



Local mass transfer rates of a first-order chemical reaction on a wall: Application to the prediction of local platelet deposition in a perfusion chamber



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ABSTRACT

In this study we derive an equation for the calculation of the local mass transfer rates generated by a first-order chemical reaction on a plane wall. The validity of the expression is discussed and analyzed. It can be used to determine the kinetic constant of the surface reaction, with the knowledge of the wall mass flux, or to predict the local mass transfer rate knowing the kinetic constant, using parallel-plate (bio-)microreactors. The application of the derived equation is illustrated in the prediction of the platelet deposition in a blood perfusion chamber. The computed local surface coverage by the platelets agrees well with the corresponding measurements found in the literature. Consequently, the equation can be used to determine the kinetic constant in perfusion experiments carried out with different drug strategies oriented to the prevention of myocardial infarction and stroke.

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1. Introduction

Many chemical and biochemical transformations occur on the surface of a solid wall. Examples are found in reactors and bioreactors where catalyzers or enzymes are immobilized on a solid support. Some of these (bio-)chemical reactions are carried out in miniaturized reactors, which have a high surface-to-volume ratio. These microreactors, typically on-chip microchannel reactors, allow an efficient use of small amounts of reactants or catalyzers and a more precise control of the flow and the heat and mass transfer processes than large scale reactors. They are used in analytical and environmental applications [1], for catalyst optimization and selection [2], in micro fuel cells [3], and, among others, for synthesis and production in the pharmaceutical industry [4]. The field is vast and extensive reviews are available in the literature. See for example [5,6].

In this study we focus on the utilization of laminar straight-microchannel-based reactors for the determination of the effects of different operating conditions on the production rates or in the determination of the kinetic constant of a first order

chemical or biochemical transformation. These microreactors have the advantage of operating under very well controlled and defined flow conditions, which allow the construction of simple models to accurately predict production rates, with the knowledge of the kinetic, or to determine the kinetics, with the knowledge of the production rates. Particularly in this study, we derive a simple equation to compute the local mass transfer rates on a plane surface generated by a first-order surface chemical reaction. The equation, which is obtained from that proposed in [7] to compute the surface averaged mass transfer rate, is applied here for the prediction of the local rates of deposition of platelets in parallel-plate perfusion chambers. In these devices, blood, under controlled conditions, is pumped (mechanically or using the donor's heart) to flow over a biological or synthetic substrate. The measurement of the number of platelets deposited under certain conditions (flow, type of substrate and perfusing blood composition and/or treatment) has some important implications, for example, in thrombus formation on artificial organs, the durability of vascular prosthesis or in the fundamental studies of hemostasis, thrombosis and the development of atherosclerosis. Sakariassen et al. [8] reviews the different types of perfusion chambers reported in the literature and their use for studies on thrombosis and on different drug strategies oriented to the prevention thromboembolytic diseases, such as myocardial infarction and stroke.

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Nomenclature

<i>A</i>	area
<i>Ai, Bi</i>	Airy functions
<i>C</i>	concentration
<i>D</i>	mass diffusion coefficient
<i>Da</i>	Damkhöler number, $Da = kL/D$
<i>h</i>	channel half-width
<i>k</i>	kinetic constant
<i>K</i>	convective mass transfer coefficient, $K = N''/C_o$
<i>L</i>	length of the active portion of the wall
<i>N''</i>	molar flux at the wall
<i>Pe</i>	Péclet number, $Pe = L^2S/D$
<i>S</i>	shear rate
<i>Sh</i>	Sherwood number, $Sh = KL/D = N''L/(DC_o)$
<i>t</i>	time
<i>x, y</i>	Cartesian coordinates

<i>Greek letters</i>	
Γ	gamma function
ν	kinematic viscosity
θ	fraction of surface covered
τ	shear stress

<i>Superscripts and subscripts</i>	
*	non-dimensional quantity
<i>C</i>	infinitely fast reaction
<i>Da</i>	finite rate reaction
<i>o</i>	reference value
<i>pl</i>	platelet
<i>s</i>	substrate
<i>w</i>	wall

2. Physical and mathematical model

Fig. 1 shows the two-dimensional physical model and the coordinate system adopted. It is assumed that the flow is steady, laminar and fully developed and the fluid has constant physical properties. The concentration of the reactant outside the mass boundary layer is uniform and steady. The velocity profile within the mass transfer boundary layer generated by the active portion of the plane wall, where the first-order chemical reaction occurs, is assumed to be linear (i.e. constant shear rate). This assumption is valid if the mass transfer boundary layer thickness is much smaller than the radius or the channel-half width (*h*) of the channel (i.e. high Schmidt number). Pallares and Ferré [9] reported that the adoption of this hypothesis produces errors in the mass transfer coefficients of less than 1% if $h > 10(DL/S)^{1/3}$ (see for example Fig. 4 in [9]).

The simplified mass transfer governing equation can be written as,

$$Sy \frac{\partial C}{\partial x} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (1)$$

The boundary conditions are: at $x = 0$ and $y \geq 0$; $C = C_o$ and $\partial C/\partial x = 0$, at $y = 0$ and $0 < x < L$; $kC = D \partial C/\partial x$ and at $y \rightarrow \infty$ and $x > 0$; $C = C_o$.

Analytical solutions to Eq. (1), together with the boundary conditions, were reported by Apelblat neglecting the axial diffusion term in the mass transport equation [10] and considering the axial diffusion [11]. The corresponding local Sherwood numbers are, respectively,

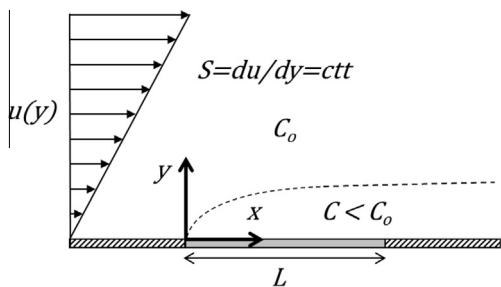


Fig. 1. Physical model and coordinate system.

$$Sh_{Da}(x^*) = Da \frac{3/2}{2\pi} \int_0^\infty \frac{\exp(-u\alpha)}{1+u+u^2} du \left\{ \right. \\ \left. \alpha = \frac{\Gamma(1/3)}{3^{1/3}\Gamma(2/3)} Da \left(\frac{x^*}{Pe} \right)^{1/3} \right. \quad (2)$$

and

$$Sh_{Da}(x^*) = \frac{Da^2}{\pi^2 Pe^{1/2}} \int_0^\infty \frac{\exp(-uPe^{1/2}x^*)}{u^{2/3}(M_1^2 + M_2^2)} du \left\{ \right. \\ \left. M_1 = u^{1/3} Ai'(-u^{4/3}) + \frac{Da}{Pe^{1/2}} Ai(-u^{4/3}) \right. \\ \left. M_2 = u^{1/3} Bi'(-u^{4/3}) + \frac{Da}{Pe^{1/2}} Bi(-u^{4/3}) \right. \quad (3)$$

Pallares and Grau [7] proposed a simple equation (Eq. (4)) to compute the surface averaged Sherwood number as a function of the Damkhöler number (*Da*) and the surface averaged Sherwood number corresponding to an infinitely fast surface reaction (\overline{Sh}_C).

$$\overline{Sh}_{Da} = \int_0^1 Sh_{Da}(x^*) dx^* = \left(\frac{1}{Da} + \frac{1}{\overline{Sh}_C} \right)^{-1} \quad (4)$$

In Eq. (4), x^* is the non-dimensional axial coordinate that is defined as $x^* = x/L$.

For an infinitely fast surface reaction the local and the surface averaged Sherwood numbers are, according to the Lévêque's solution [12],

$$Sh_C(x^*) = \frac{N''(x)L}{D} = \frac{3^{1/3}}{\Gamma(1/3)} \left(\frac{Pe}{x^*} \right)^{1/3} \approx 0.5384 \left(\frac{Pe}{x^*} \right)^{1/3} \quad (5)$$

and

$$\overline{Sh}_C = \int_0^1 Sh_C(x^*) dx^* \approx 0.8075 Pe^{1/3} \quad (6)$$

respectively.

The ranges of applicability of Eq. (4) are analyzed in [7]. Differences with respect to the exact expression considering the axial diffusion are less than 5% for $Pe > 10^5$, independently of the Damkhöler number (see Fig. 2 in [7] to evaluate the error for other ranges of Péclet numbers).

3. Results and discussion

The approximate local Sherwood numbers for a first-order surface reaction can be obtained rewriting Eq. (4) in its local form (Eq. (7)) and taking its derivative (Eq. (8)).

$$\int_0^{x^*} Sh_{Da}(x^*) dx^* = \left(\frac{1}{Da x^*} + \frac{1}{\int_0^{x^*} Sh_C(x^*) dx^*} \right)^{-1} \quad (7)$$

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