Preliminary Study on Dimensionless Expression of Bacterial Chemotaxis in Simulated Contaminated System

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Abstract. The use of chemotactic bacteria in bioremediation may improve the efficiency and decrease the cost of restoration of contaminated groundwater system. However, most previous studies focused at the laboratory scale and could hardly apply to the field scale. In this study, a dimensionless equation was formulated to solve this problem. First, the main influential factors were extracted from previous researches and then one set of dimensionless numbers was obtained based on Buckingham theory. After collecting parameter values and supplementing missing data, Chemotaxis number (Ch), the ratio of accumulated bacterial concentration to its initial value, was correlated with a combination of dimensionless numbers. For a Chemotaxis number greater than one, the bioremediation strategy is expected to be effective, and chemotactic bacteria are expected to accumulate around nonqueous phase liquid (NAPL) contaminant sources efficiently.

1. Introduction

Soil and groundwater polluted by refined petroleum products such as gasoline, kerosene, diesel, and lubricating oil has been frequently reported, like the oil spill in Gulf of Mexico, requiring appropriate measures to counteract their harmful effects on ecology and human health \cite{1}. Conventional physical and chemical treatments and remediation of petroleum refinery waste have been shown inefficient in eliminating genotoxicity of these pollutants. The use of chemotactic bacteria in bioremediation is theoretically a potential efficient and low-cost technology in restoring contaminated soils and groundwater. They have perceptions of contaminant concentration gradients in water and can make response to it by preferentially swim towards regions of higher contaminant concentration \cite{2}.

Bacteria can swim through aqueous media at speeds comparable to typical groundwater flow rates. At particularly low flow rates, chemotaxis may be the main influence factor on bacterial transport through advection-dominated systems, and direct microbial populations towards contaminants retained in regions of low permeability \cite{2}. In this study, we aim to acquire a Chemotaxis number, like Reynolds number, that can incorporate experimental results to evaluate the efficiency of chemotaxis and direct chemotactic biodegradation in the field application. We first extracted influential parameters in
bioremediation [3]-[5], and then would combine them into a dimensionless number based on Buckingham theory. When Ch number greater than one, chemotactic bacteria show greater accumulation near contaminated regions and can effectively degrade contaminant chemicals into nontoxic byproducts.

2. Dimensionless Analysis
This section presents the dimensionless analysis for all the parameters that controls bacterial chemotaxis in contaminated porous media as shown in Table 1. Parameters are extracted from previous researches about bacterial chemotaxis [2]-[5], and their values can be directly obtained from experimental results except for contaminant distribution and concentration gradient.

Table 1. Influential parameters in bioremediation.

| Factors          | Parameters          | Dimensional unit |
|------------------|---------------------|------------------|
| Media            | porosity, \( \varepsilon \) | \([-\] \) |
|                  | permeability, \( K \) | \([L^{-1}]\) |
|                  | tortuosity, \( \tau \) | \([-\] \) |
|                  | groundwater velocity, \( v_i \) | \([LT^{-1}]\) |
|                  | concentration, \( a \) | \([\text{Mol. } L^{-3}]\) |
| Chemoattractant  | concentration gradient, \( \Delta a/\Delta l \) | \([\text{Mol. } L^{-2}]\) |
|                  | diffusion coefficient, \( D \) | \([L^2T^{-2}]\) |
|                  | concentration, \( b \) | \([\text{Mol. } L^{-2}]\) |
|                  | motility coefficient, \( \mu \) | \([L^2T^{-1}]\) |
|                  | chemotactic sensitivity coefficient, \( \chi_c \) | \([\text{Mol. } L^{-1}]\) |
| Bacteria         | swimming speed, \( v \) | \([LT^{-1}]\) |

According to Buckingham theory, a function including all the parameters above can be written as,

\[
F(\varepsilon, K, \tau, a, \Delta a/\Delta l, D, b, \mu, \chi_c, K_v, v, \chi_a) = 0
\]

(1)

Then \( \chi_a \), \( K_v \) and \( \Delta a/\Delta l \) are selected as recurring parameters by means of linear algebra, and all the other parameters can be expressed as dimensionless \( \pi \) numbers accordingly,

\[
\pi_1 = \frac{K_v^2}{K(\Delta a/\Delta l)^2}, \pi_2 = \frac{K_v}{a}, \pi_3 = \frac{\chi_a}{D}, \pi_4 = \frac{K_v}{b}, \pi_5 = \frac{\chi_a}{\mu_{\text{eff}}}, \pi_6 = \frac{vK_v}{\chi_a (\Delta a/\Delta l)}, \pi_7 = \frac{v_i K_v}{\chi_a (\Delta a/\Delta l)}
\]

where tortuosity and porosity are incorporated into motility coefficient \( \mu_{\text{eff}} = \frac{\varepsilon}{\tau} \mu_0 \) [2]. Combine these dimensionless groups, and we can get the main dimensionless numbers that have influence on bacterial transport\(^6\) and may help us predict the bacterial distribution in contaminated layers.

\[
P_1 = \pi_1 = \frac{K_v^2}{K(\Delta a/\Delta l)^2}, P_2 = \pi_2 = \frac{\chi_a}{D}, P_3 = \pi_3 = \frac{vK_v}{\mu_{\text{eff}}}, P_4 = \pi_4 = \frac{K_v}{a}
\]

especially \( P_3 \) can further adopted to explain the difference in diffusion between chemotactic and nontochmotactic bacteria. As for \( P_5 \), researchers have found that bacterial chemotaxis is significant with typical groundwater velocity [2], [4]. In \( P_5 \), \( K_v \) and \( a \) are normally considered in the same order of magnitudes. \( P_1 \) combines the factors of bacteria, porous media and chemoattractant, and requires further studies to explore its significance on directing bacterial towards sources of contaminant.

Here we define Chemtaxis number \( \text{Ch} = \frac{b_{\text{bac}}}{b_0} \) as the ratio of accumulated bacterial concentration near contaminants to its initial value, and it is a combination of the influential parameters as the following [6],

\[
\text{Ch} = f(P_1, P_2, P_3, P_4) = \varepsilon P_1^a P_2^b P_3^c P_4^d
\]

(2)

3. Results and Discussion
In this study, we selected three papers about bacterial chemotaxis out of data integrity, and Table 2 displays the parameters available in X.Wang 2016 as an example.
Table 2. All the parameters available in X.Wang 2016.

| Bacteria       | $v_f$ (m/d) | $\varepsilon_p$ | $K$ (m$^3$) | $a$ (Mol/m$^3$) | $D$ (m$^2$/s) |
|----------------|-------------|-----------------|-------------|-----------------|---------------|
| *P. putida F1* | 0.25        | 0.43            | $1 \times 10^{-11}$ | 5.65            | $9.5 \times 10^{-10}$ |

3.1. Chemoattractant Concentration Gradient Acquisition via Numerical Simulation

However, we still need to get chemoattractant concentration distribution before we can figure out the exponents $x_1$, $x_2$, $x_3$ and $x_4$ in equation (2). We rebuilt numerical modules of the experimental devices in references within COMSOL and solved the distribution of attractant concentration.

3.1.1. Heterogeneous Contaminated Porous Media

Figure 1(a) is the rebuilt numerical module of microfluidic device used in X.Wang 2016 and steady chemoattractant distribution under specific groundwater velocity. NAPL droplets were trapped within a fine pore network, and bacterial suspension was injected through a highly conductive adjacent macrochannel. We exported the distribution along series of cut lines parallel to black dash line in Figure 1(a) and got concentration distributions of attractant as shown in the Figure 1(b).

![Figure 1](image1.png)

**Figure 1.** (a) Attractant distribution under 0.25 m/d; (b) Attractant distribution along black dash line.

It can be found the plotted data points around $y=0$ tend to be two lines with different slopes. $y=0$ represents the interface between porous media and groundwater flow path in the experiments, and we took the slope of line when $y<0$ as the concentration gradient $\Delta a/\Delta l$ in pore network.

3.1.2. Pore-scale Chamber with NAPL Source

Wang used microfluidic device to study the dissolution of an organic-phase contaminant from a single pore into a larger macropore and migration of microorganisms that were carried along by groundwater flow. Figure 2(a) is a magnification of region near NAPL/water interface. We simulated the chemoattractant concentration distribution in the vicinity of NAPL/water interface shown in Figure 2(b). Similar to the calculation of $\Delta a/\Delta l$ in X.Wang 2016, and we also obtained $\Delta a/\Delta l$ under different groundwater flow rates as shown in Figure 2(c).

![Figure 2](image2.png)

**Figure 2.** (a) Magnification of region near NAPL/water interface; (b) Chemoattractant concentration distribution in the vicinity of NAPL/water interface; (c) Chemoattractant concentration distribution in the vicinity of NAPL/water interface.

3.1.3. T-shaped Channel

Lanning used a T-shaped microfluidic device shown in Figure 3(a) to study chemotaxis transverse to advective flow. Two fluid streams, namely bacteria and attractant, were brought into contact by impinging flow, and then flowed adjacent to each other along a transparent channel. Figure 3(b) shows the attractant concentration distributes at specific flow rate, and (c) is chemoattractant concentration distribution vertical to the direction of stream flow.

![Figure 3](image3.png)
Figure 2. (a) NAPL/water interface; Attractant distribution in ROI (b) and along black dash line (c).

Figure 3. (a) T-shaped sensor; (b) T-shaped model; (c) Attractant distribution along black dash line.

Table 3 gives the concentration gradients of chemoattractant under different groundwater flow rates in discussed three papers.

|                  | \( v_f \) (m/s) | \( a_0 \) (mM) | \( \Delta a/\Delta l \) (Mol/m^4) |
|------------------|-----------------|----------------|----------------------------------|
| X.Wang 2016      | 0               | 5.79 \times 10^{-6} | 62.430 |
|                  | 5.79 \times 10^{-3} | 5.65             | 4.64 \times 10^{4}              |
| X.Wang 2012      | 5.79 \times 10^{-5} | 1.16 \times 10^{-3} | 3.13 \times 10^{4} |
|                  | 5.79 \times 10^{-5} | 5.65             | 3.51 \times 10^{4}              |
|                  | 1.16 \times 10^{-4} | 5.65             | 3.86 \times 10^{4}              |
| L.Lanning 2008   | 5.5 \times 10^{-3} | 0.1              | 20.041                          |
|                  | 5.5 \times 10^{-4} | 0.1              | 21.566                          |

3.2. Solution of Chemotaxis Number

The four dimensionless numbers \( P_1, P_2, P_3, P_4 \) are calculated accordingly and shown in Table 4, together with chemotaxis numbers directly obtained from published researches.

Table 4. Four dimensionless numbers and chemotaxis number in published articles.

|        | \( P_1 \)     | \( P_2 \) | \( P_3 \) | \( P_4 \) | \( Ch \) |
|--------|--------------|----------|----------|----------|--------|
| X.Wang 2016 | 3.79\times 10^6 | 7.17\times 10^3 | 0.177 | 0.132 | 826.83 | 1.05 |
|         | 4.64\times 10^3 |          | 1.315   |          |        | 1.02 |
| X.Wang 2012 | 1.307\times 10^3 | 1.135\times 10^3 | 0.177 | 0.132 | 826.83 | 1.05 |
|         | 1.038\times 10^3 |          | 1.315   |          |        | 1.02 |
|         | 8.570\times 10^{-4} |        | 2.630   |          |        | 1.02 |
| L.Lanning 2008 | 2.543\times 10^3 | 2.196\times 10^3 | 1.25  | 2.412 | 2232.56 | 1.788 |
|         | 1.25          |          | 24.123  |          |        | 1.7    |

The exponents and constant can be determined by fitting experimental and simulated results in previous section, and the chemotaxis number is solved.
From $P_3$ and its exponent, we found that accumulation of chemotactic bacteria will decrease with the increasing of groundwater velocity, which agrees with experimental results shown in Figure 4. In Figure 4, the groundwater flow rate increases steadily from left to right in each reference, and Ch number, namely the accumulated bacteria concentration around contaminants, all shows a decline trend. $P_1$ is under the influence of groundwater, and its exponent also accords with the trend in Table 4.

\[ Ch = 0.266 P_1^{0.2248} P_2^{0.0031} P_3^{0.0858} P_4^{0.4852} \]  

\[ (3) \]

**Figure 4.** Ch number under different groundwater rates in references

However, we are still not sure about the effects of $P_2$ and $P_4$ on the bacterial chemotaxis. Available research results are difficult to be put together since they were obtained under different experimental conditions. At this moment, we have designed microfluidic devices with three parts of different geological properties, resembling different layers in realistic groundwater system. Next we will conduct experiments on the devices to verify the Chemotaxis number, and study systematically the influential factors on chemotactic bioremediation.

4. References

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