

**Modeling Reactive Flows in Porous
Media Under Important Peclet's and
Damkohler's Numbers, Using
Homogenization**

Talk at *SIAM Conference on Mathematical
and Computational Issues in the
Geosciences*, Avignon, France, June 8,
2005

by

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Thanks:

This research was supported in part by the GDR MOMAS (Modélisation Mathématique et Simulations numériques liées aux problèmes de gestion des déchets nucléaires: 2439 - ANDRA, BRGM, CEA, EDF, CNRS) as a part of the project "*Modélisation micro-macro des phénomènes couplés de transport-chimie-déformation en milieux argileux*"

This research is in collaboration with C.J. van Duijn and I. S. Pop (TU Eindhoven, The Netherlands).

In many processes arising in chemical engineering it is important to study the diffusion of a solute transported by a fluid flowing through a porous medium. In addition, there are reactions or adsorption occurring at the solid/fluid interfaces.

Examples are chromatographic systems, heterogeneous reactors from chemical and catalytic reaction engineering, the use of surfactants in tertiary oil recovery processes, environmental problems

These systems are analyzed in terms of **dispersion equations** for momentum, energy and mass transfer in continua. In fact averaging of the physical first principles should give us the dispersion coefficients (=effective coefficients). Nevertheless, there are difficulties:

Even the simplest models contain the transport terms of the form $\vec{v} \cdot \nabla c$. Since both the velocity and the concentration gradient are oscillatory, in general the average of the product is different from the product of the averages.

Par example, in Taylor's dispersion the velocity field contributes, after averaging, to the effective diffusion and one obtains Taylor's mechanical dispersion term. Presence of the chemical reactions complicates additionally determination of the effective coefficients since they can depend on the reaction term or on the adsorption isotherm in a complicated way. It is fairly complicated to determine this dependence using just **laboratory experiments** .

In order to start with a simple situation, we consider a porous medium comprised of a bundle of capillary tubes. The disadvantage is that a bundle of capillary tubes represents a geometrically oversimplified model of a porous medium. Nevertheless, there is considerable insight to be gained from such analysis.

We start with a toy problem:

We study the diffusion of the solute particles transported by the Poiseuille velocity profile in a semi-infinite 2D channel. Solute particles are participants in a first-order chemical reaction with the boundary of the channel. They don't interact between them. The simplest example, borrowed from *[Mau:91], is described by the following model for the solute concentration c^*

$$\frac{\partial c^*}{\partial t^*} + q(z) \frac{\partial c^*}{\partial x^*} - D^* \Delta_{x^*, z} c^* = 0 \text{ in } \mathbb{R}_+ \times (-H, H), \quad (1)$$

where $q(z) = Q^*(1 - (z/H)^2)$ and Q^* (**velocity**) and D^* (**molecular diffusion**) are positive constants. At the lateral boundaries $z = \pm H$ the first-order chemical reaction with the solute particles is modeled through the following boundary condition :

$$D^* \partial_z c^* + k^* c^* = 0 \text{ on } z = \pm H, \quad (2)$$

where k^* is the **surface reactivity coefficient**.

This case is the mathematical equivalent of an **irreversible, first order, heterogeneous chemical reaction with equilibrium being maintained between the fluid and adsorbed species**.

*[Mau:91] R. Mauri, *Dispersion, convection and reaction in porous media*, Phys. Fluids A (1991), p. 743-755.

The natural way of analyzing this problem is to introduce the appropriate scales.

They would come from the characteristic concentration \hat{c} , the characteristic length L_R , the characteristic velocity Q_R , the characteristic diffusivity D_R and the characteristic time T_c . The characteristic length L_R coincides in fact with the "observation distance". Problem involves the following time scales:

$$T_L = \text{characteristic longitudinal time scale} = \frac{L_R}{Q_R}$$

$$T_T = \text{characteristic transversal time scale} = \frac{H^2}{D_R}$$

$$T_R = \text{superficial chemical reaction time scale} = \frac{H}{k_R}$$

and the following characteristic non-dimensional numbers

$$\mathbf{Pe} = \frac{L_R Q_R}{D_R} \quad (\text{Peclet's number})$$

$$\mathbf{Da} = \frac{L_R^2 k_R}{H D_R} \quad (\text{Damkohler's number})$$

Further we set $\varepsilon = \frac{H}{L_R} \ll 1$ and choose $T_c = T_L$. Solving the full problem for arbitrary values of coefficients is costly and practically impossible. Consequently, **one would like to find the effective (or averaged) values of the dispersion coefficient and the transport velocity and an effective corresponding 1D parabolic equation for the effective concentration.**

In *[Tay:53] Taylor obtained an explicit effective expression for the enhanced diffusion coefficient and it is called in literature *Taylor's dispersion formula*.

We choose $Q = \frac{Q^*}{Q_R} = \mathcal{O}(1)$, and

$$\frac{T_T}{T_L} = \frac{HQ_R}{D_R} \varepsilon = \mathcal{O}(\varepsilon^{2-\alpha}) = \varepsilon^2 \mathbf{Pe}.$$

Then the situation from Taylor's article corresponds to the case when $\alpha = 1$, i.e. Peclet's number is equal to $\frac{1}{\varepsilon}$ and $k = 0$ (no chemistry).

*[Tay:53] G.I. Taylor, *Dispersion of soluble matter in solvent flowing slowly through a tube*, Proc. Royal Soc. A, Vol. 219 (1953), p. 186-203.

Our equations in their non-dimensional form are

$$\frac{\partial c}{\partial t} + Q(1 - y^2) \frac{\partial c}{\partial x} = D\varepsilon^\alpha \partial_{xx}c + D\varepsilon^{\alpha-2} \partial_{yy}c$$

$$\text{in } \mathbb{R}_+ \times (0, 1) \times (0, T) \quad (3)$$

$$c(x, y, 0) = 1, \quad (x, y) \in \mathbb{R}_+ \times (0, 1), \quad (4)$$

$$-D\varepsilon^{\alpha-2} \partial_y c|_{y=1} = -D \frac{1}{\varepsilon^2 \mathbf{Pe}} \partial_y c|_{y=1} =$$

$$k_0 \frac{\mathbf{Da}}{\mathbf{Pe}} c|_{y=1} = k_0 \varepsilon^{\alpha+\beta} c|_{y=1} \quad (5)$$

$$\partial_y c(x, 0, t) = 0, \quad (x, t) \in \mathbb{R}_+ \times (0, T) \quad (6)$$

$$\text{and } c(0, y, t) = 0, \quad (y, t) \in (0, 1) \times (0, T), \quad (7)$$

where it was used that c is antisymmetric in y and Damkohler number was set to $k_0 \varepsilon^\beta$. Our domain is now the infinite strip $Z^+ = \mathbb{R}_+ \times (0, 1)$. We study the behavior of the solution to (3) -(7), with square integrable gradient in x and y , when $\varepsilon \rightarrow 0$. Clearly, the most interesting case is $\beta = -\alpha$ and $0 \leq \alpha < 2$ and we restrict our considerations to this situation.

Effective problem with Taylor's dispersion coefficient:

$$\begin{cases} \partial_t c^{Tay} + \frac{2}{3} \partial_x c^{Tay} = \varepsilon \left(D + \frac{8}{945} \frac{Q^2}{D} \right) \partial_{xx} c^{Tay}, \\ \text{in } \mathbb{R}_+ \times (0, T), \quad c^{Tay}|_{x=0} = 1, \\ c^{Tay}|_{t=0} = 0, \quad \partial_x c^{Tay} \in L^2(\mathbb{R}_+ \times (0, T)), \end{cases} \quad (8)$$

What is known concerning derivation of (8) ?

◇ Formal derivation using the **method of moments**, see * [Aris:56].

◇ " Near rigorous " derivation using the centre manifold theory, see † [MerRob:90] : The initial value problem is studied and the Fourier transform with respect to x is applied. The resulting PDE is written in the form $\dot{u} = \mathcal{A}u + F(u)$, with $u = (k, \hat{c})$. Then the **centre manifold theory** is applied to obtain effective equations at various orders. Since the corresponding centre manifold isn't finite dimensional, the results aren't rigorous.

*[Aris:56] R. Aris: On the dispersion of a solute in a fluid flowing through a tube, Proc. Roy. Soc. London Sect A., 235 (1956), pp. 67-77.

†[MerRob:90] G.N. Mercer, A.J. Roberts, *A centre manifold description of contaminant dispersion in channels with varying flow profiles* , SIAM J. Appl. Math. , Vol. 50 (1990), p. 1547-1565.

◇ When the chemistry is added (e.g. having an irreversible, 1st order, chemical reaction with equilibrium at $y = 1$, as we have), then there is a paper * [PCW:83]. They noted that the equation for the difference between the physical and averaged concentrations is not closed, since it contains a dispersive source term $\frac{\partial}{\partial x} \langle \bar{q}_x \bar{c} \rangle$. Then they multiplied the equation for \bar{c} by \bar{q}_x and got an equation for $\langle \bar{q}_x \bar{c} \rangle$. Nevertheless, a dispersive transport term $\frac{\partial}{\partial x} \langle \bar{q}_x^2 \bar{c} \rangle$ and clearly the procedure enters the same difficulty as the method of moments: there is an infinite system of equations.

Paine et al used the "single-point" closure schemes of turbulence modeling by Launder to obtain a closed model for the averaged concentration.

*[PCW:83] M.A. Paine, R.G. Carbonell, S. Whitaker, *Dispersion in pulsed systems – I, Heterogeneous reaction and reversible adsorption in capillary tubes*, Chemical Engineering Science, Vol. 38 (1983), p. 1781-1793.

Our technique is motivated by the paper * [RuMa:86], where the analysis is based on the hierarchy of time scales. In our knowledge the only rigorous result concerning the effective dispersion, in the presence of high Peclet's numbers (and no chemistry), is in the recent paper † [BoJuPi:03]. Nevertheless, their approach is based on the regular solutions for compatible data for the underlying linear transport equation. This compatibility isn't acceptable for the reactive transport.

For the bounds on convection enhanced diffusion we refer to papers by Fannjiang, Papanicolaou, Zhikov, Kozlov, Piatnitskii

In collaboration with C.J. van Duijn and I. S. Pop (Eindhoven), we obtained several **mathematically rigorous** results on Taylor's dispersion, with and without chemical reactions and I'll present one of them.

*[RuMa:86] J. Rubinstein, R. Mauri, *Dispersion and convection in porous media*, SIAM J. Appl. Math., Vol. 46 (1986), p. 1018 - 1023.

†[BoJuPi:03] A. Bourgeat, M. Jurak, A.L. Piatnitski, *Averaging a transport equation with small diffusion and oscillating velocity*, Math. Meth. Appl. Sci., Vol. 26 (2003), pp. 95-117.

A simple L^2 error estimate

The simplest way to average the problem (3)-(7) is to take the mean value with respect to y . Let $c_0^{eff} = \langle c^\varepsilon \rangle = \int_0^1 c^\varepsilon dy$. Supposing that the mean of the product is the product of the means, which is in general wrong, we get the following problem for the "averaged" concentration $c_0^{eff}(x, t)$:

$$\begin{cases} \frac{\partial c_0^{eff}}{\partial t} + \frac{2Q}{3} \frac{\partial c_0^{eff}}{\partial x} + k_0 c_0^{eff} = \varepsilon^\alpha D \frac{\partial^2 c_0^{eff}}{\partial x^2} & \text{in} \\ \mathbb{R}_+ \times (0, T), \quad \partial_x c_0^{eff} \in L^2(\mathbb{R}_+ \times (0, T)) \\ c_0^{eff}|_{t=0} = 1, \quad c_0^{eff}|_{x=0} = 0. \end{cases} \quad (9)$$

Let the operator \mathcal{L}^ε be given by

$$\mathcal{L}^\varepsilon \zeta = \frac{\partial \zeta}{\partial t} + Q(1-y^2) \frac{\partial \zeta}{\partial x} - D\varepsilon^\alpha \left(\partial_{xx} \zeta + \varepsilon^{-2} \partial_{yy} \zeta \right) \quad (10)$$

We want to approximate c^ε by c_0^{eff} . Then

$$\mathcal{L}^\varepsilon(c_0^{eff}) = -k_0 c_0^{eff} + Q \partial_x c_0^{eff} \left(\frac{1}{3} - y^2 \right) = R^\varepsilon$$

$$\begin{aligned} \mathcal{L}^\varepsilon(c^\varepsilon - c_0^{eff}) &= -R^\varepsilon & \text{in } Z^+ \times (0, T) \text{ and} & \quad (11) \\ -D\varepsilon^{\alpha-2} \partial_y(c^\varepsilon|_{y=1} - c_0^{eff}) &= k_0 c^\varepsilon|_{y=1} & \text{on } \mathbb{R}_+ \times (0, T) & \quad (12) \end{aligned}$$

Let $\Psi(x) = 1/(x + 1)$. Then $(\partial_x \Psi^2)^2/\Psi^2 \leq 4\Psi^2$. We have the following proposition, which will be useful in getting the estimates :

Proposition 1 Let $g^\varepsilon \in H_{loc}^1(Z^+ \times (0, T))$ and $\xi_0^\varepsilon \in L_{loc}^2(Z^+)$. Let $\xi \in C([0, T]; L_{loc}^2(Z^+))$, $\nabla_{x,y}\xi \in L^2(Z^+ \times (0, T))$ satisfies the system

$$\mathcal{L}^\varepsilon(\xi) = -R^\varepsilon \text{ in } Z^+ \times (0, T) \quad (13)$$

$$-D\varepsilon^{\alpha-2}\partial_y\xi|_{y=1} = k_0\xi|_{y=1} + g^\varepsilon|_{y=1} \quad (14)$$

$$\partial_y\xi|_{y=0} = 0 \text{ on } \mathbb{R}_+ \times (0, T) \quad (15)$$

$$\xi|_{t=0} = \xi_0^\varepsilon \text{ on } Z^+ \quad (16)$$

$$\xi|_{x=0} = 0 \text{ on } (0, 1) \times (0, T). \quad (17)$$

Then we have the following energy estimate

$$\begin{aligned} \mathcal{E}(\xi, t) &= \frac{1}{2} \int_{Z^+} \Psi(x)^2 \xi^2(t) \, dx dy + \\ &\frac{D}{2} \varepsilon^\alpha \int_0^t \int_{Z^+} \Psi(x)^2 \left\{ \varepsilon^{-2} |\partial_y \xi|^2 + |\partial_x \xi|^2 \right\} \, dx dy d\tau \\ &+ k_0 \int_0^t \int_{\mathbb{R}_+} \xi^2|_{y=1} \Psi^2(x) \, dx d\tau \leq - \int_0^t \int_{Z^+} \Psi(x)^2 \cdot \\ &R^\varepsilon \xi \, dx dy d\tau - \int_0^t \int_{\mathbb{R}_+} g^\varepsilon|_{y=1} \xi|_{y=1} \Psi^2(x) \, dx d\tau + \\ &2D\varepsilon^\alpha \int_0^t \int_{Z^+} \Psi(x)^2 \xi^2 \, dx dy d\tau. \quad (18) \end{aligned}$$

Let $O_T = (0, T) \times Z^+$. After estimating R^ε in $L^2((0, T) \times \mathbb{R}_+; (H^1(0, 1) \cap L_0^2(0, 1))')$, we get

Proposition 2 In the setting of this section we have

$$\|(c^\varepsilon - c_0^{eff})\Psi\|_{L^\infty(0, T; L^2(Z^+))} \leq \varepsilon^{1-\alpha/2} \frac{F^0}{\sqrt{D}} \quad (19)$$

$$\|\partial_x(c^\varepsilon - c_0^{eff})\Psi\|_{L^2((0, T) \times Z^+)} \leq \varepsilon^{1-\alpha} \frac{F^0}{D} \quad (20)$$

$$\|\partial_y(c^\varepsilon - c_0^{eff})\Psi\|_{L^2((0, T) \times Z^+)} \leq \varepsilon^{2-\alpha} \frac{F^0}{D}, \quad (21)$$

But $\|\partial_x c_0^{eff}\|_{L^2(O_T)}^2 = \int_0^T \int_0^{+\infty} |\partial_x c_0^{eff}|^2 = C\varepsilon^{-\alpha/4}$
and

$$F^0 = C_1^F \|\partial_x c_0^{eff}\|_{L^2(O_T)} + C_2^F k_0 \leq C_3^F \varepsilon^{-\alpha/4} \quad (22)$$

Hence in fact

$$\|c^\varepsilon - c_0^{eff}\|_{L^\infty(0, T; L_{loc}^2(\mathbb{R}_+ \times (0, 1)))} \leq C\varepsilon^{1-3\alpha/4} \quad (23)$$

NOT BRILLANT AS APPROXIMATION. FOR $\alpha > 4/3$ IT DOESN'T GIVE CONVERGENCE

IS THERE A BETTER APPROXIMATION ?

Paine et al propose the following effective model

$$\begin{cases} \partial_t c^{Pai} + Q\left(\frac{2}{3} + A_1\right) \partial_x c^{Pai} + C_2 c^{Pai} = K^* \partial_{xx} c^{Pai}, \\ \text{in } \mathbb{R}_+ \times (0, T), \partial_x c^{Pai} \in L^2(\mathbb{R}_+ \times (0, T)) \\ c^{Pai}|_{x=0} = 0, c^{Pai}|_{t=0} = 1, \end{cases} \quad (24)$$

where A_1 depends on the zeroth order moments of c^{Pai} and qc^{Pai} and K^* depends on the zero, first and second order moments of the same quantities and Peclet's number.

This is a non-local problem, hence difficult solve. Even worse: it was derived using an **ad hoc** closure assumption.

We did a different derivation of the effective model. The model we got is the following:

$$\left\{ \begin{array}{l} \partial_t c^{Mau} + Q \left(\frac{2}{3} + \frac{4k_0}{45D} \varepsilon^{2-\alpha} \right) \partial_x c^{Mau} + \\ k_0 \left(1 - \frac{k_0}{3D} \varepsilon^{2-\alpha} \right) c^{Mau} = (D\varepsilon^\alpha + \frac{8Q^2}{945D} \varepsilon^{2-\alpha}) \partial_{xx} c^{Mau} \\ \text{in } \mathbb{R}_+ \times (0, T), \quad c^{Mau}|_{x=0} = 0, \\ c^{Mau}|_{t=0} = 1, \quad \partial_x c^{Mau} \in L^2(\mathbb{R}_+ \times (0, T)). \end{array} \right. \quad (EFF)$$

For $k_0 = 0$ and $\alpha = 1$ this is exactly Taylor's dispersion model.

Our result could be restated in dimensional form:

Theorem 1 Let us suppose that

$$L_R > \max\{D_R/Q_R, Q_R H^2/D_R, H\}.$$

Then the upscaled *dimensional* approximation for (1) reads

$$\begin{aligned} \frac{\partial c^{*,eff}}{\partial t^*} + \left(\frac{2}{3} + \frac{4}{45} \mathbf{Da}_T \right) Q^* \frac{\partial c^{*,eff}}{\partial x^*} + \frac{k^*}{H} \left(1 - \right. \\ \left. \frac{1}{3} \mathbf{Da}_T \right) c^{*,eff} = D^* \left(1 + \frac{8}{945} \mathbf{Pe}_T^2 \right) \frac{\partial^2 c^{*,eff}}{\partial (x^*)^2}, \end{aligned} \quad (25)$$

where $\mathbf{Pe}_T = \frac{Q^* H}{D^*}$ is the transversal Peclet's number and $\mathbf{Da}_T = \frac{k^* H}{D^*}$ is the transversal Damkohler's number (= **Sh**, the Sherwood number).

Why our model is better than other models from the literature?

For simplicity, we compare only the physical concentration c^ε with c^{Mau} . Throughout the talk $H(x)$ is Heaviside's function.

Theorem 2 Let c^{Mau} be given by (EFF). Then we have $\forall \delta > 0$

$$\|t^3(c^\varepsilon - c^{Mau})\|_{L^\infty(O_T)} \leq \begin{cases} C\varepsilon^{2-3\alpha/2}, & \alpha < 1, \\ C\varepsilon^{3/2-\alpha-\delta}, & \alpha \in [1, 2). \end{cases} \quad (26)$$

$$\|t^3(c^\varepsilon - c^{Mau})\|_{L^2(0,T;L^1_{loc}(Z^+))} \leq C\varepsilon^{2-\alpha} \quad (27)$$

$$\|t^3(c^\varepsilon - c^{Mau})\|_{L^2(0,T;L^2_{loc}(Z^+))} \leq C\left(\varepsilon^{2-5\alpha/4}H(1-\alpha) + \varepsilon^{3/2-3\alpha/4}H(\alpha-1)\right) \quad (28)$$

$$\|t^3\partial_y c^\varepsilon\|_{L^2(0,T;L^2_{loc}(Z^+))} \leq C\left(\varepsilon^{2-5\alpha/4}H(1-\alpha) + \varepsilon^{3/2-3\alpha/4}H(\alpha-1)\right) \quad (29)$$

$$\begin{aligned} & \|t^3 \partial_x (c^\varepsilon - c^{Mau})\|_{L^2(0,T;L^2_{loc}(Z^+))} \leq \\ & C\left(\varepsilon^{2-7\alpha/4} H(1-\alpha) + \varepsilon^{3/2-5\alpha/4} H(\alpha-1)\right) \end{aligned} \quad (30)$$

Corollary In the conditions of Taylor's article, $\alpha = 1$ and $k_0 = 0$, we have

$$\|t^3 (c^\varepsilon - c^{Mau})\|_{L^\infty(O_T)} \leq C\varepsilon^{1/2-\delta}, \quad \forall \delta > 0, \quad (31)$$

$$\|t^3 (c^\varepsilon - c^{Mau})\|_{L^2(0,T;L^1_{loc}(Z^+))} \leq C\varepsilon \quad (32)$$

We note that the solution c^{Mau} to the problem (EFF) is **not close** to the solution c_0^{eff} to the problem (9), as the simulations on the figures show:

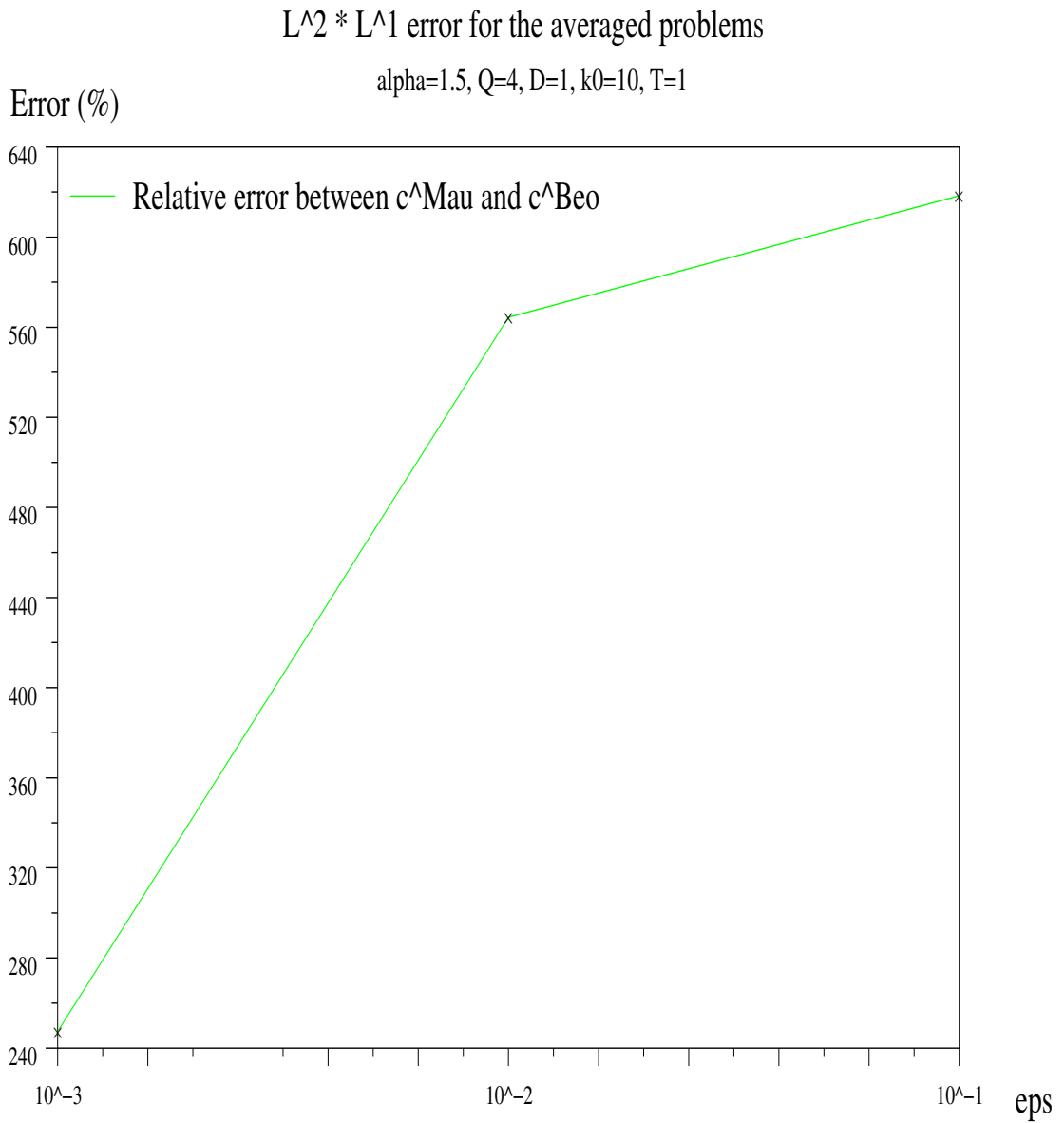


Fig. Difference between the solution to our model and c_0^{eff}

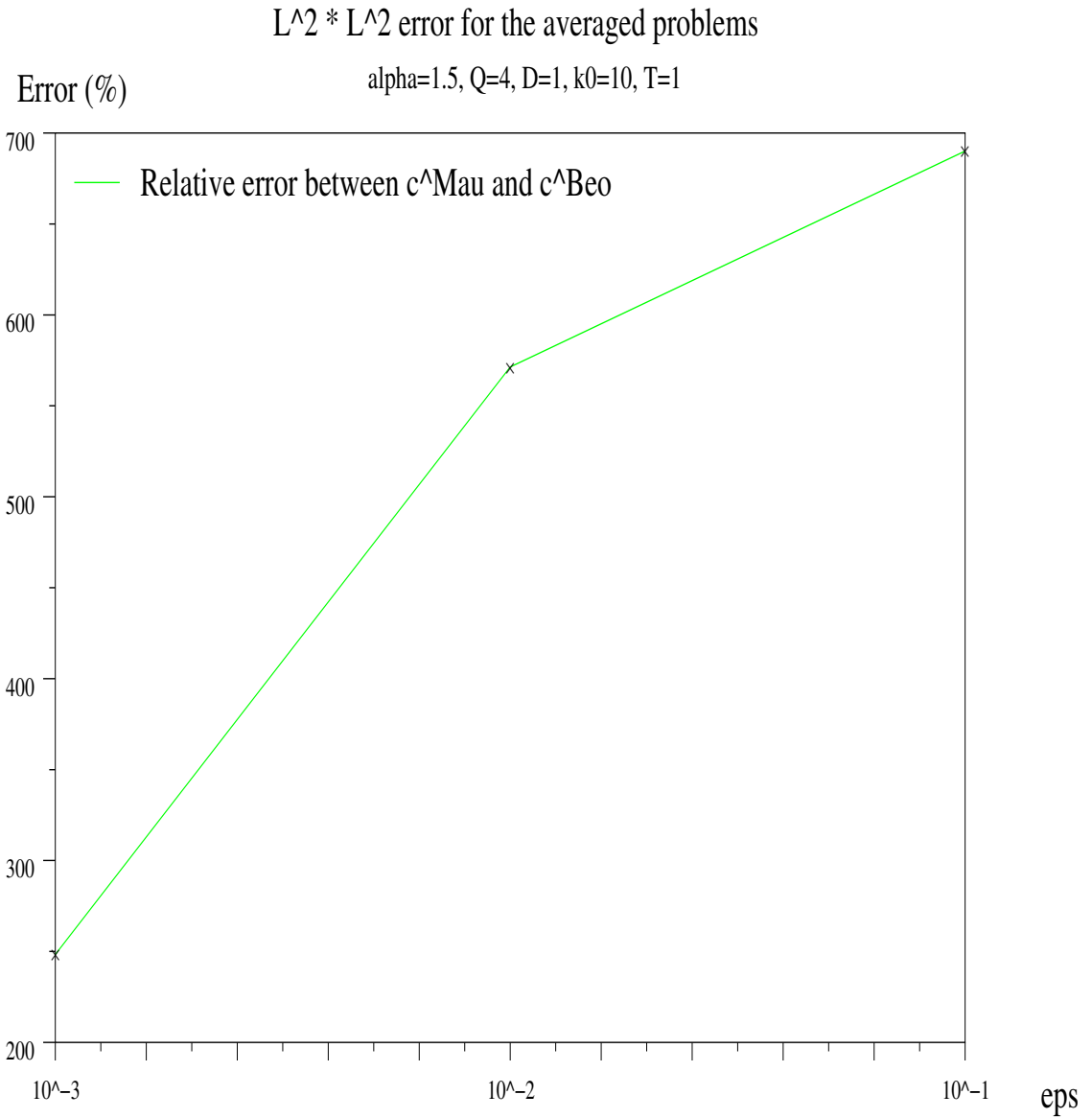


Fig. Difference between the solution to our model and c_0^{eff}

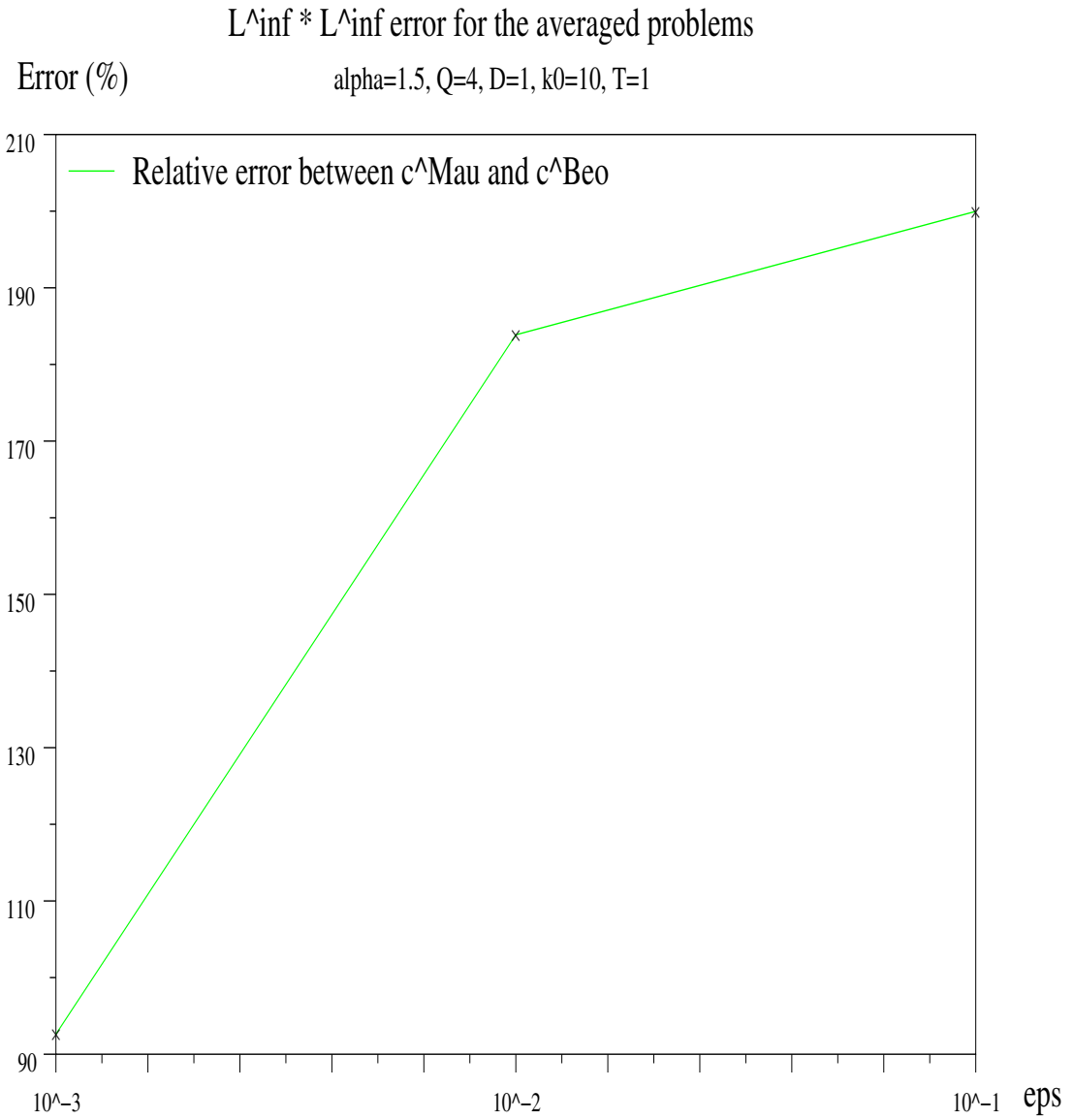


Fig. Difference between the solution to our model and c_0^{eff}

First Correction and Error estimate

The estimate (23) isn't satisfactory. In order to get a better approximation we could try the correction constructed using the formal 2-scale expansion. Unfortunately it leads to a hyperbolic equation for c^0 and, except under high compatibility, c^0 is not smooth and it is very difficult to use it for expansions. We proceed by following an idea from [RuMa:86] and suppose that

$$\partial_t c^0 + 2Q\partial_x c^0 / 3 + k_0 c^0 = \mathcal{O}(\varepsilon) \quad \text{in } (0, +\infty) \times (0, T). \quad (33)$$

Then we get the problem (48).

Let $0 \leq \alpha < 2$. We start by the $\mathcal{O}(\varepsilon^2)$ approximation and consider the function

$$c_1^{cor}(x, y, t; \varepsilon) = c^{Maui}(x, t; \varepsilon) + \varepsilon^{2-\alpha} \zeta(t) \left(\frac{Q}{D} \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} - \beta^\varepsilon \right) \frac{\partial c^{Maui}}{\partial x} + \frac{k_0}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right) c^{Maui}(x, t; \varepsilon) \right) \quad (34)$$

where $c^{Ma u}$ is the solution to the effective problem with Taylor's dispersion coefficient and reaction terms:

$$\begin{cases} \partial_t c^{Ma u} + Q\left(\frac{2}{3} + \frac{4k_0}{45D}\varepsilon^{2-\alpha}\right)\partial_x c^{Ma u} + \\ k_0\left(1 - \frac{k_0}{3D}\varepsilon^{2-\alpha}\right)c^{Ma u} = (D\varepsilon^\alpha + \frac{8Q^2}{945D}\varepsilon^{2-\alpha})\partial_{xx} c^{Ma u}, \\ \text{in } \mathbb{R}_+ \times (0, T), \partial_x c^{Ma u} \in L^2(\mathbb{R}_+ \times (0, T)) \\ c^{Ma u}|_{x=0} = 0, c^{Ma u}|_{t=0} = 1, \end{cases} \quad (35)$$

$\tilde{D} = D\varepsilon^\alpha + \frac{8}{945}\frac{Q^2}{D}\varepsilon^{2-\alpha}$ is the Taylor's dispersion coefficient. The cut-off in time ζ is given by

$$\zeta(t) = \begin{cases} \left(\frac{t}{\tilde{D}}\right)^r & \text{for } 0 \leq t \leq \tilde{D}, \\ 1 & \text{otherwise,} \end{cases} \quad (36)$$

and we use to eliminate the time-like boundary layer appearing at $t = 0$. These effects are not visible in the formal expansion.

$\beta^\varepsilon(x, y) = \beta\left(\frac{x}{\varepsilon}, y\right)$ is the boundary layer function.

NEXT it should be noted that **the second term** in c_1^{cor} is of order $\varepsilon^{2-5\alpha/4}H(1-\alpha) + \varepsilon^{3(2-\alpha)/4}H(\alpha-1)$ in L^2 . \Downarrow

CONVERGENCE RESULT:

Theorem: Let c^{Maui} be given by (8). Then we have

$$\begin{aligned} & \|t^3(c^\varepsilon - c_1^{cor})\|_{L^\infty(0,T;L^2(\mathbb{R}_+ \times (0,1)))} \leq \\ & C\left(\varepsilon^{3-9\alpha/4}H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2}H(\alpha-1)\right) \end{aligned} \quad (37)$$

$$\begin{aligned} & \|t^3\partial_y(c^\varepsilon - c_1^{cor})\|_{L^2(0,T;L^2(\mathbb{R}_+ \times (0,1)))} \leq \\ & C\varepsilon^{1-\alpha/2}\left(\varepsilon^{3-9\alpha/4}H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2}H(\alpha-1)\right) \end{aligned} \quad (38)$$

$$\begin{aligned} & \|t^2\partial_x(c^\varepsilon - c_1^{cor})\|_{L^2(0,T;L^2(\mathbb{R}_+ \times (0,1)))} \leq \\ & C\varepsilon^{-\alpha/2}\left(\varepsilon^{3-9\alpha/4}H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2}H(\alpha-1)\right) \end{aligned} \quad (39)$$

Theorem 3 We have

$$\begin{aligned} & \|t^5(c^\varepsilon - c_1^{cor}(x, t; \varepsilon))\|_{L^\infty(0, T; L_{loc}^2(\mathbb{R}_+ \times (0, 1)))} \leq \\ & C\left(\varepsilon^{4-13\alpha/4} H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2} H(\alpha-1)\right) \end{aligned} \quad (40)$$

$$\begin{aligned} & \|t^5 \partial_y(c^\varepsilon - c_1^{cor}(x, t; \varepsilon))\|_{L^2(0, T; L_{loc}^2(\mathbb{R}_+ \times (0, 1)))} \leq \\ & C\varepsilon^{1-\alpha/2} \left(\varepsilon^{4-13\alpha/4} H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2} H(\alpha-1)\right) \end{aligned} \quad (41)$$

$$\begin{aligned} & \|t^5 \partial_x(c^\varepsilon - c_1^{cor}(x, t; \varepsilon))\|_{L^2(0, T; L_{loc}^2(\mathbb{R}_+ \times (0, 1)))} \leq \\ & C\varepsilon^{-\alpha/2} \left(\varepsilon^{4-13\alpha/4} H(1-\alpha) + \varepsilon^{3(1-\alpha/2)/2} H(\alpha-1)\right) \end{aligned} \quad (42)$$

If we give up the energy norm, then even better estimates are possible:

Theorem 4 We have

$$\begin{aligned} & \|t^5(c^\varepsilon - c_1^{cor}(x, t; \varepsilon) - c_2^{cor})\|_{L^2(0, T; L_{loc}^1(\mathbb{R}_+ \times (0, 1)))} \leq \\ & C\left(\varepsilon^{4-3\alpha} H(1-\alpha) + \varepsilon^{2-\alpha} H(\alpha-1)\right) \end{aligned} \quad (43)$$

$$\begin{aligned} & \|t^5(c^\varepsilon - c_1^{cor}(x, t; \varepsilon) - c_2^{cor})\|_{L^2(0, T; L_{loc}^2(\mathbb{R}_+ \times (0, 1)))} \leq \\ & C\left(\varepsilon^{4-3\alpha} H(1-\alpha) + \varepsilon^{2-\alpha} H(\alpha-1)\right) \end{aligned} \quad (44)$$

Next we prove the corresponding $L^\infty(L^\infty)$ -estimate. Using the technique of Nash and Moser we have

Theorem 5

$$\begin{aligned} \|t^5(c^\varepsilon - c_1^{cor}(x, t; \varepsilon) - c_2^{cor})\|_{L^\infty((0, T) \times (\mathbb{R}_+ \times (0, 1)))} \leq \\ C(\delta) \left(\varepsilon^{4-7\alpha/2-\delta} H(1-\alpha) \right. \\ \left. + \varepsilon^{3/2-\alpha-\delta} H(\alpha-1) \right), \quad \forall \delta > 0. \end{aligned} \quad (45)$$

Remark From the proof we see that $C(\delta)$ has an exponential growth when $\delta \rightarrow 0$.

PERSPECTIVES:

- Getting the effective equation for more complicated chemistry
- Generalization to realistic porous media
- Advantages of the homogenization approach over direct simulations of stiff anisotropic multidimensional convection/diffusion are obvious

The formal 2-scale expansion leading to Taylor's dispersion

The estimate obtained in the previous section isn't satisfactory. At the other hand, it is known that the Taylor dispersion model gives a very good 1D approximation. With this motivation we briefly explain how to obtain formally the higher precision effective models and notably the variant of Taylor's dispersion formula, by the 2-scale asymptotic expansion.

We start with the problem (3)-(7) and search for c^ε in the form

$$c^\varepsilon = c^0(x, t; \varepsilon) + \varepsilon c^1(x, y, t) + \varepsilon^2 c^2(x, y, t) + \dots \quad (46)$$

After introducing (33) into the equation (3) we get

$$\begin{aligned} \varepsilon^0 \left\{ \partial_t c^0 + Q(1 - y^2) \partial_x c^0 - D \varepsilon^{\alpha-1} \partial_{yy} c^1 \right\} + \\ \varepsilon \left\{ \partial_t c^1 + Q(1 - y^2) \partial_x c^1 - D \varepsilon^{\alpha-1} \partial_{xx} c^0 - \right. \\ \left. D \varepsilon^{\alpha-1} \partial_{yy} c^2 \right\} = \mathcal{O}(\varepsilon^2) \quad (47) \end{aligned}$$

In order to have (34) for every $0 < \varepsilon < \varepsilon_0$, all coefficients in front of the powers of ε should be zero.

The problem corresponding to the order ε^0 is

$$\begin{cases} -D\partial_{yy}c^1 = -\varepsilon^{1-\alpha}Q(1/3 - y^2)\partial_x c^0 - \\ \varepsilon^{1-\alpha}(\partial_t c^0 + 2Q\partial_x c^0/3) \text{ on } (0, 1), \\ \partial_y c^1|_{y=0} = 0, \quad -D\partial_y c^1|_{y=1} = k_0\varepsilon^{1-\alpha}c^0. \end{cases} \quad (48)$$

for every $(x, t) \in (0, +\infty) \times (0, T)$. By Fredholm's alternative, the problem (35) has a solution if and only if

$$\partial_t c^0 + 2Q\partial_x c^0/3 + k_0 c^0 = 0 \quad \text{in } (0, L) \times (0, T). \quad (49)$$

Unfortunately our initial and boundary data are incompatible and the hyperbolic equation (36) has a discontinuous solution. Since the asymptotic expansion for c^ε involves derivatives of c^0 , the equation (36) doesn't suit our needs. In [BoJuPi:03] the difficulty was overcome by supposing compatible initial and boundary data. We proceed by following an idea from [RuMa:86] and suppose that

$$\partial_t c^0 + 2Q\partial_x c^0/3 + k_0 c^0 = \mathcal{O}(\varepsilon) \quad \text{in } (0, +\infty) \times (0, T). \quad (50)$$

The hypothesis (??) will be justified *a posteriori*, after getting an equation for c^0 . Hence (35) reduces to

$$\begin{cases} -D\partial_{yy}c^1 = -\varepsilon^{1-\alpha}Q(1/3 - y^2)\partial_x c^0 + \\ \varepsilon^{1-\alpha}k_0c^0 \text{ on } (0, 1), \\ \partial_y c^1|_{y=0} = 0, \quad -D\partial_y c^1|_{y=1} = k_0\varepsilon^{1-\alpha}c^0, \end{cases} \quad (51)$$

for every $(x, t) \in (0, +\infty) \times (0, T)$, and

$$\begin{aligned} c^1(x, y, t) = \varepsilon^{1-\alpha} & \left(\frac{Q}{D} \left(\frac{y^2}{6} - \frac{y^4}{12} \right) \partial_x c^0 + \right. \\ & \left. \frac{k_0}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right) c^0 + C_0(x, t) \right), \end{aligned} \quad (52)$$

where C_0 is an arbitrary function.

Let us go to the next order. Then we have

$$\begin{cases} -D\partial_{yy}c^2 = -\varepsilon^{1-\alpha}Q(1 - y^2)\partial_x c^1 + D\partial_{xx}c^0 - \\ \varepsilon^{1-\alpha}\partial_t c^1 + D\varepsilon\partial_{xx}c^1 - \varepsilon^{-\alpha} \left(\partial_t c^0 + 2Q\partial_x c^0/3 + k_0c^0 \right) \\ \text{on } (0, 1), \quad \partial_y c^2|_{y=0} = 0 \text{ and} \\ -D\partial_y c^2|_{y=1} = k_0\varepsilon^{1-\alpha}c^1|_{y=1} \end{cases} \quad (53)$$

for every $(x, t) \in (0, +\infty) \times (0, T)$. The problem (40) has a solution if and only if

$$\begin{aligned}
& \partial_t c^0 + 2Q\partial_x c^0/3 + k_0(c^0 + \varepsilon c^1|_{y=1}) - \\
& D\varepsilon^{1+\alpha}\partial_{xx}\left(\int_0^1 c^1 dy\right) + \varepsilon\partial_t\left(\int_0^1 c^1 dy\right) - \varepsilon^\alpha D\partial_{xx}c^0 + \\
& Q\varepsilon\partial_x\left(\int_0^1 (1-y^2)c^1 dy\right) = 0 \text{ in } (0, +\infty) \times (0, T).
\end{aligned} \tag{54}$$

(41) is the equation for c^0 . In order to get the simplest possible equation for c^0 we choose C_0 giving $\int_0^1 c^1 dy = 0$. Now c^1 takes the form

$$c^1(x, y, t) = \varepsilon^{1-\alpha} \left(\frac{Q}{D} \left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right) \partial_x c^0 + \frac{k_0}{D} \left(\frac{1}{6} - \frac{y^2}{2} \right) c^0 \right) \tag{55}$$

and the equation (41) becomes

$$\begin{aligned}
& \partial_t c^0 + Q \left(\frac{2}{3} + \frac{4k_0}{45D} \varepsilon^{2-\alpha} \right) \partial_x c^0 + k_0 \left(1 - \right. \\
& \left. \frac{k_0}{3D} \varepsilon^{2-\alpha} \right) c^0 = \varepsilon^\alpha \tilde{D} \partial_{xx} c^0 \text{ in } (0, +\infty) \times (0, T).
\end{aligned} \tag{56}$$

with

$$\tilde{D} = D + \frac{8}{945} \frac{Q^2}{D} \varepsilon^{2(1-\alpha)} \tag{57}$$

Now the problem (40) becomes

$$\left\{ \begin{array}{l} -D\partial_{yy}c^2 = -\varepsilon^{2-2\alpha}\frac{Q^2}{D}\partial_{xx}c^0 \left\{ \frac{8}{945} + (1-y^2)\left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}\right) \right\} - \varepsilon^{2-2\alpha}\partial_x c^0 \frac{Qk_0}{D} \left\{ -\frac{2}{45} + (1-y^2)\left(\frac{1}{6} - \frac{y^2}{2}\right) \right\} + \frac{2k_0Q}{45D}\varepsilon^{2-2\alpha}\partial_x c^0 - \varepsilon^{2-2\alpha}\frac{k_0^2}{3D}c^0 \\ -\varepsilon^{2-2\alpha}\left(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}\right)(\partial_{xt}c^0\frac{Q}{D} - \varepsilon^\alpha Q\partial_{xxx}c^0) \\ -\varepsilon^{2-2\alpha}\left(\frac{1}{6} - \frac{y^2}{2}\right)(\partial_t c^0\frac{k_0}{D} - \varepsilon^\alpha k_0\partial_{xx}c^0) \text{ on } (0, 1), \\ \partial_y c^2 = 0 \text{ on } y = 0 \text{ and } -D\partial_y c^2 = \\ \frac{Qk_0}{D}\varepsilon^{2-2\alpha}\partial_x c^0\frac{2}{45} - \frac{k_0^2}{3D}\varepsilon^{2-2\alpha}c^0 \text{ on } y = 1. \end{array} \right. \quad (58)$$

If we choose c^2 such that $\int_0^1 c^2 dy = 0$, then

$$\begin{aligned} c^2(x, y, t) = \varepsilon^{2-2\alpha} \left\{ -\frac{Q^2}{D^2}\partial_{xx}c^0 \left(\frac{281}{453600} + \frac{23}{1512}y^2 - \frac{37}{2160}y^4 + \frac{1}{120}y^6 - \frac{1}{672}y^8 \right) + \left(\frac{Q}{D^2}\partial_{xt}c^0 - \varepsilon^\alpha\frac{Q}{D}\partial_{xxx}c^0 \right) \right. \\ \left(\frac{31}{7560} - \frac{7}{360}y^2 + \frac{y^4}{72} - \frac{y^6}{360} \right) + \frac{Qk_0}{D^2}\partial_x c^0 \left(\frac{y^6}{60} - \frac{y^4}{18} \right. \\ \left. + \frac{11y^2}{180} - \frac{11}{810} \right) - \left(\frac{k_0}{2D^2}\partial_t c^0 - \frac{k_0}{2D}\varepsilon^\alpha\partial_{xx}c^0 \right) \left(\frac{y^4}{12} - \frac{y^2}{6} + \frac{7}{180} \right) \\ \left. + \left(\frac{Qk_0}{45D^2}\partial_x c^0 - \frac{k_0^2}{6D^2}c^0 \right) \left(\frac{1}{3} - y^2 \right) \right\} \quad (59) \end{aligned}$$