A DIFFUSION MODEL OF BATH WASHING EXTRACTION OF A POROUS MATERIAL AND AN EVALUATION OF ITS CONFORMITY WITH THE REAL PROCESS

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Abstract

In this paper, the focus is on the definition of the mathematical conditions needed to ensure that the presented diffusion model of the extraction of a bound biopolymer impurity into the wash liquid during the bath-washing process of that porous material will be in satisfactory accordance with the real washing process from a certain calculated time. The numerical computation of the space-time volume concentration field course in the porous material by means of a diffusion model, which is mentioned in the contribution, is very helpful for the optimization of the washing processes in the chemical and tanning industries.

Keywords: diffusion, extraction of impurity, porous material, washing process

1 Introduction

In the contribution we deal with the numerical computation of the volume concentration of washed out component from a porous material, such as, into the wash liquid by means of Maple software. The calculation is based on analytic solution of the washing process model. We visualized the derived dependence of the removed component concentration for dimensionless variables in the mentioned porous material on the operating time. Experts from working practice strictly demanded - for their needs, only a solution that is obtained by the Laplace transform, since proved very useful to them in the optimization of many washing processes.

2 Statement of the problem

In the bath washing process, the wash liquid neither flows in - nor flows out of the bath into which the biopolymer is placed in the form of a porous material. For simplification purposes, one considers the bound impurity content in the biopolymer to be lower than its solubility in the same volume of wash liquid at the given temperature; and the influence of flanges on diffusion inside the biopolymer sample is neglectable. If these assumptions are realized, one can formulate a one-dimensional space model of bath-washing a biopolymer by the diffusion model of the translocation of the washed-out bound biopolymer impurity by means of the under-mentioned partial differential equation (1) of a parabolic type with the following initial and boundary conditions. The conditions ensure the existence as well as the unicity of the given problem.

The solution of the model is given by the field of concentration \( c(x,t) \) of washed-out component on a half-stripe domain where \( G = \{(x,t) \in \mathbb{R} \times \mathbb{R}^+ \mid 0 \leq x \leq b \ , \ t > 0 \} \). We want to determine the function \( c(x,t) \) that satisfies the initial boundary problem [1]

\[
D \frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial t} + \frac{\partial c_A}{\partial t} \\
(1)
\]

\[
c_A = \frac{Ac}{Be+1} \\
(2)
\]

\[
c(x,0) = c_p \\
(3)
\]
\[ \frac{\partial c}{\partial x}(0, t) = 0 \]  \hspace{1cm} (4)
\[ c(b, t) = \epsilon \cdot c_0(t) \]  \hspace{1cm} (5)
\[ \frac{\partial c}{\partial x}(b, t) = -\frac{V_0}{D \cdot S} \cdot \frac{dc}{dt}(t) \]  \hspace{1cm} (6)
\[ c_0(0) = 0 . \]  \hspace{1cm} (7)

The conditions ensure the existence and unicity of the solution of the under-mentioned problem. The following table depicts the requisite extraction diffusion formulation using mathematical symbols.

<table>
<thead>
<tr>
<th>x</th>
<th>space coordinate</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>half thickness of a porous material</td>
<td>m</td>
</tr>
<tr>
<td>t</td>
<td>time</td>
<td>s</td>
</tr>
<tr>
<td>c</td>
<td>concentration of the washed-out component in the porous material</td>
<td>kg \cdot m^{-3}</td>
</tr>
<tr>
<td>c_A</td>
<td>concentration of bound component in the porous material</td>
<td>kg \cdot m^{-3}</td>
</tr>
<tr>
<td>c_0</td>
<td>concentration of washed-out component in the bath</td>
<td>kg \cdot m^{-3}</td>
</tr>
<tr>
<td>c_p</td>
<td>washed-component initial concentration in the porous material</td>
<td>kg \cdot m^{-3}</td>
</tr>
<tr>
<td>D</td>
<td>effective diffusion coefficient of the washed-out component in the porous material</td>
<td>m^2 \cdot s^{-1}</td>
</tr>
<tr>
<td>D_A</td>
<td>modified washing diffusion coefficient</td>
<td>m^2 \cdot s^{-1}</td>
</tr>
<tr>
<td>A</td>
<td>sorption balance constant (from Langmuir’s sorption isotherm)</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>sorption balance constant (from Langmuir’s sorption isotherm)</td>
<td>m^3 \cdot kg^{-1}</td>
</tr>
<tr>
<td>\epsilon</td>
<td>material porosity (ratio of pores’ volume to material volume)</td>
<td>1</td>
</tr>
<tr>
<td>V_0</td>
<td>volume of washing water as a washing solvent in the washing equipment</td>
<td>m^3</td>
</tr>
<tr>
<td>V</td>
<td>volume of the porous material sample in the washing equipment used</td>
<td>m^3</td>
</tr>
<tr>
<td>S</td>
<td>area of porous material (of one-side)</td>
<td>m^2</td>
</tr>
<tr>
<td>C</td>
<td>dimensionless concentration of washed-out component in the porous material</td>
<td>1</td>
</tr>
<tr>
<td>C_0</td>
<td>dimensionless concentration of washed-out component in the bath</td>
<td>1</td>
</tr>
<tr>
<td>Fo</td>
<td>Fourier criterion (dimensionless time)</td>
<td>1</td>
</tr>
<tr>
<td>X</td>
<td>dimensionless space coordinate</td>
<td>1</td>
</tr>
<tr>
<td>Na</td>
<td>soak number (the V_0/V ratio)</td>
<td>1</td>
</tr>
<tr>
<td>q_n</td>
<td>n-th root of a certain transcendent equation</td>
<td>1</td>
</tr>
<tr>
<td>n</td>
<td>number of terms of a series in a numerical model of washed-out component concentration in a porous material</td>
<td>1</td>
</tr>
</tbody>
</table>

Tab. 1: List of symbols

Suppose that the considered concentration field \( c(x, t) \) of washed undesirable solid component is very low, i.e. \( Bc \ll 1 \), we can define a domain in which the sorption isotherm assumes a linear form and thus relation (2) will be in a simpler form

\[ c_A = A \cdot c \]  \hspace{1cm} (8)

and the system of equations will be as follows

\[ \frac{\partial c}{\partial t} - D \cdot \frac{\partial^2 c}{\partial x^2} = 0 \quad \text{where constant} \quad D^* = \frac{D}{1+1+1} . \]  \hspace{1cm} (9)

For simplification of the solution of equation (9) with additional conditions (3–7), dimensionless variables are introduced

\[ C = \frac{c}{c_p} \quad c_0 = \frac{c_0}{c_p} \quad Fo = \frac{D \cdot t}{b^2 \cdot (1+A)} \quad X = \frac{x}{b} \quad Na = \frac{V_0}{V} . \]  \hspace{1cm} (10)

The analytic solution is obtained by means of the Laplace transform. The final solution given by the dimensionless concentration field \( C(X, Fo) \) can be expressed as follows

\[ C(X, Fo) = \frac{\epsilon(1+A)}{\epsilon(1+A)+Na} - 2 \sum_{n=1}^{N_a} \frac{\cos(q_n X) \exp(-q_n^2Fo)}{\epsilon(1+A) \cos(q_n) - \frac{\epsilon(1+A)}{q_n^2} \sin(q_n) - Na \cdot q_n \sin(q_n)} . \]  \hspace{1cm} (11)

In this equation, \( q_n \) is the \( n \)-th positive root of the following transcendent equation...
\[-\frac{Na \cdot q}{\varepsilon \cdot (1 + A)} = \tan(q)\]  

which is solved by some of the approximate methods.

3 Main results

THE PRACTICAL CRITERION FOR CONFORMITY EVALUATION OF THE WASHING MODEL WITH THE CORRESPONDING REAL PROCESS

Let us approximate the mathematical model of the concentration field \( C(X, Fo) \) - given by the infinite functional series (11), by using the respective numerical approximation with the finite sum of \( n \) terms of this series; and let us briefly call this approximation the “Concentration Field Model” in the following text. Let us represent then that model with some 3D graphics. Further, let \( n, Na, \varepsilon, A, b, D \) be the constants. Then, one can say that the displayed 3D concentration field model is in conformity with the real washing process only from the instant of the start time \( Fo_{\text{start}} \) of an already running washing process when the corresponding 2D concentration field model is \( C(X, Fo) \) at time \( Fo_{\text{start}} \), that is to say, that the concentration

\[ C(0 \leq X \leq 1, Fo = Fo_{\text{start}}) \]

represented by the function of one independent variable \( X \), satisfies the following conformity condition

\[ C(0 \leq X < 0.9, Fo = Fo_{\text{start}}) \leq 1.05 \quad C(0.9 \leq X < 1, Fo = Fo_{\text{start}}) \leq 1.12. \]  

The figures below represent the dimensionless 3D and 2D concentration field courses at the chosen value of the sorption constant \( A \). Apart from the \( Fo \) constant, there is also the corresponding real time \( t \). Fig. 1 shows the concentration field of washed-out impurity in a bath-washed porous material as 3D plots (Left) and 2D plots (Right). Near the dimensionless time \( Fo = 0 \), oscillations of the concentration field are evident. For calculation, the following parameters were used: \( n = 100, A = 5, b = 0.002 \text{ m}, D = 6.10^{-9} \text{ m}^2/\text{s}, \varepsilon = 0.5, Na = 4.\)

![Figure 1: Concentration fields of washed-out porous material impurity as a 3D plot (L) and 2D plot (R).](image)

Fig. 2 shows the concentration fields of washed-out porous material impurity near the dimensionless time \( Fo = 0 \). The red curve shows the limit progress in dimensionless start time \( Fo_{\text{start}} = 0.0001 \); which satisfies the condition (14). The right-hand graph in Fig. 2 shows a detail of the concentration field in the dimensionless start time. The start time \( Fo_{\text{start}} \), or respectively, \( t_{\text{start}} \), depends on the sorption constant \( A \). In our example, when the value of sorption constant \( A = 5 \); the start time \( t_{\text{start}} = 1 \text{ s}. \)

THE MOTIVATION FOR THE CRITERION

given by (14) was the result of the progressive refinement of practitioners’ requirements. The values of the right sides of both inequalities, i.e. 1.05 and 1.12, and also the range for \( X \) are given by material type, etc. The second of the inequalities is very important since, according to researchers in practice, so as to partially eliminate undesirable "shock" effects near the surface. For the solution (11) of our problem to be sufficiently accurate, \( n \) must be large enough dependent on the resolved model. The accuracy condition of our model adequately meets the constant value \( n = 100. \) The problem with the oscillation of the solution accuracy for fast processes. For the most part, the processes which we deal with in our workplaces are slow, thus oscillations can only occur at the beginning of the process.
4 Conclusion

This paper formulates the criterion in the form of inequalities resulting from the 2D space concentration field model of undesirable solid substance extracted from a porous material in the washing process in order to ensure that the appropriate 3D evolutionary concentration field model would be satisfactory in accordance with the real washing process. We show that the above-mentioned conformity is possible starting from a certain time - which we define as the start-time, and all that, on the basis of the evaluation of the above-mentioned 2D concentration models; or, more precisely, the concentration cross profiles thickness. From the set start time - which we are able to determine, we can consider the evolutionary 3D washing model presented in this paper as being conformable with the real process. It must be emphasized that the negative effect of solutions’ oscillations (11) of the diffusion equation in proximity with its characteristics \( t = 0 \), is caused by the number of members of \( n \); so it is analogous to a Gibbs phenomenon. Simply put, our criterion and figures demonstrate that the solution acquired through using the Laplace transform sufficiently precisely approximates the real bath-washing process from a certain point in time. This point in time is called the start-time, and is designated as \( t_{\text{start}} \). This short timeframe does not play a significant role in the overall course of the slow, real washing process.

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