MODELLING OF BATH WASHING CONCENTRATION FIELD IN BIOPOLYMER AT THE START OF WASHING

Miloslav Fialka

Tomas Bata University in Zlín, Faculty of Applied Informatics,
Department of Mathematics, Zlín
Hana Charvátová
Tomas Bata University in Zlín, Faculty of Applied Informatics,
Department of Automation and Control Engineering

Abstract
The contribution deals with a mathematic model of biopolymer washing by water for times near to zero. Here, the solid phase – the biopolymer is represented by the pelt. Influence of the times about $t \approx 0$ on difference between the real and a modelled course of calcium hydroxide concentration field in delimed biopolymer is studied. The mentioned model of the process is developed by the computer algebraic system Maple. The modelling of the washing process is very important from the economic point of view.

Keywords: Mathematic model, bath washing, calcium hydroxide concentration field, deliming of biopolymer, start of washing, compatibility criterion, system Maple.

1. Mathematic model of the biopolymer bath washing process

In this process, the solid phase – the biopolymer is put into the washing liquid water. The washing water neither flows in nor flows out the bath. Let us consider, for simplification, the calcium hydroxide ions content in biopolymer is lower than its solubility in the same volume of clean water at the given temperature and the influence of flanges on diffusion inside of the biopolymer sample is neglectable. Under these assumptions we can formulate one-dimensional space model of bath washing of biopolymer sample by diffusion model of transport of washed out calcium inside of the biopolymer sample by means of partial differential equation (1) of parabolic type with following initial boundary conditions. The conditions ensure existence and unicity of solution of the undermentioned problem.

The solution of model is given by the field of concentration $c(x,t)$ of calcium on half-stripe domain $G = \left\{ (x,t) \in \mathbf{R} \times \mathbf{R}^+ \mid 0 \le x \le b,\ t > 0 \right\}$.

We want to find the concentration $c(x, t)$ which satisfies the initial boundary problem

$$D \frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial t} + \frac{\partial c_A}{\partial t} \tag{1}$$

$$c_A = \frac{Ac}{Bc+1} \tag{2}$$

$$c(x, 0) = c_p \tag{3}$$

$$\frac{\partial c}{\partial x}(0, t) = 0 \tag{4}$$

$$c(b, t) = \varepsilon \cdot c_0(t) \tag{5}$$

$$\frac{\partial c}{\partial x}(b, t) = - \frac{V_0}{D \cdot S} \cdot \frac{\mathrm{d} c_0}{\mathrm{d} t}(t) \tag{6}$$

$$c_0(0) = 0 . \tag{7}$$

Now, we show signs and sense of symbols used in this contribution.

Symbol	Sense	Measuring unit
A	sorption constant (from Langmuir's sorption isotherm)	1
B	sorption constant (from Langmuir's sorption isotherm)	$m^3 \cdot kg^{-1}$
b	half thickness of solid phase (i.e. biopolymer)	
C	dimensionless volume concentration of calcium hydroxide in biopolymer	1
C_0	dimensionless volume concentration of calcium hydroxide in bath	1
c	volume concentration of calcium hydroxide in biopolymer	$kg \cdot m^{-3}$
c_A	volume concentration of bound calcium hydroxide in biopolymer	$kg \cdot m^{-3}$
c_p	initial concentration of calcium hydroxide in biopolymer	$kg \cdot m^{-3}$
c_0	volume concentration of calcium hydroxide in bath	$kg \cdot m^{-3}$
D	effective diffusion coefficients of washing component from solid phase	$m^2 \cdot s^{-1}$
D^*	modified diffusion coefficient	$m^2 \cdot s^{-1}$
F_o	Fourier number (dimensionless time)	1
Na	soak number (dimensionless volume of washing water)	1
q_n	n^{th} root of a certain transcendent equation	1
S	area of biopolymer	m^2
t	time	s
V	volume of biopolymer	m^3
V_0	volume of washing water as a deliming reagent	m^3
X	dimensionless space coordinate	1
x	space coordinate	m
ε	porosity (ratio of poroses volume to biopolymer volume)	1

Equation (1) represents calcium ion diffusion from biopolymer sample in the direction of water bath. The expression of the right hand side last therm of equation (1) depends on desorption mechanism of washing component from solid phase. Suppose that diffusion is determining for change rate of concentration, it is possible to express the dependence of c_A (of fixed component) on the free component c by relation of Langmuir's sorption isotherm (2). Condition (3) shows initional distribution of concentration in solid phase.

Boundary conditition (4) denotes that field of concentration in solid phase is symmetric.

Relation (5) holds under condition of a perfectly mixed liquid phase. Balance condition (6) denotes the equality of the diffusion flux at the boundary between the solid and liquid phases with the speed of accumulation of the diffusing element in the surrounding. Relation (7) describes that we use clean water for biopolymer bath washing.

Suppose that considered concentration $c(x, t)$ of calcium is very low, i.e. $B \cdot c \ll 1$, we can define domain in which sorption isotherm comes into the linear form and thus relation (2) will be in more simple form

$$c_A = A \cdot c \tag{8}$$

and system of equations will be in linear form

$$\frac{\partial c}{\partial t} - D^* \frac{\partial^2 c}{\partial x^2} = 0 \quad (\text{where constant } D^* = \frac{D}{A+1}). \tag{9}$$

For simplification of solution of equation (9) with additional conditions (3–7) we introduce dimensionless variables

$$C = \frac{c}{c_p}, \quad C_0 = \frac{c_0}{c_p}, \quad F_o = \frac{D \cdot t}{b^2 \cdot (A+1)}, \quad X = \frac{x}{b}, \quad Na = \frac{V_0}{V}.$$

By means of Laplace transformation we obtain analytic solution. Final solution given by dimensionless concentration field $C(X, F_o)$ in biopolymer holds

$$C(X, F_o) = \frac{\varepsilon(A+1)}{\varepsilon(A+1)+Na} - 2\,Na \cdot \sum_{n=1}^{\infty} \frac{\cos(q_n X)\,\exp(-q_n^2 F_o)}{\varepsilon(A+1)\cos(q_n) - \frac{\varepsilon(A+1)}{q_n}\sin(q_n) - Na \cdot q_n \sin(q_n)}. \tag{10}$$

Where q_n is the n-th positive root of following transcendent equation

$$-\frac{Na \cdot q}{\varepsilon \cdot (A+1)} = \tan(q).$$ (11)

2. The influence of the time values on course of the bath washing process

During the study of washing process we observed that the used model is characterized by a distinctive oscillating feature of concentration field c around the highest possible initial concentration c_p in dependence on the space variable x until a certain time, in other words, in dependence on distance from the centre of biopolymer. In reality, the concentration should monotonically decrease on a concave curve with increasing distance and in addition the oscillating values should not exceed c_p. Oscillatory feature appears at time $t = 0$ most often and from the mathematical point of view it is caused by the cosine term $\cos(q_n X)$ of series (10), of course.

For the assessment of dimensionless F_{oc} and real t_c respectively initial time of compatibility, by which we consider the real process course to be compatible with a mathematic model, we formulated the following

Compatibility criterion of concentration field model with a real process

We consider the mathematic model to be compatible with a real process course under the condition that we find by modelling the dimensionless F_{oc} and to it corresponding the real t_c initial time of compatibility respectively such that despite the space an oscillatory unreal course of concentration $C(X, F_o = F_{oc})$ and $c(x, t = t_{oc})$ respectively around maximum possible initial concentration $C = 1$ and $c = c_p$ respectively, it occurs the situation when for every times $F_o \geq F_{oc}$ and $t \geq t_{oc}$ respectively, yet any local maximum of the concentration at the points near the surface of biopolymer, including the point nearest to the surface (on the 2D figures there the point of local maximum always lies nearest to the value $X = 1$ and $x = b$ respectively), has a value not exceeding the maximum possible value $C = 1$ and $c = c_p$ respectively, i.e., it holds the following relations at above mentioned points of these local maxima displayed in 2D

$$C(X \leq X_{sur}, F_o = F_{oc}) \leq 1 \quad \text{and} \quad c(x \leq x_{sur}, t = t_c) \leq c_p \quad \text{respectively.} \quad (12)$$

The figures follow, which represent the dimensionless 2D and 3D respectively concentration field course $C(X, F_o = const.)$ at chosen value of the sorption constant A. Besides the constant F_o there is also the corresponding real time t shown in seconds.

We can see that the oscillatory feature of concentrations in 3D graphics on the right is suppressed owing to the displaying software.
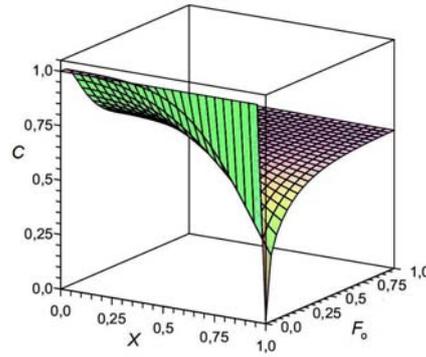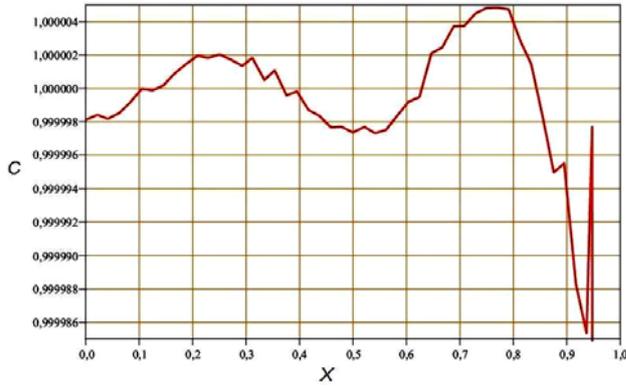

$A = 6$

$F_o = 0.0000000 \quad t = 0.0000 \text{ s}$
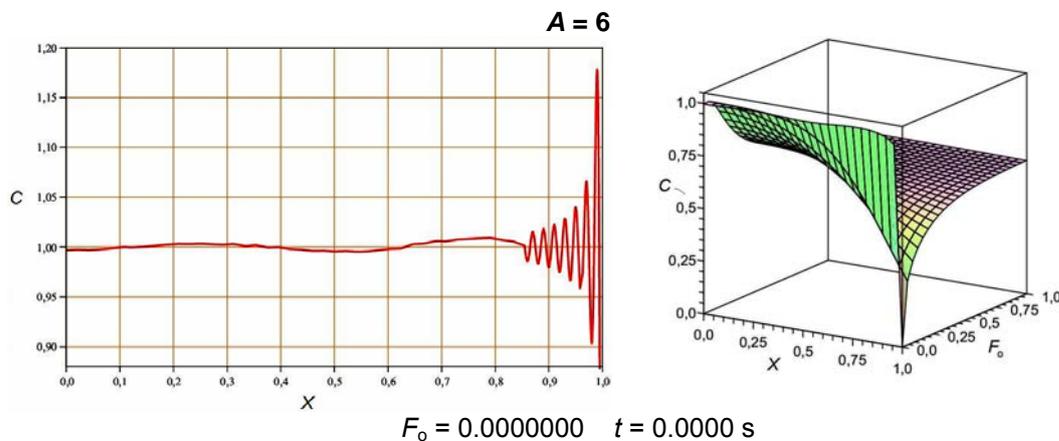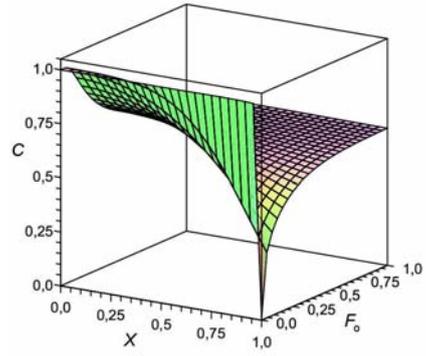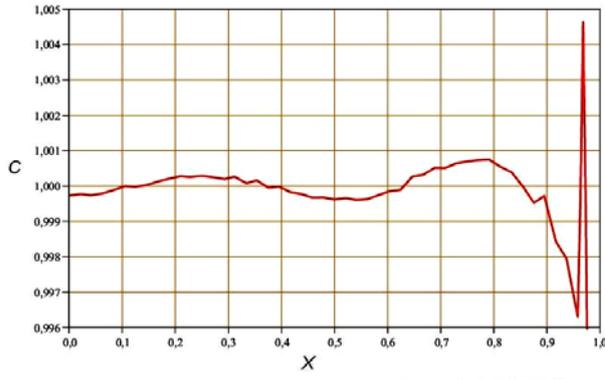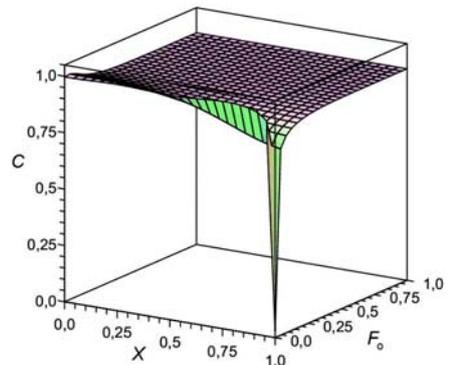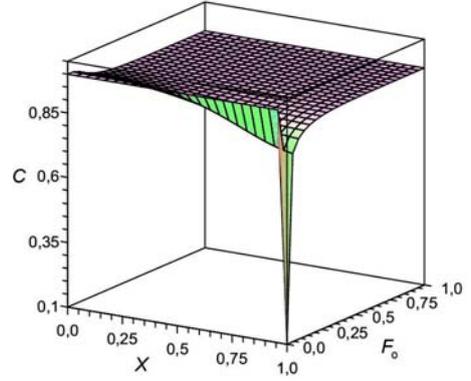
$F_o = 0.0000251$ $t = 0.3515$ s
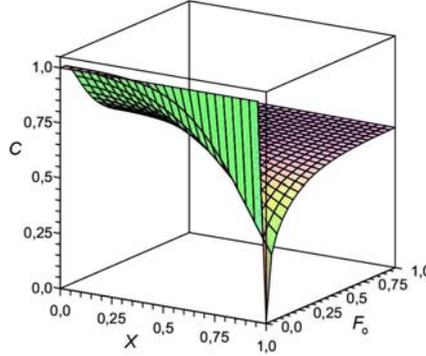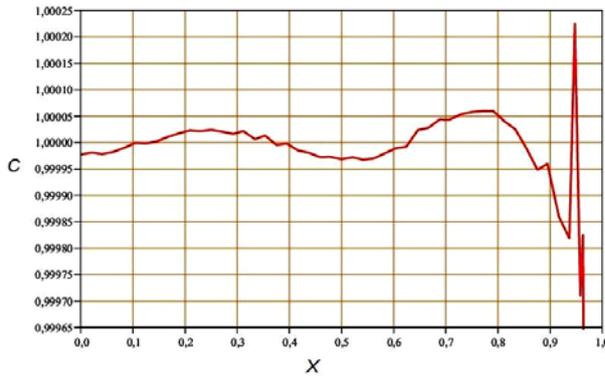
$F_o = 0.0000502$ $t = 0.7029$ s

$F_o = 0.0000753$ $t_c = 1.0544$ s

A = 60
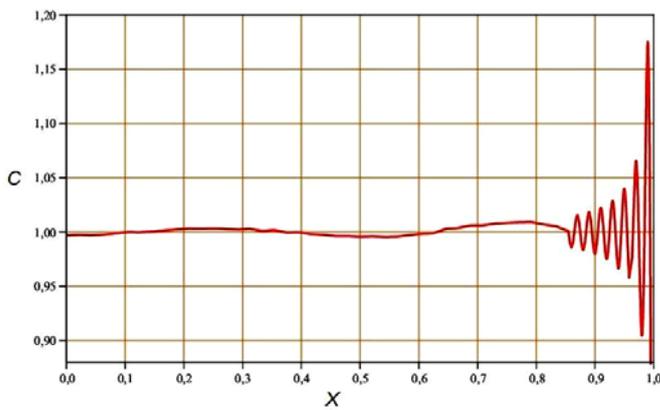
$F_o = 0.0000000$ $t = 0.0000$ s
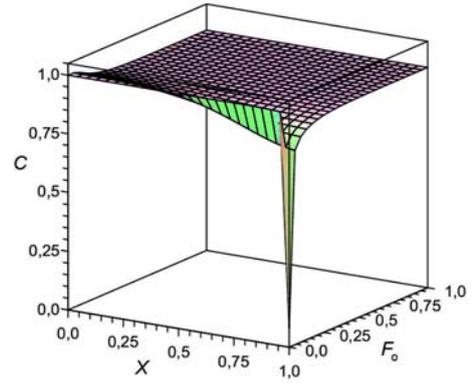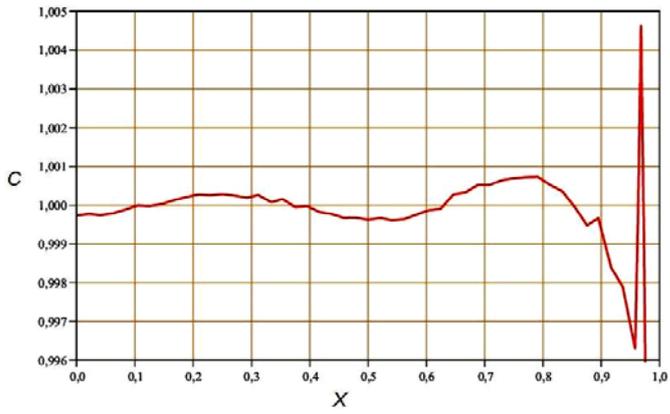
$F_\text{o} = 0.0000251$ $t = 3.0627$ s
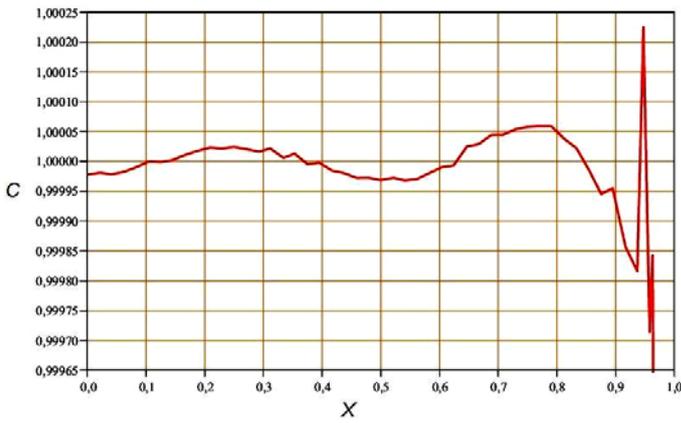
$F_\text{o} = 0.0000502$ $t = 6.1254$ s
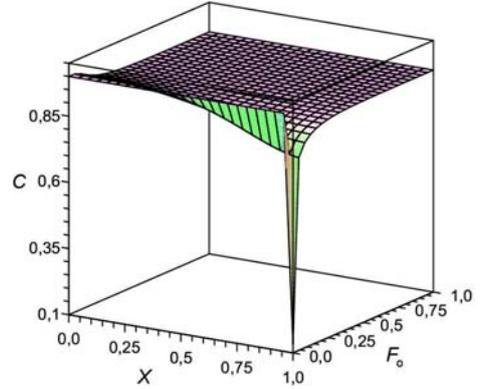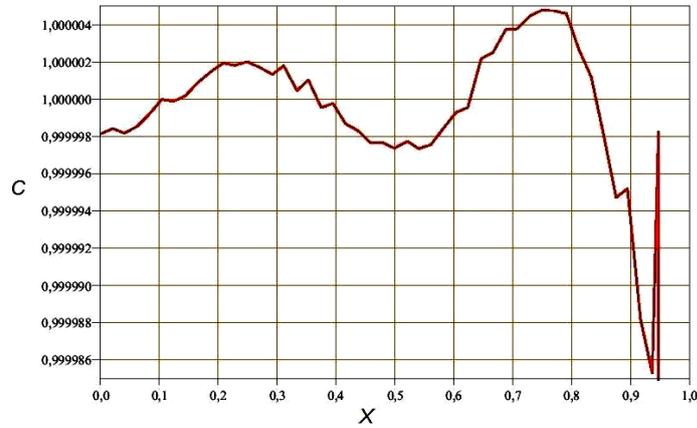
$F_\text{o} = 0.0000753$ $t_c = 9.1881$ s
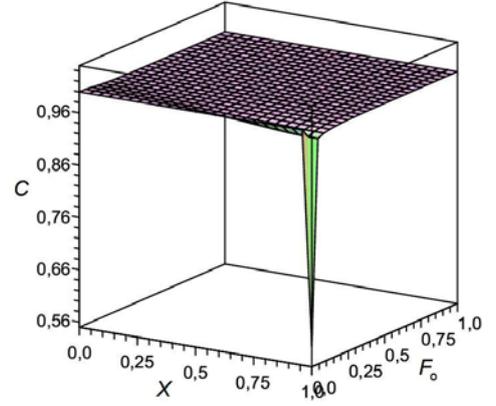
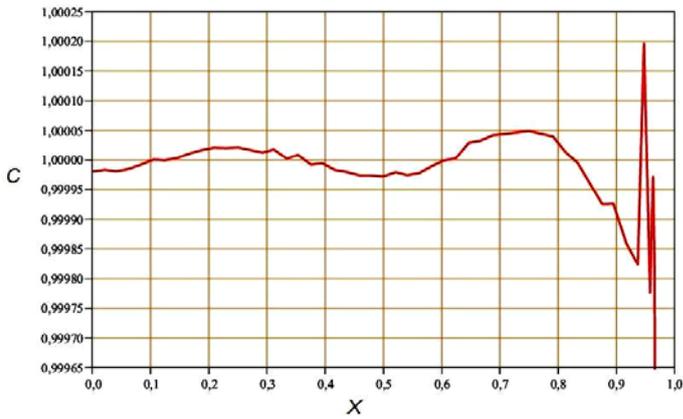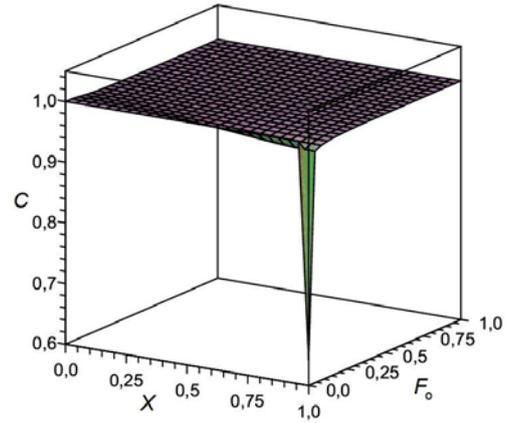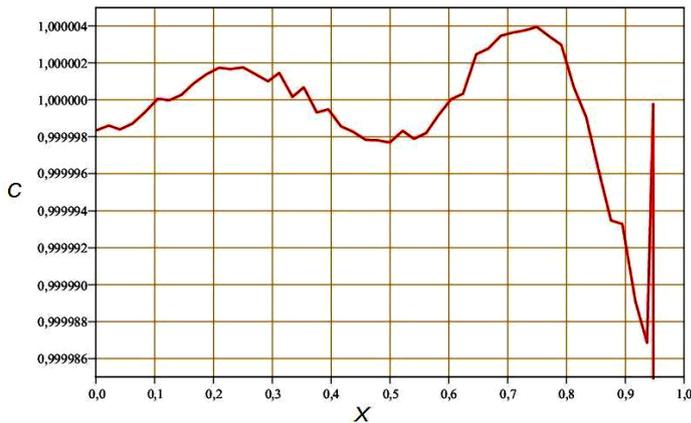**A = 600**
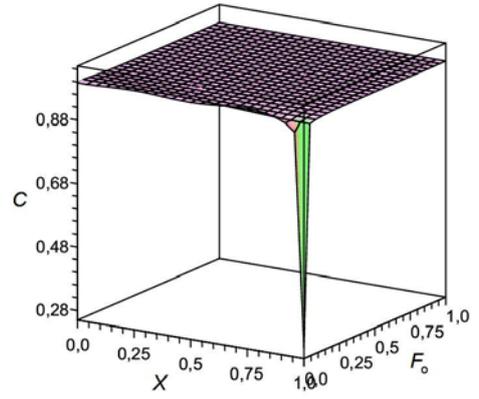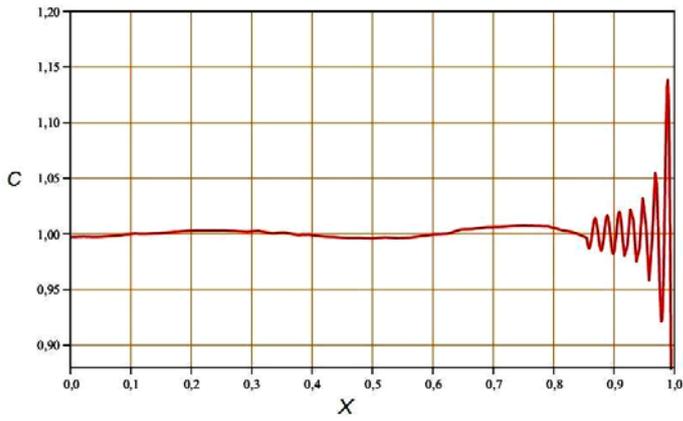
F_o = 0.0000000 t = 0.0000 s
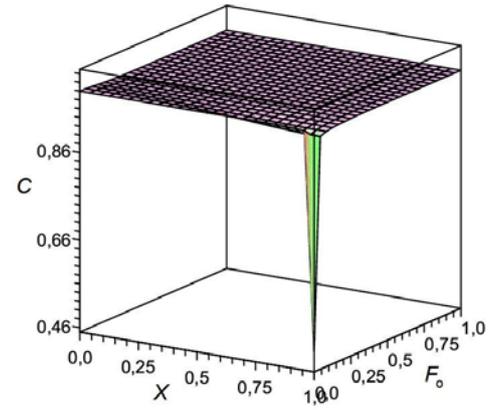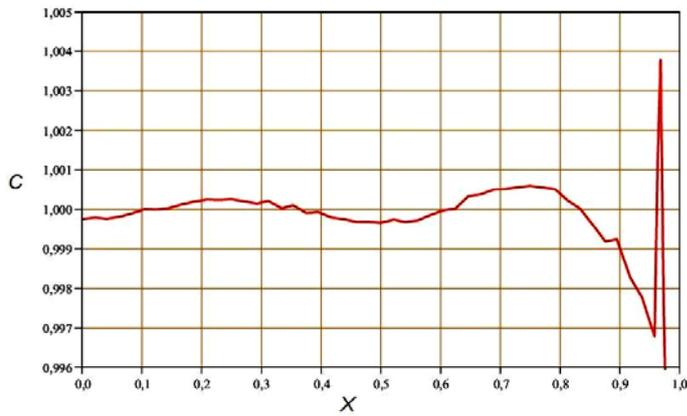
F_o = 0.0000251 t = 30.1752 s

F_o = 0.0000502 t = 60.3504 s

$F_o = 0.0000753$ $t_c = 90.5256$ s

Summary

In the paper we present the first test to find a practical criterion that defines a certain time, by which the space-time 3D concentration field course in a model will be regarded as corresponding to the studied real process. We show that one alternative for the formulation of such a practical criterion is sufficient use 2D course of concentration field in which the concentrations otherwise still oscillate, however their course already is not too in contradiction with the real process.

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