APPLICATION OF THE PENETRATION THEORY FOR GAS–LIQUID MASS TRANSFER WITHOUT LIQUID BULK

Differences with Systems with a Bulk

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Abstract: Frequently applied micro models for gas–liquid mass transfer all assume the presence of a liquid bulk. However, some systems are characterized by the absence of a liquid bulk, a very thin layer of liquid flows over a solid surface. An example of such a process is absorption in a column equipped with structured packing elements. The penetration model was slightly modified, so that it can describe systems without liquid bulk. A comparison is made between the results obtained with the modified model and the results that would be obtained when applying the original penetration theory for systems with liquid bulk. Both physical absorption and absorption accompanied by first and second order chemical reaction have been investigated. It is concluded that the original penetration theory can be applied for systems without liquid bulk, provided that the liquid layer has sufficient thickness ($\delta > d^*_{\mathrm{pen}}$). For packed columns this means, in terms of Sherwood number, $Sh \geq 4$. In case of a 1,1-reaction with $Ha > 0.2$ an additional second criterion is $Sh \geq 4\sqrt{D_\mathrm{b}/D_\mathrm{a}}$ For very thin liquid layers ($Sh < 4$ or $Sh < 4\sqrt{D_\mathrm{b}/D_\mathrm{a}}$), the original penetration model may give erroneous results, depending on the exact physical and chemical parameters, and the modified model is required.

Keywords: penetration theory; mass transfer; film; liquid layer; packed columns; structured packing.

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INTRODUCTION

Mass transfer from a gas phase to a liquid phase proceeds via the interfacial area. Micro models are required to model this interphase transport of mass that often takes place in combination with a chemical reaction.

Frequently applied micro models are the stagnant film model in which mass transfer is postulated to proceed via stationary molecular diffusion in a stagnant film of thickness δ (Whitman, 1923), the penetration model in which the residence time θ of a fluid element at the interface is the characteristic parameter (Higbie, 1935), the surface renewal model in which a probability of replacement is introduced (Danckwerts, 1951) and the film-penetration model which is a two-parameter model combining the stagnant film model and the penetration model (Dobbins, 1956; Toor and Marchello, 1958).

All micro models mentioned above assume the presence of a well mixed liquid bulk. This may limit the application of these models to systems where a liquid bulk is present, for example absorption in a tray column or mass transfer in a stirred tank reactor. The question arises whether it is also possible to apply the micro models for systems where no liquid bulk is present, for example absorption in a column with structured or random packing elements, where thin liquid layers flow over the packing.

In this paper, the penetration model approach is adapted, so that it can describe systems without a liquid bulk. Next, a comparison is made between the results obtained with the modified model and the results that would be obtained when applying the original penetration theory for systems with a liquid bulk.

THEORY

Introduction

The problem considered is gas–liquid mass transfer followed by an irreversible first or second order reaction:

$$A(g) + \gamma_\mathrm{b} B(l) \longrightarrow \gamma_\mathrm{c} C(l) + \gamma_\mathrm{d} D(l) \qquad (1)$$

with the following overall reaction rate equation:

$$R_\mathrm{a} = k_\mathrm{R}[A][B]^n \qquad (2)$$

where $\gamma_b = n = 0$ in case of a first order reaction and $\gamma_b = n = 1$ in case of a second order reaction.

The mathematical model used is based on the following assumptions:

(1) Mass transfer of component A takes place from the gas phase to a liquid layer that flows over a vertical contact surface (i.e., a packing or a reactor wall).
(2) The mass transfer in the gas phase is described with the stagnant film model. The conditions are chosen so that the gas phase mass transfer is no limiting factor.
(3) The mass transfer in the liquid phase is described according to the penetration model approach.
(4) The reaction takes place in the liquid phase only.
(5) The liquid phase components are non-volatile.
(6) Axial dispersion in the liquid layer can be neglected.
(7) The velocity profile in the liquid layer is either plug flow or a fully developed parabolic (laminar flow).
(8) Temperature effects on micro scale are neglected.

Higbie Penetration Model

First, the standard penetration model is discussed (Figure 1). The phenomenon of mass transfer accompanied by a chemical reaction is governed by the equations:

$$\frac{\partial[A]}{\partial t} = D_a \frac{\partial^2[A]}{\partial x^2} - R_a \tag{3}$$

$$\frac{\partial[B]}{\partial t} = D_b \frac{\partial^2[B]}{\partial x^2} - \gamma_b R_a \tag{4}$$

To permit a unique solution of the non-linear partial differential equations (3) and (4) one initial (5) and two boundary conditions (6) and (7) are required:

$$t = 0 \text{ and } x \geq 0{:}\ [A] = [A]_{l,\mathrm{bulk}},\ [B] = [B]_{l,\mathrm{bulk}} \tag{5}$$

$$t > 0 \text{ and } x = \infty{:}\ [A] = [A]_{l,\mathrm{bulk}},\ [B] = [B]_{l,\mathrm{bulk}} \tag{6}$$

$$J_a = -D_a\left(\frac{\partial[A]}{\partial x}\right)_{x=0} = k_g\left([A]_{g,\mathrm{bulk}} - \frac{[A]_{x=0}}{m_a}\right)$$

$$\left(\frac{\partial[B]}{\partial x}\right)_{x=0} = 0 \tag{7}$$

Species C and D do not need to be considered because, due to the irreversibility of the reaction (1), they do not influence the mass transfer. Assuming that the mixture density is not affected, also the total flow of the is not affected.

Penetration Model for Systems Without Liquid Bulk

In this section it is assumed that mass transfer takes place from a continuous gas phase to a liquid layer that flows down over a vertical contact surface (Figure 2). The model can however be modified easily to apply for non-vertical surfaces or for systems without contact surface.

Mass transport in the *x* direction takes place by diffusion, as is the case with the penetration model. Mass transport in the vertical (*y*) direction takes place primarily due to the flow in the liquid layer over the contact surface. The contribution of diffusion or axial dispersion to the mass transport is neglected.

$$v_y \frac{\partial[A]}{\partial y} = D_a \frac{\partial^2[A]}{\partial x^2} - R_a \tag{8}$$

$$v_y \frac{\partial[B]}{\partial y} = D_b \frac{\partial^2[B]}{\partial x^2} - \gamma_b R_a \tag{9}$$

Please note that these equations are similar to the penetration model [equations (3) and (4)]. The vertical velocity v_y and the vertical position *y* have replaced the time *t*.

To permit a unique solution of the non-linear partial differential equations (8) and (9) one boundary condition (10) and two boundary conditions (11) and (12) are required:

$$y = 0 \text{ and } x \geq 0{:}\ [A] = [A]_{l,0}, [B] = [B]_{l,0} \tag{10}$$

$$y > 0 \text{ and } x = \delta{:}\ \frac{\partial[A]}{\partial x} = 0, \frac{\partial[B]}{\partial x} = 0 \tag{11}$$

$$J_a = -D_a\left(\frac{\partial[A]}{\partial x}\right)_{x=0} = k_g\left(\frac{[A]_{g,\mathrm{bulk}} - [A]_{x=0}}{m_a}\right)$$

$$\left(\frac{\partial[B]}{\partial x}\right)_{x=0} = 0 \tag{12}$$

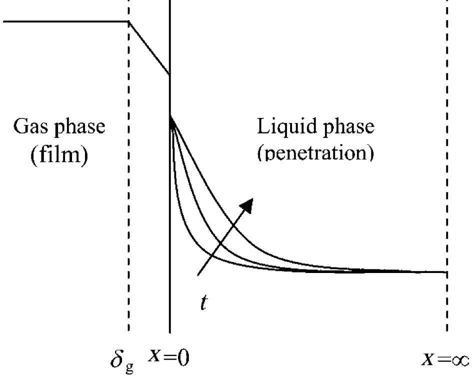

Figure 1. Penetration model for systems with liquid bulk.

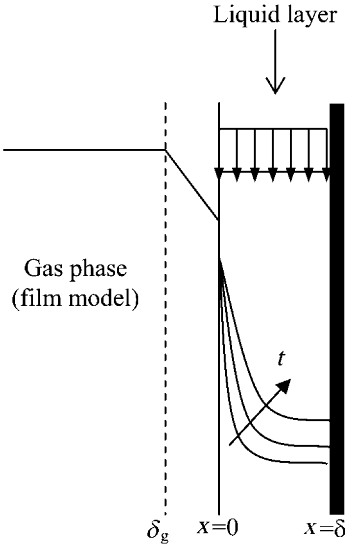

Figure 2. Penetration model for systems without liquid bulk.