Mathematical Modeling, Laboratory Experiments, and Sensitivity Analysis of Bioplug Technology at Darcy Scale

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Summary

In this paper we study a Darcy-scale mathematical model for biofilm formation in porous media. The pores in the core are divided into three phases: water, oil, and biofilm. The water and oil flow are modeled by a generalized version of Darcy’s law and the substrate is transported by mechanical dispersion, diffusion, and convection in the water phase. Initially, there is biofilm on the pore walls. The biofilm consumes substrate for production of biomass and modifies the pore space which changes the rock permeability. The model includes detachment of biomass due to water flux and death of bacteria, and it is implemented in the MATLAB Reservoir Simulation Toolbox (MRST). We discuss the capability of the numerical simulator to capture results from laboratory experiments. We perform a novel sensitivity analysis based on sparse-grid interpolation and multi-wavelet expansion to identify the critical model parameters. Numerical experiments using diverse injection strategies are performed to study the impact of different porosity/permeability relationships in a core saturated with water and oil.

Introduction

After primary and secondary production, up to 85% of the oil remains in the reservoir (Patel et al. 2015). Microbial improved and enhanced oil recovery (MIEOR) is one of the secondary and tertiary methods to increase the oil production using microorganisms (Wood 2019). Bioplug technology is an MIEOR strategy that comprises plugging the most permeable zones in the reservoir, which provokes water to flow through new paths, and recovering the oil in these new zones. However, microorganisms could also form biofilms in undesirable zones in the reservoir leading to negative effects such as reduction of water injectivity. Therefore, understanding the mechanisms involved in the development of biofilms is important to control their formation.

The bioplug technology is intended for use on the field scale, but to perform field scale experiments is both time consuming and economically infeasible. Experiments in microsystems allow us to observe processes in greater detail, which leads to improvement of the experimental methods in core-scale experiments prior to field applications. For example, in Liu et al. (2019) the effects of flow velocity and substrate (also referred to as nutrients/food) concentration on biofilm in a microchannel was studied, finding values of substrate concentration and flow velocity for a strong plugging effect. Core samples from reservoirs can be used to study changes in permeability due to biofilm formation, e.g., in Suthar et al. (2009) two-phase flow experiments were performed to study the selective plugging strategy for MIEOR. In that study, the MIEOR effects increased the oil recovery around 25%.

Mathematical models of bioplug technology are important as they help to predict the applicability of this MIEOR strategy and to optimize its benefits. In Kim (2006) a mathematical model for single-phase flow was proposed which includes changes of rock porosity and permeability as a result of biofilm growth. The author calibrated the model using data from experiments in silica sand columns and performed a simple sensitivity analysis (one-at-a-time technique) of a few model parameters. Li et al. (2011) built a mathematical model for two-phase flow including the effects of bio-surfactants and biomass on improving the oil recovery. The authors also performed a simple sensitivity analysis of a few model parameters and compared the numerical results for two different porosity/permeability relationships. They concluded that MIEOR could enhance the oil recovery substantially if a larger capillary number is achievable. Nielsen et al. (2016) built a two-phase flow mathematical model for MIEOR that included reduction of oil-water interfacial tension by produced surfactants and selective plugging by microbes and metabolic products. The authors studied the oil recovery for diverse injection strategies changing the pore volumes injected and substrate concentration at a fixed flow rate. In Dzianach et al. (2019) the authors present a recent review of mathematical models of biofilms for diverse purposes. They concluded that the cooperation between various disciplines is required to develop novel models. In this work, we present a two-phase core-scale model of bioplug technology. To our knowledge, this is the first mathematical model for two-phase flow and permeable biofilm. This mathematical model is the result of a research project where microbiologists,
physicists, chemists, and mathematicians were involved. A detailed description of this project and previous publications can be found in Landa-Marbán (2019). In contrast to Li et al. (2011), in this work we perform simulations to find at which part (low, medium, or high porosity) of five porosity/permeability relationships the oil recovery is more sensitive. Unlike Nielsen et al. (2016), we study the oil recovery for several injection strategies changing the substrate concentration, flow rate, and injection direction.

Sensitivity studies of mathematical models are of great interest because they provide estimates of the influence of the inputs (e.g., physical parameters) on a quantity of interest (e.g., biofilm formation). In Brockmann et al. (2006) a regional steady-state sensitivity analysis was performed to identify parameters with the largest impact on a mathematical model for deammonification in biofilm systems. Sensitivity analysis by means of Sobol decomposition provides rigorous estimates of parameter dependencies, but are prohibitively expensive to compute if the number of parameters is large. This is remedied for smooth problems by first computing spectral (generalized polynomial chaos) expansions in the parameters, which then leads to efficient evaluation of the sensitivity indices via post-processing of spectral coefficients (Sudret 2008). The latter method was employed in Landa-Marbán et al. (2019), where a global sensitivity analysis was performed using Sobol indices to identify the critical parameters of a pore-scale model for permeable biofilm. In this paper, we introduce a different approach which can be also used for nonsmooth mathematical models in the dependent parameters, where spectral expansions with global smooth basis functions are not a robust choice. We propose a two-stage method where we first use sparse grids to estimate a piecewise linear interpolant of the function of interest, which yields a surrogate that can be further sampled at negligible cost. Secondly, we compute a multi-wavelet representation of the interpolant, from which the sensitivities can be directly evaluated.

The mathematical model consists of equations for the mass balance equations for two flowing phases (water and oil), the transport of substrate (nutrients/food for the bacteria), and the formation of biofilm. In addition, mathematical relationships between different variables (like the porosity/permeability relationship) are assumed, resulting in a coupled system of nonlinear partial and ordinary differential equations, or algebraic equations. Two-point flux approximation (TPFA) and backward Euler (BE) are used for the space and time discretization respectively. To solve the resulting nonlinear algebraic system, Newton’s method is used. The scheme is implemented in the MATLAB Reservoir Simulation Toolbox (MRST), a free open-source software for reservoir modeling and simulation (Lie 2019).

To summarize, the new contributions of this work are:

- The formulation of a core-scale mathematical model for two-phase flow and permeable biofilms.
- The description, publication of data, and comparison to numerical simulations of a core-scale experiment including biofilm formation.
- The introduction of a robust sensitivity analysis for nonsmooth mathematical models.
- The study of the impact of diverse porosity/permeability relationships and substrate injection strategies on the bioplug technology.
- The application of the proposed sensitivity analysis in the mathematical model.

The paper is structured as follows. Firstly, we introduce and describe the implementation of the core-scale mathematical model for two-phase flow including the effects of biofilm formation. Secondly, we present a comparison of numerical simulations to laboratory experiments of this core-scale model. Thirdly, we introduce a novel method for sensitivity analysis and apply it to the mathematical core-scale model. Diverse numerical experiments for different porosity/permeability relationships and injection strategies are also explained. Finally, we present the conclusions.

Core-Scale Model

We consider a core sample of radius $r$ and length $L$ initially filled with oil and water and a given biofilm distribution. Fig. 1 shows the schematic representation of this system. As water and substrate are injected, some biomass is detached due to erosion (shear forces caused by the water flow). The biofilm consumes substrate to produce metabolites (i.e., gases) and to grow, which modifies the rock porosity and hence the rock permeability. Consequently, the flow pattern is modified in the sense that pores where oil was replaced by water, and which were forming a preferential path for water flow, become less permeable. Therefore water enters other pores, mobilizing the oil present there and leading to improved oil production. The mathematical model presented in this section aims to describe the following processes in a core after bacterial inoculation: two-phase flow, substrate transport, substrate consumption by the bacteria, permeability changes due to porosity modification, and biofilm growth, detachment, and death.
We assume that the fluids are immiscible and incompressible. We consider that the biofilm has water (θ_w) and biomass (θ_b) (bacterial cells and extracellular polymeric substances (EPS)) as the only two components, and that the biofilm porosity (Φ_b) and biofilm permeability (k_b) are constants. Thus, θ_w and θ_b are also constants and Φ_b = θ_w. In this work we use θ_w for referring both biofilm water content and biofilm porosity indistinctly, as the two are equal and constant. In order to determine the amount of fluid outside the biofilm in the representative element volume (REV), we introduce the saturation of a fluid S_α (for oil α = o and for water α = w) given by the ratio of volume of fluid α outside the biofilm over the volume of voids outside the biofilm (in REV). For this two-phase flow model, we have that S_o + S_w = 1. Fig. 2 shows the nomenclature and the biofilm representation at different scales.

Fig. 1—Core sample for laboratory experiments after inoculation of bacteria.

![Diagram](image-url)

**Fig. 2**—Biofilm representation at different scales.

The mass conservation and generalized Darcy’s law for the oil phase are given by

$$\frac{\partial}{\partial t}(\rho_f S_o) + \nabla \cdot (\rho_o \vec{v}_o) = Q_o, \quad \vec{v}_o = -\frac{k_{r,o}}{\mu_o} (\nabla p_o - \rho_o g),$$  

(1)

and for the water phase

$$\frac{\partial}{\partial t}[\rho_w (\phi_f S_w + \phi_b \theta_w)] + \nabla \cdot (\rho_w \vec{v}_w) = Q_w, \quad \vec{v}_w = -\frac{k_{r,w}}{\mu_w} (\nabla p_w - \rho_w g),$$  

(2)

where φ_f is the porosity outside the biofilm, v_o the flow velocity, k_{r,o} the relative permeability, ρ_o the fluid density, k the absolute rock permeability, g the gravity, μ_o the viscosity, φ_b the volume fraction of biofilm in the REV, θ_w the biofilm water content, and Q_o is a source/sink term. The minimum value of φ_b is zero while the maximum value of φ_b is equal to the initial porosity of the rock φ_0, corresponding to the case when the pores are filled with biofilm. The first term in Eq. 2 gives the changes over time for the total water mass in the REV, i.e., the water outside the biofilm (ρ_w φ_f S_w) plus the water inside the biofilm (ρ_w φ_b θ_w).

Several porosity/permeability relationships have been proposed during the last decades. One possibility is to derive such relationships by upscaling, starting with models valid at the pore scale (see e.g. Golfier et al. (2009); Landa-Marbán et al. (2020); Schulz and Knabner (2016); van Noorden et al. (2010); Wood and Ford (2007)). Alternatively, such relationships have also been proposed directly at the Darcy scale, based on experimental evidence. We refer to Hommel et al. (2018) for a recent review of these relationships. Three porosity/permeability
relationships commonly used in modeling are the following:

\(
\frac{k_p}{k_0} = \left( \frac{\phi_f}{\phi_0} \right)^\eta, \quad \frac{k_{vp}}{k_0} = \left( \frac{\phi_f - \phi_{crt}}{\phi_0 - \phi_{crt}} \right)^\eta, \quad \frac{k_b}{k_0} = a \left( \frac{\phi_f - \phi_{crt}}{\phi_0 - \phi_{crt}} \right)^3 + (1 - a) \left( \frac{\phi_f - \phi_{crt}}{\phi_0 - \phi_{crt}} \right)^2,
\)

where \(k_0\) is the absolute rock permeability in the clean pores. The first one \((k_p)\) is called the power law (Carman 1937; Ives and Pieuvichir 1965), where \(\eta\) is a fitting factor calibrated either from experimental data or taken from a process-specific literature. The second relationship \((k_{vp})\) is a variation of the power law known as the Verma-Pruess relationship (Verma and Pruess 1988), where \(\phi_{crt}\) is a critical porosity when the permeability becomes zero, which value is between 70 and 90% of the initial porosity. The third relationship \((k_b)\) is proposed by Thullner et al. (2002), where \(a\) is a weighting factor between -1.7 and -1.9. These three relationships do not include the biofilm permeability. Since the biofilm is considered to be a porous medium, it is assumed to have permeability and a porosity, which are related through a porosity/permeability relationship. An example is the Brooks-Corey relationship (Brooks and Corey 1964)

\[
P_r(S_w^*) = p_e(S_w^*)^{-1/\beta}, \quad k_{r,w}(S_w^*) = (S_w^*)^{(3+2/\beta)}, \quad k_{r,o}(S_o^*) = (S_o^*)^{(1+2/\beta)},
\]

where \(p_e\) is the entry pressure and \(\beta\) is a fitting parameter. The effective water \(S_w^*\) and oil \(S_o^*\) saturations are given by

\[
S_w^* = \frac{S_w - S_{wi}}{1 - S_{or} - S_{wi}}, \quad S_o^* = \frac{S_o - S_{or}}{1 - S_{or} - S_{wi}},
\]

where \(S_{wi}\) is the irreducible water saturation and \(S_{or}\) the residual oil saturation. Given that water is a biofilm component and we consider permeable biofilms, there is water flux inside the biofilm even when there is only residual water saturation outside the biofilm. Then, the previous relationship does not provide an accurate representation because for \(S_w^* = S_{wi}\) it results in \(k_{r,w}(0) = 0\) which leads to zero water velocity. Recalling that the relative permeabilities are used to extend Darcy’s law to multiphase flow, we look for relationships which account for the water saturation and volume fraction of biofilm. These relationships need to fulfill the following criteria: when there is only oil and residual water saturation outside the biofilm, then \(k_{r,w}(S_w^* = 0, 0 < \phi_b < \phi_0) > 0\); when there is only biofilm in the pores of the rock, then \(k_{r,w}(S_w^* = 0, \phi_b = \phi_0) = 1\) and \(k_{r,o}(S_o^* = 0, \phi_b = \phi_0) = 0\). Here, we recall that the effect of the biofilm on the absolute rock permeability is given by porosity/permeability relationships and the effect on the flow of each phase by the presence of the other phases is given by the relative permeabilities. Then, we propose the following two relative permeability relationships:

\[
k_{r,w}(S_w^*, \phi_b) = (S_w^*)^{(3+2/\beta)} \left( 1 - \frac{\phi_b}{\phi_0} \right) + \left( \frac{\phi_b}{\phi_0} \right), \quad k_{r,o}(S_w^*, \phi_b) = (1 - S_w^*)^{(1+2/\beta)} \left( 1 - \frac{\phi_b}{\phi_0} \right).
\]

These relationships are proposed as a first effort to extend the concept of relative permeabilities in two-phase flow to include the effects of permeable biofilm in porous media. To formally derive effective relationships for two-phase flow at the Darcy scale (such as relative permeabilities and capillary pressures), we can apply upscaling.
techniques from pore-scale two-phase flow models including biofilms which is part of our future work. As an alternative approach, not involving upscaling from the pore to core scale, the dual-permeability formulation could be used to model this system (Barenblatt et al. 1960; Warren and Root 1963).

To describe the movement of substrate, assuming that the aqueous phase density does not depend on the substrate concentration, we consider the following convection-dispersion-reaction transport equations:

$$\frac{\partial}{\partial t} [C_n(\phi_f S_w + \phi_b \theta_w)] + \nabla \cdot \vec{j}_n = R_n, \quad \vec{j}_n = -D_n(\phi_f S_w + \phi_b \theta_w)\nabla C_n + C_n \vec{v}_w. \quad (9)$$

In the previous equations, $C_n$ is the substrate concentration (mass over volume) in the water, $\vec{j}_n$ the substrate flux in water, and $D_n$ the substrate dispersion tensor which includes mechanical dispersion plus diffusion given by (Bear 1972)

$$D_n = \alpha_T ||\vec{v}|| I + (\alpha_L - \alpha_T) \frac{\vec{v} \otimes \vec{v}}{||\vec{v}||^2} + D_n I \quad (10)$$

where $\alpha_L$ and $\alpha_T$ are the longitudinal and transverse dispersion coefficients, respectively, $\vec{v} = \vec{v}_w/(\phi_f S_w + \phi_b \theta_w)$ is the fluid velocity of the aqueous phase, and $D_n$ the molecular diffusion coefficient of substrate. In Landà-Marbán et al. (2020) Eq. 9 is derived by homogenization after starting from a pore-scale mathematical model for a permeable biofilm, and including only molecular diffusion. The conditions at the biofilm-fluid interface taken there are the conservation of mass (the Rankine-Hugoniot condition) and the continuity of the substrate concentration. Therefore, at both sides of the interface, the substrate concentrations in the water inside and outside the biofilm are the same and the substrate mass transfer into biofilm is determined by the conservation of mass across a moving interface.

The reaction term $R_n$ is given by (Monod 1949)

$$R_n = -\mu_n \frac{C_n}{K_n + C_n} \rho_b \phi_b \quad (11)$$

where $\mu_n$ is the maximum rate of substrate utilization, $\rho_b$ the biomass density, and $K_n$ is the Monod half-velocity coefficient.

The following equation describes the biofilm evolution (Landa-Marbán et al. 2020; Taylor and Jaffé 1990; Thullner et al. 2004):

$$\frac{\partial}{\partial t} (\rho_b \phi_b) = \begin{cases} f^- (Y_{bn} \mu_n \frac{C_n}{K_n + C_n} \rho_b \phi_b - K_d \rho_b \phi_b), & \phi_b = \phi_0 \\ y_{bn} \mu_n \frac{C_n}{K_n + C_n} \rho_b \phi_b - K_d \rho_b - K_{str} \phi_f S_w || \nabla p_w - \rho_w \vec{g} || \rho_w \phi_b, & 0 < \phi_b < \phi_0 \\ 0, & \phi_b = 0. \end{cases} \quad (12)$$

Here, we assume that only a part of the consumed substrate is used to produce biomass, as given by the yield coefficient $Y_{bn}$. Further, the bacterial death rate is linear and given by $K_d$, and the bacterial erosion depends on the pressure gradient and on the gravity times a biofilm constant $K_{str}$. The negative cut-off function ($f^-(x) = \min(0, x)$) appearing in Eq. 12 guarantees that the biofilm does not cross the pore walls. Thus, in the case of plugging, the biofilm decreases its volume only when bacterial death surpasses the biofilm growth. After biomass has been detached, in this model we assume that the detached biomass flows out of the core and does not affect the rock properties; therefore, we do not include a transport equation for the detached biomass.

The porosity in the porous medium changes in time as a function of the biofilm volume fraction $\phi_b(t)$. When there is no biofilm, the porosity $\phi_f(t)$ is equal to the initial porosity. In the case when the porous medium is filled with biofilm ($\phi_f(t) = 0$), the porosity in the REV is equal to the biofilm porosity $\theta_w$. The porosity/permeability relationships in Eqs. 4 and 5 are given as a function of the rock porosity and do not include the biofilm porosity. The porosity/permeability relationships $k_c$ and $k_t$ do include the biofilm porosity. Using the definitions of $\phi_f(t)$ and $\phi_b(t)$, we have the following relationship for the void space outside the biofilm

$$\phi_f(t) = \phi_0 - \phi_b(t). \quad (13)$$

For the numerical simulations based on the model proposed here we use the EOR module in MRST, a MATLAB®-based open source software for reservoir modeling and simulation (Lie 2019). A comprehensive discussion of the solution of the polymer model can be found in Bao et al. (2017). The mathematical model is solved in a 3D domain with cell-centered grids. Two-point flux approximation (TPFA) and backward Euler (BE) are used for the space and time discretization respectively. The resulting system of equations is linearized using the Newton-Raphson method and the porosity value is taken from the previous time step. In contrast to the polymer model, we implement diffusion and dispersion of the transported component, permeability changes due to biofilm formation, and biofilm detachment due to shear forces. This mathematical model has been upscaled.
from a pore-scale model based on pore-scale laboratory experiments. Discretization of field-scale domains into core-scale grids is computationally infeasible. Then, upscaling techniques can be applied to derive coarser models in order to reduce the computational time of simulations which remains an area of active research. The general idea is to replace several cells and their physical properties (e.g., porosity, permeability) by a single cell covering the same space than all smaller cells, where this larger cell represents in some averaged sense the different physical properties of the smaller cells. Then, the simulations can be performed on coarse models which have significant advantages in terms of using the available computational resources running a larger number of model realizations to perform sensitivity analysis, the upscaled models are easier to calibrate (fewer parameters), and their numerical predictions may be enough to make a certain business decision (Lie 2019).

**Model Test**

Core-scale experiments under controlled conditions are performed in the laboratory for studying the effect on biofilm growth in porous media. These experiments aim to provide a better understanding of different features, e.g., the relationship between biofilm composition and growth conditions, the plugging potential of different bacteria, and the adaptability of biofilm at diverse substrate flux.

In this section, we describe an experiment performed by NORCE Norwegian Research Centre AS for Equinor ASA. The aim of the study was to assess the bioplug potential in porous media while flooding with brine qualities differing in nutrient load and ion composition. The biofilm originated from inoculation of fresh native seawater, thus allowing natural selection of biofilm composition as respond to injected brine. The core has a length of 29.50 cm and a radius of 1.90 cm. Initially, the core has an approximately homogeneous porosity of φ₀ = 0.23 and permeability k₀ = 1528 md. The core sample is introduced inside a core holder, fully saturated with brine. Heating cables wrapped around the exterior of the core holder are used to conduct the experiments at a constant temperature (30°C). Starting from the core inlet, the length of the different core sections are 2.30, 5.10, 5.00, 10.60, and 6.50 cm respectively. A backpressure regulator (BPR) is used to control the line pressure. The inoculum from fresh native seawater was injected into the core filling the entire pore volume. The core was left standstill overnight to allow the bacteria to attach themselves to the pore walls. Fig. 3 shows a diagram of the experimental set-up.

**Fig. 3—Scheme of an experimental set up for laboratory experiments. BPR = backpressure regulator.**

The core is injected with two types of brines with different substrate compositions of glucose and organic acids (carbon source). The substrate composition in the brines are B₁ = 0.48 kg/m³ (glucose) and B₂ = 0.72 kg/m³ (glucose + organic acids). The brines were flushed with nitrogen to reduce oxygen content before injection. Both brines contained low amounts of sulphate as only available electron acceptor for anaerobic respiration. The two different brines are injected at a constant flow rate of 8.33×10⁻¹⁰ m³/s (Darcy velocity of 6.4 cm/d). The injection strategy is the following: B₁ is injected during 53 days, then B₂ is injected during 82 days, and finally B₁ is injected again during 61 days. The core permeability is estimated at different times, using the measurement of the pressure difference along the core divided by the pressure drop on the clean core. This ratio is known as the resistance factor Rₜ and it is given by Rₜ(t) = Δpₑ(t)/Δpₑ(0). When changes in brine viscosity and density are small and the injection rate is kept constant over time, the resistance factor gives an estimate of the current
rock permeability \( k(t) \approx k(0)/R_f(t) \). In this experiment, the changes of viscosity and density for the brine were small as result of the short running time for the experiment, low injection rate, and initial biofilm formation.

In the previous section we introduced the model equations for permeable biofilm growth and two-phase flow in porous media. We simplify the mathematical model to compare to the experiment. This experiment can be modeled as a 1D single-phase flow system, where in addition we consider that the biofilm is impermeable and we neglect the mechanical dispersion to reduce the number of parameters. Table 1 presents this simplified version of the mathematical model which includes only six variables: the water velocity \( v_w \), water pressure \( p_w \), permeability \( k \), porosity \( \phi \), substrate concentration \( C_n \), and volume fraction of biomass \( \phi_b \).

### Table 1—Scale single-phase equations.

<table>
<thead>
<tr>
<th>Name</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Darcy</td>
<td>( v_w = -(k/\mu_w)\partial_x p_w, \quad \partial_t \phi_f + \partial_x v_w = 0 )</td>
</tr>
<tr>
<td>Permeability</td>
<td>( k = k_0[(\phi_f - \phi_{\text{crit}})/(\phi_0 - \phi_{\text{crit}})]^n )</td>
</tr>
<tr>
<td>Porosity</td>
<td>( \phi_f = \phi_0 - \phi_b )</td>
</tr>
<tr>
<td>Substrate</td>
<td>( \partial_t (C_n \phi_f) + \partial_x (v_w C_n - D_n \phi_f \partial_x C_n) = -\mu_n \phi_0 \phi_b C_n/(K_n + C_n) )</td>
</tr>
<tr>
<td>Biofilm</td>
<td>( \partial_t \phi_b = Y_{bn} \mu_n \phi_b C_n/(K_n + C_n) - K_d \phi_b - K_{\text{str}} \phi_f \partial_x p_w \phi_b )</td>
</tr>
</tbody>
</table>

Eleven parameters are needed to solve the mathematical model in Table 1. To obtain a better estimate of the model parameters, it is necessary to perform various experiments under controlled input quantities. However, these experiments are expensive and time consuming. In Landa-Marbán et al. (2019) a pore-scale mathematical model is calibrated based on the experiments performed by Liu et al. (2019), where measurements of the biofilm amount over time are taken for different flux velocities. For the core-scale system described in this section, only one experiment is performed. Then, we select parameter values from the literature in order to run numerical simulations and compare qualitatively the results to the experimental observations. Table 2 shows the selected values of these parameters.

### Table 2—Model parameters for the verification study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bacterial death rate</td>
<td>( K_d )</td>
<td>5.8\times10^{-7} \text{ s}^{-1}</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Biomass density (dry)</td>
<td>( \rho_b )</td>
<td>60 kg/m³</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Maximum growth rate</td>
<td>( \mu_n )</td>
<td>10^{-5} \text{ s}^{-1}</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Monod-half velocity</td>
<td>( K_n )</td>
<td>5\times10^{-3} \text{ kg/m}³</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Yield coefficient (biomass/substrate)</td>
<td>( Y_{bn} )</td>
<td>0.1</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Substrate diffusion coefficient</td>
<td>( D_n )</td>
<td>5\times10^{-10} \text{ m}²/\text{s}</td>
<td>Hommel et al. (2013)</td>
</tr>
<tr>
<td>Critical porosity</td>
<td>( \phi_{\text{crit}} )</td>
<td>0.1</td>
<td>Hommel et al. (2018)</td>
</tr>
<tr>
<td>Fitting parameter</td>
<td>( \eta )</td>
<td>3</td>
<td>Landa-Marbán et al. (2019)</td>
</tr>
<tr>
<td>Stress coefficient</td>
<td>( K_{\text{str}} )</td>
<td>5\times10^{-10} \text{ m/Pa·s}</td>
<td>Landa-Marbán et al. (2019)</td>
</tr>
<tr>
<td>Water density</td>
<td>( \rho_w )</td>
<td>10^3 \text{ kg/m}³</td>
<td>Standard</td>
</tr>
<tr>
<td>Water viscosity</td>
<td>( \mu_w )</td>
<td>10^{-3} \text{ Pa·s}</td>
<td>Standard</td>
</tr>
</tbody>
</table>

These parameter values have the same order of magnitude as the ones used in mathematical modeling (Alpkvist and Klapper 2007; Duddu et al. 2009; Hommel et al. 2018; Landa-Marbán et al. 2019). In addition to the model parameters and core dimensions, initial and boundary conditions are needed to complete the model. The initial porosity and permeability are \( \phi_0=0.23 \) and \( k_0=1528 \text{ md} \) respectively. Initially, we assume that there is no substrate in the brine and the pressure is set to zero (in this system, we are only interested in pressure differences that affect the detachment and transport of substrate). The initial volume fraction of biofilm is left as a free input value to best match the experimental data. Recalling that the time after inoculation and before starting the substrate injection is roughly half a day, we assume that the initial volume fraction of biofilm is distributed uniformly along the core. Then, we performed numerical simulations using the same injection strategy of substrate. In the simulations, the core is divided into 1000 elements. After simulations, the initial volume fraction of biofilm that best fits the experimental data is \( \phi_b(x, 0) = 5 \times 10^{-3} \). Fig. 4 shows the experimental data and numerical results of the average resistance factor for the whole core sample over time and the final permeability reduction of each of the core sections.

From the numerical simulation and experimental data, we observe that the resistance factor changes over time, which means that the permeability is affected by the biofilm. We can distinguish between the three different periods of substrate injection. For the injection of B_1, both simulations and experimental measures show that the resistance factor does not increase significantly. When increasing the substrate concentration to B_2, we observe that the resistance factor increases due to major biofilm activity. When the substrate injection is set back to B_1, we observe a steady state where the resistance factor has increased by a factor of three. From the simulation,
is possible to observe how the resistance factor decreases from changing the substrate injection \( B_2 \) to \( B_1 \), which means a sensible response of the biofilm to substrate input. From Fig. 4b we observe that the core sections three and five show negative experimental values. This is attributed to the pressure transducer, as the combination of high permeability, low injection rate, and the length of core sections is challenging for even the most sensitive pressure transducer to distinguish between noise and real pressure response. From the experimental data of the average resistance factor we observe fluctuations on the measurements. This behavior is attributed (besides noise) to the dynamical attachment and detachment of biomass, a complex process not included in the mathematical model. Fig. 5 shows values of the simulations for biofilm, pressure, permeability reduction, and substrate along the core. Given the initial homogeneous volume fraction of biofilm, from subplot (a) we observe that the biofilm formation is mainly located at the inlet of the core. This leads to the steep pressure drop close to the inlet of the core in subplot (b). The assumed porosity/permeability relationship predicts a permeability reduction around 90% close to the inlet of the core as shown in subplot (c). Finally, from subplot (d) we observe that the substrate is completely consumed by the biofilm in the inlet.

Fig. 5—(a) Volume fraction of biofilm, (b) pressure, (c) permeability reduction, and (d) substrate concentration along the core at \( t=196 \) days.
Based on the experimental and simulation results, we conclude that this reduced mathematical model is simple enough to have a few input parameters but complex enough to capture processes such as dynamical changes on the resistance factor, mainly biofilm formation on the core inlet, and a steady state where the biofilm growth is balanced with the detachment and death of bacteria. One of the natural questions arising from these mathematical models is the impact of variability and uncertainty of its inputs on the numerical results. To answer this, in the following section we introduce a novel sensitivity analysis and in the section Numerical Experiments we present the results of this sensitivity analysis applied to the biofilm model parameters of this simulation.

Sensitivity Analysis

Sensitivity studies of mathematical models are of great interest because they provide estimates of the influence of input data (physical parameters, initial conditions, boundary values) on a quantity of interest, i.e., the effect of the variability and/or uncertainty of input values on the quantity of interest. This ensures that critical parameters are identified. For example, a sensitivity analysis can be performed in mathematical models for porous media to determine to which variations of rock properties (e.g., permeability and porosity) the predicted oil recovery is more sensitive (quantity of interest). In this section we introduce a novel two-stage method that can also be applied to nonsmooth models in the dependent parameters. For the interested reader in the theory and technicalities behind this method, we describe them in the following paragraphs. An example of how to use and interpret the outcomes of this analysis is given at the end of this section.

We keep the exposition on sensitivity analysis general to emphasize that the methodology is not restricted to the problems presented in this paper. Let \( q(\vec{y}) \) be a scalar multidimensional function with \( \vec{y} = (y_1, \ldots, y_n) \in \Omega \subset \mathbb{R}^n \), defined by a range of independent parameters, i.e. \( \Omega = (a_1, b_1) \cap \cdots \cap (a_n, b_n) \). We associate a nonnegative weight \( w_j(y_j) = 1/(b_j - a_j) \) with each parameter \( y_j \in [a_j, b_j] \) for \( j = 1, \ldots, n \) and use the product measure \( w = \prod_{j=1}^n w_j \). This means that all parameters and values are equally likely within their ranges of variation. More general weight functions are possible, including non-product measures corresponding to inter-dependence between the parameters (Rahman 2014). In this paper we do not aim to quantify uncertainty by stochastic models, but sensitivities in outputs given bounds on the input parameters.

To determine the relative effect of each of the \( n \) input parameters on the output quantity of interest \( q \), we perform a global sensitivity analysis in terms of a Sobol decomposition (Sobol 2001). The function \( q \) is decomposed as a series expansion in all subsets of variables; the sum of contributions from the individual variables in isolation, all combinations of pairs of variables and so on, leading to the expression:

\[
q(\vec{y}) = q^0 + \sum_{i=1}^n q^{(i)}(y_i) + \sum_{i=1,j>i}^n q^{(i,j)}(y_i, y_j) + \cdots + q^{(1,\ldots,n)}(\vec{y}),
\]

where the terms are defined recursively by

\[
q^0 = \int_{\Omega} q(\vec{y})w(\vec{y})d\vec{y},
\]

\[
q^{(i)}(y_i) = \int_{\Omega_{-i}} q(\vec{y})w_{-i}(\vec{y}_{-i})d\vec{y}_{-i} - q^0, \quad 1 \leq i \leq n,
\]

\[
q^{(i,j)}(y_i, y_j) = \int_{\Omega_{-i,j}} q(\vec{y})w_{-i,j}(\vec{y}_{-i,j})d\vec{y}_{-i,j} - q^{(i)}(y_i) - q^{(j)}(y_j) - q^0, \quad 1 \leq i < j \leq n,
\]

and so on for higher-order terms. The superscript set notation refers to the subset of input parameters that are varying, while the explicit dependence on the remaining ones have vanished due to averaging. The subscript \( \sim i \) means that the \( i \)th index is omitted, e.g., \( w_{-i} = \prod_{j \neq i} w_j \), and \( \vec{y}_{-i} = (y_1, \ldots, y_{i-1}, y_{i+1}, \ldots, y_n) \). For instance, it means that the contribution from the \( i \)th parameter, \( q^{(i)} \) is obtained by averaging over all parameters except for \( y_i \) itself. The terms subtracted in Eqs. 16-17 make sure that we do not account for the same effects more than once. The term \( q^0 \) (i.e. Eq. 15) is the mean value function. As an illustration of Eqs. 14-17, we provide two examples of two-dimensional functions with their Sobol decompositions. For simplicity, in these cases we assume the parameter range to be the unit interval and the weight function \( w = 1 \). In Example 1, there is no combined effect of \( y_1 \) and \( y_2 \), which can be inferred directly from the function \( q = y_1^2 + y_2^2 \). Excluding the mean value term, all other terms are scaled to integrate to 0. Example 2 includes joint dependence from \( y_1 \) and \( y_2 \). One can still observe that each component function corresponds to a term in the expanded square, but transformed differently to integrate to 0.

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Example 1

\[
q(y_1, y_2) = y_1^2 + y_2^2
\]
\[
q = \frac{2}{3}
\]
\[
q^{(1)}(y_1) = y_1^2 - \frac{1}{3}
\]
\[
q^{(2)}(y_2) = y_2^2 - \frac{1}{3}
\]
\[
q^{(1,2)}(y_1, y_2) = 0
\]

Example 2

\[
q(y_1, y_2) = (y_1 + y_2)^2
\]
\[
q = \frac{7}{6}
\]
\[
q^{(1)}(y_1) = y_1^2 + y_1 - \frac{5}{6}
\]
\[
q^{(2)}(y_2) = y_2^2 + y_2 - \frac{5}{6}
\]
\[
q^{(1,2)}(y_1, y_2) = 2y_1y_2 - y_1 - y_2 + \frac{1}{2}
\]

Starting with the Sobol decomposition, one can compute the relative effect of each parameter combination to the total variance. The Sobol index for the \(s\)-parameter combination \(\{y_{i_1}, y_{i_2}, \ldots, y_{i_s}\}\) is given by

\[
S_{\{i_1, \ldots, i_s\}} = \frac{1}{\text{Var}(q)} \int_{\Omega_{i_1, \ldots, i_s}} \left|q^{\{1, \ldots, i_s\}}(y_{i_1}, \ldots, y_{i_s})\right|^2 w_{i_1}(y_{i_1}) \ldots w_{i_s}(y_{i_s}) dy_{i_1} \ldots dy_{i_s}.
\] (18)

The total variability in \(q\) due to variable \(i\) is obtained by summing over all subsets of parameters including parameter \(i\), denoted \(I_i\), which yields the total Sobol index for parameter \(i\),

\[
S_i = \sum_{s=1}^{n} \sum_{\{i_1, \ldots, i_s\} \in \{1, \ldots, s\}} S_{\{i_1, \ldots, i_s\}}.
\] (19)

In the analytical examples above, the Sobol indices can be computed exactly by integrating the square of each component function over its domain of dependence, and divide by the total variance. For Example 1, we get \(S_{\{1\}} = S_{\{2\}} = 0.5\) and \(S_{\{1,2\}} = 0\), i.e., each input parameter contributes equally to the variance, and there is no joint effect. As a comparison, we have for Example 2 that \(S_{\{1\}} = S_{\{2\}} = 61/127 \approx 0.48\) and \(S_{\{1,2\}} = 5/127 \approx 0.04\). The mixed term \(2y_1y_2\) in the expansion of \(q\) clearly indicates a nonzero joint effect from \(y_1\) and \(y_2\), but it may not be intuitively clear that it only contributes around 4% of the total variance.

In practical applications, the integrals in Eqs. 15-18 cannot be computed by analytical means, and using numerical integration in some dimensions while letting others vary is not straightforward. Directly computing global sensitivities of a computationally complex function, e.g., a computer model, over a domain of only moderately high dimensionality is often infeasible due to the computational cost. As an additional challenge, we are interested in nonsmooth \(q\), excluding the use of Sobol decomposition based on generalized polynomial chaos for smooth problems (Sudret 2008). As a remedy, we approximate the function of interest with an interpolant on a Clenshaw-Curtis-type sparse grid, using the software in Klimke and Wohlmuth (2005). Subsequently, a multiwavelet decomposition of the interpolant is performed, and the global sensitivity indices are evaluated directly from the multi-wavelet coefficients. The accuracy in the sensitivity indices as determined by the computer model is thus largely determined by two kinds of errors: interpolation error and basis truncation error introduced when replacing the interpolant by a series expansion in a finite set of multi-wavelets.

**Interpolation by the Multi-Linear Method.** The outline of multi-linear collocation closely follows the exposition in Klimke and Wohlmuth (2005), which also provides the source code for the numerical implementation. We perform interpolation of possibly nonsmooth (but continuous) functions and therefore rely on localized basis functions. For discontinuous functions, we refer to the adaptive sparse grid methods introduced in Ma and Zabaras (2009). Multidimensional collocation on sparse grids is built from tensor products of low-order single dimensional collocation rules. In other words, simple integration methods are combined to form more complex integration rules that are versatile and efficient. Temporarily assume that \(n = 1\) (i.e., we consider a single parameter for integration), denote \(y = \tilde{y}\) and let \(Y_\ell\) be a set of interpolation nodes in the parameter space, for which the function \(q\) is evaluated. The index \(\ell\) refers to a refinement level: the higher \(\ell\), the bigger the set of interpolation nodes. An interpolant of \(q\) is given by

\[
I_\ell(q) = \sum_{y_\ell \in Y_\ell} q(y_\ell) \psi_{y_\ell}(y),
\] (20)

where \(\psi_{y_\ell}(y)\) are nodal basis functions with the property

\[
\psi_{y_\ell}(y_\ell') = \begin{cases} 
1 & \text{if } \ell = \ell', \\
0 & \text{otherwise.}
\end{cases}
\] (21)
In this work we employ the piecewise linear ‘hat’ functions for level $\ell > 1$

$$\psi_{\ell}(y) = \begin{cases} 
1 - 2^{1-\ell}|y - y_\ell| & \text{if } |y - y_\ell| < 2^{1-\ell}, \\
0 & \text{otherwise},
\end{cases}$$

supplemented with the unit function (level $\ell = 1$). The collocation nodes are nested, i.e., $Y_\ell \subset Y_{\ell+1}$, so existing function evaluations are recycled on the next level of refinement of the interpolant. Rather than expressing the interpolant as a function of the nodes in some sufficiently refined set $Y_\ell$, it can be expressed as a sum of hierarchical surpluses, i.e., differences between the interpolants at successive levels,

$$\Delta_{\ell}(q) = I_\ell(q) - I_{\ell-1}(q), \quad I_0(q) \equiv 0.$$

Then, Eq. 20 can be expressed

$$I_\ell(q) = \sum_{j=1}^{\ell} \Delta_j(q) = \sum_{j=1}^{\ell} \sum_{y_j \in Y_j \backslash Y_{j-1}} q(y_j) \psi_{\ell,j}(Y),$$

where the superscript ($j$) is used to emphasize that the basis functions are level specific. Using this construction, one may use the local difference between the interpolant and the true function as a measure to determine where further refinement in terms of more nodes are needed.

In multiple dimensions ($n > 1$), a tensor-product formula would lead to very large sets of nodes even for moderate $n$. As a remedy, a sparse grid based on Smolyak’s construction (Smolyak 1963) is used, adding only a subset of the tensor product Clenshaw-Curtis nodes at each new level. The hierarchical multidimensional interpolant of $q = q(y_1, \ldots, y_n)$ on total level $\ell \geq n$, is given by

$$I_{\ell,n}(q) = I_{\ell-1,n}(q) + \Delta I_{\ell,n}(q), \quad (25)$$

with $I_{n-1,n} = 0$ and

$$\Delta I_{\ell,n}(q) = \sum_{|\vec{i}|=\ell} (\Delta_{i_1} \otimes \cdots \otimes \Delta_{i_n})(q) = \sum_{|\vec{i}|=\ell} \sum_j \left( \psi^{(j)}_{i_1} \otimes \cdots \otimes \psi^{(j)}_{i_n} \right) \cdot \left( q(y^{(j)}_j) - I_{\ell-1,n}(q)(y^{(j)}_j) \right),$$

For more details on the multi-linear collocation method we refer to Klimke and Wohlmuth (2005). The hierarchical multi-linear interpolant (Eq. 25) is a surrogate from which we can obtain approximations of $q$. The Smolyak algorithm yields the multidimensional interpolant at low computational cost, but the global sensitivity indices are not directly available. Next, we introduce a series expansion of $I_{\ell,n}$ in multi-wavelets to obtain the Sobol decomposition of $I_{\ell,n}$.

### Sobol Indices via Multi-Wavelet Expansions.

An alternative representation of $q$ is via a spectral expansion in a set of multidimensional orthogonal basis functions $\{\varphi_j\}$,

$$q(Y) = \sum_{j=1}^{\infty} c_j \varphi_j(Y), \quad (27)$$

where the infinite sum is truncated to some finite set in practical application. This is known as generalized polynomial chaos expansion if the basis functions are orthogonal polynomials (Xiu and Karniadakis 2002), and it has been demonstrated that the Sobol indices can be directly identified from the expansion coefficients, once these have been computed (Sudret 2008). Nonsmooth functions can be represented by means of multi-resolution analysis where the basis functions are piecewise polynomial multi-wavelets (Le Maître et al. 2004), and the identification of the Sobol indices is straightforward.

A piecewise linear multi-wavelet expansion of sufficient resolution can exactly represent the piecewise linear interpolant, provided that the support nodes are aligned with the support of the multi-wavelets. The advantage of using the multi-wavelet expansions rather than trying to directly evaluate the Sobol component functions, is that we may rely on a single interpolation of the function of interest itself (and not its square, conditional on some subset of the variables, and so on).

Let $\{\varphi_k^{(\ell)}(y)\}_{k \in I_{\ell}^{\text{MW}}}$ be a finite-dimensional basis of multi-wavelets indexed by some set of nonnegative integers $I_{\text{MW}} \subset \mathbb{N}_0^n$. Ideally, the number of basis functions should be limited but chosen in order to be a good approximation of the interpolant $I_{\ell,n}(q)$ of the function of interest. The approximation properties of the multi-wavelet basis are determined by the order of the piecewise polynomial multi-wavelets ($\ell$) and the resolution level ($L$) that governs the localization in parameter space. Analogous to the hierarchical surplus defined for the multi-linear interpolant,
the hierarchical surplus of the multi-wavelet expansion is given by the contribution captured by the finest resolution level. The multi-wavelet basis is hierarchical, and can be enriched by adding multi-wavelets to regions labeled important due to large surpluses.

We may now either project the interpolant \( I_{\ell,n}(q) \) onto the basis \( \{\varphi_k(\vec{y})\}_{k\in \text{Isaw}} \), or interpolate the product \( q\vec{c} \), and then perform the projection by computing the expected value. The latter is simpler, as it only involves integration of a piecewise linear function to compute each multi-wavelet coefficient. However, we do not know a priori what multi-wavelets should be included in the truncated basis, and will therefore settle for a simple strategy that also admits adaptivity. Unlike \( q \) itself, the interpolant \( I_{\ell,n}(q) \) can be sampled repeatedly at moderate computational cost. Given \( N \) random samples of the parameters \( \vec{y} \), and a tentative multi-wavelet basis of size \( P \), we form the linear system for the \( P \)-vector of multi-wavelet coefficients \( \vec{c} \)

\[
\Phi \vec{c} = \vec{q},
\]

where the matrix \( \Phi \in \mathbb{R}^{N \times P} \) is defined by \( [\Phi]_{k,j} = \varphi_j(\vec{y}^{(k)}) \), and \( \vec{q} \in \mathbb{R}^N \) contains the evaluations of \( I_{\ell,n}(q) \) in the samples \( y^j, j = 1, \ldots, N \). The ordinary least squares solution to Eq. 28 gives the multi-wavelet coefficients of the tentative bases. If the hierarchical surplus (defined as the difference between the interpolants of two successive grid levels) is above a user specified threshold, the approximation of \( I_{\ell,n}(q) \) is not sufficiently resolved, and we may increase the tentative multi-wavelet basis functions in unresolved regions of parameter space. This is done by solving Eq. 28 with an extended basis. As a further measure of how well we represent \( I_{\ell,n}(q) \), we may compare the variance predicted by the multi-wavelet expansion with the sample variance of \( I_{\ell,n}(q) \). The novelty in the proposed framework for sensitivity analysis is the combination of mathematical tools: hierarchical sparse interpolation to form a surrogate (proxy) method, which is projected onto a wavelet basis at low cost using linear regression. The resulting wavelet expansion can be used in a manner similar to how polynomial chaos expansions are used to directly evaluate sensitivity indices.

Once a suitable multi-wavelet expansion has been identified, the sensitivity indices can be estimated by grouping the multi-wavelets according to what parameters they depend on. The sensitivity index of parameter \( j \) is the relative amount of variation explained by \( Y_j \) compared to the total amount of variation. The total variance equal the sum of squares of all multi-wavelet coefficients \( (c_j \text{ in Eq. 27}) \). The relative variance due to parameter \( Y_j \) is equal to the sum of squares of all coefficients for which the corresponding multiwavelets are functions of \( Y_j \).

**Example.** We present the following example to illustrate the application of this sensitivity analysis. Let us consider the expression for the void space outside the biofilm \( \phi_f = \phi_0 - \phi_b \), the Thullner et al. (2002) relationship \( k_{th}/k_0 = \left( (\phi_f - \phi_{\text{crit}})/(\phi_0 - \phi_{\text{crit}}) \right)^9 + k_b/k_0 \) and Darcy’s law in one dimension \( v = k_{th} \partial_x p_w/\mu_w \) in the interval \([0, 1]\) m. We consider the Darcy velocity \( v \) as the quantity of interest. Let \( \phi_f = 0.2, \phi_0 = 0.1, \phi_{\text{crit}} = 0.1 \), \( k_b = 10^{-14} \) m², \( k_0 = 10^{-13} \) m², \( \mu = 10^{-3} \) Pa·s, \( p_w(x = 0) = 10^6 \) Pa, \( p_w(x = 1 \) m) = 0 Pa be the numerical values of the model inputs. We only consider two model inputs for the sensitivity study to be able to illustrate with plots the steps of the analysis. Let the biofilm volume fraction \( \phi_f \) and fitting parameter \( \eta \) be these model inputs in the intervals \( Y_1 = [0.05, 0.15] \) and \( Y_2 = [1, 2] \) (Beckingham 2017) respectively. Fig. 6a shows the function, its interpolant using three levels of interpolation (13 points), and the error. Fig. 6b shows the \((L = 1, o = 2)\) multi-wavelet expansion of the same function (using its interpolant), also including the error in the approximation. For this multi-wavelet basis, the total sensitivity indices for the two parameters are respectively 0.97 and 0.062. The sum is slightly larger than 1, as there is a small joint effect from the two parameters (0.0353) that counts towards both the sensitivity indices.

**Numerical Experiments**

In the section Model Test we show the simulation results of a simplified 1D system for comparison with experimental results. In this section we perform more detailed 3D simulations of the complete two-phase flow mathematical model. For the numerical experiments, we consider a core-sample saturated with water and oil. We consider a three-dimensional cylindrical domain with the same dimensions of the core used for experiments (0.019 m radius and 0.30 m length). The computational domain is discretized into 15 × 15 × 30 elements. We consider homogeneous porosity of 0.2 and homogeneous permeability in the core (10⁻¹³ m²) except in the middle part where the permeability is anisotropic \( (k_{xx} = 10⁻⁸ \text{ m²} \text{ and } k_{yy} = k_{zz} = 10⁻¹³ \text{ m²}) \), as shown in Fig. 7a. This more permeable zone is set to study the effects of biofilm on oil recovery when it modifies the rock properties in a thief zone. We consider that initially there is only biofilm in the middle part of the thief zone with a volume fraction of 10⁻², as shown in Fig. 7b. The core has an initial water saturation of 0.2 and an oil saturation of 0.8. The substrate is injected in the middle cell on the left side of the core at a concentration of \( C_i = 2 \times 10² \) kg/m³ and rate of \( Q_w = 10⁻⁶ \) m³/day. We consider the porosity/permeability relationship \( k_{th} \) (Eq. 5) for this study. The initial oil pressure is set equal to the entry pressure. Table 3 lists the parameters for the numerical simulations. These
boundary conditions, initial conditions, and parameters are selected to perform the diverse numerical studies in a computational time of order of hours.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Values</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bacterial death rate</td>
<td>(K_d)</td>
<td>(5.8 \times 10^{-7}) s(^{-1})</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Biomass density (dry)</td>
<td>(\rho_b)</td>
<td>60 kg/m(^3)</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Monod-half velocity</td>
<td>(K_n)</td>
<td>(5 \times 10^{-3}) kg/m(^3)</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Yield coefficient (biomass/substrate)</td>
<td>(Y_{bn})</td>
<td>0.1</td>
<td>Alpkvist and Klapper (2007)</td>
</tr>
<tr>
<td>Longitudinal dispersivity</td>
<td>(\alpha_L)</td>
<td>(10^{-3}) m</td>
<td>Benekos et al. (2006)</td>
</tr>
<tr>
<td>Transverse dispersivity</td>
<td>(\alpha_T)</td>
<td>(4 \times 10^{-4}) m</td>
<td>Benekos et al. (2006)</td>
</tr>
<tr>
<td>Substrate diffusion coefficient</td>
<td>(D_n)</td>
<td>(5 \times 10^{-10}) m(^2)/s</td>
<td>Hardy and Sarko (1993)</td>
</tr>
<tr>
<td>Critical porosity</td>
<td>(\phi_{crit})</td>
<td>0.1</td>
<td>Hommel et al. (2013)</td>
</tr>
<tr>
<td>Fitting parameter</td>
<td>(\eta)</td>
<td>3</td>
<td>Hommel et al. (2018)</td>
</tr>
<tr>
<td>Stress coefficient</td>
<td>(K_{str})</td>
<td>(5 \times 10^{-10}) m/Pa-s</td>
<td>Landa-Marbán et al. (2019)</td>
</tr>
<tr>
<td>Maximum growth rate</td>
<td>(\mu_n)</td>
<td>(1.59 \times 10^{-4}) s(^{-1})</td>
<td>Linville et al. (2013)</td>
</tr>
<tr>
<td>Entry pressure</td>
<td>(p_e)</td>
<td>(5 \times 10^{-5}) Pa-s</td>
<td>Pini and Benson (2013)</td>
</tr>
<tr>
<td>Fitting parameter</td>
<td>(\alpha)</td>
<td>2.36</td>
<td>Pini and Benson (2013)</td>
</tr>
<tr>
<td>Irreducible water saturation</td>
<td>(S_{wi})</td>
<td>0.1</td>
<td>Pini and Benson (2013)</td>
</tr>
<tr>
<td>Residual oil saturation</td>
<td>(S_{or})</td>
<td>0.1</td>
<td>Pini and Benson (2013)</td>
</tr>
<tr>
<td>Critical point</td>
<td>(B_c)</td>
<td>0.35</td>
<td>Vandevivere (1995)</td>
</tr>
<tr>
<td>Biofilm permeability</td>
<td>(k_b)</td>
<td>(10^{-15}) m(^2)</td>
<td>Assumed</td>
</tr>
<tr>
<td>Biofilm water content</td>
<td>(\theta_w)</td>
<td>0.1</td>
<td>Assumed</td>
</tr>
<tr>
<td>Oil density</td>
<td>(\rho_o)</td>
<td>800 kg/m(^3)</td>
<td>Standard</td>
</tr>
<tr>
<td>Oil viscosity</td>
<td>(\mu_o)</td>
<td>(3.92 \times 10^{-3}) Pa-s</td>
<td>Standard</td>
</tr>
<tr>
<td>Water density</td>
<td>(\rho_w)</td>
<td>(10^3) kg/m(^3)</td>
<td>Standard</td>
</tr>
<tr>
<td>Water viscosity</td>
<td>(\mu_w)</td>
<td>(10^{-3}) Pa-s</td>
<td>Standard</td>
</tr>
</tbody>
</table>

Table 3—Table of model parameters for the numerical studies.

**Fig. 8** shows the simulation results for biofilm, substrate, permeability reduction, and substrate along the core after 2 days of injection. Given the initial homogeneous volume fraction of biofilm, this has increased more on the injection side like observed on the single-phase flow experiments. Subplot (b) shows the substrate concentration which is in a limited amount as it is mostly consumed by the biofilm. The reduction in permeability is nearly 100% as for this system we include the biofilm permeability which is different to zero (\(10^{-15}\) m\(^2\)). Finally, we observe that the oil has been mostly displaced where the biofilm grows.

In the following subsections we show numerical results for the following studies: injection strategies, impact of
porosity/permeability relationships, sensitivity analysis of the biofilm parameters, and sensitivity analysis of the biofilm initial configuration. To reduce the computational time, we consider a 2D rectangular domain with 0.30 m (length) × 0.038 m (width). The computational domain is divided into 9000 elements (300 × 30). In addition, we neglect the capillary pressure and substrate dispersion to further reduce the computational time as we need to perform more than thousands of simulations for the sensitivity studies. We consider a less permeable thief zone (in comparison to the previous study) with isotropic permeability value (10⁻¹¹ m²) for the following two studies. We set the initial water saturation and oil saturation as described at the beginning of this section and model parameters from Table 3.

Injection Strategies. The study of injection strategies is important for the optimization of the bioplug technology. Comparison of oil recovery for different injection techniques is possible through numerical experiments. In this work, we compare the oil recovery for different substrate injection strategies for the same initial conditions after a week. For this study, we use the $k_c$ porosity/permeability relationship. The initial volume fraction of biofilm is set to $10^{-3}$ and we set the flow rate from the 3D study as the reference injection rate ($Q_w$). Fig. 9 shows a reference profile where only water is injected and the five different strategies tested.

The reference strategy consists in injecting only water at a constant flux rate. Strategy A consists in injecting water at a higher flux rate 10 times higher after half the time of the experiment. Strategy B is found commonly in the literature. Water and substrate are injected continuously at a fixed flux rate and after increasing the water flow to diverge the water flow. This injection strategy allows to the biofilm to growth by consuming substrate under low flow rate (i.e., less detachment) until is larger to support higher flow rates to increase the oil recovery. Strategy C consists of inverting the direction of the high flux to study the effect on the oil recovery in comparison with

**Fig. 7**—(a) Initial permeability in the x-direction and (b) volume fraction of biofilm.

**Fig. 8**—(a) Volume fraction of biofilm, (b) substrate concentration, (c) permeability reduction, and (d) oil ($\rho_o \phi_f S_o$) along the core.
Strategy B. This injection strategy represents the conversion of oil production wells to injectors at the field scale (Sayyafzadeh et al. 2010). For Strategy E, first substrate is injected at a fixed flux rate and double concentration. The system is then closed in order to let the bacteria consume the suspended substrate. Afterwards, the water flux is reactivated at the high rate. We observe that Strategy B and Strategy E use the same amount of substrate. 

Fig. 10 shows the different oil predictions for the different injection strategies.

Fig. 10—Comparison of oil recoveries for the different injection strategies over time.

From the previous plot we observe that Strategy C predicts the largest oil recovery. The explanation for this result is that the reduction of permeability by the biofilm diverges the water at the inlet of the core recovering some of the surrounding oil. Strategies A and D give similar predictions of oil recovery. Then, changing the side of substrate injection affects the growth of the biofilm as the time of substrate injection is short. This leads to low impact of the biofilm in the oil recovery. Comparing Strategies B and E we observe that the flow rate is low for this system as the biofilm in Strategy B has an impact on oil recovery similar to that of Strategy E. We recall that the best injection strategy could change for different cores depending on the in situ conditions. Field-scale simulations could be performed to compare the results of these injection strategies in core samples to actual oil reservoirs.

**Impact of Porosity/Permeability Relationships.** We compare the oil recovery for four porosity/permeability relationships: Vandevivere $k_v$ (Eq. 4), Thullner $k_{th}$ (Eq. 5), channel $k_c$ (Appendix A), and tube $k_t$ (Appendix A). These four relationships include the biofilm permeability. The critical porosity ($\phi_{crit}$) is set to 0 for this
study and the remaining parameter values are taken from Table 3. **Fig. 11** shows the profiles of these four porosity/permeability relationships for a highly permeable biofilm and a less permeable biofilm respectively.

![Fig. 11—Porosity/permeability relationships of (a) \( k_b = 10^{-1} k_0 \) and (b) \( k_b = 10^{-3} k_0 \).](image)

From **Fig. 11** we can observe that these porosity/permeability relationships give different values of permeability for the same values of rock porosity. Then, we perform simulations to find at which part of the porosity/permeability relationships (low, medium, or high porosity) the oil recovery is more sensitive. The studied ratios of initial to reduce porosity intervals are [0.1,0.3], [0.4,0.6], and [0.7,0.9] respectively. We consider corresponding volume fractions of biofilm for the different intervals and inject only water at a rate of \( 10 Q_w \) for half a week. In **Table 4** we show the difference of percentage of oil recovery (\( \Delta_{oil} \)) for the different porosity intervals.

<table>
<thead>
<tr>
<th>Relationship</th>
<th>Notation</th>
<th>( \Delta_{oil} ) (Low Porosity)</th>
<th>( \Delta_{oil} ) (Medium Porosity)</th>
<th>( \Delta_{oil} ) (High Porosity)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power law</td>
<td>( k_p )</td>
<td>11.0489 %</td>
<td>8.1282 %</td>
<td>1.4791 %</td>
</tr>
<tr>
<td>Vandevivere</td>
<td>( k_v )</td>
<td>4.6873 %</td>
<td>10.6946 %</td>
<td>3.9872 %</td>
</tr>
<tr>
<td>Thullner</td>
<td>( k_{th} )</td>
<td>11.0046 %</td>
<td>8.1176 %</td>
<td>1.4785 %</td>
</tr>
<tr>
<td>Channel</td>
<td>( k_t )</td>
<td>10.9996 %</td>
<td>7.9141 %</td>
<td>1.4515 %</td>
</tr>
<tr>
<td>Tube</td>
<td>( k_t )</td>
<td>12.3801 %</td>
<td>2.2275 %</td>
<td>0.5098 %</td>
</tr>
</tbody>
</table>

**Table 4**—Variation of oil extraction prediction at different porosity ratio intervals for four porosity/permeability relationships.

From Table 4, we observe that after three days and a half of water injection the tube porosity/permeability relationship is the most sensitive and the Vandevivere the least sensitive in the low porosity range. However, the Vandevivere relationship is the most sensitive in the medium porosity and high porosity ranges while the tube relationship is the least sensitive. The sensitivities for the power law and Thullner relationships are very similar as the biofilm permeability for this study is low. From these results, we observe that the oil recovery could be significantly over- or underestimated depending on the assumed porosity/permeability relationship and porosity range. This sensitivity measurement is an indicator only for the impact of one model input at a time. In the next example, we apply the method introduced in the previous section to study sensitivities including the joint effect of several parameters in a quantity of interest.

**Sensitivity Analysis: Numerical Results.** Sensitivity analysis is performed for two test cases based on the methodology presented in a previous section.

**Case I: Mean Permeability with Variability in Six Parameters.** We consider the single-phase core-scale mathematical model in Table 1 and the same boundary, initial conditions, and domain discretization as in
Model Test. The quantity of interest \( q \) is the mean permeability of the core after 100 days of water injection, divided by the initial mean permeability of the core, and we investigate its sensitivity with respect to the six biofilm parameters (i.e., \( n = 6 \)) with ranges shown in Table 5. In this study we focus on the effect of the variability (± 10%) of parameter values on the permeability reduction. The interpolant \( \tilde{I}_{\ell,n}(q) \) is computed for \( \ell = n + 0, \ldots, n + 6 \). The relative interpolation error is estimated as the \( L_2 \) norm of the hierarchical surplus at the finest level over the norm of \( \tilde{I}_{\ell,n}(q) \) itself. The interpolant at level \( \ell = n + 6 \) requires 30,241 evaluations of \( q \), and results in an estimated relative error of less than 2\( \times 10^{-2} \).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Range</th>
<th>Total Sobol Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum growth rate</td>
<td>( \rho_n )</td>
<td>([0.9, 1.1] \times 10^{-3} ) s(^{-1} )</td>
<td>0.660</td>
</tr>
<tr>
<td>Bacterial death rate</td>
<td>( K_d )</td>
<td>([5.22, 6.38] \times 10^{-7} ) s(^{-1} )</td>
<td>0.035</td>
</tr>
<tr>
<td>Stress coefficient</td>
<td>( K_{str} )</td>
<td>([4.5, 5.5] \times 10^{-10} ) m/Pa s</td>
<td>0.001</td>
</tr>
<tr>
<td>Yield coefficient</td>
<td>( Y_{in} )</td>
<td>([0.09, 0.11] )</td>
<td>0.160</td>
</tr>
<tr>
<td>Monod-half velocity</td>
<td>( K_n )</td>
<td>([4.5, 5.5] \times 10^{-3} ) kg/m(^3)</td>
<td>0.002</td>
</tr>
<tr>
<td>Biomass density (dry)</td>
<td>( \rho_b )</td>
<td>([54, 66] ) kg/m(^3)</td>
<td>0.190</td>
</tr>
</tbody>
</table>

Table 5—Total variability contribution of input parameters to percentage of oil extraction.

The surrogate function \( \tilde{I}_{\ell,n}(q) \) is subsequently sampled \( N = 10^5 \) times and the multi-wavelet coefficients are computed by solving Eq. 28 for varying polynomial orders \( o \) and resolution levels \( \mathcal{L} \). The fraction of the total sampling variance explained by the retained multi-wavelet coefficients are shown in Table 6. For this problem, the convergence is faster in the order \( o \) of the piecewise polynomials than in the resolution level \( \mathcal{L} \) of the multi-wavelets, suggesting that \( q \) is relatively smooth. Only combinations of multi-wavelets of total polynomial order \( o \) and total resolution level \( \mathcal{L} \) have been included in the bases used to generate the numerical results. The observed accuracy with respect to capturing the total sample variance suggests that this basis truncation is indeed a suitable strategy to reduce the computational cost of solving the linear system in Eq. 28.

<table>
<thead>
<tr>
<th>( \mathcal{L} )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ell )</td>
<td></td>
<td>0.934</td>
<td>0.987</td>
<td>0.996</td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>0.700</td>
<td>0.949</td>
<td>0.989</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>0.912</td>
<td>0.951</td>
<td>0.989</td>
</tr>
</tbody>
</table>

Table 6—Fraction of sample variance in test Case I represented by multi-wavelet expansion of polynomial order \( o \) and resolution level \( \mathcal{L} \).

The accuracy in the variance captured by the multi-wavelet expansion is used as a proxy to estimate the accuracy in the sensitivity indices. We choose the smallest basis that captures at least 99% of the sample variance (i.e., \( \mathcal{L} = 0, o = 3 \)) and use that in the computation of the sensitivities. The total contribution of each material parameter, isolated, and in combination with the others, are shown in Table 5. The very small sensitivity indices for the stress coefficient and Monod half velocity indicate that the variability in these two parameters has negligible effect on the permeability reduction.

**Case II: Two-Phase Flow with Three Variable Parameters.** We now consider the case of two-phase flow (oil and water). The injected water rate changes after 3.5 days from \( Q_w \) to a higher rate of \( 10Q_w \) (Strategy B in the Injection Strategies subsection). Due to the computational complexity, only three parameters are considered in the sensitivity study: initial volume fraction, position, and length of the biofilm, as presented in Table 7. The quantity of interest is the percentage of oil extraction compared to the initial oil in the core (0-100%). We expect nonsmooth parameter dependence due to sharp changes in velocity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Range</th>
<th>Total Sobol Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume fraction of the biofilm</td>
<td>( \phi_b )</td>
<td>([0.8, 1.2] \times 10^{-3} )</td>
<td>0.039</td>
</tr>
<tr>
<td>Length of the biofilm</td>
<td>( L_b )</td>
<td>([2, 20]) cm</td>
<td>0.910</td>
</tr>
<tr>
<td>Position of the biofilm centre</td>
<td>( X_b )</td>
<td>([12, 18]) cm</td>
<td>0.070</td>
</tr>
</tbody>
</table>

Table 7—Total contribution of each initial parameter.

A sparse grid interpolant on 7 levels yields an estimated error of \( 10^{-3} \) between the two finest levels of resolution, where the relative error has again been estimated as the \( L^2 \) norm of the hierarchical surplus divided by the norm of the solution itself. A set of \( N = 10^5 \) samples are drawn from the interpolant surrogate model to fit a multi-wavelet model through ordinary least squares. As shown in Table 8, the smallest multi-wavelet basis that captures at
least 99% of the variance has total level $L = 2$ and polynomial order $o = 3$. The total Sobol indices for this multi-wavelet representation are shown in Table 7. For the parameter ranges investigated, the variability in oil extraction is dominated by the initial length of the biofilm. The volume fraction and position of the biofilm should however not be entirely ignored.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$o$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-</td>
<td>0.967</td>
<td>0.984</td>
<td>0.985</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.713</td>
<td>0.970</td>
<td>0.986</td>
<td>0.989</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.925</td>
<td>0.971</td>
<td>0.989</td>
<td>0.991</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.971</td>
<td>0.974</td>
<td>0.991</td>
<td>0.993</td>
<td></td>
</tr>
</tbody>
</table>

Table 8—Fraction of sample variance in test Case II represented by multi-wavelet expansion of polynomial order $o$ and resolution level $L$.

The methods used for the sensitivity analysis are numerically robust and accurate but it should be emphasized that the results pertain to the assumed input parameter ranges. Ideally, randomly sampled parameter values would be the preferred format of input values to build confidence in the sensitivity estimates for the problem under investigation. Provided that sufficiently wide input parameter ranges are assumed, the results from the sensitivity analysis give information about the relative importance of the parameters, and should be employed to decide on where to focus further parameter measurements.

Conclusions

In this work we integrate laboratory studies, mathematical modeling, numerical simulations, and sensitivity analysis for biofilm formation in core samples. To our knowledge, this is the first mathematical model for two-phase flow and permeable biofilm. The numerical simulations capture the following processes observed in the laboratory experiments: dynamical changes on the resistance factor, mainly biofilm formation on the core inlet, and a steady state where the biofilm growth is balanced with the detachment and death of bacteria.

Based on this work conclusions are as follows:

1. The simulated oil recovery could be significantly over- or underestimated depending on the assumed porosity/permeability relationship.
2. The best oil recovery strategy for the studied system is to inject the substrate on one side of the core and inject water at a higher rate on the opposite side.
3. The sensitivity analysis for the single-phase core-scale model shows that two parameters have negligible effect on the permeability reduction: stress coefficient and Monod half-velocity coefficient.
4. The sensitivity analysis for the two-phase core-scale model demonstrates less impact on the total variability in oil extraction from the initial position of biofilm and volume fraction as compared to the length of the biofilm.

Further work is to apply upscaling techniques to conduct field-scale studies.

Nomenclature

- $a$: weighting factor, dimensionless
- $B_c, B_r$: critical and relative porosity, dimensionless
- $B_1, B_2$: injected brine concentrations, $m/L^3, kg/m^3$
- $C_i, C_n$: injected substrate concentration and substrate concentration, $m/L^3, kg/m^3$
- $d$: core diameter, $L, m$
- $D_n$: substrate diffusion-dispersion tensor, $L^2/t, m^2/s$
- $D_n$: substrate diffusion coefficient, $L^2/t, m^2/s$
- $E, F, G, V, W, X$: integration coefficients, dimensionless
- $g$: gravity, $L/t^2, m/s^2$
- $h_b$: biofilm thickness, dimensionless
- $I$: identity matrix, dimensionless
- $I_i$: all subsets of parameters including parameter $i$ for global sensitivity analysis, dimensionless
- $I_{\ell,n}(q)$: hierarchical multidimensional interpolant of $q$ on total level $\ell \geq n$, dimension depends on $q$
\( I_{MW} = \) multi-wavelet index set of nonnegative integers
\( j_0 = \) substrate flux, \( \text{m/t} \), \( \text{L}^2 \), \( \text{kg/s} \cdot \text{m}^2 \)
\( J_\nu = \) Bessel function of order \( \nu \) of first kind, dimensionless
\( k, k_0, k_b = \) rock permeability, initial rock permeability, and biofilm permeability, \( \text{L}^2 \), \( \text{md} \) \( \text{m}^2 \]
\( k_p, k_h, k_{vp} = \) power law, weighted, and Verma-Pruess permeability relationships, \( \text{L}^2 \), \( \text{md} \) \( \text{m}^2 \]
\( k_c, k_t, k_{th}, k_{vp} = \) channel, tube, Thullner et al., and Verma-Pruess permeability relationships, \( \text{L}^2 \), \( \text{md} \) \( \text{m}^2 \]
\( \tilde{k}_b = \) biofilm permeability, dimensionless
\( K_d = \) bacterial death rate, \( \text{t}^{-1} \), \( \text{s}^{-1} \)
\( K_{str} = \) stress coefficient, \( \text{L}^2 \cdot \text{t/m} \), \( \text{m/s} \) \( \cdot \text{Pa} \)
\( K_n = \) Monod half-velocity coefficient, \( \text{m/L}^3 \), \( \text{kg/m}^3 \)
\( \ell, \tilde{\ell} = \) refinement level, dimensionless
\( \mathcal{L} = \) number of resolution levels, dimensionless
\( L, L_b = \) core and biofilm length, \( \text{L} \), \( \text{cm} \)
\( n = \) number of stochastic dimensions, dimensionless
\( \mathbb{N}_0^n = \) set of \( n \)-tuples of nonnegative integers, dimensionless
\( o = \) polynomial order of the multi-wavelet expansion, dimensionless
\( P_c, p_e, p_o, p_w = \) capillary, entry, oil, and water pressure, \( \text{m/L}^2 \), \( \text{Pa} \)
\( p = \) size of multi-wavelet basis
\( q = \) quantity of interest for global sensitivity analysis, varying dimension
\( r = \) core radius, \( \text{L} \), \( \text{cm} \)
\( R_f = \) resistance factor, dimensionless
\( R_n = \) substrate reaction term, \( \text{m/t} \cdot \text{L}^3 \), \( \text{kg/s} \cdot \text{m}^3 \)
\( S_o, S_w = \) saturation of oil and water, dimensionless
\( S_o^*, S_w^* = \) effective saturation of oil and water, dimensionless
\( S_{or}, S_{wi} = \) residual oil saturation and irreducible water saturation, dimensionless
\( S_i = \) total Sobol index for parameter \( i \), dimensionless
\( t = \) time, \( \text{t} \), \( \text{days} \) \( \text{[hours]} \)
\( T = \) temperature, \( \text{T} \), \( °\text{C} \)
\( v_i, v_o, v_w = \) injected water velocity, oil, and water velocity, \( \text{L/t} \), \( \text{m/s} \)
\( w = \) variable depending on the biofilm thickness, dimensionless
\( X_b = \) position of the biofilm centre along the core, \( \text{L} \), \( \text{cm} \)
\( y_j = \) general parameter for global sensitivity analysis, dimensionless
\( Y = \) interpolation nodes in the parameter space
\( Y_{bn} = \) yield coefficient (biomass/substrate), dimensionless
\( Y_{\nu} = \) Bessel function of order \( \nu \) of second kind, dimensionless
\( Y_{r} = \) set of interpolation nodes in the parameter space, dimensionless
\( \alpha = \) subscript (\( \alpha = o \) for oil and \( \alpha = w \) for water), dimensionless
\( \alpha_L, \alpha_T = \) longitudinal and transverse dispersion coefficients, \( \text{L} \), \( \text{m} \)
\( \beta = \) fitting factor (Brooks-Corey relationships), dimensionless
\( \eta = \) fitting factor (power law), dimensionless
\( \theta_b = \) biofilm biomass content, dimensionless
\( \theta_w = \) biofilm water content, dimensionless
\( \mu_n = \) maximum specific biomass production rate, \( \text{t}^{-1} \), \( \text{s}^{-1} \)
\( \mu_o, \mu_w = \) water and oil viscosity, \( \text{m/L-t} \), \( \text{Pa-s} \)
\( \xi = \) variable dependent on biofilm permeability and porosity, dimensionless
\( \rho_b, \rho_o, \rho_w = \) density of biomass, oil, and water, \( \text{m/L}^3 \), \( \text{kg/m}^3 \)
\( \phi, \phi_{crit} = \) rock porosity and critical porosity, dimensionless
\( \phi_b, \phi_f = \) volume fraction of biofilm and void space outside the biofilm, dimensionless
\( \Phi_b = \) porosity of the biofilm, dimensionless
\( \varphi_j = \) \( j \)th orthogonal basis function, dimensionless
\( \psi_{lw} = \) piecewise linear interpolation functions, dimensionless
\( \Omega = \) range of independent parameters for global sensitivity analysis, dimensionless

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References


Appendix A — Effective Porosity/Permeability Relationships

A detailed description of the following two porosity/permeability relationships can be found in Landa-Marbán et al. (2020), where both relationships are derived by homogenization of a pore-scale model. To this aim we let \( \tilde{h}_b \) be the dimensionless thickness of the biofilm layer, \( \phi_b \) the volume fraction of biofilm, \( \phi_0 \) the initial porosity, \( \theta_w \) the biofilm water content, and \( k_b \) the biofilm permeability. The thickness of the biofilm \( \tilde{h}_b \) is given as a function of the volume fraction of biofilm \( \phi_b \) and the initial porosity \( \phi_0 \) for the thin channels as \( \tilde{h}_b = \phi_b/\phi_0 \), whereas for the thin tubes \( \tilde{h}_b = 1 - \sqrt{1 - \phi_b/\phi_0} \). We use the notation \( w = 1 - \tilde{h}_b \) and \( \tilde{k}_b = k_b/k_0 \).

The effective porosity/permeability relationship for a porous medium modeled as a stack of thin channels is given by

\[
\frac{k_t}{k_0} = -\frac{w^3}{6} - wV - \frac{W \exp(-\lambda) \left[ \exp(\tilde{h}_b \lambda) - 1 \right] - X \exp(\lambda) \left[ \exp(-\tilde{h}_b \lambda) - 1 \right]}{\lambda} + \tilde{k}_b \hat{h}_b, \tag{A-1}
\]

where

\[
V = \left( w^2 + 2\tilde{k}_b \right) \left[ \exp(-\tilde{h}_b \lambda) + \exp(\tilde{h}_b \lambda) \right] + 2w\sqrt{\tilde{k}_b \theta_w} \left[ \exp(\tilde{h}_b \lambda) - \exp(-\tilde{h}_b \lambda) \right] - 4\tilde{k}_b
\]

\[
W = \tilde{k}_b \exp(w \lambda) - w\sqrt{\tilde{k}_b \theta_w} \exp(\lambda), \tag{A-2}
\]

\[
X = \tilde{k}_b \exp(-w \lambda) + w\sqrt{\tilde{k}_b \theta_w} \exp(-\lambda), \tag{A-3}
\]

\[
\lambda = \sqrt{\theta_w/\tilde{k}_b}.
\]

The effective porosity/permeability relationship for a porous medium modeled as a stack of thin tubes is given by

\[
\frac{k_t}{k_0} = -\frac{w^4}{8} - w^2E + \frac{2(Y_1(-\xi) F - J_1(\xi) G - wY_1(-w\xi) F + wJ_1(w\xi) G)}{\xi} + \tilde{k}_b \left( 1 - w^2 \right), \tag{A-5}
\]
where

\[
E = \frac{2w\theta_w [J_0 (\xi) Y_0 (-w\xi) - J_0 (w\xi) Y_0 (-\xi)] + \xi \tilde{k}_b [J_0 (w\xi) Y_1 (-w\xi) + Y_0 (-w\xi) J_1 (w\xi)]}{4 [\xi J_0 (\xi) Y_1 (-w\xi) + \xi Y_0 (-\xi) J_1 (w\xi)]} \\
- \frac{\xi \left( 4\tilde{k}_b + w^2 \right) [J_0 (\xi) Y_1 (-w\xi) + Y_0 (-\xi) J_1 (w\xi)]}{4 [\xi J_0 (\xi) Y_1 (-w\xi) + \xi Y_0 (-\xi) J_1 (w\xi)]},
\]

(A-6)

\[
F = \frac{2\tilde{k}_b \xi J_1 (w\xi) + w\theta_w Y_0 (-\xi)}{2 [\xi J_0 (\xi) Y_1 (-w\xi) + \xi Y_0 (-\xi) J_1 (w\xi)]},
\]

(A-7)

\[
G = \frac{2\tilde{k}_b \xi J_1 (w\xi) + w\theta_w J_0 (\xi)}{2 [\xi J_0 (\xi) Y_1 (-w\xi) + \xi Y_0 (-\xi) J_1 (w\xi)]},
\]

(A-8)

where \( \xi = i \sqrt{\theta_w / \tilde{k}_b} \) and \( i \) is the imaginary number. Here, \( J_\nu (z) \) and \( Y_\nu (z) \) are the Bessel function of order \( \nu \) of first and second kind respectively.