Technical Note

Effect of thermal diffusion on absorption during dissolution of short gas plugs

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Abstract

We study a nonisothermal gas absorption from a rising short gas plug using an approximation of the infinite dilution of absorbate and taking into account the effect of thermal diffusion on the rates of heat and mass transfer. Short contact time solutions of energy and mass conservation equations are obtained by a similarity method. It is shown that for absorption of ammonia and hydrogen chloride by water and water vapor by aqueous solution of LiBr neglecting effect of thermal diffusion results in overestimating the rate of mass transfer during absorption.
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1. Introduction

Coupled heat and mass transfer during nonisothermal gas absorption by liquid from gas plugs has been analyzed in a number of studies (see [1–3]). It was shown that for absorption accompanied by a thermal effect, the concentration and temperature fields are interdependent. The expression obtained in [2] for mass transfer coefficient during nonisothermal absorption, in the limiting case of absorption without thermal effect, recovers the formulas derived previously by van Heuven and Beek [4]. In all these studies, the effect of thermal diffusion was assumed to be negligibly small. At the same time, thermal diffusion may become important for gas plugs with short time of gas–liquid contact whereby large concentration and temperature gradients occur. In this study we develop a model of heat and mass transfer during gas plug dissolution, for evaluating the contribution of thermal diffusion to the rate of absorp-

tion. A short-exposure time solution is obtained by a similarity method.

2. Description of the model

Consider a gas plug rising with a constant velocity U in a vertical channel filled with a liquid. Schematic view of a gas plug and the system of coordinates, attached to a rising gas plug, are shown in Fig. 1. Gas plug is assumed to be short, i.e. $L_B \leqslant 2d_{ch}$. In the vicinity of the nose and at the lateral surface of a gas plug, where mass and heat transfer occur, we adopt the usual assumption of a streamline flow. Consider the coupled mass and heat transfer during absorption of a pure soluble gas from a rising gas plug in a channel accompanied by a thermal effect. The problem is solved in the approximation of the infinite dilution of absorbate in the absorbent. The thermodynamic parameters of the system are assumed to be constant, and only the resistance to mass and heat transfer in the liquid phase is taken into account. Assume that heat released during absorption is dissipated in a liquid phase, where it causes an increase of the liquid temperature. A difference between

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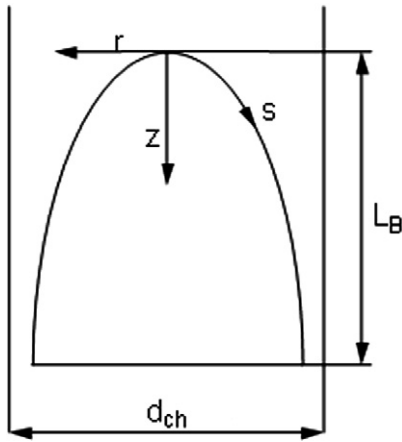
Fig. 1. Schematic view of a short gas plug.

the interface temperature and the temperature in the bulk of liquid appears due to the thermal effect of gas absorption. In the further analysis we take into account the contribution of thermal diffusion to the rate of absorption. Consequently, there is coupling between mass and heat transfer. The equilibrium condition at the gas–liquid interface is described by linear dependence of concentration on temperature (see [5]). Assume that development of thin diffusion and temperature boundary layers in a liquid begins at the leading edge of a gas plug, and convective diffusion and heat transfer are determined by fluid velocity at the gas plug surface. The gas plug–liquid interface is assumed to be a surface of revolution obtained by the rotation of a curve $r(z)$ around a z-axis. The equation of this curve $r(z)$ was derived in [6]. A differential mass balance equation for the absorbing component in cylindrical coordinates read

$$\frac{\partial N_{A_z}}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(rN_{A_r}) = 0, \tag{1}$$

where r – radial coordinate, z – axial coordinate. Expressions for mass flux density of absorbate in radial and axial directions in Eq. (1), N_{A_r} and N_{A_z}, accounting for thermal diffusion effect read (see [7,8])

$$N_{A_r} = -D\rho\frac{\partial x_A}{\partial r} - D'\cdot\rho\cdot x_A\frac{\partial T}{\partial r} + x_A\rho v_r, \tag{2}$$

$$N_{A_z} = -D\rho\frac{\partial x_A}{\partial z} - D'\rho\cdot x_A\frac{\partial T}{\partial z} + x_A\rho v_z, \tag{3}$$

where D is the molecular diffusion coefficient, D' is the thermal diffusion coefficient of the solution, x_A is the weight fraction of the absorbate, ρ is the density of solution, v_r, v_z, are the velocity components and T is the temperature of the liquid. Equation of continuity written in cylindrical coordinates reads

$$\frac{\partial v_z}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(rv_r) = 0. \tag{4}$$

Substituting expressions for N_{A_r} and N_{A_z} (Eqs. (2) and (3)) into Eq. (1) and using Eq. (4) we arrive at the following equation of convective diffusion:

$$v_r\frac{\partial x_A}{\partial r} + v_z\frac{\partial x_A}{\partial z}$$
$$= D\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right) + \frac{\partial^2 x_A}{\partial z^2} + \sigma\frac{\partial x_A}{\partial r}\frac{\partial T}{\partial r} + \sigma\frac{\partial x_A}{\partial z}\frac{\partial T}{\partial z}\right), \tag{5}$$

where $\sigma = D'/D$ is Soret coefficient. Energy conservation equation can be written as follows:

$$v_r\frac{\partial T}{\partial r} + v_z\frac{\partial T}{\partial z} = a\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right), \tag{6}$$

where a is the coefficient of thermal diffusivity of a liquid. For small rates of mass transfer the velocity components v_r and v_z in Eqs. (5) and (6) can be determined from the solution of the hydrodynamic equations with zero mass flux at the interface. In order to simplify Eq. (5) we introduce the stream function ψ and velocity potential ϕ as follows:

$$v_z = \frac{1}{r}\frac{\partial\psi}{\partial r} = \frac{\partial\phi}{\partial z}, v_r = -\frac{1}{r}\frac{\partial\psi}{\partial z} = \frac{\partial\phi}{\partial r}. \tag{7}$$

Equation of continuity, and the requirement that vorticity in the potential flow vanishes, yield

$$\frac{\partial^2\phi}{\partial z^2} + \frac{\partial^2\phi}{\partial r^2} + \frac{1}{r}\frac{\partial\phi}{\partial r} = 0, \frac{\partial^2\psi}{\partial z^2} + \frac{\partial^2\psi}{\partial r^2} - \frac{1}{r}\frac{\partial\psi}{\partial r} = 0. \tag{8}$$

Taking into account that Peclet number $Pe \gg 1$, where $Pe = Ud_{ch}/D$, U – velocity of a gas plug rising in a stagnant fluid, d_{ch} – channel diameter, neglecting molecular diffusion along the streamlines, and following the approach suggested in [9], Eq. (5) can be rewritten as follows:

$$\frac{\partial x_A}{\partial\phi} = D\left\{r^2\frac{\partial^2 x_A}{\partial\psi^2} + \sigma r^2\frac{\partial x_A}{\partial\psi}\frac{\partial T}{\partial\psi}\right\}. \tag{9}$$

Since the diffusion boundary layer is very thin, it can be assumed that r is a function of ϕ only. Then following the procedure suggested in [9], let us introduce a new variable μ defined by the following relation: $\frac{\partial\mu}{\partial\phi} = r^2$. Function μ is determined by integration along the gas plug surface, s is the length of the arc measured from the gas plug nose (see Fig. 1) and $v = \partial\phi/\partial s$, where $v^2 = v_r^2 + v_z^2$ (for details see [9]):

$$\mu(z) = \int_{\phi_0}^{\phi} r^2\,\mathrm{d}\phi' = \int_0^s r^2 v\,\mathrm{d}s'. \tag{10}$$

Using simple geometric arguments we find that

$$\mu_0 = \mu(L_B) = \int_0^{L_B} (r(z))^2\sqrt{1 + \left(\frac{\mathrm{d}r(z)}{\mathrm{d}z}\right)^2}\sqrt{2gz}\cdot\mathrm{d}z, \tag{11}$$

where g – acceleration of gravity, μ_0 – shape factor of a gas plug which was introduced in [4] and tabulated in [9]. Combining Eqs. (9) and (10) yields

$$\frac{\partial x_A}{\partial\mu} = D\left\{\frac{\partial^2 x_A}{\partial\psi^2} + \sigma\frac{\partial x_A}{\partial\psi}\frac{\partial T}{\partial\psi}\right\}. \tag{12}$$

The last term in the r.h.s. of Eq. (12) accounts for the effects of thermal diffusion. Following similar approach we arrived at the energy conservation equation taking into account that Lewis number is small, $Le = D/a \ll 1$:

$$\frac{\partial T}{\partial \mu} = a \frac{\partial^2 T}{\partial \psi^2}. \tag{13}$$

The initial and boundary conditions to Eqs. (12) and (13) read

$$T = T_0, \quad x_A = x_{A_0} \quad \text{at } \mu = 0 \text{ and at } \psi \to \infty, \tag{14}$$

$$T = T_s, \quad x_A = x_{A_s} \quad \text{at } \psi = 0. \tag{15}$$

Introducing a new variables

$$\eta_c = \frac{\psi}{2\sqrt{D\mu}}, \eta_T = Le^{1/2} \cdot \eta_c, \tag{16}$$

Eqs. (12)–(15) can be rewritten as follows (for details see [10,11]):

$$\frac{d^2 x}{d\eta_c^2} + \sigma \frac{dx}{d\eta_c} \frac{dT}{d\eta_c} + 2\eta_c \frac{dx}{d\eta_c} = 0, \tag{17}$$

$$\frac{d^2 T}{d\eta_T^2} + 2\eta_T \frac{dT}{d\eta_T} = 0, \tag{18}$$

$$x = x_{A_s}, \quad T = T_s \quad \text{at } \eta_c = \eta_T = 0, \tag{19}$$

$$x = x_{A_0}, \quad T = T_0 \quad \text{at } \eta_c \to \infty \text{ and } \eta_T \to \infty, \tag{20}$$

where x_{A_s} – weight fraction of the absorbate at the gas–liquid interface, x_{A_0} – weight fraction of the absorbate at the inlet, T_s – temperature of liquid at the gas–liquid interface, T_0 – temperature in the bulk of liquid. Solution of Eq. (18) with boundary conditions (19) and (20) reads

$$T = (T_s - T_0)\text{erfc}(\eta_T) + T_0. \tag{21}$$

During gas absorption in a liquid, $Le \ll 1$ and the thickness of the diffusion boundary layer is much smaller than the thickness of the temperature boundary layer. The latter condition allows us to expand the solution for temperature in Taylor series of η_T in the vicinity of $\eta_T = 0$ and to substitute this expansion in Eq. (17). The first two terms of expansion of Eq. (21) are as follows:

$$T = T_s - \frac{2(T_s - T_0)}{\sqrt{\pi}} \eta_T. \tag{22}$$

Eqs. (17) and (22) yield

$$\frac{d^2 x}{d\eta_c^2} - \frac{2\sigma(T_s - T_0)Le^{1/2}}{\sqrt{\pi}} \frac{dx}{d\eta_c} + 2\eta_c \frac{dx}{d\eta_c} = 0. \tag{23}$$

Solution of Eq. (23) reads

$$\frac{x - x_0}{x_s - x_0} = 1 - \frac{\int_0^{\eta_c} \exp(-[\alpha^2 - k\alpha])d\alpha}{\int_0^{\infty} \exp(-[\alpha^2 - k\alpha])d\alpha}, \tag{24}$$

where $k = \frac{2\sigma(T_s - T_0)Le^{1/2}}{\sqrt{\pi}}$. For small k ($k \ll 1$) Eq. (24) can be expanded in Taylor series of the parameter k. Keeping only the first two terms in the expansion yields

$$\frac{x - x_0}{x_s - x_0} = 1 - \frac{\int_0^{\eta_c} \exp(-\alpha^2)d\alpha + k\int_0^{\eta_c} \alpha \cdot \exp(-\alpha^2)d\alpha}{\int_0^{\infty} \exp(-\alpha^2)d\alpha + k\int_0^{\infty} \alpha \cdot \exp(-\alpha^2)d\alpha}. \tag{25}$$

For the case of nonisothermal absorption, the unknown values of concentration and temperature at the gas–liquid interface are found from the following equations:

$$x_A = dT + b \quad \text{at } \eta_c = \eta_T = 0 \tag{26}$$

and

$$\lambda \int_0^{\mu_0} \left(\frac{\partial T}{\partial \psi}\right)_{\psi=0} d\mu = L\rho D \int_0^{\mu_0} \left(\frac{\partial x_A}{\partial \psi}\right)_{\psi=0} d\mu \quad \text{at } \eta_c = \eta_T = 0, \tag{27}$$

where at λ is a thermal conductivity of a liquid, b is a nondimensional coefficient, d is a dimensional coefficient $[T^{-1}]$, L – heat of absorption. Eq. (26) describes a condition of equilibrium at the gas–liquid interface (see, e.g. [5]), and Eq. (27) implies that all the heat which is released during absorption is dissipated in the liquid phase. Note that for most gases the coefficient d in Eq. (26) is negative. Eqs. (21), (24) and (26), (27) yield expressions for T_s and x_{A_s}:

$$T_s - T_0 = \frac{T'_0 - T_0}{1 - \frac{K}{\sqrt{Le}}}, \quad x_{A_s} - x_{A_0} = \frac{x'_{A_0} - x_{A_0}}{1 - \frac{\sqrt{Le}}{K}}, \tag{28}$$

where $Le = \frac{D}{a}, K = \frac{c_p}{dL}, c_p$ – specific heat, $x'_{A_0} = dT_0 + b$ is the equilibrium concentration at the initial temperature, $T'_0 = (x_{A_0} - b)/d$ is the equilibrium temperature at the initial concentration. Note that coefficients d and b can be expressed through T'_0 and x'_{A_0}:

$$d = \frac{x_{A_0} - x'_{A_0}}{T'_0 - T_0}, \quad b = \frac{x'_{A_0} \cdot T'_0 - x_{A_0} \cdot T_0}{T'_0 - T_0}. \tag{29}$$

Eq. (25) yields the following formula for the normalized mass flux:

$$\frac{Q_c}{Q_{c0}} = \left[1 + \frac{2\Omega Le^{1/2}}{1 - \sqrt{\pi} \cdot K/\sqrt{Le}}\right]^{-1}, \tag{30}$$

where (see [3])

$$Q_{c0} = \frac{4\pi^{1/2}\rho \cdot D^{1/2}\mu_0^{1/2}}{1 - \sqrt{Le}/K}(x'_{A_0} - x_{A_0}), \tag{31}$$

$\Omega = \sigma(T'_0 - T_0)$ is the dimensionless parameter which characterizes the sensitivity of a system to thermal diffusion, Q_c – mass flux from a gas plug, while taking into account the effect of thermal diffusion, Q_{c0} – mass flux from a gas plug during nonisothermal absorption, while neglecting thermal diffusion. Note that the thermal effect of absorption of ammonia and hydrogen chloride by water and water vapor by aqueous solution of LiBr is positive ($L > 0$). At the same time, for all these gases the concentration of saturation decreases with temperature increase ($d < 0$), and the normalized heat of absorption K is negative ($K < 0$). For gas absorption in water at normal temperature and pressure, $T'_0 > T_0$, Soret coefficient σ is always positive (see, e.g.

[12]) and the parameter Ω is also positive. Consequently, Eq. (30) implies that ignoring the effect of thermal diffusion results in overestimating the rate of mass transfer during nonisothermal absorption. We evaluated the normalized mass flux using Eq. (30) for ammonia–water, hydrogen chloride–water and water vapor-aqueous solution of LiBr. The values of the normalized mass fluxes for these systems are equal to 0.998, 0.996 and 0.999, respectively. Consequently, the relative differences of the mass fluxes $[(Q_{c0} - Q_c)/Q_{c0}] \times 100\%$ for these systems are equal to 0.2%, 0.4% and 0.1%, correspondingly.

3. Conclusions

We studied analytically the effect of thermal diffusion on heat and mass transfer during gas absorption from a rising short gas plug for short time of contact using a similarity method. The obtained results show that the temperature and concentration distributions in thermal and diffusion boundary layers in a liquid surrounding a gas plug depend on three dimensionless parameters: the Lewis number, Le, the normalized heat of absorption, K, and the thermal diffusion parameter, Ω. These three parameters determine the rate of mass transfer during gas plug dissolution in liquid. It is shown that for absorption of ammonia and hydrogen chloride by water and water vapor by aqueous solution of LiBr, neglecting thermal diffusion results in overestimating the rate of mass transfer during nonisothermal absorption. Overestimating the rate of mass transfer becomes more pronounced with the increase of Lewis number (Le), the difference between the equilibrium temperature at the initial concentration and initial temperature ($T'_0 - T_0$), Soret

coefficient (σ) and with the decrease of the normalized heat of absorption K.

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