

AN ANALYTIC SOLUTION FOR THE TRANSIENT DIFFUSION PROBLEM IN A MULTI-LAYER SYSTEM

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Abstract

An analytic solution for the dynamic diffusive transport in a multi-layer system has been developed. The partial differential equations of the model are subjected to boundary conditions, which may be chosen as any function of the time. The methodology followed here, exploits the simplicity of the separation of variables method and the superposition concept and, an eigenvalue or Sturm-Liouville problem is generated. The computation of the eigenvalues associated to the Sturm-Liouville problem is presented. The analytic solution is evaluated using three different time functionality of the bulk fluid concentration. The results show that the type of time functionality at the boundaries strongly affects the shape of the concentration profile inside of the multi-layer system. In some case, the time functionality of the concentration does not lead to any steady state. The main advantage of the analytic solution, when it is compared with that obtained numerically, is the lower CPU time used to evaluate the solution of the problem with the same accuracy.

Keywords: analytic solution, multi-layer system, dynamic diffusive transport, Sturm-Liouville problem.

Resumen

Se ha desarrollado una solución analítica para el problema de transporte difusivo dinámico. Las ecuaciones diferenciales parciales del modelo están sujetas a condiciones de frontera que pueden ser seleccionadas como cualquier función del tiempo. La metodología seguida en el presente trabajo explota la simplicidad del método de separación de variables y el concepto de superposición y con esto se genera un problema de Sturm-Liouville. El cómputo de los valores propios asociado al problema de Sturm-Liouville también es presentado. La solución analítica es evaluada usando tres funcionalidades de la concentración del seno del fluido con respecto al tiempo. Los resultados muestran que el tipo de funcionalidad con el tiempo afecta fuertemente la forma de los perfiles de concentración dentro del sistema multi-capas. En algunos casos, la funcionalidad con respecto al tiempo de la concentración no conduce a un estado estacionario. La principal ventaja de la solución analítica, cuando ésta es comparada con la obtenida numéricamente, es la reducción en tiempo de CPU usado para evaluar la solución del problema con la misma exactitud.

Palabras clave: solución analítica, sistema de capa múltiple, transporte difusivo dinámico, problema de Sturm-Liouville.

1. Introduction

Many of the transient models obtained from transport phenomena principles are in terms of partial differential equations (PDE's). In recent years, the rapid advances in the computational area have promoted a high development of the numerical methods for the solution of partial differential equations. However, despite the improvements in the numerical techniques, the analytic solutions of PDE's can be very useful, because:

- i) they provide the correct trend of solution for any numerical method, this is, they state the reliability limits of the numerical methods;
- ii) they reveal clearly the importance of the different parameters involved in the model, and they are desired for intensive process simulation tasks (i.e. computations involving thousands of local and global mass and energy balances).

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More about the convenience of analytic solutions in comparison with numerical solutions can be found in the work by Lewellen *et al.* (1982).

Of particular interest for process simulation is the solution of problems that involve parabolic PDE's that arise in the modeling of dynamic separation processes and in the representation of transient heat transfer normal to a layered wall. This type of models can be important to evaluate separation schemes and heat transfer systems. The exact solutions of the linear case of the described problems have been obtained independently by Ramkrishna and Amundson (1974) and Mikhailov and Ozisik (1984). The methodology to obtain the exact solution presented by Ramkrishna and Amundson (1974) is based on the use of the Sturm-Liouville operator. Their mathematical formalism leads to an elegant solution, but they do not show any case where their analytic solution is evaluated. A similar comment can be expressed about the work presented by Mikhailov and Ozisik (1984). The methodology of Ramkrishna and Amundson (1974) has been applied successfully to formally solve problems of diffusion in particles immersed in mixed fluids (Gandek *et al.*, 1989; Hatton *et al.*, 1979, 1982; Hatton, 1985).

The objective of the present work is to obtain an analytic solution for the dynamic diffusive transport in a system consisting of two different layers subjected to boundary conditions, which may be chosen as any function of the time. The methodology followed in this work exploits the simplicity of the separation of variables method and the superposition concept. Thus, an eigenvalue or Sturm-Liouville problem is generated. It should be noted that the analytic solution obtained in this work is completely equivalent to that found by Ramkrishna and Initial condition:

Amundson (1974) and Mikhailov and Ozisik (1984). However, the simplicity of the methodology followed here allows a quicker evaluation of the solution. In this work, the analytic solution obtained is evaluated and the calculation of the eigenvalues associated to the Sturm-Liouville problem is discussed. Results for three different boundary conditions sets are reported and compared with the numerical solution.

2. Definition of the problem

2.1. Transient diffusion through a two layer system

Fig.1 shows a film in contact with two well mixed fluids that have controlled solute concentration. This film is composed by two layers with different transport properties. The transient diffusion problem for this system is defined by the following two partial differential equations:

$$\frac{\partial C_{(1)}^S}{\partial t} = \mathcal{D}_{(1)} \frac{\partial^2 C_{(1)}^S}{\partial x^2}, \quad \text{for } 0 < x < x_1 \quad (1)$$

$$\frac{\partial C_{(2)}^S}{\partial t} = \mathcal{D}_{(2)} \frac{\partial^2 C_{(2)}^S}{\partial x^2}, \quad \text{for } x_1 < x < x_2 \quad (2)$$

Boundary conditions:

at $x = 0$

$$+\mathcal{D}_{(1)} \frac{\partial C_{(1)0}^S}{\partial x} = k_0 (C_{(1)0}^F - C_{(1)0}^S), \quad \text{for } t > 0 \quad (3)$$

at $x = x_2$

$$-\mathcal{D}_{(2)} \frac{\partial C_{(2)0}^S}{\partial x} = k_2 (C_{(2)0}^F - C_{(2)0}^S), \quad \text{for } t > 0 \quad (4)$$

at $x = x_1$

$$-\mathcal{D}_{(1)} \frac{\partial C_{(1)}^S}{\partial x} = -\mathcal{D}_{(2)} \frac{\partial C_{(2)}^S}{\partial x}, \quad \text{for } t > 0 \quad (5)$$

$$\text{at } x = x_1, \quad C_{(1)}^S = K_{eq} C_{(2)}^S, \quad \text{for } t > 0 \quad (6)$$

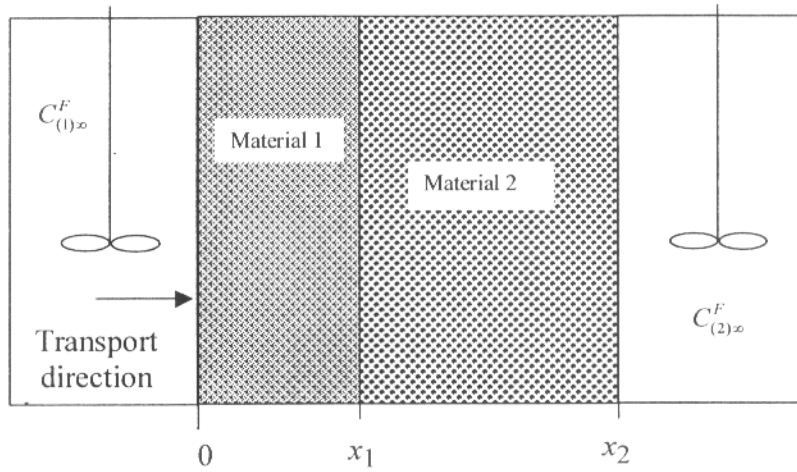


Fig. 1. System formed by two layers with different transport coefficient that are in contact with two well mixed fluids.

at $t=0$

$$C_{(1)}^S = f_1(x), \quad \text{para } 0 < x < x_1 \quad (7)$$

$$C_{(2)}^S = f_2(x), \quad \text{para } x_1 < x < x_2 \quad (8)$$

A brief explanation of the nomenclature is required due to the presence of two phases and because an extension of the solution considering N layers will be attempted later. Therefore, the superscript (S or F) indicates the phase to which the concentration is referred, the subscript (i) refers to the layer i in the multi-layer film S , and finally the right-side subscript j indicates the position x_j . For example, $C_{(1)j}^S$ is the solute concentration in the layer (1) of the multi-layer film S , corresponding to the position x_j . In addition, we have designated the solute concentrations in the bulk fluid phases as $C_{(1)\infty}^F$ y $C_{(2)\infty}^F$ respectively. The rest of the variables are defined in the nomenclature section.

Fig. 2 shows the expected profile for a situation where the transport direction is from left to right. By using the following dimensionless variables:

$$U_{(1)} = \frac{C_{(1)}^S}{C_{ref}^S}$$

$$U_{(2)} = \frac{K_{eq} C_{(2)}^S}{C_{ref}^S}$$

$$\tau = \frac{t \mathcal{D}_1}{x_2^2}$$

$$X = \frac{x}{x_2} \quad (9)$$

The problem defined by Eqs. (1-8) can be written in dimensionless form as:

$$\frac{\partial U_{(1)}}{\partial \tau} = \frac{\partial^2 U_{(1)}}{\partial X^2}, \quad \text{for } 0 < X < X_1 \quad (10)$$

$$\frac{\partial U_{(2)}}{\partial \tau} = \gamma_{(2)} \frac{\partial^2 U_{(2)}}{\partial X^2}, \quad \text{for } X_1 < X < 1 \quad (11)$$

Equations (10) and (11) must be solved together with the following dimensionless boundary conditions:

at $X=0$

$$+\frac{\partial U_{(1)}}{\partial X} = \alpha_o (U_{(1)} - U_{(1)\infty}), \quad \text{for } \tau > 0 \quad (12)$$

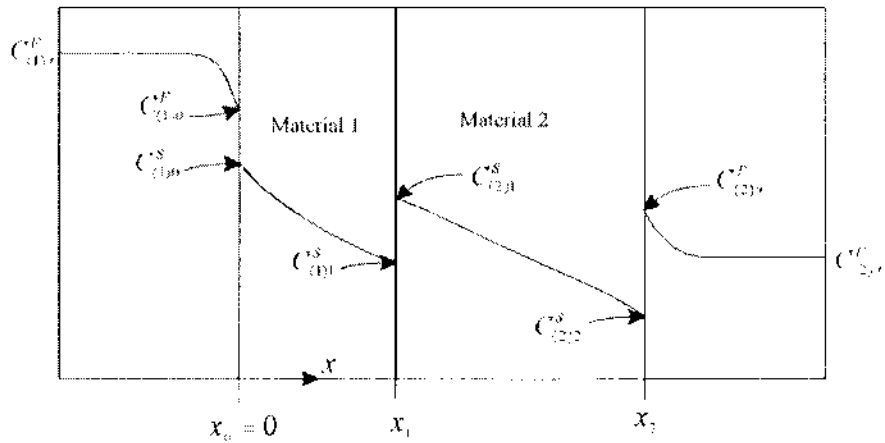


Fig. 2. Schematic diagram of the concentration profiles for a system with two layer in contact with two fluids of controlled concentration.

at $X = 1$

$$-\frac{\partial U_{(2)}}{\partial X} = \alpha_N (U_{(2)} - U_{(2)\infty}), \text{ for } \tau > 0 \quad (13)$$

at $X = X_1$

$$U_{(1)} = U_{(2)}, \text{ for } \tau > 0 \quad (14)$$

at $X = X_1$

$$-\frac{\partial U_{(1)}}{\partial X} = -\beta_1 \frac{\partial U_{(2)}}{\partial X}, \text{ for } \tau > 0 \quad (15)$$

and the initial condition:

at $\tau = 0$

$$U_{(1)} = F_{(1)}(X) \text{ for } 0 < X < X_1 \quad (16)$$

$$U_{(2)} = F_{(2)}(X) \text{ for } X_1 < X < 1 \quad (17)$$

All dimensionless parameters and functions used in equations (10)-(17) can be found in the nomenclature section. However, it is necessary to remark that, in Eqs. (12) and (13), $U_{(1)\infty}$ and $U_{(2)\infty}$ are given by

$$U_{(1)\infty} = \frac{K_0 C_{(1)\infty}^F}{C_{ref}^S}$$

$$U_{(1)\infty} = \frac{K_2 K_{eq} C_{(2)\infty}^F}{C_{ref}^S}$$

Where K_0 and K_2 are the distribution coefficient between the solid layer in contact with the fluid at $x = 0$ and $x = x_2$ respectively.

3. Methodology of solution

The solution of the PDE's, Eqs. (10)-(11), together with the boundary conditions, Eqs. (12)-(15) and the initial condition, Eqs. (16)-(17) requires a methodology that allows, step by step, to obtain an analytic solution in a way that this procedure could be easily extended to a multi-layer system. In general, the methodology to solve analytically the problem is based on the expansion in terms of the eigenfunctions generated by a Sturm-Liouville problem.

This problem is stated considering homogeneous boundary conditions for the original PDE problem. The main steps of the method of solution are as follows:

a) Perform the superposition $U_{(i)} = \tilde{U}_{(i)} + g_{(i)}$, where the functions $g_{(i)}$ may be any function which satisfy the inhomogeneous boundary conditions [Eqs. (12)-(13)] for $U_{(i)}$. This generates homogeneous boundary conditions for $\tilde{U}_{(i)}$ but as consequence the PDE are transformed to inhomogeneous.

b) Apply the method of separation of variables to the transformed partial differential equations (inhomogeneous PDE for $\tilde{U}_{(i)}$), with homogeneous boundary conditions, and obtain a Sturm-Liouville problem. The solution of the Sturm-Liouville problem leads to a set of eigenfunctions $\varphi_{(i)}$ together with eigenvalues $\lambda_{(i)}$.

c) Solve the inhomogeneous partial differential equations for $\tilde{U}_{(i)}$ through an expansion in terms of the eigenfunction $\varphi_{(i)}$.

3.1. Superposition

In order to simplify the boundary conditions of the partial differential equations the following superposition is introduced

$$U_{(i)} = \tilde{U}_{(i)} + g_{(i)} \quad \text{for } i=1,2 \quad (18)$$

Here the functions $g_{(i)}(X, \tau)$ are chosen such that they satisfy the inhomogeneous boundary conditions of the original problem for $U_{(i)}$. This requirement does not force the $g_{(i)}(X, \tau)$ functions to satisfy the differential equations. Thus, it is possible to propose any function which satisfy the inhomogeneous part of Eqs. (12)-(15). A convenient proposition is the following pair of linear relations in X :

$$g_{(1)}(X, \tau) = (U_{(2)\infty} - U_{(1)\infty}) \frac{\beta_1 \alpha_2 [\alpha_0 X + 1]}{\alpha_0 + \alpha_2 \alpha_0 [1 + X_1(\beta_1 - 1)] + \alpha_2 \beta_1} + U_{(1)\infty}, \quad 0 < X < X_1 \quad (19)$$

$$g_{(2)}(X, \tau) = (U_{(2)\infty} - U_{(1)\infty}) \frac{\alpha_2 \alpha_0 [X + X_1(\beta_1 - 1)] + \beta_1 \alpha_2}{\alpha_0 + \alpha_2 \alpha_0 [1 + X_1(\beta_1 - 1)] + \alpha_2 \beta_1} + U_{(1)\infty}, \quad X_1 < X < 1 \quad (20)$$

These relations are similar to those found if the original problem it is solved for the case in which $U_{(1)\infty}$ and $U_{(2)\infty}$ are kept constant. Replacing Eq. (18) into Eqs. (10-17), and the use of the $g_{(i)}$ functions, yields the following problem for $\tilde{U}_{(i)}$:

Transformed partial differential equations:

$$\frac{\partial \tilde{U}_{(i)}}{\partial \tau} = \frac{\partial^2 \tilde{U}_{(i)}}{\partial X^2} - \frac{\partial g_{(i)}}{\partial \tau}$$

for $0 < X < X_1$ (21)

$$\frac{\partial \tilde{U}_{(2)}}{\partial \tau} = \gamma_{(2)} \frac{\partial^2 \tilde{U}_{(2)}}{\partial X^2} - \frac{\partial g_{(2)}}{\partial \tau}$$

for $X_1 < X < 1$ (22)

Homogeneous boundary conditions:

$$\text{at } X = 0 \quad + \frac{\partial \tilde{U}_{(1)}}{\partial X} = \alpha_0 \tilde{U}_{(1)}$$

for $\tau > 0$ (23)

$$\begin{aligned} \text{at } X = 1 \quad & -\frac{\partial \tilde{U}_{(2)}}{\partial X} = \alpha_2 \tilde{U}_{(2)} \\ \text{for } \tau > 0 \end{aligned} \quad (24)$$

$$\begin{aligned} \text{at } X = X_1 \quad & \tilde{U}_{(1)} = \tilde{U}_{(2)} \\ \text{for } \tau > 0 \end{aligned} \quad (25)$$

$$\begin{aligned} \text{at } X = X_1 \quad & -\frac{\partial \tilde{U}_{(1)}}{\partial X} = -\beta_1 \frac{\partial \tilde{U}_{(2)}}{\partial X} \\ \text{for } \tau > 0 \end{aligned} \quad (26)$$

Initial condition

$$\begin{aligned} \text{at } \tau = 0 \\ \tilde{U}_{(1)} = F_1(X) - g_{(1)}(X, 0) \\ \text{for } 0 < X < X_1 \end{aligned} \quad (27)$$

$$\begin{aligned} \tilde{U}_{(2)} = F_2(X) - g_{(2)}(X, 0) \\ \text{for } X_1 < X < 1 \end{aligned} \quad (28)$$

3.2. Generation and solution of the Sturm-Liouville problem

The Sturm-Liouville problem associated with the functions $\tilde{U}_{(i)}$ can be obtained by applying the method of separation of variables to equations (21)-(26), where for convenience the inhomogeneous terms are cancelled.

If the experience of the reader allows it, the Sturm-Liouville problem could be obtained by inspection of the equations (21)-(26). Otherwise, it may be obtained by proposing solutions of the form $\tilde{U}_{(i)} = \varphi_{(i)}(X)G(\tau)$, where it is important to

recognize that the time contribution is the same for both layers. Therefore, the Sturm-Liouville problem obtained for this case is:

Ordinary differential equations (ODE):

$$\begin{aligned} \frac{d^2 \varphi_{(1)n}}{dX^2} = -\lambda_{(1)n}^2 \varphi_{(1)n} \\ \text{for } 0 < X < X_1 \end{aligned} \quad (29)$$

$$\begin{aligned} \gamma_{(2)} \frac{d^2 \varphi_{(2)n}}{dX^2} = -\lambda_{(1)n}^2 \varphi_{(2)n} \\ \text{for } X_1 < X < 1 \end{aligned} \quad (30)$$

Boundary conditions

$$\text{at } X = 0 \quad + \frac{d \varphi_{(1)n}}{dX} = \alpha_o \varphi_{(1)n} \quad (31)$$

$$\text{at } X = 1 \quad - \frac{d \varphi_{(2)n}}{dX} = \alpha_N \varphi_{(2)n} \quad (32)$$

$$\text{at } X = X_1 \quad \varphi_{(1)n} = \varphi_{(2)n} \quad (33)$$

$$\begin{aligned} \text{at } X = X_1 \\ -\frac{d \varphi_{(1)n}}{dX} = -\beta_1 \frac{d \varphi_{(2)n}}{dX} \end{aligned} \quad (34)$$

The solution of the boundary value problem defined by Eqs. (29)-(34) renders the eigenfunctions $\varphi_{(1)n}(X)$, $\varphi_{(2)n}(X)$ and the equations to find the eigenvalues $\lambda_{(1)n}$:

Eigenfunctions

$$\varphi_{(1)n}(X) = K_{(1)n} \left[\frac{\alpha_o}{\lambda_{(1)n}} \sin(\lambda_{(1)n} X) + \cos(\lambda_{(1)n} X) \right], \quad \text{for } 0 < X < X_1 \quad (35)$$

$$\varphi_{(2)n}(X) = K_{(2)n} \left[\alpha_N \frac{\sin[\lambda_{(2)n}(1-X)]}{\lambda_{(2)n}} + \cos[\lambda_{(2)n}(1-X)] \right], \quad \text{for } X_1 < X < 1 \quad (36)$$

$$\text{Where, } \lambda_{(2)n} = \frac{\lambda_{(1)n}}{\sqrt{\gamma_{(2)}}} \quad (37)$$

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$$K_{(1)n} = \frac{\alpha_N \frac{\sin[\lambda_{(2)n}(1-X_1)]}{\lambda_{(2)n}} + \cos[\lambda_{(2)n}(1-X_1)]}{\left[\alpha_N \frac{\sin(\lambda_{(2)n})}{\lambda_{(2)n}} + \cos(\lambda_{(2)n}) \right] \left[\frac{\alpha_o}{\lambda_{(1)n}} \sin(\lambda_{(1)n} X_1) + \cos(\lambda_{(1)n} X_1) \right]} \quad (38)$$

$$K_{(2)n} = \frac{1}{\alpha_N \frac{\sin(\lambda_{(2)n})}{\lambda_{(2)n}} + \cos(\lambda_{(2)n})} \quad (39)$$

Condition for the eigenvalues

$$\left\{ \frac{\alpha_N \sin[\lambda_{(2)n}(1-X_1)]}{\lambda_{(2)n}} + \cos[\lambda_{(2)n}(1-X_1)] \right\} \left\{ \alpha_o \cos(\lambda_{(1)n} X_1) - \lambda_{(1)n} \sin(\lambda_{(1)n} X_1) \right\} + \beta_1 \left\{ \alpha_N \cos[\lambda_{(2)n}(1-X_1)] - \lambda_{(2)n} \sin[\lambda_{(2)n}(1-X_1)] \right\} \left\{ \frac{\alpha_o \sin(\lambda_{(1)n} X_1)}{\lambda_{(1)n}} + \cos(\lambda_{(1)n} X_1) \right\} = 0 \quad (40)$$

A consequence of obtaining the Sturm-Liouville problem is the orthogonality of its solutions, this is, the orthogonality property of the eigenfunctions. In this case, the *Orthogonality condition* is

$$\int_0^{x_1} \varphi_{(1)n} \varphi_{(1)m} dX + \frac{\beta_1}{\gamma_{(2)}} \int_{x_1}^1 \varphi_{(2)n} \varphi_{(2)m} dX = 0$$

for $m \neq n$ (41)

The deduction of this equation is similar to that obtained for the solution of a Sturm-Liouville problem in a homogeneous medium. However, in the case of multiple layers the interfacial conditions are involved.

3.3. *Solution of the inhomogeneous problem for $\tilde{U}_{(i)}$*

The solution process starts with the expansion of $\tilde{U}_{(i)}$ and the inhomogeneous

part of equations (21)-(22) in terms of the eigenfunctions, that is

$$\tilde{U}_{(i)} = \sum_{n=1}^{\infty} C_n(\tau) \varphi_{(i)n} \quad \text{for } i=1,2 \quad (42a)$$

$$-\frac{\partial g_{(i)}}{\partial \tau} = \sum_{n=1}^{\infty} A_n(\tau) \varphi_{(i)n} \quad \text{for } i=1,2 \quad (42b)$$

The expressions for $\tilde{U}_{(i)}$ satisfy the homogeneous boundary conditions given by equations (23) to (26), but not the differential equations (21) and (22). This fact will be used to obtain the unknown time coefficients $C_n(\tau)$. The coefficients $A_n(\tau)$ are obtained through the application of the orthogonality condition, given by Eq. (41), to the equation (42b). This produces:

$$A_n(\tau) = \frac{-\int_0^{x_1} \frac{\partial g_{(1)}}{\partial \tau} \varphi_{(1)n} dX - \frac{\beta_1}{\gamma_{(2)}} \int_{x_1}^1 \frac{\partial g_{(2)}}{\partial \tau} \varphi_{(2)n} dX}{\int_0^{x_1} \varphi_{(1)n}^2 dX + \frac{\beta_1}{\gamma_{(2)}} \int_{x_1}^1 \varphi_{(2)n}^2 dX} \quad (43)$$

Substitution of Eqs. (42) into Eqs. (21) or (22) and the use of Eqs. (31)-(32) leads to a first order differential equation for $C_n(\tau)$, whose solution is

$$C_n(\tau) = \exp(-\lambda_{(1)n}^2 \tau) \left\{ C_n(0) + \int_0^{\tau} \exp(+\lambda_{(1)n}^2 \zeta) A_n(\zeta) d\zeta \right\} \quad (44)$$

The constant $C_n(0)$ is given by:

$$C_n(0) = \frac{\int_0^{x_1} [F_{(1)}(X) - g_{(1)}(X,0)] \varphi_{(1)n} dX + \frac{\beta_1}{\gamma_{(2)}} \int_{x_1}^1 [F_{(2)}(X) - g_{(2)}(X,0)] \varphi_{(2)n} dX}{\int_0^{x_1} \varphi_{(1)n}^2 dX + \frac{\beta_1}{\gamma_{(2)}} \int_{x_1}^1 \varphi_{(2)n}^2 dX} \quad (45)$$

This expression is obtained from the initial condition given by Eqs. (27)-(28), the proposed solutions, Eqs. (42a), and the orthogonality condition, Eq. (41). At this point, we have an analytic solution for the original problem defined by Eqs. (10)-(17).

4. Evaluation of the analytical solution

For the evaluation of the solution, it is convenient to write the coefficients $C_n(0)$ and $A_n(\tau)$, given by Eqs. (43) and (45), in the following form

$$A_n(\tau) = -\frac{\alpha_0 \varphi_{1n}(0)}{\mathcal{J}_n} \frac{dU_{1\infty}}{d\tau} - \frac{\beta_1 \alpha_N \varphi_{2n}(1)}{\mathcal{J}_n} \frac{dU_{2\infty}}{d\tau} \tag{46a}$$

$$C_n(0) = \frac{I_{1n}(0) - I_{2n}(0)}{\mathcal{J}_n} \tag{46b}$$

where

$$2\mathcal{J}_n = \varphi_{(2)n}^2(X_1) \left\{ X_1 + \frac{\beta_1}{\gamma_{(2)}} (1 - X_1) \right\} + \frac{1}{\lambda_{(1)n}^2} \left(\frac{d\varphi_{(2)n}}{dX} \right)^2 \Bigg|_{X_1} \{ X_1 \beta_1^2 + \beta_1 (1 - X_1) \} + \frac{1}{\lambda_{(1)n}^2} \{ \alpha_0 \varphi_{(1)n}^2(0) + \alpha_N \beta_1 \varphi_{(2)n}^2(1) \} \tag{47}$$

$$I_{(1)n}(0) = \frac{U_0}{\lambda_{(1)n}^2} [\alpha_0 \varphi_{(1)n}(0) + \alpha_N \beta_1 \varphi_{(2)n}(1)] \tag{48}$$

$$I_{(2)n}(0) = [\alpha_0 \varphi_{(1)n}(0) U_{(1)\infty}(0) + \alpha_N \beta_1 \varphi_{(2)n}(1) U_{(2)\infty}(0)] \frac{1}{\lambda_{(1)n}^2} \tag{49}$$

The term $I_{1n}(0)$ has been restricted to the case of $F_1(X) = F_2(X) = U_0$. The rest of the formulas are general. To obtain the equations (46)-(49), integration by parts together with the boundary conditions given by Eqs. (31)-(34), have been used.

In Table 1 the specific expressions for the coefficients $C_n(\tau)$ and $A_n(\tau)$ for three different functions of the dimensionless concentration of the well mixed fluids in contact with the end of the layers are shown. It should be noted that the coefficients

$C_n(0)$ given by Eq. (46b) are the same as long the initial condition is U_0 . However, the coefficients $A_n(\tau)$, given by Eq. (46a), require the direct substitution of the time derivatives of $U_{(1)\infty}$ and $U_{(2)\infty}$.

4.1. Eigenvalues computation

In Fig. 3 it is shown the algorithm to evaluate the complete analytic solution. In order to evaluate the required coefficients, it

is necessary to compute the eigenvalues from Eq. (40).

In the present work, the method of Muller have been used to find the multiple real roots of Eq. (40), this is, find the values of the eigenvalues $\lambda_{(1)n}$ for each set of parameters α_0, α_N, X_1 , and β_1 .

Table 2 shows the first seven roots or eigenvalues of $\lambda_{(1)n}$ for different values of α_0, α_N and $X_1=0.5$, and $\beta_1=10$.

5. Results and discussion

The values for the parameters used in the evaluation of the analytic solution are $\alpha_0 = 10, \alpha_N = 10, X_1 = 0.5, \gamma_{(2)} = 2$, and $\beta_1 = 10$. Once the eigenvalues $\lambda_{(1)n}$ have been determined, the expressions for $U_{(1)\infty}$

and $U_{(2)\infty}$ as functions of time and their derivatives must be known to complete the evaluation of the analytic solution. In the present work the initial condition was fixed as $U_0 = 1$ and three different time functions for $U_{(1)\infty}$ and $U_{(2)\infty}$ have been used.

5.1. Case I

The dimensionless concentration at the bulk phases $U_{(1)\infty}$ and $U_{(2)\infty}$ are considered constant. Thus, we have:

$$U_{(1)\infty} = U_{10} = 1 \tag{50}$$

$$U_{(2)\infty} = U_{20} = 2 \tag{51}$$

and as consequence $A_n(\tau) = 0$.

Table 1. Coefficients $A_n(\tau)$ and $C_n(\tau)$ for three sets of fluid concentrations $U_{(2)\infty}(\tau)$ and $U_{(2)\infty}(\tau)$.

Case I		$U_{1\infty} = U_{10}$ and $U_{2\infty} = U_{20}$
$A_n(\tau)$	0	
$C_n(\tau)$	$C_n(0) \exp(-\lambda_{(1)n}^2 \tau)$	
Case II		$U_{(1)\infty} = U_{10} - \sigma_1 \exp(-\mu_1 \tau)$ and $U_{(2)\infty} = U_{20} - \sigma_2 \exp(-\mu_2 \tau)$
$A_n(\tau)$	$-\frac{\alpha_0 \varphi_{(1)n}(0)}{\mathcal{J}_n} \mu_1 \sigma_1 \exp(-\mu_1 \tau) - \frac{\beta_1 \alpha_N \varphi_{(2)n}(1)}{\mathcal{J}_n} \mu_2 \sigma_2 \exp(-\mu_2 \tau)$	
$C_n(\tau)$	$C_n(0) \exp(-\lambda_{(1)n}^2 \tau)$ $+ \frac{\mu_1 \sigma_1 K_{3n}}{\lambda_{(1)n}^2 - \mu_1} [\exp(-\mu_1 \tau) - \exp(-\lambda_{(1)n}^2 \tau)]$ $+ \frac{\mu_2 \sigma_2 K_{4n}}{\lambda_{(1)n}^2 - \mu_2} [\exp(-\mu_2 \tau) - \exp(-\lambda_{(1)n}^2 \tau)]$	
Case III		$U_{(1)\infty} = U_{10}$ and $U_{(2)\infty} = U_{20} - \sigma_2 \sin(\omega_2 \tau)$
$A_n(\tau)$	$\frac{\beta_1 \alpha_N \varphi_{(2)n}(1)}{\mathcal{J}_n} \omega_2 \sigma_2 \cos(\omega_2 \tau)$	
$C_n(\tau)$	$C_n(0) \exp(-\lambda_{(1)n}^2 \tau)$ $- \frac{\omega_2 \sigma_2 K_{4n}}{\lambda_{(1)n}^4 + \mu_2^2} [\lambda_{(1)n}^2 \cos(\omega_2 \tau) + \omega_2 \sin(\omega_2 \tau) - \lambda_{(1)n}^2 \exp(-\lambda_{(1)n}^2 \tau)]$	

- Step 1.** Fix the dimensionless parameters α_0 , α_N , X_1 , $\gamma_{(2)}$, β_1
- Step 2.** Solve Eq. (40) and find the eigenvalues $\lambda_{(1)n}$'s
- Step 3.** Use Eqs. (38) and (39) to evaluate K_{1n} and K_{2n} .
- Step 4.** Use Eq. (46b) to obtain $C_n(0)$.
- Given the time τ :
- Step 5.** Use Eq. (44) to obtain $C_n(\tau)$, for the specific boundary conditions $U_{1\infty}(\tau)$ and $U_{2\infty}(\tau)$.
- Given the position X :
- Step 6.** Evaluate $g_{(1)}(X, \tau)$ or $g_{(2)}(X, \tau)$ using Eqs. (19) or (20)
- Step 7.** Use Eqs. (35)-(36) to evaluate $\varphi_{(1)n}(X)$ or $\varphi_{(2)n}(X)$.
- Step 8.** Evaluate $U_{(i)}$ using Eqs. (18) and (42a).

Fig. 3. Sequence of evaluation of the dimensionless concentration for a given position X and time τ . The eigen values are function of the physicochemical parameters α_0 , α_N , $\gamma_{(2)}$ and β_1 and the geometric parameter X_1 . Steps 1 through 4 are independent of time, position and of the concentrations at the ends of the layers.

Table 2. Eigen values as function of the Biot numbers α_0 and α_N . The rest of the parameters was kept constant as $X_1 = 0.5$, $\gamma_{(2)} = 2$, and $\beta_1 = 10$.

α_0	$\alpha_N = 0.1$						
	$\lambda_{(1)1}$	$\lambda_{(1)2}$	$\lambda_{(1)3}$	$\lambda_{(1)4}$	$\lambda_{(1)5}$	$\lambda_{(1)6}$	$\lambda_{(1)7}$
0.1	0.542655	3.653414	7.579777	10.86589	14.90612	18.33004	22.07767
10	1.581771	5.069331	8.47392	11.71197	15.6005	18.83039	22.62591
100	1.726318	5.60954	9.086742	12.66536	16.55307	19.82057	23.82477
	$\alpha_N = 10.0$						
0.1	1.941782	4.960962	8.72008	11.96756	15.61712	19.21222	22.6102
10	3.168221	6.073589	9.643738	12.63095	16.31502	19.66286	23.12891
100	3.421458	6.654249	10.34915	13.47666	17.3577	20.55433	24.33621
	$\alpha_N = 100.0$						
0.1	2.075618	5.347884	9.197526	12.82708	16.30623	20.27395	23.53558
10	3.412271	6.436911	10.18778	13.45381	16.99288	20.75325	27.96293
100	3.712369	7.045245	11.02348	14.26765	18.12832	21.67424	25.15356

Fig. 4 shows the results of the evaluation of the analytic solution for this case. The dimensionless concentration profiles in both layers are presented as a function of the dimensionless distance (X) in the film and the dimensionless time (τ). In Figure 4, it can be noted that as the time τ is

increased the concentration profiles change from a non-linear behavior with respect to the position to a defined linear steady state. In addition, it can be seen that the concentration at the edges of the film change with the time until they reach their steady state values.

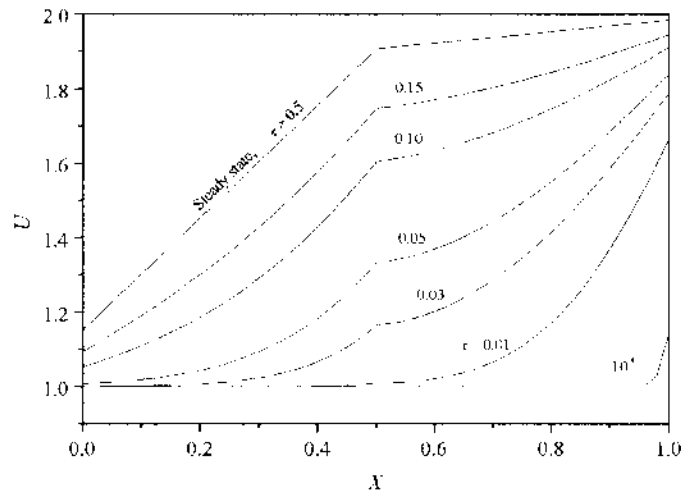


Fig. 4 Evolution of the dimensionless concentration profile for a system subject to the fluid constant concentrations $U_{(1)\infty} = 1$ and $U_{(2)\infty} = 2$. Other parameters are $\alpha_0 = 10$, $\alpha_N = 10$, $X_1 = 0.5$, $\gamma_{(2)} = 2$, and $\beta_1 = 10$.

It should be noted that, because of the transport resistance offered by the fluid, the steady state values at the ends of the film are different from $U_{10} = 1$ and $U_{20} = 2$. The change in the slope of the profiles for both layers (1 and 2) at $X=0.5$ is due to the differences between the diffusion coefficients of both phases and the inclusion of the equilibrium distribution coefficient, which renders $\beta_1 = 10$. Table 3 shows the comparison between the numerical solution

of the problem (finite differences method) and the analytical solution. It should be noted in Table 3, that the error is null at the initial condition ($\tau = 0$), and when the steady state has been achieved. Also, it can be seen that the error decreases as the time is increased. It is obvious that the computing time used for the solution of the problem is smaller for the case of the analytical solution.

Table 3. Comparison of the concentration or temperature profiles and computing times between the numerical solution and the analytical solution. The boundary conditions were kept constant: $U_{(1)\infty} = 1$ and $U_{(2)\infty} = 2.0$. The parameter combination is $\alpha_0 = 10$, $\alpha_N = 10$, $X_1 = 0.5$, $\gamma_{(2)} = 2$, and $\beta_1 = 10$.

τ	Position X								
	0.25			0.50			0.75		
	Num.	Analytic	Error	Num.	Analytic	Error	Num.	Analytic	Error
0.000	1.000	1.000	0.000%	1.000	1.000	0.000%	1.000	1.000	0.000%
0.200	1.560729	1.543920	1.089%	1.844744	1.833050	0.638%	1.892920	1.885115	0.414%
0.400	1.761317	1.754934	0.364%	1.944132	1.940976	0.163%	1.965206	1.963074	0.109%
0.600	1.794908	1.793294	0.090%	1.958793	1.958042	0.038%	1.975619	1.975107	0.026%
0.800	1.800269	1.799912	0.020%	1.961103	1.960940	0.008%	1.977256	1.977143	0.006%
1.000	1.801121	1.801047	0.004%	1.961469	1.961436	0.002%	1.977515	1.977492	0.001%
Est. Esta	1.801282	1.801282	0.000%	1.961539	1.961539	0.000%	1.977564	1.977564	0.000%
CPU time	Numerical Solution			69 s					
	Analytic Solution			4 s					

5.2. Case II

The dimensionless concentration at the bulk phases $U_{(1)\infty}$ and $U_{(2)\infty}$ are the exponential functions of the dimensionless time given by

$$U_{(1)\infty} = 1 - \exp(-10\tau) \quad (52)$$

$$U_{(2)\infty} = 2 - \exp(-10\tau) \quad (53)$$

The values for the parameters $\alpha_0, \alpha_N, X_1, \gamma_{(2)}$, and β_1 used in the evaluation of the analytic solution are the same as for case I. In this case both concentrations, at the bulk of the fluid phases change continuously with time until they reach a constant value for $\tau \gg 1$.

Fig. 5 shows the results of the evaluation of the analytic solution for this case. It can be noted two different behaviors of the profiles. As the time τ is increased the

concentration profile in the layer 1 decreases and it changes from a parabolic behavior with respect to the position to a defined linear steady state. On the other hand, for the layer 2, it can be seen that the concentration profile is linear and it continuously increases as time is increased. It is interesting to note that for short times ($\tau \approx 0.01$) the concentration in the layer 2 remains constant and the effect of the equilibrium and the diffusion coefficients is not observed. The steady state profiles are reached at $\tau = 0.7$. As in case I, it can be seen that the concentration at the edges of the film change with the time until they reach their steady state values. Because of the transport resistance of the fluids the steady state values at the ends of the fluids are different from $U_{10} = 1$ and $U_{20} = 2$.

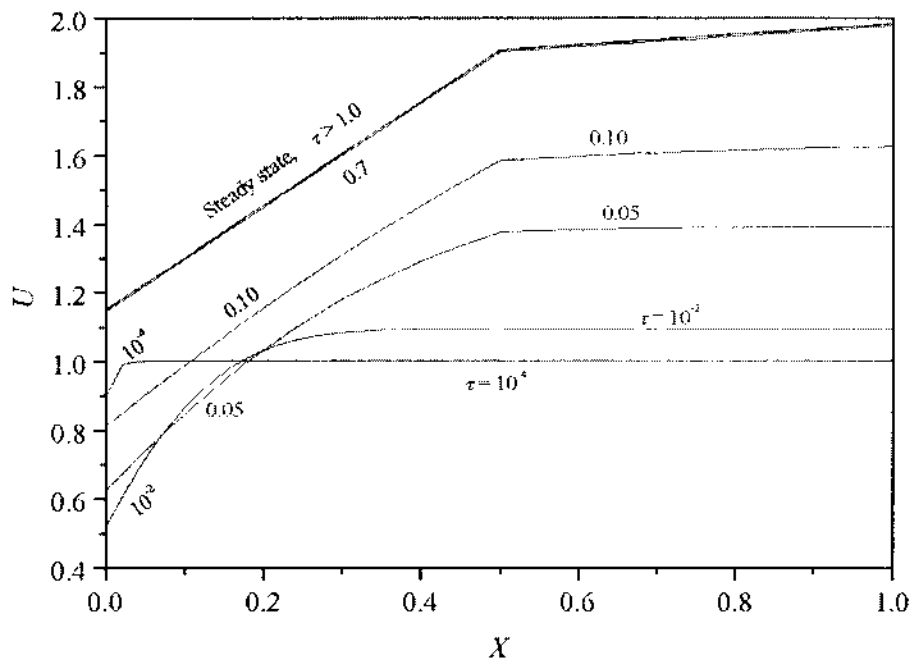


Fig. 5 Evolution of the dimensionless concentration profile for a system subject to the fluid variable concentrations $U_{(1)\infty} = 1 - \exp(-10\tau)$ and $U_{(2)\infty} = 2 - \exp(-10\tau)$. Other parameters are $\alpha_0 = 10, \alpha_N = 10, X_1 = 0.5, \gamma_{(2)} = 2$, and $\beta_1 = 10$.

5.3. Case III

The dimensionless concentration at the bulk phase $U_{1\infty}$ is considered constant and $U_{2\infty}$ is a periodic function of the dimensionless time. Thus, we have:

$$U_{(1)\infty} = U_{10} \quad (54)$$

$$U_{(2)\infty} = U_{20} - \sigma_2 \sin(\omega_2 \tau) \quad (55)$$

The values for the parameters α_0 , α_N , X_1 , $\gamma_{(2)}$, and β_1 used in the evaluation of the analytic solution are the same as for case I and $\sigma_2 = 1$, $\omega_2 = 1$. This type of functionality indicates that the concentration

at the bulk $U_{(2)\infty}$ change periodically with the time.

Fig. 6 shows the results of the evaluation of the analytic solution for this case. It should be noted that in this case a steady state is not achieved. However, two different behaviors of the profiles can be noted. At the beginning, when the time τ is increased, the concentration profile in both layers goes up. Latter, when time is large enough, the concentration profile decreases, this behavior is a consequence of the periodic nature of the bulk concentration of the fluid in contact with layer 2. It can also be seen that for a large time ($\tau \approx 1.5$) the concentration in the layer 2 remains constant and the effect of the differences in the diffusion coefficients and the equilibrium constant is not observed.

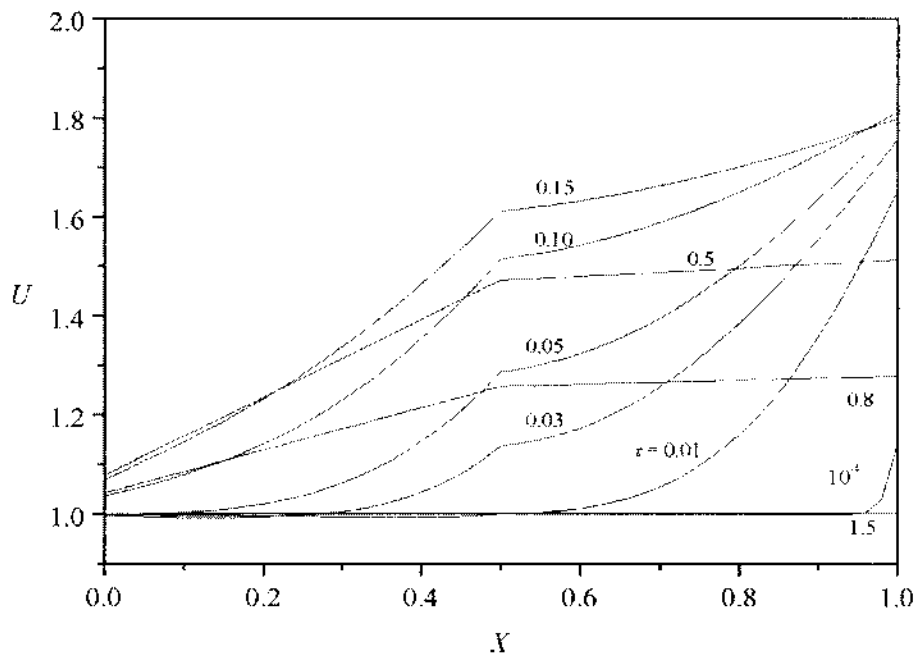


Fig. 6 Evolution of the dimensionless concentration profile for a system subject to the fluid concentrations $U_{(1)\infty} = 1$ and $U_{(2)\infty} = 2 - \sin(\tau)$. Other parameters are $\alpha_0 = 10$, $\alpha_N = 10$, $X_1 = 0.5$, $\gamma_{(2)} = 2$, and $\beta_1 = 10$.

Conclusions

An analytic solution for the transient diffusion problem for a two-layer system has been developed.

This solution has been obtained by using the superposition concept and the application of the method of separation of variables. The main advantage of the analytic solution, when it is compared with that obtained numerically, is the CPU time used to evaluate the solution of the problem for the same accuracy. This fact, confirm the value of having an analytic solution in problems concerning intensive simulation tasks. In this work three different expressions for the concentration of the well mixed fluid phases $U_{(1)\infty}$ and $U_{(2)\infty}$ have been considered. The results show that the type of time functionality for $U_{(1)\infty}$ and $U_{(2)\infty}$ will affect the shape of the concentration (U) profile inside of the multi-layer system. In some case, the effect of the fluid concentration functionality will not lead to a steady state (case III). The different parameter values used in the evaluation of the analytic solution were chosen such that they cover a wide range of real conditions. It should be pointed out that the methodology of solution for a dynamic diffusion in a multi-layer problem presented in this paper, could be exploited for systems where chemical reactions of zero order may occur. Currently, an extension of the analytic solution is being carried out in the study of the time dependence of the global mass transfer coefficients.

Nomenclature

$A_n(\tau)$ = Function defined in Eq. (46a), dimensionless.

$C_n(\tau)$ = Function defined in Eq. (44), dimensionless.

$C_{(i)j}^S$ = Solute concentration in layer i at position x_j , mol/m³.

$C_{(i)j}^F$ = Solute concentration in fluid phase in contact with layer i at position x_j , mol/m³.

C_{ref}^S = Reference concentration of solid fase, mol/m³.

$\mathcal{D}_{(i)}$ = Diffusion coefficient of material i , m²/s.

$f_i(x)$ = Initial condition distribution at layer i , mol/m³.

$F_i(X)$ = Dimensionless initial condition distribution at layer i , mol/m³.

$g_{(i)}$ = Dimensionless function that satisfy the non-homogeneous boundary conditions.

K_{eq} = Equilibrium distribution coefficient between the two solid layers, dimensionless.

$K_{(i)n}$ = Dimensionless constant in eigen function $\varphi_{(i)n}(X)$, Eqs. (38)-(39).

K_i = Distribution coefficient between the solid and the fluid at x_i , dimensionless

k_i = Film fluid mass transfer coefficient at x_0 , m/s.

$I_{1n}(0)$ = Function defined by Eq. (48), dimensionless.

$I_{2n}(0)$ = Function defined by Eq. (49), dimensionless.

\mathcal{D}_n = Denominator in Eqs. (46), dimensionless.

t = Time, s.

$U_{(i)}$ = Dimensionless concentration in layer (i), Eq. (9).

$U_{(i)\infty}$ = Dimensionless bulk fluid concentration that is in contact with layer i .

$\tilde{U}_{(i)}$ = Dimensionless concentration function obtained by the solution of homogeneous boundary value problem.

X = Dimensionless position.

x = Position, m.

x_i = Thickness of layer i , m.

Greek letters

α_0	=	Fluid Biot number at x_0 ,
$k_0 x_2 / K_0 \mathcal{L}_{(1)}$		
α_N	=	Fluid Biot number at x_2 ,
$k_2 x_2 / K_2 \mathcal{L}_{(2)}$		
β_1	=	permability ratio of solid layers,
$\mathcal{D}_{(i)} K_{eq} / \mathcal{D}_{(1)}$		
$\gamma_{(i)}$	=	Diffusion coefficient ratio,
$\mathcal{D}_{(i)} / \mathcal{D}_{(1)}$		
ζ	=	Dummy variable, dimensionless.
$\lambda_{(i)}$	=	Eigen value, dimensionless.
τ	=	Dimensionless time.
$\varphi_{(i)}$	=	Eigen function, dimensionless.

Subscripts

i	=	Indicates material layer.
0	=	Initial condition
∞	=	Bulk fluid phase.

Superscripts

S	=	Solid
F	=	Fluid

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