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Solution of counter diffusion problem with position dependent diffusion coefficent by using variational methods

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ABSTRACT

Unsteady state counter diffusion problem with position dependent diffusion coefficient can be modeled using Fick's second law. A mathematical model was constructed and solved to quantitatively describe the dynamic behavior of solute diffusion through non-homogeneous materials where diffusion coefficient is a function of position. The eigenfunction expansion approach was utilized to solve the model. The eigenvalues and eigenfunction of the system were obtained using a variational method. It has been shown that position dependency of the material can be neglected if the thickness of the material is relatively small. Mathematical models were solved for different thicknesses and different diffusion coefficient functions.

1. Introduction

Diffusion of a substance may occur in all three phases such as gas, liquid and solid, but diffusion in solids is far more complex than diffusion in gases and liquids. The reason is that a diffusing substance may be diffusing through a liquid or a gas contained within the pores of the solid. Also, some solids such as crystals, polymeric films, and solids with capillaries, have irregular pore size distributions and pores connectivity, in which the diffusing molecules have preferential direction of movement [1]. The diffusion in both gases and liquids can be successfully predicted by some theories, but predicting diffusion in solids where the diffusion coefficient can differ more than a factor of 10^{10} is much more complex [2]. Studying diffusion process, and especially diffusion in solids, has been attracted many scientists and researchers, because diffusion in solids is one the most common transport mechanisms in nature. Solution of diffusion equation for a variety of initial and boundary conditions and for a different geometry with a constant diffusion coefficient, which is the case for many processes, has been reported [3]. Studying diffusion in solids with a variable diffusion coefficient is crucial because of diffusion in non-uniform solid and counter diffusion process.

Sadikoglu et al. [4] studied the diffusion of potassium sorbate through whey protein films where the diffusion coefficient depended on the diffusion coefficient potassium sorbate at the equilibrium, and the ratio of solvent adsorption. They obtained the ratio of solvent adsorption as a function of time by solving the solvent diffusion equation. They used the ratio of solvent adsorption equation to define the time-dependent potassium sorbate diffusion coefficient through the whey protein films. They solved the diffusion equations with the time-dependent diffusion coefficient analytically to obtain the fractional potassium sorbate release. They obtained excellent agreement between the experimental and the theoretical values.

Liu and Simpson [5] analyzed the diffusion of a substance in capillary porous solids where the diffusion coefficient was an exponential function of concentration. Yamamoto [6] studied the concentration dependent diffusivity in liquid foods

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and polymer solution, and developed a simple method for determining the diffusion coefficient. Islam et al. [7] studied the diffusion of water in liquid phase in a drying material and developed a liquid diffusion model with moisture and temperature dependent effective mass diffusivity and thermal conductivity. Elbert et al. [8] proposed a mathematical model for moisture diffusion in a solid sphere with variable diffusion coefficient. Diffusion also depends heavily on the shape (geometry) of the materials where diffusion of substances takes place. Li et al. [9] analyzed and modeled the diffusion in ellipsoidal solids, which is considered to be the geometrical shape for the most food materials. Abd-el-Malek et al. [10] studied the diffusion of a drug through a skin-like membrane by using the method of transformation group theory. The heat diffusion problem in a spherical medium with nonlinear boundary conditions is solved by Abd-el-Malek and Helal [11] using the finite integral transform technique.

In this work, a mathematical model for counter diffusion problem with a position dependent diffusion coefficient is solved to describe the diffusion of a solute to the solvent inside a solid material, which is the case for many industrial processes such as drying, membrane separations, frying, drug delivery, etc.

2. Mathematical model

This work considers semi-analytical solution of diffusion equation with the position dependent diffusion coefficient. First it was assumed that the diffusion of a substance takes place from a thin film of a material where the concentration distribution is homogeneous, free of solvent, and its boundary was brought into contact with a solvent at ends (i.e. at $x = 0$ and $x = L$). The solvent absorption and solute diffusion of a material begins simultaneously. The diffusion through a swelling thin sheet can be derived from the Fick's second law of diffusion in one dimension (thickness of the film is relatively small compared with the surface area) with a time dependent diffusion coefficient:

$$\begin{aligned} &\frac{\partial C}{\partial t} = D(t)\frac{\partial^2 C}{\partial x^2}, \quad 0 < x < L, \quad t > 0 \\ &C = 0, \qquad x = 0, \quad t > 0 \\ &C = 0, \qquad x = L, \quad t > 0 \\ &C = C_0 \qquad t = 0, \quad 0 < x < L \end{aligned} \tag{1}$$

where C is the solute concentration in the film, $D(t)$ is the time-dependent diffusion coefficient of the solute, x is the coordinate along the diffusion direction, and t is the time. Good [12], Korsmeyer and Peppas [13] and Sadikoglu et al. [4] have shown that the diffusion coefficient for the solute is proportional to the degree of the solvent absorption by neglecting any changes in thickness of the thin film due to the solvent swelling. The diffusion coefficient of solute in the film varies with the solvent absorption and it always has a higher value at the surface than the center of the thin film. Since the amount of the solvent absorption increases with time, the solute diffusion coefficient in the film can be expressed as follows [12–14,4]:

$$D(t) = D_p(M^*/M^*_\infty) \tag{2}$$

where D_p represents solute diffusion coefficient at the equilibrium solvent absorption and (M^*/M^*_∞) represents the ratio of solvent absorption. The ratio of solvent absorption can be calculated from the solution of the solvent absorption equation that can be derived from Fick's second law. In this particular work, a non-uniform material is considered where the diffusion coefficient is a function of position. The position dependent diffusion has a wide range of applications in separation processes. The mathematical model for the solvent absorption by a thin film where the diffusion coefficient depends on position can be given as:

$$\begin{aligned} &\frac{\partial C^*}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial C^*}{\partial x}\right) \quad 0 < x < L, t > 0 \\ &C^* = C_0^*, \qquad x = 0, \quad t > 0 \\ &C^* = C_0^*, \qquad x = L, \quad t > 0 \\ &C^* = 0, \qquad t = 0, \quad 0 < x < L. \end{aligned} \tag{3}$$

In Eq. (3), C^*, C_0^*, and $D(x)$ represent the solvent concentration, the final solvent concentration, and the position dependent solvent diffusion coefficient, respectively. In general, the position dependent diffusion coefficient can be expressed as [3]:

$$D(x) = D_0(1 + f(x)). \tag{4}$$

Eq. (3) is an inhomogeneous (i.e. boundary conditions are inhomogeneous) linear parabolic partial differential equation with a variable coefficient and has no analytical solution due to the variable solvent diffusion coefficient. The variational method proposed in this work for the solution of the Eq. (3) is a semi-analytical method.

The solution of the time and position dependent solvent concentration equation, given in Eq. (3) can be written in the following form:

$$C^*(x, t) = V(x, t) + K(x, t). \tag{5}$$

In Eq. (5) $V(x, t)$ and $K(x, t)$ represent related homogeneous and inhomogeneous part of the solution of Eq. (3). The inhomogeneous part the solution, $K(x, t)$ is a known function and can be chosen freely to satisfy the Eq. (3).