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1 Introduction

Many chemical engineering processes are based on the absorption or desorption of gaseous material into a liquid phase. During glass melting, bubbles are created due to chemical reactions between raw materials and undergo, further, mass transfer due to fining process enhancing the rate of bubbles removal [7].

The main purpose of our work is to provide a comprehensive understanding of the interplay between diffusion, advection and chemical reaction during mass transfer across the bubble interface. More precisely, we focus on the determination of the enhancement factor due to the chemical reaction on the rate of mass transfer.

2 Problem statement

A rising bubble in a liquid at rest is considered for which its radius, a, is assumed constant even in the presence of mass transfer according to [4]. The interface between the bubble and the liquid is assumed completely mobile (shear free boundary condition) according to previous works [2, 3]. Assuming that the Reynolds number is small, the general solution provided by Hadamard [1] or Rybczynski [6] is used to describe the flow motion around the bubble for which the terminal velocity is

$$V_t = \frac{ga^2}{3\nu}, \tag{1}$$

where g is the gravity acceleration, $\nu = \mu/\rho$ is the kinematic viscosity of the liquid and ρ the liquid density.

Two chemical species are considered : A, and B consumed and produced by a homogeneous reversible chemical reaction in the liquid

$$\mathrm{A} \rightleftarrows \mathrm{B}, \tag{2}$$

with the equilibrium constant equal to

$$K_{\mathrm{eq}} = \frac{C_{\mathrm{B_{eq}}}}{C_{\mathrm{A_{eq}}}}. \tag{3}$$

The quantities C_{A} and C_{B} are the molar concentrations of the solutes A and B in the liquid, respectively.

The general equations for the transport of C_{A} and C_{B} in the liquid experiencing advection, diffusion and chemical reaction are :

$$\frac{\partial C_{\mathrm{A}}}{\partial t} + u_r \frac{\partial C_{\mathrm{A}}}{\partial r} + u_z \frac{\partial C_{\mathrm{A}}}{\partial z} = \mathcal{D}_{\mathrm{A}} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_{\mathrm{A}}}{\partial r} \right) + \frac{\partial^2 C_{\mathrm{A}}}{\partial z^2} \right] - k^+ \left(C_{\mathrm{A}} - \frac{C_{\mathrm{B}}}{K_{\mathrm{eq}}} \right), \tag{4}$$

$$\frac{\partial C_{\mathrm{B}}}{\partial t} + u_r \frac{\partial C_{\mathrm{B}}}{\partial r} + u_z \frac{\partial C_{\mathrm{B}}}{\partial z} = \mathcal{D}_{\mathrm{B}} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_{\mathrm{B}}}{\partial r} \right) + \frac{\partial^2 C_{\mathrm{B}}}{\partial z^2} \right] + k^+ \left(C_{\mathrm{A}} - \frac{C_{\mathrm{B}}}{K_{\mathrm{eq}}} \right), \tag{5}$$

where t is the time, $\mathcal{D}_{\mathrm{A}}$ and $\mathcal{D}_{\mathrm{B}}$ are the diffusion coefficients of A and B, respectively. The quantity k^+ is the kinetic constant of reaction (2) towards production of B.

The bubble-liquid interface is assumed permeable to A and impermeable to B (zero flux boundary condition). In the bulk, at the infinity, the chemical equilibrium between A and B is achieved. To summarize, the boundary conditions are the following

$$C_{\mathrm{A}} = C_{\mathrm{A}}^S, \text{ on } \Gamma_{\mathrm{b}}, \; C_{\mathrm{A}} = C_{\mathrm{A}}^{\infty}, \text{ when } ||\boldsymbol{x}|| \to \infty, \tag{6}$$

$$\frac{\partial C_{\mathrm{B}}}{\partial n} = 0, \text{ on } \Gamma_{\mathrm{b}}, \; C_{\mathrm{B}} = K_{\mathrm{eq}} C_{\mathrm{A}}^{\infty}, \text{ when } ||\boldsymbol{x}|| \to \infty, \tag{7}$$

in which $\boldsymbol{x}$ represents the position of a point in the domain given by the coordinates (r, z) in the cylindrical polar coordinate system.

Equations (4-5) are solved numerically with a finite element technique. A boundary layer approach is also proposed and solved with a coupled technique of finite difference and Chebyshev-spectral method (see for more details [5]).

We show that the equilibrium constant and the ratio of diffusion coefficients have a strong influence on the coupling between the chemical reaction and mass transfer leading to an increase of the mass transfer. The interaction between the chemical reaction and advection is clearly established by the simulations.

Références

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