Estimation of Boundary Properties Using Stochastic Differential Equations and COMSOL

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Abstract

The inverse diffusion problems deal with the estimation of many crucial parameters such as the diffusion coefficient, source properties, and boundary conditions. Such algorithms are widely applied in many design problems in different physical [1–4], chemical [5–11], and biological fields [12]. Recently, the estimation of the boundary properties, of the diffusion process, have attracted researchers[1, 2]. However, due to the complexity of the problem, the work accomplished in not yet satisfactory. On the other hand, most of the analytical and numerical methods proposed for such problems have only been used to deal with one- or at most two-dimensional problems with simple and symmetric geometries. Limited work has been achieved on three-dimensional problems, at which simplified problems are solved. Moreover, the major purpose was to estimate the properties of a pre-determined boundary position. Nevertheless, they only account for the classical nature of the diffusion, neglecting its stochastic (random) nature described by the stochastic differential equations (SDE) and the Fokker-Planck equation [13].

Our previous work [7, 8, 10] did not deal with boundaries. In this paper we extend previous results and propose a model that can deal with arbitrary boundaries. We are addressing the issue where we estimate the absorbtion property of the boundary. We propose computationally efficient framework for estimating the boundary properties using stochastic differential equations. The main advantage of this technique lies in the fact that it accounts for both drift and random effects such as Brownian motion which are not accounted for in commonly used classical techniques based on Fick's law of diffusion. The extension to realistic geometry is straight forward since it can be dealt with using Finite Element Method. Absorbing and reflecting boundaries are often encountered in realistic problems such as drug delivery where the organ surfaces represent reflecting/absorbing boundaries for the dispersion of drug particles.

In this work, we introduce a Fokker-Planck based algorithm in order to estimate the position and the length of the absorbing region of the boundary. We first utilize Fokker-planck equation with the corresponding boundary conditions to derive the forward model, at which, we utilize the COMSOL Multiphysics package to solve for the position density function of the particle undergoing diffusion. Next, we deduce the corresponding statistical model for the measurement of the number of particles. Finally, we show numerical examples to illustrate the proposed algorithm.

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