Simulation of Exudation by Root Hairs

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Abstract.

Modelling and simulation is an important tool in describing and analysing plant and soil interactions. In this work we investigate the release of organic compounds (exudation) from roots with root hairs. Exudation by root hairs is thought to increase the bioavailability of nutrients. Therefore they represent a major factor for plant uptake of nutrients which have low mobility in soil, such as phosphorus. In this paper we use the method of homogenisation to analyse the effect of root hair geometry on exudation in the root hair zone. The resulting effective homogenised equations for the root hair zone are used to develop a new exudation model. We solve the model with Comsol Multiphysics and investigate exudation patterns in a hydroponic culture.

1 Introduction

Root hairs are lateral extensions of root epidermal cells and are known to be of great importance to plant phosphorus nutrition. The average root hair length is 0.7 mm in maize and 1.3 mm in rape [1]. Root hair diameter ranges from 5-17 μm and the number of root hairs ranges from 2-100 per mm^2 root surface area [2]. The formation of root hairs is thought to be influenced by environmental conditions such as the soil phosphorus concentration [3] and by plant genetics.

Modelling multiscale problems on increasingly complex 3-dimensional structures becomes more and more computationally challenging and even intractable. For such problems, the method of homogenisation [4] represents a tool to transform the spatial heterogeneities into a tractable homogenous description. Effective equations can thus be derived which still contain the relevant information about the geometry implicitly. The method of homogenisation is particularly suitable for domains with a periodic microstructure as illustrated in figure 1. We consider a composite material whose properties change rapidly compared to the macroscopic length scale L, which is in the order of the root length (cm). On the microscale we consider individual root hairs surrounded by water. The different properties of water and root hairs are illustrated in the right graph of figure 1 by periodic changes of colour between a dark and light blue. The characteristic length scale of the heterogeneities l is given by the distance between the root hairs (in the order of μm). If the ratio between the characteristic microscopic and macroscopic scales is small *i.e.,* $\varepsilon = \frac{l}{L} << 1$, it is possible to find effective macroscopic properties. This idea is illustrated in figure 1: In the graph on the right side the heterogeneities in colour can be distinguished. If we look at it from far away, as in the left graph, the average colour of the square is a medium blue.

When the characteristic macroscopic length scale is of order one, the microscale is equal to the period of heterogeneity [5]. Scaling the macroscopic space variable x with ε^{-1} defines a new microscopic space variable $y = x\varepsilon^{-1}$. Since ε is small the scaling blows up the domain such that the microscopic heterogeneities can be distinguished with respect to y. One of the fundamental assumptions of the theory of homogenisation is that the two variables x and y can be treated as independent of each other when ε becomes small [4]. A famous example is the derivation of the macroscopic Darcy law from the microscopic Navier-Stokes equations [6].

In this work, we introduce an effective equation for exudate transport in the root hair zone of roots which contains the relevant information about the root hair geometry implicitly. Its derivation is based on the method of homogenisation. In a first step, we consider a root with root hairs in hydroponics culture, thereby avoiding diffusion limitation due to soil properties. Our aim is to analyse the development of exudate patterns around a root with root hairs for different morphological and physiological root properties.

2 Model description

We consider one single root with a root hair zone. Water flows top-down along the root. Within the water, nutrients or exudates move by diffusion and convection. In the model the geometry is simplified in the following way: The cylindrical root is unrolled yielding a rectangular domain with periodic boundary conditions on two sides, which contains a smaller rectangular domain representing the root hair zone, see figure 2. This is justified as long as the distance between the root hairs ε is small and the ratio between root hair length and root radius is not larger than order one. In this case the distance between the tips of the root hairs is of order ε. The resulting domain

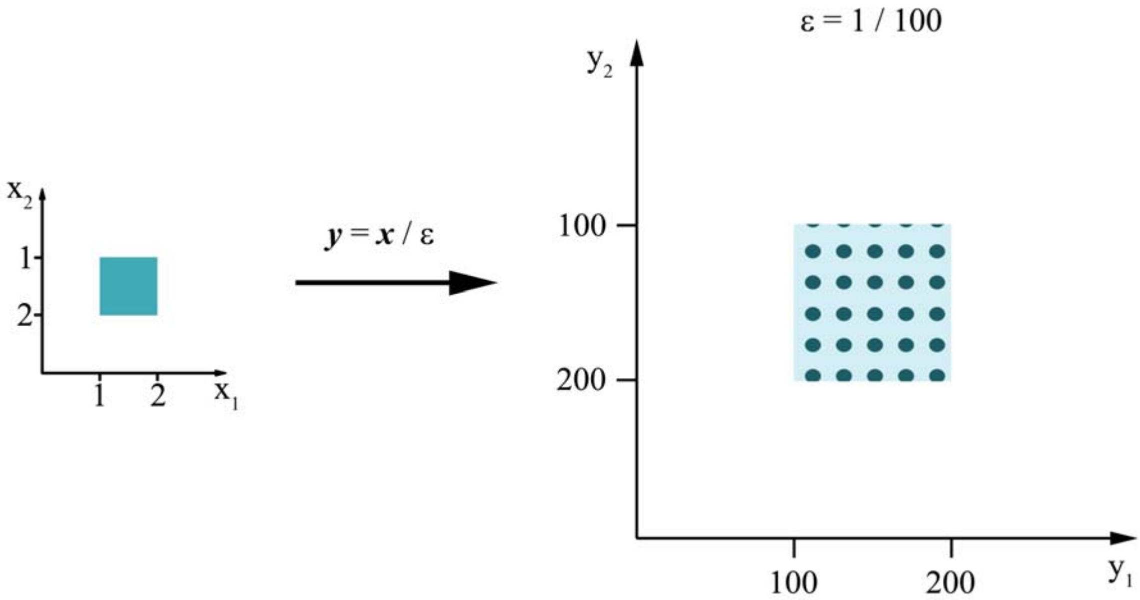

Figure 1: The left square seen with respect to x coordinates has a medium blue colour. The microstructure (periodically distributed dark blue circles on a lighter background) can be seen in the right square, blown up to y coordinates.

contains cylindrical root hairs orthogonal to the root, which have small radii and are close to each other. The distance between the root hairs $\varepsilon << 1$ is the characteristic microscopic length scale and the root length $L = \mathscr{O}(1)$ is the characteristic macroscopic length scale. Root and root hairs are surrounded by a fluid domain denoted as Ω^ε. Furthermore the domain Ω^ε is 1-periodic in x_1, thus the flow u^ε, the pressure p^ε and the concentration c^ε are 1-periodic in x_1. The superscript ε denotes that the microscopic geometry is explicitly considered.

Figure 3 shows a cross section of the domain, illustrating the bounding surfaces: the root surface, the outer boundary and the in- and outlet for water which are denoted as Γ_{in} and Γ_{out}.

For low Reynolds numbers the water flow velocity u^ε along the root is described with the Stokes equations.

$$\begin{aligned} -\Delta u^\varepsilon + \nabla p^\varepsilon &= 0, \\ \nabla \cdot u^\varepsilon &= 0, \end{aligned} \tag{1}$$

with the flow u^ε and the pressure p^ε defined in the domain Ω^ε. We assume that water uptake by the root is negligibly small compared to water flow along the root. Furthermore, we assume that the root hairs don't take up water. Thus, at the root surface, outer boundary and root hair surfaces, a no-flux condition is applied. At top (Γ_{in}) and bottom (Γ_{out}) of the domain a constant pressure is predetermined.

The nutrient concentration is described by the convection diffusion equation

$$\frac{\partial}{\partial t} c^\varepsilon - \nabla \cdot (D \nabla c^\varepsilon) + u^\varepsilon \cdot \nabla c^\varepsilon = 0, \tag{2}$$

with c^ε defined on the domain Ω^ε, the scalar constant diffusion coefficient D and the flow velocity u^ε from equation (1). The limitation on D is reasonable because the diffusion coefficient in free water can assumed to be constant [7]. The boundary conditions are chosen in the following way: There is no flux at the root surface and at the outer boundary. At the inlet Γ_{in} a constant concentration is predetermined. At Γ_{out} solutes can leave the domain with the water flow, thus at Γ_{out} the advective flux boundary condition is applied:

$$D \nabla c^\varepsilon \cdot n = 0. \tag{3}$$

The vector n is the outer normal of Γ_{in} and Γ_{out}. Uptake or exudation only occurs at the root hair surface and is described by

$$-D \nabla c^\varepsilon \cdot n^\varepsilon = \varepsilon f^\varepsilon, \tag{4}$$

where f^ε describes the uptake or exudation behaviour at a single root hair and n^ε is the outer normal of the root hairs.

When $\varepsilon << 1$ the geometry becomes complex and it is not possible to solve the above equations in reasonable time. Thus we seek a homogenised solution for $\varepsilon \to 0$. This means that we do not explicitly consider every single root hair but the cumulative effect of all root hair surfaces. The macroscopic effective model for water flow and nutrient

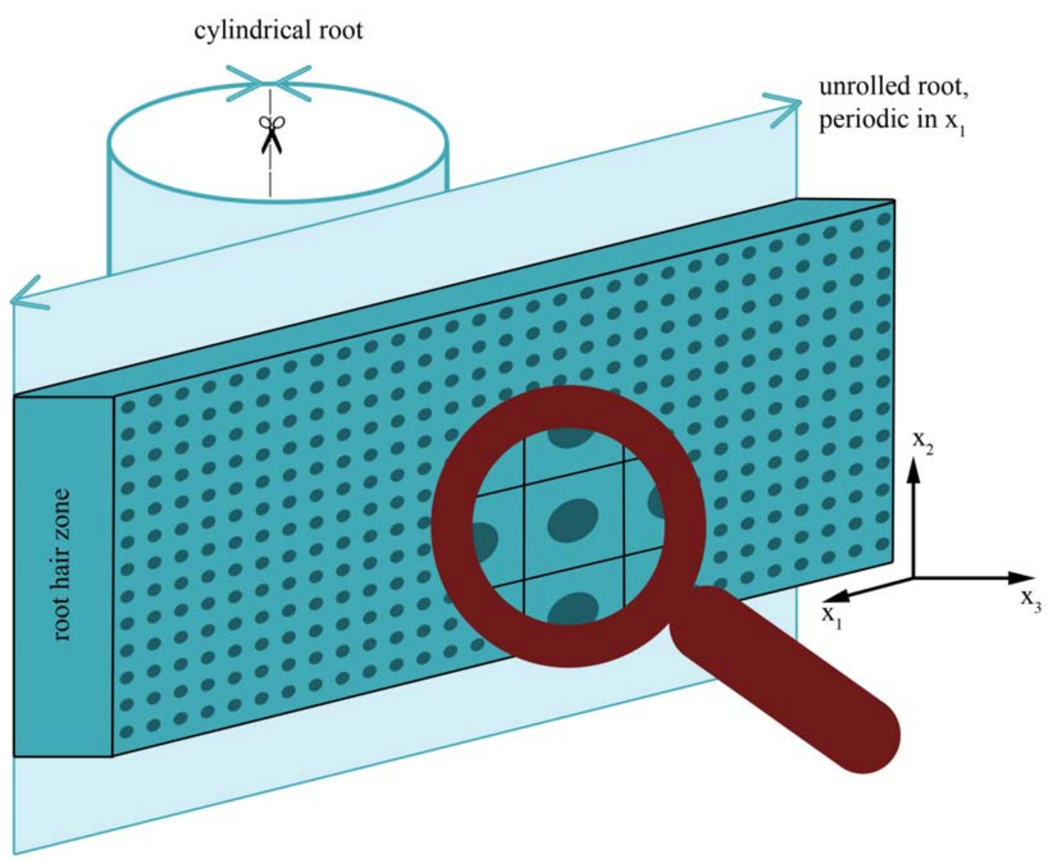

Figure 2: Geometry of a root with a root hair zone

concentration is derived in [8] using two-scale convergence. In order to give an idea how to obtain macroscopic equations we present in section 3 the derivation of the effective equations for nutrient concentration using formal asymptotic expansion.

When the root hairs are very close to each other they represent a large resistance to the water flow. In fact, [8] shows that for small ε the flow vanishes in the root hair zone Ω_a. In the fluid domain Ω_b outside the root hair zone the flow is given by the Stokes equations. Thus

$$\begin{aligned} -\Delta u_0 + \nabla p_0 &= 0, \\ \nabla \cdot u_0 &= 0, \end{aligned} \tag{5}$$

for $x \in \Omega_b$ and $u_0 = 0$ for $x \in \Omega_a$.

The concentration outside the root hair zone Ω_b is then given by

$$\frac{\partial}{\partial t} c_b - \nabla \cdot (D \nabla c_b) + u_0 \cdot \nabla c_b = 0, \tag{6}$$

with $c_b : \Omega_b \to \mathbb{R}$.

Since the convection vanishes inside the root hair zone Ω_a, [8] further shows that the concentration in this domain is described by an effective diffusion equation with a reaction term describing the cumulative uptake or exudation by the root hairs:

$$\frac{\partial}{\partial t} c_a - \frac{1}{|Y|} \nabla \cdot (\overline{D} \nabla c_a) + \frac{1}{|Y|} \int_S f dS = 0, \tag{7}$$

with $c_a : \Omega_a \to \mathbb{R}$, where Y is the fluid domain in the unit cell, S is the root hair surface in the unit cell where the uptake or exudation occurs. $\overline{D}$ is the effective diffusion tensor, which includes the cumulative effect of the root hairs to the diffusion. We expect that the effective diffusion is slower than the one in free solution. $\overline{D}$ is given by

$$\overline{D}_{ij} = \int_Y \delta_{ij} D + D \frac{\partial}{\partial y_i} \chi_j dy. \tag{8}$$

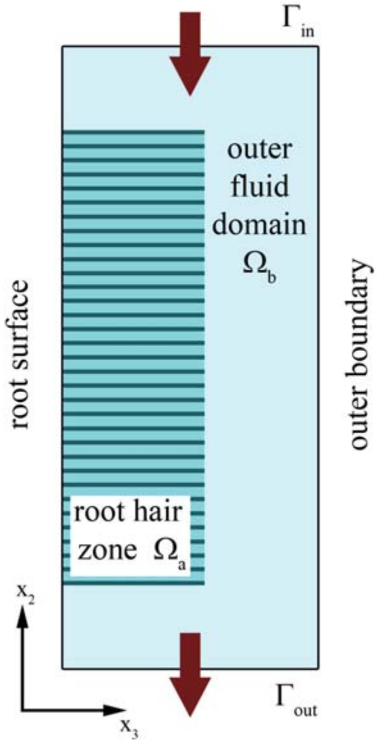

Figure 3: Boundary surfaces of the domain $\Omega = \Omega_a \cup \Omega_b$

The vector field χ is called first order corrector and describes the effect of the root hair geometry. It is sufficient to describe the effects of the root hairs in two dimensions, because the diffusion along y_3 is not effected. Therefore the corrector $\chi_3 = 0$ (in direction x_3); χ_1 and χ_2 are the solutions to the cell problem:

$$\nabla_y \cdot (\nabla_y \chi_k) \quad = \quad 0 \quad k \in \{1,2\}, \tag{9}$$

with $\chi : Y \to \mathbb{R}^2$, where $Y \subset \mathbb{T}^2$ and $\mathbb{T}^2$ is the unit torus in two dimensions. This represents the periodicity inside the root hair zone Ω_a, see figure 4. On the root hair surface S the boundary condition to the cell problem is given by

$$(\nabla_y \chi_k + e_k) \cdot n = 0 \quad k \in \{1,2\}, \tag{10}$$

where e_k is the unit vector in direction k. Between the two domains Ω_a and Ω_b a continuous flux boundary condition is applied. In the following a short derivation of the effective equations and the corresponding cell problem is given.

3 Model derivation

We look for a solution of the solute concentration c_a in the root hair zone. We derive the effective diffusion tensor in a similar manner like in chapter 13 of [4], but in contrast a constant diffusion coefficient and boundaries within the unit cells (e.g.: one root hair) are assumed.

We use the power series expansion

$$c^\varepsilon(x) = c_0(x,y) + \varepsilon c_1(x,y) + \varepsilon^2 c_2(x,y) + \ldots, \tag{11}$$

where $y = x\varepsilon^{-1}$, $y \in Y$ and $x \in \Omega_a \cap \Omega^\varepsilon$. We assume that c_0, c_1 and c_2 all are 1-periodic in y, thus the unit cell can be represented as an unit torus $\mathbb{T}^2$ with $Y \subset \mathbb{T}^2$. Furthermore x and y can be treated as independent of each other when $\varepsilon \to 0$, which is a fundamental assumption in homogenization theory.

For our formal derivation we neglect convection term in the equation for nutrient concentration c^ε

$$\frac{\partial}{\partial t} c^\varepsilon - \nabla \cdot (D \nabla c^\varepsilon) \quad = \quad 0, \tag{12}$$

$$-D \nabla c^\varepsilon \cdot n^\varepsilon \quad = \quad \varepsilon f^\varepsilon. \tag{13}$$

We denote the relevant differential operators as

$$\mathscr{L}^\varepsilon \quad := \quad -\nabla \cdot (D \nabla), \tag{14}$$

$$\mathscr{B}^\varepsilon \quad := \quad -D\nabla. \tag{15}$$

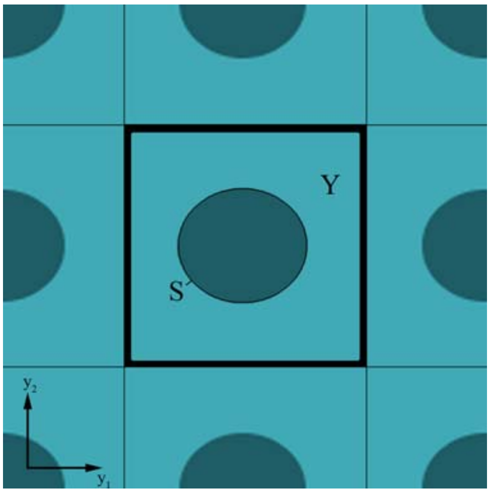

Figure 4: The periodic two dimensional unit cell, Y

With $y = x\varepsilon^{-1}$ the partial derivatives become

$$\nabla \to \nabla_x + \frac{1}{\varepsilon}\nabla_y, \tag{16}$$

with $\nabla_y = (\partial_{y_1}, \partial_{y_2}, 0)$ and the differential operators can be rewritten in the form

$$\mathscr{L}^\varepsilon = \frac{1}{\varepsilon^2}\mathscr{L}_0 + \frac{1}{\varepsilon}\mathscr{L}_1 + \mathscr{L}_2, \tag{17}$$

$$\mathscr{B}^\varepsilon = \frac{1}{\varepsilon}\mathscr{B}_0 + \mathscr{B}_1, \tag{18}$$

where

$$\mathscr{L}_0 := -\nabla_y \cdot (D\nabla_y), \tag{19}$$

$$\mathscr{L}_1 := -\nabla_y \cdot (D\nabla_x) - \nabla_x \cdot (D\nabla_y), \tag{20}$$

$$\mathscr{L}_2 := -\nabla_x \cdot (D\nabla_x), \tag{21}$$

$$\mathscr{B}_0 := -(D\nabla_y), \tag{22}$$

$$\mathscr{B}_1 := -(D\nabla_x). \tag{23}$$

Using the operators (19)-(23), equations (12) and (13) can be written in the following form:

$$\frac{\partial}{\partial t}c^\varepsilon + \frac{1}{\varepsilon^2}\mathscr{L}_0 c^\varepsilon + \frac{1}{\varepsilon}\mathscr{L}_1 c^\varepsilon + \mathscr{L}_2 c^\varepsilon = 0, \tag{24}$$

$$\left(\frac{1}{\varepsilon^2}\mathscr{B}_0 c^\varepsilon + \frac{1}{\varepsilon}\mathscr{B}_1 c^\varepsilon\right) \cdot n = f. \tag{25}$$

Substituting (11) into (24) and (25), equating coefficients of equal powers of ε and disregarding all terms of oder higher than 1 yields the following sequence of problems:

$$\mathscr{O}\left(\varepsilon^{-2}\right) \qquad \mathscr{L}_0 c_0 = 0 \ , \tag{26}$$

$$\mathscr{O}\left(\varepsilon^{-1}\right) \qquad \mathscr{L}_0 c_1 = -\mathscr{L}_1 c_0 \ , \tag{27}$$

$$\mathscr{O}(1) \qquad \mathscr{L}_0 c_2 = -\mathscr{L}_1 c_1 - \mathscr{L}_2 c_0 - \tfrac{\partial}{\partial t} c_0 \ , \tag{28}$$

with the boundary conditions:

$$\mathscr{O}\left(\varepsilon^{-2}\right) \qquad \mathscr{B}_0 c_0 \cdot n = 0 \ , \tag{29}$$

$$\mathscr{O}\left(\varepsilon^{-1}\right) \qquad \mathscr{B}_0 c_1 \cdot n = -\mathscr{B}_1 c_0 \cdot n \ , \tag{30}$$

$$\mathscr{O}(1) \qquad \mathscr{B}_0 c_2 \cdot n = -\mathscr{B}_1 c_1 \cdot n + f \ . \tag{31}$$

From the $\mathscr{O}(\varepsilon^{-2})$ equation (26) and periodicity in y we derive that c_0 is only dependent on x, so that we have $c_0 = c_0(x)$.

When the diffusion coefficient D is scalar and constant the $\mathscr{O}(\varepsilon^{-1})$ equation (27) simplifies to

$$\mathscr{L}_0 c_1 = 0, \tag{32}$$

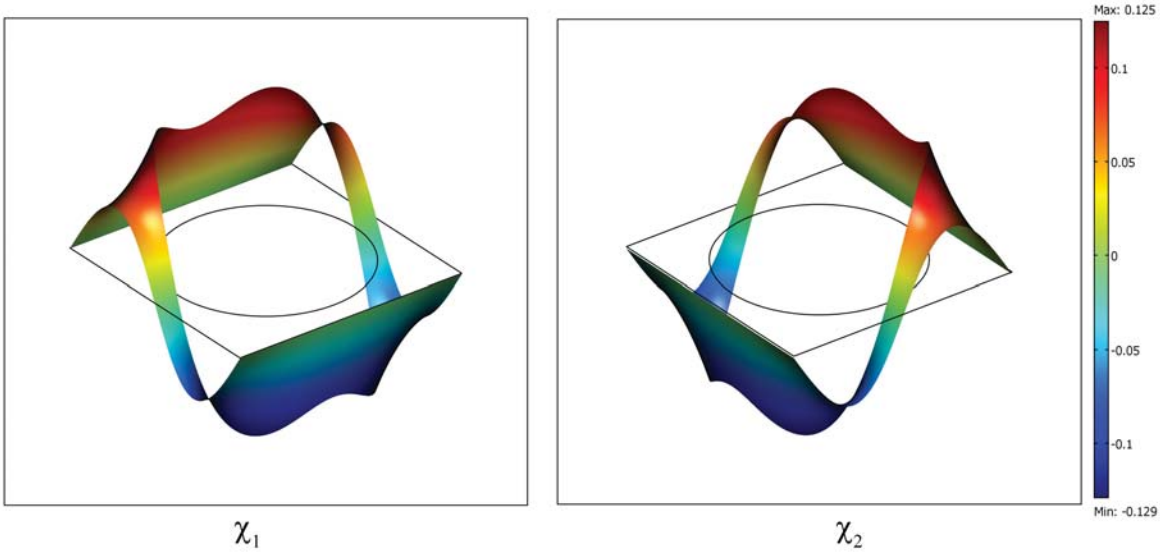

Figure 5: The first order corrector χ

where c_1 satisfies the boundary condition (30). We choose separation of variables as ansatz to define c_1 as

$$c_1(x,y) = \chi(y)\cdot\nabla_x c_0(x), \tag{33}$$

where χ is called the first order corrector, which only depends on y and hence is 1-periodic. Inserting (33) into equation (32) and into the corresponding boundary condition (30) yields the cell problem:

$$\begin{aligned} \nabla_y\cdot(\nabla_y\chi_k) &= 0, && (34)\\ (\nabla_y\chi_k+e_k)\cdot n &= 0 \quad k\in\{1,2\}, && (35)\\ \chi_3 &= 0. && (36)\end{aligned}$$

The cell problem is stationary and independent of the constant diffusion coefficient D, but highly dependent on the geometry of the boundaries. It can be easily solved numerically on a single cell, see figure 5.

Next the effective equations are obtained by analyzing the $\mathscr{O}(1)$ equation (28) with the boundary condition (31). First equation (28) is integrated over the fluid domain Y on the unit torus $\mathbb{T}^2$. By using the divergence theorem and inserting the boundary condition, the left hand side of the equation becomes:

$$\begin{aligned}\int_Y \mathscr{L}_0 c_2 dy &= -\int_Y \nabla_y\cdot(D\nabla_y c_2)dy = -\int_S (D\nabla_y c_2)\cdot n dS\\ &= \int_S \mathscr{B}_0 c_2\cdot n dS = \int_S f dS - \int_S \mathscr{B}_1 c_1\cdot n dS. \end{aligned}\tag{37}$$

As a result the integral of the $\mathscr{O}(1)$ equation (28) over Y becomes:

$$-\int_Y \mathscr{L}_2 c_0 dy - \int_Y \mathscr{L}_1 c_1 dy = |Y|\frac{\partial}{\partial t}c_0 + \int_S f dS - \int_S \mathscr{B}_1 c_1\cdot n dS. \tag{38}$$

The first integrand is already an expression in the slow variable x:

$$-\int_Y \mathscr{L}_2 c_0 dy = |Y|\nabla_x\cdot(D\nabla_x c_0) = \nabla_x\cdot\int_Y D dy \nabla_x c_0. \tag{39}$$

The last expression is according to the form needed for the effective diffusion coefficient. The second integral yields

$$\begin{aligned} -\int_Y \mathscr{L}_1 c_1 dy = \int_Y (\nabla_y\cdot(D\nabla_x)+\nabla_x\cdot(D\nabla_y))(\chi\cdot\nabla_x c_0)dy &= \\ \int_S (D\nabla_x(\chi\cdot\nabla_x c_0))\cdot n dS + \nabla_x\cdot D\int_Y (\nabla_y\chi)^T dy\nabla_x c_0 &= \\ -\int_S \mathscr{B}_1 c_1\cdot n dS + \nabla_x\cdot D\int_Y (\nabla_y\chi)^T dy \nabla_x c_0. & \end{aligned}\tag{40}$$

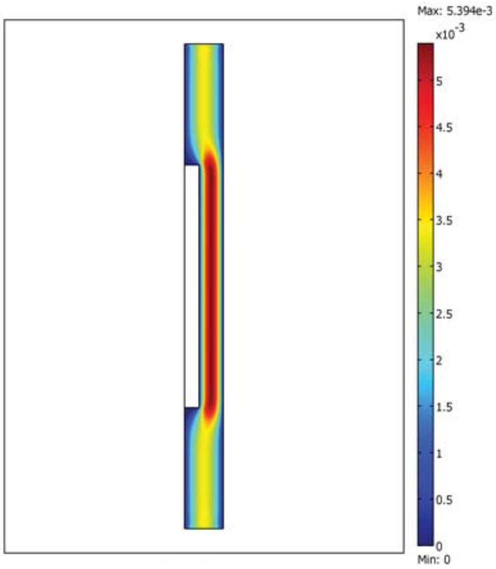

Figure 6: The static water flow u_0

Inserting the two integrals into equation (38) gives

$$\frac{1}{|Y|}\nabla_x \cdot (\underbrace{\int_Y DI + D(\nabla_y \chi)^T dy}_{\overline{D}} \nabla_x c_0) \quad = \quad \frac{\partial}{\partial t} c_0 + \frac{1}{|Y|}\int_S f dS, \tag{41}$$

which is effective diffusion equation (7) with the effective diffusion tensor $\overline{D}$ given in equation (8).

4 Results

The model is implemented in Comsol Multiphysics. First the cell problem is solved in two dimensions as described in the last section, see figure 4, yielding χ as presented in figure 5. We assume an interhair distance of 1e-4 cm and root hair radius of 4e-5 cm. With equation (8) the effective diffusion tensor is calculated from the constant scalar diffusion coefficient D which is equal to 1e-5 cm^2 s^{-1}. Since $\chi_3 = 0$ the numerical values of the effective diffusion tensor are given by

$$\overline{D} \approx \begin{pmatrix} 3.2209 \cdot 10^{-6} & -2.3238 \cdot 10^{-14} & 0 \\ -2.3238 \cdot 10^{-14} & 3.2209 \cdot 10^{-6} & 0 \\ 0 & 0 & 10^{-5} \end{pmatrix} \tag{42}$$

The homogenised problem is periodic in x_1. It is sufficient to consider one cross section (x_3, x_2), see figure 3. The stationary flow is calculated in this geometry with the domain size of 0.4 cm x 5 cm with a root hair zone of 0.15 cm x 2.5 cm. At the inlet and outlet, constant pressures of 2 and 0 bayres, respectively, are prescribed, resulting in a flow with maximum velocity of approximately 5×10^{-3} cm s^{-1}, see figure 6.

With the static flow field u_0, the convection diffusion equation can be solved on the whole domain, with the effective diffusion coefficient $\overline{D}$ on Ω_a and the scalar diffusion coefficient D on Ω_b.

The boundary conditions for concentration are set to no-flux on the left and right boundary, at the in- and outlet an advective flux boundary condition is predetermined. Between the domains Ω_a and Ω_b a continuous flux is assumed.

We calculate the exudation of the root hairs zone and assume that the exudation of the root hairs is constant per root hair surface area and time. The resulting concentration of the exudate is given in figure 7 (a). Figure 7 (b) shows how the exudate moves by convection along the flow field after leaving the root hair zone by diffusion. In figure 7 (c) the diffusion of exudate is illustrated. Diffusion mainly occurs between the domains Ω_a and Ω_b because the exudate diffuses from the high concentration in the root hair zone to the lower concentration in the solution.

This example shall demonstrate how the proposed model can be applied to experimental settings.

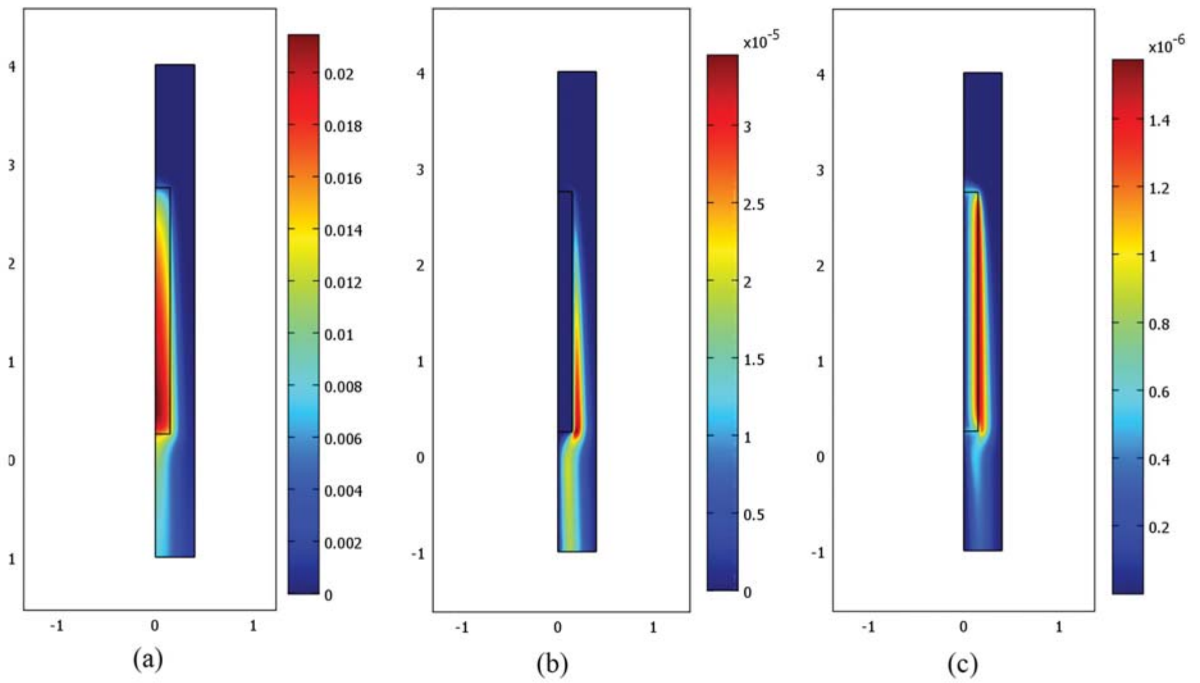

Figure 7: (a) Exudate concentration (b) Convective flux of exudates (c) Diffusive flux of exudates

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