Prolate Spheroidal Coordinate: An Approximation To Modeling Of Ellipsoidal Drops In Rotating Disc Contractor Column

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Abstract

In many situations the shape of the drops contained in a liquid or porous media is not perfectly spherical. Accurate modeling of the process extraction in Rotating Disc Contractor (RDC) column is only possible with accurate description of the geometry of the drop. In this research, the diffusion equation given in prolate spheroidal coordinate system is used for a two-dimensional case. An analytical solution of the unsteady diffusion equation describing mass transfer for prolate spheroidal drops, considering a constant diffusion coefficient is presented. The resulting equations are analytically solved by using the separation method. The solution describes that the concentration of the drop decreases with the increases of drop shapes. This model can be used to study the mass transfer process of liquid-liquid extraction in RDC Column for spheroidal drop.

Keywords: Diffusion equation, prolate spheroidal coordinate, separation method.

1.   INTRODUCTION

The study of liquid-liquid extraction is an important subject to be discussed not just amongst chemical engineers but mathematicians as well. This type of extraction is one of the important separation technologies in the process industry and is widely used in the chemical, biochemical and environmental fields. The principle of liquid-liquid extraction process is the separation of components from a homogeneous solution by using another solution which is known as a solvent [7] [13]. There are many types of equipments used for the processes of liquid-liquid extraction. The concern of this research is only with the column extractor type, namely the Rotating Disc Contactor (RDC) column.

Several models have been developed for modeling of extraction processes in RDC column. The model shows that the drop size distribution and the mass transfer processes are important factors for the column performances. Since the behavior of the drop breakage and the mass transfer process involve complex interactions between relevant parameters, the need to get as close as possible to the reality of the processes is evident. Several researchers namely Korchinsky and Azimzadih [8], Talib [12], Ghalehchian [6] and Arshad [1] had been working in the area of modeling of mass transfer in RDC column. Most of these models are based on the assumption of spherical drops. The problem of spherical drop or bubble is known as the simplest and ideal case in which the problem can be considered in spherical coordinate system [3]. However there are many physical situations the shape of the drops contained in liquid or porous media is not perfectly spherical and may be classified as prolate or oblate spheroids [3]. Accurate modeling of the process extraction in RDC column is only possible with accurate description of the geometry of the drop. The objective of this paper is to develop the model of mass transfer for ellipsoidal drops in RDC column by using prolate spheroidal coordinate as an approximation.

2.   PROLATE SPHEROIDAL COORDINATE

A prolate spheroid is generated by rotating an ellipse about its major axis contrasted with oblate spheroid. The boundary value problems involving prolate spheroid bodies may be treated in prolate spheroidal coordinates (μ, ϕ, ω). In this system the coordinate surfaces are two families of orthogonal surfaces of revolution. The surfaces of constant are a family of confocal prolate spheroids, and the surfaces of constant are a family of confocal hyperboloids of revolution. The prolate spheroidal coordinate related to the Cartesian

coordinate was presented by [10], [5] and [14] through the transformation equations ϕ

$$x = L \sinh \mu \sin^{\phi} \cos \omega \quad (1a)$$
$$y = L \sinh \mu \sin^{\phi} \sin \omega \quad (1b)$$
$$z = L \cosh \mu \cos^{\phi} \quad\quad (1c)$$

where $L=\sqrt{L_2{}^2-L_1{}^2}$ is the focal distance of the prolate spheroidal drop measured from the coordinate origin, and L_1 and L_2 are the major and minor axes, respectively. To show the significance of μ geometrically, take μ be a constant and let

$$a_1 = L\cosh \mu \quad\quad (2a)$$

$$a_2 = L\sinh \mu \quad\quad (2b)$$

From (1) and (2) we can obtain

$$\frac{x^2+y^2}{a_2{}^2}+\frac{z^2}{a_1{}^2}=1 \quad\quad\quad (3)$$

Eq (3) represents a prolate spheroid in Cartesian coordinates. On the other hand, to show the significance of ϕ geometrically, take ϕ be a constant and let

$$b_1 = L \cos^{\phi} \quad\quad (4a)$$

$$b_2 = L \sin^{\phi} \quad\quad (4b)$$

Again from (1) and (4) we can obtain

$$-\frac{x^2+y^2}{b_2{}^2}+\frac{z^2}{b_1{}^2}=1 \quad\quad\quad (5)$$

This equation represents a family of hyperboloids. An ellipsoid of revolution scheme is shown in figure 1.
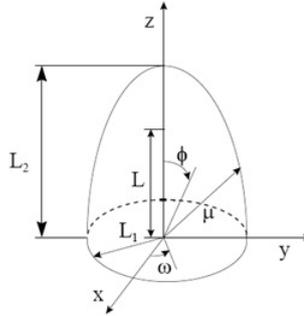
Fig1. Characteristics of a prolate spheroidal drop

Acording to Elkamel [4] there are other equivalent transformations obtained from (1) by defining $\xi = \cosh \mu$ and $\eta = \sinh f$

$$x = L\sqrt{(\xi^2 - 1)(1 - \eta^2)} \; cos \; \omega \qquad (6a)$$
$$y = L\sqrt{(\xi^2 - 1)(1 - \eta^2)} \; sin \; \omega \qquad (6b)$$
$$z = L\xi\eta \qquad (6c)$$

Where $\xi > 1$, $-1 < \eta < 1$, $0 < \omega < 2\pi$, μ, ϕ are called the radial and angular variables, respectively. Mou and Howe [10] also introduced the scale factors for the prolate spheroidal coordinates system. These factors can be calculated from equation (6)

$$h_\xi = \left|\frac{\partial r}{\partial \xi}\right| = L\sqrt{\frac{\xi^2 - \eta^2}{\xi^2 - 1}} \qquad (7a)$$

$$h_\eta = \left|\frac{\partial r}{\partial \eta}\right| = L\sqrt{\frac{\xi^2 - \eta^2}{1 - \eta^2}} \qquad (7b)$$

$$h_\phi = \left|\frac{\partial r}{\partial \phi}\right| = L\sqrt{\xi^2 - 1)(1 - \eta^2)} \qquad (7c)$$

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Where $\bar{r}$ is the Cartesian position vector of $r = xi + yj + zk$. The unit vectors $\bar{\xi}, \bar{\eta}$ and $\bar{\phi}$ are defined as

$$\bar{\xi} = \frac{\dfrac{\partial r}{\partial \xi}}{h_\xi} \tag{8a}$$

$$\bar{\eta} = \frac{\dfrac{\partial r}{\partial \eta}}{h_\eta} \tag{8b}$$

$$\bar{\phi} = \frac{\dfrac{\partial r}{\partial \phi}}{h_\phi} \tag{8c}$$

The gradient operator ∇ and Laplacian ∇^2 in the prolate spheroidal coordinate can be written as

$$\nabla = \bar{\xi}\frac{1}{h_\xi}\frac{\partial}{\partial \xi} + \bar{\eta}\frac{1}{h_\eta}\frac{\partial}{\partial \eta} + \bar{\phi}\frac{1}{h_\phi}\frac{\partial}{\partial \phi} \tag{9}$$

$$\nabla = \frac{1}{L}\left[\bar{\xi}\sqrt{\frac{\xi^2-1}{\xi^2-\eta^2}}\frac{\partial}{\partial \xi} + \bar{\eta}\sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}}\frac{\partial}{\partial \eta} + \bar{\phi}\sqrt{\frac{1}{(\xi^2-1)(1-\eta^2)}}\frac{\partial}{\partial \phi}\right] \tag{10}$$

$$\nabla^2 = \frac{1}{L^2(\xi^2-\eta^2)}\left\{\frac{\partial}{\partial \xi}\left[(\xi^2-1)\frac{\partial}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[(1-\eta^2)\frac{\partial}{\partial \eta}\right] + \frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial \phi^2}\right\} \tag{11}$$

Eq. (11) will be used later to derive the diffusion equation in prolate spheroidal coordinates.

3. GOVERNING DIFFUSION EQUATION IN PROLATE SPHEROIDAL COORDINATE

The governing equation for the diffusion process based on Fick's second law of diffusion can be written in simplified notation in any three dimensional coordinates and in the Cartesian coordinate system as

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) = D\nabla^2 u \tag{12}$$

where V^2 is known as the standard Laplacian operator which is the second order partial derivative. Eq. (12) is an appropriate equation to predict mass diffusion in bodies with a rectangular shape, such as plates and parallelepipeds [2] and [9]. To predict the phenomenon in ellipsoidal drops, it is necessary to transform this equation into an appropriate coordinate system, in this case , the prolate spheroid coordinate system. By using (11) and considering the constant diffusion coefficient, (12) can be written in prolate spheroidal coordinates as follows:

$$\frac{\partial u}{\partial t} = \frac{D}{L^2(\xi^2 - \eta^2)} \left\{ \frac{\partial}{\partial \xi}\left[(\xi^2 - 1)\frac{\partial u}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[(1 - \eta^2)\frac{\partial u}{\partial \eta}\right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)}\frac{\partial^2 u}{\partial \phi^2} \right\} \quad (13)$$

4. MATHEMATICAL MODEL AND SOLUTION

The new model to predict mass transfer in prolate spheroidal coordinates, for a situation with symmetry around the axes is given by

$$\frac{\partial u}{\partial t} = \frac{D}{L^2(\xi^2 - \eta^2)} \left\{ \frac{\partial}{\partial \xi}\left[(\xi^2 - 1)\frac{\partial u}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[(1 - \eta^2)\frac{\partial u}{\partial \eta}\right] \right\}, \quad (14)$$

$$\xi \geq 1, -1 \leq \eta \leq 1, t \geq 0$$

Where D is the coefficient of diffusion u is the concentration and t is the time. The initial condition of equation (10) is:

$$u(\xi, \eta, 0) = u_0 \quad (15)$$

and the convective boundary condition , also called boundary condition of the third kind or still Cauchy boundary condition is :

$$-\frac{D}{L}\sqrt{\frac{\xi^2 - 1}{\xi^2 - \eta^2}}\frac{\partial u}{\partial \xi} = h_m\left[u(\xi = \xi_f, \eta, t) - u_e\right] \text{ for } \xi = \xi_f = \frac{L_2}{L} \quad (16)$$

Here, h_m is the mass transfer coefficient, $u(\xi, \eta, t)$ is the concentration and u_e is the equilibrium concentration.

The solution $u(\xi, \eta, t)$ of Eq. (10) with uniform initial concentration u_0 and Cauchy boundary condition defined by Eq. (12) can be obtained by using the method of separation of variables [9]. Setting $u(\xi, \eta, t) = \Phi(\xi, \eta)\theta(t)$, the solution of Eq. (10) can be written as:

$$u(\xi, \eta, t) = \Phi(\xi, \eta)\exp\left(-\frac{c^2 Dt}{L^2}\right) \quad (17)$$

where c is a constant. Assuming that the diffusion coefficient is constant and substituting Eq. (17) to Eq. (14), we get:

$$\nabla^2 \Phi + \left(\frac{c^2}{L^2}\right)\Phi = 0. \qquad (18)$$

Setting $\Phi(\xi, \eta) = \chi(\xi)\lambda(\eta)$, we get two ordinary differential equations:

$$\left[\frac{d}{d\xi}\left((1-\xi^2)\frac{d\chi}{d\xi}\right)\right] + (b - c^2\xi^2)\chi = 0 \qquad (19)$$

$$\left[\frac{d}{d\eta}\left((1-\eta^2)\frac{d\lambda}{d\eta}\right)\right] + (b - c^2\eta^2)\lambda = 0 \qquad (20)$$

where c is the separation constant. The solution of the Eq. (19) and (20) are given by:

$$\chi_m(c, \xi) = \left[\sum_{n=0}^{\infty} d_{n,m}\right]^{-1} \sum_{n=0}^{\infty}(-1)^{\frac{n-m}{2}} d_{n,m} j_n(c\xi) \qquad (22)$$

$$\lambda_m(c, \eta) = \sum_{n=0}^{\infty} d_{n,m}(c)P_n(\eta) \qquad (23)$$

where P_n is the Legendre function series of the first kind and j_n is the spherical Bessel functions series of the first kind of order n. The formal solution of the problem is given by:

$$u(\xi, \eta, t) = \sum_{m=0,2}^{\infty}\sum_{k=1}^{\infty} A_{mk}e^{-c^2_{mk}\frac{Dt}{L^2}}\chi_m(c, \xi)\lambda_m(c, \eta) \qquad (24)$$

where

$$A_{mk} = \frac{\int_0^1\int_0^{\frac{L2}{L}}\chi_m(c_{mk}, \xi)\lambda_m(c_{mk}, \eta)(\xi^2 - \eta^2)(u_0 - u_e)d\xi d\eta}{\int_0^1\int_0^{\frac{L_2}{L}}[\chi_m(c_{mk}, \xi)\lambda_m(c_{mk}, \eta)]^2(\xi^2 - \eta^2)d\xi d\eta}. \qquad (25)$$

Fig.3 shows profile of the concentration (u) of the drop as a function of time for different value of the shape. For a prolate spheroidal drop, as the shape decreases the concentration of the drop increases.
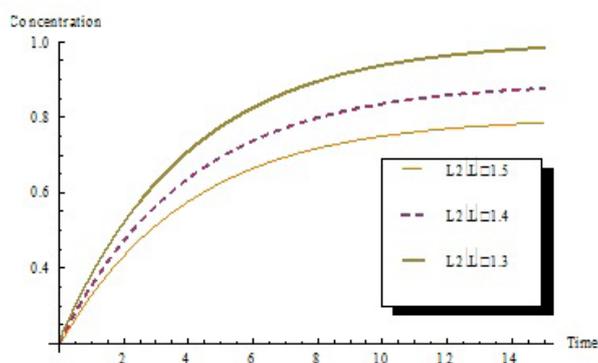
Fig. 2. Profile the concentration as a function of time of a prolate spheroidal drop for L2/L = 1.3, 1.4, and 1.5

To validate the analytical solution presented here can be compared with [2] and [12] that had been developed successfully by the previous researchers.

CONCLUSIONS

It has been presented the analytical solution for two dimensional diffusion equation in prolate spheroidal coordinate. This model can be used to describe mass transfer for prolate spheroidal drops in RDC column.

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