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Coupling simulation of microbial growth and MICP phenomena based on reaction-diffusion system

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ABSTRACT

Microbially induced carbonate precipitation (MICP) has been recognized as that microbial metabolism may induce a generation of calcium carbonates in the pores and/or on the surface of sand particles. However, only actual observations approach of inner structures by microscopes are difficult to understand the MICP process. In the current work, we propose a mathematical and numerical simulation model based on the reaction-diffusion system and finite difference method, respectively in order to understand dynamically calcium carbonate precipitation process and relationship between bacterial growth and precipitation. As a result, some temporal and spatial precipitation structures of calcium carbonate such as active and inactive bonds structures were obtained through some numerical examples, which are in good agreement with the existing experimental results.

Keywords: MICP, microbial growth, ureolytic bacteria, reaction-diffusion system, coupling simulation

1 INTRODUCTION

In recent years, natural geo-disasters such as landslides, rock falls, and liquefaction have occurred frequently around the world, causing substantial damage to buildings and endangering human lives. Thus, soil improvement techniques have received widespread attention in both academic and industrial fields.

Against liquefaction, there are many practical soil improvement techniques such as sand compaction piles and chemical grouting, which could improve ground stability. However, these techniques have some environmental problems such as noise and vibration during construction, so that better soil improvement techniques are required.

Bio-mediated soil improvement techniques called as Microbially Induced Carbonate Precipitation (MICP) using microorganisms (e.g. cyanobacteria and ureolytic bacteria) have received substantial research attention (DeJong et al., 2006). It is reported that some species of microorganisms have induced to generate carbonate rock in natural environment around the world (Danjo and Kawasaki, 2016; Oshiro and Matsubara, 2018).

From previous study, it is well known that MICP induced by ureolytic bacteria is represented as shown in Fig. 1. In the urea hydrolysis reaction, \( \text{CO}_2^+ + \text{NH}_3 \rightarrow \text{CO}_2^- + 2\text{NH}_3 \).

Calcium carbonate from MICP phenomena can be observed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray microtomography (Terzis and Laloui, 2018). For example, previous research has shown that calcium carbonates are precipitated on the sand surface and between sand particles during the initial stage of solidification. However, the laboratory experiment and the microscopic observation might not reveal the dynamic behaviour of calcium carbonate because of some problems such as reaction time and/or spatial restrictions.

In contrast, Matsubara and Yamada (2020) proposed a mathematical simulation model of the urea hydrolysis reaction system based on the reaction–diffusion system, which dynamically reproduces the precipitation process of calcium carbonates during MICP. The simulated precipitation patterns on the sand particles were extremely similar to those obtained microscope observations. Moreover, both active and inactive bond patterns observed in X-ray microtomography (Terzis and Laloui, 2018) were successfully reproduced by this mathematical model. However, it is difficult to reveal precise precipitation phenomena from experimental results and compare them quantitatively because the
mathematical and numerical models were formulated under the dimensionless field. Additionally, the models were not consideration of growth of the bacteria in soil, so that it is difficult to understand detailed MICP phenomena. Therefore, in order to understand the relationship between MICP and growth of the bacteria, it is necessary to combine the models of chemical precipitation and bacterial growth, simultaneously.

In this study, a novel numerical scheme is proposed to combine the mathematical models for bacterial growth and chemical reaction system for metabolism of ureolytic bacteria, and elucidate the relationship between growth of the bacteria and MICP. Where to evaluate more detailed MICP phenomena, although, need to consider some factors (e.g., temperature and pH), temperature and pH is not considering in order to focused on calcium carbonate precipitation by bacterial growth in this study.

2 MATHEMATICAL MODELS

2.1 Growth of bacteria

In the field of mathematical biology, it is well known that the certain characteristics of bacterial colonies growing depend on agar plates and/or nutrition concentrations, colony patterns change greatly when the concentration changes (Matsushita et al., 1999). Also, bacterial colony patterns on an agar medium can be described by a mathematical model based on the reaction–diffusion system (Golding et al., 1998). Moreover, many bacteria are well known to exhibit chemotaxis to various substances, and move in the direction of a large or small concentration gradient of a substance.

Under such situation, the mechanism of colony formation has been elucidated by mathematical models based on the reaction-diffusion system (El-Sayed et al., 2009). Although many mathematical models have been proposed to date, the following mathematical model was employed as the governing equation of bacterial grows because the effect of both growth and chemotaxis are considered in this model (El-Sayed et al., 2009):

\[
\frac{\partial u}{\partial t} = D_u \nabla^2 u - \gamma \nabla \left( \frac{v c}{(c + 1)^2} u \right) + (\varepsilon - \mu)u
\]  

(1)

where \( D_u \) is the diffusion coefficient of ureolytic bacteria, \( \gamma \) is the coefficient of chemotaxis, \( c \) is the concentration of chemotaxis substance, \( \varepsilon \) is the growth rate of ureolytic bacteria, \( \mu \) is the competition coefficient. In this study, we assume that the chemotaxis substance of ureolytic bacteria is the urea.

2.2 Metabolism of ureolytic bacteria

The MICP phenomena is the chemical precipitation process of calcium carbonate, which is induced by a metabolic reaction (i.e. urea hydrolysis reaction) in the ureolytic bacteria. Hence, mathematical models of MICP phenomena should also focus on the urea hydrolysis reaction and the chemical precipitation reaction of calcium carbonate (Matsubara and Yamada, 2020).

MCIP by the urea hydrolysis reaction is described by the following equations (Matsubara and Yamada, 2020):

\[
\begin{align*}
\frac{k_1}{k_2} & \text{ COO(NH}_2\text{)}_2 + \text{H}_2\text{O} \rightleftharpoons \text{CO}_3^{2-} + 2\text{NH}_3 \\
\frac{k_3}{k_4} & \text{Ca}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{CaCO}_3
\end{align*}
\]

(2)

(3)

Eq. (2) denotes the urea hydrolysis reaction due to metabolism of ureolytic bacteria and Eq. (3) is a chemical reaction describing the precipitation of calcium carbonate. Considering the reaction, diffusion, and inflow terms in Eqs. (2) and (3), the mathematical model based on the reaction–diffusion system is described as follows (Matsubara and Yamada, 2020):

\[
\begin{align*}
\frac{\partial A}{\partial t} &= \frac{\partial}{\partial x} \left( \frac{D_A}{\partial x} A \right) - k_1 A B + k_2 C E^2 + A_{in} \\
\frac{\partial B}{\partial t} &= \frac{\partial}{\partial x} \left( \frac{D_B}{\partial x} B \right) - k_1 A B + k_2 C E^2 + B_{in} \\
\frac{\partial C}{\partial t} &= \frac{\partial}{\partial x} \left( \frac{D_C}{\partial x} C \right) - k_1 A B - k_2 C E^2 - k_3 C F_i + k_4 P \\
\frac{\partial E}{\partial t} &= \frac{\partial}{\partial x} \left( \frac{D_E}{\partial x} E \right) + k_1 A B - k_2 C E^2 \\
\frac{\partial F_i}{\partial t} &= \frac{\partial}{\partial x} \left( \frac{D_F}{\partial x} F_i \right) - k_3 C F_i + k_4 P + F_{in} \\
\frac{\partial P}{\partial t} &= k_3 C F_i - k_4 P
\end{align*}
\]

(4)

(5)

(6)

(7)

(8)

(9)

where A, B, C, E, F, F_i, and P denote the concentration of COO(NH)_2, H_2O, CO_3^{2-}, NH_3, Ca^{2+}, and CaCO_3, respectively. A_{in}, B_{in}, and F_{in} are the constant inflows of COO(NH)_2, H_2O, and Ca^{2+}, respectively. With respect to the rate-constants of the chemical reaction, \( k_1 \) and \( k_3 \) in Eqs. (2) and (3), respectively are defined as positive responses, whereas \( k_2 \) and \( k_4 \) are defined as negative responses in Eqs. (2) and (3), respectively. Moreover, \( D_i \) is the diffusion coefficient of the related variable *, which has spatially random values. It is noted that the diffusion of calcium carbonate was not considered in Eq. (9) because calcium carbonate is a solid.

In order to model a more accurate and detailed metabolic and chemical process of MICP, some chemical and environmental factors (e.g. pH, concentration of cementation solution, significance of complexation reactions and temperature) need to be considered. However, we focus on understanding of the relationship between calcium carbonate precipitation and bacterial growth, so that the influence of other factors were neglected in this study.

The rate-constant \( k_1 \) depend on the concentration of ureolytic bacteria, that is, this parameter should relate to Eq. (1). In this study, \( k_1 \) and the concentration of ureolytic bacteria u were related by the following linear equation:
\[ k_1 = \frac{k_{1,\text{max}}}{(u_{\text{max}} - u_{\text{min}})} \times u_i - \frac{k_{1,\text{max}} \times u_{\text{min}}}{(u_{\text{max}} - u_{\text{min}})} \]  

(10)

where \( k_{1,\text{max}} \), \( u_{\text{max}} \), and \( u_{\text{min}} \) are the maximum value of \( k_1 \), the maximum and minimum concentrations of ureolytic bacteria, respectively.

With respect to discretization, in this study, the diffusion operators and gradients of Eqs. (1), (4) – (8) are discretized using the finite difference method. Let us consider the following equation using a variable \( G \) and a coefficient \( D \).

\[
\frac{\partial G}{\partial t} = \nabla (D \nabla G) = \nabla D \nabla G + D \nabla^2 G 
\]  

(11)

In Eq. (11), the term on the left-hand side was calculated step by step using forward Euler integrations. The first term on the right-hand side was divided into two terms, and each term was discretized using the forward and reverse difference, respectively, as follows:

\[
\frac{G_i^{n+1} - G_i^n}{\Delta t} = \frac{1}{\Delta x^2} \left[ D_1 G_{i+1}^n - D_2 G_i^n + D_3 G_{i-1}^n \right] 
\]  

(13a)

\[
D_1 = D_{i+1} - D_i 
\]  

(13b)

\[
D_2 = D_{i+1} + 2D_i + D_{i-1} 
\]  

(13c)

\[
D_3 = D_i + D_{i-1} 
\]  

(13d)

where \( i \) is the grid number, \( \Delta t \) is the time increment, and \( \Delta x \) is the grid size.

3 NUMERICAL EXAMPLE

3.1 Simulation model and boundary conditions

Fig. 2 shows the numerical simulation model which size is 1 mm × 1 mm × 1 mm. Each axial direction (x, y, and z) of the model were divided into 64 (number of grid points: 274625). Additionally, eight spherical sand particles with a radius of 0.5 mm were set at each vertex in the model as shown in Fig. 2, and the boundary condition on the all surfaces of the model was assumed as periodic. We determined this model size assuming to understand and evaluate dynamically changing of the precipitation of calcium carbonate on the surface of 0.075 to 2.0 mm of sand particles in diameter.

In the simulation, the time increment (\( \Delta t \)) was set to 0.001 h, and the diffusion coefficients were randomly selected as \( D_A = D_C = D_E = D_B = 6.08 \times 10^{-3} \sim 2.56 \times 10^{-2} \text{ mm}^2/\text{h} \) (Boving and Grathwohl, 2001), and \( D_B = 3.60 \times 10^{-7} \sim 7.20 \times 10^{-5} \text{ mm}^2/\text{h} \). With respect to the parameters of bacterial growth in Eq. (1), the diffusion coefficient of ureolytic bacteria: \( D_u \) is \( 1.00 \times 10^{-4} \text{ mm}^2/\text{h} \), the growth rate: \( \varepsilon \) is 0.4/h, the competition coefficient: \( \mu \) is \( 2.0 \times 10^{-3} \text{ cells/h} \), and the coefficient of chemotaxis: \( \gamma \) is 2.5 mm/h.

Also, the reaction rate constants \( k_2 \), \( k_3 \), and \( k_4 \) are parameters that depend on the habitat environment of ureolytic bacteria. In this study, the \( k_2 \), \( k_3 \), and \( k_4 \) were set to the value of 0.001, 2.0, and 0.1 mm^3/μmol/h.

Further, amounts of nutrition (e.g. urea) are decided based on the experimental results by Martinez et al. (2013).

3.2 Simulation results and Discussions

Fig. 3 shows the growth of ureolytic bacteria in the model. It is observed that the bacteria are diffusing and growing on the surface of the sand particles at the initial time 2.4 h, 48 h.

Fig. 4. The concentration of calcium carbonate due to MICP at the elapsed times of 2.4 h and 48 h.

Fig. 5. Calcium carbonate distribution on a cross section of z = 0.625 mm at the elapsed times of 2.4 h and 48 h.
However, the concentration of bacteria decreases at the elapsed time of 48 h. On the other hand, according to Fig. 4, although there is hardly precipitation of calcium carbonate at the initial stage, much of calcium carbonate precipitates around the bacteria and the sand surface and pores at 48 h. Also, Fig. 5 shows the distribution of calcium carbonate precipitation on the cross section of $z = 0.625$ mm. It is observed from this figure that calcium carbonate precipitation occurs around the surface of sand particles where there are some active and inactive bonds. Many experimental studies have reported the precipitation of calcium carbonate on the surface of sand particles and/or between sand particles in the sandy soils (e.g. DeJong et al., 2010; Dadda et al., 2017). Also, it is interested that the bonding structures similar to those observed in Figs. 4(a) and 5(b) can be observed by the X-ray microtomography (Terzis and Laloui, 2018).

Fig. 6 shows the distribution of calcium carbonate concentration on the $y$-lines of three cross sections of $z = 0.625$ mm with the elapsed times 10.3, 24, and 48 h.

From these simulation results, MICP phenomena may occur around areas which the ureolytic bacteria have grown because large amounts of calcium carbonate are developed around these areas on the surfaces of sand particles. Furthermore, calcium carbonate precipitated at initial stage becomes origin points where the precipitation of calcium carbonate grows into pore region. Subsequently, the growing calcium carbonate bonds each sand particles as an active bond structure with the chemical reaction progresses.

The total amount of the calcium carbonate with elapsed time is shown in Fig. 7 where an experimental result by Martinez et al. (2013) is also illustrated. From this figure, the amount of calcium carbonate precipitation increased at initial stage, subsequently.
converges to a certain value. The convergence may be the cause that the concentration of the bacteria decreases with elapsed time. From Fig. 7(b), the simulation results would be valid because the results are close to the experimental values by Martinez et al. (2013). Although the rate constants should be determined based on experimental/field condition because these parameters depend on the habitat environment of ureolytic bacteria such as temperature, pH, and concentration of $\text{Ca}^{2+}$, the optimal values can be found through several parametric investigations as in this study.

4 CONCLUSIONS

This study provided a novel perspective on the MICP phenomena during the growth bacteria through a coupling scheme between microbial growth and chemical reaction models. Our interpretations of the simulation results are summarised as follow:

1. The proposed MICP simulation scheme considering the microbial growth can provide temporal and spatial precipitation structures of calcium carbonate and microbes.
2. The calculated concentration and spatial structures of calcium carbonate are in good agreement with existing experimental results.
3. The proposed technique can provide a growing process of an inactive and active bonds structures on the surface of sand particles and in the pores.

The proposed simulation scheme can be used to understand the relationship between the bacterial growth and MICP phenomena. However, future work will need to focus on the advection that considers bacterial movements, the electrical characteristics of the bacteria and several materials, and effecting pH, temperature, and other chemical reaction systems in the soil.

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