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Approximate analytical solutions for steady-state nonisothermal convection–diffusion–reaction in a slab

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ABSTRACT

Approximate analytical solutions for a slab undergoing a combination of convection, diffusion and reaction for nonisothermal conditions are obtained, with the reaction assumed to be first order. The solutions are developed using the perturbation method for different situations, depending on the reaction and convection parameters. The behavior of the concentration and temperature profiles inside the slab are investigated; and, the effects of controlling parameters, such as convection, on the system are studied. It was found that the maximum temperature within the slab is achieved when the reaction and convection processes dominate the system, regardless of the strength of the convection in this regime. The maximum temperature is affected by the convection in other cases.

1. Introduction

Reactive processes are present in many industrial applications; and, their behaviors in complicated systems involving convective and diffusive transport phenomena have been studied widely. Their applications include ore reduction and catalyst deactivation [1], separation and purification [2], car airbags [3,4], emergency oxygen generation [5], ceramic, semiconductor and abrasive materials [6], energy resource applications [7,8], underground coal gasification and many others. Reactions introduce a great deal of complexity and nonlinearity to systems. Many researchers have tackled reactive related problems for specific cases and applications or for situations where a transport mechanism is relaxed to simplify the problem. This also includes isothermal cases.

There is a great deal of numerical studies for various reactive systems, as well as many attempts for semi-analytical and approximate solutions. The extensive work of Aris [9] provides a comprehensive review of and insight into diffusion and reaction mechanisms in catalysts. Del Borghi et al. [1] proposed a transformation for isothermal fluid-solid reactions with diffusion that reduces coupled nonlinear differential equations to a single nonlinear equation based on a new variable. The new equation includes diffusion and reaction. They developed their method for the case where there are no changes in pore structure, volume or effective diffusivity. Fernandes and Gavalas [2] developed another approach for the same fluid-solid reaction system. They considered isothermal conditions and first-order dependency of the reaction rate. Their technique transformed the coupled nonlinear partial differential equations into a set of ordinary differential equations. They employed the integral transformation method.

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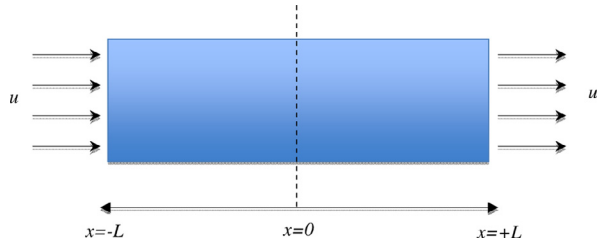

Fig. 1. Schematic of one-dimensional block considered for model development.

Gas-solid reactions have also received great attention from researchers. This class of reactions is mostly treated numerically. In this class of work, Dudukovic and Lamba [10], Ramachandran and Doraiswamy [11], Hiskakis and Hanratty [8], Rajaiah et al. [12], Dandekar et al. [6,13], Cao et al. [14] and Wang et al. [5] can be mentioned. In the majority of these works, techniques, such as integral and coordinate transformations, and more specific techniques, such as the maximum principle [14], have been used to reduce the degree of complexity of partial differential equations and convert them to ordinary ones. By inspecting the resultant equations, various criteria have been obtained for predicting the behavior of systems and influential parameters, such as criteria for the shape of the reaction front, parameters that result in instability, and reaction front velocity [2,5,6,10,12,13]. This type of simplification is usually followed by numerical studies. Some studies for the identification of the appropriate numerical techniques to obtain accurate simulation results has also been performed [15].

Researchers have also investigated solid-solid reactions [16–18]. This type of reactive system does not include convective processes. Similar to gas-solid reactions, the original partial differential equations are simplified using some transformations and generally solved numerically using different numerical schemes and techniques.

Systems that include reactions, convection, and diffusion are usually studied numerically. However, there exists a class of studies that address the problem analytically or semi-analytically. Analytical solutions are usually limited to certain conditions, such as first-order reaction and an isothermal approach [19]. Furthermore, Van Gorder [20] and Reger and Van Gorder [21] tackled similar equations for thermal explosion in various geometries and presented the qualitative behavior of such nonlinear systems. Cardoso and Rodrigues [22] provided an approximate solution for a slab of catalyst undergoing a combination of reaction, diffusion and convection processes. They used a perturbation method for their system with Dirichlet boundary conditions. The present study is an extension of this technique for a slab experiencing reactive and diffusive phenomena with Neumann boundary conditions, which are more common in industrial applications, particularly in the energy industry.

In this paper, we first present the governing equations and transform them into the dimensionless form. Then, we develop the approximate analytical solution of these equations based on the perturbation method and different values of the perturb parameter. The approximate analytical solutions for three different regimes with different mechanisms are obtained. These regimes are diffusion-convection dominant, diffusion-reaction dominant and convection-reaction dominant. For each regime, the appropriate modification to obtain the solution is presented. These sections are followed by presenting the behavior of the system under different influential parameters and variables and the corresponding interpretations.

2. Model and development

In this section, we present our model and its solution using the perturbation method and treatment of singularity issues that occur during the solution. For this purpose, a one-dimensional (1D) slab within which a chemical reaction of A → B takes place was considered. It was assumed that the reaction was a first-order Arrhenius type. The 1D assumption is for the sake of simplicity and implies that all transport and chemical phenomena solely occur along the length of the slab (i.e., in the x-direction). It is presumed that the system is in steady-state conditions. Fig. 1 demonstrates a schematic of the considered system.

The following differential equations govern the transport and reaction phenomena in the interested domain. As can be seen, mass and energy equations are coupled through the reaction term.

$$u\frac{dC}{dx} = D\frac{d^2C}{dx^2} - kC, \tag{2.1}$$

$$u\frac{dT}{dx} = \alpha\frac{d^2T}{dx^2} + \frac{(-\Delta H)}{\rho C_P}kC, \tag{2.2}$$

For this system, the following boundary conditions are considered:

$$C = C_i \text{ and } T = T_i \text{ at } x = -L, \tag{2.3}$$

$$\frac{dC}{dx} = 0 \text{ and } \frac{dT}{dx} = 0 \text{ at } x = +L, \tag{2.4}$$

where C is the concentration of reactant A, C_i is the concentration of reactant A at the inlet, T is the temperature, k is the intrinsic reaction constant, D is the effective diffusion coefficient of A, u is the superficial velocity of the fluid inside the block, α is the