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Adaptable method for estimation of parameters describing bacteria transport through porous media from column effluent data: Optimization based on data quality and quantity

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Abstract

Bacterial transport through porous media is often modeled using the colloid filtration theory with a Langmuirian blocking function (CFT-LB), with experimentally derived transport parameters being the collision efficiency, the blocking parameter, and the clean-bed breakthrough concentration. Research trends are moving towards comparing small variations in these parameters as a function of experimental conditions, and the objective of this study was to determine impact of experimental design, including number of data points and experimental duration, on the suitability of the CFT-LB model to provide sufficient resolution to permit these comparisons. The results indicate that while the CFT-LB model captures the general trends in bacterial transport data, there are cases where the CFT-LB model cannot replicate the details in the column effluent curves, and this results in the estimated transport parameters varying as a function of the experimental duration. Impacts of these variations on interpretation of the transport parameters are discussed, and a recommended procedure is provided when applying the CFT-LB model to column effluent data. Ultimately, when the CFT-LB model is used to estimate bacterial transport parameters, the process should be completely transparent, allowing the general reader to know exactly how the transport parameters were obtained from the experimental data.

Keywords: Colloid filtration theory; Langmuirian blocking; Bacterial transport; Packed bed; Collision efficiency

1. Introduction

Bacterial transport through porous media is an important process in both natural and engineered systems. Applications include enhancement of in situ biodegradation through injection of acclimated bacteria, movement of pathogenic organisms from septic tanks and leach fields to drinking water wells, and removal of pathogenic organisms from drinking water via sand filtration. The field is progressing rapidly. It has moved beyond simple experiments examining how ionic strength affects bacterial transport to research areas that include how the distribution of properties across a bacterial population affect transport [1–4] and modeling transport parameters using complex colloid interaction models, such as the secondary minimum approach with the DLVO theory [5–7].

The standard approach for interpreting bacterial transport data is to apply the colloid filtration theory (CFT), which accounts for flow of a bacterial suspension through porous media, transport of bacteria from the bulk fluid to the surface of the porous media grains, and adhesion of the bacteria to the grains. One key assumption of the CFT is that the porous media is operating under "clean bed" conditions, which means that bacteria approaching the porous media surface do not interact with bacteria already adhered to the surface. Given a well-defined system, the CFT relates the normalized clean-bed bacterial concentration, $[C/C_o]_{\text{clean-bed}}$, at a given transport distance in the porous media to the collision efficiency, depicted by the symbol α (details of the CFT are provided below in Section 2). The collision efficiency ranges from zero to one and defines the probability that a bacterium will adhere to a surface upon collision.

Many studies have viewed α as a single value and examined how α changes as a function of experimental conditions, and this is a valid approach when considering a fixed transport distance (e.g., column length). However, recent studies have found that α can often be represented as a distributed param-

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eter (e.g., bimodally or lognormally distributed), and as such the apparent collision efficiency will vary as a function of column length [2,3,8]. These studies of the distributed nature of α have provided insight into the long-distance transport of bacteria through porous media. When conducting laboratory studies using columns containing a porous media, such as sand, one means to determine α is to analyze the column bacterial effluent concentrations with the CFT. If α is assumed to be a single parameter, it can be calculated directly from $[C/C_o]_{\text{clean-bed}}$ via the CFT. If α is assumed to be a distributed parameter, the distribution variables (e.g., mean and standard deviation for the normal distribution) can be calculated given $[C/C_o]_{\text{clean-bed}}$ values from multiple columns of different lengths [8].

The clean-bed assumption of the CFT is only truly valid during the initial passage of the bacterial suspension through the porous media [9], and it is now relatively well known that adhered bacteria tend to prevent, or block, approaching bacteria from adhering to the surface [10–12]. The CFT is often modified to account for this blocking effect through use of a Langmuirian blocking term [9–12], which is a function of the amount of bacteria already deposited on the porous media at any point in the column. The key parameter that defines this process is the Langmuirian blocking parameter, β. Thus, when fitting the CFT with Langmuirian blocking (CFT-LB) model to experimental data, the experimentally derived parameters are β and either α or $[C/C_o]_{\text{clean-bed}}$. Details of the CFT-LB model are provided in Section 2 below.

Current trends in bacterial transport research are moving towards comparing small changes in the transport parameters as a function of experimental conditions. One example is the determination of the collision efficiency distribution across a bacterial population, which requires analysis based on changes in either α or $[C/C_o]_{\text{clean-bed}}$ with transport distance [2,3,8]. Another example is the effects of surfactant structure and concentration on both α and β for a given experimental system [12]. These applications require an accurate means to determine the transport parameters and their associated errors.

There are a number of practical issues that must be considered when applying the CFT-LB model to bacterial systems. First, while it has been shown that the effects of dispersion on bacterial transport at the lab-scale are negligible [13], it can impact the determination of $[C/C_o]_{\text{clean-bed}}$ when blocking occurs, especially when the blocking results in a steep rise in the column effluent after breakthrough. Second, there are instances where the column effluent concentrations over time showed a more complex relationship than can be accurately described by the Langmuirian blocking term [12,14], and the experimental duration may thus have an effect on the determination of the transport parameters. Finally, it is not well known how data quality and quantity affect the calculated parameter values and their associated confidence intervals.

Given these issues, the objectives of this study were to examine the ability of the CFT-LB model to fit bacterial transport data, and to demonstrate how data quality and quantity affect the calculated transport parameters and their 95% confidence intervals. To achieve this goal, the CFT-LB model was fit to a high-resolution, low-noise dataset, consisting of column effluent curves from eight individual bacterial transport experiments. The ability of the CFT-LB model to fit the effluent curves was assessed as a function of the number of data points and the experimental duration. Additionally, as the dataset exhibited very low noise, ±5% uniform random noise was also added to the data in order to simulate the variability often observed when direct counts are used to quantify the bacterial concentrations [15,16]. This allowed determination of how noise affects the calculated transport parameters. Finally, a recommended procedure for obtaining transport parameters from column effluent curves with the CFT-LB model is discussed.

2. Numerical model

The colloid filtration theory was developed to understand and predict colloid (bacteria) removal in packed beds. It assumes a first-order rate of removal of the form

$$\frac{\partial C}{\partial x} = -\lambda C \quad (1)$$

where C is the bacteria concentration and λ is the filter coefficient. The filter coefficient is a function of the flow conditions and the porous media, bacteria, and fluid properties and can be written as [17]:

$$\lambda = \frac{3}{2}\frac{(1-\theta)}{d_c}\alpha\eta_o \quad (2)$$

where, d_c is the collector diameter (i.e., porous media grains), θ the porosity, α the collision efficiency, and η_o is the collector efficiency. The approach of the bacteria to the collector surface is described by η_o and α describes the attachment of the bacteria to the collector. When performing bacterial transport experiments, α is typically the empirical parameter being measured, while η_o is determined from theoretical calculations. A number of expressions for η_o have been developed and excellent discussions are provided by Logan et al. [17] and Tufenkji and Elimelech [18]. The equations used to calculate η_o in this study are provided in the appendix.

In order to account for the blocking effect, where previously adhered bacteria prevent approaching bacteria from adhering to the surface, a Langmuirian term is often used to modify the filter coefficient [9–12]:

$$\lambda = \lambda_o(1 - \beta\sigma) \quad (3)$$

Here, λ_o is the filter coefficient given by Eq. (2), β is the blocking parameter and σ can either be defined as the specific deposit of bacteria on the porous media (volume of bacteria deposited per unit filter volume) [9] or the fractional collector surface coverage (projected area of deposited bacteria per unit surface area of collectors) [10,11,19].

There are a number of different ways to incorporate the colloid filtration theory with Langmuirian blocking (CFT-LB) into bacterial transport models. One is to incorporate it as a loss term in the advection-dispersion equation [20]. This allows analysis of non-steady-state bacterial transport and requires a discrete numerical model of the experimental column. Two simplifications are often used to allow an analytical solution to be obtained.