



MATHEMATICAL MODELING OF
BIOGROUT PROCESS

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Certificate

This is to certify that the project titled *Mathematical Modeling of Biogrout Process* submitted by Chinmaya Kumar Panda, Roll No. 710CE1007, in partial fulfillment of the requirements for the award of Master of Technology Degree in Civil Engineering at NIT Rourkela, is an authentic work carried out by him under our supervision and guidance.

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Chinmaya Kumar Panda

Abstract

This project deals with the mathematical formulation of flow during grouting, specifically the Biogrout process in sand. The model takes cue from the contaminant transport model, wherein both the concentration of both the aqueous species (the reactants) and the non-aqueous species (the product that acts as the cementing material) are taken into account. The porosity is variable and thus is the hydraulic conductivity of the medium. The rate of reaction is varying as it is set to depend on the initial concentration of the reactants via a time decaying relation. The governing equations are discretized using Finite Difference. The numerical scheme is implemented in MATLAB and relevant plots are obtained.

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List of Symbols

C^{urea}	Concentration of aqueous urea (kmol/m ³)
$C^{\text{Ca}^{2+}}$	Concentration of aqueous calcium ions (kmol/m ³)
$C^{\text{NH}_4^+}$	Concentration of aqueous ammonium ions (kmol/m ³)
C^{CaCO_3}	Concentration of solid calcium carbonate (kg/m ³)
θ	Porosity
θ_0	Initial porosity
\mathbf{q}	Darcy velocity (m/s)
r	Reaction rate (kmol/m ³ /s)
t	Time(s)
v_{max}	Maximum reaction rate (kmol/m ³ /s)
t_{max}	Life span of bacteria (s)
K_m	Saturation constant (kmol/m ³)
\mathbf{D}	Hydrodynamic Dispersion Tensor(m ² /s)
α_L	Longitudinal Dispersivity(m)
m_{CaCO_3}	Molecular mass of calcium carbonate (kg/kmol)
ρ_{CaCO_3}	Density of calcium carbonate (kg/m ³)
\mathbf{k}	Intrinsic permeability (m ²)
d_m	Mean particle size of the subsurface medium (m)
μ	Dynamic viscosity of the fluid (Pa s)
p	Pressure (Pa)
g	Gravity (m/s ²)
ρ	Density of the fluid (kg/m ³)

Chapter 1

Introduction

Injection of a slurry or a liquid solution into a soil or rock formation is termed grouting. Biogrout is a technology for the in-situ strengthening of unconsolidated soil using naturally occurring microorganisms. It is a new soil reinforcement method based on microbial-induced carbonate precipitation (MICP).

First the microorganisms containing the enzyme *urease* are cultivated and are then transported to the locations by water flow where the soil is to be strengthened. A fixation fluid is injected as a next step to ensure homogenous distribution of the bacteria. This fixation fluid overtakes the weakly adsorbed bacteria and fixes strongly onto the soil skeleton. Next the reactant chemicals namely urea ($\text{CO}(\text{NH}_2)_2$) and calcium chloride (CaCl_2) are injected. To get a more homogeneous distribution of calcium carbonate over a large distance and in order to prevent crystal accumulation around the point of injection, the urea ($\text{CO}(\text{NH}_2)_2$) and calcium chloride (CaCl_2) solution are supplied only after bacterial placement. The reaction involves two steps.

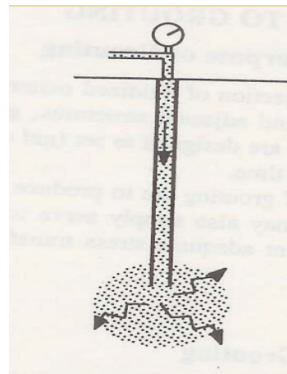
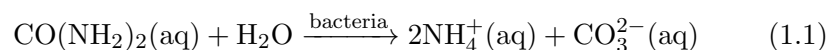


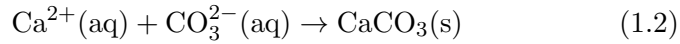
Figure 1.1: PERMEATION GROUTING

1. Hydrolysis of urea into NH_4^+ and CO_3^{2-} catalyzed by urease.

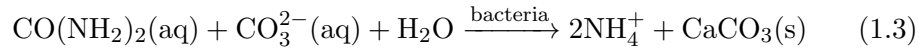


2. In the presence of CO_3^{2-} and if the solution is over-saturated The

precipitation of CaCO_3 occurs.



Combining the reaction equation for the production of carbonate,(2.1), and the reaction equation for the precipitation of calcium carbonate, (2.13), gives the overall Biogrout reaction equation:



The CaCO_3 crystals fill the void space and act as a cementing material, thus increasing the stiffness and the strength of the soil mass. As a result the porosity decreases. The decreasing porosity influences the permeability and hence affects the flow.

1.1 Objective

The objective of this project is the development of a Finite Difference model for the flow of a conservative tracer in porous media and coding for the same in MATLAB. The model simulates the permeation grouting.

1.2 Methodology

- Derivation of the relevant governing differential equations for
 - Aqueous species(the Advection-Diffusion-Reaction equation)
 - Non-aqueous species
 - Porosity
 - Flow
- Solution of the above equations by suitable numerical method (FEM/FDM) with boundary conditions typical of a grouting problem.
- MATLAB code for simulation of the model.

1.3 The Mathematical Model

The current mathematical model accounts for the following parameters:

- the concentrations of aqueous species e.g urea, calcium chloride, ammonium chloride and nonaqueous calcium carbonate, which change due to dispersion, advection and reaction;
- the density of the solution, which changes due to alteration of composition of the chemicals;

- porosity and permeability, which decrease as a result of the solid calcium carbonate precipitation;
- flow through the porous medium, which is influenced by injection, extraction and variation in density, porosity and permeability, in which the changes in the porosity and permeability are caused by the precipitation of calcium carbonate.

Chapter 2

Literature Review

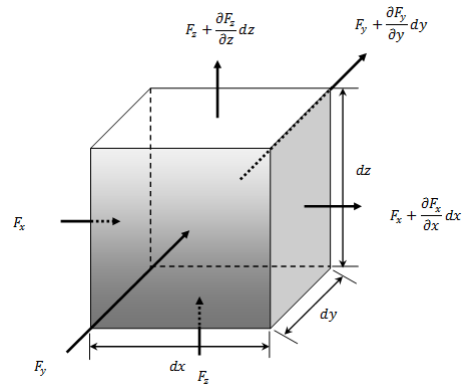
2.1 Governing Differential Equation

2.1.1 Transport of Aqueous Species

The following theories are developed from the study of [1]. Contaminants participate in several physical, chemical, and biological transformation processes during the course of their travel. The basic physical law for flow in a porous medium is derived from mass balance of the chemical tracer. Mass balance states that

the rate of change of the total mass in an arbitrary region Ω of the medium must equal the net rate of mass inflow into the region through its boundaries $\partial\Omega$, plus the rate at which mass is created, or destroyed, within Ω .

Figure 2.1: MASS BALANCE



Therefore, considering an arbitrary Ω of the medium, mass balance, written symbolically, leads directly to the integral conservation law

$$\frac{d}{dt} \int_{\Omega} C\theta \, dV = - \int_{\partial\Omega} \mathbf{Q} \cdot \mathbf{n} \, dA + \int_{\Omega} F\theta \, dV \quad (2.1)$$

where

$C(\mathbf{x}, t)$ = concentration in mass/ unit volume of liquid

$\theta(\mathbf{x}, t)$ = porosity

Rate of change of solute = $\frac{d}{dt} \int_{\Omega} C\theta \, dV$

$Q(\mathbf{x}, t)$ = flux in mass/unit area/unit time

$\mathbf{n}(\mathbf{x})$ = outward normal at \mathbf{x}

Flux of the solute through the boundary = $-\int_{\partial\Omega} \mathbf{Q} \cdot \mathbf{n} dA$

$F(\mathbf{x}, t, C)$ = reaction term/source term in mass rate/unit volume of solution

Rate of reaction = $\int_{\Omega} F\theta dV$

Using Gauss-Divergence Theorem

$$\int_{\Omega} \frac{d(\theta C)}{dt} dV = -\int_{\Omega} \nabla \cdot \mathbf{Q} dV + \int_{\Omega} \theta F dV \quad (2.2)$$

leading to the differential form (assuming that the functions are sufficiently smooth to allow application of the divergence theorem)

$$\frac{d(\theta C)}{dt} = -\nabla \cdot \mathbf{Q} + \theta F \quad (2.3)$$

At this point, a constitutive relation, usually based in empirics, must be postulated regarding the form of the flux \mathbf{Q} . There are three generally accepted ways as to how dissolved particles move from one position to another in a porous medium.

1. **advection**, which means that particles are simply carried by the bulk motion of the fluid. The Darcy velocity, therefore, is equal to the advective flux

$$\mathbf{Q}^{(a)} = C\mathbf{q}$$

\mathbf{q} .

2. **molecular diffusion**, This is the spreading caused by the random collisions and molecular motion of the particles themselves. Molecular diffusion is present regardless of whether or not the fluid is in motion. This type of motion is driven by concentration gradients and the flux due to diffusion is given by **Fick's law**. This is called the molecular diffusive flux

$$\mathbf{Q}^{(m)} = -\theta \mathbf{D}^{(m)} \nabla C$$

where $\mathbf{D}^{(m)}(\mathbf{x}, t)$ is the effective diffusion coefficient.

3. **Mechanical Dispersion**. This is the mixing phenomenon, or spreading caused by the variability of the complex microscopic velocities through the porespace in the medium. So, it is related to the heterogeneities present in the medium and is present only if the flow exists. The idea being that different flow pathways have different velocities and some have a greater than the average velocity to carry the solutes ahead of a position based only on the mean velocity. The mathematical form of the dispersion flux

$$\mathbf{Q}^{(d)} = -\theta \mathbf{D}^{(d)} \nabla C$$

In a higher-dimensional formulation of the equations, the hydrodynamic dispersion would be different in different directions, because generally it is observed that in three dimensions the spreading caused by dispersion is lower in the transverse direction of flow than in the direction of the flow.

Thus the net flux is given by

$$\mathbf{Q} = C\mathbf{q} - \theta\mathbf{D}\nabla C \quad (2.4)$$

where $\mathbf{D} = \mathbf{Q}^{(m)} + \mathbf{D}^{(d)}$ is the **hydrodynamic dispersion coefficient**. Hence the mass balance equation becomes

$$\frac{d(\theta C)}{dt} = -\nabla \cdot (C\mathbf{q}) + \nabla \cdot (\theta\mathbf{D}\nabla C) + \theta F \quad (2.5)$$

The above is the standard *reaction-advection-dispersion equation*.

The following equations are derived from the study of [3].

$$\theta \frac{\partial C^{\text{urea}}}{\partial t} = \nabla \cdot (\theta\mathbf{D} \cdot \nabla C^{\text{urea}}) - \mathbf{q} \cdot \nabla C^{\text{urea}} - \theta r \quad (2.6)$$

$$\theta \frac{\partial C^{\text{Ca}^{2+}}}{\partial t} = \nabla \cdot (\theta\mathbf{D} \cdot \nabla C^{\text{Ca}^{2+}}) - \mathbf{q} \cdot \nabla C^{\text{Ca}^{2+}} - \theta r \quad (2.7)$$

$$\theta \frac{\partial C^{\text{NH}_4^+}}{\partial t} = \nabla \cdot (\theta\mathbf{D} \cdot \nabla C^{\text{NH}_4^+}) - \mathbf{q} \cdot \nabla C^{\text{NH}_4^+} + 2\theta r \quad (2.8)$$

For Non-aqueous Species CaCO_3

Once any CaCO_3^{2-} is generated, it precipitates immediately and attaches itself onto the matrix of the porous medium. Hence, its concentration is defined in terms of weight per unit volume (and not per unit volume of the voids) and the differential equation is derived to be

$$\frac{\partial C^{\text{CaCO}_3}}{\partial t} = m_{\text{CaCO}_3} \theta r \quad (2.9)$$

2.1.2 Differential equation for porosity

As CaCO_3 fills the void the void space, hence the porosity decreases by an equal amount. The change in porosity $\Delta\theta$ in time Δt is

$$\Delta\theta = \frac{\Delta V_v}{V} = -\frac{\Delta C^{\text{CaCO}_3}}{\rho_{\text{CaCO}_3}}$$

The rate of change of porosity can be expressed as follows

$$\frac{\partial \theta}{\partial t} = -\frac{1}{\rho_{\text{CaCO}_3}} \frac{\partial C^{\text{CaCO}_3}}{\partial t}$$

2.1.3 Differential Equation for flow

The head h available for flow

$$h = p + \rho g z \quad (2.10)$$

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu} \nabla h = -\frac{\mathbf{k}}{\mu} (\nabla p + \rho g \mathbf{e}_z) \quad (2.11)$$

2.1.4 Differential Equation for Pressure

The fluid has been assumed incompressible and it is also assumed that the hydrolysis of urea and precipitation of CaCO_3 has no effect on the total volume of fluid. Hence the amount of fluid transported through any closed surface(S) must be equal to the change in volume of the domain(Ω) enclosed by the closed surface. Thus the following results.

$$\int_S \mathbf{q} \cdot \mathbf{n} \, dS = - \int_{\Omega} \frac{\partial \theta}{\partial t} \, d\Omega$$

Using Gauss divergence theorem

$$\int_{\Omega} \nabla \cdot \mathbf{q} \, d\Omega = - \int_{\Omega} \frac{\partial \theta}{\partial t} \, d\Omega$$

As this is true for any subdomain of Ω

$$\nabla \cdot \mathbf{q} = - \frac{\partial \theta}{\partial t}$$

Hence the resulting differential equation is

$$-\nabla \cdot \left(\frac{\mathbf{k}}{\mu} (\nabla p + \rho g \mathbf{e}_z) \right) = \frac{m_{\text{CaCO}_3} \theta r}{\rho_{\text{CaCO}_3}} \quad (2.12)$$

2.1.5 Expression for Reaction

$$r = v_{max} \frac{u}{K_m + u} \left(1 - \frac{t}{t_{max}} \right) \quad (2.13)$$

for $0 \leq t \leq t_{max}$ and is zero else.

In the above equation a linear decay with time has been assumed : in t_{max} seconds the reaction rate decreases from a maximum reaction rate, v_{max} , to zero. Further, the reaction rate becomes zero, if there is no chemical present and is maximum if an abundant amount of reactant chemical is present.

2.1.6 Expression for Intrinsic Permeability

The intrinsic permeability is determined, using the Kozeny–Carman relation: an empiric relation between the intrinsic permeability and the porosity that is commonly used in ground water flow modelling,

$$k_x = k_y = k_z = \frac{d_m^2}{180} \frac{\theta^3}{(1 - \theta)^2} \quad (2.14)$$

Chapter 3

One Dimensional Case: Constant Coefficients

The 1D form of the general equation is given below.

$$\theta \frac{\partial u}{\partial t} = -q \frac{\partial u}{\partial x} + \frac{\partial}{\partial x} (\theta D \frac{\partial u}{\partial x}) - \theta r \quad (3.1)$$

where

$$D = \alpha_L \frac{|q|}{\theta}$$

α_L =longitudinal dispersivity

Constant θ and q

As θ and q are constants D is also a constant and hence can be taken outside of the derivative.

$$\frac{\partial u}{\partial t} = -\frac{q}{\theta} \frac{\partial u}{\partial x} + D \frac{\partial^2 u}{\partial x^2} - r \quad (3.2)$$

The above equation is of second order and is *non-linear* because of r .

3.1 Finite Difference Discretization

The one dimensional spacial domain x is replaced by a grid of N_x+1 equidistant points indexed $i = 0, 1, 2, \dots, N_x - 1, N_x$. The time domain is similarly replaced by a grid $j = 0, 1, 2, \dots, N_t - 1, N_t$.

Now $\Delta x = \frac{x_{N_x} - x_0}{N_x}$ and $\Delta t = \frac{x_{N_t} - t_0}{N_t}$.

The discretization is done by **Crank-Nicholson scheme**, which is obtained by taking the average of the explicit and implicit schemes. This method is unconditionally stable and is accurate to second order in both space and

time.

$$\begin{aligned} \frac{u_i^{j+1} - u_i^j}{\Delta t} = & \frac{D}{2} \left(\frac{(u_{i-1}^{j+1} - 2u_i^{j+1} + u_{i+1}^{j+1}) + (u_{i-1}^j - 2u_i^j + u_{i+1}^j)}{\Delta x^2} \right) \\ & - \frac{q}{2\theta} \left(\frac{(u_{i+1}^{j+1} - u_{i-1}^{j+1}) + (u_{i+1}^j + u_{i-1}^j)}{2\Delta x} \right) - r_i^j \end{aligned} \quad (3.3)$$

Rearranging and taking $c = \frac{q\Delta t}{4\theta\Delta x}$ and $s = \frac{D\Delta t}{4\Delta x^2}$ we get

$$\begin{aligned} (-c - s)u_{i-1}^{j+1} + (1 + 2s)u_i^{j+1} + (c - s)u_{i+1}^{j+1} \\ = (c + s)u_{i-1}^j + (1 - 2s)u_i^j + (-c + s)u_{i+1}^j - r_i^j \Delta t \end{aligned} \quad (3.4)$$

These equations hold only for $1 \leq i \leq N_x - 1$. In matrix form the above equation can be written as

$$\begin{aligned} \begin{bmatrix} -c - s & 1 + 2s & c - s & 0 & \dots\dots\dots \\ 0 & -c - s & 1 + 2s & c - s & 0 & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & -c - s & 1 + 2s & c - s & 0 \\ \dots\dots\dots & \dots\dots\dots & 0 & -c - s & 1 + 2s & c - s \end{bmatrix} \begin{Bmatrix} u_0^{j+1} \\ u_1^{j+1} \\ \vdots \\ u_{N_x-1}^{j+1} \\ u_{N_x}^{j+1} \end{Bmatrix} = \\ \begin{bmatrix} c + s & 1 - 2s & -c + s & 0 & \dots\dots\dots \\ 0 & c + s & 1 - 2s & -c + s & 0 & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & c + s & 1 - 2s & -c + s & 0 \\ \dots\dots\dots & \dots\dots\dots & 0 & c + s & 1 - 2s & -c + s \end{bmatrix} \begin{Bmatrix} u_0^j \\ u_1^j \\ \vdots \\ u_{N_x-1}^j \\ u_{N_x}^j \end{Bmatrix} - \begin{Bmatrix} r_1^j \\ r_2^j \\ \vdots \\ r_{N_x-2}^j \\ r_{N_x-1}^j \end{Bmatrix} \Delta t \end{aligned} \quad (3.5)$$

where r_i^j is obtained by putting u_i^j in (2.13).

There are $N_x - 2$ equations in N_x unknowns. The boundary conditions provide the two missing equations.

3.2 Boundary conditions

This specific problem is to be solved with a Dirichlet boundary condition at x_0 and a Neumann boundary condition at x_{N_x} .

1. Dirichlet: $(x_0, j) = u_0$ for $j = 0, 1, \dots, Nt$

2. Neumann: $\left(\frac{\partial u}{\partial x}\right)_{x_{N_x}} = 0$. Now applying a Backward difference at x_{N_x}

$$\frac{u_{N_x}^j - u_{N_x-1}^j}{2} = 0 \implies u_{N_x}^j = u_{N_x-1}^j$$

3.3 Equations in Matrix Form

The matrix equation (3.5) can now be modified by applying the boundary conditions.

$$\begin{aligned}
 & \begin{bmatrix} 1+2s & c-s & 0 & \dots\dots\dots \\ -c-s & 1+2s & c-s & 0 & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & -c-s & 1+2s & c-s & \dots\dots\dots \\ \dots\dots\dots & 0 & -c-s & 1+c+s & \dots\dots\dots \end{bmatrix} \begin{pmatrix} u_1^{j+1} \\ u_2^{j+1} \\ \vdots \\ u_{N_x-2}^{j+1} \\ u_{N_x-1}^{j+1} \end{pmatrix} + \begin{pmatrix} (-c-s)u_0^{j+1} \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} = \\
 & \begin{bmatrix} 1-2s & -c+s & 0 & \dots\dots\dots \\ c+s & 1-2s & -c+s & 0 & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & c+s & 1-2s & -c+s & \dots\dots\dots \\ \dots\dots\dots & 0 & c+s & 1-c-s & \dots\dots\dots \end{bmatrix} \begin{pmatrix} u_1^j \\ u_2^j \\ \vdots \\ u_{N_x-2}^j \\ u_{N_x-1}^j \end{pmatrix} + \begin{pmatrix} (c+s)u_0^j \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} r_1^j \\ r_2^j \\ \vdots \\ r_{N_x-2}^j \\ r_{N_x-1}^j \end{pmatrix} \Delta t
 \end{aligned} \tag{3.6}$$

In a compact form the above equation can be written as

$$\mathbf{M}_l \mathbf{u}^{j+1} + \mathbf{b}_l^{j+1} = \mathbf{M}_r \mathbf{u}^j + \mathbf{b}_r^j - \mathbf{r}^j \tag{3.7}$$

$$\Rightarrow \boxed{\mathbf{u}^{j+1} = \mathbf{M}_l^{-1} \left(\mathbf{M}_r \mathbf{u}^j + (\mathbf{b}_r^j - \mathbf{b}_l^{j+1}) - \mathbf{r}^j \right)} \tag{3.8}$$

Chapter 4

One Dimensional Case: General Formulation

4.1 Finite Difference Discretization

The one dimensional spacial domain x is replaced by a grid of $N_x + 1$ equidistant points indexed $i = 0, 1, 2, \dots, N_x - 1, N_x$. The time variable t is nondimensionalized using $t = \tau t_m$ to avoid difficulties during numerical computation as long term behavior of the model is sought. Then the τ domain is similarly replaced by a grid $j = 0, 1, 2, \dots, N_\tau - 1, N_\tau$.

Now $\Delta x = \frac{x_{N_x} - x_0}{N_x}$ and $\Delta \tau = \frac{\tau_{N_\tau} - \tau_0}{N_\tau}$.

For Pressure

$$-\frac{d}{dx} \left(\frac{k}{\mu} \frac{dp}{dx} \right) = \frac{m_{\text{CaCO}_3}}{\rho_{\text{CaCO}_3}} \theta$$

At each time-grid point $j = 1, 2, \dots, N_t$

$$\begin{aligned} \frac{k_{i+\frac{1}{2}}}{\mu} \frac{dp}{dx} \Big|_{i+\frac{1}{2}} - \frac{k_{i-\frac{1}{2}}}{\mu} \frac{dp}{dx} \Big|_{i-\frac{1}{2}} &= - \frac{m_{\text{CaCO}_3}}{\rho_{\text{CaCO}_3}} \theta_i \Delta x \\ \frac{k_{i+\frac{1}{2}}}{\mu} (p_{i+1} - p_i) - \frac{k_{i-\frac{1}{2}}}{\mu} (p_i - p_{i-1}) &= - \frac{m_{\text{CaCO}_3}}{\rho_{\text{CaCO}_3}} \theta_i \Delta x^2 \\ \frac{k_{i-\frac{1}{2}}}{\mu} p_{i-1} - \left(\frac{k_{i-\frac{1}{2}}}{\mu} + \frac{k_{i+\frac{1}{2}}}{\mu} \right) p_i + \frac{k_{i+\frac{1}{2}}}{\mu} p_{i+1} &= - \frac{m_{\text{CaCO}_3}}{\rho_{\text{CaCO}_3}} \theta_i r_i \Delta x^2 \end{aligned} \quad (4.1)$$

The superscript j is omitted for compactness as it is a differential equation of only x .

For Flow

$$q = -\frac{k}{\mu} \frac{dp}{dx}$$

$$q_0 = -\frac{k_0}{\mu} \frac{p_1 - p_0}{\Delta x} \quad (4.2)$$

$$q_i = -\frac{k_i}{\mu} \frac{p_{i+1} - p_{i-1}}{2\Delta x} \quad \text{for } 1 \leq i \leq N_x - 1 \quad (4.3)$$

$$q_{N_x} = -\frac{k_{N_x}}{\mu} \frac{p_{N_x} - p_{N_x-1}}{\Delta x} \quad (4.4)$$

For Concentration of Aqueous Specis

$$\theta \frac{\partial u}{\partial t} = -q \frac{\partial u}{\partial x} + \frac{\partial}{\partial x} \left(d \frac{\partial u}{\partial x} \right) - \theta r$$

where $d = \theta D = \theta \alpha_L \frac{|q|}{\theta} = \alpha_L |q|$

$$\implies \theta \frac{\partial u}{\partial \tau} = -e \frac{\partial u}{\partial x} + \frac{\partial}{\partial x} \left(f \frac{\partial u}{\partial x} \right) - \theta g \quad (4.5)$$

where $e = qt_m$ $f = dt_m$ $g = rt_m$

The discretization is done by **Crank-Nicholson scheme**, which is obtained by taking the average of the explicit and implicit schemes. This method is unconditionally stable and is accurate to second order in both space and time.

$$\theta_i \frac{u_i^{j+1} - u_i^j}{\Delta \tau} = -\frac{e_i^j}{2} \left(\frac{(u_{i+1}^{j+1} - u_{i-1}^{j+1}) + (u_{i+1}^j + u_{i-1}^j)}{2\Delta x} \right)$$

$$+ \frac{1}{2} \left\{ \frac{\left(f_{i-\frac{1}{2}}^j u_{i-1}^{j+1} - (f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j) u_i^{j+1} + f_{i+\frac{1}{2}}^j u_{i+1}^{j+1} \right)}{\Delta x^2} \right.$$

$$\left. + \frac{\left(f_{i-\frac{1}{2}}^j u_{i-1}^j - (f_{i-\frac{1}{2}}^j + f_{i+\frac{1}{2}}^j) u_i^j + f_{i+\frac{1}{2}}^j u_{i+1}^j \right)}{\Delta x^2} \right\} - \theta_i^j g_i^j$$

$$\begin{aligned}
&\Rightarrow \left(-\frac{e_i^j \Delta \tau}{4\Delta x} - \frac{f_{i-\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_{i-1}^{j+1} + \left(\theta_i^j + \frac{f_{i-\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} + \frac{f_{i+\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_i^{j+1} \\
&\quad + \left(\frac{e_i^j \Delta \tau}{4\Delta x} - \frac{f_{i+\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_{i+1}^j \\
&= \left(\frac{e_i^j \Delta \tau}{4\Delta x} + \frac{f_{i-\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_{i-1}^j + \left(\theta_i^j - \frac{f_{i-\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} - \frac{f_{i+\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_i^j \\
&\quad + \left(-\frac{e_i^j \Delta \tau}{4\Delta x} + \frac{f_{i+\frac{1}{2}}^j \Delta \tau}{2\Delta x^2} \right) u_{i+1}^j - \theta_i^j g_i^j \Delta \tau
\end{aligned} \tag{4.6}$$

Concentration of CaCO_3

$$\begin{aligned}
\frac{\partial u^{\text{CaCO}_3}}{\partial t} &= m_{\text{CaCO}_3} \theta r \\
u_i^{j+1} &= u_i^j + m \theta_i^j r_i^{j+1} \Delta t = u_i^j + m \theta_i^j g_i^{j+1} \Delta \tau
\end{aligned} \tag{4.7}$$

For Porosity

$$\begin{aligned}
\frac{\partial \theta}{\partial t} &= -\frac{1}{\rho_{\text{CaCO}_3}} \frac{\partial u^{\text{CaCO}_3}}{\partial t} \\
\theta_i^j &= \theta_i^0 - \frac{u_i^j - u_i^0}{\rho}
\end{aligned} \tag{4.8}$$

Updating Values of r and k

$$r_i^j = v_{\max} \frac{u_i^j}{K_m + u_i^j} \left(1 - \frac{t}{t_{\max}} \right) \tag{4.9}$$

$$k_i^j = \frac{d_m^2}{180} \frac{\theta^3}{(1-\theta)^2} \tag{4.10}$$

4.2 Boundary Conditions

	p	C^{urea}	$C^{\text{Ca}^{2+}}$	$C^{\text{NH}_4^+}$
x_0	$p = p_1$ (pressure driven case)	$C^{\text{urea}} = c_{in}$	$C^{\text{Ca}^{2+}} = c_{in}$	$C^{\text{NH}_4^+} = 0$
x_{N_x}	$p = p_2$	$\frac{\partial C^{\text{urea}}}{\partial n} = 0$	$\frac{\partial C^{\text{Ca}^{2+}}}{\partial n} = 0$	$\frac{\partial C^{\text{NH}_4^+}}{\partial n} = 0$

The Neumann Boundary Condition at x_{N_x} , $\left(\frac{\partial u}{\partial x} \right)_{x_{N_x}} = 0$ can be dealt with by applying a Backward difference at x_{N_x}

$$\mathbf{M}_r = \begin{bmatrix}
\theta_1^j - \frac{f_1^j \Delta \tau}{2\Delta x^2} - \frac{f_3^j \Delta \tau}{2\Delta x^2} & -\frac{e_1^j \Delta \tau}{4\Delta x} + \frac{f_3^j \Delta \tau}{2\Delta x^2} & 0 & \dots & \dots & \dots \\
\frac{e_2^j \Delta \tau}{4\Delta x} + \frac{f_3^j \Delta \tau}{2\Delta x^2} & \theta_2^j - \frac{f_3^j \Delta \tau}{2\Delta x^2} - \frac{f_5^j \Delta \tau}{2\Delta x^2} & -\frac{e_2^j \Delta \tau}{4\Delta x} + \frac{f_5^j \Delta \tau}{2\Delta x^2} & 0 & \dots & \dots \\
\dots & \dots & \dots & \dots & \dots & \dots \\
\dots & \frac{e_{N_x-2}^j \Delta \tau}{4\Delta x} + \frac{f_{N_x-5}^j \Delta \tau}{2\Delta x^2} & \theta_{N_x-2}^j - \frac{f_{N_x-5}^j \Delta \tau}{2\Delta x^2} - \frac{f_{N_x-3}^j \Delta \tau}{2\Delta x^2} & -\frac{e_{N_x-2}^j \Delta \tau}{4\Delta x} + \frac{f_{N_x-3}^j \Delta \tau}{2\Delta x^2} & \dots & \dots \\
\dots & \dots & 0 & \frac{e_{N_x-1}^j \Delta \tau}{4\Delta x} + \frac{f_{N_x-3}^j \Delta \tau}{2\Delta x^2} & \theta_{N_x-1}^j - \frac{f_{N_x-3}^j \Delta \tau}{2\Delta x^2} - \frac{e_{N_x-1}^j \Delta \tau}{4\Delta x} & \dots
\end{bmatrix}$$

Chapter 5

Computer Simulation

5.1 Algorithm

Initially, the concentration of calcium carbonate, urea, calcium and ammonium are equal to zero.

At each time step, Eqs. (4.1)-(4.10) are solved.

1. First the equation for the pressure, (4.1), is solved, using the porosity, density, intrinsic permeability and reaction rate from the previous time step.
2. Subsequently, the velocities are calculated, using Eq. (4.2),(4.3) and (4.4). Again, the density and the intrinsic permeability from the previous time step are to be used.
3. The differential equation for concentration of urea has the non-linear reaction term and it is solved using Eq. (4.6), using the porosity from the previous time step.
4. The differential equations for the concentrations of chemical species present are solved using using Eq. (4.6) and reaction r obtained from the differential equation for urea.
5. Subsequently, the equation for CaCO_3 concentration, (4.7), is solved, using the porosity from the previous time step and the reaction rate from the current one.
6. Finally, the intrinsic permeability k and the porosity θ are recalculated with Eq. (4.10) and (4.8), respectively.
7. Also the boundary conditions and the density of the fluid ρ are updated, if necessary,

5.2 Constants Used in MATLAB Program

$x_0 = 0$	$x_{N_x} = 1$
$N_x = 100$	$N_t = 10^5$
$m_{\text{CaCO}_3} = 100.1 \text{ Kg Km}^{-1}$	$\rho_{\text{CaCO}_3} = 2710 \text{ Kg m}^{-3}$
$t_{\text{max}} = 2.88 \times 10^5 \text{ s (=80h)}$	$v_{\text{max}} = 9 \times 10^{-5} \text{ kmol m}^{-3} \text{ s}^{-1}$
$\mu = 1.15 \times 10^{-3} \text{ Pa s}$	$\theta_0 = .35$
$\alpha_L = .01 \text{ m}$	$K_m = .01$
$d_m = 2 \times 10^{-4} \text{ m}$	$c_{in} = 1.0 \text{ kmol m}^{-3}$

5.3 MATLAB Codes

```
1 clear all
2
3 L=1;          %length of x domain
4 tm=288000;   %tmax
5 T=1;         %tau max
6 vm=9e-5;     %Vmax
7 Km=.01;
8 m2=100.1;    %molar mass of CaCO3
9 dm=2e-4;     %mean particle size
10 mu=1.15e-3;
11 rho2=2710;  %density of mass of CaCO3
12 Cin=1;
13 p1=100854;
14 p2=1e5;
15 Nx=100;
16 Nt=100000;
17 dx=L/Nx;
18 dt=T/Nt;
19 alpha=.01;  %horizontal dispersivity
20
21 %C1=concentration of urea
22 %C2=concentration of CaCO3
23 %initial condition
24 for i=1:Nx+1
25     x(i)=(i-1)*dx;
26     C1(i,1)=0;
27     C2(i,1)=0;
28 end
29
30 %boundary conditions at X0(Dirichlet)
31 for j=1:Nt+1
32     t(j)=(j-1)*dt;
33 end
34 C1(1,1:Nt+1)=Cin;
35 C2(1,1:Nt+1)=0;
```



```

36 p(1,1:Nt+1)=p1;
37 p(Nx+1,1:Nt+1)=p2;
38
39 g(:,1)=tm*vm*(1-t(1))*C1(:,1)/(Km+C1(:,1));% initial ...
    reaction rate
40 por(1:Nx+1,1)=.35;
41 k(:,1)=dm^2/180*por(:,1).^3./(1-por(:,1).^2);%intrinsic ...
    permeability
42
43 for j=1:Nt
44
45 %-----
46 %Solution for pressure
47 for i=1:Nx
48     kk(i)=(k(i,j)+k(i+1,j))/2;
49 end
50
51 Q=-m2/rho2*por(2:Nx,j).*g(2:Nx,j)*dx*dx/(tm);
52 Q(1)=Q(1)-p1*kk(1);
53 Q(Nx-1)=Q(Nx-1)-p2*kk(Nx);
54 aa(1:Nx-2)=kk(2:Nx-1);
55 for i=1:Nx-1
56     bb(i)=-(kk(i)+kk(i+1));
57 end
58 cc(1:Nx-2)=kk(2:Nx-1);
59 MMP=diag(bb,0)+diag(aa,-1)+diag(cc,1);
60 p(2:Nx,j)=MMP\Q;
61 %-----
62
63 %-----
64 %solution for flow
65 q(1,j)=-k(1,j)/mu*(p(2,j)-p(1,j))/dx;%forward diff.
66 for i=2:Nx
67     q(i,j)=-k(i,j)/mu*(p(i+1,j)-p(i-1,j))/(2*dx);%central ...
        diff.
68 end
69 q(Nx+1,j)=-k(Nx+1,j)/mu*(p(Nx+1,j)-p(Nx,j))/dx;%backward diff.
70 %-----
71
72 %-----
73 %solution for urea concentration(C1)
74 e=tm*q(:,j);
75 f=tm*alpha*abs(q(:,j));
76 ff=zeros(Nx,1);
77 for i=1:Nx
78     ff(i)=(f(i)+f(i+1))/2;
79 end
80
81 aal(1:Nx-2)=-(ff(2:Nx-1)/(2*dx^2)+e(3:Nx)/(4*dx))*dt;
82 for i=1:Nx-2
83     bbl(i)=por(i+1,j)+(ff(i)+ff(i+1))*dt/(2*dx^2);
84 end
85 bbl(Nx-1)=por(Nx,j)+dt/(2*dx^2)*ff(Nx-1)+e(Nx)*dt/(4*dx);
86 ccl(1:Nx-2)=-(ff(2:Nx-1)/(2*dx^2)-e(2:Nx-1)/(4*dx))*dt;

```

```

87 Mm1=diag(aal,-1)+diag(bbl,0)+diag(ccl,1);
88 r1=zeros(Nx-1,1);
89
90 aar(1:Nx-2)=(ff(2:Nx-1)/(2*dx^2)+e(3:Nx)/(4*dx))*dt;
91 for i=1:Nx-2
92 bbr(i)=por(i+1,j)-(ff(i)+ff(i+1))*dt/(2*dx^2);
93 end
94 bbr(Nx-1)=por(Nx,j)-dt/(2*dx^2)*ff(Nx-1)-e(Nx)*dt/(4*dx);
95 ccr(1:Nx-2)=(ff(2:Nx-1)/(2*dx^2)-e(2:Nx-1)/(4*dx))*dt;
96 MMr=diag(bbr,0)+diag(aar,-1)+diag(ccr,1);
97 rr=zeros(Nx-1,1);
98
99 r1(1)=-dt*(ff(1)/(2*dx^2)+e(2)/(4*dx))*C1(1,j+1);
100 rr(1)=dt*(ff(1)/(2*dx^2)+e(2)/(4*dx))*C1(1,j);
101 uu=C1(2:Nx,j);
102 C1(2:Nx,j+1)=(Mm1)\(rr-r1+MMr*uu-por(2:Nx,j).*g(2:Nx,j)*dt);
103 % -----
104
105 % -----
106 %calculation of reaction-rate,CaCO3 concentration(C2) and ...
    porosity
107
108 g(:,j+1)= ...
    tm*vm*(1-t(j+1))*C1(:,j+1)./(Km+C1(:,j+1));%reaction rate
109 C2(1:Nx,j+1)=C2(1:Nx,j)+dt*m2*por(1:Nx,j).*g(1:Nx,j+1);
110 por(:,j+1)=por(:,1)-(C2(:,j+1)-C2(:,1))/rho2;
111 k(:,j+1)=dm^2/180*por(:,j+1).^3./(1-por(:,j+1)).^2;
112 j
113 end
114
115 %Neumann Boundary Conditions at Xn
116 C1(Nx+1,:)=C1(Nx,:);
117
118 %Plots
119 %urea-x
120 figure(1);
121 plot(x,C1(:,ceil(72000/2.88+1)),'-',x,...
122      C1(:,ceil(144000/2.88+1)),'-',x,C1(:,ceil(216000/2.88+1)),'-',...
123      x,C1(:,ceil(288000/2.88+1)),'-');
124
125 %urea-T
126 figure(2);
127 time=tm*t;
128 plot(time,C1(1,:),'-',time,C1(ceil(0.2/.01+1),:),'-',time,...
129      C1(ceil(0.5/.01+1),:),time,C1(ceil(1/.01+1),:))
130
131 %CaCO3-X
132 figure(3)
133 plot(x,C2(:,ceil(72000/2.88+1)),'-',x,...
134      C2(:,ceil(144000/2.88+1)),'-',x,C2(:,ceil(216000/2.88+1)),...
135      '- ',x,C2(:,ceil(288000/2.88+1)),'-')
136
137 %porosity
138 figure(4)

```

```
139 plot(x,por(:,Nt+1))
140 %permeability
141 plot(x,k(:,Nt+1))
```

5.4 Plots

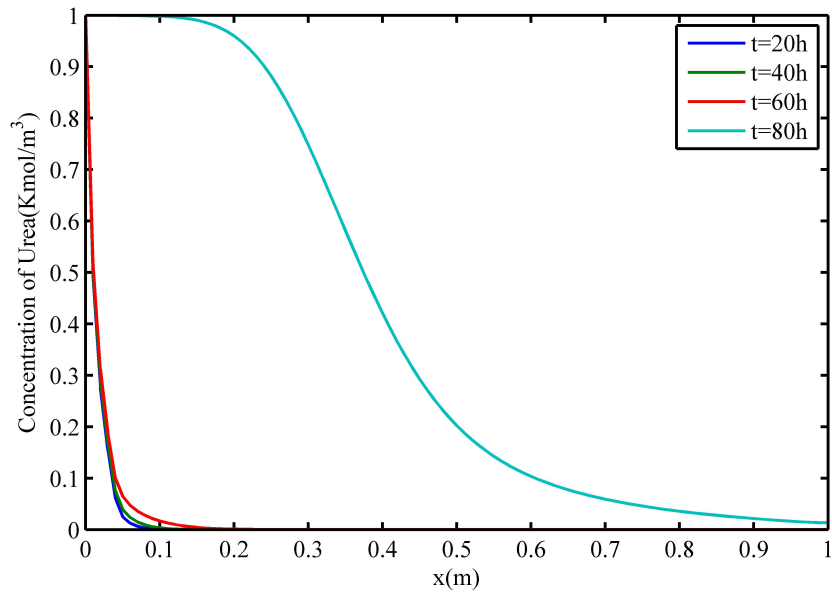


Figure 5.1: The urea concentration as a function of x at several times.

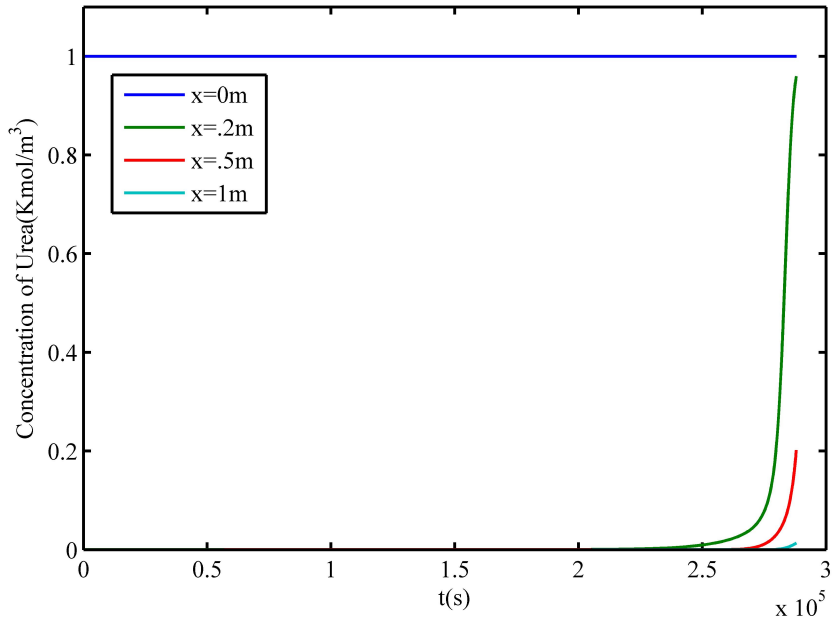


Figure 5.2: The urea concentration as a function of t at several positions

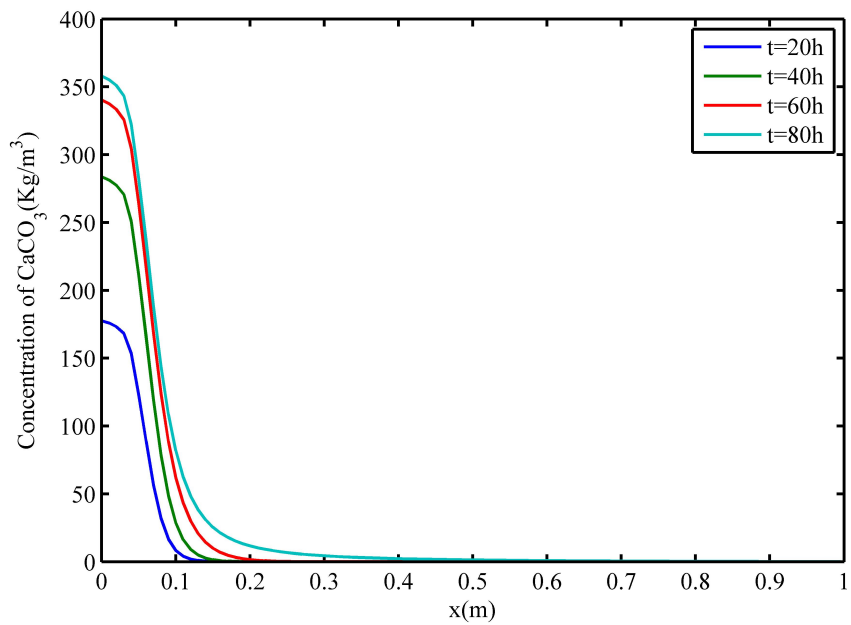


Figure 5.3: The concentration of calcium carbonate as a function of x at several times.

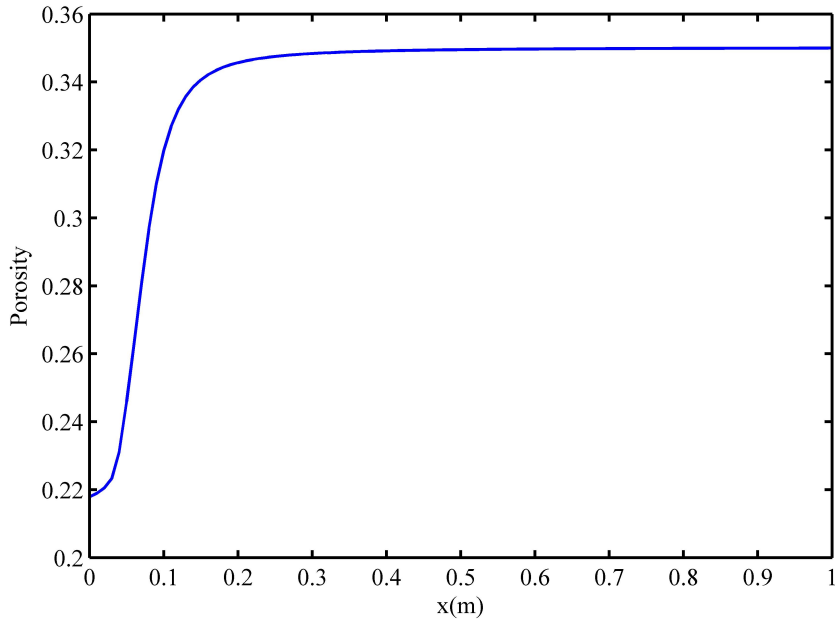


Figure 5.4: the porosity as a function of the position at $t = t_{max}$

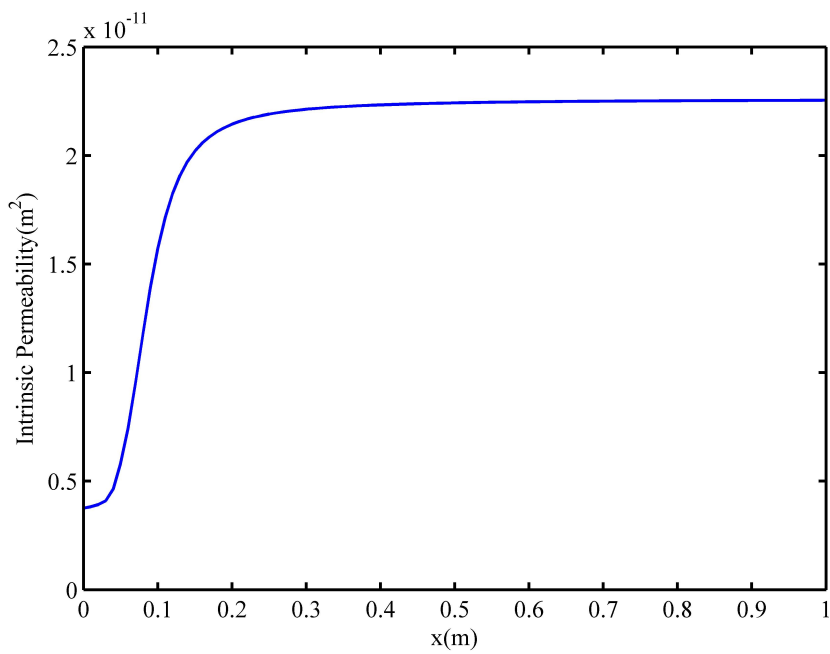


Figure 5.5: the intrinsic permeability as a function of the position at $t = t_{max}$

Chapter 6

Inference

In the pressure driven case modelled above, initially, the inflow velocity is high. Both the porosity and the permeability decrease due to the precipitation of calcium carbonate. Since the pressure at the inflow and outflow boundary remain constant, the inflow velocity decreases.

The calcium carbonate concentration in the domain at several times for the pressure driven case. For example, in the first 80 hours, in about 20 % of the domain, calcium carbonate has been formed in the pressure driven case. Eventually, the inflow velocity became so low that the urea molecules could not reach the end of the column. As a result no calcium carbonate has been formed in the remaining part of the domain.

An increase of the generated calcium carbonate concentration, gives a decrease of both intrinsic permeability and the porosity. This phenomenon is confirmed in the above figures.

Conclusion

A model has been formulated to describe the Biogrout process. The model gives insight into several aspects of the Biogrout process. The Biogrout process influences several properties of the subsoil. The precipitation of the solid calcium carbonate decreases the porosity and the permeability. A consequence of a decreasing permeability is that the pressure should increase to keep up the same flow rate, or, if the pressure is constant, that the flow rate decreases. The model contains the concentrations of the dissolved species that are present in the biochemical reaction. These concentrations can be solved from a advectiondispersionreaction equation with a variable porosity. Other model equations involve the bacteria, the solid calcium carbonate concentration, the (decreasing) porosity, the flow and the density of the fluid.

Scope for Future Study

The model has been created under several assumptions. These assumptions should be validated using experiments.

- The first assumption was that the process is governed by the given biochemical reaction. In reality, however, this reaction happens in several steps, some of which being equilibrium reactions that depend on the pH.
- The retardation factors have been assumed to be 1 and it is also assumed that the total volume of the fluid remain unaltered due to the hydrolysis of urea and the precipitation of calcium carbonate.
- It has also been assumed that calcium carbonate precipitates locally and will not be transported. Calcium carbonate can precipitate in several ways e.g. it can attach to sand grains but can also form crystals. When these crystals are large enough, they will stick in the porespace and it can be assumed that they are not transported. However, when these crystals are small, they should be considered to be transported.
- Another assumption was that of the distribution of bacteria being homogeneous and that the reaction rate has a linear decay with time.
- To calculate the intrinsic permeability the Kozeny-Carman relation has been used, the validity of which is to be verified in case of Biogrout process.
- The viscosity has been assumed to be constant and independent on the concentrations of various chemicals involved.

Only pressure driven case has been discussed. The flow driven case can be investigated where the flow is constant at the boundary points.

The model deals with only one dimensional case. Similar models can be developed for two and three dimensional cases.

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