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An inverse problem in estimating the reaction functions and solute concentration simultaneously in a reversible process

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ABSTRACT

An inverse algorithm basing on the Iterative Regularization Method (IRM) is applied in this study in determining the unknown time-dependent reaction functions and solute concentration in the solution, i.e. three unknown time-dependent functions, simultaneously in a reversible process by using measurements of concentration components. It is assumed that no prior information is available on the functional form of the unknown functions in the present study, it can thus be classified as function estimation for the inverse calculations. The accuracy of this inverse problem is examined by using the simulated exact and inexact concentration measurements in the numerical experiments. Results show that the estimation of the time-dependent reaction functions and solute concentration in the solution can be obtained in a very short CPU time on a HP d2000 2.66 GHz personal computer. Moreover, the sensors should be placed as close to the boundary as possible to obtain better estimations.

1. Introduction

Simultaneously diffusion with chemical reaction has numerous applications, for instance, in diffusion through a gel, some of the diffusing molecules are attracted to fixed sites within the medium, hence considered immobilized, or in a problem of diffusion into a textile fiber in which there are a number of active groups, the diffusing molecules can become attached to them and thus become immobilized [1,2].

In such problems, depending on the relative rates of diffusion and chemical reaction, certain extreme cases can be examined. When the reaction rate is very rapid so that the immobilized component can be assumed to be always in equilibrium with the component free-to-diffuse. When the diffusion is so rapid, the diffusing substance and the immobilized product are considered uniform throughout the medium. The solution for these two extreme cases is easy. However, when the reaction and diffusion rates are comparable, the solution becomes rather involved [3].

The reaction rate play an important role in the field of chemistry, chemical engineering, combustion and other related physical problems, so the measurement or estimation of reaction functions becomes important. For instance, Storozhev [4] used Langmuir approach to estimate the maximum values of the reaction coefficient for various reactions relevant to atmospheric chemistry. Cartry et al [5] considered the estimation of surface reaction coefficient values for atomic oxygen recombination on a glass surface in connection with atomic sources development. Harrison and Collins [6] measured the reaction coefficients of nitrogen dioxide and nitrous acid with monodisperse sodium chloride and ammonium sulphate aerosols in a flow reactor at atmospheric pressure. The above research works are based on the assumption that the reaction rates are constant. When such assumption is not valid, the algorithms presented above can not be used to estimate the reaction coefficients.

The reaction function should be a function of temperature and temperature is function of time. If the temperature distribution for the solution exhibits large variation during the reacting process, the reaction coefficient becomes function of time. For this reason an inverse algorithm basing on the Iterative Regularization Method (IRM) [7,8] is developed for the model of a reversible process in estimating the time-dependent reaction functions and solute concentration in the solution.

The direct diffusion problem with chemical reaction in a reversible process is concerned with the determination of concentrations of free-to-diffuse and immobilized solutes when the initial conditions, reaction functions and the concentration of the solute in the solution are specified. In contrast, the inverse problem considered here involves the determination of the unknown time-dependent reaction functions and solute concentration in the solution for a reversible process from the knowledge of the concentration measurements taken within the domain.

The main result of the IRM is that the Conjugate Gradient Method (CGM) together with the regularizing discrepancy principal as a stopping criterion for inverse problems gives a regularization method in the Tikhonov sense where the last iteration index is

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Nomenclature

A	surface
$C(t)$	free-to-diffuse solute concentration
$C_s(t)$	solute concentration in the solution
D	diffusion coefficient
f	dimensionless solute concentration in the solution
F	rate of solute concentration change
J	functional defined by Eq. (4)
J'	gradient of functional defined by Eq. (17)
K_δ	dimensionless forward reaction rate function
K_η	dimensionless backward reaction rate function
P	direction of descent defined by Eq. (6)
$S(t)$	immobilized solute concentration
t	dimensional time
V	volume
x	dimensional coordinate
Y_1, Y_2	dimensionless measured concentration
Greek letters	
$\delta(t)$	forward reaction rate function
$\eta(t)$	backward reaction rate function
ξ	dimensionless coordinate
τ	dimensionless time
β	search step size
γ	conjugate coefficient
$\Lambda(\bullet)$	Dirac delta function
λ_1, λ_2	Lagrange multiplier defined by Eq. (14)
$\theta_1(\xi,\tau)$	dimensionless estimated free-to-diffuse solute concentration
$\theta_2(\xi,\tau)$	dimensionless estimated immobilized solute concentration
$\Delta\theta_1$, $\Delta\theta_2$	sensitivity function defined by Eq. (8)
ε	stopping criterion
Superscript	
n	iteration index

the regularization parameter. This technique has been proven to be a very powerful algorithm in handling the inverse problems and has been applied to many different applications.

For instance, Orlande and Ozisik [9] determined the reaction function in a reaction-diffusion parabolic problem. Huang and Wang [10] used IRM in estimating surface heat fluxes for a three-dimensional inverse heat conduction problem. Huang [11] applied the IRM in a nonlinear inverse vibration problem in estimating the unknown external forces for a system with displacement-dependent parameters. Jin [12] discussed a non-linear inverse problem associated with the Laplace equation to identify the Robin coefficient from boundary measurements. Prud'homme and Nguyen [13] applied the convergence and regularization mechanism of the conjugate gradient algorithm to an inverse heat conduction problem to determine an unknown time-dependent heat flux. Huang and Kim [14] estimated the time-dependent reaction coefficient in an autocatalytic reaction pathway. Huang and Chen [15] determined the boundary temperatures for a double-layer nanoscale thin-film in an inverse phonon radiative transport problem. Huang and Lin [16] applied the IRM in an inverse hyperbolic conduction problem to estimate two unknown surface heat fluxes simultaneously. Huang et al. [17] determined the spatial and temporal-dependent external forces for cutting tools in an inverse vibration problem. Recently, Huang and Chung [18] used IRM in a non-linear fin design Problem to determine the optimal shapes of longitudinal and spine fully wet fins.

The objective of the present study is to utilize IRM to solve this inverse problem in estimating the time-dependent reaction functions and solute concentration in a reversible process. To the best knowledge of the authors, to estimate simultaneously three unknown functions (not three parameters) in the inverse problem is very limited in the literature. The Conjugate Gradient Method derives its basis from the variational principles [7] and transforms the original direct problem to the solution of two subproblems, namely, the sensitivity problem and the adjoint problem, which will be discussed in detail in the next few sections.

2. Direct problem

To illustrate the methodology for developing expressions for use to determine simultaneously the forward and backward reaction rate functions $\delta(t)$ and $\eta(t)$ as well as the concentration of the solute in the solution $C_s(t)$ in a reversible reaction, the following inverse problem is considered. An infinite plate of thickness $2a$ immersed into a solution of finite volume and the solute allowed to diffuse into the material region. The concentration of the solute in the solution is assumed as a function of time, i.e. $C_s(t)$.

For time $t > 0$, the diffusion of the solute into the material volume proceeds and a first order, reversible reaction occurs inside the material volume. As a result, a nondiffusing product is formed, i.e. some of the solute is immobilized. Due to symmetry, the material volume confined to the region $0 \leqslant x \leqslant a$.

Let $C(x,t)$ be the concentration of the solute free-to-diffuse within the body and $S(x,t)$ be that of immobilized solute, each being expressed as an amount of mass per unit volume of the body. The mathematical formulation of this mass diffusion problem is given by [19]

$$\frac{\partial C(x,t)}{\partial t} + \delta(t)C(x,t) - \eta(t)S(x,t) = \frac{\partial^2 C(x,t)}{\partial x^2} \quad \text{in } 0 < x < a, \quad t > 0 \tag{1a}$$

$$\frac{\partial S(x,t)}{\partial t} = \delta(t)C(x,t) - \eta(t)S(x,t) \text{ in } 0 < x < a, \quad t > 0 \tag{1b}$$

Subjected to the following boundary and initial conditions

$$\frac{\partial C(x,t)}{\partial x} = 0 \quad \text{at } x = 0 \tag{1c}$$

$$V\frac{\partial C(x,t)}{\partial t} + AD\frac{\partial C(x,t)}{\partial x} = AD\frac{\partial C_s(t)}{\partial t}; \quad \text{at } x = a \tag{1d}$$

$$C(x,t) = C_0 \text{ in } 0 < x < a, \quad t = 0 \tag{1e}$$

$$S(x,t) = S_0 \text{ in } 0 < x < a, \quad t = 0 \tag{1f}$$

where $\delta(t)$ and $\eta(t)$ are the forward and backward time dependent reaction rate functions, respectively. The concentration of the solute in the solution is taken as $C_s(t)$. D is the diffusion coefficient, V and A represent the volume and surface, respectively.If the following dimensionless quantities are defined