



## Technical Note

## Mass transfer rate of a first-order chemical reaction on a wall at high Schmidt numbers



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## ABSTRACT

In this study, we propose a simple formula to calculate the steady-state surface averaged Sherwood number at high Schmidt numbers when a first-order chemical reaction occurs on a wall. The formula uses the surface averaged Sherwood number corresponding to the mass transfer rate with an infinitely fast kinetic and the Damköhler number. The validity of the prediction is analyzed. It has been found that it predicts the surface averaged Sherwood number of the analytical solution within 5% for wide ranges of Reynolds and Damköhler numbers. The mathematical form of the prediction is suitable to compute the initial transient of the time evolution of the surface averaged Sherwood number in unsteady state conditions. The validity of this time evolution is determined by comparing it with numerical simulations.

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## 1. Introduction

The wall mass transfer rate is a key quantity in many technological and natural processes. Heterogeneous reactions on catalytic surfaces, electrochemical reactions on the surface of an electrode and the exchange of chemicals in biological surfaces are examples of situations in which the mass fluxes of chemical species on boundaries play an important role. These mass fluxes can be originated by a defect of a specific reacting chemical produced by a chemical or electrochemical reaction on the boundary or by the deposition of biological molecules or cells onto surfaces. For example, many microfluidic devices for biomolecular detection are based on the reaction between the analytes that are transported in solution by a fluid flow and the receptors that are located on a surface [1].

Some of these processes follow, or can be modeled considering, a first-order kinetic law. The overall rate at which the chemical or the biochemical transformation occurs at the wall depends on the rate at which the chemicals are advected and diffused and on the kinetic rate. The ratio between the time scales of diffusion and reaction is usually expressed as the Damköhler number ( $Da \equiv$  diffusion time/reaction time). If  $Da \ll 1$  the process is kinetically limited and if  $Da \rightarrow \infty$  (i.e. fast chemical reaction) the process is considered diffusion limited.

A wide variety of surface reactions occurring in the above mentioned applications, take place in liquid phase. In this case the typical Schmidt numbers may range from about  $10^3$  to  $10^5$  considering the kinematic viscosity of the water ( $\nu \approx 10^{-6} \text{ m}^2/\text{s}$ ) and diffusivities of chemical species in liquids of  $D = 10^{-9} \text{ m}^2/\text{s}$  [2], diffusivities of large biomolecules [3] or diffusivities of cells or platelets [4] of about  $D = 10^{-11} \text{ m}^2/\text{s}$ . Even in microfluidic applications with liquid flows in conduits with small hydraulic diameters, the large value of the Schmidt number produces very thin mass transfer boundary layers in comparison with the momentum boundary layer [5] and the mass transfer rate depends mainly on the velocity gradient at the wall.

The analytical solution to the two-dimensional steady state heat/mass transfer boundary layer equations at large Prandtl/Schmidt numbers was first reported by Lévêque [6]. The expression of the surface averaged wall transfer rate is the conventional design relation for mass-transfer wall gauges used to measure the wall shear stress [7]. Unsteady state analytical solutions to the two-dimensional mass transfer boundary layer equations were given by Soliman and Chambré [8]. Mass transfer with a finite rate first order chemical reaction was considered by Apelblat [9,10] who reported analytical solutions for the steady state boundary layer equations neglecting the streamwise diffusion [9] and considering the streamwise diffusion [10]. The approach used by Apelblat [9] was generalized by Elperin and Fominykh [11] for the case of flow past a wedge.

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**Nomenclature**

Ai, Bi	Airy functions
C	concentration (mol m <sup>-3</sup> )
c <sub>n</sub>	zeros of the function Ai(-x)
d	diameter (m)
D	mass diffusion coefficient (m s <sup>-2</sup> )
Da	Damkhöler number, Da = k δ/D
H	height (m)
K	convective mass transfer coefficient (m s <sup>-1</sup> )
k	kinetic constant (m s <sup>-1</sup> )
L	length (m)
N''	molar flux density (mol m <sup>-2</sup> s <sup>-1</sup> )
Re <sub>τδ</sub>	Reynolds number, Re <sub>τ</sub> = u <sub>τ</sub> δ/ν
S	velocity gradient (s <sup>-1</sup> )
Sc	Schmidt number, Sc = ν/D
Sh	Sherwood number, Sh = K δ/D
t	time (s)
U	average velocity (m s <sup>-1</sup> )

x, y Cartesian coordinates (m)

*Greek letters*

Γ	Gamma function
δ	length of the active portion of the wall (m)
δ <sub>c</sub>	mass transfer boundary layer thickness (m)
μ	dynamic viscosity (kg m <sup>-1</sup> s <sup>-1</sup> )
ν	kinematic viscosity (m s <sup>-2</sup> )
ρ	density (kg m <sup>-3</sup> )

*Superscripts and subscripts*

*	non-dimensional quantity
ad	axial diffusion
O	reference value
w	wall

The objective of this study is to propose simple correlations to compute easily the surface averaged wall mass transfer rates produced by a first-order chemical reaction occurring on a wall. The validity of the proposed correlations is analyzed comparing the predicted Sherwood numbers with those corresponding to the full analytical expression for the steady state situations and to those obtained from numerical simulations for the unsteady mass transfer problem.

**2. Model**

Fig. 1 shows a sketch of the two dimensional physical model and the coordinate system adopted. It is assumed that the fluid has constant physical properties. The flow is incompressible, steady and fully developed. The mass transfer boundary layer is much more thin than the momentum boundary layer (Sc ≫ 1) to, reasonably, assume that the velocity profile within the mass transfer boundary layer is linear (S = du/dy = constant). This assumption is valid if the hydraulic diameter of the conduit (d) is much larger than the mass transfer boundary layer thickness (δ<sub>c</sub>). The first-order chemical reaction with kinetic constant, k, occurs on a portion of the wall with length δ. The concentration of the reacting chemical specie outside the mass transfer boundary layer is constant, C<sub>o</sub>. Under these hypotheses, the non-dimensional unsteady concentration distribution is governed by

$$\frac{\partial C^*}{\partial t^*} + \text{Re}_{\tau\delta}^2 \text{Sc} y^* \frac{\partial C^*}{\partial x^*} = \left( \frac{\partial^2 C^*}{\partial x^{*2}} + \frac{\partial^2 C^*}{\partial y^{*2}} \right) \tag{1}$$

The scales of concentration, length and time used to obtain the non-dimensional variables are C<sub>o</sub>, δ, and δ<sup>2</sup>/D, respectively. In Eq. (1), Re<sub>τδ</sub> = (S/ν)<sup>1/2</sup> δ is the Reynolds number based on the velocity gradient, S, and Sc = ν/D is the Schmidt number. Note that the in the second term on the left had side of Eq. (1) the term Re<sub>τδ</sub><sup>2</sup> Sc y\* corresponds to the streamwise velocity component that varies linearly along the vertical direction within the mass transfer boundary layer.

The boundary conditions in terms of the non-dimensional variables are:

$$\frac{\partial C^*}{\partial y^*} \Big|_w = \text{Da} C^* \Big|_w \tag{2}$$

on the active portion of the wall and

$$\frac{\partial C^*}{\partial y^*} \Big|_w = 0 \tag{3}$$

on the inactive portions of the wall. In Eq. (2) Da = kδ/D is the Damkhöler number. At the inlet (x\* = 0) and far from the wall (y\* → ∞) the concentration is constant and C\* is set to 1. Additionally, ∂C\*/∂x\* = 0 is set at x\* = 0 if the streamwise diffusion term is considered (i.e. ∂<sup>2</sup>C\*/∂x\*<sup>2</sup> ≠ 0 in Eq. (1)).

The local Sherwood number or the local non-dimensional wall mass transfer rate at the wall can be defined as,

$$\text{Sh}(x^*) = \frac{N''(x) \delta}{C_o D} = \frac{\partial C^*}{\partial y^*} \Big|_w \tag{4}$$

Using the definition of the local Sherwood number and the boundary condition expressed in Eq. (2) the concentration at the active portion of the wall is

$$C_w^*(x^*) = \frac{\text{Sh}(x^*)}{\text{Da}} \tag{5}$$

Correspondingly, the surface averaged Sherwood number and the surface averaged concentration on the active portion of the wall are

$$\overline{\text{Sh}} = \frac{\overline{N''} \delta}{C_o D} = \int_0^1 \text{Sh}(x^*) dx^* \tag{6}$$

and

$$\overline{C}_w^* = \frac{\overline{\text{Sh}}}{\text{Da}} \tag{7}$$

respectively.

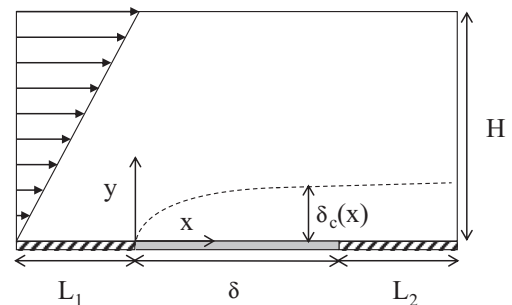


Fig. 1. Physical model and coordinate system.

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