

Modelling the New Soil Improvement Method Biogrout: Extension to 3D

W.K. van Wijngaarden, F.J. Vermolen, G.A.M. van Meurs, and C. Vuik

Abstract Biogrout is a new soil improvement method based on microbial induced carbonate precipitation. Bacteria and reactants are flushed through the soil, resulting in calcium carbonate precipitation and consequent soil reinforcement. A mathematical model was created to describe the process. The model contains the concentrations of the dissolved species that are present in the precipitation reaction. These concentrations can be solved from a convection-dispersion-reaction equation with a variable porosity. Other model equations involve the concentrations of the bacteria and of the solid calcium carbonate, the decreasing porosity (due to precipitation) and the flow. The partial differential equations are solved by the Standard Galerkin Finite Element Method. The subject of this paper is the extension of the mathematical model to 3D.

1 Introduction

Biogrout is a new soil reinforcement method based on microbial induced carbonate precipitation [7]. Bacteria are placed and subsequently reactants (urea ($\text{CO}(\text{NH}_2)_2$) and calcium chloride (CaCl_2)) are flushed through the soil, resulting in calcium carbonate (CaCO_3) precipitation, causing an increase in strength and stiffness of the soil.

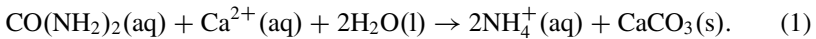
Biogrout can be applied to a wide variety of situations, in which it is desirable to change the properties of the subsoil [2]. We briefly mention the following examples

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- reinforcement of the soil underneath railway-tracks;
- soil stabilization prior to tunnelling;
- reinforcement of dunes to decrease effects of wave erosion, and hence to protect delicate coastlines;
- prevention of liquefaction of the subsoil resulting from earthquakes.

The Biogrout process consists of two parts: the microbial induced production of carbonate (CO_3^{2-}) due to the hydrolysis of urea (with ammonium (NH_4^+) as a side-product) and the precipitation of calcium carbonate. In [7], the corresponding reaction equations are given. Combining these reactions gives the overall Biogrout reaction equation:



The solid calcium carbonate strengthens the subsoil by connecting the sand grains. As a result of the precipitation of calcium carbonate, the porosity and the permeability of the soil decrease. This phenomenon influences the flow.

In [5] a model has been derived to describe the Biogrout process. Thus far, only simulations for 1D and 2D configurations have been done. In this paper, a simulation will be carried out for a 3D configuration.

This paper contains the following sections. Section 2 summarizes the model for the Biogrout process that was derived in [5]. Section 3 is devoted to the numerical methods, used to solve the model equations. Section 4 contains some computer simulations for a 3D configuration and in Sect. 5 conclusions and discussions can be found.

2 The Mathematical Model

In this section, the (differential) equations that are needed to describe the Biogrout process are given, together with a short explanation. In [5] the derivation can be found. These (differential) equations were derived in respect with the following assumptions:

- Only dissolved species do react;
- The biochemical reaction of the Biogrout process is the only reaction that takes place and this reaction is governed by reaction (1);
- The concentration of the bacteria is constant in time and homogeneous;
- Calcium carbonate is not transported but it precipitates on the matrix of the porous medium;
- The precipitation of calcium carbonate has no influence on the total volume of the fluid over the entire domain of computation;
- The flow is incompressible;
- The viscosity is constant.

The biochemical reaction of the Biogrout process is given by (1). We will start by giving the differential equations for the aqueous species in this equation.

The differential equation for the concentration of urea is given by:

$$\theta \frac{\partial C^{urea}}{\partial t} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C^{urea}) - \mathbf{q} \cdot \nabla C^{urea} - \theta r. \quad (2)$$

In this equation, θ is the porosity, C^{urea} is the dissolved concentration of urea, \mathbf{D} is the dispersion tensor, \mathbf{v} is the pore water velocity and r is the reaction rate of the production of calcium carbonate, which is a non-linear function of the urea concentration and the time.

The term at the left-hand side represents the accumulation. The first term at the right-hand side represents the effect of dispersion and diffusion, the second term models advection and the last term stands for the biochemical reaction. The minus-sign comes from the fact that urea is consumed at the same rate as calcium carbonate is formed, see (1).

In three dimensions, the coefficients of the dispersion tensor \mathbf{D} equal $D_{ij} = (\alpha_L - \alpha_T) \frac{v_i v_j}{|\mathbf{v}|} + \delta_{ij} \alpha_T \sum_i \frac{v_i^2}{|\mathbf{v}|}$, see [8]. The quantity α_L is the longitudinal dispersivity and α_T is the transverse dispersivity.

Analogously, we have the following differential equation for the concentrations of calcium and ammonium:

$$\theta \frac{\partial C^{Ca^{2+}}}{\partial t} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C^{Ca^{2+}}) - \mathbf{q} \cdot \nabla C^{Ca^{2+}} - \theta r, \quad (3)$$

$$\theta \frac{\partial C^{NH_4^+}}{\partial t} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C^{NH_4^+}) - \mathbf{q} \cdot \nabla C^{NH_4^+} + 2\theta r. \quad (4)$$

Note the $+2$ in the biochemical reaction term in the differential equation for ammonium: for each produced mole of calcium carbonate, two moles of ammonium are generated.

For the non-aqueous species in reaction (1), calcium carbonate, we have the following differential equation:

$$\frac{\partial C^{CaCO_3}}{\partial t} = m_{CaCO_3} \theta r. \quad (5)$$

In this equation, m_{CaCO_3} is the molar mass of calcium carbonate and is used to convert number of molecules (moles) into mass (kilograms). The right-hand side of this differential equation only contains the reaction term since it has been assumed that calcium carbonate is not transported.

We have the following relation between the concentration of calcium carbonate and the porosity:

$$\theta(t) = \theta(0) - \frac{C^{CaCO_3}(t) - C^{CaCO_3}(0)}{\rho_{CaCO_3}}, \quad (6)$$

where ρ_{CaCO_3} is the density of calcium carbonate.

The flow is calculated from Darcy's Law, given in [8]:

$$q_x = -\frac{k_x}{\mu} \frac{\partial p}{\partial x}, q_y = -\frac{k_y}{\mu} \frac{\partial p}{\partial y}, q_z = -\frac{k_z}{\mu} \left(\frac{\partial p}{\partial z} + \rho g \right). \quad (7)$$

In Darcy's Law, p is the pressure, k_i is the intrinsic permeability in the various coordinate directions ($i = x, y, z$), μ is the viscosity that is assumed to be constant in the Biogroout case, ρ is the density of the solution and g is the gravitational constant.

The intrinsic permeability k is determined, using the Kozeny–Carman relation: an empirical relation between the intrinsic permeability and the porosity that is commonly used in ground water flow modelling (see [1]):

$$k = \frac{(d_m)^2}{180} \frac{\theta^3}{(1 - \theta)^2}. \quad (8)$$

In this relation, d_m is the mean particle size of the subsurface medium. If the porosity is small, it might be that the pores are not connected. Hence, the permeability is zero. This phenomenon is not directly incorporated in the Kozeny–Carman relation. Since in our simulations the porosity is not that small, we assume that the Kozeny–Carman relation is a good relation between the permeability and the porosity.

The density of the solution (at 20 °C), ρ , will be calculated with the following experimental relation:

$$\rho = 1000 + 15.4996C^{urea} + 86.7338C^{Ca^{2+}} + 15.8991C^{NH_4^+}. \quad (9)$$

For the pressure, the following differential equation was derived in [5] by the use of Darcy's Law (7):

$$-\nabla \cdot \left(\frac{k}{\mu} (\nabla p + \rho g \mathbf{e}_z) \right) = \frac{mCaCO_3}{\rho CaCO_3} \theta r. \quad (10)$$

Differential equation (2), (3), (4), (5) and (10) contain the reaction rate r of the biochemical reaction (1). This rate decreases in time as is shown in experiments, see [6]. In [5] a linear reduction had been assumed, combined with Monod kinetics, [3]. In this paper, we will combine Monod kinetics with an exponential reduction, since this is commonly used as a first approximation (see [4]):

$$r = v_{max} \frac{C^{urea}}{K_m + C^{urea}} e^{-bt}. \quad (11)$$

In this equation, v_{max} is the initial activity, K_m is the saturation constant and b is some constant, representing the reduction in bacterial activity in the course of time.

As initial conditions, the concentration of calcium carbonate, urea, calcium and ammonium are equal to zero and the porosity equals θ_0 .

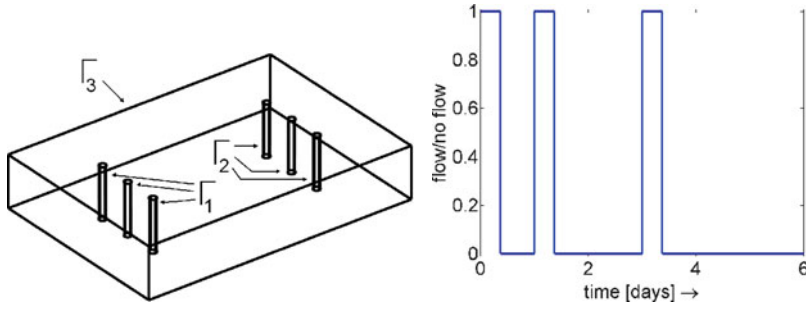


Fig. 1 Experimental set-up. *Left*: Configuration, *Right*: Flow strategy

Table 1 Boundary conditions for the pressure and the concentration of urea, calcium and ammonium

	p	C^{urea}	$C^{Ca^{2+}}$	$C^{NH_4^+}$
Γ_1 (during injection)	$-\frac{k}{\mu}(\nabla p + \rho g \mathbf{e}_z) \cdot \mathbf{n} = q_{in}$	$C^{urea} = c_{in}$	$C^{Ca^{2+}} = c_{in}$	$C^{NH_4^+} = 0$
Γ_1 (during rest)	$p = p_2 + \int_z^{1.5} \rho g \bar{z} d\bar{z}$	$\frac{\partial C^{urea}}{\partial n} = 0$	$\frac{\partial C^{Ca^{2+}}}{\partial n} = 0$	$\frac{\partial C^{NH_4^+}}{\partial n} = 0$
Γ_2	$p = p_2 + \int_z^{1.5} \rho g \bar{z} d\bar{z}$	$\frac{\partial C^{urea}}{\partial n} = 0$	$\frac{\partial C^{Ca^{2+}}}{\partial n} = 0$	$\frac{\partial C^{NH_4^+}}{\partial n} = 0$
Γ_3	$-\frac{k}{\mu}(\nabla p + \rho g \mathbf{e}_z) \cdot \mathbf{n} = 0$	$\frac{\partial C^{urea}}{\partial n} = 0$	$\frac{\partial C^{Ca^{2+}}}{\partial n} = 0$	$\frac{\partial C^{NH_4^+}}{\partial n} = 0$

As a model experiment, a container (8 m×5.6 m×1.5 m) has been taken, having closed boundaries (represented by boundary Γ_3). In this container injection and extraction wells have been placed (Fig. 1). The injection wells are represented by boundary Γ_1 , whereas the extraction wells are represented by boundary Γ_2 . The following flow strategy has been chosen: there are three batches, starting with nine hours of injection and no injection during the rest of the batch. The duration of the batches is respectively 1, 2 and 3 days, see Fig. 1.

Table 1 displays the boundary conditions that are chosen.

Since we have the same differential equation, initial condition and boundary conditions for both the concentration of urea and calcium chloride, these concentrations are equal. Hence it is sufficient to calculate only the urea concentration.

3 Numerical Method

The differential equations for the pressure, the velocity and the concentration of the aqueous species are solved by the Standard Galerkin Finite Element Method. The weak formulation is derived by multiplication by a test function $\eta \in H^1(\Omega)$ and integration over the domain Ω . For the time integration, an IMEX-scheme is used: all components are solved implicitly, except for the porosity θ , the intrinsic permeability k and the density of the solution ρ . Solving the differential equation for the pressure, the reaction rate r is also computed explicitly. While solving

the differential equation for the urea concentration, Newton's method is used, because of the non-linearity in the reaction term (11). The Newton-Cotes quadrature rules have been used for the approximation of the element matrices and vectors. Tetrahedral elements have been used, in combination with linear basis functions.

Since the differential equation for the concentration of calcium carbonate, (5), is an ordinary differential equation (in each grid point), it is not necessary to use the Finite Element Method. For the time integration, an IMEX-scheme is used: solving all components implicitly, except for the porosity.

At each time step, the differential equations for the following components are solved successively: the pressure, the flow and the concentration of urea, calcium, ammonium and calcium carbonate. For more details, see [5].

Finally, the porosity (θ), the intrinsic permeability (k) and the density of the fluid (ρ) are recalculated with (6), (8) and (9), respectively. Also the boundary conditions are updated.

Since the porosity, the permeability and the density of the solution (may) vary, at each time step all the matrices are rebuilt. That means, calculate for each element a 4×4 element matrix and add them to the large matrix. This is done for 10 different matrices + the number of Newton-iterations, since in each Newton-iteration a new matrix is built.

4 Results

In this section, the results of the simulation with the model for a 3D configuration are shown. Matlab has been used to do the numerical simulations. The linear systems are solved by a direct method. The time step $\Delta t = 1$ h, $q_{in} = 2.29 \times 10^{-4} \text{ m s}^{-1}$, $v_{max} = 1.621 \times 10^{-2} \text{ mol m}^{-3} \text{ s}^{-1}$ and $b = 7.15 \times 10^{-6} \text{ s}^{-1}$. The values of the other constants can be found in [5].

All the three batches start with nine hours of injection with inflow velocity q_{in} . During injection, the amount of urea in the domain increases, although this phenomenon is diminished by the hydrolysis of urea. During rest, the total amount of urea decreases, due to the hydrolysis of urea. The reaction rate (11) decreases in time. As a consequence, the total amount of urea decreases slower during the period of rest as time proceeds.

The urea/calcium chloride solution is heavier than water and is also heavier than the solution of the reaction product ammonium chloride as can be seen from formula (9). As a result, in the lower parts of the domain a higher urea and calcium chloride concentration are expected. This will result in a higher calcium carbonate concentration in the lower parts of the domain. Figure 2 confirms these expectations and also gives some quantitative details.

At each time step, new matrices are built, since porosity, permeability and density of the solution (may) vary. In this paper, the relation between the CPU time for the building part and for the solving part has been investigated. Seven different meshes have been taken, with increasing number of elements. With each mesh 10 time steps

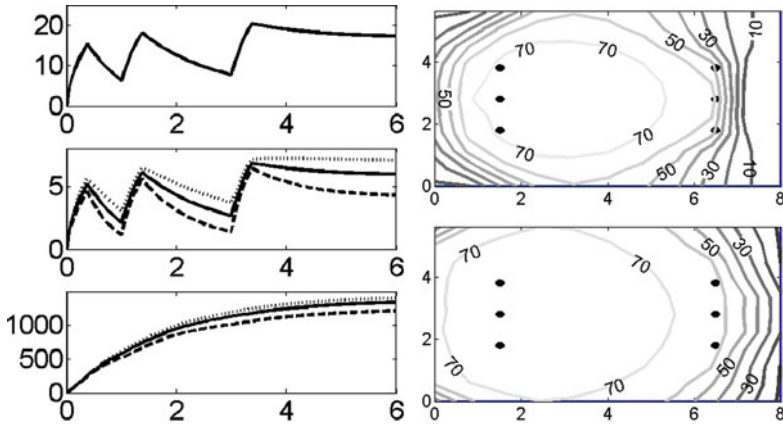


Fig. 2 Some results of the 3D model experiment. *Top left*: total amount of urea (kmol) in time (days) in the whole domain; *Middle left*: amount of urea (kmol) in time (days) in several parts of the domain: --- upper part, - middle part, ··· lower part; *Bottom left*: the amount of calcium carbonate (kg) in the same parts of the domain: --- upper part, - middle part, ··· lower part. *Top right*: a contour plot of the calcium carbonate concentration (kg/m^3) after the three batches at $z = 1.5$ m (top domain), $x[\text{m}]$ and $y[\text{m}]$ on the x -axis and y -axis; *Bottom right*: a contour plot of the calcium carbonate concentration (kg/m^3) after the three batches at $z = 0$ m (bottom domain), $x[\text{m}]$ and $y[\text{m}]$ on the x -axis and y -axis

Table 2 CPU time per time step, subdivided in the building part and the solving part for seven different meshes, with increasing number of elements and the relative error

Number of Elements (approximately)	CPU time			Percentage Solving part	Relative Error
	Per time step (s)	Building part (s)	Solving part (s)		
2500	0.344	0.242	0.102	30%	24%
5000	0.715	0.459	0.255	36%	15%
10000	1.58	0.921	0.661	42%	10%
20000	4.28	1.88	2.39	56%	6.3%
40000	13.9	3.80	10.1	73%	3.5%
80000	46.8	8.23	38.6	82%	1.1%
160000	182	17.0	165	91%	(0%)

have been taken, registering the average CPU time per time step and the average CPU time per time step for the building part and the solving part. The results can be found in Table 2. This table also contains the percentage solving time/total time.

From this table, it can be seen that, if the number of elements increases with a factor 2, so does the CPU time for the building part. This is what is expected: for each element a 4×4 element matrix is created and is added to the large matrix. If the number of elements doubles, the amount of work doubles, too.

If the number of elements doubles, the amount of solving work increases with a factor 2.5, 2.6, 3.6, 4.2, 3.8 and 4.3, respectively. So the amount of work increases with more than a factor 2, what can also be expected from the analysis of a band

matrix solver. For a mesh with 2500 elements only 30% of the CPU time is spent in the solving part. For a mesh with 160000 elements this is even 91%. If the number of elements increases further, it will be necessary to use an iterative method instead of a direct method.

The discretization error is $O(\Delta x^2 + \Delta t)$. If the number of elements is increased with a factor 2, Δx^2 is decreased with a factor $2^{2/3}$. If the time step is also decreased with a factor $2^{2/3}$, then, in the limit, the error should decrease with a factor $2^{2/3}$ (≈ 1.6). The last column of Table 2 contains the relative error in the concentration after six hours in an arbitrary point in the domain with respect to the finest mesh. For the coarsest mesh, a time step of $\Delta t = 0.5$ h has been taken and this time step has been decreased while doubling the number of elements. The relative error decreases with a factor 1.6, 1.5, 1.6, 1.8 and 3.2, respectively. So in the limit, the error decreases with even more than a factor 1.6.

5 Conclusions and Discussion

An extension to 3D of the Biogrout model has been made. The results of the numerical simulation with the 3D configuration with three injection lances and three extraction lances look promising. Also the error analysis gives a good result.

For a small number of elements, building matrices takes more CPU time than solving the matrix vector systems. For a large number of elements it is the other way around. In building matrices, the amount of work increases linearly with the number of elements. If the number of elements increases further, it will be necessary to use an iterative method instead of a direct method.

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