Parameter estimation in biofilm models

Alma Masic, Niels Chr. Overgaard, Anders Heyden

Applied Mathematics Group, Malmo University, 20506 Malmo, Sweden;
alma.masic@ts.mah.se, nco@ts.mah.se, heyden@ts.mah.se

Keywords: biofilm models, parameter estimation, moving bed reactor, detachment

Mathematical modeling of biofilm development has been an active research topic during the latest years. The main purpose of these models is to understand and predict biofilm growth and development. One of the first mathematical model was the so called Wanner-Gujer model, presented in [4], where a one-dimensional model capable of describing multiple species development was proposed. Later on, more advanced models, incorporating more dimensions, eps-production, cell-to-cell-signalling and other properties have been developed. cf. [2]. The major obstacle when trying to predict biofilm development using these mathematical models is that a huge number of parameters are needed, such as parameters in the bacterial metabolism, growth and detachment rates. Some of these parameters are possible to measure in experimental conditions, but others are more difficult, such as the detachment rate. In this paper, we will propose a methodology for estimating parameters in mathematical models of biofilm development from comparison of model prediction and experimental data. The proposed method is based on parameter identification methods used in automatic control theory, see [3]. We will especially focus on the determination of the detachment rate in the Wanner-Gujer model.

The model proposed in [4] considers a one-dimensional biofilm growth in the direction $z > 0$. The biofilm consists of $N_B$ bacterial species and $N_S$ different substrates, where $f_i$ denote the volume fractions of the different species. The model is based on a conservation law for both the substrates and the biomass, which results in

$$\frac{\partial f_i}{\partial t} + u \frac{\partial f_i}{\partial z} = (\mu_{Oi} - \bar{\mu}_O)f_i, \quad i = 1, \ldots, N_B ,$$

(1)

where $\mu_{Oi}$ denote the specific growth rate, $\bar{\mu}_O$ denotes the average growth rate and $u$ denotes the velocity field, defined by

$$u = \int_0^z \bar{\mu}_O(z')dz' ,$$

(2)

and the corresponding equations for the substrates

$$\frac{\partial S_k}{\partial t} + \frac{\partial}{\partial z}(D_k \frac{\partial S_k}{\partial z}) = r_k, \quad k = 1, \ldots, N_S ,$$

(3)

where $D_k$ denote the diffusivities and $r_k$ the consumption rates. The thickness of the biofilm, $L(t)$ evolves according to

$$\frac{d}{dt}L = u(t, L) - \sigma L^2 ,$$

(4)

where $\sigma$ denotes the detachment rate.

We propose to estimate parameters by observing substrate concentrations, $S_k$, from real experiments and compare them with substrate concentrations predicted from the mathematical model, $\hat{S}_k(p_1, \ldots, p_n)$, where $p_i$ denote the unknown parameters, obtained from (1)–(4) under $N_C$ different running conditions. The optimal estimate of the parameters is obtained by minimizing the functional

$$\min_{p_1, \ldots, p_n} V(S_k, \hat{S}_k) = \min_{p_1, \ldots, p_n} \sum_{j,k} (S^j_k - \hat{S}^j_k)^2 ,$$

(5)
where the index $j$ denotes the different running conditions. In continuous time the functional in (5) can be replaced by the corresponding integral. The actual optimum is found by calculating the first order variation, $dV$ of the functional in (5) and applying a gradient descent method resulting in the following differential equation

$$\frac{dp_i}{d\tau} = -dV(p_i(\tau)),$$

where $\tau$ denotes artificial time.

The proposed method will be used to estimate the detachment rate in a moving bed biofilm reactor for waste water treatment presented in [1], see Fig. 1 for an illustration of the predicted and measured nitrification rates. Based on the Wanner-Gujer model in (1)–(4) and the gradient descent scheme for solving (5), we will estimate the detachment rate.

**References**


