1}{\tau_R}(C_J^n-C_0^n)-\frac{k_La}{\varepsilon}\frac{P_2-P_1}{He}\frac{1}{\tau_R} \quad (6)$$

In this way it is very easy to get the functions of A^{01} (C_0) and A^{02} (C_J) vs. t.

If a matching between the calculated and experimental results is obtained, the corresponding k_La is taken as the mass transfer coefficient. The different values of k_La under the experimental conditions in [1] for $L=21\,132$ kg m^{-2} h^{-1} and $L=33\,048$ kg m^{-2} h^{-1} respectively, will be different from 59.4 h^{-1} and 64.8 h^{-1}, which were determined with the wrong solution in [1].

4. Nomenclature

The same as in [1].

References

[1] V. Evren and A.R. Ozdural, Chem. Eng. J., 57 (1995) 67.