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Laplace transform approach to the rigorous upscaling of the infinite adsorption rate reactive flow under dominant Peclet number through a pore‡

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In this paper we undertake a rigorous derivation of the upscaled model for reactive flow through a narrow and long two-dimensional pore. The transported and diffused solute particles undergo the infinite adsorption rate reactions at the lateral tube boundary. At the inlet boundary we suppose Danckwerts' boundary conditions. The transport and reaction parameters are such that we have dominant Peclet number. Our analysis uses the anisotropic singular perturbation technique, the small characteristic parameter ε being the ratio between the thickness and the longitudinal observation length. Our goal is to obtain error estimates for the approximation of the physical solution by the upscaled one. They are presented in the energy norm. They give the approximation error as a power of ε and guarantee the validity of the upscaled model. We use the Laplace transform in time to get better estimates than in our previous article [20] and to undertake the study of important Danckwerts' boundary conditions.

Keywords: Taylor's dispersion; large Peclet number; singular perturbation; Laplace's transform; adsorption chemical reaction; Danckwerts' boundary conditions.

AMS Subject Classification: 35B25; 92E20; 76F25; 44A10

1. Introduction

We consider the transport of a reactive solute by molecular diffusion and convection in a semi-infinite two-dimensional channel. We suppose that the characteristic numbers are large (Peclet's number, Damkohler's number, ...) and study the *dispersion* effects.

Dispersion expresses the fluctuation of a quantity with respect to its mean behavior. It is induced by motion of a transported solute in a fluid (molecular diffusion,

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convection and their interaction) or by the chemical reactions which that solute undergoes.

At the pore level we have *a)* the molecular diffusion, expressed by Fick's law, *b)* the convective dispersion, which corresponds to the spreading of particles by the velocity field and *c)* the creation (or destruction) of the solute particles induced by chemical reactions.

Next, for the solute particles subject to convection and molecular diffusion, a complicated interaction of diffusion and convection is observed. The overall behavior heavily depends on the ratios of characteristic times.

In the literature usually we find three distinct regimes: a) *diffusion-dominated mixing*, b) *Taylor dispersion-mediated mixing* and c) *chaotic advection.*

Our goal is the study of reactive flows through slit channels in the regime of Taylor dispersion-mediated mixing, using anisotropic singular perturbations. Contrary to the regime *a)*, where we could quote papers [9], [10],[11], [14], [15] and [18] and references therein, and despite a vaste literature on the subject, with over 2000 citations here to date, mathematical results on the subject are rare. The derivation of the model without chemical reactions is in the original paper [24] by Taylor. It was formally justified, using the method of moments in [3]. We also mention the mathematically rigorous paper [6] and the papers with formal asymptotic expansion [17], [22] and [23]. Nevertheless, they address the mechanical dispersion in the absence of chemical reactions. In presence of chemical reactions we mention the following papers:

(i) Flow with chemistry, as described by equation (2), is considered by Paine, Carbonell and Whitaker in [21]. They noted that the equation for the difference between the physical and averaged concentrations is not closed, since it contains a dispersive source term $\dfrac{\partial}{\partial x} < \overline{q}_x \overline{c} >$. Then they multiplied the equation for $\overline{c}$ by $\overline{q}_x$ and got an equation for $< \overline{q}_x \overline{c} >$. Nevertheless, a dispersive transport term $\dfrac{\partial}{\partial x} < \overline{q}_x^2 \overline{c} >$ is present 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. We note that their effective equations contain non-local terms depending of the solution and in fact the effective coefficients are not explicitly given.

(ii) The center manifold approach of Mercer and Roberts (see the article [17] and the subsequent article [22] by Rosencrans) allowed to calculate approximations at any order for the original Taylor's model with no chemistry. Even if the error estimate was not obtained, this approach gives a very plausible argument for the validity of the effective model. This approach was applied to reactive flows in the article [4] by Balakotaiah and Chang. A number of effective models for different Damkohler numbers were obtained. Some generalizations to reactive flows through porous media are in [16] and the preliminary results on their mathematical justification are in [1] .

(iii) Another approach consisting of the Liapounov-Schmidt reduction coupled with a perturbation argument is developed in the articles [5] and [7]. It allows developing multi-mode hyperbolic upscaled models.

(iv) For the case of reactive flows with an irreversible, first order, heterogeneous chemical reaction with equilibrium between the liquid and the concentrations of adsorbed solutes, we refer to [19], where the problem is rigorously solved. It covers also the classical Taylor's dispersion, which corresponds to absence of the chemistry. The case of general chemical reactions was considered from the point of view of formal expansions in [12] and the results were justified through numerical simulations.

In this article we continue our research from the article [20], where a slit flow under dominant Peclet and Damkohler numbers was considered in the case when the adsorption rate constant is infinitely large.

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 a semi-infinite 2D channel. The solute particles do not react among themselves. Instead they undergo an adsorption process at the lateral boundary. We consider the following model for the solute concentration c^*:

a) transport through channel $\Omega^* = \{(x^*, y^*) : 0 < x^* < +\infty, |y^*| < H\}$

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

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

b) reaction at channel wall $\Gamma^* = \{(x^*, y^*) : 0 < x^* < +\infty, |y^*| = H\}$

$$-D^*\partial_{y^*} c^* = K_e \frac{\partial c^*}{\partial t^*} \quad \text{on } \Gamma^*, \tag{2}$$

where K_e is the linear adsorption equilibrium constant.

c) infiltration with a pulse of water containing a solute of concentration c_f^*, followed by solute-free water is stated using the Danckwerts boundary condition from [13]

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

The natural way of analyzing this problem is to introduce appropriate scales. This requires characteristic or reference values for the parameters in variables involved. The obvious transversal length scale is H. For all other quantities we use reference values denoted by the subscript R. Setting

$$c = \frac{c^*}{\hat{c}},\ x = \frac{x^*}{L_R},\ y = \frac{y^*}{H},\ t = \frac{t^*}{T_R},\ Q = \frac{Q^*}{Q_R},\ D = \frac{D^*}{D_R}, \tag{4}$$

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

$$-\frac{D D_R T_R}{H K_e}\frac{\partial c}{\partial y} = \frac{\partial c}{\partial t} \quad \text{on } \Gamma, \tag{6}$$

where

$$\Omega = (0, +\infty) \times (-1, 1) \text{ and } \quad \Gamma = (0, +\infty) \times \{-1, 1\}. \tag{7}$$

The equations involve the time scales:

$$T_L = \text{characteristic longitudinal time scale} = \frac{L_R}{Q_R},$$
$$T_T = \text{characteristic transversal time scale} = \frac{H^2}{D_R},$$
$$T_C = \text{superficial chemical reaction time scale} = \frac{L_R K_e}{H Q_R},$$

and the non-dimensional number $\mathbf{Pe} = \dfrac{L_R Q_R}{D_R}$ (Peclet number). In this paper we fix the reference time by setting $T_R = T_c = T_L$ and $K = K_e/H = T_C/T_L = \mathcal{O}(1)$. We are going to investigate the behavior of the two-dimensional system (5)-(6) with respect to the small parameter $\varepsilon = \dfrac{H}{L_R}$. Specifically, as in [19], we will derive expressions for the effective values of the dispersion coefficient and velocity, and an effective 1-D convection-diffusion equation for small values of ε. To carry out the analysis we need to compare the dimensionless numbers with respect to ε. For this purpose we set $\mathbf{Pe} = \varepsilon^{-\alpha}$. Introducing the dimensionless numbers in equations (5)-(6) yields the problem:

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

$$-D\varepsilon^{\alpha-2}\frac{\partial c^\varepsilon}{\partial y} = -D\frac{1}{\varepsilon^2 \mathbf{Pe}}\frac{\partial c^\varepsilon}{\partial y} = K\frac{\partial c^\varepsilon}{\partial t} \quad \text{on } \Gamma^+ \times (0,T), \tag{9}$$

$$c^\varepsilon(x,y,0) = 0 \quad \text{for } (x,y) \in \Omega^+, \tag{10}$$

$$-D\varepsilon^\alpha \partial_x c^\varepsilon + Q(1-y^2)c^\varepsilon = \begin{cases} Q(1-y^2)c_f, & \text{for } 0<t<t_0 \\ 0, & \text{for } t > t_0. \end{cases} \quad \text{at } \{x=0\}, \tag{11}$$

$$\frac{\partial c^\varepsilon}{\partial y}(x,0,t) = 0, \quad \text{for } (x,t) \in (0,+\infty) \times (0,T). \tag{12}$$

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

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

and T is an arbitrary chosen positive number.

We study the behavior of this problem as $\varepsilon \searrow 0$, while keeping the coefficients Q, D and K all $\mathcal{O}(1)$.

Continuing the work from [20], in this paper we prove that the correct upscaling of the problem (8)-(12) gives the following 1D parabolic problem :

$$(EFF) \qquad \begin{cases} \partial_t c + \dfrac{2Q}{3(1+K)}\partial_x c = \tilde{D}\varepsilon^\alpha \dfrac{\partial_{xx} c}{1+K} \text{ in } (0,+\infty)\times(0,T), \\[2ex] -D\varepsilon^\alpha \partial_x c|_{x=0} + \dfrac{2Q}{3}(c|_{x=0} - c_f \chi_{t<t_0}) = 0, \qquad c|_{t=0} = 0, \\[2ex] \partial_x c \in L^2((0,+\infty)\times(0,T)), \end{cases}$$

where

$$\tilde{D} = D + \frac{8}{945}\frac{Q^2}{D}\varepsilon^{2-2\alpha} + \frac{4Q^2}{135D}\frac{K(7K+2)}{(1+K)^2}\varepsilon^{2-2\alpha}. \tag{13}$$

We note that for $K = 0$ (absence of chemistry) this is exactly the effective model of Taylor [24]. Taylor's data correspond to $\alpha = 1.7$ and $\alpha = 1.9$. For more discussions and numerical experiments we refer to [12].

It should be noted that the real interest is to derive *dispersion equations* for reactive flows through porous media and our results are just the first step in that direction. Our technique is strongly motivated by the paper by Rubinstein and Mauri [23], where effective dispersion and convection in porous media is studied using the homogenization technique. Averaging the concentration in a tube with dissolution/precipitation occurring on the wall and with **Pe**$= \mathcal{O}(1)$, is considered in [11].

In this paper we choose a different strategy than in [20]. We explain the differences in the plan of the paper:

Plan of the paper is the following : Section §2 recalls some basic facts about applications of Laplace's transform to PDEs.

In Section §3 we study the upscaled problem. We are only interested in the case $2 > \alpha \geq 1$, since the case $\alpha \in (0, 1)$ does not pose difficulties. Contrary to the particular Dirichlet boundary conditions, which were chosen in [20] and which allow an explicit solution having the form of moving Gaussian, here we consider the general Danckwerts boundary condition. After [13], it is very important in application and more realistic than Dirichlet's boundary condition. In difference to [20], we are not able to give an explicit solution and investigate its properties when diffusion coefficient becomes small. Consequently, we use the vector-valued Laplace's transform in time. It permits to calculate the Laplace transform of the solution and to get precisely its limit behavior when ε tends to zero. The estimates depends on the compatibility between the boundary and initial data and on the direction of the flow.

Then in Section §4 we give a justification of a lower order approximation, using the energy argument. In fact such approximation does not use Taylor's dispersion formula and, for $\alpha \geq 2/3$ gives an error of the same order as the solution to the linear transport equation.

In Section §5, we use a formal derivation of the upscaled problem (EFF), obtained in [20] and [12], to set up the correction. We prove that the effective concentration satisfying the corresponding 1D parabolic problem, with Taylor's diffusion coefficient and the reactive correction, is an approximation in $C(L^2)$ for the physical concentration. We give the corresponding error estimate. We note that we were able to obtain a better approximation than in [20], without using the boundary layer correction for the Danckwerts boundary condition. Furthermore, using the elementary parabolic theory one concludes that the problem (8)-(12) has a unique bounded variational solution c^ε, with square integrable gradient in x and y. Function c^ε belongs to C^∞ for $x > 0$ and it stabilizes to 0 exponentially fast when $x \to \infty$.

Let us announce our main result.

Theorem 1.1 : *Let $\alpha \geq 1$ and let $c_f \in C_0^\infty(0, T)$. Let c be given by (EFF). Then we have*

$$\|c^\varepsilon - c\|_{\mathcal{C}([0,T];L^2(\Omega^+))} \leq C\varepsilon^{2-\alpha}, \tag{14}$$

$$\|\partial_y c^\varepsilon\|_{\mathcal{C}([0,T];L^2(\Omega^+))} \leq C\varepsilon^{3-3\alpha/2}, \tag{15}$$

$$\|\partial_x \big(c^\varepsilon - c\big)\|_{\mathcal{C}([0,T];L^2(\Omega^+))} \leq C\varepsilon^{2-3\alpha/2}. \tag{16}$$

For ill-prepared data see Corollary 5.4. Note that in estimate (15) c has disappeared since it is only x and t dependent. This estimate is superior to estimate (16) because of the large $\mathcal{O}(\varepsilon^{\alpha-2})$ transversal diffusivity. Our result could be restated in dimensional form:

Theorem 1.2: *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*

$$(1+K)\frac{\partial c^{*,eff}}{\partial t^*}+\frac{2}{3}Q^*\frac{\partial c^{*,eff}}{\partial x^*} = D^*\Big(1+(\frac{8}{945}+\frac{4}{135}\frac{K(7K+2)}{(1+K)^2})\mathbf{Pe}_T^2\Big)\frac{\partial^2 c^{*,eff}}{\partial (x^*)^2}, \quad (17)$$

where $\mathbf{Pe}_T = \dfrac{Q^* H}{D^*}$ *is the transversal Peclet number and* $K = K_e/H$ *is the transversal Damkohler number.*

We note that the powers of ε obtained in Theorem 1.1, are superior to the corresponding results in [20]. Furthermore, we obtain better functional spaces in time.

2. Vector valued Laplace transform and applications to PDEs

We start this section by recalling the basic facts about applications of Laplace's transform to linear parabolic equations. 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.

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

$$\hat{f}(\tau) = \int_0^{+\infty} f(t)e^{-\tau t}\, dt, \quad \tau = \xi + i\,\eta \in \mathbb{C}. \quad (18)$$

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

$$\hat{f}(\tau) = \mathcal{F}\big(f(t)e^{-\xi t}\big)(-\eta), \quad \xi > a, \quad (19)$$

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

$$\mathcal{F}\big(g(t)\big)(\omega) = \int_{\mathbb{R}} g(t)e^{i\omega t}\, dt, \quad \omega \in \mathbb{R}.$$

It is well-known (see *e.g.* [25] or [8]) that $\hat{f}$ defined by (18) 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 $\mathcal{D}'_+(a) = \{f \in \mathcal{D}'(\mathbb{R});\ \mathrm{supp}\, f \subset [a, +\infty)\}$. If $\mathcal{S}'(\mathbb{R})$ denotes the space of distributions of slow growth, then we introduce $\mathcal{S}'_+(\mathbb{R})$ by

$$\mathcal{S}'_+(\mathbb{R}) = \mathcal{D}'_+(0) \cap \mathcal{S}'(\mathbb{R}) \quad (20)$$

and we use the formula (19) 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 [25] by Vladimirov.

Laplace's transform is applier 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

$$\begin{aligned} H(a) = \{ \ & g \in \mathcal{H}ol\big(\{\tau \in \mathbb{C};\ \mathrm{Re}(\tau) > a\}\big) \text{ satisfying the growth condition :} \\ & \text{for any } \sigma_o > a \text{ there are real numbers } C(\sigma_o) > 0 \text{ and } m = m(\sigma_o) \geq 0 \\ & \text{such that } |g(\tau)| \leq C(\sigma_o)\,(1 + |\tau|^m),\ \mathrm{Re}(\tau) > \sigma_o \}. \end{aligned} \tag{21}$$

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

Theorem 2.1 : *([25] 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.*

$$f(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \hat{f}(z) e^{zt}\ dz. \tag{22}$$

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 [2] and we give only results directly linked to our needs. For a reflexive Banach space X we set

$$\mathcal{C}_w^\infty(\mathbb{R}_+;X) = \{r \in \mathcal{C}^\infty((0,+\infty);X);\ \|r\|_w = \sup_{n\in\mathbb{N}} \sup_{\lambda>0} \frac{\lambda^{n+1}}{n!} \big\| \frac{d^n}{d\lambda^n} r(\lambda) \big\|_X < +\infty\}. \tag{23}$$

Then we have the following result.

Theorem 2.2 : *([2], Chapter 2) Let X be a reflexive Banach space. Then the (real) Laplace's transform $f \mapsto \hat{f}$ is an isometric isomorphism between $L^\infty(\mathbb{R}_+;X)$ and $\mathcal{C}_w^\infty(\mathbb{R}_+;X)$.*

In many instances the growth condition in (23) is too difficult to check. It is easier to use the complex Laplace's transform. We have the sufficient condition by Prüss:

Theorem 2.3 : *([2], Chapter 2) Let $q : \{\mathrm{Re}(\tau) > 0\} \to X$ be analytic. If there exists a real number $M > 0$ such that $\|\lambda q(\lambda)\|_X \leq M$ and $\|\lambda^2 q'(\lambda)\|_X \leq M$ for $\mathrm{Re}(\lambda) > 0$, then there exists a bounded function $f \in \mathcal{C}(0,+\infty;X)$ such that*

$$q(\lambda) = \int_0^{+\infty} f(t) e^{-\lambda t}\ dt.$$

In particular $q \in \mathcal{C}_w^\infty(\mathbb{R}_+;X)$.

Even Theorem 2.3 represents a complicated criterium and, following ideas from [8], we will use a direct approach based on the link to Fourier's transform. We apply this approach in the study of the upscaled equations and then in the error estimates. We derive estimates for the solutions of the Laplace transformed problem. We use that if image is in L^1, the original is in $\mathcal{C}$.

3. Study of the upscaled diffusion-convection equation on the half-line

In Sections §4 and §5, we will prove that the original problem can be approximated by some upscaled 1-D diffusion-convection equation. The present section is thus devoted to the study of this type of equation in the half-line. The results of

Subsection §3.1 (respectively Subsection §3.2) are used in Section §4 (respectively Section §5).

3.1. *Danckwerts boundary condition*

For $\bar{Q}, \bar{D}$ and $\gamma > 0$, we consider the problem

$$\begin{cases} \partial_t u + \bar{Q}\partial_x u = \gamma \bar{D}\partial_{xx} u \ \text{ in } \ (0,+\infty)\times(0,T), \\ \partial_x u \in L^2((0,+\infty)\times(0,T)), \\ u(x,0) = 0 \ \text{ in } \ (0,+\infty), \quad -\gamma\bar{D}\partial_x u + \bar{Q}u = \bar{Q}g \ \text{ at } \ x=0. \end{cases} \tag{24}$$

Let $\Omega_l = \mathbb{R}_+ \times \{\mathrm{Re}(\tau) > 0\}$. After applying the Laplace transform with respect to the time variable we get the following equation for the Laplace transform $\hat{u}(x,\tau)$ of u:

$$\begin{cases} \tau\hat{u} + \bar{Q}\partial_x \hat{u} = \gamma\bar{D}\partial_{xx}\hat{u} \ \text{ in } \ \Omega_l, \\ \partial_x \hat{u} \in L^2(\mathbb{R}_+), \quad \mathrm{Re}(\tau) > 0, \\ -\gamma\bar{D}\partial_x\hat{u} + \bar{Q}\hat{u} = \bar{Q}\hat{g} \ \text{ at } \ x = 0, \end{cases} \tag{25}$$

where $\tau = \xi + i\,\eta \in \mathbb{C}$, $\xi > 0$. Problem (25) allows the following explicit solution:

$$\hat{u}(x,\tau) = \frac{2\bar{Q}}{\bar{Q} + \sqrt{\bar{Q}^2 + 4\gamma\tau\bar{D}}} e^{\frac{-2\tau x}{\bar{Q} + \sqrt{\bar{Q}^2 + 4\gamma\tau\bar{D}}}} \hat{g}(\tau). \tag{26}$$

This explicit formula allows us to find the exact behavior of u with respect to γ. For the sake of simplicity, we write

$$\hat{u}(x,\tau) = \frac{2\bar{Q}}{l(\tau)} e^{-\frac{2\tau x}{l(\tau)}} \hat{g}(\tau)$$

where

$$\begin{cases} l(\tau) = \bar{Q} + \sqrt{\bar{Q}^2 + 4\gamma\tau\bar{D}}, \quad \mathrm{Re}(\tau) = \xi > 0, \\ R(\tau) = \big(\bar{Q}^4 + (4\gamma\bar{D})^2|\tau|^2 + 8\gamma\bar{D}\xi\bar{Q}^2\big)^{1/4}, \\ \phi \in \big[-\frac{\pi}{2}, \frac{\pi}{2}\big], \ \cos\phi = \frac{\bar{Q}^2 + 4\gamma\bar{D}\xi}{R^2(\tau)}, \ \sin\phi = \frac{4\gamma\bar{D}\eta}{R^2(\tau)}. \end{cases} \tag{27}$$

Then $\cos(\phi/2) > 0$ and

$$\begin{cases} l(\tau) = \bar{Q} + R(\tau)\cos(\phi/2) + iR(\tau)\sin(\phi/2), \\ |l(\tau)|^2 = \bar{Q}^2 + R^2(\tau) + \sqrt{2}\bar{Q}\sqrt{\bar{Q}^2 + R^2(\tau) + 4\gamma\bar{D}\xi}. \end{cases} \tag{28}$$

Consequently,

$$R^2(\tau) + \bar{Q}^2 \le |l(\tau)|^2 \le 3(R^2(\tau) + \bar{Q}^2). \tag{29}$$

Furthermore, we note that for $\xi > 0$

$$\mathrm{Re}\Big(\frac{\tau}{l(\tau)}\Big) = \mathrm{Re}\Big(\frac{\tau\overline{l(\tau)}}{|l(\tau)|^2}\Big)$$

$$= \frac{\xi\bar{Q} + (\xi/\sqrt{2})\sqrt{R^2(\tau)+\bar{Q}^2+4\gamma\bar{D}\xi} + \sqrt{2}\gamma\bar{D}\eta^2/\sqrt{R^2(\tau)+\bar{Q}^2+4\gamma\bar{D}\xi}}{|l(\tau)|^2}$$

$$\geq \frac{C_1\xi}{(R(\tau)^2+\bar{Q}^2)^{1/2}} + \frac{C_2\eta^2}{(R(\tau)^2+\bar{Q}^2)^{3/2}} \geq \frac{C_1\xi}{(R(\tau)^2+\bar{Q}^2)^{1/2}} > 0. \tag{30}$$

Now we compute some explicit estimates for $\hat{u}$. First, by the maximum principle and for $0 \leq g(t) \leq C_g$, we have

$$0 \leq u(x,t) \leq C_g. \tag{31}$$

If, in addition, $\partial_t g \geq 0$, then

$$0 \leq u(x,t) \leq g(t). \tag{32}$$

Next we estimate the difference between $\hat{g}\exp\{-\dfrac{\tau x}{\bar{Q}}\}$ and $\hat{u}$. We have the following approximation result.

Lemma 3.1: *Function $\hat{u}$ satisfies the estimate*

$$\big\|\hat{g}\exp\{-\frac{\tau x}{\bar{Q}}\} - \hat{u}\big\|_{L^p((0,+\infty))} \leq \gamma\frac{C|\hat{g}(\tau)|}{\xi^{1/p}}\frac{|\tau|}{\bar{Q}+\gamma\bar{D}|\tau|}, \quad \forall 1 \leq p < +\infty. \tag{33}$$

Proof: It is enough to make the calculations with $\hat{g} = 1$. Let

$$q(x,\tau) = \hat{u}(x,\tau) - e^{-\tau x/\bar{Q}} = \frac{2\bar{Q}}{l(\tau)}e^{-2\tau x/l(\tau)} - e^{-\tau x/\bar{Q}}.$$

Then we have with (25)

$$\begin{cases} \tau q(x,\tau) + \bar{Q}\partial_x q(x,\tau) = \gamma\bar{D}\dfrac{8\tau^2\bar{Q}}{l(\tau)^3}e^{-2\tau x/l(\tau)}, \quad x \in \mathbb{R}_+, \\ q(0,\tau) = -\dfrac{4\tau\bar{D}\gamma}{l(\tau)^2}. \end{cases} \tag{34}$$

We look for the solution of (34) in the form

$$q(x,\tau) = q_H(x,\tau) + q_P(x,\tau), \tag{35}$$

with

$$q_H(x,\tau) = -\frac{4\tau\bar{D}\gamma}{l(\tau)\big(l(\tau)-2\bar{Q}\big)}e^{-\tau x/\bar{Q}}, \tag{36}$$

$$q_P(x,\tau) = \frac{8\tau\bar{D}\bar{Q}\gamma}{l(\tau)^2\big(l(\tau)-2\bar{Q}\big)}e^{-2\tau x/l(\tau)}. \tag{37}$$

Then we compute the L^p-norms, $1 \le p < +\infty$,

$$\|q_H(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} = \gamma \frac{4\bar{D}|\tau|}{|l(\tau)||l(\tau)-2\bar{Q}|}\Big(\frac{\bar{Q}}{p\xi}\Big)^{1/p}, \tag{38}$$

$$\|q_P(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} \le C\gamma \frac{|\tau|}{\big|l(\tau)^2\big(l(\tau)-2\bar{Q}\big)\big|}\,\frac{1}{\big(\mathrm{Re}(\tau/l(\tau))\big)^{1/p}}. \tag{39}$$

Since $|l(\tau)| \ge \sqrt{2/3}(R(\tau)+\bar{Q})$, $|l(\tau)-2\bar{Q}| \ge (1-\sqrt{2}/2)\sqrt{2/3}(R(\tau)+\bar{Q})$, $R(\tau)+\bar{Q} \ge C\bar{Q}+\sqrt{\gamma\bar{D}|\tau|}$ and $\mathrm{Re}(\tau/l(\tau)) \ge C\xi/(\bar{Q}+\sqrt{\gamma\bar{D}|\tau|})$, we infer from (35)-(39):

$$\|q(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} \le \frac{C\gamma}{\xi^{1/p}}\Big(\frac{|\tau|}{\bar{Q}^2+\gamma\bar{D}|\tau|} + \frac{|\tau|}{(\bar{Q}+\sqrt{\gamma\bar{D}|\tau|})^{3-1/p}}\Big). \tag{40}$$

The lemma is proved. □

The following result follows as the consequence of Lemma 3.1.

Corollary 3.2: *Let $g \in \mathcal{C}_0^\infty(\mathbb{R}_+)$, then*

$$\big\|u - g(t-\frac{x}{\bar{Q}})\big\|_{\mathcal{C}(\mathbb{R}_+;L^p(\mathbb{R}_+))} \le C\gamma, \quad 1 < p < +\infty.$$

If $g \in W^{1,\infty}(\mathbb{R}_+)$ is with compact support in $[0,+\infty)$, but $g(0) \neq 0$, then

$$\big\|u - g(t-\frac{x}{\bar{Q}})\big\|_{L^r(\mathbb{R}_+;L^p(\mathbb{R}_+))} \le C\gamma^{1-\delta}, \quad 1 < p, r < +\infty,\ 0<\delta<1,\ r(1-\delta)<1.$$

Remark 1: Presence of the contact discontinuity due to $g(0) \neq 0$ diminishes precision. Furthermore, the case of $g = 1$ on $(0,T)$ is covered by Corollary 3.2, since it could be extended to a Lipschitz function on $\mathbb{R}_+$, with compact support in $[0,+\infty)$. Hence, it is easy to compare the result of Corollary 3.2 with the corresponding results from [19] and [20] and see that we have now a more precise estimate.

We now aim to give explicit estimates with respect to τ for $\hat{u}$ in $H^p((0,+\infty))$. Since $|l(\tau)| \ge \sqrt{2/3}(R(\tau)+\bar{Q})$, $\mathrm{Re}(\tau/l(\tau)) \ge C\xi/(\bar{Q}+\sqrt{\gamma\bar{D}|\tau|})$ and $R(\tau)+\bar{Q} \ge C\bar{Q}+\sqrt{\gamma\bar{D}|\tau|}$, we begin by noting that $\hat{u}(x,\tau) = (2\bar{Q}/l(\tau))\exp(-2\tau x/l(\tau))\hat{g}(\tau)$ satisfies

$$\|\hat{u}(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} \le \frac{C|\hat{g}(\tau)|}{\xi^{1/p}}\frac{1}{\bar{Q}+\sqrt{\gamma\bar{D}|\tau|}}(\bar{Q}+\sqrt{\gamma\bar{D}|\tau|})^{1/p}. \tag{41}$$

We also compute

$$\partial_x\hat{u}(x,\tau) = -\frac{4\bar{Q}\tau}{l(\tau)^2}e^{-2\tau x/l(\tau)}\hat{g}(\tau),$$

$$\partial_x^k\hat{u}(x,\tau) = 2\bar{Q}\Big(\frac{-2\tau}{l(\tau)}\Big)^k\hat{u}(x,\tau), \quad k \in \mathbb{N}.$$

The following are then straightforward.

Lemma 3.3: *Function $\hat{u}$ satisfies the estimates*

$$\|\hat{u}(\cdot,\tau)\|_{L^2((0,+\infty))} \le \frac{C|\hat{g}(\tau)|}{\sqrt{\xi}(1+\gamma^{1/4}|\tau|^{1/4})}, \tag{42}$$

$$|\partial_x \hat{u}(\cdot,\tau)\,|_{x=0}\,| \le \frac{C|\tau\hat{g}(\tau)|}{1+\gamma|\tau|}, \tag{43}$$

$$\|\partial_x^k \hat{u}(\cdot,\tau)\|_{L^2((0,+\infty))} \le \frac{C|\hat{g}(\tau)|}{\sqrt{\xi}(1+\gamma^{1/4}|\tau|^{1/4})}\Big(\frac{|\tau|^2}{1+\gamma|\tau|}\Big)^{k/2} \quad k\ge 1, \tag{44}$$

with $\tau = \xi + i\,\eta$, $\xi > 0$.

3.2. *Perturbed Danckwerts boundary condition*

For $\bar{Q}, \bar{D}, \gamma > 0$ and $\delta \in \mathbb{R}$ such that $\bar{D} - |\delta| \ge C_0 > 0$, we consider the problem

$$\begin{cases} \partial_t u + \bar{Q}\partial_x u = \gamma\bar{D}\partial_{xx}u \ \text{ in } \ (0,+\infty), \\ \partial_x u \in L^2((0,+\infty)), \\ u(x,0) = 0 \ \text{ in } \ (0,+\infty), \quad -\gamma(\bar{D}+\delta)\partial_x u + \bar{Q}u = \bar{Q}g \ \text{ at } \ x=0. \end{cases} \tag{45}$$

We have the corresponding equation for the Laplace transform $\hat{u}(x,\tau)$ of u:

$$\begin{cases} \tau\hat{u} + \bar{Q}\partial_x\hat{u} = \gamma\bar{D}\partial_{xx}\hat{u} \ \text{ in } \ \Omega_l, \\ \partial_x\hat{u} \in L^2(\mathbb{R}_+), \quad \mathrm{Re}(\tau) > 0, \\ -\gamma(\bar{D}+\delta)\partial_x\hat{u} + \bar{Q}\hat{u} = \bar{Q}\hat{g} \ \text{ at } \ x=0, \end{cases} \tag{46}$$

where $\tau = \xi + i\,\eta \in \mathbb{C}$. Problem (46) allows the following explicit solution:

$$\begin{aligned} \hat{u}(x,\tau) &= \frac{2\bar{D}\bar{Q}}{(\sqrt{\bar{Q}^2+4\gamma\tau\bar{D}}+\bar{Q})(\bar{D}+\delta) - 2\bar{Q}\delta} e^{\dfrac{\bar{Q}-\sqrt{\bar{Q}^2+4\gamma\tau\bar{D}}}{2\gamma\bar{D}}x}\hat{g}(\tau) \\ &= \frac{2\bar{D}\bar{Q}}{l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta} e^{\dfrac{-2\tau x}{l(\tau)}}\hat{g}(\tau). \end{aligned} \tag{47}$$

The explicit formula allows us to find the exact behavior of u with respect to γ. We emphasize that we can prove similar results as in the previous subsection in spite of the δ perturbation. We follow the lines of Subsection 3.1. We bear in mind the auxiliary computations (27)-(30). We also note that

$$\begin{aligned} &\big|l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta\big|^2 \\ &= \bar{Q}^2(\bar{D}-\delta)^2 + R(\tau)^2(\bar{D}+\delta)^2 + \sqrt{2}\bar{Q}(\bar{D}^2-\delta^2)\sqrt{R(\tau)^2+\bar{Q}^2+4\gamma\bar{D}\xi} \\ &\ge (\bar{D}-|\delta|)^2(\bar{Q}^2+R(\tau)^2). \end{aligned} \tag{48}$$

Next we estimate the difference between $\hat{g}\exp\{-\frac{\tau x}{\bar{Q}}\}$ and $\hat{u}$.

Lemma 3.4: *Let $\delta \in \mathbb{R}$ be such that $\bar{D} - |\delta| \ge C_0 > 0$. Then $\hat{u}$ satisfies the* *estimate*

$$\|\hat{g}\exp\{-\frac{\tau x}{\bar{Q}}\} - \hat{u}\|_{L^p((0,+\infty)))} \leq \gamma \frac{C|\hat{g}(\tau)|}{\xi^{1/p}} \frac{|\tau|}{\bar{Q}+\gamma\bar{D}|\tau|}, \quad \forall 1 \leq p < +\infty. \tag{49}$$

Proof: It is enough to make the calculations with $\hat{g} = 1$. Let

$$q(x,\tau) = \hat{u}(x,\tau) - e^{-\tau x/\bar{Q}} = \frac{2\bar{D}\bar{Q}}{l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta} e^{-2\tau x/l(\tau)} - e^{-\tau x/\bar{Q}}.$$

In view of (46), function q is solution of

$$\begin{cases} \tau q(x,\tau) + \bar{Q}\partial_x q(x,\tau) = \gamma\bar{D}\dfrac{8\tau^2\bar{Q}\bar{D}}{l(\tau)^2(l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta)} e^{-2\tau x/l(\tau)}, \quad x \in \mathbb{R}_+, \\ q(0,\tau) = -\dfrac{4\tau\bar{D}(\bar{D}+\delta)\gamma}{l(\tau)(l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta)}. \end{cases} \tag{50}$$

We look for the solution of (50) in the form

$$q(x,\tau) = q_H(x,\tau) + q_P(x,\tau), \tag{51}$$

with

$$q_H(x,\tau) = -\frac{4\tau\bar{D}\gamma}{l(\tau)\big(l(\tau) - 2\bar{Q}\big)} e^{-\tau x/\bar{Q}}, \tag{52}$$

$$q_P(x,\tau) = \frac{8\tau\bar{D}^2\bar{Q}\gamma}{l(\tau)\big(l(\tau) - 2\bar{Q}\big)\big(l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta\big)} e^{-2\tau x/l(\tau)}. \tag{53}$$

Then we compute the L^p-norms, $1 \leq p < +\infty$,

$$\|q_H(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} = \frac{4\bar{D}\gamma|\tau|}{|l(\tau)||l(\tau) - 2\bar{Q}|} \Big(\frac{\bar{Q}}{p\xi}\Big)^{1/p}, \tag{54}$$

$$\|q_P(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} \leq \frac{C\gamma|\tau|}{\big|l(\tau)\big(l(\tau) - 2\bar{Q}\big)\big(l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta\big)\big|} \frac{1}{\big(\mathrm{Re}(\tau/l(\tau))\big)^{1/p}}. \tag{55}$$

Using $|l(\tau)| \geq \sqrt{2/3}(R(\tau)+\bar{Q})$, $|l(\tau) - 2\bar{Q}| \geq (1-\sqrt{2}/2)\sqrt{2/3}(R(\tau)+\bar{Q})$, $R(\tau) + \bar{Q} \geq C\bar{Q} + \sqrt{\gamma\bar{D}|\tau|}$, $\mathrm{Re}(\tau/l(\tau)) \geq C\xi/(\bar{Q} + \sqrt{\gamma\bar{D}|\tau|})$ and (48), we infer from (51)-(55):

$$\|q(\cdot,\tau)\|_{L^p(\mathbb{R}_+)} \leq \frac{C\gamma}{\xi^{1/p}} \Big(\frac{|\tau|}{\bar{Q}+\gamma\bar{D}|\tau|} + \frac{|\tau|}{(\bar{D}-|\delta|)(\bar{Q}+\sqrt{\gamma\bar{D}|\tau|})^{3-1/p}}\Big). \tag{56}$$

Estimate (49) follows. □

Corollary 3.5: *Let $\delta \in \mathbb{R}$ be such that $\bar{D} - |\delta| \geq C_0 > 0$. Let $g \in \mathcal{C}_0^\infty(\mathbb{R}_+)$. Then we have*

$$\big\|u - g(t - \frac{x}{\bar{Q}})\big\|_{\mathcal{C}(\mathbb{R}_+;L^p(\mathbb{R}_+))} \leq C\gamma, \quad 1 < p < +\infty.$$

If $g \in W^{1,\infty}(\mathbb{R}_+)$ is with compact support in $[0,+\infty)$, but $g(0) \neq 0$, then

$$\big\| u - g(t - \frac{x}{\bar{Q}}) \big\|_{L^r(\mathbb{R}_+;L^p(\mathbb{R}_+))} \leq C\gamma^{1-\delta}, \quad 1 < p, r < +\infty, \ 0 < \delta < 1, \ r(1-\delta) < 1.$$

We now aim to give explicit estimates with respect to τ for $\hat{u}$ in $H^p((0,+\infty))$. Following the lines of Subsection 3.1 and using (48) we get directly the following set of estimates.

Lemma 3.6: *Function $\hat{u}$ satisfies the estimates*

$$\|\hat{u}(\cdot,\tau)\|_{L^2((0,+\infty))} \leq \frac{C|\hat{g}(\tau)|}{\sqrt{\xi}(1+\gamma^{1/4}|\tau|^{1/4})}, \tag{57}$$

$$|\partial_x \hat{u}(\cdot,\tau) \ |_{x=0} \ | \leq \frac{C|\tau\hat{g}(\tau)|}{1+\gamma|\tau|}, \tag{58}$$

$$\|\partial_x^k \hat{u}(\cdot,\tau)\|_{L^2((0,+\infty))} \leq \frac{C|\hat{g}(\tau)|}{\sqrt{\xi}(1+\gamma^{1/4}|\tau|^{1/4})} \Big(\frac{|\tau|^2}{1+\gamma|\tau|} \Big)^{k/2} \quad k \geq 1, \tag{59}$$

with $\tau = \xi + i\,\eta$, $\xi > 0$.

4. A simple L^2 error estimate

The simplest way to average the problem (8)-(12) is to take the mean value with respect to y. 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 $c_0^{L,eff}(x,\tau)$:

$$\begin{cases} (1+K)\tau c_0^{L,eff} + \dfrac{2Q}{3}\dfrac{\partial c_0^{L,eff}}{\partial x} = \varepsilon^\alpha D \dfrac{\partial^2 c_0^{L,eff}}{\partial x^2} \quad \text{in } (0,+\infty), \\ \partial_x c_0^{L,eff} \in L^2((0,+\infty)), \\ -D\varepsilon^\alpha \partial_x c_0^{L,eff} + 2Q c_0^{L,eff}/3 = 2Q\hat{c}_f/3, \qquad \text{for } \ x = 0. \end{cases} \tag{60}$$

This is the problem (24) with $\hat{g} = \hat{c}_f$, $\bar{Q} = \dfrac{2}{3}\dfrac{Q}{1+K}$ and $\bar{D} = \dfrac{D}{1+K}$. The small parameter γ is equal to ε^α. We will call this problem the "**simple closure approximation**".

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

$$\mathcal{L}^\varepsilon \zeta = \tau\zeta + Q(1-y^2)\frac{\partial \zeta}{\partial x} - D\varepsilon^\alpha \Big(\frac{\partial^2 \zeta}{\partial x^2} + \varepsilon^{-2}\frac{\partial^2 \zeta}{\partial y^2} \Big). \tag{61}$$

The non-dimensional physical concentration c^ε satisfies (8)-(12). Its Laplace transform $\hat{c}^\varepsilon$ is thus solution of

$$\mathcal{L}^\varepsilon \hat{c}^\varepsilon = 0 \quad \text{in } (0,+\infty)\times(0,1) \tag{62}$$

$$-D\varepsilon^\alpha \partial_x \hat{c}^\varepsilon + Q(1-y^2)\hat{c}^\varepsilon = Q(1-y^2)\hat{c}_f, \quad \text{for } (x,y) \in \{0\}\times(0,1), \tag{63}$$

$$-D\varepsilon^{\alpha-2}\partial_y \hat{c}^\varepsilon(x,1,\tau) = K\tau\hat{c}^\varepsilon(x,1,\tau) \quad \text{in } (0,+\infty). \tag{64}$$

We want to approximate $\hat{c}^\varepsilon$ by $c_0^{L,eff}$. Then, if

$$\mathcal{L}^\varepsilon(c_0^{L,eff}) = -K\tau c_0^{L,eff} + Q\partial_x c_0^{L,eff}(1/3 - y^2) = R^\varepsilon,$$

we have to consider

$$\mathcal{L}^\varepsilon(\hat{c}^\varepsilon - c_0^{L,eff}) = -R^\varepsilon \quad \text{in} \quad (0,+\infty)\times(0,1), \tag{65}$$

$$-D\varepsilon^{\alpha-2}\partial_y(\hat{c}^\varepsilon(x,1,\tau) - c_0^{L,eff}) = K\tau\hat{c}^\varepsilon(x,1,\tau) \quad \text{on} \quad (0,+\infty), \tag{66}$$

$$\begin{aligned}&-D\varepsilon^\alpha\partial_x(\hat{c}^\varepsilon - c_0^{L,eff}) + Q(1-y^2)(\hat{c}^\varepsilon - c_0^{L,eff})\\ &= Q(1/3 - y^2)(\hat{c}_f - c_0^{L,eff}), \quad \text{on} \quad \{0\}\times(0,1).\end{aligned} \tag{67}$$

The weak formulation for the system (65)-(67) reads: for any $\tau = \xi + i\eta$, find $\hat{c}^\varepsilon - c_0^{L,eff} = w \in H^1(\Omega^+)$ such that

$$\begin{aligned}&\int_{\Omega^+}\tau w\varphi\ dxdy - \int_{\Omega^+}Q(1-y^2)\partial_x\varphi w\ dxdy + \int_{\Omega^+}D\varepsilon^\alpha(\partial_x w\partial_x\varphi + \varepsilon^{-2}\partial_y w\partial_y\varphi)\ dxdy\\ &+K\int_0^{+\infty}\tau w|_{y=1}\varphi|_{y=1}\ dx = -\int_{\Omega^+}Q\partial_x c_0^{L,eff}(1/3-y^2)\varphi\ dxdy\\ &-\int_0^1 Q(1/3-y^2)(\hat{c}_f - c_0^{L,eff}|_{x=0})\varphi|_{x=0}\ dy\\ &+K\int_0^{+\infty}\tau c_0^{L,eff}\int_0^1(\varphi - \varphi|_{y=1})\ dydx, \quad \forall\,\varphi\in H^1(\Omega^+).\end{aligned} \tag{68}$$

Next we test (68) by $\varphi = \overline{w} = \overline{\hat{c}^\varepsilon - c_0^{L,eff}}$. The real part of the corresponding relation is

$$\begin{aligned}&\int_{\Omega^+}\xi|w|^2\ dxdy + \int_{\Omega^+}D\varepsilon^\alpha(|\partial_x w|^2 + \varepsilon^{-2}|\partial_y w|^2)\ dxdy + K\int_0^{+\infty}\xi|w|_{y=1}|^2\ dx\\ &-\text{Re}\int_{\Omega^+}Q(1-y^2)\partial_x\overline{w}w\ dxdy = -\text{Re}\int_{\Omega^+}Q\partial_x c_0^{L,eff}(1/3-y^2)\overline{w}\ dxdy\\ &-\text{Re}\int_0^1 Q(1/3-y^2)(\hat{c}_f - c_0^{L,eff}|_{x=0})\overline{w}\ |_{x=0}\ dy\\ &+K\text{Re}\int_0^{+\infty}\tau c_0^{L,eff}\int_0^1(\overline{w} - \overline{w}|_{y=1})\ dydx.\end{aligned} \tag{69}$$

We find out immediately that

$$-\text{Re}\int_{\Omega^+}Q(1-y^2)\partial_x\overline{w}w\ dxdy = \frac{1}{2}\int_0^1 Q(1-y^2)|w\ |_{x=0}\ |^2\ dy \geq 0.$$

The terms in the right hand side of (69) are estimated as follows. Using

$$\int_0^{+\infty}\int_0^1 Q\partial_x c_0^{L,eff}(1/3-y^2)\overline{w}\ dxdy \\ = -\int_0^{+\infty}\int_0^1 Q\partial_x c_0^{L,eff}(y/3-y^3/3)\partial_y\overline{w}\ dxdy, \tag{70}$$

we obtain

$$\Big|\mathrm{Re}\int_0^{+\infty}\int_0^1 Q\partial_x c_0^{L,eff}(1/3-y^2)\overline{w}\Big| \le \Big|\int_0^{+\infty}\int_0^1 Q\partial_x c_0^{L,eff}(1/3-y^2)\overline{w}\Big| \\ \le C\|\varepsilon^{\alpha/2-1}\partial_y w\|_{L^2(\Omega^+)}\varepsilon^{1-\alpha/2}\|\partial_x c_0^{L,eff}\|_{L^2((0,+\infty))}. \tag{71}$$

Next, let $\omega = \hat{c}_f - c_0^{L,eff}|_{x=0}$. We have

$$\Big|\int_0^1 Q(1/3-y^2)(\hat{c}_f - c_0^{L,eff}|_{x=0})\overline{w}\ |_{x=0}\ \ dy\Big| \\ = \Big|\int_{\Omega^+} Q(1/3-y^2)\omega\partial_x(\overline{w}e^{-x/\varepsilon})\ dxdy\Big| \\ \le \Big|\int_{\Omega^+} Q(1/3-y^2)\omega\partial_x\overline{w}e^{-x/\varepsilon}\ dxdy\Big| + \varepsilon^{-1}\Big|\int_{\Omega^+} Q(y/3-y^3/3)\omega\partial_y\overline{w}e^{-x/\varepsilon}\ dxdy\Big| \\ \le C|\omega|\varepsilon^{-\alpha/2}\|e^{-x/\varepsilon}\|_{L^2(\Omega^+)}\big(\|\varepsilon^{\alpha/2}\partial_x w\|_{L^2(\Omega^+)} + \|\varepsilon^{\alpha/2-1}\partial_y w\|_{L^2(\Omega^+)}\big).$$

We bear in mind that $\|e^{-x/\varepsilon}\|_{L^2(\Omega^+)} \le C\varepsilon^{1/2}$. We also compute ω using (26) and obtain

$$|\omega| = \big|\gamma\frac{-4\tau\bar{D}}{l(\tau)^2}\hat{c}_f\big| \le C\varepsilon^\alpha|\partial_x c_0^{L,eff}\ |_{x=0}\ |.$$

We get

$$\Big|\int_0^1 Q(1/3-y^2)(\hat{c}_f - c_0^{L,eff}|_{x=0})\overline{w}\ |_{x=0}\ \ dy\Big| \\ \le C\varepsilon^{(1+\alpha)/2}|\partial_x c_0^{L,eff}\ |_{x=0}\ |\ \big(\|\varepsilon^{\alpha/2}\partial_x w\|_{L^2(\Omega^+)} + \|\varepsilon^{\alpha/2-1}\partial_y w\|_{L^2(\Omega^+)}\big). \tag{72}$$

The last term in the right hand side of (69) is treated as follows.

$$\Big|K\int_0^{+\infty}\tau c_0^{L,eff}\int_0^1(\overline{w}-\overline{w}|_{y=1})\ dydx\Big| = \Big|K\int_{\Omega^+}\tau c_0^{L,eff}\big(\int_1^y\partial_y\overline{w}\,dz\big)\ dxdy\Big| \\ \le C\|\varepsilon^{\alpha/2-1}\partial_y w\|_{L^2(\Omega^+)}\varepsilon^{1-\alpha/2}|\tau|\ \|c_0^{L,eff}\|_{L^2((0,+\infty))}. \tag{73}$$

Inserting estimates (71)-(73) in (69), we obtain

$$\int_{\Omega^+} \xi |w|^2 \, dxdy + \int_{\Omega^+} D\varepsilon^\alpha (|\partial_x w|^2 + \varepsilon^{-2} |\partial_y w|^2) \, dxdy + K \int_0^{+\infty} \xi |w|_{y=1}|^2 \, dx$$
$$+ \frac{1}{2} \int_0^1 Q(1-y^2) |w\,|_{x=0}\,|^2 \, dy \le C\varepsilon^{(1+\alpha)/2} |\partial_x c_0^{L,eff}\,|_{x=0}\,| \, \|\varepsilon^{\alpha/2} \partial_x w\|_{L^2(\Omega^+)}$$
$$+ \varepsilon^{1-\alpha/2} \big(C\varepsilon^{\alpha-1/2} |\partial_x c_0^{L,eff}\,|_{x=0}\,| + C|\tau| \|c_0^{L,eff}\|_{L^2((0,+\infty))}$$
$$+ C \|\partial_x c_0^{L,eff}\|_{L^2((0,+\infty))} \big) \|\varepsilon^{\alpha/2-1} \partial_y w\|_{L^2(\Omega^+)}.$$

The terms $|\partial_x c_0^{L,eff}\,|_{x=0}\,|$, $\|c_0^{L,eff}\|_{L^2((0,+\infty))}$ and $\|\partial_x c_0^{L,eff}\|_{L^2((0,+\infty))}$ are estimated through (42)-(44). We thus infer from the latter relation the following error estimates.

Proposition 4.1:

$$\|\hat{c}^\varepsilon - c_0^{L,eff}\|_{L^2(I\!R_+ \times (0,1))} \le \varepsilon^\beta \frac{C|\tau||\hat{c}_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}, \tag{74}$$

$$\|\partial_x (\hat{c}^\varepsilon - c_0^{L,eff})\|_{L^2(I\!R_+ \times (0,1))} \le \varepsilon^{\beta-\alpha/2} \frac{C|\tau||\hat{c}_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}, \tag{75}$$

$$\|\partial_y (\hat{c}^\varepsilon - c_0^{L,eff})\|_{L^2(I\!R_+ \times (0,1))} \le \varepsilon^{\beta+1-\alpha/2} \frac{C|\tau||\hat{c}_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}, \tag{76}$$

where $\beta = 1 - \alpha/2$ if $\alpha \ge 1/2$ and $\beta = (1+\alpha)/2$ if $\alpha < 1/2$.

Note that the presence of the given source term $\hat{c}_f$ is sufficient to control the behavior in τ of the right hand side terms.

Corollary 4.2: *Let $c_f \in \mathcal{D}(0,T)$ and let c_0^{eff} be such that $\hat{c}_0^{eff} = c_0^{L,eff}$. Let β be defined as in Proposition 4.1. Then we have*

$$\|c^\varepsilon - c_0^{eff}\|_{\mathcal{C}(\mathbb{R}_+; L^2(\Omega^+))} \le C\varepsilon^\beta.$$

Next let $c_f \in W^{1,\infty}(\mathbb{R}_+)$ with compact support in $[0,+\infty)$, such that $c_f(0) \ne 0$. Then for $1 < r < +\infty$, we have

$$\|c^\varepsilon - c_0^{eff}\|_{L^r(\mathbb{R}_+; L^2(\Omega^+))} \le \begin{cases} C\varepsilon^{1-\alpha/2-\alpha\delta}, & 2 > \alpha \ge 1/2, \; 0 < \delta < 1/4, \; r(1-\delta) < 1. \\ C\varepsilon^{(1+\alpha)/2}, & 1/2 > \alpha \ge 0. \end{cases}$$

Remark 1: Presence of the contact discontinuity due to $c_f(0) \ne 0$ diminishes precision. Furthermore, the case of $c_f = 1$ on $(0,T)$ is covered by Corollary 4.2, since it could be extended to a Lipschitz function on $\mathbb{R}_+$, with compact support in $[0,+\infty)$. Hence, it is easy to compare the result of Corollary 4.2 with the corresponding results from [19] and [20] and see that we have now a more precise estimate, which gives convergence for any $\alpha \in [0,2)$. Other possible comparaison is with the case $\alpha = 0$ from [11], but they have more complex chemical reactions.

In the next section we provide another "average" problem which leads to better error estimates.

5. Next order corrector

We now limit ourself to the more realistic and critical case $\alpha \geq 1$. A formal asymptotic expansion of a solution c^ε of system (8)-(12) (see [19] or [20] for the details of the corresponding computation) leads to consider the following function for approximating $\hat{c}^\varepsilon$:

$$c_1^{L,eff}(x,y;\varepsilon) = c_0(x;\varepsilon) + \varepsilon^{2-\alpha}\frac{Q}{D}\Big(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} - \frac{2}{45}\frac{K(7K+2)}{(1+K)^2}\Big)\partial_x c_0(x;\varepsilon)$$
$$+\varepsilon^{2-\alpha}\frac{K}{D}\Big(\frac{1}{6} + \frac{K}{3(1+K)} - \frac{y^2}{2}\Big)\tau c_0(x;\varepsilon) \tag{77}$$

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

$$\begin{cases} (1+K)\tau c_0 + \dfrac{2Q}{3}\partial_x c_0 - \varepsilon^\alpha \tilde{D}\partial^2_{xx} c_0 = 0 & \text{in } (0,+\infty), \\ -D\varepsilon^\alpha \partial_x c_0 + \dfrac{2Q}{3} c_0 = \dfrac{2Q}{3}\hat{c}_f & x = 0, \end{cases} \tag{78}$$

with

$$\tilde{D} = D + \frac{8}{945}\frac{Q^2}{D}\varepsilon^{2(1-\alpha)} + \frac{4Q^2}{135D}\frac{K(7K+2)}{(1+K)^2}\varepsilon^{2(1-\alpha)}.$$

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

$$\mathcal{L}^\varepsilon(\hat{c}^\epsilon - c_1^{L,eff}) = -\Phi^\varepsilon \quad \text{in } \Omega^+, \tag{79}$$

$$-D\varepsilon^{\alpha-2}\partial_y(\hat{c}^\epsilon - c_1^{L,eff})\mid_{y=1} = K\tau(\hat{c}^\epsilon - c_1^{L,eff})\mid_{y=1} + g^\varepsilon\mid_{y=1} \quad \text{in } (0,+\infty), \tag{80}$$

$$\partial_y(\hat{c}^\epsilon - c_1^{L,eff})\mid_{y=0} = 0 \quad \text{in } (0,+\infty), \tag{81}$$

$$-D\varepsilon^\alpha\partial_x(\hat{c}^\epsilon - c_1^{L,eff})\mid_{x=0} + Q(1-y^2)(\hat{c}^\epsilon - c_1^{L,eff})\mid_{x=0}$$
$$= Q(\frac{1}{3} - y^2)(\hat{c}_f - c_0\mid_{x=0}) + \eta_0^\varepsilon\mid_{x=0}, \tag{82}$$

where functions Φ^ε, g^ε and η_0^ε are defined by

$$\Phi^\varepsilon = \sum_{i=1}^{5} F_i^\varepsilon - g^\varepsilon, \tag{83}$$

$$F_1^\varepsilon = \varepsilon^{2-\alpha}\partial^2_{xx}c_0\frac{Q^2}{D}\Big(\frac{8}{945} + (1-y^2)(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180})\Big), \tag{84}$$

$$F_2^\varepsilon = \varepsilon^{2-\alpha}\tau\partial_x c_0\frac{QK}{D}\Big(-\frac{2}{45} + (1-y^2)(\frac{1}{6} - \frac{y^2}{2})\Big), \tag{85}$$

$$F_3^\varepsilon = \varepsilon^{2-\alpha}\tau\partial_x c_0\frac{Q}{D}\Big(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}\Big), \tag{86}$$

$$F_4^\varepsilon = \varepsilon^{2-\alpha}\tau^2 c_0\frac{K}{D}\Big(\frac{1}{6} - \frac{y^2}{2}\Big), \tag{87}$$

$$F_5^\varepsilon = -\varepsilon^{2-\alpha}\frac{Q}{D}\big(\frac{1}{3}-y^2\big)\Big(\frac{2Q}{45}\partial^2_{xx}c_0\frac{K(7K+2)}{(1+K)^2} - \frac{K^2}{3(1+K)}\tau\partial_x c_0\Big), \tag{88}$$

$$g^\varepsilon = \varepsilon^{2-\alpha}\frac{K\tau}{D}\Big(\frac{2Q}{45}\partial_x c_0\big(1-\frac{K(7K+2)}{(1+K)^2}\big) - \frac{K}{3(1+K)}\tau c_0\Big), \tag{89}$$

$$\begin{aligned}\eta_0^\varepsilon = {}& \varepsilon^{2-\alpha}\frac{Q^2}{D}(1-y^2)\partial_x c_0\big(\frac{y^2}{6}-\frac{y^4}{12}-\frac{7}{180}-\frac{2}{45}\frac{K(7K+2)}{(1+K)^2}\big)\\ & +\varepsilon^{2-\alpha}\frac{QK}{D}(1-y^2)\tau c_0\big(\frac{1}{6}-\frac{y^2}{2}+\frac{K}{3(1+K)}\big)\\ & -\varepsilon^2\Big(K\tau\partial_x c_0\big(\frac{1}{6}-\frac{y^2}{2}+\frac{K}{3(1+K)}\big)\\ & +Q\partial^2_{xx}c_0\big(\frac{y^2}{6}-\frac{y^4}{12}-\frac{7}{180}-\frac{2}{45}\frac{K(7K+2)}{(1+K)^2}\big)\Big).\end{aligned} \tag{90}$$

The variational formulation corresponding to problem (79)-(82) is

$$\begin{aligned}&\int_{\Omega^+}\tau w\phi\ dxdy + \int_{\Omega^+} D\varepsilon^\alpha(\partial_x w\partial_x\phi + \varepsilon^{-2}\partial_y w\partial_y\phi)\ dxdy\\ &+K\int_0^{+\infty}\tau w|_{y=1}\phi\ |_{y=1}\ \ dx + \int_{\Omega^+} Q(1-y^2)\phi\partial_x w\ dxdy\\ &+\int_0^1 Q(1-y^2)w\ |_{x=0}\ \phi\ |_{x=0}\ \ dy\\ =& -\int_0^1 Q(1/3-y^2)(\hat{c}_f - c_0\ |_{x=0})\phi\ |_{x=0}\ \ dy + \int_0^1 \eta_0^\varepsilon\ |_{x=0}\ \phi\ |_{x=0}\ \ dy\\ & -\int_{\Omega^+}\sum_{i=1}^5 F_i^\varepsilon\phi\ dxdy + \int_0^{+\infty} g^\varepsilon\int_0^1(\phi-\phi|_{y=1})\ dydx.\end{aligned} \tag{91}$$

We note that the source terms Φ^ε and g^ε satisfy the following properties.

Lemma 5.1: *Let $\phi \in H^1(\Omega^+)$. The following estimates hold true.*

$$\Big|\int_{\Omega^+}\sum_{i=1}^5 F_i^\varepsilon\phi\ dxdy\Big| \le C\varepsilon^{3(1-\alpha/2)}\mathcal{C}(c_0)\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}, \tag{92}$$

$$\Big|\int_0^{+\infty} g^\varepsilon\big(\int_0^1 \phi - \phi\ |_{y=1}\ \ dy\big)\ dx\Big| \le C\varepsilon^{3(1-\alpha/2)}\mathcal{C}(c_0)\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}, \tag{93}$$

where the quantity $\mathcal{C}(c_0)$ is defined by

$$\mathcal{C}(c_0) = \|\partial^2_{xx}c_0\|_{L^2((0,+\infty))} + (1+|\tau|)\|\partial_x c_0\|_{L^2((0,+\infty))} + |\tau|^2\|c_0\|_{L^2((0,+\infty))}.$$

Proof: On the one hand, we note that $\sum_{i=1}^5 F_i^\varepsilon$ can be written as

$$\sum_{i=1}^5 F_i^\varepsilon = \varepsilon^{2-\alpha}\big(\partial_y(P_0(y))\tau^2 c_0 + \partial_y(P_1(y))\tau\partial_x c_0 + \partial_y(P_2(y))\partial^2_{xx}c_0\big)$$

where the polynomials P_j, $0 \le j \le 2$, have zero traces in $y = 0, 1$. We thus have

$$
\begin{aligned}
&\Big|\int_{\Omega^+} \sum_{i=1}^{5} F_i^\varepsilon \phi \; dxdy\Big| \\
&= \Big|\int_{\Omega^+} \varepsilon^{2-\alpha}\big(\partial_y(P_0(y))\tau^2 c_0 + \partial_y(P_1(y))\tau\partial_x c_0 + \partial_y(P_2(y))\partial^2_{xx}c_0\big)\phi \; dxdy\Big| \\
&= \Big|-\int_{\Omega^+} \varepsilon^{2-\alpha}\big(P_0(y)\tau^2 c_0 + P_1(y)\tau\partial_x c_0 + P_2(y)\partial^2_{xx}c_0\big)\partial_y\phi \; dxdy\Big| \\
&\le C\varepsilon^{2-\alpha}\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}\varepsilon^{1-\alpha/2}\big(|\tau|^2\|c_0\|_{L^2((0,+\infty))} + |\tau|\|\partial_x c_0\|_{L^2((0,+\infty))} \\
&+\|\partial^2_{xx}c_0\|_{L^2((0,+\infty))}\big).
\end{aligned}
$$

Estimate (92) is proved. On the other hand, we write

$$
\begin{aligned}
&\Big|\int_0^{+\infty} g^\varepsilon\big(\int_0^1 \phi - \phi\,|_{y=1} \; dy\big)\,dx\Big| = \Big|\int_{\Omega^+} g^\varepsilon\big(\int_1^y \partial_y\phi \, dz\big)\,dxdy\Big| \\
&\le C\varepsilon^{2-\alpha}(\|\partial_x c_0\|_{L^2((0,+\infty))} + |\tau|\|c_0\|_{L^2((0,+\infty))})\varepsilon^{1-\alpha/2}\|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}.
\end{aligned}
$$

This ends the proof of the lemma. □

Let us now study the terms in (91) coming from the boundary condition at $x = 0$.

Lemma 5.2: *The following estimates hold true.*

$$
\begin{aligned}
&\Big|\int_0^1 Q(1/3 - y^2)(\hat{c}_f - c_0\,|_{x=0})\phi\,|_{x=0} \; dy\Big| \\
&\le C\varepsilon^{(1+\alpha)/2}|\partial_x c_0\,|_{x=0}|(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)} + \|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}), \qquad (94)
\end{aligned}
$$

$$
\begin{aligned}
&\Big|\int_0^1 \eta_0^\varepsilon\,|_{x=0}\,\phi\,|_{x=0} \; dy\Big| \le C\varepsilon^{2-\alpha}\|\sqrt{1-y^2}\phi\,|_{x=0}\,\|_{L^2(0,1)}\big(|\partial_x c_0\,|_{x=0}\,| + |\tau||c_0\,|_{x=0}\,|\big) \\
&+C\varepsilon^{2-\alpha/4}\big(|\partial^2_{xx}c_0\,|_{x=0}\,| + |\tau||\partial_x c_0\,|_{x=0}\,|\big)\big(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)} + \|\phi\|_{L^2(\Omega^+)}\big). \qquad (95)
\end{aligned}
$$

Proof: Let $\omega = |\hat{c}_f - c_0\,|_{x=0}\,|$. We have

$$
\begin{aligned}
&\Big|\int_0^1 Q(1/3 - y^2)(\hat{c}_f - c_0\,|_{x=0})\phi\,|_{x=0} \; dy\Big| = \Big|\int_{\Omega^+} Q(1/3 - y^2)\,\omega\,\partial_x(\phi e^{-x/\varepsilon}) \; dxdy\Big| \\
&\le C|\omega|\int_{\Omega^+}\Big|\frac{1}{3} - y^2\Big||\partial_x\phi|e^{-x/\varepsilon}\,dxdy + C|\omega|\Big|\int_{\Omega^+}\varepsilon^{-1}\big(\frac{1}{3} - y^2\big)\phi e^{-x/\varepsilon} \; dxdy\Big| \\
&\le C|\omega|\Big(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)}\varepsilon^{-\alpha/2}\|e^{-x/\varepsilon}\|_{L^2(\Omega^+)} + \Big|\int_{\Omega^+}\varepsilon^{-1}\big(\frac{y}{3} - \frac{y^3}{3}\big)\partial_y\phi e^{-x/\varepsilon} \; dxdy\Big|\Big) \\
&\le C|\omega|\varepsilon^{(1-\alpha)/2}\big(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)} + \|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}\big).
\end{aligned}
$$

Then, using the explicit solution of problem (78) given in (3.2) with $\bar{Q} = \dfrac{2}{3}\dfrac{Q}{1+K}$, $\bar{D} = \dfrac{D}{1+K}$, $\hat{g} = \hat{c}_f$, $\gamma = \varepsilon^\alpha$ and $\delta = -\varepsilon^{2(1-\alpha)}(8Q^2/(945D) + (4Q^2/135D)K(7K +$

$2)/(1+K)^2)$, we compute

$$|\omega| = |\hat{c}_f - c_0 \mid_{x=0} | = \Big|\frac{2\bar{D}\bar{Q} - l(\tau)(\bar{D}+\delta) + 2\bar{Q}\delta}{l(\tau)(\bar{D}+\delta) - 2\bar{Q}\delta}\Big||c_f| \leq C\varepsilon^{\alpha}|\partial_x c_0 \mid_{x=0} |.$$

We thus get

$$\Big|\int_0^1 Q(1/3 - y^2)(\hat{c}_f - c_0 \mid_{x=0})\phi \mid_{x=0} \ dy\Big|$$
$$\leq C\varepsilon^{(1-\alpha)/2}\varepsilon^{\alpha}|\partial_x c_0 \mid_{x=0} |(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)} + \|\varepsilon^{\alpha/2-1}\partial_y\phi\|_{L^2(\Omega^+)}).$$

Estimate (94) is proved.

We now prove (95). We write

$$\Big|\int_0^1 \varepsilon^{2-\alpha}(1-y^2)\frac{Q}{D}\Big(Q\partial_x c_0\big(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180} - \frac{2}{45}\frac{K(7K+2)}{(1+K)^2}\big)$$
$$+K\tau c_0\big(\frac{1}{6} - \frac{y^2}{2} + \frac{K}{3(1+K)}\big)\Big) \mid_{x=0} \cdot\phi \mid_{x=0} \ dy\Big|$$
$$\leq C\varepsilon^{2-\alpha}\|\sqrt{1-y^2}\phi \mid_{x=0} \|_{L^2(0,1)}\big(|\partial_x c_0 \mid_{x=0} | + |\tau||c_0 \mid_{x=0} |\big). \tag{96}$$

The remaining term to estimate is

$$\int_0^1 \varepsilon^2\Big(K\tau\partial_x c_0\big(\frac{1}{6} - \frac{y^2}{2} + \frac{K}{3(1+K)}\big) + Q\partial^2_{xx}c_0\big(\frac{y^2}{6} - \frac{y^4}{12} - \frac{7}{180}$$
$$-\frac{2}{45}\frac{K(7K+2)}{(1+K)^2}\big)\Big) \mid_{x=0} \phi \mid_{x=0} \ dy$$
$$= \int_0^1 \varepsilon^2(p_1(y)\tau\partial_x c_0 + p_2(y)\partial^2_{xx}c_0) \mid_{x=0} \phi \mid_{x=0} \ dy,$$

with

$$\Big|\int_0^1 \varepsilon^2(p_1(y)\tau\partial_x c_0 + p_2(y)\partial^2_{xx}c_0) \mid_{x=0} \phi \mid_{x=0} \ dy\Big|$$
$$=\Big|\int_{\Omega^+} \varepsilon^2(p_1(y)\tau\partial_x c_0 + p_2(y)\partial^2_{xx}c_0) \mid_{x=0} \partial_x(\phi e^{-x/\varepsilon^{\alpha/2}}) \ dxdy\Big|$$
$$\leq \varepsilon^2\Big|\int_{\Omega^+} (p_1(y)\tau\partial_x c_0 + p_2(y)\partial^2_{xx}c_0) \mid_{x=0} \partial_x\phi e^{-x/\varepsilon^{\alpha/2}} \ dxdy\Big|$$
$$+\varepsilon^{2-\alpha/2}\Big|\int_{\Omega^+} (p_1(y)\tau\partial_x c_0 + p_2(y)\partial^2_{xx}c_0) \mid_{x=0} \phi e^{-x/\varepsilon^{\alpha/2}} \ dxdy\Big|$$
$$\leq C\varepsilon^{2-\alpha/4}\big(|\partial^2_{xx}c_0 \mid_{x=0} | + |\tau||\partial_x c_0 \mid_{x=0} |\big)\big(\|\varepsilon^{\alpha/2}\partial_x\phi\|_{L^2(\Omega^+)} + \|\phi\|_{L^2(\Omega^+)}\big). \tag{97}$$

Estimate (95) follows from (96)-(97).

□

Now let $w = \hat{c}^{\varepsilon} - c_1^{L,eff}$. We write the variational formulation (91) for the test function $\phi = \overline{w}$. We obtain

$$\int_{\Omega^+} \xi |w|^2 \, dxdy + \int_{\Omega^+} D\varepsilon^\alpha (|\partial_x w|^2 + \varepsilon^{-2} |\partial_y w|^2) \, dxdy + K \int_0^{+\infty} \xi |w|_{y=1}|^2 \, dx$$
$$+ \frac{1}{2} \int_0^1 Q(1-y^2) |w\,|_{x=0}\,|^2 \, dy = -\mathrm{Re} \int_0^1 Q(1/3 - y^2)(\hat{c}_f - c_0\,|_{x=0}) \overline{w}\,|_{x=0} \, dy$$
$$+ \mathrm{Re} \int_0^1 \eta_0^\varepsilon \,|_{x=0} \, \overline{w}\,|_{x=0} \, dy - \mathrm{Re} \Big(\int_{\Omega^+} \sum_{i=1}^5 F_i^\varepsilon \overline{w} \, dxdy - \int_0^{+\infty} g^\varepsilon \int_0^1 (\overline{w} - \overline{w}|_{y=1}) \, dydx \Big).$$

The terms in the right hand side of the latter relation are estimated in Lemmas 5.1 and 5.2. The L^2 error estimate is thus

$$\|w\|_{L^2(\Omega^+)} = \|\hat{c}^\epsilon - c_1^{L,eff}\|_{L^2(\Omega^+)} \leq C\varepsilon^{2-\alpha} \Big(\varepsilon^{1-\alpha/2} \big(\|\partial_{xx}^2 c_0\|_{L^2((0,+\infty))}$$
$$+ (1+|\tau|) \|\partial_x c_0\|_{L^2((0,+\infty))} + |\tau|^2 \|c_0\|_{L^2((0,+\infty))} \big) + |\partial_x c_0\,|_{x=0}\,| + |\tau| |c_0\,|_{x=0}\,|$$
$$+ \varepsilon^{3\alpha/4} \big(|\partial_{xx}^2 c_0\,|_{x=0}\,| + |\tau| |\partial_x c_0\,|_{x=0}\,| \big) \Big).$$

The terms containing c_0 are estimated in Subsection 3.2. Problem (78) is indeed Problem (46) where $\bar{Q}\dfrac{2Q}{3(1+K)}$, $\bar{D} = \dfrac{\tilde{D}}{1+K}$, $\hat{g} = \hat{c}_f$, $\gamma = \varepsilon^\alpha$ and $\delta = -\varepsilon^{2(1-\alpha)} \big(\dfrac{8}{945} \dfrac{Q^2}{D} + \dfrac{4Q^2}{135D} \dfrac{K(7K+2)}{(1+K)^2} \big)$. We thus claim the following result.

Proposition 5.3:

$$\|(\hat{c}^\varepsilon - c_1^{L,eff})(\tau)\|_{L^2(\mathbb{R}_+ \times (0,1))} \leq C\varepsilon^{2-\alpha} \frac{|\tau^2 c_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}, \tag{98}$$

$$\|\partial_x (\hat{c}^\varepsilon - c_1^{L,eff})\|_{L^2(\mathbb{R}_+ \times (0,1))} \leq C\varepsilon^{2-3\alpha/2} \frac{|\tau^2 c_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}, \tag{99}$$

$$\|\partial_y (\hat{c}^\varepsilon - c_1^{L,eff})\|_{L^2(\mathbb{R}_+ \times (0,1))} \leq C\varepsilon^{3-3\alpha/2} \frac{|\tau^2 c_f|}{1 + (\varepsilon^\alpha |\tau|)^{1/4}}. \tag{100}$$

Corollary 5.4: *Let $c_f \in \mathcal{D}(0,T)$ and let c_0^{eff} be such that $\hat{c}_0^{eff} = c_0^{L,eff}$. Let β be defined as in Proposition 5.3. Then we have*

$$\|c^\varepsilon - c_0^{eff}\|_{\mathcal{C}(\mathbb{R}_+; L^2(\Omega^+))} \leq C\varepsilon^{2-\alpha}.$$

Next let $c_f \in W^{1,\infty}(\mathbb{R}_+)$ with compact support in $[0,+\infty)$, such that $c_f(0) \neq 0$. Then for $1 < r < +\infty$, we have

$$\| \int_0^t (c^\varepsilon - c_0^{eff}) \, dt \|_{L^r(\mathbb{R}_+; L^2(\Omega^+))} \leq C\varepsilon^{2-\alpha-\alpha\delta}, \ 0 < \delta < 1/4, \ r(1-\delta) < 1.$$

Remark 1: As before, presence of the contact discontinuity due to $c_f(0) \neq 0$ diminishes precision. Nevertheless, main deterioration of the approximation comes from the boundary condition. Without inlet boundary, we would have an approximation of order $\varepsilon^{3-3\alpha/2}$. The case of $c_f = 1$ on $(0,T)$ is covered by the Corollary

5.4, since it could be extended to a Lipschitz function on $\mathbb{R}_+$, with compact support in $[0, +\infty)$. Hence, it is easy to compare the result of the Corollary 5.4 with the corresponding results from [19] and [20] and see that we have now a better estimate, even without constructing boundary layers.

Theorem 1.1 follows from Corollary 5.4.

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