Nonlinear Analysis: Real World Applications 11 (2010) 4586–4596

Contents lists available at ScienceDirect

Nonlinear Analysis: Real World Applications

journal homepage: www.elsevier.com/locate/nonrwa

Derivation of a macroscopic model for nutrient uptake by hairy-roots ☆

Mariya Ptashnyk

Mathematical Institute, University of Oxford, 24-29 St Giles', Oxford, OX1 3LB, UK

ARTICLE INFO

Article history:
Received 26 January 2008
Accepted 27 October 2008

Keywords:
Homogenization
Reaction-diffusion equations
Flow in porous medium
Partially perforated domain
Stokes equations

ABSTRACT

In this article the process of nutrient uptake by a single root branch is studied. We consider diffusion and active transport of nutrients dissolved in water. The uptake happens on the surface of thin root hairs distributed periodically and orthogonal to the root surface. Water velocity is defined by the Stokes equations. We derive a macroscopic model for nutrient uptake by a hairy-root from microscopic descriptions using homogenization techniques. The macroscopic model consists of a reaction-diffusion equation in the domain with hairs and a diffusion-convection equation in the domain without hairs. The macroscopic water velocity is described by the Stokes system in the domain without hairs, with no-slip condition on the boundary between domain with hairs and free fluid.

1. Introduction

As a result of root damage, certain species of plant can be genetically transformed by the bacterium *Agrobacterium rhizogenes*. This transformation causes the plant to produce "hairy-roots" — dense, highly branched root structures. Of particular interest is that hairy-roots can produce certain metabolites, which have beneficial pharmaceutical properties. In an attempt to intensify the production of these metabolites, experiments concerning the growth of hairy-roots in bioreactors are now underway. In order to optimize this process, it is necessary to obtain a better understanding the metabolism and growth of these root structures. Here, as a first step, we develop and analyse a mathematical model for the nutrient uptake by a single branch of a hairy-root. The surface of a hairy-root is covered with fine "hairs" (micro-scale roots), which enlarge the active surface area of roots and thus increase the uptake of nutrients. However, due to their high density, the hairs are a significant obstacle to the flow of water. The model we propose is defined in a partially perforated domain. We consider water flow around the root structure and diffusion of nutrient molecules dissolved in water. Substrates diffuse and are transported by the flow in the fluid part and are absorbed on the surface of the hairs, i.e. on the boundary of the microstructure. Flow velocity of the water can be defined by the Stokes system. The scale of hairs is too small for accurate numerical computation of the full problem and the derivation of a macroscopic model is required.

The derivation of macroscopic equations for the fluid flow in partially perforated domains was considered in [1–3]. As a zero order approximation, a solution of Stokes or Navier–Stokes system in a free fluid domain with no-slip boundary conditions on the interface between two domains was obtained. Higher order approximations and effective boundary conditions at the interface between homogeneous and perforated domains were derived using boundary layers. In this work, these ideas are applied to a more general geometry. To derive macroscopic equations for the velocity field we have to assume C^2 regularity of the interface between free fluid and perforated domain, which implies the regularity of a Stokes solution needed for the analysis. As a macroscopic model, we obtain Stokes equations in the domain without hairs with no-slip condition on the interface between two domains. A better approximation for the water velocity requires the construction of boundary layers, see [3]. For the more complicated geometry considered here, boundary layer correction can be constructed

☆ Supported by by the BMBF project "Modeling, simulation, and optimization of the hairy-roots reactor", University of Heidelberg.
E-mail address: mariya.ptashnyk@iwr.uni-heidelberg.de.

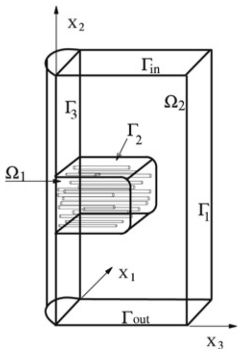
1468-1218/$ – see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.nonrwa.2008.10.063

only locally and hence will not be considered further here. A macroscopic model for the nutrient concentration consists of a diffusion equation with a reaction describing the uptake process on hair surfaces in the perforated domain and a diffusion-convection equation in the homogeneous domain. Both the partial heterogeneity of the domain and the convective term make the analysis of the equations for the concentration proposed here, non-standard. In the estimates for the convective term, the regularity of the velocity field and the error estimate for the difference of microscopic and macroscopic velocities are used. To derive a macroscopic equation for the nutrient concentration we use the technique of two-scale convergence, which was introduced in [4,5] and extended to sequences of functions defined on surfaces in [6,7]. This extension and a compactness argument are used here to obtain the convergence of the nonlinear function defined on the surface of the microstructure. There are many results on homogenization of parabolic equations defined in completely perforated domains. The two-scale convergence was used in [7] to homogenize diffusion-reaction processes in a catalyst consisting of periodic distributed bars. A similar model with convection defined in a porous medium was studied in [8] using an energy method. A macroscopic model describing diffusion, convection and nonlinear reaction in a periodic array of cells was derived in [9]. Two-scale convergence coupled with monotonicity methods and compensated compactness were used there to show the convergence in the nonlinear terms. Homogenization of reaction-diffusion and reaction-diffusion-convection equations coupled with linear or nonlinear ordinary differential equations on the surface of the microstructure was studied in [10,11]. Macroscopic equations for reaction-diffusion between periodic distributed soil grain with nonlinear monotone kinetics on the grain surface and for reaction-diffusion processes both inside and outside grains were derived in [12,13]. The effective behavior of solutions of Laplace equation in a partially perforated domain and the contact problem between a porous medium and a non-perforated domain were studied in [14,15]. Derivation of macroscopic equations in a domain with a microstructure consisting of thick junctions is based on the construction of a proper extension operator, [16].

The paper is organized as follows: First, we present a description of the considered geometry, define a microscopic model, and formulate existence and uniqueness results for solutions of the microscopic model. In Section 3 we show a priori estimates for the water velocity and derive macroscopic equations for the velocity field. In Section 4 we prove a priori estimates for the nutrient concentration and, after extension of the solutions from the perforated domain to the whole domain, using there estimates, we show the convergence of solutions of the microscopic problem to a solution of a macroscopic model.

2. Problem formulation

We consider a single root with hairs orthogonal to the root surface and distributed periodically. For the sake of simplicity we replace the cylindrical geometry of a root surface by a rectangle and pose periodic boundary conditions on the sides. We define a domain $\Omega = (0,1) \times (0,M)^2$ with inflow boundary $\Gamma_{\text{in}} = (0,1) \times \{M\} \times (0,M)$, outflow boundary $\Gamma_{\text{out}} = (0,1) \times \{0\} \times (0,M)$, and $\Gamma_1 = (0,1) \times (0,M) \times \{M\}$, $\Gamma_3 = (0,1) \times (0,M) \times \{0\}$. For $0 < m_1 < m_2 < M$ and a smooth (C^2), positive, 1-periodic in x_1 function $G : (0,1) \times (m_1, m_2) \to \mathbb{R}$ with $\sup_{x_1,x_2} G < M$, $G = 0$ for $x_2 = m_1$, $x_2 = m_2$, we define $\Omega_1 = \{(x_1,x_2,x_3) \in (0,1) \times (m_1,m_2) \times (0, G(x_1,x_2))\}$, $\Omega_2 = \Omega \setminus \Omega_1$, $\Gamma_2 = \partial\Omega_1 \setminus \Gamma_3$. We can extend G to $\mathbb{R}^2$ by zero in x_2 and periodically in x_1. We define also



- Unit cell $Z = [0,1]^2$, repeated periodically over $\mathbb{R}^2$, $Y_0 \subset Z$, an open compactly included in Z subset with a smooth boundary $R = \partial Y_0$, $Y = Z \setminus \bar{Y}_0$.
- $Z^k = Z + \sum_{i=1}^2 k_i e_i$, $Y_0^k = Y_0 + \sum_{i=1}^2 k_i e_i$, $Y^k = Y + \sum_{i=1}^2 k_i e_i$, $R^k = R + \sum_{i=1}^2 k_i e_i$ for $k \in \mathbb{Z}^2$; $Z^* = \cup\{Z^k,\ k \in \mathbb{Z}^2\}$; $\Gamma^* = \cup\{R^k \times (0, L^k),\ k \in \mathbb{Z}^2\}$, L^k are the lengths of the hairs, $L^k = \inf_{(x_1,x_2)\in\varepsilon Z^k} G(x_1,x_2) - \varepsilon$, and $\varepsilon > 0$ is the ratio between the radius of a root hair and the size of Ω_1.
- $Q = \cup\{\varepsilon Z^k | \varepsilon Z^k \subset \Omega_1 \cap \{x_3 = 0\}\}$; $Q^\varepsilon = \cup\{\varepsilon Y^k | \varepsilon Z^k \subset Q\}$;
  $R^\varepsilon = \cup\{\varepsilon R^k | \varepsilon Z^k \subset Q\}$; $\mathcal{R}^\varepsilon = \cup\{\varepsilon R^k \times \{x_3 = L^k\} | \varepsilon Z^k \subset Q\}$;
  $\Gamma^\varepsilon = \cup\{\varepsilon R^k \times (0, L^k) | \varepsilon Z^k \times (0, L^k) \subset \Omega_1\}$; $\Upsilon^\varepsilon = \cup\{\varepsilon \bar{Y}_0^k \times \{L^k\} | \varepsilon Z^k \subset Q\}$.
- $\Omega_0^\varepsilon = \cup\{\varepsilon Y_0^k \times (0, L^k) | \varepsilon Z^k \times (0, L^k) \subset \Omega_1\}$, $\Omega_1^\varepsilon = \Omega_1 \setminus \bar{\Omega}_0^\varepsilon$ and $\Omega^\varepsilon = \Omega_1^\varepsilon \cup \Omega_2$.