

# Rigorous derivation of a hyperbolic model for Taylor dispersion

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**PACEN**



# Thanks:

The results which I will present today are obtained in collaboration with C.J. van Duijn, from the *Dept. Math. and Comp. Sci., TU Eindhoven, The Netherlands.*

They present a continuation of the previous work:

[1] A. Mikelić, V. Devigne, C.J. van Duijn : Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers, *SIAM J. Math. Anal.*, Vol. 38, Issue 4 (2006), p. 1262-1287.

[2] C.J. van Duijn, A. Mikelić, I. S. Pop, C. Rosier : Effective Dispersion Equations For Reactive Flows With Dominant Peclet and Damkohler Numbers, In: Guy B. Marin, David West and Gregory S. Yablonsky, editors: *Advances in Chemical Engineering*, Vol 34, Academic Press, 2008, pp. 1 – 45.

[3] C. Choquet, A. Mikelić : Rigorous upscaling of the reactive flow with finite kinetics and under dominant Peclet number, *Continuum Mechanics and Thermodynamics*, Volume 21, 2009, p. 125-140.

# Thanks 2

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*"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. "*



# Intro 1

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

# Intro 2

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 exemple, 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 dependance using just **laboratory experiments**.

# Intro 3

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 the classical Taylor dispersion problem:

We study the diffusion of the solute particles transported by the Poiseuille velocity profile in a semi-infinite 2D channel. They don't interact between them. We suppose zero diffusion flux at the lateral walls. The simplest example, is described by the following model for the solute concentration  $c^*$ :

# Intro 4

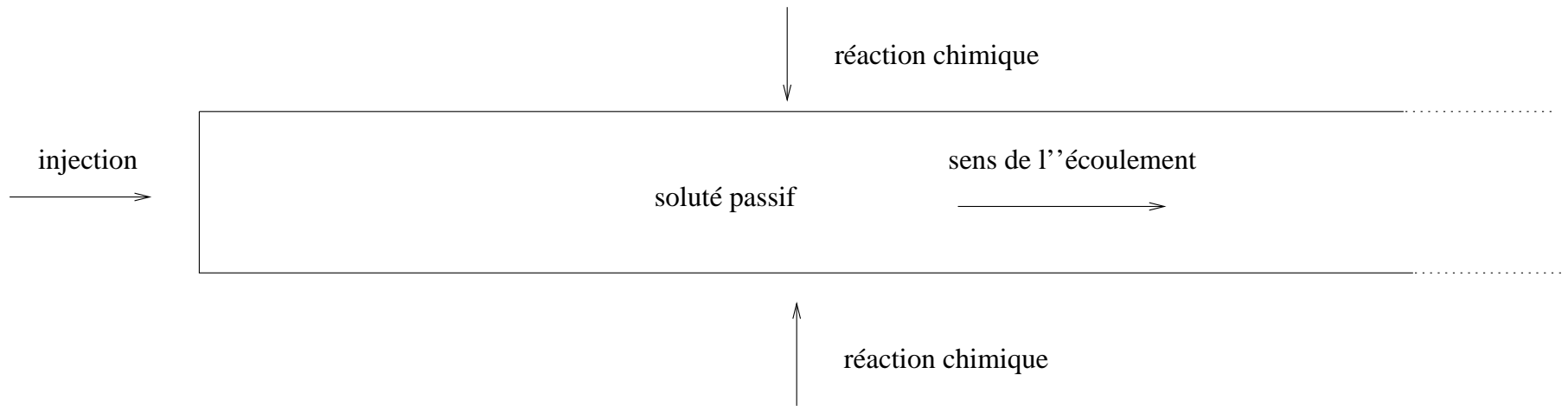
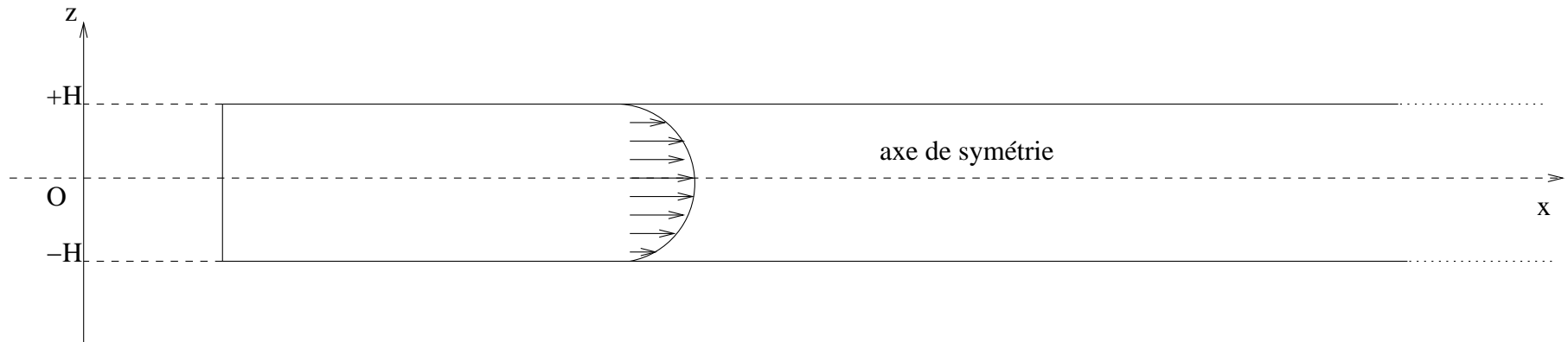


Figure 1: The tube



# Intro 5

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

where  $q(z) = Q^*(1 - (z/H)^2)$  and  $Q^*$  (**velocity**) and  $D_{mol}$  (**molecular diffusion**) are positive constants. At the lateral boundaries  $z = \pm H$  we impose zero flux:

$$-D_{mol} \partial_{y^*} c^* = 0 \text{ on } \Gamma^*, \quad (2)$$

$\Gamma^* = \{(x^*, y^*) : 0 < x^* < +\infty, |y^*| = H\}$ . At the inlet boundary, infiltration with a pulse of water containing a solute of concentration  $c_f^*$ , followed by solute-free water, is described using the Danckwerts boundary condition

$$-D_{mol} \partial_{x^*} c^* + q(y^*) c^* = \begin{cases} q(y^*) c_f^*, & \text{for } 0 < t^* < t_0^* \\ 0, & \text{for } t^* > t_0^*. \end{cases} \quad (3)$$

# Intro 6

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  $Q^*$ , the characteristic diffusivity  $D_R$  and the characteristic time  $T_R$ . The characteristic length  $L_R$  coincides in fact with the " observation distance".

**Problem involves the following time scales:**

$$T_L = \text{characteristic longitudinal time scale} = L_R / Q^*$$

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

and the non-dimensional number

$$\mathbf{Pe} = \frac{L_R Q^*}{D_R} \quad (\text{Peclet number}).$$

# Intro 7

In this presentation we fix the reference time by setting  $T_R = T_C = T_L$  and introduce  $\varepsilon = H/L_R = H/(Q^*T_L) \ll 1$ . To carry out the analysis we need to compare the dimensionless numbers with respect to  $\varepsilon$ . For this purpose we set  $\mathbf{Pe} = \varepsilon^{-\alpha}$ .

Solving the full problem for arbitrary values of coefficients is costly. 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 1953 G.I. Taylor obtained an explicit effective expression for the enhanced diffusion coefficient and it is called in literature *Taylor's dispersion formula*.

# Intro 7A

We have

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

The situation from Taylor's article corresponds to the case when  $0 \leq \alpha < 2$ , i.e. transversal Peclet's number is equal to  $(\frac{1}{\varepsilon})^{\alpha-1}$ . It is interesting to remark that in his paper Taylor has  $\alpha = 1.6$  and  $\alpha = 1.9$ .

Our domain is now the infinite strip  $\Omega^+ = \mathbb{R}_+ \times (0, 1)$ . Then using the antisymmetry of  $c$ , our equations in their non-dimensional form are

# Problem 1

$$\frac{\partial c^\varepsilon}{\partial t} + Q(1 - y^2) \frac{\partial c^\varepsilon}{\partial x} = D\varepsilon^\alpha \frac{\partial^2 c^\varepsilon}{\partial x^2} + D\varepsilon^{\alpha-2} \frac{\partial^2 c^\varepsilon}{\partial y^2} \quad \text{in } \Omega^+ \times (0, T), \quad (4)$$

$$-D\varepsilon^{\alpha-2} \frac{\partial c^\varepsilon}{\partial y} = -D \frac{1}{\varepsilon^2 \mathbf{Pe}} \frac{\partial c^\varepsilon}{\partial y} = 0 \quad \text{on } \Gamma^+ \times (0, T), \quad (5)$$

$$c^\varepsilon(x, y, 0) = 0 \quad \text{for } (x, y) \in \Omega^+, \quad (6)$$

$$\left( -D\varepsilon^\alpha \partial_x c^\varepsilon + Q(1 - y^2) c^\varepsilon \right)_{x=0} = \begin{cases} Q(1 - y^2) c_f, & \text{for } 0 < t < t_0 \\ 0, & \text{for } t > t_0. \end{cases}, \quad (7)$$

$$\frac{\partial c^\varepsilon}{\partial y}(x, 0, t) = 0, \quad \text{for } (x, t) \in (0, +\infty) \times (0, T). \quad (8)$$

## Problem 2

In the absence of chemical reactions, dimensionless version of Taylor's result for the dispersion coefficient reads:

$$\left\{ \begin{array}{l} \partial_t c^{Tay} + \frac{2Q}{3} \partial_x c^{Tay} = (D\varepsilon^\alpha + \frac{8}{945} \frac{Q^2}{D} \varepsilon^{2-\alpha}) \partial_{xx} c^{Tay}, \\ \text{in } \mathbb{R}_+ \times (0, T), \quad c^{Tay}|_{x=0} = c_f, \\ c^{Tay}|_{t=0} = 0, \quad \partial_x c^{Tay} \in L^2(\mathbb{R}_+ \times (0, T)), \end{array} \right. \quad (9)$$

What is known concerning derivation of (9) ?

# Problem 3

- ◇ For the formal derivation using the **method of moments**, see the paper of Aris from Proc. Roy. Soc. London (1956).
- ◇ Another approach is in the paper by Lungu and Moffat, J. Engng Math (1982). They used a large time and small wave number expansion, after a Fourier transform, to decipher the asymptotic behavior.
- ◇ "Near rigorous" derivation using the centre manifold theory is due to Mercer and Roberts, SIAM J. Appl. Math. (1990). The initial value problem is studied and the Fourier transform with respect to  $x$  is applied. The resulting PDE is written in the form  $\dot{u} = Au + F(u)$ , 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.

# Problem 4

◇ Rigorous derivation, with an error estimate is due to Mikelić et al (see [1], [2], [3] and related work).

Our result could be restated in dimensional form:

**Theorem 1** Let us suppose that

$L_R > \max\{D_R/Q^*, Q^*H^2/D_R, H\}$ . Then the upscaled *dimensional* approximation for (1) reads

$$\frac{\partial c^{*,eff}}{\partial t^*} + \frac{2}{3}Q^* \frac{\partial c^{*,eff}}{\partial x^*} = D_{mol} \left(1 + \frac{8}{945} \mathbf{Pe}_T^2\right) \frac{\partial^2 c^{*,eff}}{\partial (x^*)^2}, \quad (10)$$

where  $\mathbf{Pe}_T = \frac{Q^*H}{D_{mol}}$  is the transversal Peclet number.

# Problem 5

Conclusion is that modeling of dispersion for flow through tubes is classically done by using an effective convection-diffusion equation of the type

$$\frac{\partial c}{\partial t} + \langle v \rangle \frac{\partial c}{\partial x} = \tilde{D}_{eff} \frac{\partial^2 c}{\partial x^2}, \quad (11)$$

where  $\langle v \rangle$  is the transversally averaged velocity and  $\tilde{D}_{eff}$  is the effective dispersion coefficient.

$\tilde{D}_{eff}$  depends on the transversal Péclet number

$\mathbf{Pe}_T = \frac{\langle v \rangle H}{D_{mol}}$ , where  $D_{mol}$  is the molecular diffusivity and

$H$  is the tube radius.

Characteristic of all these models is that they give rise to a parabolic equation for the effective volume concentration.

# Problem 6

Parabolicity of the effective dispersion equations leads to some non-physical properties:

- i) In the starting equation the longitudinal diffusion is frequently neglected. Nevertheless, the dispersion equations have effective dispersion in the longitudinal direction. Consequently, they predict the infinite propagation speed of perturbations, which is (of course) not met in experiments.
- ii) For purely convective flows a particle follows a streamline, flow reversal does not alter the streamline and the particle returns to the starting position. In the presence of transverse diffusion particles move randomly in the transverse direction between streamlines. Consequently, after the flow reversal they do not return to their original position.

# Problem 7

The diffusion reduces the reversibility. If directly at reversal a variance decrease is observed, at least over a short time, the phenomenon is called *partial reversibility*. Physical arguing implies that one should observe at least partial reversibility. These reasons motivated Scheidegger to propose as early as in 1958 the 1D telegraph equation

$$\frac{\partial^2 c}{\partial t^2} + \frac{1}{\tau} \frac{\partial c}{\partial t} = \sigma_v^2 \frac{\partial^2 c}{\partial x^2} \quad (12)$$

as model for dispersion in porous media.

For Taylor's dispersion in a tube, Camacho developed upscaled hyperbolic models (see Physical Rev E 1993), using a viewpoint of irreversible thermodynamics and by averaging over the section the Fourier expansion of the solution in the original equation.

## Problem 8

He arrived at the following non-Fickian relaxation telegraph equation:

$$\begin{cases} \frac{\partial^2 c}{\partial t^2} + \frac{1}{\tau_{eff}} \left( \frac{\partial c}{\partial t} + \langle v \rangle \frac{\partial c}{\partial x} \right) + (2 \langle v \rangle + \beta_{eff}) \frac{\partial^2 c}{\partial x \partial t} = \\ \left( \sigma_v^2 - (\langle v \rangle + \beta_{eff}) \langle v \rangle \right) \frac{\partial^2 c}{\partial x^2}. \end{cases} \quad (13)$$

Another approach, consisting of the Liapounov-Schmidt reduction coupled with a perturbation argument is developed by Balakotaiah et al in recent years (see SIAM J. Appl Math 2003, Korean J. Chem. Eng 2004). For the setting of Taylor's result, they obtained the following dispersion equation

$$\frac{\partial c}{\partial t} + \langle v \rangle \frac{\partial c}{\partial x} + \langle v \rangle \frac{H^2}{48 D_{mol}} \frac{\partial^2 c}{\partial x \partial t} = D_{mol} \frac{\partial^2 c}{\partial x^2}. \quad (14)$$

# Problem 9

Since  $D_{mol}$  is very small, the right hand side could be neglected and we get a hyperbolic equation for  $c$ . This result indicates that dispersion could be better described using the hyperbolic dispersion model (14) than by classical Taylor's model.

In this talk we address the question of the rigorous justification of the formal results and observations from the article by Balakotaiah et al.

We have the following result:

Let  $c_0 = c_0(x)$ . As upscaled approximation of the problem (4)-(8) we introduce the following 1D Goursat's problem :

$$\partial_t c + \langle v \rangle \partial_x c - m \mathbf{Pe}_0 \varepsilon^{2-\alpha} \frac{\partial^2 c}{\partial x \partial t} = 0 \text{ in } (0, +\infty) \times (0, T), \quad (15)$$

# Problem 10

$$c|_{x=0} = c_f(t) - \int_0^t e^{\langle v \rangle (t-z)} / (\mathbf{Pe}_0 m \varepsilon^{2-\alpha}) \partial_z c_f(z) dz, \quad (16)$$

$$c|_{t=0} = c_0(x), \quad (17)$$

where  $\langle v \rangle = \int_0^1 v(y) dy = \frac{2}{3}$ ,  $m = \langle v(y) P_4(y) \rangle = -\frac{4}{315}$ ,  
 $c_f = 0$  for  $t > t_0$  and  $P_4(y)$  is the solution for

$$\left\{ \begin{array}{l} -\partial_{yy} P_4(y) = -\frac{v(y) - \langle v \rangle}{\langle v \rangle} \quad \text{on } (0, 1), \\ \partial_y P_4 = 0 \quad \text{on } y = 0 \quad \text{and} \quad -\partial_y P_4 = 0 \quad \text{on } y = 1 \\ \int_0^1 P_4(y) dy = 0. \end{array} \right. \quad (18)$$

Let us announce our main result.

# Problem 11

**Theorem 2** Let  $2 > \alpha > 4/3$ , let  $c_0 \in H^1(\mathbb{R}_+)$  and let  $c_f \in C^\infty[0, T]$ . Let  $c$  be given by (15)-(17) and let  $c^0$  be its Laplace transform. Then we have

$$\frac{\varepsilon^{\alpha-2}}{\mathbf{Pe}_0} (\hat{c}^\varepsilon - c^0) - P_4(y) (\langle c_0 \rangle - \tau c^0) \rightarrow 0 \quad \text{strongly in } L^2(\Omega^+),$$

$$\forall \tau \in \mathbb{C}, \Re \tau > 0, \quad (19)$$

where  $\hat{c}^\varepsilon$  is the Laplace transform of  $c^\varepsilon$ .

Let us suppose in addition  $c_f(0) = c_0(0)$ . Then the above convergence takes place in  $H^2(\mathbb{C}_+; L^2(\Omega^+))$  and for all  $T \in (0, +\infty)$  we have

$$\frac{\varepsilon^{\alpha-2}}{\mathbf{Pe}_0} (c^\varepsilon - c) + P_4(y) \frac{\partial c}{\partial t} \rightarrow 0 \quad \text{strongly in } L^2(\Omega^+ \times (0, T)), \quad \text{as } \varepsilon \rightarrow 0$$

(20)

# Problem 12

**Corollary 1** Let us suppose that

$L_R \gg \max\{D_{mol}/Q^*, Q^* H^2 / D_{mol}, H\}$ . Then the upscaled *dimensional* approximation for (1) reads

$$\frac{\partial c^{*,eff}}{\partial t^*} + \langle V \rangle \frac{\partial c^{*,eff}}{\partial x^*} - mH \mathbf{Pe}_T \frac{\partial^2 c^{*,eff}}{\partial x^* \partial t^*} = 0, \quad \text{in } \mathbb{R}_+ \times (0, T), \quad (21)$$

$$c^{*,eff}|_{t=0} = c_0(x), \quad (22)$$

$$c^{*,eff}|_{x=0} = c_f^* - \int_0^{t^*} e^{\langle V \rangle (t^* - z^*)} / (\mathbf{Pe}_T mH) \partial_{z^*} c_f^*(z^*) dz^*, \quad (23)$$

where  $\mathbf{Pe}_T = \frac{Q^* H}{D_{mol}}$  is the transversal Peclet number,

$\langle V \rangle = \frac{1}{H} \int_0^H V(y) dy$  and  $H \mathbf{Pe}_T$  is the mixing length.

# Proof 1

Finally, with a little more work we have the following strong convergence result **Theorem 3** Convergences in (19) and in (20) are strong.

How to get these results?

**1. STEP** We apply the Laplace transform with respect to  $t$  and get

$$\mathcal{L}^\varepsilon \hat{c}^\varepsilon = c_0 \quad \text{in } (0, +\infty) \times (0, 1) \quad (24)$$

$$-\frac{\varepsilon^\alpha}{\mathbf{Pe}_0} \partial_x \hat{c}^\varepsilon + (1 - y^2) \hat{c}^\varepsilon = (1 - y^2) \hat{c}_f, \quad \text{for } (x, y) \in \{0\} \times (0, 1), \quad (25)$$

$$-\frac{\varepsilon^{\alpha-2}}{\mathbf{Pe}_0} \partial_y \hat{c}^\varepsilon(x, y, \tau) = 0 \quad \text{on } (0, +\infty) \times (\{0\} \cup \{1\}). \quad (26)$$

# Proof 2

with

$$\mathcal{L}^\varepsilon \zeta = \tau \zeta + (1 - y^2) \frac{\partial \zeta}{\partial x} - \frac{\varepsilon^\alpha}{\mathbf{Pe}_0} \left( \frac{\partial^2 \zeta}{\partial x^2} + \varepsilon^{-2} \frac{\partial^2 \zeta}{\partial y^2} \right). \quad (27)$$

We start from the system (24)-(26) and search for  $\hat{c}^\varepsilon$  in the form

$$\hat{c}^\varepsilon = c^0(x, t; \varepsilon) + \varepsilon^{2-\alpha} c^1(x, y, t) + \varepsilon^{2(2-\alpha)} c^2(x, y, t) + \dots \quad (28)$$

After introducing (28) into the equation (24) we get

$$\varepsilon^0 \left\{ \tau c^0 + (1 - y^2) \partial_x c^0 - \frac{1}{\mathbf{Pe}_0} \partial_{yy} c^1 - c_0 \right\} + \varepsilon^{2-\alpha} \left\{ \tau c^1 + (1 - y^2) \partial_x c^1 - \frac{1}{\mathbf{Pe}_0} \partial_{yy} c^2 \right\} = O(\varepsilon^{2(2-\alpha)}) + O(\varepsilon^\alpha). \quad (29)$$

# Proof 3

In order to have (29) for every  $0 < \varepsilon < \varepsilon_0$ , all coefficients in front of the powers of  $\varepsilon$  should be zero.

The problem corresponding to the order  $\varepsilon^0$  is

$$\begin{cases} -\frac{1}{\mathbf{Pe}_0} \partial_{yy} c^1 = -(1/3 - y^2) \partial_x c^0 + c_0 - \int_0^1 c_0(x, y) dy \\ -(\tau c^0 + 2\partial_x c^0 / 3 - \int_0^1 c_0(x, y) dy) \text{ on } (0, 1), \\ \partial_y c^1 = 0 \text{ on } y = 0 \text{ and } -\partial_y c^1 = 0 \text{ on } y = 1. \end{cases} \quad (30)$$

Fredholm's alternative  $\Rightarrow$

$$\tau c^0 + 2\partial_x c^0 / 3 - \int_0^1 c_0(x, y) dy = 0 \quad \text{in } (0, L). \quad (31)$$

For  $\alpha$  close to 2, the equation (31) gives a coarse approximation and it does not suit our needs.

# Proof 4

We throw it to the next order by imposing that

$$\tau c^0 + 2\partial_x c^0 / 3 - \int_0^1 c_0(x, y) dy = O(\varepsilon^{2-\alpha}) \quad \text{in } (0, +\infty). \quad (32)$$

Since

$$\begin{aligned} & -(1/3 - y^2)\partial_x c^0 - (\tau c^0 + 2\partial_x c^0 / 3 - c_0(x)) = \\ & -\frac{3}{2}\left(\frac{1}{3} - y^2\right)(c_0(x) - \tau c^0) + O(\varepsilon^{2-\alpha}) \quad \text{in } (0, +\infty). \end{aligned} \quad (33)$$

(30) reduces to

$$\begin{cases} -\frac{1}{\mathbf{Pe}_0}\partial_{yy}c^1 = -\frac{3}{2}(1/3 - y^2)(c_0(x) - \tau c^0) \quad \text{on } (0, 1), \\ \partial_y c^1 = 0 \quad \text{on } y = 0 \quad \text{and} \quad -\partial_y c^1 = 0 \quad \text{on } y = 1 \end{cases} \quad (34)$$

# Proof 5

$$\frac{1}{\mathbf{Pe}_0} c^1(x, y, t) = \frac{3}{2} \left( \frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} \right) (c_0(x) - \tau c^0) + C_0(x, t), \quad (35)$$

where  $C_0$  is an arbitrary function.

Let us go to the next order. Then we have

$$\begin{cases} -\frac{1}{\mathbf{Pe}_0} \partial_{yy} c^2 = -(1 - y^2) \partial_x c^1 - \tau c^1 - \varepsilon^{\alpha-2} (\tau c^0 + 2\partial_x c^0 / 3 - \\ c_0(x)) \text{ on } (0, 1), \partial_y c^2|_{y=0,1} = 0 \text{ on } y = 0. \end{cases} \quad (36)$$

Finally, after straightforward calculations, Fredholm's alternative for (36) gives

$$\tau c^0 + \frac{2}{3} \partial_x c^0 + \frac{4}{315} \varepsilon^{2-\alpha} \mathbf{Pe}_0 \tau \partial_x c^0 = F \quad \text{in } (0, +\infty) \times (0, T), \quad (37)$$

# Proof 6

$$F = c_0(x) + \frac{4}{315} \varepsilon^{2-\alpha} \mathbf{Pe}_0 \partial_x c_0(x). \quad (38)$$

$c^0 + \frac{\varepsilon^{2-\alpha}}{\mathbf{Pe}_0} C_0$  satisfies the same equation at order  $O(\varepsilon^{2(2-\alpha)})$   
and we choose  $C_0 = 0$  without loosing generality.

After applying the inverse Laplace's transform we get  
Goursat's problem (15)-(17).

**HOW TO JUSTIFY THIS RESULT RIGOROUSLY?**

# Rigorous 1

**2. STEP** Function  $q^\varepsilon = \varepsilon^{\alpha-2}(\hat{c}^\varepsilon - c^0)/\mathbf{Pe}_0$  satisfies the following variational equation

$$\begin{aligned}
 \mathbf{b}(q^\varepsilon, \bar{\varphi}) &= \int_{\Omega^+} \tau q^\varepsilon \varphi + \int_0^1 v(y) q^\varepsilon |_{x=0} \varphi |_{x=0} \int_{\Omega^+} v(y) \partial_x q^\varepsilon \varphi + \\
 \frac{\varepsilon^\alpha}{\mathbf{Pe}_0} \int_{\Omega^+} (\partial_x q^\varepsilon \partial_x \varphi + \varepsilon^{-2} \partial_y q^\varepsilon \partial_y \varphi) &= \varepsilon^{\alpha-2} \int_{\Omega^+} \frac{\langle v \rangle - v(y)}{\mathbf{Pe}_0} \partial_x c^0 \varphi \\
 - \int_{\Omega^+} m \tau \partial_x c^0 \varphi + \int_{\Omega^+} m \partial_x c^0 \varphi - \frac{\varepsilon^{2(\alpha-1)}}{\mathbf{Pe}_0^2} \int_{\Omega^+} \partial_x c^0 \partial_x \varphi + \\
 \int_0^1 v(y) \frac{m(c_0|_{x=0} - \tau \hat{c}_f)}{\langle v \rangle - \mathbf{Pe}_0 m \varepsilon^{2-\alpha} \tau} \varphi |_{x=0}, \quad \forall \varphi \in H^1(\Omega^+), \quad \forall \tau \in \mathbb{C}_+.
 \end{aligned}
 \tag{39}$$

# Rigorous 2

For  $\alpha > 4/3$  we get

$$\|\partial_y q^\varepsilon\|_{L^2(\Omega^+)} \leq C \left\{ \|c_0\|_{H^1(\Omega^+)} + |c_0|_{x=0} - \tau \hat{c}_f + (1 + |\tau|^{1/2} \varepsilon^{1-\alpha/2}) \|\partial_x c^0\|_{L^2(\Omega^+)} \right\}. \quad (40)$$

Estimate (40) implies existence of a subsequence of  $\{q^\varepsilon\}$ , denoted by the same superscript, and  $Q \in L^2(\Omega^+)$ , such that  $\partial_y q^\varepsilon \rightharpoonup Q$  weakly in  $L^2(\Omega^+)$ . Passing to the limit in the variational equation (39), yields the following equation for  $Q$ :

$$\int_{\Omega^+} Q \partial_y \varphi \, dx dy = - \int_{\Omega^+} (v(y) - \langle v \rangle) \partial_x c^{0,tr} \varphi \, dx dy, \quad (41)$$

where  $c^{0,tr}$  is the solution for the problem

# Rigorous 3

$$\begin{cases} \tau c^{0,tr} + \langle v \rangle \partial_x c^{0,tr} = \langle c_0 \rangle & \text{in } \Omega^+; \\ c^{0,tr}|_{x=0} = \hat{c}_f. \end{cases} \quad (42)$$

Next we obtain that

$$\partial_y q^\varepsilon = \varepsilon^{\alpha-2} \partial_y \frac{\hat{c}^\varepsilon - c^0}{\mathbf{Pe}_0} \rightharpoonup \partial_y P_4(y) (\langle c_0 \rangle - \tau c^{0,tr}), \quad (43)$$

weakly in  $L^2(\Omega^+)$ , for every  $\tau \in \mathbb{C}_+$ . We would like to go one step forward and use the hyperbolic effective equation to prove the weak convergence of  $q^\varepsilon$  to  $P_4(y) (\langle c_0 \rangle - \tau c^{0,tr})$ .

# Rigorous 3

**3. STEP** Having in mind the estimates from **STEP 2**, we introduce the function  $w^\varepsilon$  by

$$w^\varepsilon = \frac{\varepsilon^{\alpha-2}}{\mathbf{Pe}_0} (\hat{c}^\varepsilon - c^0) - P_4(y) (\langle c_0 \rangle - \tau c^0) \quad (44)$$

and write the corresponding variational equation. After carefully estimating the terms, we obtain that

$$\begin{cases} \|\partial_y w^\varepsilon\|_{L^2(\Omega^+)} \leq C\varepsilon^{1-\alpha/2}; & \|w^\varepsilon\|_{L^2(\Omega^+)} \leq C; \\ \|\partial_x w^\varepsilon\|_{L^2(\Omega^+)} \leq C\varepsilon^{-\alpha/2}; & \|\sqrt{v}w^\varepsilon|_{x=0}\|_{L^2(0,1)} \leq C. \end{cases} \quad (45)$$

Consequently, there is  $w = w(x, \tau) \in L^2(\mathbb{R}_+)$ , for every  $\tau \in \mathbb{C}_+$  such that

# Rigorous 4

$$w^\varepsilon \rightharpoonup w \text{ in } L^2(\Omega^+) \text{ and } \partial_y w^\varepsilon \rightarrow 0 \text{ in } L^2(\Omega^+), \quad \forall \tau \in \mathbb{C}_+. \quad (46)$$

Next we find out that

$$\int_0^{+\infty} (\tau w \varphi(x) - v w \partial_x \varphi(x)) dx = 0, \quad \forall \varphi \in H^1(\mathbb{R}_+). \quad (47)$$

The equation (47) yields  $w \in H^1(\mathbb{R}_+)$  and  $w(0, \tau) = 0$ .

Therefore  $w = 0$  on  $\mathbb{R}_+$  for all  $\tau \in \mathbb{C}_+$ . This proves (19).

It remains to prove the convergence with respect to the time as well. Difficulty is that bounds in (45) depend on  $\tau$  and their integrability is to be discussed.

We use the properties of the upscaled solution. They lead to

# Rigorous 5

$$\|w^\varepsilon\|_{H^2(\mathbb{C}_+; L^2(\Omega^+))} + \varepsilon^{\alpha/2-1} \left\| \sqrt{\Re\left(\frac{1}{\tau}\right)} \partial_y w^\varepsilon \right\|_{H^2(\mathbb{C}_+; L^2(\Omega^+))} \leq C. \quad (48)$$

Now we repeat the above convergence argument but in  $H^2(\mathbb{C}_+; L^2(\Omega^+))$  and obtain (20).

**4. STEP: STRONG CONVERGENCE** We construct the corresponding boundary layer through the problem

$$v(y) \partial_z \beta = \partial_{yy} \beta \quad \text{in } \Omega^+, \quad (49)$$

$$\beta(0, y) = P_4(y) - \frac{m}{\langle v \rangle} \quad \text{on } (0, 1), \quad (50)$$

$$\partial_y \beta|_{y=0,1} = 0 \quad \text{for } x \in \mathbb{R}_+. \quad (51)$$

# Rigorous 6

Next we consider the function

$$\begin{aligned} w^{\varepsilon, full} = & \frac{\varepsilon^{\alpha-2}}{\mathbf{Pe}_0} (\hat{c}^\varepsilon - c^0) - P_4(y) (\langle c_0 \rangle - \tau c^0) \\ & + \beta \left( \frac{x}{\varepsilon^{2-\alpha} \mathbf{Pe}_0}, y \right) (\langle c_0 \rangle |_{x=0} - \tau c^0 |_{x=0}). \end{aligned} \quad (52)$$

For it we prove that for  $2 > \alpha > 4/3$

$$\|w^\varepsilon\|_{L^2(\Omega^+)} \leq C e^{\min\{3\alpha/2-2, 1-\alpha/2\}} \text{ and } w^\varepsilon \rightarrow 0 \text{ in } L^2(\Omega^+), \forall \tau \in \mathbb{C} \quad (53)$$

and the strong convergence is proved.

# Open questions

- How to get rigorously such results for reactive flows?
- How to handle nonlinearities in reactive flows?