

Analytical study of the Richards equation with a non-linear sink term of the RWU type

by
Guillermo Manns

Director
Dr. Emilio Cariaga López

Abstract

This study focuses on the comparison of analytical methods for solving the Richards equation with the presence of a non-linear sink term of the RWU type (root-water uptake for its acronym in English). This mathematical model arises from the need to model soil-water-plant systems where the term sink models the water consumption by the root. One of the main contributions of this research is to provide a more unified look at the solution of this equation given that to date there is little literature on the matter, and what does exist is very scattered. First, the quasilinearization method is presented and developed. The method consists mainly in the application of a series of variable changes that reduce the Richards equation with source term to a quasi-linear differential equation. The following is Green's method of functions. In this method, the solution of an inhomogeneous partial differential equation is obtained as a superposition of integral expressions in terms of Green's functions. Finally, some computational experiments are provided for the solutions obtained in both methods.

Keywords: Richards equation, nonlinear sink term, root-water uptake.

Simulation of the release of *Arrabidaea chica* extract from chitosan/alginate swelling membranes

by

Luis Alberto Concha Caamaño

Director

Dr. Jacobo Hernández Montelongo

Abstract

This thesis is about the mathematical simulation of *Arrabidaea chica* extract release from chitosan/alginate (Q/A) swellable membranes. The extract of the *A. chica* plant is an important source of tannins, flavonoids and anthocyanins, molecules that have different medicinal properties such as antioxidant, antiseptic, anti-inflammatory and anti-fungal activities. In order to carry out this work, in vitro experimental data of controlled release of *A. chica* were used. Data were obtained from four types of Q/A membranes: dense membrane (QA), dense and flexible membrane (QAS), porous membrane (QAP) and porous and flexible membrane (QAPS). Initially, the mechanism of the extract release kinetics was determined using five classic models from the literature: Zero Order, First Order, Higuchi, Korsmeyer-Peppas and Weibull. Subsequently, the results of these models were compared with an optimization method using the cost function. The results indicated that the model, which best fit the experimental data, during the first 8 h of release, was the Korsmeyer-Peppas model and the phenomenon was primarily by Fickian diffusion. In addition, according to the constants k_kP and n from the Korsmeyer-Peppas model, and K from the optimization model, it was determined that the release control maintained the following hierarchy according to the type of membrane: $QA < QAS < QAP < QAPS$. That is, QA presented the slowest release and QAPS the fastest one. On the other hand, as the models used from the literature are effective only for the first release times, in this case up to 8 h, a mathematical model was developed based on Fick's equations to obtain a simulation for the total release time. The model included 4 parameters, which are related to the diffusion coefficient to adjust the release: k_1 , k_2 , k_3 and k_4 , with k_1 and k_4 being the most significant. Adjusting the value of the parameters for each membrane, correct release simulations of the *A. chica* extract were obtained for the total time of 24 h. Although it can be concluded that the proposed model adequately simulated controlled release from experimental data, in this work, the simulation of the swelling of the membranes was not achieved, but the mathematical model was proposed to be solved in a future project. This thesis demonstrates the application of mathematical models for the study and evaluation of Q/A membranes with therapeutic applications.

Keywords: controlled release; *Arrabidaea chica*; chitosan/alginate swellable membranes; Fick equations; mathematical simulations; cost function.

Simulation of signals generated by tremors in Parkinson's disease, by approximation of polynomial NARMAX models

by
Lizandro García

Director
Dr. Julio Rojas

Abstract

In this work, a methodology is developed to identify the dynamics behind tremors at rest in Parkinson's disease, using acceleration records based on actual tremors present in a person suffering from the disease. A statistical and dynamic examination is carried out in order to evaluate the capacity of the polynomial NARMAX models found and evaluated by time windows, to predict and represent the underlying dynamics from the approximation of their responses to the values of the series of time of real accelerations, using the simulated annealing algorithm to optimize the parameters of the input function (input signal), and the forward orthogonal regression algorithm for the identification of the NARMAX models.

Keywords: Resting tremor, nonlinear dynamics, NARMAX, dynamical systems, chaotic dynamics systems, attractor, Lyapunov maximum exponent, simulated annealing.