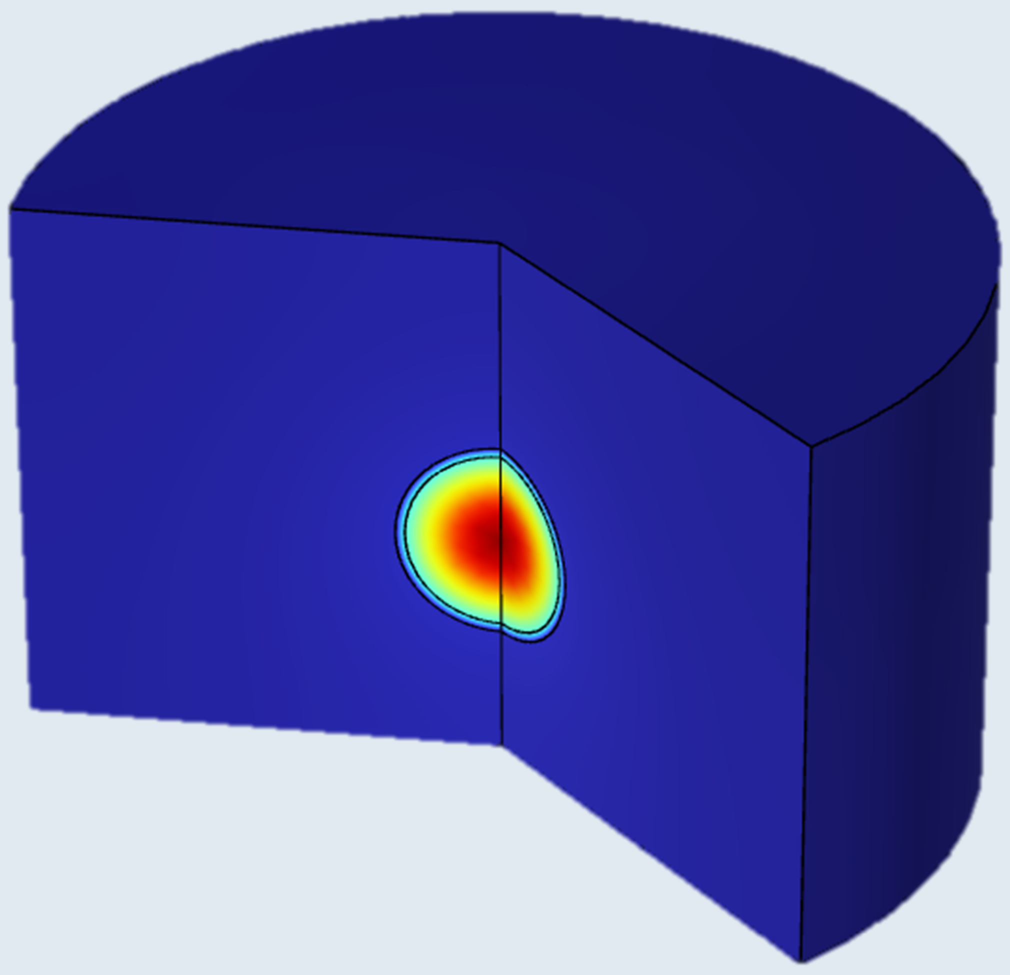

Release of the Model Substance Through the Polymer Membrane into the Biological Environment

Using the COMSOL Multiphysics® software to understand transport and physical properties to design a suitable controlled release system

D. Zhurauliova*, M. Pekař

Faculty of Chemistry, Brno University of Technology, Brno, Czech Republic

*Corresponding author: xczhurauliova@vutbr.cz

Introduction

Transport modeling, or the release of a substance from a gel system into a biological environment using the COMSOL Multiphysics tool plays an important role in understanding the processes required for proper design and optimization of a suitable model [1]. This model should have the ability to accurately simulate transport, or the release of substances from a three-dimensional gel structure in a certain biological environment (organism, soil). The goal of the project is to design a model corresponding to a real sample of fertilizer or gel sphere containing a medicinal or bioactive substance, or filled with a model dye (e.g. methylene blue) for release properties determination using appropriate experimental methods.

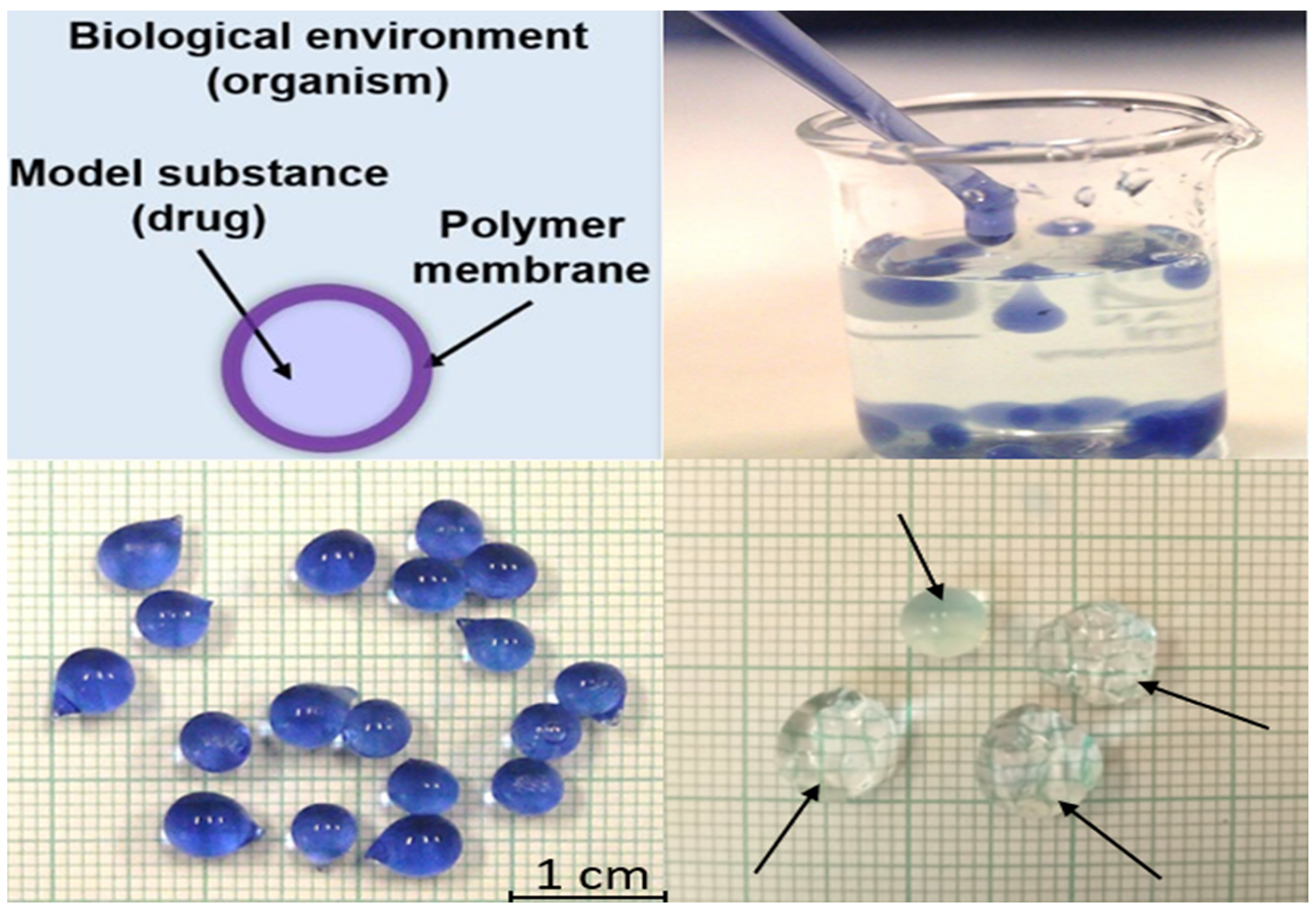

FIGURE 1. Design of model and example of gel beads based on sodium alginate filled with methylene blue

Methodology

In this work, according to the design (see FIGURE 1), a two-dimensional axisymmetric model was developed and evaluated with defined materials, for which different values of diffusion coefficient were included. The diffusion coefficient is the most interesting variable in the area of transport properties, as it is influenced by the size of the molecules and the characteristics of the polymer network. By changing this variable, the course of release of the model substance can be influenced, which makes it possible to change the properties of the designed hydrogel systems according to the required applications [1]. *Transport of Diluted Species* physics, in which the *Porous Medium* condition is included, and *Laminar Flow* physics are also present in the model, although the flow rate is zero, the gravity condition is introduced.

Results

FIGURE 2 shows the simulation of dependence of concentration on time, which shows the course of the model substance with a concentration 0.5 M release through the polymer membrane into the environment. The results for samples with a different value of the diffusion coefficient ($0.28 \cdot 10^{-9}$ m²/s (blue), $0.28 \cdot 10^{-10}$ m²/s (green), $0.28 \cdot 10^{-11}$ m²/s (red)) and with the same value of porosity indicate a different rate of release of the model substance, i.e. the rate decreases with time until it is almost constant. Considering that, by changing certain parameters of the polymer membrane, the properties of the systems can be adjusted according to the desired application.

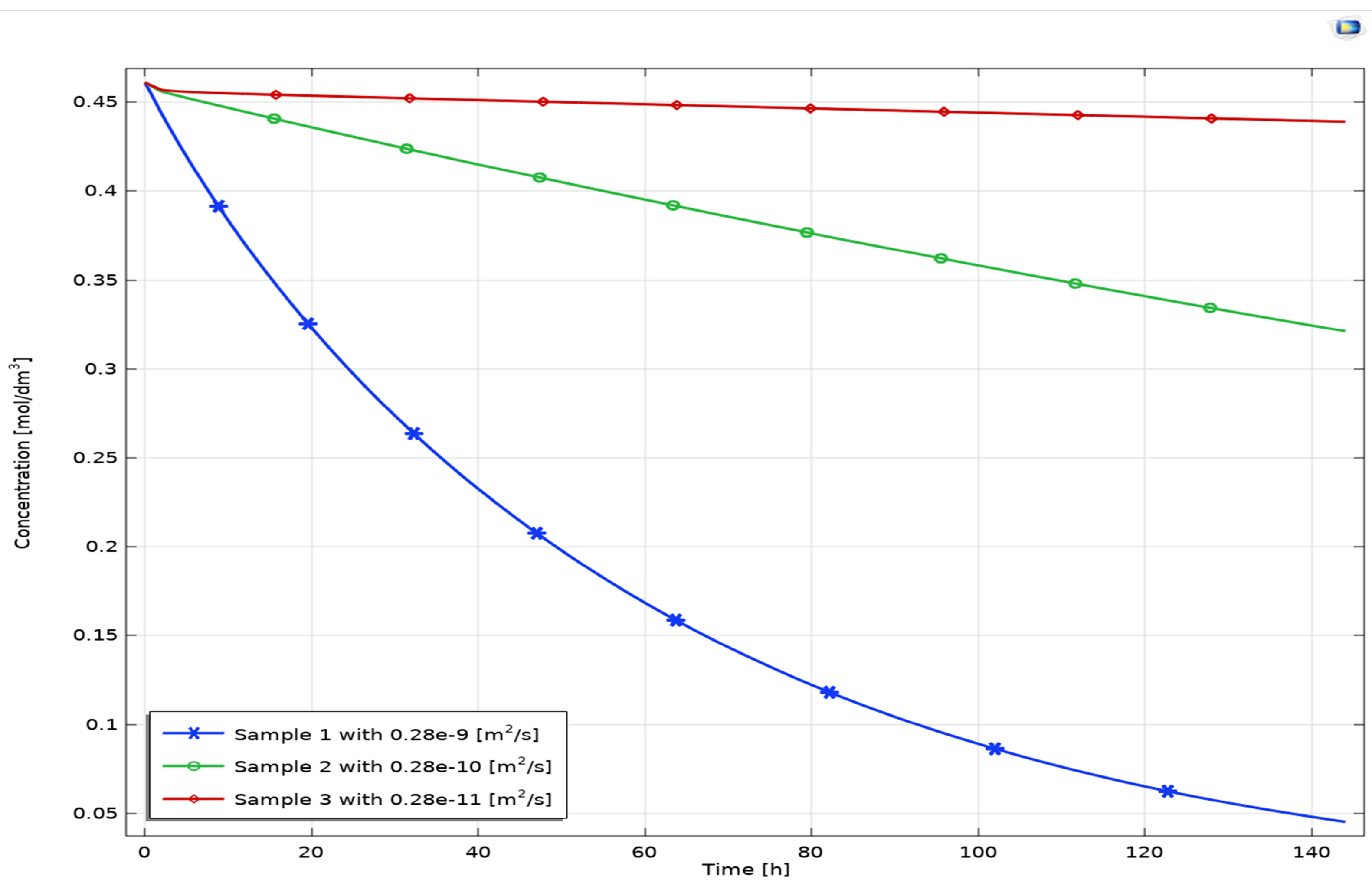

FIGURE 2. Simulation of dependence of concentration on time for samples with 0.5 porosity and the different diffusion coefficients

REFERENCES

[1] C. Lin, A. T. Metters, T. Hoare, et al. Hydrogels in controlled release formulations: Network design and mathematical modeling. *Advanced Drug Delivery Reviews*, pp. 1379-1408. 2006

BRNO UNIVERSITY OF TECHNOLOGY FACULTY OF CHEMISTRY