

Preface

This edited book on “Modeling and Simulation of Diffusive Processes: Methods and Applications” contains contributions from authors with a variety of academic backgrounds. It is an outgrowth of the International Conference on Simulation and Modeling of Diffusive Processes and Applications (ICMSDPA12) organized in Banaras Hindu University, India during October 9–12, 2012. There are contributors from outside ICMSDPA12 also to make the book more broad-based. This book addresses some of the issues in simulation modeling and simulation over a number of application areas. There are fifteen chapters in the book.

The first chapter is on diffusive processes and modeling: an introduction by Naveen Kumar and S. K. Basu. It deals briefly with a number of processes which are intimately connected with the diffusion processes, advection–diffusion equation (ADE) in different coordinate systems, mentioning different transformations generally used, different analytical and numerical methods. The effect of fractional order space derivative with skewness parameter on the mass transport has been explained through simulation using ADE for a simplified wound healing problem. Lastly, simulation study about the effect of ionic diffusion on the controlled release of nutrients from a coated spherical fertilizer granule is explained.

The second chapter on diffusion and transport of molecules in living cells by Ruchi Gaur, Lallan Mishra, and Susanta K. Sen Gupta deals with diffusion and different models of it, and relevance of different transport phenomena in living cells.

The third chapter on modeling diffusion and transport of suspended sediment in open channels, using two-phase flow theory by Sanjeev Kumar Jha and Fabián A. Bombardelli deals with a general framework of sediment transport in open channels as a two-phase flow, composed of mass and momentum equations for both phases (water and sediment). The authors discuss two levels of model complexity based on the nature of the terms involved in modeling: the complete two-fluid model (CTFM), and a partial two-fluid model (PTFM).

The fourth chapter on mathematical modeling of peristaltic transport of nanofluids by Dharmendra Tripathi and O. Anwar Bég reviews the challenges and potential of mathematical modeling in biofluid mechanics. The fundamentals of peristaltic transport and nanofluid dynamics have also been described qualitatively. A novel mathematical model has additionally been presented by the authors, to simulate

the influence of nanofluid and thermo-diffusive/diffuso-thermal characteristics on peristaltic heat and mass transfer in a two-dimensional axisymmetric channel for simulation of nanofluid peristaltic drug delivery systems.

The fifth chapter on numerical study on isotachophoretic separation of ionic samples in microfluidics by Partho P. Gopmandal and S. Bhattacharyya deals with a high resolution numerical algorithm to analyze two-dimensional isotachopheresis (ITP) of electrolytes of different mobility in a wide micro-channel based on a finite volume method over a staggered grid arrangement along with a higher-order upwind scheme. The model is based on equations for conservation of mass and charge and also electro-neutrality condition.

The sixth chapter on thermal characterization of non-homogeneous media by Helcio R. B. Orlande, Carolina P. Naveira-Cotta, Henrique Massard da Fonseca, Diego Knupp, Renato M. Cotta, and Olivier Fudym presents application of a Markov chain Monte Carlo (MCMC) method, within the Bayesian framework, for the identification of non-homogeneities or inclusions in a medium through the solution of an inverse heat conduction problem. They present two different approaches in conjunction with the MCMC method. A nodal approach which locally linearizes the inverse problem by using temperature measurements for the computation of the sensitivity matrix, and an expansion of unknown spatially-dependent thermo-physical properties in terms of eigen functions, which is used in conjunction with the Generalized Integral Transform Technique (GITT).

The seventh chapter on scale dependent porous dispersion resulting from the cumulative effects of velocity fluctuations by Wynand S. Verwoerd deals with semi-analytical stochastic model of the dispersion effects of macroscopic drift velocity fluctuations leading to significant insights like enhancement of intrinsic dispersion by a fluctuation, beyond the value associated with flow at the mean drift velocity. This enhancement manifests as a factor multiplying the spatial variance of the solute plume, so that the effects of a sequence of fluctuations accumulate as a product, implying an exponential rise of dispersion with the distance travelled as a solute plume traverses the fluctuation sequence. This behavior is tempered by an annealing effect downstream of a velocity step, which has a length scale related to plume extension.

The eighth chapter on modeling nitrogen fate and transport at the sediment-water interface by M. M. Hantush, and L. Kalin deals with analytical models describing transport and fate phenomena at media interfaces. The first problem discussed is modeling of nitrogen cycling at the sediment-water interface at the bottom of lakes. The second is modeling atmospheric input of oxygen into under-saturated lakes. The third model describes polychlorinated biphenyl redistribution at the sediment-water interface.

The ninth chapter on modeling groundwater flow in unconfined aquifers by S. N. Rai deals with groundwater flow equations to describe two dimensional groundwater flows in inhomogeneous anisotropic unconfined aquifer, inhomogeneous, isotropic unconfined aquifer, in leaky unconfined aquifer, in homogeneous isotropic sloping aquifer in response to intermittently applied time varying recharge and/or pumping from multiple basins of rectangular shapes and wells, respectively along

with the initial and boundary conditions and methods of their solutions. The governing flow equations are used for the development of analytical/numerical models to predict water table fluctuations in the flow system under consideration.

The tenth chapter on two-dimensional solute transport from a varying pulse type point source by Premrata Singh, Sanjay Kumar Yadav, and Alexander V. Perig deals with solute transport originating from a source through a heterogeneous horizontal medium assuming temporal dependence of velocity and dispersivity.

The eleventh chapter on the problems of futile cycles in metabolic flux modeling: flux space characterization and practical approaches to its solution by Wynand S. Verwoerd and Longfei Mao deals with metabolic capabilities and behaviours of an organism by development of flux models of genome scale with flux balance analysis (FBA). For elimination of futile cycles in the FBA results, the authors introduce a simple notion to cut off the circulating flux layer while obtaining the same objective value. To comprehensively elucidate the alternate optimal solutions without the interference of futile values, they present flux variability analysis with target flux minimization, a combined pipeline approach based on FBA and flux variability analysis.

The twelfth chapter on contaminant concentration prediction along unsteady groundwater flow by Mritunjay Kumar Singh and Priyanka Kumari deals with the contaminant concentration pattern of one-dimensional advection-dispersion equation along a homogeneous semi-infinite aquifer with pulse type boundary condition for different forms of velocity expressions.

The thirteenth chapter on wavelet-multigrid method for solving modified Reynolds equation modeling synovial fluid flow in a normal human knee joint by S. C. Salimath deals with modified Reynolds equation, incorporating surface roughness and poroelastic nature of articular cartilage enabling bio-medical engineers in selecting suitable design parameters, giving deeper understanding of the lubrication of knee. The results obtained could guide the new material experimentation for knee replacement with mechanical characteristics.

The fourteenth chapter on a basic concept on modeling soil organic carbon by Nimai Senapati, Subhadip Ghosh, Heiko Daniel, and Amitava Rakshit discusses SOC models as important means of improving our understanding of C turnover process as well as underlying C stabilization mechanisms in soil. The SOC models often simulate the dynamics of different macro- and micro-nutrients along with SOC dynamics inadequately. They also often do not account soil pH and do not simulate the whole process of soil aggregation and the dynamics of soil biota explicitly. Inclusion of all these process/factors/parameters in the SOC models could represent the complex real life systems in a better way and might improve the overall model performance.

The fifteenth chapter on crop growth simulation modeling by Avnish Kumar Bhatia deals with crop growth models emphasizing crop physiology, weather parameters, soil parameters, and management practices to simulate growth and yield of crops. Crop simulation models compute growth values on a day to day basis using the relations among values of crop growth and weather parameters. A generic model can be developed using common crop physiological processes. Validating and fine

tuning of crop model is an important step before using it for actual prediction tasks. The author opines that future crop models should rely on improving the mechanism of interacting with environment and society.

The editors have attempted, through these chapters from different contributors, to put in one place wide ranging areas where simulation-modeling techniques are being used for better understanding of the underlying processes. The editors feel that this volume would be quite useful for researchers and advance graduate students from multiple disciplines where simulation-modeling is of major interest.

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