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On a dissolution-diffusion model. Existence, uniqueness, regularity and simulations

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Abstract

We perform a mathematical analysis of a model for drug dissolution-diffusion in non erodible nor swellable devices. We deduce a model and obtain a coupled nonlinear system which contains a parabolic equation for the dissolved drug and an ordinary differential equation for the solid drug, which is assumed to be distributed in the whole domain into microspheres which can differ in size. We analyze existence, uniqueness, and regularity properties of the system. Existence is proved using Schauder fixed point theorem. Lack of uniqueness is shown when the initial concentration of dissolved drug is higher than the saturation density in a region, and uniqueness is obtained in the non-saturated case. A square root function appears in the equation for the solid drug, and is responsible for the lack of uniqueness in the oversaturated case. The regularity results are sufficient for the optimal a priori error estimates of a finite element discretization of the system, which is presented and analyzed here. Simulations illustrating some features of the solutions and a good agreement with laboratory experiments are presented. Finally, we obtain error estimates for the finite element method used to compute the simulations.