Continuum Mech. Thermodyn. (2009) 21: 125–140
DOI 10.1007/s00161-009-0099-z

ORIGINAL ARTICLE

Catherine Choquet · Andro Mikelić

Rigorous upscaling of the reactive flow with finite kinetics and under dominant Péclet number

Received: 7 January 2009 / Accepted: 24 February 2009 / Published online: 24 April 2009

Abstract We consider the evolution of a reactive soluble substance introduced into the Poiseuille flow in a slit channel. The reactive transport happens in presence of dominant Péclet and Damköhler numbers. We suppose Péclet numbers corresponding to Taylor's dispersion regime. The two main results of the paper are the following. First, using the anisotropic perturbation technique, we derive rigorously an effective model for the enhanced diffusion. It contains memory effects and contributions to the effective diffusion and effective advection velocity, due to the flow and chemistry reaction regime. Error estimates for the approximation of the physical solution by the upscaled one are presented in the energy norms. Presence of an initial time boundary layer allows only a global error estimate in L^2 with respect to space and time. We use the Laplace's transform in time to get optimal estimates. Second, we explicit the retardation and memory effects of the adsorption/desorption reactions on the dispersive characteristics and show their importance. The chemistry influences directly the characteristic diffusion width.

Keywords Taylor's dispersion · Asymptotic expansion · Large Péclet number · Large Damköhler's number · Anisotropic singular perturbation · Multi-scale modelling

PACS 02.30.Jr, 47.56.+r, 47.70.Fw, 47.87.lk, 82.40, 82.65.+r

Research of the authors was partially supported by the GNR MOMAS (Modélisation Mathématique et Simulations numériques liées aux problèmes de gestion des déchets nucléaires) (PACEN/CNRS, ANDRA, BRGM, CEA, EDF, IRSN) as a part of the project "*Modèles de dispersion efficace pour des problèmes de Chimie-Transport: Changement d'échelle dans la modélisation du transport réactif en milieux poreux, en présence des nombres caractéristiques dominants*".

Communicated by A. Visintin

C. Choquet
Faculté des Sciences et Techniques de Saint-Jérôme, Université P. Cézanne, LATP UMR 6632,
13397 Marseille Cedex 20, France

C. Choquet
Université de Savoie, LAMA UMR 5127, Le Bourget du Lac Cedex, France

A. Mikelić
Université de Lyon, 69003 Lyon, France

A. Mikelić (✉)
Institut Camille Jordan, Université Lyon 1, UMR CNRS 5208, Bât. Braconnier, 43, Bd du onze novembre 1918,
69622 Villeurbanne Cedex, France
E-mail: Andro.Mikelic@univ-lyon1.fr

1 Introduction

We consider the evolution of a soluble substance introduced into the Poiseuille flow in a slit channel. In fact, this problem could be studied in three distinct regimes: (a) diffusion-dominated mixing; (b) Taylor dispersion-mediated mixing; (c) chaotic advection. We focus our analysis to regime (b), corresponding to dominant Péclet's numbers, but smaller than a threshold value. The dispersion is due to the combined action of convection parallel to the axis and molecular diffusion in the radial direction. In the fundamental paper [20], Taylor found an effective axial diffusivity, proportional to the square of the transversal Péclet number and occurring in addition to the molecular diffusivity. When Taylor's effective dispersion is used in the 1D model, obtained by section averaging, as the effective diffusion coefficient, then the numerical experiences show good agreement with the solution of the complete physical problem (see, e.g. [13]). But despite a large literature on the subject, rigorous mathematical justification of the one-dimensional model from the multidimensional model was seldom addressed, especially in the presence of chemical reactions. This is the first goal of the present paper, continuing the research from the articles [10,13,16,17]. Note in particular that we obtain error estimates depending explicitly on the small parameter $\varepsilon = H/L_R$, H being the transversal length of the pipe and L_R being the observation distance.

The second goal of this paper is the analysis of the chemical effects. It is assumed that adsorption and desorption reactions occur on the walls of the channel. We consider a linear driving force model with a finite kinetics and a linear isotherm. Dominant Péclet and Damköhler numbers are supposed. We explicit the influence of the chemical kinetics on the dispersive effects. Furthermore we prove that the effective model, despite being derived from the conventional diffusive Fick law at the microscopic level, exhibits enhanced diffusive effects. Thus we show that observed memory effects and augmented diffusion and transport could be rigorously derived from the first principles, in the regime of dominant Péclet and Damköhler numbers.

We end this section with some references. In the absence of chemical reactions, Aris [2] presented a formal derivation of an effective equation using the method of moments. Flow with chemistry is considered by Paine et al. [18]. They noted that the equation for the difference between the physical and averaged concentrations is not closed, since it contains a dispersive source term $\frac{\partial}{\partial x}\langle \overline{q}_x \overline{c}\rangle$. For its determination one should go to the next order and in fact there is an infinite system of equations to solve. Paine et al used the "single-point" closure schemes of turbulence modeling by Launder to obtain a closed model for the averaged concentration. With this approach they obtain effective equations which qualitatively look like the corresponding model obtained formally by the two-scale expansion in [13]. Nevertheless, the coefficients in their equations contain four unknown parameters and they are fixed by requiring that the model fits the experimentally observed zero, first and second order moments of the area-averaged concentrations and of the adsorbed species concentrations.

The recent paper [3] by Balakotaiah et al. uses formally the center manifold approach. It is a continuation of work by Mercer and Roberts (see [15]) on Taylor's dispersion. Balakotaiah et al obtained a whole scale of effective models for reactive fluid flows through a tube, corresponding to the ones obtained by our approach. More recently, Balakotaiah et al. obtained in [4,5,9] non-parabolic models, being formally at the same order of precision. Other derivation of non-parabolic models, using statistical physics approach is in the papers [6–8] by Camacho.

Our technique is different. It is strongly motivated by the paper by Rubinstein and Mauri [19], where effective dispersion and convection in porous media is studied using the homogenization technique. We use a two-scale expansion based on anisotropic singular perturbation and control the error in energy.

Plan of the paper is as follows: in Sect. 2 we give the precise setting of the problem. Its non-dimensional form is derived. Then we present the effective problem in its non-dimensional form and the main result of the paper, with the error estimate for the approximation of the non-dimensional physical concentration by the non-dimensional upscaled one. Finally, the effective problem in its dimensional form is given. In Sect. 3 we recall some facts about the vector-valued Laplace transform and write the Laplace transform of our problem. Sect. 4 is consecrated to the rigorous derivation of the effective problem and its analysis. In Sect. 4.1 we recall the formal derivation of the effective problem. In Sect. 4.2 existence, uniqueness and estimates explicit in ε for the solution to the effective problem are obtained. It is immediately used in Sect. 4.3 to obtain the error estimate. We conclude with Sect. 4.4, where we make the inversion of the Laplace transform and derive the effective equation in its non-dimensional form.

2 Setting of the problem and main result

Let us write the precise setting of the problem. We consider the transport of a reactive solute by diffusion and convection by Poiseuille's velocity in an infinite 2D channel. The solute particles do not react among themselves. Instead they undergo an adsorption process at the lateral boundary. For a general discussion on the modeling adsorption processes in porous media we refer to [12] and [14]. Here we consider a linearized case.

We consider the following model for the solute concentration c^*:

(a) transport through channel $\Omega^* = \{(x^*, y^*) : x^* \in \mathbb{R}, |y^*| < H\}$

$$\frac{\partial c^*}{\partial t^*} + q(y^*)\frac{\partial c^*}{\partial x^*} - D^*\frac{\partial^2 c^*}{\partial (x^*)^2} - D^*\frac{\partial^2 c^*}{\partial (y^*)^2} = 0 \quad \text{in } \Omega^*, \tag{1}$$

where $q(z) = Q^*(1 - (z/H)^2)$ and where Q^* (velocity) and D^* (molecular diffusion) are positive constants.

(b) reaction at channel wall $\Gamma^* = \{(x^*, y^*) : x^* \in \mathbb{R}, |y^*| = H\}$ linking the solute concentration c^* and the adsorbed species surface concentration c_s^*:

$$-D^*\partial_{y^*}c^* = \frac{\partial c_s^*}{\partial t^*} = k_s^*\left(c^* - \frac{c_s^*}{K_e^*}\right) \quad \text{on } \Gamma^*, \tag{2}$$

where k_s^* is the adsorption rate constant (velocity), K_e^* is the linear adsorption equilibrium constant (length), the constant desorption rate being characterized by k_s^*/K_e^*. These quantities are all positive real numbers.

(c) initial infiltration with a mollified Dirac pulse of water containing a solute of volume concentration c_{00}^* and the adsorbed species surface concentration c_{s0}^*:

$$c^*(x^*, y^*, 0) = c_{00}^*(x^*), \quad c_s^*(x^*, 0) = c_{s0}^*(x^*), \tag{3}$$

where $c_{00}^* \in C_0^\infty(\mathbb{R})$, $c_{00}^* \geq 0$ and $c_{s0}^* \in C_0^\infty(\mathbb{R})$, $c_{s0}^* \geq 0$. Following Taylor's example (B1) (see [20, page 192]), we can take as c_{00}^* the mollified Dirac measure of mass M, concentrated at $x = 0$.

We now introduce appropriate scales. The obvious transversal length scale is H. For all other quantities we use reference values denoted by the subscript R. Setting

$$\begin{cases} c = \dfrac{c^*}{c_R},\ c_s = \dfrac{c_s^*}{c_{sR}},\ x = \dfrac{x^*}{L_R},\ y = \dfrac{y^*}{H},\ t = \dfrac{t^*}{T_R}, \\[2ex] Q = \dfrac{Q^*}{Q_R},\ D = \dfrac{D^*}{D_R},\ k_s = \dfrac{k_s^*}{k_{sR}},\ K_e = \dfrac{K_e^*}{K_{eR}}, \end{cases} \tag{4}$$

where L_R is the "observation distance", we obtain the dimensionless equations

$$\frac{\partial c}{\partial t} + \frac{Q_R T_R}{L_R}Q(1 - y^2)\frac{\partial c}{\partial x} - \frac{D_R T_R}{L_R^2}D\frac{\partial^2 c}{\partial x^2} - \frac{D_R T_R}{H^2}D\frac{\partial^2 c}{\partial y^2} = 0 \quad \text{in } \Omega \tag{5}$$

and

$$-\frac{D D_R c_R}{H}\frac{\partial c}{\partial y} = \frac{c_{sR}}{T_R}\frac{\partial c_s}{\partial t} = k_{sR}k_s\left(c_R c - \frac{c_{sR}}{K_e K_{eR}}c_s\right) \quad \text{on } \Gamma, \tag{6}$$

where

$$\Omega = \mathbb{R} \times (-1, 1) \text{ and } \quad \Gamma = \mathbb{R} \times \{-1, 1\}. \tag{7}$$

The equations involve the time scales:

T_L = characteristic longitudinal time scale = $\frac{L_R}{Q_R}$,
T_T = characteristic transversal time scale = $\frac{H^2}{D_R}$,

T_{De}= characteristic desorption time scale = $\frac{K_{eR}}{k_{sR}}$,
T_A= characteristic adsorption time scale = $\frac{c_{sR}}{c_R k_{sR}}$,
T_{react}= superficial chemical reaction time scale = $\frac{H}{k_{sR}}$,

and the non-dimensional numbers

$Pe = \frac{L_R Q_R}{D_R}$ (Péclet number),

$Da = \frac{L_R}{T_A Q_R}$ (Damköhler number).

We fix the reference time by setting $T_R = T_L$. We define a small parameter by $\varepsilon = \frac{H}{L_R}$ and suppose that $Pe = \varepsilon^{-\alpha}$, $1 \le \alpha < 2$. Furthermore, we assume that $K_{eR} \approx H$, and $\frac{T_T}{T_L} = \frac{HQ_R}{D_R}\varepsilon = \mathcal{O}(\varepsilon^{2-\alpha}) = \varepsilon^2 Pe$, being small. The time scales T_{De}, T_A and T_L are supposed to be of the same order. We note that this implies Damköhler's number of order one, which means that one should take care simultaneously of the flow and of the chemical reactions. Introducing the dimensionless numbers in Eqs. (5) and (6) yields the problem:

$$\frac{\partial c^\varepsilon}{\partial t} + Q(1-y^2)\frac{\partial c^\varepsilon}{\partial x} = D\varepsilon^\alpha \frac{\partial^2 c^\varepsilon}{\partial x^2} + D\varepsilon^{\alpha-2}\frac{\partial^2 c^\varepsilon}{\partial y^2} \quad \text{in } \Omega \times (0,T), \tag{8}$$

$$-D\varepsilon^{\alpha-2}\frac{\partial c^\varepsilon}{\partial y} = \frac{T_A}{T_{De}}\frac{\partial c_s^\varepsilon}{\partial t} = \frac{T_L}{T_{De}} k_s\left(c^\varepsilon - \frac{T_A}{T_{De}}\frac{c_s^\varepsilon}{K_e}\right) \quad \text{on } \Gamma^+ \times (0,T), \tag{9}$$

$$c^\varepsilon(x,y,0) = c_{00}(x), \quad c_s^\varepsilon(x,0) = c_{s0}(x) \quad \text{on } \mathbb{R}, \tag{10}$$

$$\frac{\partial c^\varepsilon}{\partial y}(x,0,t) = 0 \quad \text{for } (x,t) \in \mathbb{R} \times (0,T). \tag{11}$$

The latter condition results from the y-symmetry of the solution. Furthermore

$$\Omega = \mathbb{R} \times (0,1), \quad \Gamma^+ = \mathbb{R} \times \{1\},$$

and T is an arbitrary chosen positive number.

We study the behavior of the problem (8)–(11) as $\varepsilon \searrow 0$, while keeping the coefficients Q, D, k_s and K_e all $\mathcal{O}(1)$. We prove that the corresponding upscaled problem in $\mathbb{R}$ for the effective concentration c_0^{eff} is the following:

$$\begin{aligned}
&\partial_t c_0^{\text{eff}} + \frac{T_L}{T_{De}} k_s c_0^{\text{eff}} + \frac{2Q}{3}\partial_x c_0^{\text{eff}} - \tilde{D}\partial_{xx}^2 c_0^{\text{eff}} - \left(\frac{T_L}{T_{De}}k_s\right)^2 \frac{1}{K_e}\int_0^t \mathrm{e}^{-T_L k_s (t-\xi)/(T_{De}K_e)} c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi \\
&-\varepsilon^{2-\alpha}\frac{1}{3D}\left(\frac{T_L}{T_{De}}k_s\right)^2 \left(c_0^{\text{eff}} - 2\frac{T_L k_s}{T_{De}K_e}\int_0^t \mathrm{e}^{-T_L k_s (t-\xi)/(T_{De}K_e)} c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi\right. \\
&\left.+\left(\frac{T_L k_s}{T_{De}K_e}\right)^2 \int_0^t \mathrm{e}^{-T_L k_s (t-\xi)/(T_{De}K_e)}(t-\xi) c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi\right) + \frac{4Q}{45D}\frac{T_L}{T_{De}}k_s\varepsilon^{2-\alpha} \\
&\times\left(\partial_x c_0^{\text{eff}} - \frac{T_L k_s}{T_{De}K_e}\int_0^t \mathrm{e}^{-T_L k_s (t-\xi)/(T_{De}K_e)}\partial_x c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi\right) \\
&= \frac{T_A T_L}{T_{De}^2 K_e}\partial_x c_{s0}\mathrm{e}^{-(T_L k_s t)/(T_{De}K_e)}\frac{2Q}{45D}\varepsilon^{2-\alpha} \\
&+\frac{T_A T_L k_s}{T_{De}^2 K_e}\frac{c_{s0}}{3D}\mathrm{e}^{-(T_L k_s t)/(T_{De}K_e)}\left\{3D + \frac{T_L k_s}{T_{De}}\varepsilon^{2-\alpha}\left(\frac{T_L k_s}{T_{De}K_e}t - 1\right)\right\}.
\end{aligned} \tag{12}$$

Note that the chemical reactions on the walls produce complicated memory terms.

In fact we prove in Sect. 4.3 the following result, justifying rigorously the validity of the effective equation (12).

Theorem 1 *Let $2 > \alpha \geq 1$ and let $T_A \approx T_{DE} \approx T_L$. Assume that $c_{00}, c_{s0} \in C_0^\infty(\mathbb{R})$. Let c^ε be the solution for (8)–(11) and $c_0^{eff} \in H^1(\mathbb{R}_+; H^2(\mathbb{R}))$ the solution for (12), satisfying the initial condition $c_0^{\text{eff}}|_{t=0} = c_{00}$. Then we have*

$$\Bigg\| c^\epsilon - c_0^{\text{eff}} - \varepsilon^{2-\alpha}\frac{Q}{D}\left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}\right)\partial_x c_0^{\text{eff}} - \frac{\varepsilon^{2-\alpha}}{D}\left(\frac{1}{6} - \frac{y^2}{2}\right)\left(\frac{T_L}{T_{De}}k_s c_0^{\text{eff}} - \left(\frac{T_L}{T_{De}}k_s\right)^2 \times \frac{1}{K_e}\int_0^t \mathrm{e}^{-T_L k_s(t-\xi)/(T_{De}K_e)} c_0^{\text{eff}}(x,\xi)\mathrm{d}\xi - \frac{T_A T_L}{T_{DE}^2 K_e} c_{so}(x)\mathrm{e}^{-T_L k_s t/(T_{De}K_e)}\right)\Bigg\|_{L^2(\Omega\times(0,T))}$$
$$\leq C\varepsilon^{(2-\alpha)(3-2\delta)/(2-\delta)}\left(||c_{00}||_{H^3(\mathbb{R})} + ||c_{s0}||_{H^2(\mathbb{R})}\right), \quad \forall \delta \in (0,1). \tag{13}$$

It remains to return to the dimensional form. We kept the order one quantities Q, D, k_s and K_e just to be able to return to the dimensional form. Now we set them to be equal to one, i.e. we impose $Q^* = Q_R$, $D^* = D_R$, $k_s^* = k_{sR}$ and $K_e^* = K_{eR}$.

Using that $T_L \approx T_{DE} \approx T_A$ and $K_{eR} \approx H$, we obtain for the basic dimensional effective concentration c^{eff} the following equation:

$$\frac{\partial c^{\text{eff}}}{\partial t^*} + \frac{k_s^*}{K_e^*}c^{\text{eff}} + \frac{2}{3}Q^*\frac{\partial c^{\text{eff}}}{\partial x^*} - \left(\frac{k_s^*}{K_e^*}\right)^2\int_0^{t^*} \mathrm{e}^{-k_s^*(t^*-\xi)/K_e^*}c^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi - D^*\left(1 + \frac{8}{945}Pe_T^2\right)\frac{\partial^2 c^{\text{eff}}}{\partial (x^*)^2}$$
$$-\frac{1}{3}Pe_T\ Da_T\frac{H}{K_e^*}\frac{k_s^*}{K_e^*}\left(c^{\text{eff}} + \int_0^{t^*}\mathrm{e}^{-k_s^*(t^*-\xi)/K_e^*}\left(\left(\frac{k_s^*}{K_e^*}\right)^2(t^*-\xi) - 2\frac{k_s^*}{K_e^*}\right)c^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi\right)$$
$$+\frac{4}{45}\frac{H}{K_e^*}Pe_T k_s^*\left\{\partial_x c^{\text{eff}} - \frac{k_s^*}{K_e^*}\int_0^{t^*}\mathrm{e}^{-k_s^*(t^*-\xi)/K_e^*}\partial_x c^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi\right\}$$
$$= \frac{k_s^*}{K_e^*}\mathrm{e}^{-k_s^* t^*/K_e^*}\left\{\frac{c_{s0}}{K_e^*} + \frac{1}{3}Pe_T\ Da_T\frac{c_{s0}}{K_e^*}\frac{H}{K_e^*}\left(\frac{k_s^*}{K_e^*}t^* - 1\right)\right\} + \mathrm{e}^{-k_s^* t^*/K_e^*}\frac{4}{45}\frac{k_s^*}{K_e^*}\frac{H}{K_e^*}Pe_T\ \partial_x c_{s0}, \tag{14}$$

where the transversal Péclet et Damköhler numbers, Pe_T and Da_T are given by

$$Pe_T = \frac{Q^* H}{D^*} \quad \text{and} \quad Da_T = \frac{k_s^*}{Q^*}.$$

Corollary 1 *Under the assumptions of Theorem 1, the dimensional effective concentration reads*

$$c_{\text{eff}}^{\text{full}}(x^*,y^*,t^*) = c^{\text{eff}}(x^*,t^*) + HPe_T\partial_x c^{\text{eff}}(x^*,t^*)\left(\frac{1}{6}\left(\frac{y^*}{H}\right)^2 - \frac{1}{12}\left(\frac{y^*}{H}\right)^4 - \frac{7}{180}\right)$$
$$+\left(\frac{1}{6} - \frac{1}{2}\left(\frac{y^*}{H}\right)^2\right)Pe_T\ Da_T\frac{H}{K_e^*}\left(c^{\text{eff}}(x^*,t^*) - \frac{k_s^*}{K_e^*}\int_0^{t^*}\mathrm{e}^{-k_s^*(t^*-\xi)/K_e^*}c^{\text{eff}}(x^*,\xi)\,\mathrm{d}\xi\right)$$
$$-\left(\frac{1}{6} - \frac{1}{2}\left(\frac{y^*}{H}\right)^2\right)\frac{c_{s0}}{K_e^*}\mathrm{e}^{-k_s^* t^*/K_e^*}Pe_T\ Da_T, \tag{15}$$

$$c_s^{\text{eff}}(x^*,t^*) = c_{s0}\mathrm{e}^{-k_s^* t^*/K_e^*} + T_L k_s^*\int_0^{t^*}\mathrm{e}^{-k_s^*(t^*-\xi)/K_e^*}c_{\text{eff}}^{full}(x^*,\xi)\mathrm{d}\xi \tag{16}$$

and it gives an approximation of order $O((\varepsilon Pe_T)^{3/2})$.

Remark 1 The characteristic parameters, based on the data from Taylor's article [20], could be found in [13]. We mention two important Taylor's examples, one with $\alpha = 1.614$, $H = 2.6 \cdot 10^{-4}$ m, the longitudinal Péclet number $Pe = 0.95 \cdot 10^5$ and $Pe_T = 78$ and the second one with $\alpha = 1.96$, $H = 2.6 \cdot 10^{-4}$ m, the longitudinal Péclet number $Pe = 4.14 \cdot 10^6$ and $Pe_T = 173$. Obviously, in Taylor's situation, our derived contributions are important and using them is necessary in order to simulate correctly the reactive flows.

In his fundamental work [20], Taylor showed that, for sufficiently large time, any point discharge of tracer in laminar pipe Poiseuille flow evolves to a symmetric gaussian distribution moving longitudinally with the mean speed of the flow. This type of flow is usually called Taylor regime where the characteristic diffusion width is $\sigma \sim \sqrt{D^*(1 + \frac{8}{945} Pe_T^2)t}$.

Informations on the regime for the effective concentration c_0^{eff} can be obtained from the first moments, defined by

$$M_k(t) = \int_{-\infty}^{+\infty} x^k c_0^{\text{eff}}(x,t)\,\mathrm{d}x, \quad 0 \le k \le 2.$$

Direct calculation gives for the characteristic diffusion width $\sigma \sim \sqrt{Ct}$, where C depends not only on Taylor's diffusion coefficient, but also nonlinearly on $C_k = \frac{T_L}{T_{De}} k_s$, $C_0 = \frac{T_L k_s}{T_{De} K_e}$ and $C_{g1} = \frac{T_A T_L k_s}{T_{De}^2 K_e}$.

3 Vector valued Laplace transform and applications to PDEs

The Laplace's transform method is widely used in solving engineering problems. In applications it is usually called the operational calculus or Heaviside's method. Note that if we apply the Laplace transform on the equation

$$\frac{T_A}{T_{De}} \frac{\partial c_s^\varepsilon}{\partial t} = \frac{T_L}{T_{De}} k_s \left(c^\varepsilon|_{y=1} - \frac{T_A}{T_{De}} \frac{c_s^\varepsilon}{K_e} \right),$$

being a part of (9), we compute easily

$$\frac{T_A}{T_{De}} \hat{c}_s^\varepsilon = \frac{1}{\tau + (T_L k_s)/(T_{De} K_e)} \left(\frac{T_L}{T_{De}} k_s \hat{c}^\varepsilon|_{y=1} + \frac{T_A}{T_{De}} c_{s0} \right). \tag{17}$$

It follows that the Laplace transform of the problem (8)–(11) reads

$$\tau \hat{c}^\varepsilon + Q(1-y^2) \frac{\partial \hat{c}^\varepsilon}{\partial x} - D\varepsilon^\alpha \frac{\partial^2 \hat{c}^\varepsilon}{\partial x^2} - D\varepsilon^{\alpha-2} \frac{\partial^2 \hat{c}^\varepsilon}{\partial y^2} = c_{00} \quad \text{in } \mathbb{R} \times (0,1), \tag{18}$$

$$-D\varepsilon^{\alpha-2} \frac{\partial \hat{c}^\varepsilon}{\partial y}|_{y=1} = k(\tau) \hat{c}^\varepsilon|_{y=1} - g(\tau) \quad \text{in } \mathbb{R}, \tag{19}$$

$$k(\tau) = \frac{(T_L/T_{De}) k_s \tau}{\tau + (T_L k_s)/(T_{De} K_e)}, \qquad g(\tau) = \frac{1}{T_{De}^2 K_e} \frac{T_A T_L k_s c_{s0}}{\tau + (T_L k_s)/(T_{De} K_e)}, \tag{20}$$

$$\frac{\partial \hat{c}^\varepsilon}{\partial y}|_{y=0} = 0 \quad \text{in } \mathbb{R}. \tag{21}$$

In the sequel, we work on the Laplace's form (18)–(21) of the original problem. In this section we thus recall some basic facts about applications of Laplace's transform to linear parabolic equations. These results will be used in particular to assert that our error estimates in the "Laplace's world" can be straightforward interpreted as error estimates in the "real world".

For locally integrable function $f \in L^1_{loc}(\mathbb{R})$ such that $f(t) = 0$ for $t < 0$ and $|f(t)| \le Ae^{at}$ as $t \to +\infty$, the Laplace transform of f, denoted $\hat{f}$, is defined as

$$\hat{f}(\tau) = \int_0^{+\infty} f(t) \mathrm{e}^{-\tau t} \mathrm{d}t, \quad \tau = \xi + i\eta \in \mathbb{C}. \tag{22}$$

It is closely linked with Fourier's transform in $\mathbb{R}$. We note that

$$\hat{f}(\tau) = \mathcal{F}\left(f(t)e^{-\xi t}\right)(-\eta), \quad \xi > a, \tag{23}$$

where the Fourier's transform of a function $g \in L^1(\mathbb{R})$ is given by

$$\mathcal{F}\left(g(t)\right)(\omega) = \int_{\mathbb{R}} g(t)\mathrm{e}^{i\omega t}\,\mathrm{d}t, \quad \omega \in \mathbb{R}.$$

It is well-known (see, e.g. [21] or [11]) that $\hat{f}$ defined by (22) is analytic in the half-plane $\{\mathrm{Re}(\tau) = \xi > a\}$ and it tends to zero as $\mathrm{Re}(\tau) \to +\infty$.

For real applications, Laplace's transform of functions is not well-adapted and it is natural to use Laplace's transform of distributions. It is defined for distributions with support on $[a, +\infty)$ i.e. for $f \in \mathcal{D}'_+(a)$, where $\mathcal{D}'_+(a) = \{f \in \mathcal{D}'(\mathbb{R});\ \operatorname{supp} f \subset [a, +\infty)\}$. If $\mathcal{S}'(\mathbb{R})$ denotes the space of distributions of slow growth, then we introduce $\mathcal{S}'_+(\mathbb{R})$ by

$$\mathcal{S}'_+(\mathbb{R}) = \mathcal{D}'_+(0) \cap \mathcal{S}'(\mathbb{R}) \tag{24}$$

and we use the formula (23) to define Laplace's transform for $f \in \mathcal{D}'_+(a)$ such that $fe^{-\xi t} \in \mathcal{S}'_+(\mathbb{R})$ for all $\xi > a$. This approach permits the rigorous operational calculus. For details we refer to classical textbooks as [21] by Vladimirov.

Laplace's transform is applied to linear ODEs and PDEs, the transform problem is solved and its solution $\hat{f}$ is calculated. Then the important question is how to inverse the Laplace's transform. First we need a suitable space for image functions. It is the algebra $H(a)$ defined by

$$\begin{aligned} H(a) = \{g \in \mathcal{H}ol\,(\{\tau \in \mathbb{C};\ \mathrm{Re}(\tau) > a\}) &\text{ satisfying the growth condition:} \\ &\text{for any } \sigma_o > a \text{ there are real numbers } C(\sigma_o) > 0 \text{ and } m = m(\sigma_o) \geq 0 \\ &\text{such that } |g(\tau)| \leq C(\sigma_o)\,(1 + |\tau|^m),\ \mathrm{Re}(\tau) > \sigma_o\}. \end{aligned} \tag{25}$$

For elements of $H(a)$ we have the following classical result.

Theorem 2 [21, pp. 162–165] *Let $\hat{f} \in H(a)$ be absolutely integrable with respect to η on $\mathbb{R}$ for certain $\xi > a$. Then the following formula holds true.*

$$f(t) = \frac{1}{2\pi i}\int_{\xi - i\infty}^{\xi + i\infty} \hat{f}(z)\mathrm{e}^{zt}\,\mathrm{d}z. \tag{26}$$

These classical results are not sufficient for our purposes. We need results for reflexive Sobolev space X valued Laplace's transform. Furthermore we need an inversion theorem in $L^p((0, +\infty); X)$. The corresponding theory could be found in Arendt [1] and we give only results directly linked to our needs.

Let X be a Hilbert space, $\mathbb{C}_+ = \{\lambda \in \mathbb{C}:\ \mathrm{Re}\ \lambda > 0\}$ and let $H^2(\mathbb{C}_+, X)$ be the subset of the space of holomorphic functions defined by

$$H^2(\mathbb{C}_+, X) = \left\{ h : \mathbb{C}_+ \to X \text{ such that } ||h||_{H^2(\mathbb{C}_+, X)} = \sup_{x>0} \int_{\mathbb{R}} ||h(x + is)||^2_X\,\mathrm{d}s < +\infty \right\}.$$

Then we have

Theorem 3 (Vector valued Paley–Wiener theorem from [1, page 48]) *Let X be a Hilbert space. Then the map $f \to \hat{f}|_{\mathbb{C}}$ is an isometric isomorphism of $L^2(\mathbb{R}_+, X)$ onto $H^2(\mathbb{C}_+, X)$.*

In our situation, we have to deal with $\mathbb{C}_+$ replaced by $\{\lambda \in \mathbb{C}:\ \mathrm{Re}\ \lambda > \tau_0 > 0\}$. But this means just replacing f by $e^{-\tau t} f$ in Theorem 3. Other, more direct way to proceed is to follow ideas from [11] and use a direct approach based on the link to Fourier's transform. We apply this result in the study of the upscaled equations and then in the error estimates. We derive estimates for the solutions of the Laplace transformed problem.

4 Rigorous derivation and analysis of the effective problem

4.1 Formal asymptotic expansion

We suppose $\alpha \geq 1$ and look for a solution c^ε of the problem, in the form

$$c^\varepsilon = c_0(x;\varepsilon) + \varepsilon^{2-\alpha} c_1(x,y) + \varepsilon^{2(2-\alpha)} c_2(x,y) + \cdots$$

where $\varepsilon^{2-\alpha}$ is the transversal Péclet number. Introducing this expansion in the equation, we get

$$\begin{aligned} &\tau c_0 + Q(1-y^2)\partial_x c_0 - D\partial^2_{yy} c_1 + \varepsilon^{2-\alpha}\Big(\tau c_1 + Q(1-y^2)\partial_x c_1 - D\varepsilon^{2(\alpha-1)}\partial^2_{xx} c_0 - D\varepsilon^\alpha \partial^2_{xx} c_1 - D\partial^2_{yy} c_2\Big) \\ &\quad = c_{00} + \mathcal{O}(\varepsilon^{2(2-\alpha)}). \end{aligned} \tag{27}$$

We then write the cascade of equations corresponding to each power of the transversal Péclet number. For the order 1, we get for every $x \in \mathbb{R}$

$$\begin{aligned} &\tau c_0 + \frac{2Q}{3}\partial_x c_0 + Q\left(\frac{1}{3} - y^2\right)\partial_x c_0 = D\partial^2_{yy} c_1 + c_{00} \quad \text{on } (0,1), \\ &\partial_y c_1|_{y=0} = 0, \quad -D\partial_y c_1|_{y=1} = k(\tau)c_0 - g(\tau). \end{aligned} \tag{28}$$

By Fredholm's alternative, the latter problem has a solution if and only if c_0 is a solution of a given hyperbolic equation. Our initial and boundary data being incompatible, we choose to relax the hyperbolic equation into the following assumption

$$k(\tau)c_0 - g(\tau) = -\tau c_0 - \frac{2Q}{3}\partial_x c_0 + c_{00} + \mathcal{O}(\varepsilon^{2-\alpha}). \tag{29}$$

This assumption is justified at the end of the present subsection when we get the equation satisfied by c_0. Because of (29), problem (28) now is

$$\begin{aligned} k(\tau)c_0 - g(\tau) - Q\left(\frac{1}{3} - y^2\right)\partial_x c_0 &= -D\partial^2_{yy} c_1 \quad \text{in } \mathbb{R}\times(0,1), \\ \partial_y c_1|_{y=0} = 0, \quad -D\partial_y c_1|_{y=1} &= k(\tau)c_0 - g(\tau). \end{aligned}$$

If we choose the solution c_1 of the latter problem such that $\int_0^1 c_1 \mathrm{d}y = 0$, it reads

$$c_1(x,y) = \frac{Q}{D}\left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}\right)\partial_x c_0 + \frac{1}{2D}\left(\frac{1}{3} - y^2\right)(k(\tau)c_0 - g(\tau)). \tag{30}$$

Bearing in mind (29), we now study the next order terms in (27), that is

$$\begin{aligned} &\tau c_1 + Q(1-y^2)\partial_x c_1 - D\varepsilon^{2(\alpha-1)}\partial^2_{xx} c_0 - D\varepsilon^\alpha \partial^2_{xx} c_1 + \varepsilon^{\alpha-2}\left((\tau + k(\tau))\,c_0 + \frac{2Q}{3}\partial_x c_0 - g(\tau) - c_{00}\right) \\ &\quad = D\partial^2_{yy} c_2, \qquad \partial_y c_2|_{y=0} = 0, \quad -D\partial_y c_2|_{y=1} = k(\tau)c_1|_{y=1}. \end{aligned} \tag{31}$$

Using once again the Fredholm alternative, we ensure that this problem has a solution if and only if

$$\begin{aligned} &\tau c_0 + \frac{2Q}{3}\partial_x c_0 + k(\tau)\big(c_0 + \varepsilon^{2-\alpha} c_1|_{y=1}\big) - \varepsilon^\alpha D\partial^2_{xx} c_0 + \varepsilon^{2-\alpha}\tau \int_0^1 c_1 \mathrm{d}y \\ &+\varepsilon^{2-\alpha} Q \int_0^1 (1-y^2)\partial_x c_1 \mathrm{d}y - D\varepsilon^2 \partial^2_{xx} \int_0^1 c_1 \mathrm{d}y = g(\tau) + c_{00} \end{aligned}$$

is satisfied in $\mathbb{R}$. Because c_1 is chosen such that $\int_0^1 c_1 \mathrm{d}y = 0$, the zero order term c_0 is characterized by

$$\tau c_0 + \frac{2Q}{3}\partial_x c_0 + k(\tau)(c_0 + \varepsilon^{2-\alpha} c_1|_{y=1}) - \varepsilon^\alpha D \partial_{xx}^2 c_0 + \varepsilon^{2-\alpha} Q \int_0^1 (1-y^2)\partial_x c_1 \mathrm{d}y = g(\tau) + c_{00} \quad \text{in } \mathbb{R}. \tag{32}$$

We compute

$$\int_0^1 (1-y^2)\partial_x c_1 dy = -\frac{8Q}{945D}\partial_{xx}^2 c_0 + \frac{2}{45D}(k(\tau)\partial_x c_0 - \partial_x g(\tau)),$$
$$c_1|_{y=1} = \frac{2Q}{45D}\partial_x c_0 - \frac{1}{3D}(k(\tau)c_0 - g(\tau)).$$

Equation (32) thus reduces to

$$\left(\tau + k(\tau) - \frac{k(\tau)^2}{3D}\varepsilon^{2-\alpha}\right)c_0 + \left(\frac{2Q}{3} + \frac{4Q}{45D}k(\tau)\varepsilon^{2-\alpha}\right)\partial_x c_0$$
$$-\left(D\varepsilon^\alpha + \frac{8Q^2}{945D}\varepsilon^{2-\alpha}\right)\partial_{xx}^2 c_0 = c_{00} + g(\tau)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha}\right) + \frac{2Q}{45D}\varepsilon^{2-\alpha}\partial_x g(\tau),$$

in $\mathbb{R}$. For convenience we set

$$F_0(\tau) = \tau + k(\tau) - \frac{k(\tau)^2}{3D}\varepsilon^{2-\alpha}, \tag{33}$$
$$F_1(\tau) = \frac{2Q}{3} + \frac{4Q}{45D}k(\tau)\varepsilon^{2-\alpha}, \tag{34}$$
$$\tilde{D} = D\varepsilon^\alpha + \frac{8Q^2}{945D}\varepsilon^{2-\alpha}. \tag{35}$$

We finally claim that the effective equation governing c_0 is

$$F_0(\tau)c_0 + F_1(\tau)\partial_x c_0 - \tilde{D}\partial_{xx}^2 c_0 = c_{00} + g(\tau)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha}\right) + \frac{2Q}{45D}\varepsilon^{2-\alpha}\partial_x g(\tau). \tag{36}$$

4.2 Existence and uniqueness result for the effective equation

The present subsection is devoted to the analysis of the effective problem (36) derived in Sect. 4.1. Since the problem (36) is posed in $\mathbb{R}$, we search for a solution $c_0 \in H^2(\mathbb{R})$, for every $\tau \in \mathbb{C}$, Re $\tau \geq \tau_0$. Let $w = \mathcal{F}_x(c_0) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} c_0(x,\tau)\mathrm{e}^{i\omega x}\,\mathrm{d}x$. Then it is determined by the following equation

$$\left(F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2\right) w(\omega) = \mathcal{F}(c_{00})(\omega) + \mathcal{F}(g)(\omega)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha} + i\omega\frac{2Q}{45D}\varepsilon^{2-\alpha}\right) \quad \text{in } \mathbb{R}. \tag{37}$$

Solution to (37) is formally given by

$$w(\omega) = \frac{\mathcal{F}(c_{00})(\omega) + \mathcal{F}(g)(\omega)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha} + i\omega\frac{2Q}{45D}\varepsilon^{2-\alpha}\right)}{F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2}, \quad \omega \in \mathbb{R}, \tag{38}$$

and in order to prove that $c_0 \in H^2(\mathbb{R})$, we need to check properties of the denominator. We have

$$\begin{aligned}
\left|F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2\right|^2 &= (\tilde{D}\omega^2)^2 + 2\tilde{D}\omega^2 \mathrm{Re}(F_0(\tau) + i\omega F_1(\tau)) + |F_0(\tau) + i\omega F_1(\tau)|^2 \\
&= (\tilde{D}\omega^2)^2 + 2\tilde{D}\omega^2 \mathrm{Re} F_0(\tau) - 2\tilde{D}\omega^3 \mathrm{Im} F_1(\tau) \\
&\quad + (\mathrm{Re} F_0(\tau) - \omega \mathrm{Im} F_1(\tau))^2 + (\mathrm{Im} F_0(\tau) + \omega \mathrm{Re} F_1(\tau))^2 \\
&= \frac{1}{2}\tilde{D}\omega^2 \left(\sqrt{\tilde{D}}\omega - \frac{2\mathrm{Im} F_1(\tau)}{\sqrt{\tilde{D}}}\right)^2 + \left\{\tilde{D}\mathrm{Re} F_0(\tau) - 2(\mathrm{Im} F_1(\tau))^2\right\}\omega^2 \\
&\quad + \frac{1}{2}(\tilde{D}\omega^2)^2 + \tilde{D}\omega^2 \mathrm{Re} F_0(\tau) + (\mathrm{Re} F_0(\tau) - \omega \mathrm{Im} F_1(\tau))^2 \\
&\quad + (\mathrm{Im} F_0(\tau) + \omega \mathrm{Re} F_1(\tau))^2 \\
&\geq \frac{1}{2}(\tilde{D}\omega^2)^2 + (\mathrm{Re} F_0(\tau) - \omega \mathrm{Im} F_1(\tau))^2 \\
&\quad + (\mathrm{Im} F_0(\tau) + \omega \mathrm{Re} F_1(\tau))^2 + \tilde{D}\omega^2 \mathrm{Re} F_0(\tau),
\end{aligned} \tag{39}$$

where we have used that Re $F_0 \geq \tau_0/2$, $\varepsilon << 1$ and Im $F_1(\tau) = O(\tilde{D})$. Now, using (39), for $c_{00} \in L^2(\mathbb{R})$ and $c_{s0} \in H^1(\mathbb{R})$, we get $w \in L^2(\mathbb{R})$, $\omega w \in L^2(\mathbb{R})$ and $\omega^2 w \in L^2(\mathbb{R})$, is a unique solution for (37). We conclude that there exists a unique solution $c_0 = \mathcal{F}_x^{-1}(w) \in H^2(\mathbb{R})$ of the effective Laplace-transformed problem (36) for any τ such that $\mathrm{Re}(\tau) \geq \tau_0 > 0$. As $c_{00}, c_{s0} \in C_0^\infty(\mathbb{R})$, we have $c_0 \in \mathcal{S}(\mathbb{R})$. Unfortunately, in (39) the leading term contains $\tilde{D}$ and the regularization comes along with estimates which explode when $\varepsilon \to 0$. It confirms difficulties already observed in [16]. Precise lower bound for the denominator is given in the following lemma:

Lemma 1 *Under the above assumptions, we have*

$$\left|F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2\right| \geq C\left\{\tilde{D}\omega^2 + \mathrm{Re}\tau + \sqrt{\tilde{D}}|\mathrm{Im}\tau| + 1\right\}, \tag{40}$$

where C does not depend on $\tilde{D}$, τ and ω.

Proof We start from (39) and use that Re $F_0 \geq \tau_0/2$, $\varepsilon << 1$ and Im $F_1(\tau) = O(\tilde{D})$. We have

$$(\mathrm{Re} F_0(\tau) - \omega \mathrm{Im} F_1(\tau))^2 + \frac{1}{4}\tilde{D}\omega^2 \mathrm{Re} F_0(\tau) > \frac{1}{2}(\mathrm{Re} F_0)^2. \tag{41}$$

The remaining term is estimated as

$$\frac{1}{4}\tilde{D}\omega^2 \mathrm{Re} F_0(\tau) + \frac{1}{4}(\mathrm{Re} F_0)^2 + (\mathrm{Im} F_0(\tau) + \omega \mathrm{Re} F_1(\tau))^2 \geq \frac{(\mathrm{Im} F_0(\tau))^2 \tilde{D} \mathrm{Re} F_0(\tau)}{\tilde{D}\mathrm{Re} F_0(\tau) + 4(\mathrm{Re} F_1(\tau))^2}. \tag{42}$$

After inserting (41) and (42) into (39), we get (40). □

Proposition 1 *Let* $2 > \alpha \geq 1$. *Then for any* $\tau \in \mathbb{C}$ *such that* $\mathrm{Re}(\tau) \geq \tau_0 > 0$ *we have*

$$||c_0(\tau)||_{L^2(\mathbb{R})} \leq C\frac{||c_{00}||_{H^1(\mathbb{R})} + ||c_{s0}||_{L^2(\mathbb{R})}}{1 + |\tau|}, \tag{43}$$

$$||\partial_x c_0(\tau)||_{L^2(\mathbb{R})} \leq C\frac{||c_{00}||_{H^2(\mathbb{R})} + ||c_{s0}||_{H^1(\mathbb{R})}}{1 + |\tau|}, \tag{44}$$

$$||\partial^2_{xx} c_0(\tau)||_{L^2(\mathbb{R})} \leq C\frac{||c_{00}||_{H^3(\mathbb{R})} + ||c_{s0}||_{H^2(\mathbb{R})}}{1 + |\tau|}. \tag{45}$$

Proof The difficulty is that any decay in τ is accompanied by the presence of the negative powers of $\tilde{D}$ in the estimates. Main difficulty is the presence of c_{00}. In order to handle it we decompose w as $w = U + \mathcal{F}_x(c_{00})/(1+\tau)$. Then for U we have

$$\begin{aligned}
\left(F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2\right) U(\omega) &= \mathcal{F}_x(c_{00})(\omega)(1 - \frac{F_0(\tau)}{1+\tau}) - i\omega F_1(\tau)\mathcal{F}_x(c_{00})(\omega) - \frac{\tilde{D}\omega^2}{1+\tau}\mathcal{F}_x(c_{00})(\omega) \\
&\quad + \mathcal{F}(g)(\omega)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha} + i\omega\frac{2Q}{45D}\varepsilon^{2-\alpha}\right), \quad \text{in } \mathbb{R}.
\end{aligned} \tag{46}$$

Using that $\tilde{D} = C\varepsilon^{2-\alpha}$, we have

$$\left\| \frac{\tilde{D}\omega^2 \mathcal{F}_x(c_{00})(\omega)/(1+\tau)}{F_0(\tau) + i\omega F_1(\tau) + \tilde{D}\omega^2} \right\|_{L^2(\mathbb{R})} \leq \frac{\|c_{00}\|_{L^2(\mathbb{R})}}{1+|\tau|}.$$

Summing up the estimates gives (43)–(45). □

4.3 Error estimates

As before, we limit ourselves to the case $\alpha \geq 1$. As described in Sect. 4.1, the formal asymptotic expansion of a solution c^ε of system (8)–(11) leads to consider the following function for approximating $\hat{c}^\varepsilon$:

$$\begin{aligned} c_1^{L,\mathrm{eff}}(x, y; \varepsilon) &= c_0(x; \varepsilon) + \varepsilon^{2-\alpha} \frac{Q}{D} \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right) \partial_x c_0(x; \varepsilon) \\ &\quad + \frac{\varepsilon^{2-\alpha}}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right) (k(\tau) c_0(x; \varepsilon) - g(\tau)), \end{aligned} \tag{47}$$

where $c_0 \in H^1(\Omega)$ is the solution of the following effective equation

$$\begin{aligned} &\left(\tau + k(\tau) - \frac{k(\tau)^2}{3D} \varepsilon^{2-\alpha} \right) c_0 + \left(\frac{2Q}{3} + \frac{4Q}{45D} k(\tau) \varepsilon^{2-\alpha} \right) \partial_x c_0 - \left(D\varepsilon^\alpha + \frac{8Q^2}{945D} \varepsilon^{2-\alpha} \right) \partial_{xx}^2 c_0 \\ &= c_{00} + g(\tau) \left(1 - \frac{k(\tau)}{3D} \varepsilon^{2-\alpha} \right) + \frac{2Q}{45D} \varepsilon^{2-\alpha} \partial_x g(\tau). \end{aligned} \tag{48}$$

After some computations, we assert that $\hat{c}^\epsilon - c_1^{L,\mathrm{eff}}$ satisfies the following problem.

$$\mathcal{L}^\varepsilon \left(\hat{c}^\epsilon - c_1^{L,\mathrm{eff}} \right) = -\Phi^\varepsilon \quad \text{in } \Omega, \tag{49}$$

$$-D\varepsilon^{\alpha-2} \partial_y \left(\hat{c}^\epsilon - c_1^{L,\mathrm{eff}} \right) \Big|_{y=1} = k(\tau) \left(\hat{c}^\epsilon - c_1^{L,\mathrm{eff}} \right) \Big|_{y=1} - b^\varepsilon \quad \text{in } \mathbb{R}, \tag{50}$$

$$\partial_y \left(\hat{c}^\epsilon - c_1^{L,\mathrm{eff}} \right) \Big|_{y=0} = 0 \quad \text{in } \mathbb{R}, \tag{51}$$

where functions Φ^ε and b^ε are defined by

$$\Phi^\varepsilon = \sum_{i=1}^{5} F_i^\varepsilon + \sum_{i=1}^{3} S_i^\varepsilon + b^\varepsilon, \tag{52}$$

$$F_1^\varepsilon = \varepsilon^{2-\alpha} \partial_{xx}^2 c_0 \frac{Q^2}{D} \left(\frac{8}{945} + (1-y^2) \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right) \right), \tag{53}$$

$$F_2^\varepsilon = \varepsilon^{2-\alpha} \partial_x c_0 \frac{Qk(\tau)}{D} \left(-\frac{2}{45} + (1-y^2) \left(\frac{1}{6} - \frac{y^2}{2} \right) \right), \tag{54}$$

$$F_3^\varepsilon = \varepsilon^{2-\alpha} \tau \partial_x c_0 \frac{Q}{D} \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right), \tag{55}$$

$$F_4^\varepsilon = \varepsilon^{2-\alpha} c_0 \frac{\tau k(\tau)}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right), \tag{56}$$

$$F_5^\varepsilon = -\varepsilon^2 k(\tau) \partial_{xx}^2 c_0 \left(\frac{1}{6} - \frac{y^2}{2} \right) - \varepsilon^2 Q \partial_{xxx}^3 c_0 \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right), \tag{57}$$

$$S_1^\varepsilon = -\varepsilon^{2-\alpha} \frac{\tau g(\tau)}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right), \tag{58}$$

$$S_2^\varepsilon = -\varepsilon^{2-\alpha} \frac{Q}{D} \partial_x g \left(-\frac{2}{45} + (1-y^2)\left(\frac{1}{6} - \frac{y^2}{2}\right)\right), \tag{59}$$

$$S_3^\varepsilon = \varepsilon^2 \partial_{xx}^2 g \left(\frac{1}{6} - \frac{y^2}{2}\right), \tag{60}$$

$$b^\varepsilon = \varepsilon^{2-\alpha} \frac{k(\tau)^2}{3D} c_0 - \varepsilon^{2-\alpha} \frac{2Q}{45D} k(\tau) \partial_x c_0 - \varepsilon^{2-\alpha} \frac{k(\tau)}{3D} g(\tau). \tag{61}$$

Let $w = \hat{c}^\varepsilon - c_1^{L,\mathrm{eff}}$. The variational formulation corresponding to problem (49)–(51) is

$$\int_\Omega \tau w \phi \mathrm{d}x\, \mathrm{d}y + \int_\Omega D\varepsilon^\alpha (\partial_x w \partial_x \phi + \varepsilon^{-2} \partial_y w \partial_y \phi) \mathrm{d}x\, \mathrm{d}y + \int_{\mathbb{R}} k(\tau) w|_{y=1} \phi|_{y=1}\, dx + \int_\Omega Q(1-y^2)\phi \partial_x w\, \mathrm{d}x\, \mathrm{d}y$$

$$= -\int_\Omega \sum_{i=1}^5 F_i^\varepsilon \phi\, \mathrm{d}x\, \mathrm{d}y - \int_\Omega \sum_{i=1}^3 S_i^\varepsilon \phi\, \mathrm{d}x\, \mathrm{d}y - \int_{\mathbb{R}} b^\varepsilon \int_0^1 (\phi - \phi|_{y=1})\, \mathrm{d}y\, \mathrm{d}x. \tag{62}$$

We now look for estimates of the terms in the right hand side of (62). We state and prove the following result:

Lemma 2 *Let $\phi \in H^1(\Omega)$. Then the following estimates hold true*:

$$\left| \int_\Omega \sum_{i=1}^5 F_i^\varepsilon \phi\, \mathrm{d}x\, \mathrm{d}y \right| \le C\varepsilon^{3(1-\alpha/2)} \mathcal{C}(c_0) \left\| \varepsilon^{\alpha/2-1} \partial_y \phi \right\|_{L^2(\Omega)} + C\varepsilon^{2-\alpha/2} \|\partial_x c_0\|_{L^2(\mathbb{R})} \left\| \varepsilon^{\alpha/2} \partial_x \phi \right\|_{L^2(\Omega)}, \tag{63}$$

$$\left| \int_\Omega \sum_{i=1}^3 S_i^\varepsilon \phi\, \mathrm{d}x\, \mathrm{d}y \right| \le C\varepsilon^{3(1-\alpha/2)} \mathcal{C}(c_{s0}) \left\| \varepsilon^{\alpha/2-1} \partial_y \phi \right\|_{L^2(\Omega)}, \tag{64}$$

$$\left| \int_{\mathbb{R}} b^\varepsilon \left(\int_0^1 \phi - \phi|_{y=1}\, \mathrm{d}y \right) \mathrm{d}x \right| \le C\varepsilon^{3(1-\alpha/2)} \frac{\mathcal{C}(c_0) + \mathcal{C}(c_{s0})}{1+|\tau|} \left\| \varepsilon^{\alpha/2-1} \partial_y \phi \right\|_{L^2(\Omega)}, \tag{65}$$

where the quantities $\mathcal{C}(c_0)$ and $\mathcal{C}(c_{s0})$ are defined by

$$\mathcal{C}(c_0) = (1+|\tau|)\left(\|c_0\|_{L^2(\mathbb{R})} + \|\partial_x c_0\|_{L^2(\mathbb{R})}\right) + \|\partial_{xx}^2 c_0\|_{L^2(\mathbb{R})},$$
$$\mathcal{C}(c_{s0}) = \|c_{s0}\|_{L^2(\mathbb{R})} + \frac{1}{1+|\tau|} \|\partial_x c_{s0}\|_{L^2(\mathbb{R})}.$$

Proof First, we note that all F_i^ε have zero mean with respect to y. Therefore, $\sum_{i=1}^4 F_i^\varepsilon$ can be written as

$$\sum_{i=1}^4 F_i^\varepsilon = \varepsilon^{2-\alpha} \partial_y \left(P_0(y)\tau k(\tau) c_0 + (P_1(y)\tau + P_2(y)k(\tau))\partial_x c_0 + P_3(y)\partial_{xx}^2 c_0 \right),$$

where the polynomials P_j, $0 \le j \le 3$, have zero traces in $y = 0, 1$. We thus have

$$\left| \int_\Omega \sum_{i=1}^4 F_i^\varepsilon \phi\, \mathrm{d}x\, \mathrm{d}y \right|$$
$$= \left| \int_\Omega \varepsilon^{2-\alpha} \left(P_0(y)\tau k(\tau) c_0 + (P_1(y)\tau + P_2(y)k(\tau))\partial_x c_0 + P_3(y)\partial_{xx}^2 c_0 \right) \partial_y \phi\, \mathrm{d}x\, \mathrm{d}y \right|$$
$$\le C\varepsilon^{2-\alpha} \|\varepsilon^{\alpha/2-1} \partial_y \phi\|_{L^2(\Omega)} \varepsilon^{1-\alpha/2} \left(|\tau k(\tau)| \|c_0\|_{L^2(\mathbb{R})} + |\tau + k(\tau)| \|\partial_x c_0\|_{L^2(\mathbb{R})} + \|\partial_{xx}^2 c_0\|_{L^2(\mathbb{R})} \right). \tag{66}$$

Next, for the second term in F_5^ε, in order to avoid using the estimate for $\partial_{xxx}c_0$, we use the partial integration with respect to x and get the following estimate:

$$\left|\int_\Omega \varepsilon^2\partial_y\mathcal{P}_4(y)\partial^3_{xxx}c_0\phi\,\mathrm{d}x\mathrm{d}y\right| = \left|\int_\Omega \varepsilon^2\partial_y\mathcal{P}_4(y)\partial^2_{xx}c_0\partial_x\phi\,\mathrm{d}x\mathrm{d}y\right|$$
$$\le C\varepsilon^{2-\alpha/2}\|\partial_{xx}c_0\|_{L^2(\mathbb{R})}\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega)}. \quad (67)$$

The first term in F_5^ε is easily estimated by the same bound. Estimates (66) and (67) imply estimate (63). Analogously, the term $\sum_{i=1}^2 S_i^\varepsilon$ can be written as

$$\sum_{i=1}^2 S_i^\varepsilon = \varepsilon^{2-\alpha}\left(\partial_y(P_{g0}(y))\tau g(\tau) + \partial_y(P_{g1}(y))\partial_x g\right)$$

where the polynomials P_{gj}, $0 \le j \le 1$, have zero traces in $y = 0, 1$. We thus have

$$\left|\int_\Omega \sum_{i=1}^2 S_i^\varepsilon\phi\,\mathrm{d}x\mathrm{d}y\right| \le C\varepsilon^{2-\alpha}\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega)}\varepsilon^{1-\alpha/2}\left(\|c_{s0}\|_{L^2(\mathbb{R})} + \frac{1}{1+|\tau|}\|\partial_x c_{s0}\|_{L^2(\mathbb{R})}\right). \quad (68)$$

In analogy with (67), for the term S_3^ε we have

$$\left|\int_\Omega S_3^\varepsilon\phi\,\mathrm{d}x\mathrm{d}y\right| \le C\varepsilon^{2-\alpha/2}\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega)}\frac{1}{1+|\tau|}\|\partial_x c_{s0}\|_{L^2(\mathbb{R})}. \quad (69)$$

Finally, for the term b^ε, we proceed using Poincaré's inequality:

$$\left|\int_\mathbb{R} b^\varepsilon\left(\int_0^1 \phi(x,\xi)\,\mathrm{d}\xi - \phi|_{y=1}\right)\mathrm{d}x\right|$$
$$= \left|\int_\Omega y b^\varepsilon\partial_y\phi\,\mathrm{d}x\mathrm{d}y\right|$$
$$\le C\varepsilon^{3-3\alpha/2}\left(|k(\tau)|^2\|c_0\|_{L^2(\mathbb{R})} + |k(\tau)|\|\partial_x c_0\|_{L^2(\mathbb{R})} + |k(\tau)||g(\tau)|\|c_{s0}\|_{L^2(\mathbb{R})}\right)\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega)}. \quad (70)$$

Now (68)–(69) implies (64) and (70) gives (65). This completes the proof of the lemma. □

Using Hölder's inequalities in the latter proof, we have the following result:

Corollary 2 *Let* $\gamma \in [0, 1]$ *and* $\alpha \in [1, 2)$. *Then, under the assumptions of Lemma 2, the left hand sides of the estimates (63)–(65) could be replaced by*

$$C\varepsilon^{(2+\gamma)(1-\alpha/2)}(\mathcal{C}(c_0) + \mathcal{C}(c_{s0}))\left(\|\varepsilon^{\alpha/2-1}\partial_y\phi\|^\gamma_{L^2(\Omega)} + \|\varepsilon^{\alpha/2}\partial_x\phi\|^\gamma_{L^2(\Omega)}\right)\|\phi\|^{1-\gamma}_{L^2(\Omega)}.$$

Now we test the variational formulation (62) by the function $\phi = \overline{w}$. After taking the absolute value, we obtain

$$\int_\Omega |\tau||w|^2\,\mathrm{d}x\mathrm{d}y + \int_\Omega D\varepsilon^\alpha(|\partial_x w|^2 + \varepsilon^{-2}|\partial_y w|^2)\,\mathrm{d}x\mathrm{d}y + \int_\mathbb{R} |k(\tau)||w|_{y=1}|^2\mathrm{d}x$$
$$\le \left|\left(\int_\Omega\left(\sum_{i=1}^5 F_i^\varepsilon + \sum_{i=1}^3 S_i^\varepsilon\right)\overline{w}\,\mathrm{d}x\mathrm{d}y - \int_\mathbb{R} b^\varepsilon\int_0^1(\overline{w} - \overline{w}|_{y=1})\,\mathrm{d}y\mathrm{d}x\right)\right|. \quad (71)$$

The terms in the right hand side of the later relation are estimated in Lemma 2. The L^2 error estimate is thus

$$\begin{aligned} \|w\|_{L^2(\Omega)} &= \|\hat{c}^{\epsilon} - c_1^{L,\text{eff}}\|_{L^2(\Omega)} \\ &\le C\varepsilon^{3(1-\alpha/2)} \Big((1+|\tau|) \left(\|c_0\|_{L^2(\mathbb{R})} + \|\partial_x c_0\|_{L^2(\mathbb{R})} \right) \\ &\quad + \|\partial_{xx}^2 c_0\|_{L^2(\mathbb{R})} + \|c_{s0}\|_{L^2(\mathbb{R})} + \frac{\|\partial_x c_{s0}\|_{L^2(\mathbb{R})}}{1+|\tau|} \Big). \end{aligned} \tag{72}$$

The terms containing c_0 are estimated in Sect. 4.2. We thus got the following result:

Proposition 2

$$\left\| (\hat{c}^{\varepsilon} - c_1^{L,\text{eff}})(\tau) \right\|_{L^2(\Omega)} \le C\varepsilon^{3(1-\alpha/2)} \left(\|c_{00}\|_{H^3(\mathbb{R})} + \|c_{s0}\|_{H^2(\mathbb{R})} \right), \tag{73}$$

$$\left\| \partial_x (\hat{c}^{\varepsilon} - c_1^{L,\text{eff}}) \right\|_{L^2(\Omega)} \le C\varepsilon^{3-2\alpha} \left(\|c_{00}\|_{H^3(\mathbb{R})} + \|c_{s0}\|_{H^2(\mathbb{R})} \right), \tag{74}$$

$$\left\| \partial_y (\hat{c}^{\varepsilon} - c_1^{L,\text{eff}}) \right\|_{L^2(\Omega)} \le C\varepsilon^{4-2\alpha} \left(\|c_{00}\|_{H^3(\mathbb{R})} + \|c_{s0}\|_{H^2(\mathbb{R})} \right). \tag{75}$$

$$\left\| (\hat{c}^{\varepsilon} - c_1^{L,\text{eff}})(\tau) \right\|_{L^2(\Omega)} \le C\varepsilon^{(2-\alpha)(3-2\delta)/(2-\delta)} \left(\|c_{00}\|_{H^3(\mathbb{R})} + \|c_{s0}\|_{H^2(\mathbb{R})} \right) |\tau|^{-1/(2-\delta)}, \quad \forall \delta \in (0,1). \tag{76}$$

Proof Estimates (73)–(75) follow immediately from Lemma 2, estimate (72) and inequality (71). It remains to prove the estimate (76).

Let $1 > \delta > 0$. Then by Young's inequality we have

$$\begin{aligned} &\left\{ \left(|\tau| \|w\|_{L^2(\Omega)}^2 \right)^{1/(2-\delta)} \right\}^{2-\delta} + \left\{ \left(\|\varepsilon^{\alpha/2-1} \partial_y w\|_{L^2(\Omega)}^2 \right)^{(1-\delta)/(2-\delta)} \right\}^{(2-\delta)/(1-\delta)} \\ &\quad \ge C \left(|\tau| \|w\|_{L^2(\Omega)}^2 \right)^{1/(2-\delta)} \left(\|\varepsilon^{\alpha/2-1} \partial_y w\|_{L^2(\Omega)}^2 \right)^{(1-\delta)/(2-\delta)}, \end{aligned} \tag{77}$$

$$\begin{aligned} &\left\{ \left(|\tau| \|w\|_{L^2(\Omega)}^2 \right)^{1/(2-\delta)} \right\}^{2-\delta} + \left\{ \left(\|\varepsilon^{\alpha/2} \partial_x w\|_{L^2(\Omega)}^2 \right)^{(1-\delta)/(2-\delta)} \right\}^{(2-\delta)/(1-\delta)} \\ &\quad \ge C \left(|\tau| \|w\|_{L^2(\Omega)}^2 \right)^{1/(2-\delta)} \left(\|\varepsilon^{\alpha/2} \partial_x w\|_{L^2(\Omega)}^2 \right)^{(1-\delta)/(2-\delta)}, \end{aligned} \tag{78}$$

After inserting (77) and (78) into (71) and using Corollary 2 with $\gamma = 2(1-\delta)/(2-\delta)$, we obtain

$$\begin{aligned} |\tau|^{1/(2-\delta)} \|w\|_{L^2(\Omega)}^{2/(2-\delta)} &\le C \Big((1+|\tau|) \left(\|c_0\|_{L^2(\mathbb{R})} + \|\partial_x c_0\|_{L^2(\mathbb{R})} \right) + \|\partial_{xx}^2 c_0\|_{L^2(\mathbb{R})} \\ &\quad + \|c_{s0}\|_{L^2(\mathbb{R})} + \frac{\|\partial_x c_{s0}\|_{L^2(\mathbb{R})}}{1+|\tau|} \Big) \|w\|_{L^2(\Omega)}^{\delta/(2-\delta)}. \end{aligned} \tag{79}$$

Now we use the estimates for c_0 from Sect. 4.2 and the estimate (76) follows immediately. □

Proof of Theorem 1 Theorem 1 now follows directly from the estimate (76) and the Paley–Wiener theorem 3. □

4.4 Inverse Laplace transform for the effective problem

In order to prove that (12) is the effective equation, it remains to go from the "Laplace world" to the "real world". Let c_0^{eff} be the inverse Laplace transform of c_0. We recall that c_0 is the unique solution of

$$F_0(\tau)c_0 + F_1(\tau)\partial_x c_0 - \tilde{D}\partial_{xx}^2 c_0 = c_{00} + g(\tau)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha}\right) + \frac{2Q}{45D}\varepsilon^{2-\alpha}\partial_x g(\tau),$$

where

$$F_0(\tau) = \tau + k(\tau) - \frac{k(\tau)^2}{3D}\varepsilon^{2-\alpha},$$
$$F_1(\tau) = \frac{2Q}{3} + \frac{4Q}{45D}k(\tau)\varepsilon^{2-\alpha}, \quad \tilde{D} = D\varepsilon^{\alpha} + \frac{8Q^2}{945D}\varepsilon^{2-\alpha}$$
$$k(\tau) = C_k\frac{\tau}{\tau + C_0} = C_k - \frac{C_k C_0}{\tau + C_0}, \quad \text{with } C_k = \frac{T_L}{T_{De}}k_s \quad \text{and} \quad C_0 = \frac{T_L k_s}{T_{De}K_e};$$
$$g(\tau) = C_{g1}\frac{c_{s0}}{\tau + C_0}, \quad \text{with } C_{g1} = \frac{T_A T_L k_s}{T_{De}^2 K_e}.$$

Using elementary properties of Laplace's transform, notably the Heaviside expansion theorem, and with notations of the operational calculus (see, e.g. [21]), we have

$$\tau c_0 - c_{00} \leftrightarrow \frac{\partial c_0^{\text{eff}}}{\partial t};$$
$$k(\tau)c_0 \leftrightarrow C_k c_0^{\text{eff}} - C_k C_0 \int_0^t \mathrm{e}^{-C_0(t-\xi)} c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi;$$
$$k(\tau)^2 c_0 \leftrightarrow C_k^2 c_0^{\text{eff}} - 2C_k^2 C_0 \int_0^t \mathrm{e}^{-C_0(t-\xi)} c_0^{\text{eff}}(\cdot,\xi)\mathrm{d}\xi + C_k^2 C_0^2 \int_0^t \mathrm{e}^{-C_0(t-\xi)} c_0^{\text{eff}}(\cdot,\xi)(t-\xi)\mathrm{d}\xi.$$

For the right hand side we have

$$g(\tau)\left(1 - \frac{k(\tau)}{3D}\varepsilon^{2-\alpha}\right) = \frac{C_{g1}}{3D}c_{s0}\frac{(3D - C_k\varepsilon^{2-\alpha})\tau + 3DC_0}{(\tau + C_0)^2} \leftrightarrow \frac{C_{g1}}{3D}c_{s0}\mathrm{e}^{-C_0 t}\left(3D - C_k\varepsilon^{2-\alpha} + C_0 C_k \varepsilon^{2-\alpha} t\right);$$
$$\frac{2Q}{45D}\varepsilon^{2-\alpha}\partial_x g(\tau) = \frac{2Q}{45D}\varepsilon^{2-\alpha}C_{g1}\frac{\partial_x c_{s0}}{\tau + C_0} \leftrightarrow \frac{2Q}{45D}\varepsilon^{2-\alpha}C_{g1}\partial_x c_{s0}\mathrm{e}^{-C_0 t}.$$

In view of these equalities, we obtain the effective equation (12) for c_0^{eff}:

For the non-dimensional surface concentration $\hat{c}_s^{\varepsilon}$, we recall that

$$\hat{c}_s^{\varepsilon} = \frac{T_{De}}{T_A}\left(\frac{T_L k_s}{T_{De}}\hat{c}^{\varepsilon} + \frac{T_A}{T_{De}}c_{s0}\right)\frac{1}{\tau + \frac{T_L k_s}{T_{De}K_e}}$$

and it is easy to write the effective non-dimensional surface concentration c_s^{eff} using c_0^{eff} and expansion for c^{ε}.

References

1. Arendt, W., Batty, C.J.K., Hieber, M., Neubrander, F.: Vector-valued Laplace Transforms and Cauchy Problems. Birkhäuser, Basel (2001)
2. Aris, R.: On the dispersion of a solute in a fluid flowing through a tube. Proc. Roy. Soc. Lond. Sect. A **235**, 67–77 (1956)
3. Balakotaiah, V., Chang, H.-C.: Dispersion of chemical solutes in chromatographs and reactors. Phil. Trans. R. Soc. Lond. A **351**(1695), 39–75 (1995)
4. Balakotaiah, V., Chang, H.-C.: Hyperbolic homogenized models for thermal and solutal dispersion. SIAM J. Appl. Math. **63**, 1231–1258 (2003)
5. Balakotaiah, V.: Hyperbolic averaged models for describing dispersion effects in chromatographs and reactors. Korean J. Chem. Eng. **21**(2), 318–328 (2004)
6. Camacho, J.: Thermodynamics of Taylor dispersion: constitutive equations. Phys. Rev. E **47**(2), 1049–1053 (1993)
7. Camacho, J.: Purely global model for Taylor dispersion. Phys. Rev. E **48**(1), 310–321 (1993)
8. Camacho, J.: Thermodynamics functions for Taylor's dispersion. Phys. Rev. E **48**(3), 1844–1849 (1993)
9. Chakraborty, S., Balakotaiah, V.: Spatially averaged multi-scale models for chemical reactions. Adv. Chem. Eng. **30**, 205–297 (2005)
10. Choquet, C., Mikelić, A.: Laplace transform approach to the rigorous upscaling of the infinite adsorption rate reactive flow under dominant Peclet number through a pore. Appl. Anal. **87**(12), 1373–1395 (2008)

11. Dautray, R., Lions, J.L.: Analyse mathématique et calcul numérique pour les sciences et techniques, vol. 7. Evolution: Fourier, Laplace, Masson, Cea, Paris (1984)
12. van Duijn, C.J., Knabner, P.: Travelling waves in the transport of reactive solutes through porous media: adsorption and binary ion exchange—Part 1. Transp. Porous Media **8**, 167–194 (1992)
13. van Duijn, C.J., Mikelić, A., Pop, I.S., Rosier, C.: Effective dispersion equations for reactive flows with dominant Peclet and Damkohler numbers. In: Marin, G.B., West, D., Yablonsky, G.S. (eds.) Advances in Chemical Engineering, vol. 34, pp. 1–45. Academic Press, New York (2008)
14. Knabner, P., van Duijn, C.J., Hengst, S.: An analysis of crystal dissolution fronts in flows through porous media. Part 1. Compatible boundary conditions. Adv. Water Resour. **18**, 171–185 (1995)
15. Mercer, G.N., Roberts, A.J.: A centre manifold description of contaminant dispersion in channels with varying flow profiles. SIAM J. Appl. Math. **50**, 1547–1565 (1990)
16. Mikelić, A., Devigne, V., van Duijn, C.J.: Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers. SIAM J. Math. Anal. **38**(4), 1262–1287 (2006)
17. Mikelić, A., Rosier, C.: Rigorous upscaling of the infinite adsorption rate reactive flow under dominant Peclet number through a pore. Ann. Univ. Ferrara Sez. VII Sci. Mat. **53**, 333–359 (2007)
18. Paine, M.A., Carbonell, R.G., Whitaker, S.: Dispersion in pulsed systems. I. Heterogeneous reaction and reversible adsorption in capillary tubes. Chem. Eng. Sci. **38**, 1781–1793 (1983)
19. Rubinstein, J., Mauri, R.: Dispersion and convection in porous media. SIAM J. Appl. Math. **46**, 1018–1023 (1986)
20. Taylor, G.I.: Dispersion of soluble matter in solvent flowing slowly through a tube. Proc. R. Soc. A **219**, 186–203 (1953)
21. Vladimirov, V.S.: Equations of mathematical physics. URSS, Moscow (1996)