mathematics

MDPI

Article

Application of Fractional Differential Equations for Modeling Bacteria Migration in Porous Medium

Vladimir Chugunov [1] and Sergei Fomin [2,*]

[1] Institute of Mathematics, Informatics and Natural Sciences, Moscow City University, 129226 Moscow, Russia; chugunovva@mgpu.ru
[2] Department of Mathematics and Statistics, California State University, Chico, CA 95928, USA
* Correspondence: sfomin@csuchico.edu

Abstract: One of the modern, recently developed mathematical approaches for modeling various complex chaotic processes (the bacteria migration is apparently one of them), is the application of fractional differential equations. Introduction of fractional derivatives is also a very effective approach for investigation of the reactive processes (growth of bacteria in our case). Our recent advances in application of fractional differential equations for modeling the anomalous transport of reactive and non-reactive contaminants (see our recent publications in the References) allow us to expect that the anomalous transport of growing bacteria can also be effectively described by the models with fractional derivatives. Based on these modern approaches, utilizing fractional differential equations, in this paper we developed a reliable mathematical model that could be properly calibrated and, consequently, provide an adequate description of the growing bacteria transport. This model accounts for the memory effects in the bacteria transport due to the random character of bacteria trapping and release by the porous matrix. Two types of bacteria in the saturated porous medium are considered: mobile and immobile bacteria. Bacteria in the mobile phase are migrating in the fluid and have the velocity of the bulk flow, whereas bacteria in the immobile phase are the bacteria that are captured by the porous matrix. These bacteria have zero velocity and can cause clogging of some pores (therefore, porosity is possibly not constant). Examining different conventional models and comparing computations based on these models, we show that this extremely complex character of bacteria transport cannot be described by the traditional approach based on classical partial differential equations. In this paper we suggest fractional differential equations as a simple but very effective tool that can be used for constructing the proper model capable of simulating all the above-mentioned effects associated with migration of alive bacteria. Using this approach, a reliable model of the growing bacteria transport in the porous medium is developed and validated by comparison with experimental laboratory results. We proved that this novel model can be properly linearized and calibrated, so that an excellent agreement with available experimental results can be achieved. This simple model can be used in many applications, for example, as a part of more general mathematical models for predicting the outcomes of the bioremediation of contaminated soils.

Keywords: fractional equation; bacteria migration; mathematical model; active bacteria; porous medium

MSC: 35R11

Citation: Chugunov, V.; Fomin, S. Application of Fractional Differential Equations for Modeling Bacteria Migration in Porous Medium. *Mathematics* **2024**, *12*, 685. https://doi.org/10.3390/math12050685

Academic Editors: Ying Luo, Fudong Ge and Jorge Muñoz

Received: 11 January 2024
Revised: 12 February 2024
Accepted: 21 February 2024
Published: 26 February 2024

1. Introduction

An increased subsurface pollution, especially due to organic wastes, oil discharges, and leakages from chemical and petroleum plants, is a serious environmental problem for every country. Bioremediation is an effective practical approach based on the application of bacteria to the subsurface systems for eliminating hazardous waste. Therefore, the proper understanding of the peculiarities of bacteria migration in a porous medium is an important factor for the development and implementation of bioremediation technology.

Experimental studies by Simamura et al. [1] and Yang et al. [2] were focused on peculiarities of the bacteria transport in a porous medium simultaneously with the cell growth (bacteria reproduction). The experiments showed that mass transport of non-active bacteria as a suspension of particles can be well described by the conventional advection-dispersion equation. However, if the injected bacteria are active and capable for reproduction, then the application of conventional advection-dispersion equation, even with added term that models bacteria growth, does not provide an agreement with experimentally observed behavior. The maximal values of bacteria concentration in the exit cross-section of the experimental set up (see Figure 1) were much lower than the computed concentration. Moreover, the experimentally obtained concentration curve is shifted towards the origin of the Cartesian coordinates from the computed concentration curve. The reduction of the maximal values of concentration within the experimental studies in comparison to the computed concentration can be attributed to the fact that theoretical model does not account for capture of the bacteria in the fluid phase by the porous matrix. The key conclusion based on analysis of the experimental data was that migration of the growing bacteria in the porous media exhibits an anomalous behavior and, therefore, cannot be described by existing traditional models based on advection-dispersion equations, even if these equations are coupled with the first type kinetic equations for modeling the adsorption-desorption phenomena (bacteria capture-release), which are normally used for modeling the bacteria transport. The target of this paper is to construct a mathematical model of bacteria transport by the flow of nutrient solution in the porous medium capable to adequately describe the experimentally observed in [1,2] behavior.

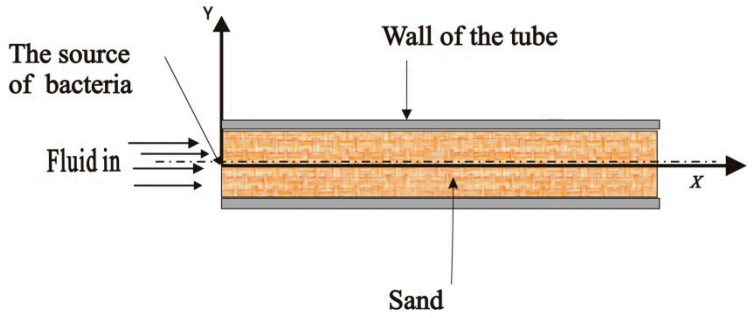

Figure 1. A schematic of the process (an experimental setup).

Concentration of the alive bacteria in the active state can increase due to the bacteria reproduction. Herewith, the growing bacteria can gather in groups which size exceed the size of the singular cell. This behavior can trigger such situations when these groups (colonies) of bacteria fill the part of the pore space within the porous medium that may lead to the capture by the porous matrix a certain number of bacteria. Similar phenomena can be observed in the flows of colloid solutions. In the latter case, the mechanism of particles capture is well documented [3–7]. Another group of researchers, using analogies with the adsorption processes, describe the bacteria capture using the approach, which is typically used for modeling the solution flow with effects of adsorption [8–10].

The process of capture of bacteria by the porous matrix is normally accompanied by the process of detachment by the fluid flow of some bacteria that have already settled in the porous medium. In order to account for bacteria capture-detachment prompt researchers, in a view of similarities of bacteria transport with particulate solutions flow, to incorporate in the model of bacteria transport the equations of kinetics of the first order [6,11].

Obviously, it could be suggested that the behavior of bacteria has the stochastic character and, therefore, can be described in terms of stochastic physics. At least for the passive solutes, in [12] it is shown that within the framework of stochastic physics the process of the complex mass transport can be described by the classic advection-dispersion equation, but with incorporation of the complex law of concentration distribution in the fluid phase and particles captured by the porous matrix. This law is presented in the form

convolution integral for the bacteria concentration in the fluid phase with some coefficient of distribution, which values define the mechanism of interaction of the particles in the fluid phase with particles settled in the porous matrix. For the active particles, such as active growing bacteria, mass transport is more complex and, therefore, the equation used for its description can be different from the classical advection-dispersion equation. In the publications [13–15] it is noted that for description of the anomalous types of diffusive processes, it is meaningful to consider the so-called fractional kinetic equations, in which the fractional operator with respect to time is applied to the mass flux. In the publication [16] it is demonstrated that the temporal fractional derivative is a very promising tool, especially for modeling and analyzing the reactive solute transport. In the publications [17–19] equations with fractional derivatives for describing the solute transport in the porous rocks were used and theoretically obtained results were in a good agreement with laboratory and field experiments.

Further on, following the ideas suggested in [13–15], we will assume that transport of bacteria in the porous medium is described by the fractional equation and correlation between the immobile and active bacteria in the nutrient liquid solution is defined by the convolution equation, as suggested in [12,20–23]. One of the recently developed mathematical approaches for modeling various complex chaotic processes (bacteria migration is apparently one of them), is the application of fractional differential equations. Our recent advances in application of fractional differential equations for modeling the anomalous transport of the non-reactive and reactive contaminants [24–27] allow us to expect that the anomalous transport of growing bacteria can also be well approximated by the models with fractional derivatives. Our preliminary efforts to develop the adequate model based on these modern approaches brought us to the conclusion that the problem of growing bacteria transport should be modeled by accounting for the memory effects in the bacteria transport due to the random character of bacteria trapping and release by the porous matrix. Two phases (mobile and immobile) of bacteria existence in the flow should be considered. Bacteria in a mobile phase have the velocity of the bulk flow, whereas bacteria in the immobile phase, which are trapped by the porous matrix, have zero velocity and can clog some of the pores.

2. System Model and Analysis

The description of the experimental set-up (see Figure 1), as outlined in [1]. Silica sand was packed into the column in which the nutrient solution with suspended cells was injected. The *Lactobacillus casei* (ATCC 15883) was used as a model bacterium. The size of a cell is around 1 μm in diameter and 2 μm in length (approximately the volume of the cell $V_0 \approx 10^{-12}$ cm^3). Two types of bacterial cells, growing (at temperatures comfortable for bacteria reproduction) and resting (no growth, due to the lower temperature), were prepared. This allowed testing in different experiments two types of bacteria behavior when the bacteria were active and mobile, which rapidly increase their population, and immobile, which population does not grow (resting cells). In the laboratory experiment the growth and transport of bacteria was performed in the sand with a granule diameter of 600–850 μm and a porosity of $m_0 = 0.4$ packed in the tube with non-permeable walls, which length $l = 14$ cm and diameter $d = 4.6$ cm, cross sectional area S and volume $V = Sl$. In both cases (growing or resting bacteria) concentration of bacteria in a suspension at the input c^* was 2.1×10^8 cell/mL and the average flow rate in the porous medium $v = 10$ cm/h. The length of the injection period τ_0 was equal to 0.5 pore volume, $\tau^* = l/v$. In the experiments, the bacteria specific growth rate μ was in the range from 0.12 to 0.16 h^{-1}. We will denote by c_m and c_i the concentrations of mobile (in the fluid) and immobile (trapped by pores) bacteria, respectively, so that the porosity m is a function of the concentration c_i, and v_f is a fluid velocity.

Obviously, porosity and concentration are coupled by the following equation in increments:

$$mS\Delta x = m_0 S\Delta x - (c_i m_0 S\Delta x)V_0, \quad (1)$$

which represents the simple fact that the volume occupied of the liquid phase is equal to the difference of initial porous volume and the volume occupied by immobile bacteria. From the above equation it follows that:

$$m = m_0(1 - c_i V_0). \tag{2}$$

Here, $c_i V_0$ is the volumetric fraction of the porous medium occupied by the by immobile bacteria. From Equation (2) it follows that the maximal value of c_i should not exceed V_0^{-1}. So, the equality $c_i = V_0^{-1}$ means that all pores within the porous medium cross-section are totally filled with bacteria. Denoting by c the sum of all bacteria at the cross-section x of the porous medium, we can obviously write:

$$c = mc_m + m_0 c_i \tag{3}$$

The conservation law for c, which expresses the fact that the rate of change of c depends on the influx of bacteria to the cross-section x and growth of the bacteria population at this cross-section, can be presented in the following standard form:

$$\frac{\partial c}{\partial \tau} = -\frac{\partial q}{\partial x} + j \tag{4}$$

In the latter equation it is assumed that the bacteria transport takes place in the direction of x-axis only, which is quite reasonable for the experimental set-up presented in Figure 1, q is the mass flux, τ is a temporal variable, and j is the bacteria source (sink) term.

The approaches for modeling the bacteria growth are well documented. For example, the behavior of bacteria population can be described by Monod kinetics [9,28,29]. Based on this approach, it can be written that:

$$j_g^{(i)} = \mu_g c_i,\ j_d^{(i)} = k_d c_i,\ j_g^{(m)} = \mu_g c_m,\ j_d^{(m)} = k_d c_m, \tag{5}$$

where $j_g^{(i)}$ and $j_d^{(i)}$ are the specific mass discharges due to the growth and decay of the immobile (captured) bacteria, respectively; $j_g^{(m)}$ and $j_d^{(m)}$ are the specific mass discharges due to the growth and decay of the mobile bacteria, respectively; μ_g is the bacteria growth constant and k_d is the bacteria decay constant.

Obviously, accounting for Equation (3), the overall specific discharge j for the mobile and immobile species can be defined as follows:

$$j = \mu(mc_m + m_0 c_i) = \mu c, \tag{6}$$

where $\mu = \mu_g - k_d$ is the specific constant of the rate of growth of the bacteria colony.

The magnitude of the bacteria flux q depends on the bacteria transport in the solution and its form should be determined by the mechanisms of the mass transport in the solution and mass exchange between mobile bacteria in the solution and captured bacteria. The final expression for q will be derived later, following the consideration of the equation for the bacteria transport in the nutrient liquid medium.

The conservation law for c_i can be presented as follows:

$$\frac{\partial c_i m_0}{\partial \tau} = q_{im} + \mu m_0 c_i, \tag{7}$$

where q_{im} represents the bacteria participating in the exchange between the mobile and immobile phases per unit time and μ is the specific constant of the rate of growth of the bacteria colony.

According to Dentz and Bercovitz [12], in the sufficiently general case, it can be assumed that the correlation between the mobile and immobile phases can by modeled by the following convolution equation:

$$m_0 c_i = \int_0^\tau k(\tau - \xi) m c_m(\xi, x) d\xi, \tag{8}$$

where $k(\tau)$ is a memory function which correlates the mobile and immobile concentrations by a convolution with respect to time. If $k(\tau)$ in Equation (8) is known, then Equation (7) can be used for obtaining the correlation between the flux of mobile–immobile exchange q_{im} and concentration of bacteria in the fluid. If there is no bacteria growth (no bacteria reproduction), i.e., $\mu = 0$, but bacteria in the solution are sufficiently big, so that the bacteria capture can occur, then the bio-clogging effect may take place. In this case, the behavior of the mobile bacteria can be modeled by the equation with the fractional time derivative, which is often used for modeling complex random processes [13]:

$$\frac{\partial c_m m}{\partial \tau} = k_\alpha \mathcal{D}_\tau^{1-\alpha} \left[\alpha_d v_f m \frac{\partial^2 c_m}{\partial x^2} - m v_f \frac{\partial c_m}{\partial x} \right] \tag{9}$$

where $\mathcal{D}_\tau^{1-\alpha} c = \frac{\partial^{1-\alpha} c}{\partial \tau^{1-\alpha}} = \int_0^\tau \frac{(\tau-\xi)^{-(1-\alpha)}}{\Gamma(1-1+\alpha)} \frac{\partial c}{\partial \xi} d\xi$ is the fractional time derivative of Riemann-Liouville [30], k_α is a parameter which depends on properties of the porous medium and bacteria in the fluid phase and α_d is the coefficient of dispersion.

Due to the geometry of the experimental set-up (long and narrow channel filled with porous medium), it is convenient to proceed in terms of mean over the cross section of the porous medium velocities, $v = m v_f$, so that Equation (9) can be rewritten in the following form:

$$\frac{\partial c_m m}{\partial \tau} = k_\alpha \mathcal{D}_\tau^{1-\alpha} (L_v c_m), \tag{10}$$

where

$$L_v c_m = \alpha_d v \frac{\partial^2 c_m}{\partial x^2} - v \frac{\partial c_m}{\partial x} \tag{11}$$

It should be noted that Equation (10) does not contain the term q_{im} from Equation (7), which represent the exchange between mobile and immobile bacteria. Instead, this exchange between the mobile and immobile bacteria (captured by the pores) is accounted for by the form of fractional derivative and the values of parameters k_α and α.

Summing Equations (7) and (10), we should obtain the conservation equation for the total concentration c, i.e., Equation (4) when $j = 0$. Hence, accounting for Equation (8), Equation (7) will take the following form:

$$\frac{\partial q}{\partial x} = -\frac{\partial}{\partial \tau} \int_0^\tau k(\tau - \xi) m c_m(\xi, x) d\xi - k_\alpha \mathcal{D}_\tau^{1-\alpha} (L_v c_m) \tag{12}$$

If function k is known, then Equation (12) defines the spatial variation of the mass flux which affects the concentration of the bacteria in the porous medium. On the other hand, we can consider the inverse problem of defining the distribution $k(\tau)$ for the given $\frac{\partial q}{\partial x}$. In the latter case, it would be natural to assume that function $\frac{\partial q}{\partial x}$ has the same structure as the term that represents the variation of c_i in Equation (10), i.e., the variation of the total concentration can be also modeled by the equation of anomalous diffusion (fractional equation), but with its own values of parameters k_β, β (instead of k_α and α_d):

$$\frac{\partial q}{\partial x} = -k_\beta \mathcal{D}_\tau^{1-\beta} (L_v c_m) \tag{13}$$

Introduction of the fractional Equation (13) is quite reasonable, because for the active bacteria, even if there are no bacteria capture by the porous matrix, diffusion (dispersion) can be anomalous, since bacteria tend to gather in groups (micro colonies) and the rate of

their displacement by the fluid flow will be different from the velocity of this flow. This can affect the diffusivity (dispersity) constant as well.

To obtain $k(\tau)$, we will apply the Laplace transform to Equations (12) and (13). As a result, excluding $\frac{\partial q}{\partial x}$, we have:

$$k_\beta s^{1-\beta}\overline{(L_v c_m)} = s\bar{k}\overline{mc_m} + k_\alpha s^{1-\alpha}\left(\overline{L_v c_m}\right) \tag{14}$$

where a bar above the variable denotes the Laplace transform of this variable and s is the parameter of Laplace transformation, e.g., $\bar{c}(s,x) = \int_0^\infty e^{-s\tau}c(\tau,x)d\tau$.

From Equation (10) it follows that:

$$\overline{L_v c_m} = \frac{1}{k_\alpha}s^\alpha(\overline{mc_m}). \tag{15}$$

Substituting Equation (15) into (14), yields:

$$\bar{k} = \frac{k_\beta}{k_\alpha}s^{\alpha-\beta} - 1. \tag{16}$$

Applying the inverse Laplace transform to Equation (16), gives:

$$k(\tau) = \frac{k_\beta}{k_\alpha}\frac{\tau^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)} - \delta(\tau), \tag{17}$$

where $\delta(\tau)$ is Dirac delta function and Γ(x) is Gamma function.

Thus, if variation of k is defined by the Formula (17) and concentration of the particles in the liquid phase of the porous medium is defined by the by the equation of anomalous diffusion (10), then in the equation for the total concentration c, spatial variation of the mass flux is also modeled by the fractional derivative.

Accounting for Equations (6), (7) and (12), equation for the total concentration will have the following form:

$$\frac{\partial c}{\partial \tau} = \frac{\partial}{\partial \tau}\int_0^\tau k(\tau-\xi)mc_m(\xi,x)d\xi + k_\alpha \mathcal{D}_\tau^{1-\alpha}(L_v c_m) + \mu c, \tag{18}$$

where $k(\tau)$ is defined by (17). Applying to (7) ($\mu = 0$) Laplace transform and accounting for (8) and (16), the mass flux $\overline{q_{im}}$ can be presented in following form:

$$\overline{q_{im}} = s\overline{m_0 c_i} = s\bar{k}\cdot\overline{mc_m} = \frac{k_\beta}{k_\alpha}s^{\alpha-\beta+1}\cdot\overline{mc_m} - s\cdot\overline{mc_m}. \tag{19}$$

From the above:

$$\overline{q_{im}} = \frac{k_\beta}{k_\alpha}s^{\alpha-\beta+1}\cdot\overline{mc_m} - s\cdot\overline{mc_m}. \tag{20}$$

The bar above the variables in (19) and (20), same as before, denotes the Laplace transformation of these variables. Applying the inverse Laplace transform to the Formula (20), yields:

$$q_{im}(\tau) = \frac{k_\beta}{k_\alpha}D_\tau^{1-(\beta-\alpha)}(mc_m) - \frac{\partial(mc_m)}{\partial\tau}. \tag{21}$$

In the case of the growing bacteria ($\mu \neq 0$), Equation (7) in Laplace transforms leads to

$$\overline{q_{im}} = (s-\mu)\overline{m_0 c_i}. \tag{22}$$

Comparing Equation (20) with Equation (22), which corresponds to $\mu \neq 0$, we see that instead of the factor s in Equation (20), Equation (22) contains the factor $(s-\mu)$. Therefore, following this analogy, in the case when $\mu \neq 0$, we can assume that in Laplace transforms,

$$\bar{k}(s) = \bar{k}(s-\mu) = \frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta} - 1. \tag{23}$$

Then, using Equations (22) and (23), we can obtain:

$$\overline{q_{im}} = [\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta+1} - (s-\mu)]\overline{mc_m} \tag{24}$$

Also, in this case,

$$\overline{m_0 c_i} = [\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta} - 1]\overline{mc_m}, \tag{25}$$

and, accounting for Equation (6), Equation (4) can be rewritten as follows,

$$\overline{\frac{\partial q}{\partial x}} = (s-\mu)\bar{c}. \tag{26}$$

So, instead of s, as it occurs in the case of $\mu = 0$, in the present case, the right-hand side contains the factor $(s-\mu)$. Therefore, accounting for Equation (13), in the case when $\mu \neq 0$, we should write:

$$\overline{\frac{\partial q}{\partial x}} = -k_\beta (s-\mu)^{1-\beta}\overline{(L_v c_m)}. \tag{27}$$

From Equations (26) and (27) it follows that:

$$s\bar{c} = k_\beta (s-\mu)^{1-\beta}\overline{(L_v c_m)} + \mu\bar{c}\,. \tag{28}$$

Accounting for Equation (24), Equation (7) in Laplace transforms can be rewritten as follows:

$$s\overline{m_0 c_i} = \left[\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta+1} - (s-\mu)\right]\overline{mc_m} + \mu\overline{m_0 c_i}. \tag{29}$$

Subtracting Equation (29) from Equation (28), we obtain an equation in Laplace transforms for the concentration of the particles in the fluid phase, $s\overline{mc_m} = k_\beta (s-\mu)^{1-\beta}\overline{(L_v c_m)} - \left[\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta+1} - (s-\mu)\right]\overline{mc_m} + \mu\overline{mc_m}$, which can be reduced to the following form:

$k_\beta (s-\mu)^{1-\beta}\overline{(L_v c_m)} - \left[\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta+1}\right]\overline{mc_m} = 0$. The latter equation, after division by $\frac{k_\beta}{k_\alpha}(s-\mu)^{\alpha-\beta}$, can be rewritten as follows:

$$(s-\mu)\ \overline{c_m m} = k_\alpha (s-\mu)^{1-\alpha}\overline{L_v c_m}. \tag{30}$$

Applying the inverse Laplace transform to Equation (30) leads to the following equation for the mobile bacteria concentration in the liquid nutrient medium:

$$\frac{\partial c_m m}{\partial \tau} = e^{\mu\tau}\mathcal{D}_\tau^{1-\alpha}\left[k_\alpha e^{-\mu\tau} L_v c_m\right] + \mu m c_m. \tag{31}$$

Equation (8) is the equation for the concentration of bacteria in immobile stage, where the factor k is defined by the Formula (23). Application of inverse Laplace transform to the expression (23) gives:

$$k(\tau) = \frac{k_\beta}{k_\alpha}\frac{\tau^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}e^{\mu\tau} - \delta(\tau). \tag{32}$$

The value of q_{im}, which determines the number of bacteria participating in the mobile-immobile interexchange, can be obtained from the Formulae (24) or (22), where the former couples q_{im} with concentration c_m and the latter with c_i. Applying the inverse Laplace transform to the expression (24) and accounting for the Riemann-Liouville definition of fractional derivative, yields:

$$q_{im} = \frac{k_\beta}{k_\alpha}e^{\mu\tau}\mathcal{D}_\tau^{1+\beta-\alpha}\left[e^{-\mu\tau}(mc_m)\right] - \frac{\partial(mc_m)}{\partial\tau} + \mu m c_m. \tag{33}$$

The system of Equations (31)–(33) along with Equation (8) completely defines the behavior of active (mobile) and passive (immobile) bacteria in the porous medium. It should be noted that by choosing the certain forms of the functions $k(\tau)$ and $\frac{\partial q}{\partial x}$ we can obtain from the above system, as the particular cases, different well-known conventional models, which are typically used for computation of concentrations of the bacteria (or particles) in the solution flows within porous media. For example, let's assume that in Formula (32), $k_\alpha = k_\beta = 1$, $\beta = 1$, $\alpha \to \beta$. Then, for $\mu \neq 0$, we have:

$$k(\tau) = 0, \tag{34}$$

$$-\frac{\partial q}{\partial x} = L_v c_m. \tag{35}$$

Accounting for (34) and (5), equation for the total concentration (18) will take the following form:

$$\frac{\partial c}{\partial \tau} = (L_v c_m) + \mu c. \tag{36}$$

Assuming that $m_0 c_i = k_a m c_m$, we obtain:

$$c = k_a m c_m + m c_m = m c_m (1 + k_a), \tag{37}$$

where the coefficient k_a defines the rate of bacteria capture.

Then, accounting for (37), Equation (36) can be rewritten as follows:

$$(1 + k_a)\frac{\partial c_m m}{\partial \tau} = \alpha_d v \frac{\partial^2 c_m}{\partial x^2} - v\frac{\partial c_m}{\partial x} + \mu(1 + k_a) m c_m \tag{38}$$

Equations (36)–(38) are well-known in the literature as an adsorption model [5,8,11,28,31].

One more model, which will be used in the further numerical analysis, can be obtained, if we assume that

$$k(\tau) = k_m e^{(\mu - k_i)\tau}. \tag{39}$$

In the above formula, k_m is the parameter that defines the rate of particle capture from the liquid phase and parameter k_i defines the rate of release of the previously captured particles, i.e., the transition of particles from the immobile to mobile status. The value of $\frac{\partial q}{\partial x}$, as in the previous case, is defined by the expression (35). In this case, the formula for q_{im} can be presented as follows:

$$q_{im} = k_m m c_m - k_i m_0 c_i. \tag{40}$$

It should be noted that Equations (4), (6)–(8) and (39) constitute the well-known adsorption–desorption model, where the exchange between phases is described by the kinetics of the first order [11,12]. In the case of any arbitrary function $k(\tau)$, expression for q_{im} can be presented as follows:

$$q_{im} = \frac{\partial}{\partial \tau}\int_0^\tau k(\tau - \xi) m c_m(\xi, x) d\xi - \mu \int_0^\tau k(\tau - \xi) m c_m(\xi, x) d\xi. \tag{41}$$

If we introduce a so-called memory function $\varphi(\tau)$, Formula (41) can be rewritten in a more compact form. Let us assume that Laplace transform of this memory function has the following form:

$$\overline{\varphi}(s) = \frac{(s - \mu)}{s}\overline{k}(s), \tag{42}$$

where, as before, the bar above the variable denotes the Laplace transform of this variable.

Utilizing Formula (42), expression (41) can be rewritten as follows:

$$q_{im} = \frac{\partial}{\partial \tau}\int_0^\tau \varphi(\tau - \xi) m c_m(\xi, x) d\xi. \tag{43}$$

In the particular case, when $k(\tau)$ is defined by the Formula (23),

$$\varphi(\tau) = \frac{k_\beta}{k_\alpha}\varphi_0(\tau) + \mu - \delta(\tau), \tag{44}$$

where

$$\varphi_0(\tau) = \frac{\tau^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}e^{\mu\tau} - \frac{\mu}{\Gamma(\beta-\alpha)}\int_0^\tau \tau^{\beta-\alpha-1}e^{\mu\tau}d\tau. \tag{45}$$

Note that for the particular case when $\beta = 1$, formula for $\varphi_0(\tau)$ coincides with the memory function obtained in the study presented in [24], which is related to interaction of the radioactive contaminants in the fracture and surrounding porous medium. If, as in the work presented in (45) we assume that $\beta = 1$, $\mu = 0$, then we obtain another well documented particular case, when $\varphi_0(\tau)$ describes the interaction of the solute between the blocks of the porous medium without chemical reactions [25]. The system of the above equations completely defines the behavior of active (mobile) and passive (immobile) bacteria in the porous medium. This system should be supplemented by the proper initial and boundary conditions. For example for the experimental setup illustrated in Figure 1, we can assume that

$$\tau = 0, \;\; c_m = c_i = 0, \qquad m = m_0; \tag{46}$$

$$x = 0, c_m = c_{m0}(\tau) = \begin{cases} c_0 - const., & 0 < \tau < \tau_0 \\ 0, & \tau > \tau_0 \end{cases}; \tag{47}$$

where in the laboratory experiments, the constant c_0 is taken as 3.6×10^8 cells/mL, 2.1×10^8 cells/mL, and 0.8×10^8 cells/mL and τ_0 is the length of bacteria injection period. In the infinity,

$$x \to \infty, \;\; c_m = c_i = 0, \; m = m_0. \tag{48}$$

For the further analysis it is convenient to introduce the following non-dimensional variables:

$$\begin{gathered} C_i = \tfrac{c_i}{c_0}, \; C_m = \tfrac{c_m}{c_0}, \; t = \tfrac{\tau}{\tau^*}, \; t_0 = \tfrac{\tau_0}{\tau^*}, \; \psi = \tfrac{m}{m_0}, \; X = \tfrac{x}{l}, \; Pe = \tfrac{l}{\alpha_d}, \; D_a = \mu\tau^*, \\ K_\alpha = k_\alpha\left(\tau^*\right)^{\alpha-1}, \; K_\beta = k_\beta\left(\tau^*\right)^{\beta-1}, \; K(t) = \tfrac{k(\tau)}{k_0}, \; C_0(t) = \tfrac{c_{m0}(\tau)}{c_0}, \; Q_{im} = \tfrac{q_{im}}{q_0}, \end{gathered} \tag{49}$$

where $\tau^* = \frac{l}{v}, k_0 = \frac{1}{\tau^*}, q_0 = \frac{c_0}{\tau^*}$.

In non-dimensional variables the governing equations will take the following form:

$$\frac{\partial C_m\psi}{\partial t} = e^{D_a t}\mathcal{D}_t^{1-\alpha}\left[K_\alpha e^{-D_a t}(L_{Pe}C_m)\right] + D_a\psi C_m, \tag{50}$$

where $L_{Pe}C_m = -\frac{\partial C_m}{\partial X} + \frac{1}{Pe}\frac{\partial^2 C_m}{\partial X^2}$,

$$C_i = \int_0^t K(t-\tau)\psi C_m(\tau, x)d\tau, \tag{51}$$

$$Q_{im} = \frac{\partial}{\partial t}\int_0^t K(t-\tau)\psi C_m(\tau, x)d\tau - D_a\int_0^t K(t-\tau)\psi C_m(\tau, x)d\tau, \tag{52}$$

$$K(t) = \frac{K_\beta}{K_\alpha}\frac{t^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}e^{D_a t} - \delta(t), \tag{53}$$

$$\psi = 1 - V_0\, c_0 C_i \;\;, \tag{54}$$

$$t = 0, \quad C_m = C_i = 0, \quad \psi = \psi_0;$$

$$X = 0, C_m = C_0(t) = \begin{cases} 1, & 0 < t < t_0 \\ 0, & t > t_0 \end{cases}; \tag{55}$$

$$X \to \infty, C_m = C_i = 0.$$

In general, the system of Equations (50)–(54) is non-linear, since porosity ψ depends on C_i. Furthermore, the experimental results show that parameter α depends on the rate of the bacteria colony growth. If the bacteria reproduction in the porous medium is ignored, then Equation (50) should be reduced to the traditional diffusion-advection equation, which effectively models the behavior of non-active bacteria. Hence, in this case, $D_a = 0$, $K_\beta = K_\alpha = 1$, $\beta = \alpha = 1$. When bacteria are active, then $D_a \neq 0$, and $\alpha < 1$. The rate of growth of bacteria population is proportional to the concentration of bacteria in the fluid medium. This fact can be denoted as

$$\alpha = \alpha(D_a \psi C_m). \tag{56}$$

Let us assume that concentration in the inlet of the porous medium c_0 varies in the range $[0, c_0^{max}]$. Denoting by $C_\gamma = c_0/c_0^{max}$ and approximating α in the vicinity of C_γ (while keeping only the leading term in this approximating expansion), we can write $\alpha = \alpha(D_a \psi C_\gamma)$. Further, assuming that $D_a C_\gamma < 1$, approximation for (56) yields:

$$\alpha = 1 - \alpha_0 D_a \psi C_\gamma + O\Big((D_a \psi C_\gamma)^2\Big) \tag{57}$$

Similarly, for the parameter $K_\alpha = K_\alpha(D_a \psi C_m)$, we can write, $K_\alpha = 1 + K_0 D_a \psi C_\gamma + O((D_a \psi C_\gamma)^2)$. The same reasonings can be used for approximating the parameters K_β and β.

According to the experimental data, the values of c_0 varied from its minimum 0.8×10^8 cells/mL to maximum of 3.6×10^8 cells/mL. For these values of initial concentration in expression (54) the value of the product $c_0 V_0 \sim 10^{-4}$. Assuming that within the considered period of time the value of the non-dimensional concentration of immobile bacteria is the order of 1, then approximately we can assume that $\psi \approx 1$. Obviously, this assumption works within a certain finite period of time. For the longer periods of time, due to the growth of the bacteria colony, concentration C_i can reach rather high magnitudes, then $\psi < 1$ and the variation of porosity cannot be ignored. In this paper, we will consider the situation when the porosity variation is rather small and, therefore, $\psi \approx 1$.

3. Solution of the Governing Equations

For solving the system of Equations (50)–(54) we will apply the method of Laplace transforms with respect to the variable t. Note, that it is sufficient to solve equations for the case when $C_0(t) = 1$. After obtaining this solution, application of the Duhamel's theorem immediately gives:

$$C_m(t, X) = \frac{\partial}{\partial t} \int_0^t C_0(\tau) \hat{C_m}(t - \tau, x) d\tau, \tag{58}$$

where $\hat{C_m}$ is the solution of the system (50)–(54) for $C_0(t) = 1$.

Application of Laplace transform to Equations (51)–(53) leads to the following equations in terms of Laplace transforms (denoted by the bar on the top):

$$\overline{K}(S) = \frac{K_\beta}{K_\alpha} (S - D_a)^{-\beta + \alpha} - 1, \tag{59}$$

$$\overline{C_i}(S, X) = \overline{K}(S) \overline{C_m}(S, X), \tag{60}$$

$$\overline{Q_{im}}(S, X) = (S - D_a) \overline{K}(S) \overline{C_m}(S, X). \tag{61}$$

Fractional differential Equation (50) with the corresponding boundary conditions (55) will be reduced to the following boundary-value problem for the ordinary differential equation:

$$\frac{1}{Pe} \frac{\partial^2 \overline{C_m}}{\partial X^2} - \frac{\partial \overline{C_m}}{\partial X} - \overline{C_m} g(S) = 0, \tag{62}$$

$$X = 0, \quad \overline{C_m} = 1/S, \tag{63}$$

$$X \to \infty, \quad \overline{C_m} \to 0, \tag{64}$$

where

$$g(S) = \frac{1}{K_\alpha}(S - D_a)^\alpha. \tag{65}$$

It can be readily shown that the conventional adsorption–desorption models for the flows of particles in the liquids are constituted by the same Equations (62)–(64), but with functions g different from the function given by Equation (65).

Solution of the problem (62)–(65) can presented in the following form:

$$\overline{C_m}(S, X) = \frac{1}{S} e^{\frac{Pe}{2}X} e^{-\sqrt{\left(\frac{Pe}{2}\right)^2 + Pe\,g(S)}X}. \tag{66}$$

For performing the inversion of this solution, it is convenient to utilize the following representation of the exponential function:

$$e^{-2z} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\xi^2 - \left(\frac{z}{\xi}\right)^2} d\xi. \tag{67}$$

Accounting for the Formula (67), solution (66) can be presented as

$$\overline{C_m}(S, X) = \frac{2}{S\sqrt{\pi}} \int_0^\infty e^{\frac{Pe}{2}X - \xi^2 - \frac{Pe}{4}Z}\, e^{-Z g(S)} d\xi, \tag{68}$$

where $Z = -\frac{X^2 Pe}{4\xi^2}$.

If in Equation (62) we assume that $Pe \to \infty$, then Equations (62)–(64) will describe (in terms of Laplace transforms) concentration of bacteria in a fluid phase when dispersion is ignored. Solution of this truncated equation can be readily obtained in the following form:

$$\overline{C_\infty}(S, X) = \frac{1}{S} e^{-X g(S)}. \tag{69}$$

Applying to (69) the inverse Laplace transformation, we can obtain the concentration $C_\infty(t, X)$. If this function is obtained, then applying the inverse Laplace transform to Equation (68), yields:

$$\hat{C_m}(t, X) = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{\frac{Pe}{2}X - \xi^2 - \frac{Pe}{4}Z}\, C_\infty(t, Z) d\xi. \tag{70}$$

When $\hat{C_m}(t, X)$ is known and, hence $C_m(t, X)$ can be obtained by the Formula (58), the corresponding values of C_i and Q_{im} can be readily computed from the expressions (60) and (61) by taking the inverse Laplace transform. Let us consider three different particular models, which can be determined by the different forms of the function $K(t)$.

(a) Model of adsorption, which accounts for the growth of bacteria population

This model is presented by Equations (34)–(38). Converting these formulae to the non-dimensional form and accounting for the approximation $\psi \approx 1$, yields: $C_i = k_a C$, $R\frac{\partial C_m}{\partial t} = \frac{1}{Pe}\frac{\partial^2 C_m}{\partial X^2} - \frac{\partial C_m}{\partial X} + D_a R C_m$, where $R = 1 + k_a$. Applying the Laplace transform to the latter aquation, we obtain: $\overline{C}_i = k_a \overline{C}$, $RS\overline{C}_m = \frac{1}{Pe}\frac{\partial^2 \overline{C}_m}{\partial X^2} - \frac{\partial \overline{C}_m}{\partial X} + D_a R \overline{C}_m$, or $\frac{1}{Pe}\frac{\partial^2 \overline{C_m}}{\partial X^2} - \frac{\partial \overline{C_m}}{\partial X} - \overline{C_m} g(S) = 0$, where $g(S) = R(S - D_a)$. Obviously, the boundary conditions will be the same as those that were used in the more general case of (63), (64), i.e., for $X = 0$, $\overline{C_m} = 1/s$, and for $X \to \infty$, $\overline{C_m} \to 0$.

The obtained boundary-value problem for the Laplace transformations has the same structure as the problem (62)–(64) discussed above. The only difference is in function $g(S)$, which justifies the application of Equations (66)–(70). Using these equations, we obtain:

$$\overline{C_\infty}(S,X) = \frac{1}{S} e^{-XR(S-D_a)}, \tag{71}$$

Applying to the expression (71) the inverse Laplace transform, yields:

$$C_\infty(t,X) = e^{XRD_a} H(t-XR), \tag{72}$$

where H is a Heaviside unit step function.

Substituting C_∞ into the Formula (70) yields:

$$\hat{C_m}(t,X) = \frac{X}{2}\sqrt{\frac{PeR}{\pi}} e^{\frac{Pe}{2}X} \int_0^t e^{-\frac{X^2 PeR}{4\tau} - \frac{Pe\tau}{4R} + D_\alpha \tau} \frac{1}{\sqrt{\tau^3}} d\tau. \tag{73}$$

If $\frac{Pe}{4R} - D_\alpha > 0$, then an integral in (73) can be expressed through the error function $erfc(x)$ as follows:

$$\hat{C_m}(t,X) = e^{\frac{Pe}{2}X} \frac{1}{2} \left\{ e^{-X\sqrt{\frac{Pe^2}{4} - D_\alpha PeR}} erfc\left[\frac{X}{2}\sqrt{\frac{PeR}{t}} - \sqrt{\left(\frac{Pe}{4R} - D_\alpha\right)t} \right] + e^{X\sqrt{\frac{Pe^2}{4} - D_\alpha PeR}} erfc\left[\frac{X}{2}\sqrt{\frac{PeR}{t}} + \sqrt{\left(\frac{Pe}{4R} - D_\alpha\right)t} \right] \right\}. \tag{74}$$

For $C_0(t)$ given by (55), it can be readily shown that

$$C_m(t,X) = \hat{C_m}(t,X) - \hat{C_m}(t-t_0,X) H(t-t_0). \tag{75}$$

Obviously, in this case:

$$C_i(t,X) = k_a C_m(t,X) \text{ and } Q_{im} = k_a \left[\frac{\partial C_m}{\partial t} - D_\alpha C_m \right], \tag{76}$$

where k_a is the parameter used in Equation (38), which defines the rate of bacteria capture in the fluid phase.

(b) Adsorption-desorption model, which accounts for the growth of bacteria population

In this case, $k(t)$ is defined by the expression (39). The Laplace transform of this function can be easily calculated:

$$\overline{k}(S) = K_i \frac{1}{S - (D_\alpha - K_m)}, \tag{77}$$

where $K_i = k_i \tau^*$, $K_m = k_m \tau^*$.

Function $g(S)$ will have the following form: $g(S) = (S - D_a)\left[1 + K_i \frac{1}{S-(D_\alpha - K_m)}\right]$ and, therefore:

$$\overline{C_\infty}(S,X) = \frac{1}{S} e^{-X(S-D_a) - XK_i e^{\frac{XK_i K_m}{S-(D_\alpha - K_m)}}}. \tag{78}$$

Applying the inverse Laplace transform, leads to the following solution:

$$C_\infty(t,X) = e^{-X(K_i - D_a)} \left[I_0\left(2\sqrt{XK_i K_m (t-X)}\right) e^{-X(K_m - D_a)(t-X)} + (K_m - D_a) \int_0^{t-X} I_0\left(2\sqrt{XK_i K_m \tau}\right) e^{-X(K_m - D_a)\tau} d\tau \right] H(t-X), \tag{79}$$

where $I_0(X)$ is the modified Bessel function of zero order.

Substituting this expression into the Formula (70), yields:

$$\hat{C_m}(t,X) = \frac{X}{2}\sqrt{\frac{Pe}{\pi t}} \int_0^1 e^{\frac{Pe}{2}X - \frac{X^2 Pe}{4(1-\xi)t} - (\frac{Pet}{4} + t(K_i - D_\alpha))(1-\xi)} \frac{V(t,\xi)}{\sqrt{(1-\xi)^3}} d\xi, \tag{80}$$

where $V(t,\xi) = I_0\left(2t\sqrt{\xi K_i K_m(1-\xi)}\right)e^{-t(K_m-D_a)\xi} + (K_m - D_a)t\int_0^\xi I_0\left(2t\sqrt{(1-\xi)K_i K_m \tau}\right)$ $e^{-t(K_m-D_a)\tau}d\tau$.

Introducing the auxiliary function $G(\tau,\xi,t) = I_0\left(2t\sqrt{K_i K_m(1-\xi)\xi\tau}\right)e^{-t\xi(K_m-D_a)}$ and denoting $B = \frac{Pe}{4} - K_f - D_\alpha$, we can rewrite Equation (80) in a more compact form:

$$\hat{C_m}(t,X) = \frac{X}{2}\sqrt{\frac{Pe}{\pi t}}\int_0^1 e^{\frac{Pe}{2}X - \frac{X^2 Pe}{4(1-\xi)t} - Bt(1-\xi)}\ \frac{V(t,\xi)}{\sqrt{(1-\xi)^3}}d\xi, \tag{81}$$

where $V(t,\xi) = G(1,\xi,t) + (K_m - D_a)t\xi\int_0^1 G(\tau,\xi,t)d\tau$.

For $C_0(t)$ given by (55), it can be readily shown that:

$$C_m(t,X) = \hat{C_m}(t,X) - \hat{C_m}(t-t_0,X)H(t-t_0). \tag{82}$$

Expressions for $C_i(t,X)$ and Q_{im} are defined by the Formulae (51) and (52), where $\hat{C_m}(t,X)$ is given by the Formula (81).

(c) Model of anomalous dispersion, which accounts for bacteria growth

In this case, the expression for $g(S)$ is given by (65) and, therefore, in Laplace transforms we have:

$$\overline{C_\infty}(S,X) = \frac{1}{S}\,e^{-\frac{X}{K_\alpha}(S-D_a)^\alpha}. \tag{83}$$

Applying to the latter equation the inverse Laplace transform, yields:

$$C_\infty(t,X) = \frac{1}{\pi}\int_0^\infty \frac{1-e^{-(\xi-D_a)t}}{(\xi-D_a)}e^{-\frac{X}{B_a}\xi^\alpha\cos(\pi\alpha)}\sin\left[\frac{X}{B_a}\xi^\alpha\sin(\pi\alpha)\right]d\xi. \tag{84}$$

Finally, substituting expression (84) into the Formula (70), we obtain the following solution:

$$\hat{C_m}(t,X) = \frac{X}{2}\sqrt{\frac{Pe}{\pi}}e^{\frac{Pe}{2}X}\int_0^\infty e^{-\frac{Pe}{2}\left(\frac{X^2}{2z}+z\right)}C_\infty(t,z)\frac{1}{\sqrt{z^3}}dz. \tag{85}$$

Note that, if in the latter solution we assume that $K_\alpha = 1/R$, $K_\beta = 1$, $\beta = \alpha = 1$, then expressions (84) and (85) provide the solution of the model (a), as a particular case. Formulae (82), (84) and (85) define the concentration of bacteria in the fluid phase within the porous medium. Using these solutions, the values of $C_i(t,X)$ and Q_{im} can be readily obtained from the Formulae (51) and (52).

4. Comparison of Mathematical Models (a), (b), and (c) with Experimentally Obtained Data

Let us consider the situation when bacteria are in non-active state, so that the rate of bacteria growth $D_a = 0$ and there is no bacteria capture. In this case, all three models provide the same solution for bacteria concentration in liquid phase. From Equation (74), assuming there $D_a = 0$ and $K = 0$, we obtain:

$$\hat{C_m}(t,X) = e^{\frac{Pe}{2}X}\frac{1}{2}\left\{e^{-\frac{Pe}{2}X}erfc\left[\frac{X}{2}\sqrt{\frac{PeR}{t}} - \sqrt{\left(\frac{Pet}{4}\right)}\right] + e^{\frac{XPe}{2}}erfc\left[\frac{X}{2}\sqrt{\frac{Pe}{t}} + \sqrt{t\frac{Pe}{4}}\right]\right\}. \tag{86}$$

Hence,

$$C_m(t,X) = \hat{C_m}(t,X) - \hat{C_m}(t-t_0,X)H(t-t_0) \tag{87}$$

and, correspondingly, $C_i(t,X) = 0$ and $Q_{im} = 0$.

Figure 2 illustrates the results of computations by the Formulae (86) and (87) (solid lines) and experimental data (dots) obtained for non-active bacteria. It is obvious that the traditional advection–dispersion equation provides a sufficiently effective instrument for modeling the behavior of non-active bacteria.

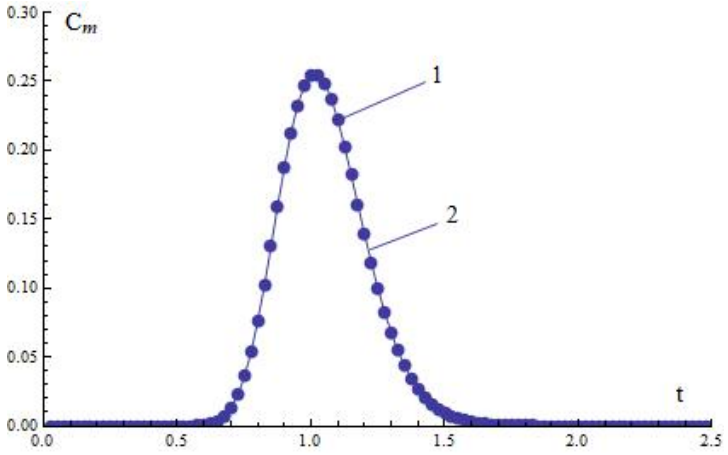

Figure 2. Non-active bacteria migration. Mathematical model (a) which is based on conventional advection–dispersion equations (2—solid line), experimental data (1—dots) measured at low temperatures when bacteria are non-active.

Now, let us consider the situation when the injection of active bacteria in the porous medium takes place with growth rate $D_a = 0.14$. Figure 3 contains the results of computation by model (a) that accounts for adsorption (solid line) and experimental data for the active bacteria (dots). In the computations presented in Figure 3, it is assumed that retardation parameter R is equal to 1 ($k_a = 0$). It corresponds to the situation when concentration of bacteria in immobile state is equal to 0, i.e., there is no capture of bacteria by the porous matrix. In this case, as it is illustrated in the figure, the maximal computed values of concentration are greater than experimentally measured values. It proves that the conventional model does not provide the proper description of the active bacteria migration. If the coefficient k_a is not equal to 0 (Figure 4), then the greater value of coefficient k_a will model the situation when some bacteria in the fluid phase will be captured by the porous matrix and will be transferred to the colony of immobile bacteria. Obviously, in this case the maximal concentration of the mobile bacteria will decline with growth of k_a. On the other hand, the increase of k_a will significantly affect the retardation, which leads to translation of the computed curve to the right from the experimentally obtained values. This discrepancy of the computed and experimental data (Figures 3 and 4) occurs due to the limitations of the model (a), which accounts for capture of the mobile bacteria only. In reality, the process of mobile bacteria capture should be accompanied by detachment of the immobile bacteria from immobile mass and transition them to the mobile population.

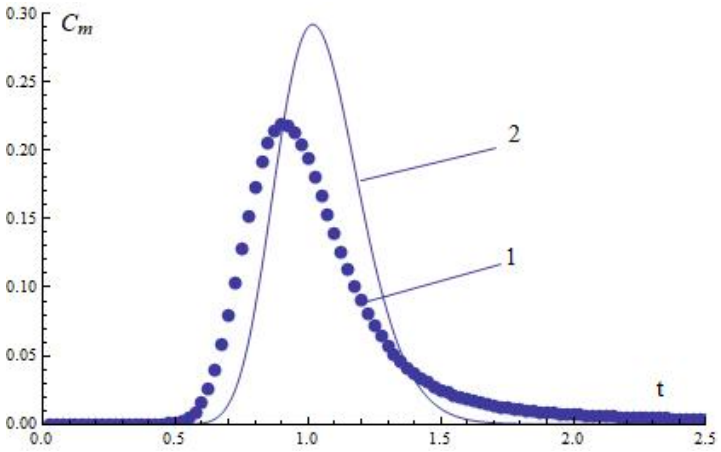

Figure 3. Active bacteria migration. Mathematical model (a) which is based on conventional advection–dispersion equations (2—solid line), experimental data (1—dots) measured at high temperatures when bacteria are active, and bacteria reproduction takes place. ($D_a = 0.14$, $Pe = 80$, $X = 1$, $k_a = 0$).

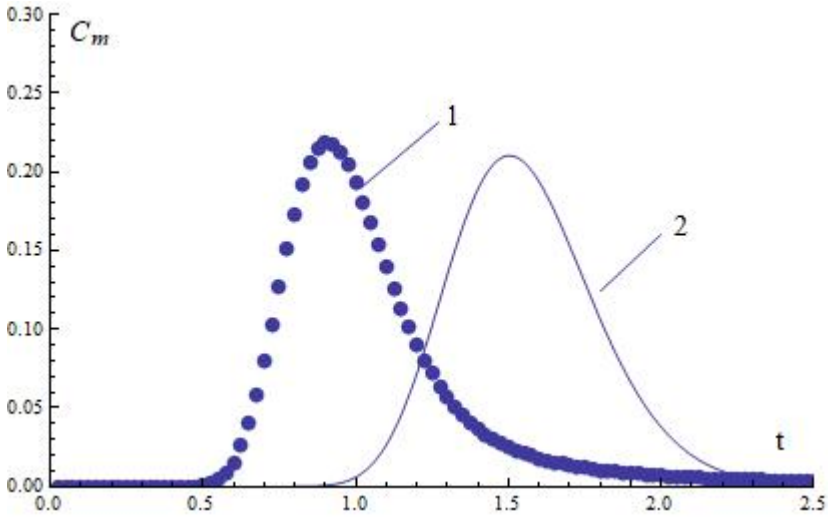

Figure 4. Active bacteria migration. Mathematical model (a) which is based on conventional advection–dispersion equations (2—solid line), experimental data (1—dots) measured at high temperatures when bacteria are active, and bacteria reproduction takes place. ($D_a = 0.14$, $Pe = 80$, $X = 1$, $k_a = 0.5$).

Figure 5 illustrates the results of computation obtained from model (b) based on kinetics of the first order. Obviously, model (b) provides the better description of the bacteria behavior, since it accounts for both capture of the mobile bacteria by the porous matrix and avulsion of the immobile (trapped by the porous matrix) bacteria by the fluid flow. However, as can be seen in Figure 5, the computed curve is substantially translated to the right from the experimental data. Our numerical experiments with the first order kinetic equation for adsorption–desorption process also indicates that this approach does not provide the adequate description of the transport of the active growing bacteria and matching with the experimental data is rather poor. All these attempts were unsuccessful, since the theoretically obtained curve could not be shifted to the left by variation of the controlling parameters. So, our attempts to attain the better agreement with experiments by choosing different values of constant parameters did not improve the mismatch of computed and experimental results depicted in Figure 5. For example, increasing of the value of the parameter K_m leads to the reduction of the number of immobile bacteria and, consequently, to the growth of the mobile bacteria in a fluid phase C_m. This behavior is understandable, since the higher values of K_m correspond to enhancing the mechanisms of avulsion of bacteria by the fluid flow. It is interesting to note that the slight increments of K_m lead to the increase of C_m mostly at the tail region of the curve, where the overall flux of interaction between the mobile bacteria and captured bacteria becomes negative. The further increment of K_m leads to the reduction of immobile bacteria C_i and to decrease of the flux Q_{im}, which causes the growth of the maximal value of C_m. These features of the model are illustrated in Figures 6 and 7. The poor agreement of computed and experimental results implies that the mobile–immobile bacteria exchange is more complex than suggested by the model (b), which is based on the conventional advection–dispersion equation and kinetics of the first order.

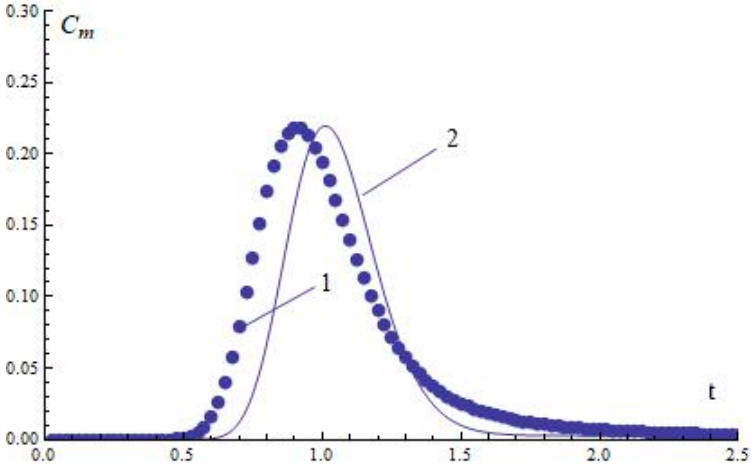

Figure 5. Active bacteria migration. Mathematical model (b) which is based on conventional advection–dispersion equations supplemented by kinetics of the first order (solid line—2), experimental data (dots—1) measured at high temperatures when bacteria are active and bacteria reproduction takes place.

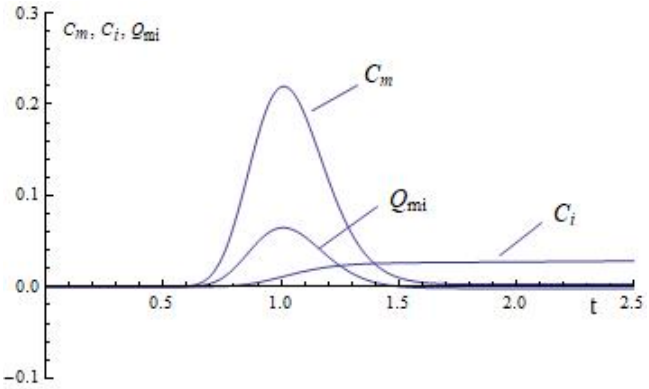

Figure 6. Temporal variations of C_m, C_i, Q_{mi} computed by model (b) for $K_m = 0.1$; $Pe = 80$; $t_0 = 0.1$; $K_i = 0.3$; $x = 1$; $\alpha = \beta = 1$; $D_a = 0.14$.

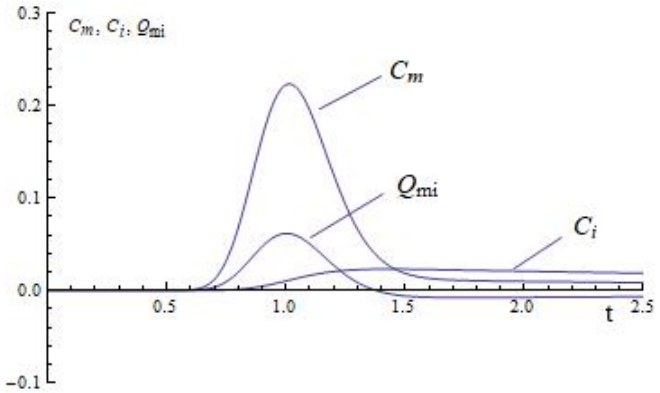

Figure 7. Temporal variations of C_m, C_i, Q_{mi} computed by model (b) for $K_m = 0.5$; $Pe = 80$; $t_0 = 0.1$; $K_i = 0.3$; $x = 1$; $\alpha = \beta = 1$; $D_a = 0.14$.

Results of computations based on the model (c) are depicted in Figure 8. The initial values of parameters for these computations are determined by the experimental set-up, whereas the values of parameters α_0 and B_0 were properly selected to calibrate the model in order to attain the agreement with experimental data. Obviously, model (c) provides rather good agreement of computed and experimentally obtained results. So, accounting

for the effects of anomalous dispersion by incorporating into the model fractional differential equations, allows us to calibrate the model and attain the perfect agreement with experimental data. We can use this model for description of the alive bacteria migration in the porous medium, which accounts for bacteria capture and detachment, clogging and de-clogging of pores by the growing reproductive bacteria carried by the flow of the liquid nutrient within the porous medium. Figure 9 illustrates the effect of initial concentration on bacteria behavior using the same model (c). It can be readily seen that the greater values of initial concentration C_0 amplify the anomalous character of bacteria dispersion. This happens due to the intensification of bacteria capture, which leads to the decrease of the non-dimensional bacteria concentration in liquid phase (mobile bacteria). Furthermore, the capture intensification leads to the slight shift of the calculated curve towards the origin of the Cartesian system of coordinates. This behavior of the bacteria in the liquid nutrient agrees with experimental findings.

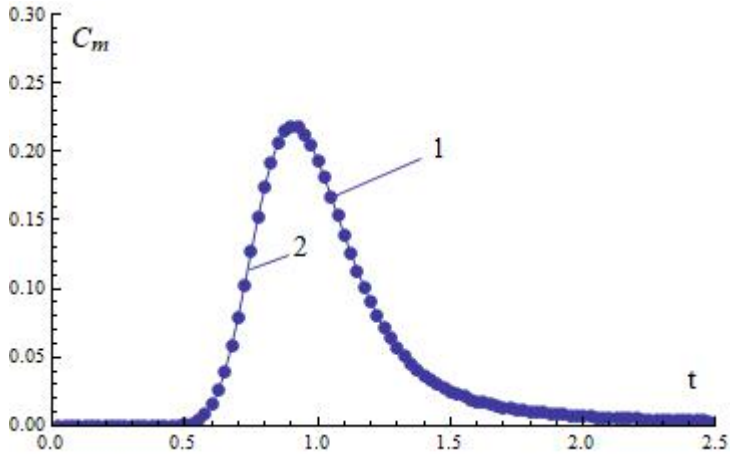

Figure 8. Active bacteria migration. Computations were made by the mathematical model (c), which is based on fractional differential equation and accounts for anomalous dispersion supplemented by kinetics of the first order (2—solid line). Experimental data (1—dots) measured at high temperatures when bacteria are active, and bacteria reproduction takes place.

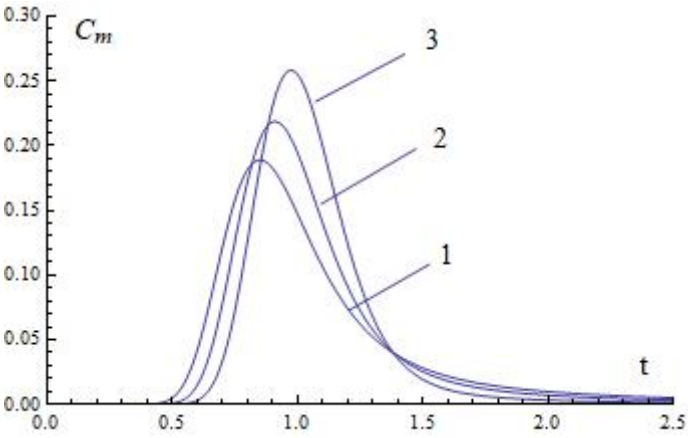

Figure 9. Concentration C_m obtained by mathematical model (c), which is based on fractional differential equation and accounts for anomalous dispersion, computed for different values of initial concentration c_0. Computations are done for the following values of controlling parameters: 1—$\alpha = 0.92$, $c_0 = 1$; 2—$\alpha = 0.95$, $c_0 = 0.58$; 3—$\alpha = 0.98$, $c_0 = 0.22$.

Figure 10 illustrates the dynamics of the bacteria concentrations in the liquid flow C_m, in the immobile state C_i and also variation of function Q_{im}, which characterizes the interaction between the mobile and immobile bacteria. It was assumed that $\beta = \alpha$, $K_\alpha = 1.2K_\beta$,

whereas the other constants are the same as in previous computations. As it can be seen in Figure 10, at the beginning of the process an active capture of bacteria from the solution is taking place. This process is significantly more intense than in the case of the conventional model (b) based on kinetics of the first order. Obviously, accounting for the anomalous dispersion phenomenon and incorporating the fractional derivatives in the model, allows us to describe the complex behavior of the alive bacteria, which cannot be correctly described by the kinetics of the first order only.

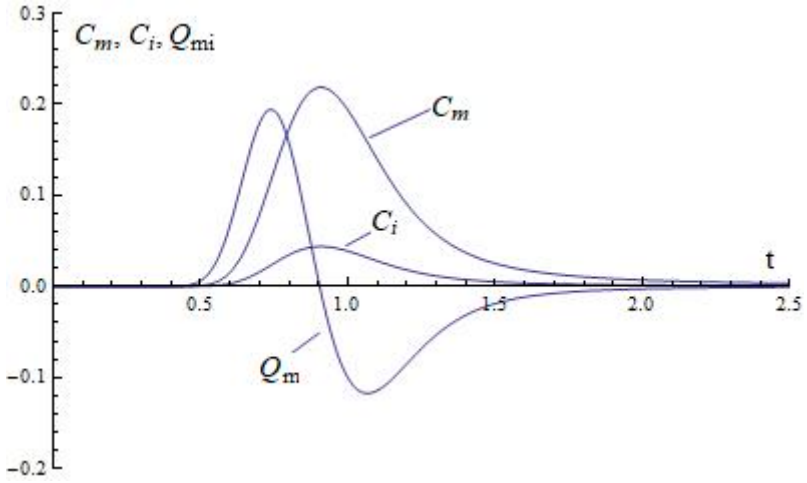

Figure 10. Temporal variation of the functions C_m, C_i, Q_{mi} obtained by mathematical model (c) which is based on fractional differential equation and computed for $\alpha = 0.95$, $c_0 = 0.58$.

5. Conclusions

The numerical results of the bacteria migration based on conventional dispersion-advection equations appeared to be in perfect agreement with results of laboratory experiments for the non-active, resting bacteria (due to low temperatures of liquid nutrient when bacteria are non-active).

However, if bacteria are in an active stage capable of growth and reproduction, the traditional model, even being supplemented with the terms that account for the bacteria growth, does not provide the adequate description of the bacteria behavior observed in the experiments. For the growing bacteria, the experimentally obtained curve of bacteria concentration is shifted to the left from the concentration curve for the resting bacteria. We attempted to use different conventional models based on traditional advection-dispersion equation with incorporated the first order kinetic equations, which account for the adsorption-desorption process (i.e., trapping and detaching bacteria) and tried to calibrate these mathematical models by choosing different values of the controlling parameters. All our numerical computations for these models indicate that this approach does not provide an adequate description of the transport of the active growing bacteria in the nutrient solution. It occurred that the theoretically obtained curves could not be shifted to the left along the x-axis by variation of the controlling parameters.

Our analysis shows that the mathematical model, which is based on fractional advection–dispersion equation and incorporates a convolution equation for modeling the mobile–immobile bacteria interaction, can be very promising tools for solving the problems of bacteria migration and associated problems of bioremediation of polluted soils.

Furthermore, more general models of bacteria migration can be developed by introducing different forms of the coefficients of bacteria distribution, k, within the convolution equation that models the bacteria interaction. These new mathematical models can be effectively used for describing the behavior of the various types of bacteria within the different porous media and nutrient solutions.

Author Contributions: Conceptualization, S.F.; Methodology, V.C.; Validation, V.C.; Formal analysis, V.C.; Investigation, S.F.; Writing—original draft, S.F. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: No new data were created or analyzed in this study. Data sharing is not applicable to this article.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Simomura, D.; Suto, K.; Inoue, C.; Chida, T. Behaviors of Bacteria in Porous Materials under the Growth Condition. In Proceedings of the 2002 International Symposium on Subsurface Microbiology, Copenhagen, Denmark, 8–13 September 2002; pp. 58–59.
2. Yang, Y.-G.; Niibori, Y.; Inoue, C.; Chida, T. Modeling of Growth and Transport of Bacteria in Porous Media. In Proceedings of the International Conference on Applied Modeling and Simulation, IASTED International Conference, AMS'99, Cairns, QLD, Australia, 1–3 September 1999; pp. 589–594.
3. Ryan, J.N.; Elimelech, M. Colloid mobilization and transport in groundwater. *Colloids Surf. A Physicochem. Eng. Asp.* **1996**, *107*, 1–56. [CrossRef]
4. Kretzschmar, R.; Barmettler, K.; Grolimund, D.; Yan, Y.D.; Borkovec, M.; Sticher, H. Experimental determination of colloid deposition rates and collision efficiencies in natural porous media. *Water Resour. Res.* **1997**, *33*, 1129–1137. [CrossRef]
5. Harter, T.; Wagner, S.; Atwill, E.R. Colloid Transport and Filtration of Cryptosporidium parvum in Sandy Soils and Aquifer Sediments. *Environ. Sci. Technol.* **2000**, *34*, 62–70. [CrossRef]
6. Harvey, R.W.; Garabedian, S.P. Use of Colloid Filtration Theory in Modeling Movement of Bacteria through a Contaminated Sandy Aquifer. *Environ. Sci. Technol.* **1991**, *25*, 178–185. [CrossRef]
7. Johnson, W.P.; Blue, K.A.; Logan, B.E.; Arnold, R.G. Modeling bacterial detachment during transport through porous media as a resident-time-dependent process. *Water Resour. Res.* **1995**, *31*, 2649–2658. [CrossRef]
8. Jin, Y.; Chu, Y.; Li, Y. Virus removal and transport in saturated and unsaturated sand columns. *J. Contam. Hydrol.* **2000**, *43*, 111–128. [CrossRef]
9. Corapcioglu, M.Y.; Kim, S. Modeling Facilitated Contaminant Transport by Mobile Bacteria. *Water Resour. Res.* **1995**, *31*, 2639–2647. [CrossRef]
10. Sim, Y.; Chrysikopoulos, C.V. Virus transport in unsaturated porous media. *Water Resour. Res.* **2000**, *36*, 173–179. [CrossRef]
11. Scheibe, T.D.; Wood, B.D. A particle-based model of size or anion exclusion with application to microbial transport in Porous Media. *Water Resour. Res.* **2003**, *39*, 1080. [CrossRef]
12. Dentz, M.; Berkowitz, B. Transport behavior of a passive solute in continuous time random walks and multirate mass transfer. *Water Resour.* **2003**, *39*, 1111. [CrossRef]
13. Metzler, R.; Compte, A. Generalized diffusion–advection schemes and dispersive sedimentation: A fractional approach. *J. Phys. Chem. B* **2000**, *104*, 3858–3865. [CrossRef]
14. Metzler, R.; Klafter, J. The random walks guide to anomalous diffusion: A fractional dynamics approach. *Phys. Rep.* **2000**, *339*, 1–77. [CrossRef]
15. Barkai, E.; Metzler, R.; Klafter, J. From continuous time random walks to the fractional Fokker–Planck equation. *Phys. Rev. E* **2000**, *61*, 132–138. [CrossRef]
16. Meerschaert, M.M.; Benson, D.A.; Scheffler, H.-P. Stochastic solution of space–time fractional diffusion equations. *Phys. Rev. E* **2002**, *65*, 041103. [CrossRef]
17. Benson, D.A.; Wheatcraft, S.W.; Meerschaert, M.M. Application of a fractional advection–dispersion equation. *Water Resour. Res.* **2000**, *36*, 1403–1412. [CrossRef]
18. Herrick, M.; Benson, D.; Meerschaert, M.; McCall, K. Hydraulic conductivity, velocity, and the order of the fractional dispersion derivative in a highly heterogeneous system. *Water Resour. Res.* **2002**, *38*, 1227–1239. [CrossRef]
19. Benson, D.A.; Schumer, R.; Meerschaert, M.M.; Wheatcraft, S.W. Fractional dispersion, Levy motion, and the MADE tracer tests. *Transp. Porous Media* **2001**, *42*, 211–240. [CrossRef]
20. Berkowitz, B. Characterizing flow and transport in fractured geological media: A review. *Adv. Water Resour.* **2002**, *25*, 861–884. [CrossRef]
21. Berkowitz, B.; Scher, H. Anomalous transport in random fracture networks. *Phys. Rev. Lett.* **1997**, *79*, 4038–4041. [CrossRef]
22. Berkowitz, B.; Scher, H. Theory of anomalous chemical transport in random fracture networks. *Phys. Rev. E* **1998**, *57*, 5858–5869. [CrossRef]
23. Berkowitz, B.; Scher, H.; Silliman, S.E. Anomalous transport in laboratory scale, heterogeneous porous media. *Water Resour. Res.* **2000**, *36*, 149–158. [CrossRef]
24. Chugunov, V.; Fomin, S. Effect of adsorption, radioactive decay and fractal structure of matrix on solute transport in fracture. *Phil. Trans. R. Soc. A* **2020**, *378*, 20190283. [CrossRef] [PubMed]

25. Fomin, S.; Chugunov, V.; Hashida, T. Non-Fickian mass transport in fractured porous media. *Adv. Water Resour.* **2011**, *34*, 205–214. [CrossRef]
26. Fomin, S.; Chugunov, V.; Hashida, T. Application of fractional differential equations for modeling the anomalous diffusion of contaminant from fracture into porous rock matrix with bordering alteration zone. *Transp. Porous Media* **2010**, *81*, 187–205. [CrossRef]
27. Fomin, S.; Chugunov, V.; Hashida, T. The effect of non-Fickian diffusion into surrounding rocks on contaminant transport in fractured porous aquifer. *Proc. R. Soc. A* **2005**, *461*, 2923–2939. [CrossRef]
28. Thullner, M.; Schroth, M.H.; Zeyer, J.; Kinzelbach, W. Modeling of a microbial growth experiment with bio clogging in a two-dimensional saturated porous media flow field. *J. Contam. Hydrol.* **2004**, *70*, 37–62. [CrossRef]
29. Kim, S.; Corapcioglu, M.Y. A Kinetic Approach to Modeling Mobile Bacteria-Facilitated Groundwater Contaminant Transport. *Water Resour. Res.* **1996**, *32*, 321–331. [CrossRef]
30. Samko, S.G.; Kilbas, A.A.; Marichev, O.I. *Fractional Integrals and Derivatives: Theory and Applications*; Gordon and Breach: London, UK, 1993.
31. Tang, D.H.; Frind, E.O.; Sudicky, E.A. Contaminant transport in fractured porous media: Analytical solution for a single fracture. *Water Resour. Res.* **1981**, *17*, 555–564. [CrossRef]