

# Modeling solute transport through unsaturated porous media using homogenization I\*

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**Abstract.** In this paper we consider homogenization of the diffusion, adsorption and convection of chemical species in porous media, that are transported by unsaturated single phase flows. The unsaturated flow is described by the Richards' equation. We present in details a rigorous derivation of the corresponding dual porosity model. Then we give the derivation by homogenization of first-order kinetic models for the evolution of the chemical species. Finally, numerical simulations for the Freundlich and Langmuir isotherms are presented.

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**Key words:** homogenization, Richards equation, dual porosity.

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## 1 Introduction

The underground solute transport involves a complex interplay among hydrological, physical, geochemical and biochemical processes. The geometry plays an important role in modeling. Usually the primary solid particles are assumed to be aggregated into porous pellets (aggregates). The inter-aggregate pore space is such that bulk flow of water only takes place between the aggregates. Consequently, solutes move inside the porous pellets only because of molecular

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diffusion. On the surface of the pellets the chemical species undergo adsorption or exchange processes.

In the article [23] there is a classification of the computationally significant types of reactions into homogeneous, heterogeneous sorption or ion exchange, and classical heterogeneous dissolution/precipitation reactions.

Our goal is to obtain the upscaled equations, valid at the macro level, starting from the mesoscopic geometry described above. We expect to justify the models from [23] and [15], at least for adsorption processes, and to obtain more precise modeling for dissolution/precipitation reactions involving free boundaries. Direct application of our results is to the hydrochemical computer codes which are of interest for ANDRA.

In this article we concentrate to the case when the chemical species undergo adsorption. A direct modeling approach to this problem is in [14], where the mathematical analysis of a model from the general paper of Rubin [23] is undertaken. Since the first difficulty is with the unsaturated flow, we concentrate our efforts mainly on the obtaining of the dual porosity Richards model and leave the more detailed considerations of the transport, diffusion and adsorption of chemical species to the subsequent papers. That's reason why "I" appears in the title.

For simplicity we suppose the porous media  $\Omega$  be a unit cube.

Let  $Y = ]0, 1[^n$ ,  $n = 2, 3$  be the unit cell and let  $\partial\Omega = \overline{\Gamma^1} \cup \overline{\Gamma^2}$ ,  $\Gamma^1 \cap \Gamma^2 = \emptyset$ , where each  $\Gamma^1$  and  $\Gamma^2$  is a  $n - 1$ -dimensional manifold (with boundary).

We assume then that the geometry of the cell  $Y$  defined as follows.

◊  $Y_m$ , the pellet, is a connected open subset of  $\mathbb{R}^n$ ,  $\overline{Y}_m \subset Y$ , with Lipschitz boundary;  $Y_f = Y \setminus \overline{Y}_m$ , the unit inter-aggregate pore is connected.

Now for a given bounded open set  $\Omega \subset \mathbb{R}^n$  and  $\varepsilon > 0$  we define the union of the pore spaces

$$\Omega_f^\varepsilon = \Omega \cap \bigcup_{k \in \mathbb{Z}^n} \varepsilon(Y_f + k).$$

Then  $\Omega_m^\varepsilon$  is the union of all pellets and  $\Gamma^\varepsilon$  is the boundary between  $\Omega_m^\varepsilon$  and  $\Omega_f^\varepsilon$ .  $\Omega^\varepsilon = \Omega_f^\varepsilon \cup \Omega_m^\varepsilon \cup \Gamma^\varepsilon$ .

Under the above assumptions, the theory from [1] implies that there exists a linear and continuous extension operator  $\Pi_\varepsilon : W^{1,q}(\Omega_f^\varepsilon) \rightarrow W_{loc}^{1,q}(\Omega)$ , and three constants  $k_0, k_1, k_2 > 0$ , such that  $\forall u \in W^{1,q}(\Omega_f^\varepsilon)$  we have

$$\Pi_\varepsilon u = u \quad (\text{a.e.}) \quad \text{in} \quad \Omega_f^\varepsilon \quad (1)$$

$$\int_{\Omega(\varepsilon k_0)} |\Pi_\varepsilon u|^q dx \leq k_1(Y_f, n, q) \int_{\Omega_f^\varepsilon} |u|^q dx \quad (2)$$

$$\int_{\Omega(\varepsilon k_0)} |\nabla(\Pi_\varepsilon u)|^q dx \leq k_2(Y_f, n, q) \int_{\Omega_f^\varepsilon} |\nabla u|^q dx. \quad (3)$$

Finally,  $\Omega(\varepsilon k_0) = \{x \in \Omega : \text{dist}(x, \partial\Omega) > \varepsilon k_0\}$ .

## 2 Modeling of the filtration

In the modeling of the underground transport, first question is how to handle the fluid flow. In all models reviewed in [23] and [15], and further studied in [14], we remark that the concentration of the transported contaminants is such that the flow is not affected. This means that we should study the effective flow before looking at the mass balance equations for the transported species. All flows could be considered as incompressible.

For the saturated single phase flows we know that the filtration velocity is given by the Darcy's law. This situation is fairly well understood and using homogenization it is possible to obtain Darcy's law from the microscopic momentum equation. For more details in the case of periodic porous media we refer to the original contribution by Tartar [25] in the book [24] and to the review papers [4] and [20]. Let us note that that the derivation of the Darcy's law for random porous media is in [8]. Consequently, for the mesoscopic model we'll have the Darcy's law but with different permeabilities, corresponding to the pellets and to the inter-aggregate pores.

The homogenization of the mesoscopic model is straightforward if the permeabilities are of the same order, since it reduces to study of the convergence of the homogenization process for a scalar elliptic equation for the pressure, when the characteristic size of the inter-aggregate pores  $\varepsilon$  tends to zero. If the permeability ratio between the pellets and the pore space is of order  $\varepsilon^2$  then one obtains the

dual-porosity model widely present in the oil literature. For its derivation in the case of a periodic porous medium we refer to [6]. Derivation for random porous media is in [13].

For the multiphase flows, we can't say much about the derivation of the mesoscopic models from the first principles. We refer to the review paper of Bourgeat [12] and to the calculations for the flow through a single pore in [19]. To the contrary, homogenization of the mesoscopic models was studied with success in many papers. We refer to [9] and [18] for the 2-phase flows in periodic geometries and with the permeabilities of same order, to the article [10] for the random case and to [11] for the 2-phase dual-porosity model.

Very frequently, solutes are transported by an unsaturated flow. Single phase unsaturated flows are described by the Richards' equation. Even if it seems that the equations describing the 2-phase flow of water and air are more realistic, the Richards's equation is widely used and in the hydrochemical computer codes one should solve it in a heterogeneous medium.

Hence in order to have an effective equation for the velocity and the pressure, we study the homogenization of the Richards equation. The Richards equation in the dual porosity case reads as follows (see e.g. [7])

$$\frac{\partial \vartheta_f(P^\varepsilon)}{\partial t} = \operatorname{div} (k_f(\vartheta_f(P^\varepsilon))(\nabla P^\varepsilon - e_3)) \quad \text{in } \Omega_f^\varepsilon \times (0, T) \tag{4}$$

$$\frac{\partial \vartheta_m(p^\varepsilon)}{\partial t} = \varepsilon^2 \operatorname{div} (k_m(\vartheta_m(p^\varepsilon))(\nabla p^\varepsilon - e_3)) \quad \text{in } \Omega_m^\varepsilon \times (0, T) \tag{5}$$

$$P^\varepsilon = p^\varepsilon \quad \text{on } \Gamma^\varepsilon \times (0, T) \tag{6}$$

$$k_f(\vartheta_f(P^\varepsilon))(\nabla P^\varepsilon - e_3) \cdot \nu = \varepsilon^2 k_m(\vartheta_m(p^\varepsilon))(\nabla p^\varepsilon - e_3) \cdot \nu \quad \text{on } \Gamma^\varepsilon \times (0, T) \tag{7}$$

$$P^\varepsilon = P^D \quad \text{on } \Gamma^1 \times (0, T) \tag{8}$$

$$k_f(\vartheta_f(P^\varepsilon))(\nabla P^\varepsilon - e_3) \cdot \nu = g \frac{(P^\varepsilon - \vartheta^{-1}(\theta_0) - \delta)_+}{|P^\varepsilon - \vartheta^{-1}(\theta_0)|} \quad \text{on } \Gamma^2 \times (0, T) \tag{9}$$

$$\chi_{\Omega_f^\varepsilon} P^\varepsilon(x, 0) + \chi_{\Omega_m^\varepsilon} p^\varepsilon(x, 0) = P^D(x, 0) \quad \text{on } \Omega \tag{10}$$

where  $\delta$  is a small positive number,  $P^\varepsilon, p^\varepsilon$  are the unknown (scaled) pressures,

$\vartheta$  is the water content and  $k$  is the hydraulic conductivity. Let us note that we have two functions  $\vartheta$  and  $k$ . Each  $\vartheta$  is a  $C^1$  strictly monotone increasing positive function on  $\mathbb{R}$ , equal to  $\delta s$  for  $s > 0$ . Each  $k$  is a  $C^1$  increasing function defined on  $[0, 1]$ . They are positive and strictly monotone increasing for  $\vartheta > \theta_0$ . They could be zero on  $[0, \theta_0)$ . Let  $V = \{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma^1\}$ .

**Proposition 1.** *Let  $P^D \in H^1(0, T; L^\infty(\Omega)) \cap L^2(0, T; H^1(\Omega))$ ,  $P^D \geq \vartheta^{-1}(\theta_0) + \delta$ ,  $\delta > 0$ . Let  $g \in L^2(\Gamma^2 \times (0, T))$ . Then there exists at least one solution  $\tilde{p}^\varepsilon = \chi_{\Omega_f^\varepsilon} P^\varepsilon + \chi_{\Omega_m^\varepsilon} p^\varepsilon \in (P^D + L^2(0, T; V)) \cap L^\infty(\Omega \times (0, T))$ ,  $\tilde{p}^\varepsilon \geq \vartheta^{-1}(\theta_0) + \delta$  and  $\frac{\partial \vartheta_f(P^\varepsilon)}{\partial t} \chi_{\Omega_f^\varepsilon} + \frac{\partial \vartheta_m(p^\varepsilon)}{\partial t} \chi_{\Omega_m^\varepsilon} \in L^2(0, T; V')$  satisfying*

$$\begin{aligned} & \int_0^T \left\langle \frac{\partial}{\partial t} (\vartheta_f(P^\varepsilon) \chi_{\Omega_f^\varepsilon} + \vartheta_m(p^\varepsilon) \chi_{\Omega_m^\varepsilon}), \varphi \right\rangle_\Omega \\ & + \int_0^T \int_\Omega \left( \chi_{\Omega_f^\varepsilon} k_f(\vartheta_f(P^\varepsilon)) (\nabla P^\varepsilon - e_3) \right. \\ & \left. + \chi_{\Omega_m^\varepsilon} \varepsilon^2 k_m(\vartheta_m(p^\varepsilon)) (\nabla p^\varepsilon - e_3) \right) \cdot \nabla \varphi \\ & = \int_0^T \int_{\Gamma^2} g \frac{(P^\varepsilon - \vartheta^{-1}(\theta_0) - \delta)_+}{|P^\varepsilon - \vartheta^{-1}(\theta_0)|} \varphi, \quad \forall \varphi \in L^2(0, T; V) \end{aligned} \quad (11)$$

and satisfying the initial condition (10). Furthermore, it satisfies the a priori estimates

$$\|\tilde{p}^\varepsilon\|_{L^\infty(\Omega \times (0, T))} + \|\nabla P^\varepsilon\|_{L^2(\Omega_f^\varepsilon \times (0, T))} \leq C \quad (12)$$

$$\|\nabla p^\varepsilon\|_{L^2(\Omega_m^\varepsilon \times (0, T))} \leq \frac{C}{\varepsilon} \quad (13)$$

$$\begin{aligned} & \int_0^{T-h} \int_\Omega \left( (\vartheta_f(P^\varepsilon) \chi_{\Omega_f^\varepsilon} + \vartheta_m(p^\varepsilon) \chi_{\Omega_m^\varepsilon})(x, t+h) \right. \\ & \left. - (\vartheta_f(P^\varepsilon) \chi_{\Omega_f^\varepsilon} + \vartheta_m(p^\varepsilon) \chi_{\Omega_m^\varepsilon})(x, t) \right) \\ & (\tilde{p}^\varepsilon(x, t+h) - \tilde{p}^\varepsilon(x, t)) \leq Ch, \quad \forall h \in (0, 1) \end{aligned} \quad (14)$$

where constants are independent of  $\varepsilon$ .

**Proof.** Proof of the proposition follows the lines of the article [5]. It should be noted that the conditions on the data guarantee the non-degeneracy of the coefficients.  $\square$

Next we use the results from [1] presented in the introduction and extend  $P^\varepsilon$  to  $\Omega$ . The extension  $\Pi_\varepsilon P^\varepsilon$  satisfies

**Lemma 2.** *We have*

$$\|\Pi_\varepsilon P^\varepsilon\|_{L^\infty(\Omega \times (0, T))} + \|\nabla \Pi_\varepsilon P^\varepsilon\|_{L^2(\Omega \times (0, T))} \leq C \tag{15}$$

$$\int_0^{T-h} \int_\Omega (\vartheta_f(\Pi_\varepsilon P^\varepsilon)(x, t+h) - \vartheta_f(\Pi_\varepsilon P^\varepsilon)(x, t)) (\Pi_\varepsilon P^\varepsilon(x, t+h) - \Pi_\varepsilon P^\varepsilon(x, t)) \leq Ch, \quad \forall h \in (0, 1) \tag{16}$$

Using the a priori estimates derived in proposition 1 and lemma 2 and the concept of two scale convergence as in [3], we get the following compactness results

**Proposition 3.** *There exists a subsequence such that*

$$\Pi_\varepsilon P^\varepsilon \longrightarrow P \in L^2((0, T); H^1(\Omega)) \quad \text{in the two-scale sense} \tag{17}$$

$$\begin{aligned} \nabla(\Pi_\varepsilon P^\varepsilon) &\longrightarrow \nabla P + \nabla_y P_1(t, x, y) \quad \text{in the two-scale sense, where} \\ P_1 &\in L^2((0, T) \times \Omega; H^1_{per}(Y)) \end{aligned} \tag{18}$$

$$\tilde{p}^\varepsilon \longrightarrow p \in L^2((0, T) \times \Omega; H^1_{per}(Y)) \quad \text{in the two scale-sense} \tag{19}$$

$$\Pi_\varepsilon P^\varepsilon \longrightarrow P \quad \text{strongly in } L^q((0, T) \times \Omega), \quad \forall q < +\infty \tag{20}$$

$$\varepsilon \nabla \tilde{p}^\varepsilon \longrightarrow \nabla_y p \in L^2((0, T) \times \Omega \times Y) \quad \text{in the two scale-sense} \tag{21}$$

**Proof.** The proof is a direct consequence of the a priori estimates and of theorem 1.2 and proposition 1.4 in [3].  $\square$

Again as in [3] we plug into (11) a test function of the form  $\varphi(x, t) + \varepsilon \varphi_1(x, x/\varepsilon, t) + \Psi(x, x/\varepsilon, t)$ , where  $\varphi \in C^\infty_0(Q_T)$ ,  $\varphi_1 \in C^\infty_0(Q_T; C^\infty_{per}(Y))$  and

$\Psi \in C_0^\infty(Q_T; C_{per}^\infty(Y))$  with  $\Psi = 0$  for  $y \in \Omega_f$ . Passing to the two-scale limit yields:

$$\begin{aligned} & \int_0^T \int_\Omega \int_{Y_f} \vartheta_f(P) \frac{\partial \varphi(x, t)}{\partial t} \\ & + \int_0^T \int_\Omega \int_{Y_m} \Theta_m \cdot \left[ \frac{\partial \varphi(x, t)}{\partial t} + \frac{\partial}{\partial t} \Psi(x, y, t) \right] \\ & - \int_0^T \int_\Omega \int_{Y_f} k_f(\vartheta_f(P)) [\nabla P + \nabla_y P_1 - e_3] [\nabla \varphi + \nabla_y \varphi_1(x, y, t)] \\ & - \lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Omega_m^\varepsilon} k_m(\vartheta_m(p^\varepsilon)) \nabla p^\varepsilon \nabla_y \Psi^\varepsilon = 0, \end{aligned} \quad (22)$$

where  $\Theta_m$  is the two-scale limit of the (sub)sequence of  $\vartheta_m(p^\varepsilon) \chi_{\Omega_m^\varepsilon}$ . Let  $\xi_j$ ,  $\int_{Y_f} \xi_j = 0$ , be the 1-periodic solution to

$$\Delta_y \xi_j = 0 \text{ in } Y_f, \quad \nabla_y \xi_j \cdot \nu = -e_j \cdot \nu \text{ on } \partial Y_m. \quad (23)$$

and  $\Xi$  the tensor whose  $(i, j)$  component is the average of  $\partial \xi_j / \partial y_i$ . Then  $P_1 = \sum_j \xi_j(y) (\partial P / \partial x_j - \delta_{j3})$  and the choice  $\Psi = 0$  gives

$$\begin{aligned} & |Y_f| \frac{\partial \vartheta_f(P)}{\partial t} + \frac{\partial}{\partial t} \int_{Y_m} \Theta_m dy \\ & - \operatorname{div}_x \{ k_f(\vartheta_f(P)) (I + \Xi) [\nabla_x P - e_3] \} = 0 \text{ in } Q_T \end{aligned} \quad (24)$$

We note that by Lemma 4.2 from [11],  $\partial_t \int_{Y_m} \Theta_m dy \in L^2(\Omega \times (0, T))$ .

The real difficulty is in identifying  $\Theta_m$ . Let us note that  $\chi_{\Omega_m^\varepsilon} p^\varepsilon$  doesn't converge strongly and oscillations are likely to persist. We proceed by using the method of periodic modulation as in [11]. It was introduced in [6] and we repeat the definition:

**Definition 4.** For a given  $\varepsilon > 0$ , we define a dilation operator  $D^\varepsilon$  mapping measurable functions on  $\Omega_m^\varepsilon \times (0, T)$  to measurable functions on  $\Omega \times Y_m \times (0, T)$  by

$$(D^\varepsilon u)(x, y, t) = u(c^\varepsilon(x) + \varepsilon y, t), \quad y \in Y_m, \quad (x, t) \in \Omega \times (0, T) \quad (25)$$

where  $c^\varepsilon(x)$  denote the lattice translation point of the  $\varepsilon$ -cell domain containing  $x$ . We extend  $D^\varepsilon u$  from  $Y_m$  to  $\cup_k(Y_m + k)$  periodically.

It is easy to see that

**Lemma 5** (see [6] pp 828–831). For  $\forall u \in L^2(0, T; W^{1,q}(\Omega_m^\varepsilon))$  we have

$$\begin{cases} \| D^\varepsilon u \|_{L^q(Q_T \times Y_m)} = \| u \|_{L^q(Q_T)}, & 1 \leq q < +\infty \\ \nabla_y D^\varepsilon u = \varepsilon D^\varepsilon \nabla_x u & \text{(a.e.) in } Q_T \times Y_m. \end{cases} \quad (26)$$

Furthermore, let  $\varphi, \psi \in L^2(0, T; H^1(\Omega_m^\varepsilon))$ . Then

$$(D^\varepsilon \varphi, D^\varepsilon \psi)_{L^2(Q_T \times Y_m)} = (\varphi, \psi)_{L^2(\Omega_m^\varepsilon \times (0, T))} \quad (27)$$

$$\| \nabla_y D^\varepsilon \varphi \|_{L^2(Q_T \times Y_m)^3} = \varepsilon \| D^\varepsilon \nabla_x \varphi \|_{L^2(\Omega_m^\varepsilon \times (0, T))^3} \quad (28)$$

$$(D^\varepsilon \varphi, \psi)_{L^2(Q_T \times Y_m)} = (\varphi, D^\varepsilon \psi)_{L^2(Q_T \times Y_m)} \quad (29)$$

**Proposition 6** ([11]). Let  $\{u^\varepsilon\}$  be a uniformly bounded sequence in  $L^2(\Omega_m^\varepsilon \times (0, T))$  which satisfy the conditions

$$\begin{aligned} D^\varepsilon u^\varepsilon &\rightharpoonup u^0 \text{ weakly in } L^2(Q_T; L^2_{per}(Y_m)) \text{ and} \\ \chi_{\Omega_m^\varepsilon} u^\varepsilon &\longrightarrow u^* \in L^2(Q_T; L^2_{per}(Y)) \text{ in the two-scale sense.} \end{aligned}$$

Then we have

$$u^0 = u^* \text{ (a.e.) in } Q_T \times Y_m. \quad (30)$$

**Proposition 7.** With the above notations we have

$$\| D^\varepsilon p^\varepsilon \|_{L^2(Q_T; L^2_{per}(Y_m))} \leq C \quad (31)$$

Let  $\varepsilon > 0$  and let  $D^\varepsilon p^\varepsilon$  be defined by (25). Then  $D^\varepsilon p^\varepsilon = \bar{p}^\varepsilon$  satisfies in  $L^2(0, T; H^{-1}(Y_m))$  the equation

$$\partial_t \vartheta_m(D^\varepsilon p^\varepsilon) - \operatorname{div}_y \{k_m(\vartheta_m(\bar{p}^\varepsilon))(\nabla_y \bar{p}^\varepsilon - \varepsilon e_3)\} = 0 \quad (32)$$

$$\text{for (a.e.) } x \in \Omega_m^\varepsilon \text{ and } (D^\varepsilon p^\varepsilon)(x, y, 0) = D^\varepsilon P^D(x, 0) \text{ on } \Omega \times Y_m \quad (33)$$



We consider the problem:

$$\left\{ \begin{aligned} &\text{Find } p^* \in L^2(Q_T; L^2_{per}(Y_m)) \cap L^\infty(Q_T \times Y_m), \vartheta^{-1}(\theta_0) + \delta \\ &\leq p^* \text{ (a.e.) on } Q_T \times Y_m, \nabla_y p^* \in L^2(Q_T; L^2_{per}(Y_m))^n, \\ &\partial_t p^* \in L^2(Q_T; H^{-1}_{per}(Y_m)) \text{ such that } \int_0^t \int_{Y_m} \vartheta_m(p^*(x, y, \tau)) \partial_t \psi \\ &- \int_0^t \int_{Y_m} k_m(\vartheta_m(p^*)) \nabla_y p^* \nabla_y \psi = \int_{Y_m} \vartheta_m(p^*(x, y, t)) \psi(y, t) dy \\ &- \int_{Y_m} \vartheta_m(P^D(x, 0)) \psi(y, 0) dy \text{ for (a.e.) } (x, t) \in Q_T, \\ &\forall \psi \in H^1((0, T) \times Y_m), \psi = 0 \text{ on } \partial Y_m \times (0, T) \\ &p^* = P \text{ in } L^2(0, T; H^{1/2}(\partial Y_m)) \text{ for (a.e.) } x \in \Omega \end{aligned} \right. \quad (34)$$

$$\left. \begin{aligned} &p^* = P \text{ in } L^2(0, T; H^{1/2}(\partial Y_m)) \text{ for (a.e.) } x \in \Omega \end{aligned} \right. \quad (35)$$

For fixed  $P \in L^2(0, T; H^1(\Omega)) \cap L^\infty(Q_T)$ ,  $\vartheta^{-1}(\theta_0) + \delta \leq P$  (a.e.) on  $Q_T$  and  $P^0 \in L^\infty(\Omega)$ ,  $\vartheta^{-1}(\theta_0) + \delta \leq P^D(\cdot, 0)$  (a.e.) on  $\Omega$ , the theory from [5] and [21] gives existence of a unique solution  $p^*$  for (34)–(35).

Our final step is to compare the problems (34)–(35) and (32)–(33). We have the following result:

**Proposition 8.** *Let  $D^\varepsilon s^\varepsilon$  be defined by (25) and let  $p^*$  be a solution for (34)–(35). Then we have*

$$\begin{aligned} D^\varepsilon p^\varepsilon &\longrightarrow p^* \text{ in } L^2(\Omega \times Y_m \times (0, T)) \text{ and} \\ p^* &= p \text{ (a.e.) on } \Omega \times Y_m \times (0, T) \end{aligned} \quad (36)$$

where  $p$  is defined by (19).

**Proof.** We choose the test function by a change of pivot. Therefore, we introduce for (a.e.)  $(x, t) \in Q_T$  a function  $w^\varepsilon \in H^1_0(Y_m)$  by

$$-\Delta_y w^\varepsilon = \vartheta_m(D^\varepsilon p^\varepsilon) - \vartheta_m(p^*) \text{ in } Y_m. \quad (37)$$

Obviously,  $w^\varepsilon \in H^1(Q_T \times Y_m)$ ,  $\|\nabla_y w^\varepsilon(x, y, 0)\|_{L^2(Q_T \times Y_m)} \leq C\varepsilon$  and

$$\|\nabla_y w^\varepsilon\|_{L^2(Q_T; L^2(Y_m))} \leq C \|D^\varepsilon p^\varepsilon - p^*\|_{L^2(Q_T \times Y_m)}.$$

Now we introduce the function  $\zeta^\varepsilon$  by  $\zeta^\varepsilon = \vartheta_m(D^\varepsilon p^\varepsilon) - \vartheta_m(p^*)$  and  $K_m(s)$  by  $K_m(s) = \int_0^s k_m(\vartheta_m(\eta)) d\eta$ . Obviously,  $\zeta^\varepsilon$  satisfies the variational equation

$$\begin{aligned} & \int_0^T \int_{Y_m} \int_{\Omega} \zeta^\varepsilon \partial_t \Psi - \int_{Q_T} \int_{Y_m} \nabla_y \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \nabla_y \Psi \\ & \quad - \int_{\Omega} \int_{Y_m} (\zeta^\varepsilon(\cdot, T) \Psi(\cdot, T) - \zeta^\varepsilon(\cdot, 0) \Psi(\cdot, 0)) \\ & = -\varepsilon \int_{Q_T} \int_{Y_m} k_m(\vartheta_m(D^\varepsilon p^\varepsilon)) \frac{\partial \Psi}{\partial y_3}, \\ & \quad \forall \Psi \in H^1(Q_T \times Y_m), \Psi = 0 \text{ on } \partial Y_m \end{aligned} \tag{38}$$

and the boundary condition

$$\zeta^\varepsilon = \vartheta_m(D^\varepsilon P^\varepsilon) - \vartheta_m(P) \text{ in } L^2(0, T; H^{1/2}(\partial Y_m)) \text{ for (a.e.) } x \in \Omega.$$

In order to estimate the  $L^2$ -norm of  $\zeta^\varepsilon$  we choose  $\Psi = w^\varepsilon$  as the test function. We have

$$\begin{aligned} & \int_{Q_T} \int_{Y_m} \zeta^\varepsilon \partial_t w^\varepsilon - \int_{\Omega} \int_{Y_m} (\zeta^\varepsilon(\cdot, T) w^\varepsilon(\cdot, T) - \zeta^\varepsilon(\cdot, 0) w^\varepsilon(\cdot, 0)) \\ & \quad - \int_{Q_T} \int_{Y_m} \left( \nabla_y \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \nabla_y w^\varepsilon \right. \\ & \quad \left. + \varepsilon k_m(\vartheta_m(D^\varepsilon p^\varepsilon)) \frac{\partial w^\varepsilon}{\partial y_3} \right) = 0. \end{aligned} \tag{39}$$

Using the uniform bound for  $\nabla_y w^\varepsilon$  in  $L^2(Q_T \times Y_m)$  we find out that the right hand side is bounded by  $C\varepsilon$ .

Furthermore

$$\begin{aligned} & \int_{Q_T} \int_{Y_m} \partial_t w^\varepsilon \zeta^\varepsilon = \int_{Q_T} \int_{Y_m} \nabla_y w^\varepsilon \nabla_y \partial_t w^\varepsilon \\ & = \frac{1}{2} \int_{\Omega} \int_{Y_m} |\nabla_y w^\varepsilon(\cdot, T)|^2 - \frac{1}{2} \int_{\Omega} \int_{Y_m} |\nabla_y w^\varepsilon(\cdot, 0)|^2, \\ & \int_{\Omega} \int_{Y_m} \zeta^\varepsilon(\cdot, T) w^\varepsilon(\cdot, T) = \int_{\Omega} \int_{Y_m} |\nabla_y w^\varepsilon(\cdot, T)|^2 \text{ and} \\ & \int_{\Omega} \int_{Y_m} \zeta^\varepsilon(\cdot, 0) w^\varepsilon(\cdot, 0) = \int_{\Omega} \int_{Y_m} |\nabla_y w^\varepsilon(\cdot, 0)|^2. \end{aligned}$$

Therefore, we write (39) in the form

$$\begin{aligned} & \left| \int_{Q_T} \int_{Y_m} \nabla_y \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \nabla_y w^\varepsilon \right| \\ & \leq C\varepsilon + \frac{1}{2} \int_{\Omega} \int_{Y_m} |\nabla_y w^\varepsilon(\cdot, 0)|^2 \leq C\varepsilon. \end{aligned}$$

It remains to find an estimate from below for the diffusion term. We have

$$\begin{aligned} & \int_{Q_T} \int_{Y_m} \nabla_y \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \nabla_y w^\varepsilon \\ & = \int_{Q_T} \int_{\partial Y_m} \{K_m(D^\varepsilon p^\varepsilon) - K_m(P)\} \nabla_y w^\varepsilon \cdot \nu \\ & \quad - \int_{Q_T} \int_{Y_m} \{K_m(D^\varepsilon p^\varepsilon) - K_m(P)\} \Delta_y w^\varepsilon \\ & = \int_{Q_T} \int_{Y_m} \nabla_y K_m(\Pi_\varepsilon D^\varepsilon P^\varepsilon) \nabla_y w^\varepsilon \\ & \quad + \int_{Q_T} \int_{Y_m} \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \zeta^\varepsilon \end{aligned}$$

Therefore

$$\begin{aligned} & \int_{Q_T} \int_{Y_m} \{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \{\vartheta_m(D^\varepsilon p^\varepsilon) - \vartheta_m(p^*)\} \leq C\varepsilon \\ & \quad + C \| (D^\varepsilon P^D - P^D)(x, y, 0) \|_{L^2(\Omega \times Y_m)} \\ & \quad + C \| \nabla_y K_m(\Pi_\varepsilon D^\varepsilon P^\varepsilon) \|_{L^2(Q_T \times Y_m)^n} \\ & = C\varepsilon + C\varepsilon \| \nabla_x K_m(\Pi_\varepsilon D^\varepsilon P^\varepsilon) \|_{L^2(Q_T \times Y_m)^n} \end{aligned}$$

and consequently,

$$\{K_m(D^\varepsilon p^\varepsilon) - K_m(p^*)\} \{\vartheta_m(D^\varepsilon p^\varepsilon) - \vartheta_m(p^*)\} \rightarrow 0 \text{ (a.e.) in } Q_T \times Y_m.$$

Hence, after passing to a subsequence,  $D^\varepsilon p^\varepsilon - p^* \rightarrow 0$  (a.e.) in  $Q_T \times \Omega_m$  and  $D^\varepsilon p^\varepsilon - p^* \rightarrow 0$  (a.e.) in  $L^q(Q_T \times Y_m)$  for  $\forall q \in [1, +\infty[$  by Lebesgue's dominated convergence theorem.  $\square$

Therefore the sequence  $\{P^\varepsilon, p^\varepsilon\}$  converge to the unique<sup>1</sup> solution  $\{P, p\}$  of

<sup>1</sup>It should be noted that the uniqueness follows from the energy equality.

the problem

$$|Y_f| \frac{\partial \vartheta_f(P)}{\partial t} + \frac{\partial}{\partial t} \int_{Y_m} \vartheta_m(p) dy = \operatorname{div}_x \{k_f(\vartheta_f(P))(I + \Xi)[\nabla_x P - e_3]\}$$

in  $Q_T$  (40)

$$P = P^D \quad \text{on } \Gamma^1 \times (0, T) \tag{41}$$

$$k_f(\vartheta_f(P))(I + \Xi)[\nabla_x P - e_3] \cdot \nu = g \frac{(P - \vartheta^{-1}(\theta_0) - \delta)_+}{|P - \vartheta^{-1}(\theta_0)|}$$

on  $\Gamma^2 \times (0, T)$  (42)

$$P(x, 0) = P^D(x, 0) \quad \text{on } \Omega \quad \text{and} \quad p(x, y, 0) = P^D(x, 0)$$

on  $\Omega \times Y_m$  (43)

$$\partial_t \vartheta_m(p) - \operatorname{div}_y \{k_m(\vartheta_m(p)) \nabla_y p\} = 0 \quad \text{on } \Omega \times Y_m \times (0, T) \tag{44}$$

$$p = P \quad \text{on } \Omega \times \partial Y_m \times (0, T) \tag{45}$$

### 3 Modeling transport, diffusion and adsorption of chemical species

We are going to assume that certain chemical species are dissolved in the fluid. Their concentration is sufficiently small and the fluid flow is not affected. For simplicity of notation we write the equations for just one specie; the generalization to  $m$  substances is straightforward. The conservation of mass law is

$$\frac{\partial(\vartheta_f(P^\varepsilon)u^\varepsilon)}{\partial t} - \operatorname{div}_x \{D\nabla u^\varepsilon - v^\varepsilon u^\varepsilon\} = f(u^\varepsilon) \quad \text{in } \Omega_f^\varepsilon \times (0, T) \tag{46}$$

where  $v^\varepsilon = k_f(\vartheta_f(P^\varepsilon))(\nabla P^\varepsilon - e_3)$  is the filtration velocity,  $v^\varepsilon u^\varepsilon$  is the convection term,  $-D\nabla u^\varepsilon$  is the dispersion and diffusion term and  $f(u^\varepsilon)$  represents the chemical reactions.

The simplest way to include adsorption effects is to introduce the concentration  $U^\varepsilon$  of the substance absorbed on the pellet surface. It is reasonable to suppose that the actual adsorption rate  $b^\varepsilon$  depends on  $u^\varepsilon$  and  $U^\varepsilon$ . Thus we have

$$(D\nabla u^\varepsilon - v^\varepsilon u^\varepsilon) \cdot \nu = \varepsilon b(x, u^\varepsilon, U^\varepsilon) \quad \text{on } \Gamma^\varepsilon \times (0, T), \tag{47}$$

where  $b$  is a Hölder continuous function of  $u$  and  $U$ . In order to complete the model we add an equation describing the dynamics of the adsorbed concentration  $U^\varepsilon$  which reads

$$\partial_t U^\varepsilon = b(x, u^\varepsilon, U^\varepsilon) \quad (48)$$

Using the results from [17] we find out that  $\{u^\varepsilon, U^\varepsilon\}$  converges in 2-scales to the solution  $\{u, U\}$  of the following problem

$$\begin{aligned} |Y_f| \frac{\partial(\vartheta_f(P)u)}{\partial t} + \frac{\partial}{\partial t} (|\partial Y_m|U) - \operatorname{div}_x \{D(I + \Xi)\nabla_x u - vu\} \\ = |Y_f|f(u) \quad \text{in } Q_T \end{aligned} \quad (49)$$

$$v = k_f(\vartheta_f(P))(I + \Xi)[\nabla_x P - e_3] \quad \text{in } \Omega \times (0, T) \quad (50)$$

$$u = u_g \quad \text{on } \Gamma^1 \times (0, T) \quad (51)$$

$$\{D(I + \Xi)\nabla_x u - vu\} \cdot \nu = g_1 \quad \text{on } \Gamma^2 \times (0, T) \quad (52)$$

$$u(x, 0) = u_g(x, 0) \quad \text{on } \Omega \quad \text{and} \quad U(x, 0) = U_g(x, 0) \quad \text{on } \Omega \quad (53)$$

$$\partial_t U = b(x, u, U) \quad \text{on } \Omega \times (0, T) \quad (54)$$

We suppose

$$g_1 \in L^2(\Gamma^2 \times (0, T)) \quad \text{and} \quad U_g, u_g \in H^1(0, T; L^\infty(\Omega)) \cap L^2(0, T; H^1(\Omega)).$$

Well-known examples of nonlinear adsorption rates are the Freundlich isotherm  $b(u, U) = \gamma(u^p - U)$ ,  $\gamma > 0$ ,  $0 < p \leq 1$  and the Langmuir isotherm  $b(u, U) = \gamma(\alpha u / (1 + \beta u) - U)$ ,  $\alpha, \beta, \gamma > 0$ .

The next step would be to add the *surface diffusion* as in [16] or to consider the nonlinear transmission to the pellet, as in [17]. Getting more complicated models from [23] would be subject of our subsequent publications.

#### 4 Numerical simulations

We would like to point out the effects of chemical reactions. Consequently, without losing generality, we consider only a saturated flow in  $\Omega = (0, 2\pi)^2$  and the periodic boundary conditions for the concentrations.

To obtain a precise approximation to the saturations, we approximate the spatial derivatives using the pseudo-spectral method. More precisely, we write  $u$  and  $U$  in terms of the corresponding spectral Fourier basis. The unknown functions in the nonlinear terms are evaluated in the collocation points, coming from Fourier's grid of the size  $256 \times 256$ . Then using the inverse FFT, the nonlinear terms are written in the spectral basis.

In the time discretization, we integrate exactly the linear terms: (a) the diffusion-convection term in (50) and (b) the linear term containing  $U$  in the adsorption rate  $b$ . For the nonlinear terms we use a third order explicit Adams-Bashforth scheme for  $f(u)$  in (50) and an implicit third order Adams-Bashforth scheme for  $b(\cdot, u, \cdot)$  in (54). After scaling the equations with the characteristic time  $T_c = 2 \times 10^4$ , we take the time step  $10^{-3}$ .

This numerical approach was developed in 2D turbulence simulation by Robert and Rosier (see [22]) and the method is very robust for the non-linear coupled transport and diffusion.

We present two numerical experiments. They are with same data, but with different isotherms. The data are given by the following table:

<i>Parameters</i>	<i>Values</i>
Porosity: $ Y_f $	0.35
Characteristic surface: $ \partial Y_m $	4
Molecular diffusion: $D$	$5 \times 10^{-11} m^2/s$
Darcy's velocity: $(v, 0)$	$3.5 \times 10^{-4} m/s$
Pore size: $\ell$	$1 \times 10^{-4}$
Size of the domain: $L$	$6.28 \times 10^{-2} m$

Table 1 – Parameter values.

$f(u)$  is taken to be linear. The results are at the figures which follow. They show important effects of the transport on the evolution of the concentration profiles. Also diffusive effects depend very much on the choice of the isotherms, as visible on the figures.

After these calculations, which correspond to the simplest homogenized model, we are planning to develop a numerical method for the unsaturated flow, to add the surface diffusion in the modeling of the adsorption and to include the effects

of high Péclet number. The basic challenge is to develop fast solvers for dual-porosity models and for more details we refer to the recent article [2].

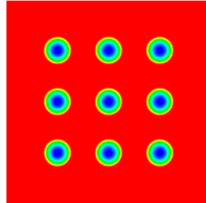


Figure 1 – Initial concentration.

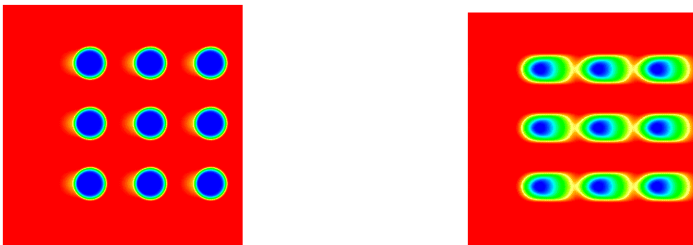


Figure 2 – Time evolution for the Freundlich's isotherm.

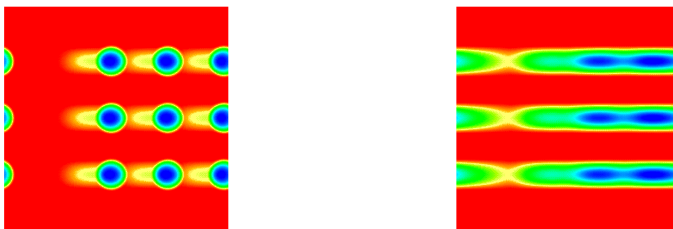


Figure 3 – Time evolution for the Langmuir's isotherm.

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