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To develop the theoretical foundation for an efficient, flexible, and reliable automatic and adaptive finite element analysis methodology to aid design automation of mechanical systems. To develop stochastic simulation models for food, agricultural, and biological products and processes which are crucial for quality evaluation, equipment and process design and the evaluation of packaging, storage and handling practices. A comprehensive numerical and parametric system for automatic and adaptive generation of finite element models for mechanical systems will be developed which is efficient, flexible, and reliable. The material model of each product will be developed using finite element method, parametric solid modeling, and computer aided design codes. Adaptive finite element formulations will be developed that will allow soil properties as random variables. Mathematical models developed so far to predict the drug release from coated controlled release products are often insufficient to predict the in-vivo dissolution and release rates reliably and precisely. To fully understand the drug-carrier and drug-cell interaction behaviors and mechanisms, study at the molecular level must be conducted in concert with the traditional macroscopic effort and with the incorporation of inherent biological and other involved variabilities. Such multi-scale methods are hindered by un-bridged gaps between the macro and molecular scales in both the spatial and temporal dimensions. A multi-scale mathematical model for drug release form polymer coated delivery systems that deliver 5-ASA to the colon has been developed. Underlying physical and biochemical principles governing the involved processes diffusion and dissolution were employed to develop the mathematical description. Finite element formulation was used to numerically solve the model equations and molecular dynamics MD simulations were used to predict macro-scale transport properties of the drug and the biologic fluid. The effect of pH variability in the gastrointestinal tract environment on the dissolution of the polymeric enteric coating was investigated using the Monte Carlo method. Results for the amount of released drug versus time in the different parts of the gastrointestinal tract GIT were obtained and analyzed. Moreover, the effect of biological variability in the GIT environment on the release profile was investigated. As a result, prediction of amount of drug that entered the systemic circulation was obtained and was comparable to clinical in vivo data from literature. This predictive model was used to better understand the in-vivo drug release process in the GIT. Additional modules of absorption and biotransformation models are being developed with prediction of additional model parameters using molecular dynamics simulation. These modules will be incorporated into the existing drug release model, improving the predictive power of the model significantly. Impacts The developed multi-scale model is expected to play a significant role in the development of novel and superior design of controlled drug release systems. The availability of reliable prediction of the drug release profile from newly discovered delivery systems would help reduce the number of trials with substantial impact on the cost and fatalities on human and animal subjects. The incorporation of absorption and biotransformation modules will expand the expediency of the model as an essential tool for physicians to choose from available delivery systems based on the physiological and pathological condition of a patient towards patient specific treatment regimen. Moreover, the model is useful for regulatory agencies for pre-clinical toxicology studies of newly introduced drugs. Multiscale drug release modeling for targeted oral drug delivery TODD. Technical proceedings of the Nanotechnology Conference and Trade Show. A stochastic mathematical drug release model for polymer coated ion-exchange resin complexes. Nashville, TN Nov , Underlying physical and biochemical principles were employed to develop the mathematical description. Prediction of amount of drug that entered the systemic circulation was obtained and was compared to clinical in vivo data from literature. In addition, application of finite element modeling techniques to microelectromechanical systems MEMS and nanoelectromechanical systems NEMS were investigated. The first numerical experiment dealt with modeling of a piezoelectric micropump. An effective description and an accurate understanding of any pumping mechanism is critical, especially at the micro scale. With the existence of a comprehensive and adaptable model, accurate preproduction predictions of performance were realized. Optimal geometries and operating parameters were determined without the need for expensive prototyping. A three-dimensional FEA approach for parametric design and optimization of a piezoelectrically actuated membrane micropump was developed. The model includes the piezoelectric material, membrane, pumping chamber, and valves. This numerical representation includes electro-mechanical coupling for piezoelectric actuation as well as consideration of fluid-structural interaction. Transient consideration of electrical, mechanical, and fluidic effects was included. Outputs included membrane deflection, flow pattern and velocities, and volumetric flow rate. Results were compared favorably with experimental data available in the literature. Impacts The developed models are expected to play a significant role in the development of novel and achievement of better design of controlled release systems. The developed finite model is expected to play a major role in the design of MEMS for drug treatment delivery systems for plants, animals, and human, as well as for targeted spatial microfluidic chemical applications for plants and soil treatment. Accurate modeling of the multiphysics processes would enable a rapid and relatively inexpensive prediction of the MEMS performance. Accurate modeling and simulation of the MEMS behavior will be a powerful and economical tool for their design and fabrication. It will help savings of prototyping costs and allows for sensitivity analysis of the system before the final production. J Drug Targeting under preparation. Characterization of coating polymers for targeted delivery systems. With the existence of a comprehensive and adaptable model, accurate preproduction predictions of performance are realized. Optimal geometries and operating parameters may be determined without the need for expensive prototyping. A three-dimensional FEA approach for parametric design and optimization of a piezoelectrically actuated membrane micropump is developed. Transient consideration of electrical, mechanical, and fluidic effects is included. The effects of independent factors such as component geometry, backpressure, and excitation voltage and frequency are each evaluated. Results are obtained by using an iterative finite element procedure. Attempts in the literature show only a 2-D pump, but results were not compared with experimental data as well as two and three dimensional valve models which are not attached to an operational pump. Outputs include membrane deflection, flow pattern and velocities, and volumetric flow rate. Results are being compared with experimental data available in the literature. Existing mathematical models that attempt to describe the drug release step from these delivery systems contain model parameters that are often estimated empirically and assumed constant. This limits the ability of the models to address underlying physical mechanisms of the transient drug delivery, relying heavily on in-vitro and in-vivo experiments. To fully understand the drug-carrier and drug-cell interaction behaviors and mechanisms, study at the molecular level must be conducted in concert with the traditional macroscopic effort. The present study deals with the development of a mathematical model of the drug release of different commercially available delayed release capsules that deliver 5-ASA to the colon, based on underlying physical and biochemical principles governing the involved processes e. It was attempted to derive macro-scale transport properties of the capsule components and their interaction with the drug molecule from their molecular descriptors. Molecular simulation work is in progress to estimate the transport properties that serve as coupling coefficients between the micro and macro-scales. Impacts The developed finite model, once validated by experimental data, is expected to play a major role in the design of MEMS for drug treatment delivery systems for plants, animals, and human, as well as for targeted spatial microfluidic chemical applications for plants and for soil treatment. The impact of drug release modeling approach is three fold. Transactions of the ASAE 46 1: Stochastic Modeling of Transient Contaminant Transport. Journal of Hydrology, Effect of viscoelastic relaxation on moisture transport in foods. Solution of general transport equation. Journal of Mathematical Biology, 49 1: Numerical Modeling of a Piezoelectric Micropump. Results will be compared with experimental data available in the literature. It will help saving prototyping costs and allows for sensitivity analysis of the system before the final production. The high degree of variability of material properties was taken into account by using effective parameters. The resulting set of stochastic models was solved using the finite element method. A computer code was developed to implement the stochastic finite element formulation. Several problems of transient unsaturated flow were modeled and simulated. The predicted mean values and their respective variances were evaluated. The results obtained using the stochastic finite element formulation was compared to experimental data. Large-scale models of contaminant transport were formulated by using two different approaches: For the stochastic approach, the spatial variability of the unsaturated hydraulic conductivity of the soil was introduced in the derivation of the effective bulk macrodispersion coefficient. For the deterministic approach, mean values of the hydraulic properties of the soil were used. To investigate the importance of accounting for the spatial variability of hydraulic soil properties in large-scale models, the stochastic results were compared to the deterministic results. Large discrepancies in the results between the two simulations were detected. A finite element code was developed to run the simulations and real field data was used to make the scenario as realistic as possible. The model was successfully applied to several specific cases and results were verified with experimental data. Numerous realistic scenarios were simulated to calibrate the model. The extensions of models into micro and nanoscale systems are under investigation. Impacts The developed finite element model, which has been validated by experimental data, is expected to play a major role in predicting the movement of water and chemicals through the vadose zone into the ground water system. Accurate modeling of the transport processes would enable a rapid and relatively inexpensive prediction of solute movement. Since reliable predictions will be available to avoid a potential contamination of the ground water, the environmental engineer will have enough time and data to decide which technique is the best and the most inexpensive to remediate the problem. The high degree of variability of soil properties was taken into account by using effective parameters such as hydraulic conductivities and moisture capacities. The resulting set of stochastic differential equations was solved using the finite element formulation. The results obtained using the stochastic finite element formulation were compared to experimental data. Both models were solved using a finite element formulation. For the stochastic approach, the spatial variability of the unsaturated hydraulic conductivity of the soil was introduced in the derivation of the effective bulk macrodispersion coefficient tensor. Model was successfully applied to several specific cases and results were verified with experimental data. Numerous realistic scenarios are being simulated and additional work on experimental validation of the model predictions. Impacts The developed finite element model, which is being validated by experimental data, is expected to play a major role in predicting the movement of water and chemicals through the vadose zone into the ground water system. Journal of Agricultural Engineering Research, 77 3:

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