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MODELLING GROUNDWATER FLOW IN AQUIFERS

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Abstract

An aquifer is a body of saturated rock, which is filled with moving water. It is a natural filter that traps sediment and other particles and provides natural purification of the ground water flow. In this work we used the $1D$ advection-diffusion equation to model the groundwater flow. For modeling the contaminants in the aquifer we consider injection of three types of bacteria at the boundary of the region. To solve the partial differential equation we use the Crank-Nicolson and sixth order Gauss method.

1   Introduction

An aquifer is an underground layer of permeable water-bearing rock, which fills with water from rain that drains into the ground. In some areas, the water passes through the soil on top of the aquifer, and in others, it enters through joints and cracks in rocks. The water moves downward until it meets less permeable rock. Aquifers act as reservoirs for groundwater. Because aquifers fill with water that drains from the surface of the Earth, they can be contaminated by any chemical or toxic substance found on the surface. Once polluted the groundwater can cause huge damages to health of people in contact and nature. Therefore it is quite important to model groundwater transport to understand how long a contaminant plume will grow, remain stable or shrink, as well as how easy or difficult it will be to remediate.
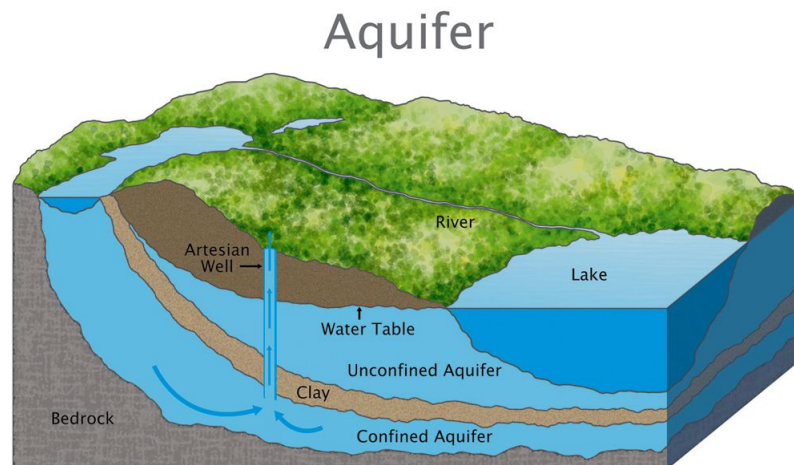
Figure 1: Solute-site-adsorbed particle reaction

2   Problem formulation

2.1   The model

In any fixed volume, the fraction of space, called the pore space, available to the water is assumed to be ω, which is called the porosity of the medium, where $0 < \omega < 1$. Let $C(x,t)$ be the concentration of the chemical or biological tracer in the liquid measured in mass per unit of volume of water and let $J(x,t)$ denote the flux, rate per unit area that the contaminant mass crosses a cross-section A at x. We further assume that the tracer is created or destroyed with a rate of $F(x,t)$, measured in mass per unit volume of porous medium, per unit time. Mass balance states that the rate of change of the total mass in an arbitrary section of the medium must be equal to the net rate that mass flows into the section through its boundaries plus the rate that mass is created or destroyed within the section. For an arbitrary interval (a,b), where $a < b$:

$$\frac{d}{dt}\int_a^b C(x,t)\ \omega A dx = J(a,t)A - J(b,t)A + \int_a^b F(x,t)A dx$$

$$\int_a^b \left[\omega\frac{dC(x,t)}{dt} + \frac{dJ(x,t)}{dx} - F(x,t)\right]A dx = 0$$

$$\implies \omega\ \frac{dC(x,t)}{dt} = -\frac{dJ(x,t)}{dx} + F(x,t).$$

We calculate the flux as the sum of three terms caused by advection, diffusion and dispersion.

$$J = J^{(A)} + J^{(M)} + J^{(D)}.$$

Particles are being carried by the bulk motion of the fluid so we define advective flux $J^{(A)}$ by

$$J^{(A)} = V\ C(x,t).$$

To calculate the flux caused by diffusion and dispersion we will use Fick's law which states that the magnitude of the flux is proportional to the concentration gradient.

$$J^{(M)} = -\omega\ D^{(M)}\ \frac{\partial C(x,t)}{\partial x}$$

$$J^{(D)} = -\omega\ D^{(D)}\ \frac{\partial C(x,t)}{\partial x}.$$

Where $D^{(M)}$ and $D^{(D)}$ are effective molecular diffusion and dispersion coefficients respectively. If we define the hydrodynamic dispersion coefficient $D = D^{(M)} + D^{(D)}$,

putting $v = \frac{V}{\omega}$ and placing it into our original equation, we get:

$$\omega \, \frac{\partial C(x,t)}{\partial t} = -V \, \frac{\partial C(x,t)}{\partial x} + \omega \, D \, \frac{\partial^2 C(x,t)}{\partial x^2} + F(x,t) \ \ / : \omega$$

$$\frac{\partial C(x,t)}{\partial t} = -v \, \frac{\partial C(x,t)}{\partial x} + D \, \frac{\partial^2 C(x,t)}{\partial x^2} + \omega^{-1} F(x,t).$$

Due to the fact that dispersion is present in moving fluids, it has been an important exercise to determine how the dispersion coefficient depends on the velocity of the flow. We assume linear constitutive relationship

$$D^{(D)} = \alpha_L |V|,$$

where α_L is the longitudinal dispersivity. In the transverse direction of the flow, the dispersion coefficient is taken to be $\alpha_T |V|$, where the traverse dispersivity $\alpha_T |V|$ is roughly an order of magnitude smaller that the longitudinal dispersivity. If we make these assumptions, the hydrodynamic dispersion coefficient in one-dimensional flow can be written as

$$D = D^{(M)} + \alpha_L V.$$

2.2 Adsorption

Adsorption is a process that causes the tracer, or solute, to adhere to the surface of the solid porous fabric and thus become immobile. Let $S = S(x,t)$ denote the amount of solute adsorbed. The mass of soil per unit volume of porous medium is $\rho(1 - \omega)$ and therefore the rate of adsorption is given by

$$F(x,t) = -\rho(1 - \omega) \, \frac{\partial S(x,t)}{\partial t}.$$

We consider the case where the adsorption process is a reversible chemical reaction where one adsortpion site on the solid reacts with a solute particle in a strict sense. The law of mass action states that the reaction rate is

$$r = k_f \sigma C - k_b S,$$

where k_f, k_b are the forward and the backward rate constants, respectively, and σ denotes the density of adsorption sites on the immobile solid fabric. With the assumption that the reaction equilibrates on a fast time scale compared to that of dispersion and advection, then the reaction is always in equilibrium (r $\equiv$ 0), or

$$S = K.C,$$

where $K = \frac{k_f \sigma}{k_b}$.

Substituting F in our equating we finally get

$$\frac{\partial C(x,t)}{\partial t} = -v \frac{\partial C(x,t)}{\partial x} + D \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\rho(1-\omega)}{\omega} K \frac{\partial C(x,t)}{\partial t}$$

(1)

$$R \frac{\partial C(x,t)}{\partial t} = -V \frac{\partial C(x,t)}{\partial x} + D \frac{\partial^2 C(x,t)}{\partial x^2},$$
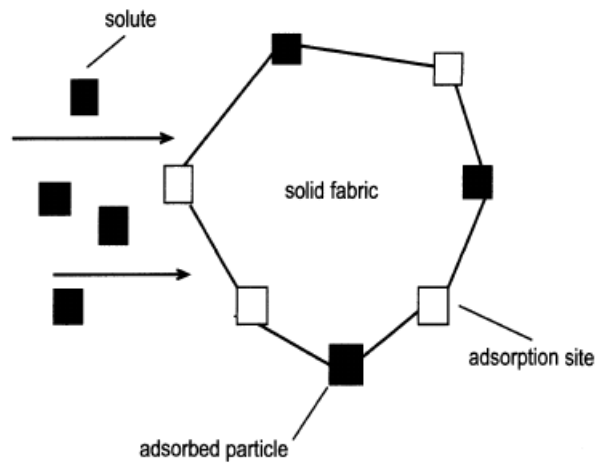
where $R = 1 + \frac{\rho(1-\omega)}{\omega} K$.

Figure 2: Solute-site-adsorbed particle reaction

2.3 Different contaminants

Depending on the type of the tracer, we can adjust the particle change rate $F(x,t)$ in (**??**). First, we consider a radioactive tracer with the decay rate λ. The change rate is $F(x,t) = -\lambda \, \omega C(x,t)$. The equation then becomes

$$R\frac{\partial C(x,t)}{\partial t} = -v \frac{\partial C(x,t)}{\partial x} + D \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t).$$

Another tracer we consider is a biological species with logistic growth rate $F(x,t) = rC(1 - \frac{C}{K})$, where r is the growth constant and K is the carrying capacity, then

$$R\frac{\partial C(x,t)}{\partial t} = -v \frac{\partial C(x,t)}{\partial x} + D \frac{\partial^2 C(x,t)}{\partial x^2} + \frac{r}{\omega} C(x,t) \left(1 - \frac{C(x,t)}{K}\right).$$

Instead of considering the source term $F(x,t)$ in the equation, we include different types of contaminant as an injection at a part of the boundary of the region (the aquifer).

Therefore, the first equation becomes

$$\frac{\partial C(x,t)}{\partial t} = -v\,\frac{\partial C(x,t)}{\partial x} + D\,\frac{\partial^2 C(x,t)}{\partial x^2} \tag{2}$$

with the boundary conditions set to be

$$C(0,t) = g(t)$$

$$\frac{dg(t)}{dt} = -\omega\lambda g(t)$$

$$C(\infty,t) = 0$$

.

Analogously, the second equation becomes

$$C(0,t) = g(t)$$

$$\frac{dg(t)}{dt} = -\frac{r}{\omega}\,g(t)\left(1 - \frac{g(t)}{K}\right)$$

$$C(\infty,t) = 0.$$

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2.4 Data

The effective diffusion coefficient varies significantly depending on the nature of the porous medium and the species diffusing itself. Bulk diffusion coefficients for some ions in water are given below; these would then have to be scaled to account for the presence of the porous medium.

The longitudinal dispesivity reflects the spatial variation in hydraulic conductivity, which can be described by use of geostatical tool. These general findings are still valid although additional studies have refined the understanding of the processes and the database with high quality observations. Some examples of findings in relevant field studies are provided here.

Ion	$D^M (10^{-6} cm^2/s)$
H^+	93.1
K^+	19.6
Na^+	13.3
Mg^{2+}	7.05
Ca^{2+}	7.93
F^-	14.6
Cl^-	20.3
HCO_3^-	11.8
SO_4^{2-}	10.7

Table 1: Bulk diffusion coefficients for some ions.

Field site	Aquifer	Longitudinal dispersivity	Transversal dispersivity
Borden air force base	Homogeneous sandy aquifer	0.43 m	0.04 m
Cape Cod	Homogeneous sandy aquifer	0.96 m	0.0018 m
Vejan	Homogeneous sandy aquifer	0.45	0.001 m
Columbus side	Heterogeneous sand and gravel aquifer	7.5 m	Not reported
Contaminant plume with chloride	Sand and gravel aquifer	Not reported	0.1 m
Grindsted landfill	Homogenous sandry aquifer	3 m	0.05 m

Table 2: Examples of dispersivity values obtained from field tracer experiments and field observations at contaminant plumes.

The velocity of the fluid varies between 1 m/day and 1 m/year, but they are much greater through caverns.

	Average velocity (m/day)	Porosity (%)
granite	0.0001	1
shale	0.0001	3
clay	0.0002	50
flagstone	5	15
sand	20	30
gravel	300	25
limestone	variable	5

Table 3: Tipical hydrological values for sedimentary rocks

For a biological contaminant, we will observe *Vibrio natriegens*, or V. natriegens for short which is a marine bacterium commonly found in the mud around estruaries. Bacterial growth data from a V. natriegens experiment are shown in the following table. The population was measured by a spectrophotometer every 16 minutes for a total of 160 minutes.

Let us now derive the three different approaches for the contaminants in the aquifer. First, we consider radium as a contaminant. The half - life of radium ^{223}Ra is $t = 11.4$ days $= 9.85 \cdot 10^5$ s, therefore the decay rate would be

Time (min)	Population density
0	0.022
16	0.036
32	0.060
48	0.101
64	0.169
80	0.266
96	0.360
112	0.510
128	0.704
144	0.827
160	0.928

Table 4: Measurements of bacterial density taken by a spectrophotometer

$$\lambda = \frac{\ln 2}{t} = 7.037 \cdot 10^{-7} \text{ s}^{-1}$$

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Solving the ODE for the boundary condition we get

$$g(t) = C_0 e^{-\omega \lambda t}$$

For the second initial boundary value problem, the boundary condition is the logistic growth model which solution has the form

$$g(t) = \frac{K}{1 + g_0 e^{-r/\omega \ t}}$$

and is used to simulate some logistic bacterial growth inside aquifers.

By using the Gauss-Newton method to fit the three unknown parameters r, K, g_0 to the data, we get $\frac{r}{\omega} = 0.545295$, $K = 1.15237$, $g_0 = 0.0209191$.

3 Discrete Model

In practice the velocity of the water can be measured. The porosity and diffusion parameter is unknown. To understand how the aquifer behaves we discretize the equation (2) and consider different parameters.

3.1 Discretization in space

First, let us discretize the differential equation in space. There are some different methods which are useful but we apply a finite different method (FDM) to

$$R \, \frac{\partial C(x,t)}{\partial t} = -V \, \frac{\partial C(x,t)}{\partial x} + D \, \frac{\partial^2 C(x,t)}{\partial x^2}$$

We assume that a solution of (2) is four time differentiable and solve the discrete problem.

Let L be the length of the aquifer, $n \in \mathbb{N}$ the number of nodes and we define the discrete space $S := \left\{ x_i = i \cdot \frac{L}{n} \,|\, i = 0, ..., n \right\}$. We write C_i for $C(x_i)$. The second derivative of C is discretized by the standard three-point stencil

$$\frac{\partial^2 C(x,t)}{\partial x^2} \approx \frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2} \tag{3}$$

and for the advection term we apply the second order central difference

$$\frac{\partial C(x,t)}{\partial x} \approx \frac{C_{i+1} - C_{i-1}}{2\Delta x}. \tag{4}$$

We insert (3) and (4) in (2) and we get for $i = 0, ..., n$

$$R \, \frac{\partial C_i}{\partial t} = -V \, \frac{C_{i+1} - C_{i-1}}{2(\Delta x)} + D \, \frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2}. \tag{5}$$

We can write (5) for each i as the linear equation system

$$R \, \frac{\partial C}{\partial t} = -\frac{V}{2\Delta x} \, \mathbf{S} \cdot C + \frac{D}{(\Delta x)^2} \, \mathbf{A} \cdot C, \tag{6}$$

where $C = (C_i)$ and

$$\mathbf{S} = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & 2 \end{pmatrix}.$$

3.2 Discretization in time

Let $[0, T]$ be the time interval. We define $\tau > 0$ as the time step's size and $\{t_j = j \cdot \tau\}$ as the discrete time space. To discretize the time derivative we integrate (6) over (t_j, t_{j+1})

$$R \int_{t_i}^{t_{i+1}} \frac{\partial C}{\partial t} \, \mathrm{d}t = -\frac{V}{2\Delta x} \int_{t_i}^{t_{i+1}} \mathbf{S} \cdot C \, \mathrm{d}t + \frac{D}{(\Delta x)^2} \int_{t_i}^{t_{i+1}} \mathbf{A} \cdot C \, \mathrm{d}t.$$

This integral means a component-wise integral of vectors and matrices. The left hand side can be directly solved. To solve the right hand side, we apply a quadrature rule. For the trapezoidal rule an easy computation shows

$$\left(Id + \frac{\tau V}{4R\Delta x}\, \mathbf{S} - \frac{\tau D}{2R(\Delta x)^2}\, \mathbf{A}\right) \cdot C^{j+1} = \left(Id - \frac{\tau V}{4R\Delta x}\, \mathbf{S} + \frac{\tau D}{2R(\Delta x)^2}\, \mathbf{A}\right) \cdot C^{j}.$$

The is equivalent to directly apply the Crank-Nicolson Method to (2). Further, we use a six order Gauss Method to compare the results.

4   Results

In this chapter we want to discuss how the concentration of the pollution behaves when we are changing the porosity and the diffusion parameter. First of all we take a look the constant pollution flow and the bacteria growth in the aquifer as in figure 3. If we are waiting long enough the bacteria growth is modeled by approximately constant boundary conditions on the left side of the aquifer. That's why changing the parameters does not change the final result. If the pollution is in the aquifer it remains permanent. It more interesting to discuss boundary conditions of the type $g(t) = C_0 e^{-\omega \lambda t}$ which model radioactive material or other material with half-life time.

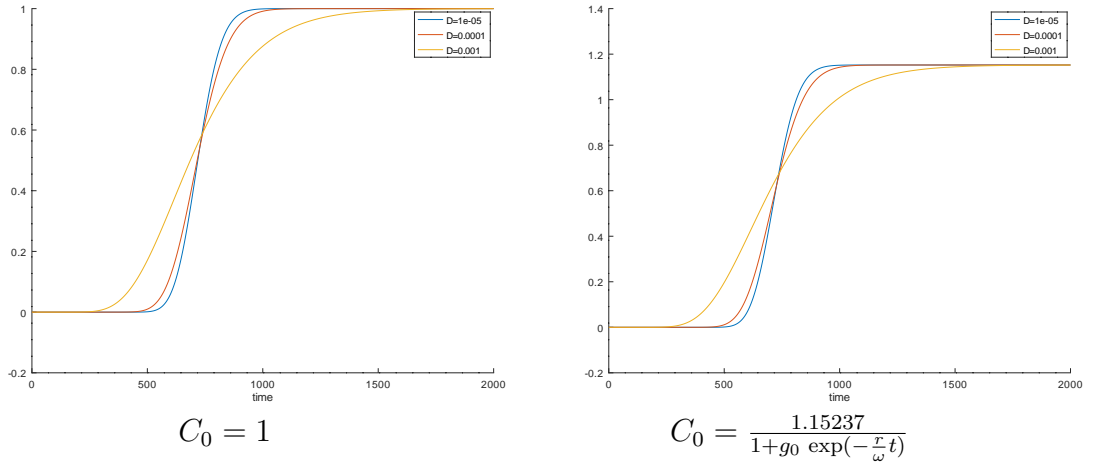$$C_0 = 1 \qquad\qquad C_0 = \frac{1.15237}{1 + g_0\, \exp(-\frac{r}{\omega}t)}$$

Figure 3: Comparison of constant pollution flow and bacteria growth

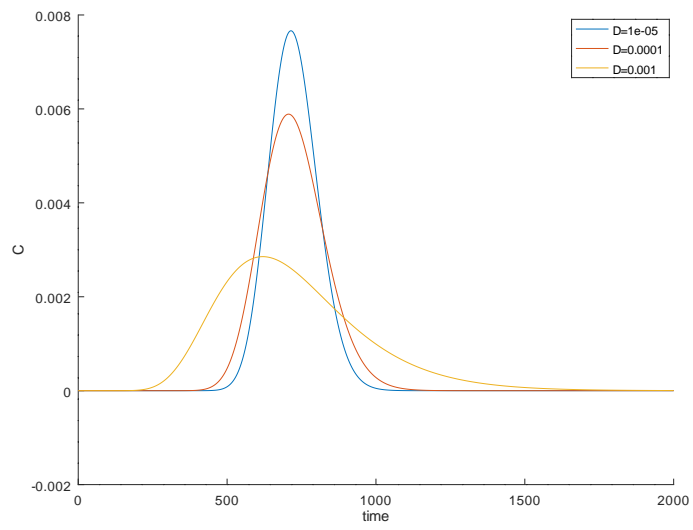Figure 4: Different diffusion parameters with boundary condition $C_0 = exp(-\frac{1}{2}t)$
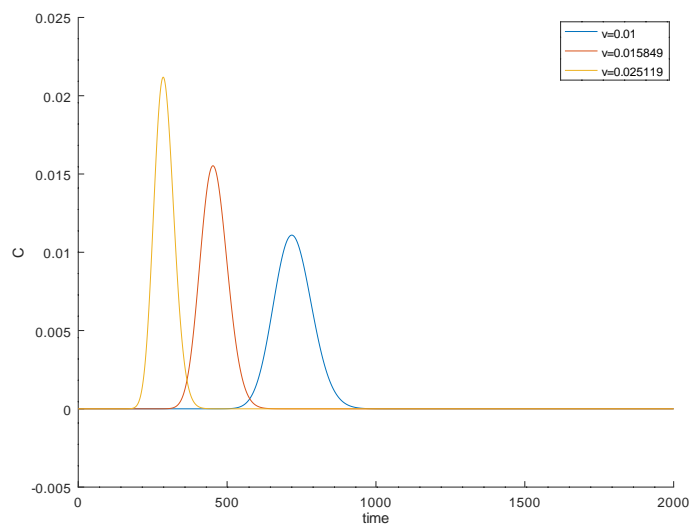

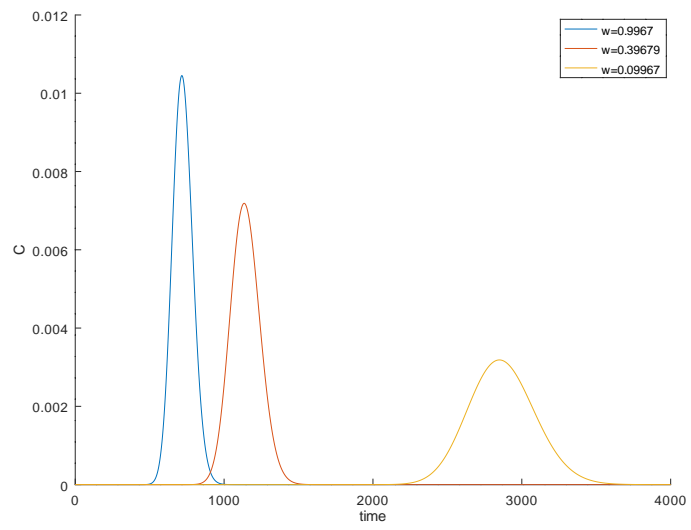Figure 5: Different velocities with boundary condition $C_0 = exp(-\frac{1}{2}t)$

Figure 6: Different porosity with boundary condition $C_0 = exp(-\frac{1}{2}t)$

5 Discussion and conclusions

Depending on the nature and scope of the study, the report ends either with the chapter "Conclusions", or two separate chapters, e.g. "Discussion" and "Conclusions". In the discussion, the author relates all of the material he or she wishes in reply to the research questions posed. Repetition with respect to the text in the report's main content should be avoided unless it is necessary. However, the discussion must be drawn up in such a way that a professional in the field can repeat the research work e.g. to check the equations, expressions, measurements, calculations or results and conclusions.

The conclusions analyze the observations and results drawn from the research, as well as examine and reflect on e.g. the compatibility of the theory and measurements, the reasons for possible differences, and summarize the conclusions drawn from the results. The need for further research and possible practical applications may also be argued here.

6 Group work dynamics

The student group should write an assessment of the group work dynamics (including both the Modeling Week time itself and the time/workload afterwards, spent on writing the report itself). In particular, you should at least answer to the following questions:

- How did you plan the work?

- How was the work distributed between the partners?

- What was beneficial or challenging about the group work?

7 Instructor's assessment

Every instructor is asked to add a brief (1–2 paragraph) summary of how the group has performed through the week, especially with respect to the problem's initial goals and the actual achievements. Here is also the place to report possible total or part-time absences of the students during the group work hours — these can be also reported by the fellow group mates.

Possible references should be included in Harvard (author and year) style.

References

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[8] Cornette JL, Ackerman RA, and Nykamp DQ, *Developing an initial model to describe bacteria growth.*, Math Insight.

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