A two-scale RD system for gas-liquid reactions with nonlinear micro-macro transmission conditions: well-posedness and fast-reaction asymptotics

Adrian Muntean

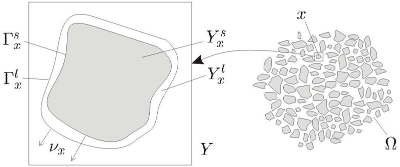
Centre for Analysis, Scientific computing and Applications (CASA)
Department of Mathematics and Computer Science, TU Eindhoven, The Netherlands

Joint work with Maria Neuss-Radu (Heidelberg, Germany)

Eindhoven, April 2010

Balance equations in heterogeneous media

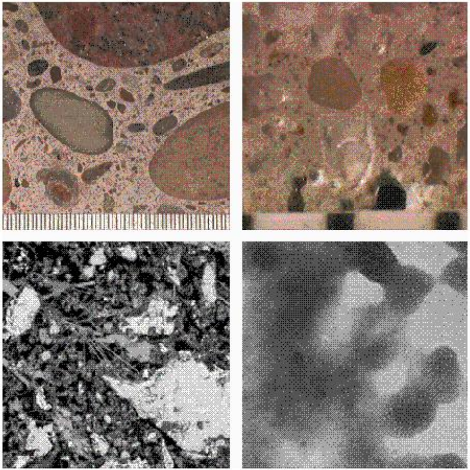
- Balance equations (PDEs) in heterogeneous media
- *x*-dependent microstructures



- *t*-dependent microstructures (evolving free boundaries)

Outline of the Talk

Length scales in heterogeneous media

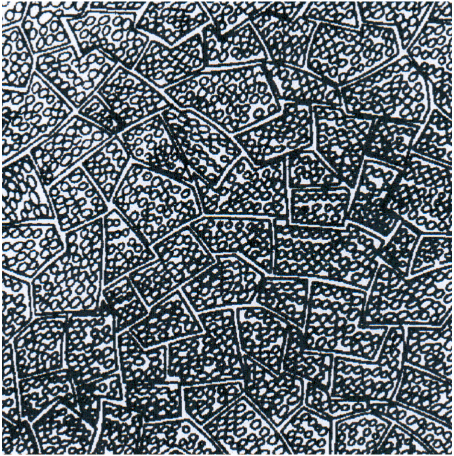


Bridging length scales

- Averaging techniques (periodic homogenization, ...)
- PDE models with distributed microstructure

1. two-scale models – A. Friedman, A. Tzavaras, P. Knabner
2. distributed-microstructure models – R. E. Showalter and co-workers (Walkington, Cook, Clark, Visarraga, ...) + M. Böhm, S. Meier
3. dual- or double-porosity models – U. Hornung, W. Jäger, T. Arbogast, ...
4. two-scale models with freely evolving micro-interfaces – C. Eck., H. Emmerich, P. Knabner, A. Muntean (2 scale phase-field models), *S. Meier, A. Muntean (2 scale fast-reaction asymptotics)*

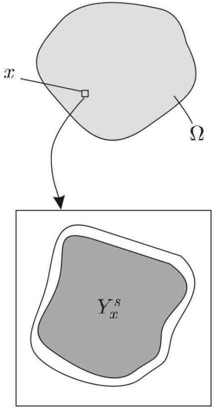
Double-porosity structure of materials



Barenblatt, Zheltov, Kochina, *PMM*, 24(1960), 5, pp. 852–864

"Structured physics": Mass-transfer at air-liquid interfaces

- Species $A(g)$ penetrates Ω and dissolves in pore water as $A(aq)$
- $A(aq) + B(aq) \rightarrow$ precipitate $+$ *water*
- $\frac{D_{A(g)}}{D_{A(aq)}} = \mathcal{O}(\epsilon^2)$



A concrete example

Sewer pipes corrosion (micro – macro)

- $H_2S(g)$ penetrates Ω and dissolves in pore water as $H_2S(aq)$
- $H_2SO_4 + CaCO_3(aq) \rightarrow$ gypsum $+$ *water*
- $\frac{D_{H_2S(g)}}{D_{H_2S(aq)}} = \mathcal{O}(\epsilon^2)$

(jointly with Tasnim Fatima (Eindhoven))

- How important is the precise shape of the microstructure?

Generic model (GM): micro – macro

$$\theta\partial_t U(t,x) - D\Delta U(t,x) = -\int_{\Gamma_R} b(U(t,x) - u(t,x,y))d\lambda_y^2 \quad \text{in } S\times\Omega,$$

$$\partial_t u(t,x,y) - d_1\Delta_y u(t,x,y) = -k\eta(u(t,x,y), v(t,x,y)) \quad \text{in } S\times\Omega\times Y,$$
$$\partial_t v(t,x,y) - d_2\Delta_y v(t,x,y) = -\alpha k\eta(u(t,x,y), v(t,x,y)) \quad \text{in } S\times\Omega\times Y,$$

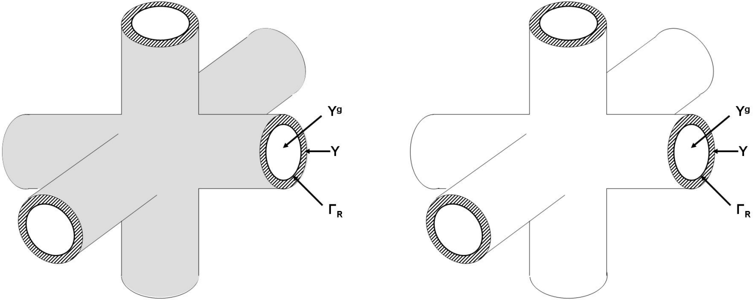
$$U(t,x) = U^{ext}(t,x) \quad \text{on } S\times\partial\Omega,$$

$$\nabla_y u(t,x,y)\cdot n_y = 0 \quad \text{on } S\times\Omega\times\Gamma_N,$$
$$\nabla_y v(t,x,y)\cdot n_y = 0 \quad \text{on } S\times\Omega\times\Gamma.$$

$$-\nabla_y u(t,x,y)\cdot n_y = -b(U(t,x) - u(t,x,y)) \quad \text{on } S\times\Omega\times\Gamma_R.$$

+ i.c.

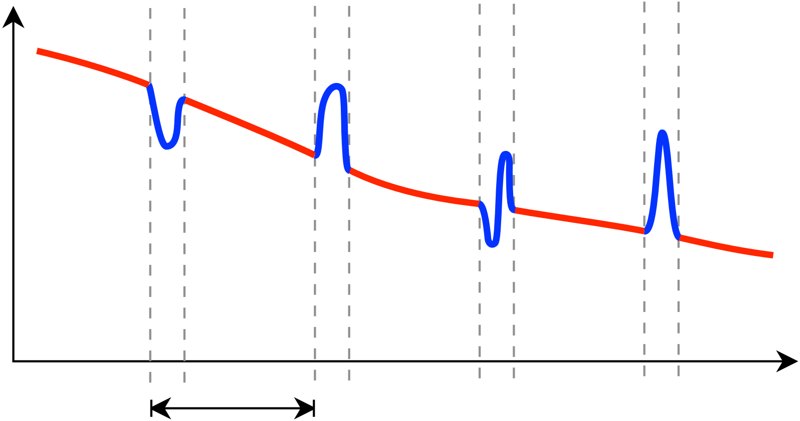
Geometry of the microstructure Y



The GM model has 3 main qualities:

1. minimal: We need 3 PDEs to model air-liquid transfer and fast reaction in the liquid phase
2. robust: Well-posedness is guaranteed
3. general: Many situations incorporating both structured transport and chemical reactions are captured by GM

Difficulties?



History-dependent processes!

Generic model (GM): micro – macro

$$\theta\partial_t U(t,x) - D\Delta U(t,x) = -\int_{\Gamma_R} b(U(t,x) - u(t,x,y))d\lambda_y^2 \quad \text{in } S\times\Omega,$$

$$\partial_t u(t,x,y) - d_1\Delta_y u(t,x,y) = -k\eta(u(t,x,y), v(t,x,y)) \quad \text{in } S\times\Omega\times Y,$$
$$\partial_t v(t,x,y) - d_2\Delta_y v(t,x,y) = -\alpha k\eta(u(t,x,y), v(t,x,y)) \quad \text{in } S\times\Omega\times Y,$$

$$U(t,x) = U^{ext}(t,x) \quad \text{on } S\times\partial\Omega,$$

$$\nabla_y u(t,x,y)\cdot n_y = 0 \quad \text{on } S\times\Omega\times\Gamma_N,$$
$$\nabla_y v(t,x,y)\cdot n_y = 0 \quad \text{on } S\times\Omega\times\Gamma.$$

$$-\nabla_y u(t,x,y)\cdot n_y = -b(U(t,x) - u(t,x,y)) \quad \text{on } S\times\Omega\times\Gamma_R.$$

+ i.c.

Assumptions on data and parameters

(A1) $D > 0, d_1 > 0, d_2 > 0$.

(A2) $b : \mathbb{R} \to \mathbb{R}_+$ is globally Lipschitz s. t. it exists a constant $\hat{c} > 0$ satisfying $b(z) \leq \hat{c}z$ if $z > 0$ and $b(z) = 0$ if $z \leq 0$.

(A3) $\eta : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$ by $\eta(r,s) := R(r)Q(s)$, where $R, Q \in C^1(\mathbb{R}, \mathbb{R}_+)$. Assume $R(r) > 0$ if $r > 0$ and $R(r) = 0$ if $r \leq 0$, and similarly, $Q(s) > 0$ if $s > 0$ and $Q(s) = 0$ if $s \leq 0$.
$k, \alpha \in \mathbb{R}, k > 0$, and $\alpha > 0$.

(A4) $U^{ext} \in H^2(S \times \Omega) \cap L^\infty_+(S \times \Omega)$, $U_I - U^{ext}(0, \cdot) \in H^1_0(\Omega) \cap L^\infty_+(\Omega)$, $u_I, v_I \in H^1(\Omega; H^1(Y)) \cap L^\infty_+(\Omega \times Y)$.

Find (U, u, v) with

$$U - U^{ext} \in L^2(S, H^1_0(\Omega)),\ (u, v) \in L^2(S, L^2(\Omega, H^1(Y)))^2$$

such that

$$\begin{aligned}
\frac{d}{dt}\int_\Omega \theta U\varphi \quad &+ \quad \int_\Omega \theta D\nabla U\nabla\varphi + \int_\Omega\int_{\Gamma_R} b(U-u)\varphi d\lambda_y^2 dx = 0\\
\frac{d}{dt}\int_{\Omega\times Y} u\phi \quad &+ \quad \int_{\Omega\times Y} d_1\nabla_y u\nabla_y\phi\\
&- \quad \int_\Omega\int_{\Gamma_R} b(U-u)\phi d\lambda_y^2 dx + k\int_{\Omega\times Y}\eta\phi = 0\\
\frac{d}{dt}\int_{\Omega\times Y} v\psi \quad &+ \quad \int_{\Omega\times Y} d_2\nabla_y v\nabla_y\psi + \alpha k\int_{\Omega\times Y}\eta\psi = 0,
\end{aligned}$$

for all $(\varphi, \phi, \psi) \in H^1_0(\Omega) \times L^2(\Omega; H^1(Y))^2$, and

$$U(0) = U_I \text{ in } \Omega, \quad u(0) = u_I,\ v(0) = v_I \text{ in } \Omega \times Y.$$

Basic estimates (1): Positivity of concentrations

Estimate the boundary term:

$$
\begin{aligned}
\int_\Omega \int_{\Gamma_R} b(U-u)(U^- - u^-)d\lambda_y^2 dx &\leq \int_\Omega \int_{\Gamma_R} b(U-u)U^- d\lambda_y^2 dx \\
&\leq \hat{c} \int_\Omega \int_{\Gamma_R} \mathcal{H}(U-u)(U-u)U^- d\lambda_y^2 dx \\
&\leq \hat{c} \int_\Omega \int_{\Gamma_R} \mathcal{H}(U-u)[UU^- - u^+U^+ + u^-U^-] d\lambda_y^2 dx \\
&\leq \hat{c}\lambda_y^2(\Gamma_R) \int_\Omega |U^-|^2 + \hat{c} \int_\Omega \int_{\Gamma_R} u^- U^- d\lambda_y^2 dx \\
&\leq \hat{c}\lambda_y^2(\Gamma_R) \int_\Omega |U^-|^2 + \left(\frac{\hat{c}\lambda_y^2(\Gamma_R)}{\sqrt{\epsilon}} \right)^2 \int_\Omega |U^-|^2 + \epsilon \int_\Omega \int_{\Gamma_R} |u^-|^2 d\lambda_y^2 dx \\
&\leq \hat{c}\lambda_y^2(\Gamma_R)(1 + \frac{\hat{c}\lambda_y^2(\Gamma_R)}{\epsilon})||U^-||^2_{L^2(\Omega)} + \epsilon \int_\Omega \int_Y ||u^-||^2_{H^1(Y)}.
\end{aligned}
$$

Basic estimates (2): L^∞-bounds on concentrations

Estimate the boundary term: Set

$$\begin{aligned} M_1 &:= \max\{||U^{ext}||_{L^\infty(S\times\Omega)}, ||U_I||_{L^\infty(\Omega)}\}, \\ M_2 &:= \max\{||u_I||_{L^\infty(\Omega\times Y)}, M_1\}, \\ M_3 &:= ||v_I||_{L^\infty(\Omega\times Y)}. \end{aligned}$$

$$\begin{aligned} & \int_\Omega\int_{\Gamma_R} b(U-u)(u-M_2)^+ d\lambda_y^2 dx \leq \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-u)(u-M_2)^+ d\lambda_y^2 dx \\ \leq\ & \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-M_1)(u-M_2)^+ d\lambda_y^2 dx - \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)|(u-M_2)^+|^2 d\lambda_y^2 dx \\ \leq\ & \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)(U-M_1)^+(u-M_2)^+ d\lambda_y^2 dx - \hat{c}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)|(u-M_2)^+|^2 d\lambda_y^2 d \\ \leq\ & \frac{\hat{c}}{2}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)|(U-M_1)^+|^2 d\lambda_y^2 dx - \frac{\hat{c}}{2}\int_\Omega\int_{\Gamma_R}\mathcal{H}(U-u)|(u-M_2)^+|^2 d\lambda_y^2 dx \\ \leq\ & \frac{\hat{c}}{2}\lambda_y^2(\Gamma_R)||(U-M_1)^+||^2_{L^2(\Omega)}. \end{aligned}$$

Uniqueness follows easily (via interpolation-trace inequality)

Two-scale Galerkin approximation

Let $\{\xi_i\}_{i\in\mathbb{N}}$ be a basis of $L^2(\Omega)$, with $\xi_j \in H_0^1(\Omega)$, o.n.s. w.r.t. $L^2(\Omega)$-norm. Let $\{\zeta_{jk}\}_{j,k\in\mathbb{N}}$ be a basis of $L^2(\Omega \times Y)$, with

$$\zeta_{jk}(x,y) = \xi_j(x)\eta_k(y),$$

where $\{\eta_k\}_{k\in\mathbb{N}}$ is a basis of $L^2(Y)$, with $\eta_k \in H^1(Y)$, forming an o.n.s. w.r.t. $L^2(Y)$-norm.

Define the projection operators on finite dimensional subspaces P_x^N, P_y^N associated to the bases $\{\xi_j\}_{j\in\mathbb{N}}$, and $\{\eta_k,\}_{k\in\mathbb{N}}$. For (φ,ψ) of the form

$$\varphi(x) = \sum_{j\in\mathbb{N}} a_j\xi_j(x), \quad \psi(x,y) = \sum_{j,k\in\mathbb{N}} b_{jk}\xi_j(x)\eta_k(y),$$

we define

$$\begin{aligned}
(P_x^N\varphi)(x) &= \sum_{j=1}^{N} a_j\xi_j(x),\\
(P_x^N\psi)(x,y) &= \sum_{j=1}^{N}\sum_{k\in\mathbb{N}} b_{jk}\,\sigma_j(x)\eta_k(y)\\
(P_y^N\psi)(x,y) &= \sum_{j\in\mathbb{N}}\sum_{k=1}^{N} b_{jk}\,\sigma_j(x)\eta_k(y).
\end{aligned}$$

- $\{\sigma_j\}_{j\in\mathbb{N}}$, and $\{\eta_k\}_{k\in\mathbb{N}}$ are chosen s.t. P_x^N, P_y^N are stable w.r.t. L^∞-norm and H^2-norm;
- The Galerkin system has a unique global solution $(\alpha^N, \beta^N, \gamma^N)$ in $C^1([0,T])^N \times C^1([0,T])^{N^2} \times C^1([0,T])^{N^2}$.

Uniform (in N) estimates

Theorem: Assume that the projection operators P_x^N, P_y^N are stable w.r.t. L^∞-norm and H^2-norm, and that (A1)–(A4) are satisfied. Then the following statements hold:

(i) The finite-dimensional approximations $U_0^N(t)$, $u^N(t)$, and $v^N(t)$ are positive and uniformly bounded. More precisely, we have for a.e. $(x,y) \in \Omega \times Y$, all $t \in S$, and all $N \in \mathbb{N}$

$$0 \leq U_0^N(t,x) \leq m_1, \quad 0 \leq u^N(t,x,y) \leq m_2, \quad 0 \leq v^N(t,x,y) \leq m_3,$$

where

$$\begin{aligned} m_1 &:= 2||U^{ext}||_{L^\infty(S\times\Omega)} + ||U_I||_{L^\infty(\Omega)}, \\ m_2 &:= \max\{||u_I||_{L^\infty(\Omega\times Y)}, m_1\}, \\ m_3 &:= ||v_I||_{L^\infty(\Omega\times Y)}. \end{aligned}$$

(ii) There exists a constant $c > 0$, independent of N, such that

$$\begin{aligned} ||U_0^N||_{L^\infty(S,H^1(\Omega))} + ||\partial_t U_0^N||_{L^2(S,L^2(\Omega))} &\leq c, \\ ||u^N||_{L^\infty(S,L^2(\Omega;H^1(Y)))} + ||\partial_t u^N||_{L^2(S,L^2(\Omega;L^2(Y)))} &\leq c, \\ ||v^N||_{L^\infty(S,L^2(\Omega;H^1(Y)))} + ||\partial_t v^N||_{L^2(S,L^2(\Omega;L^2(Y)))} &\leq c. \end{aligned}$$

Assume (A1)–(A4) to be satisfied. Then there exists a constant $c > 0$, independent of N, such that the following estimates hold

$$\begin{aligned} ||\nabla_x u^N||_{L^\infty(S,L^2(\Omega\times Y))} + ||\nabla_x v^N||_{L^\infty(S,L^2(\Omega\times Y))} &\leq c \\ ||\nabla_y \nabla_x u^N||_{L^2(S,L^2(\Omega\times Y))} + ||\nabla_y \nabla_x v^N||_{L^2(S,L^2(\Omega\times Y))} &\leq c. \end{aligned}$$

Theorem:

There exists a subsequence, again denoted by (U_0^N, u^N, v^N), and a limit $(U_0, u, v) \in L^2(S; H^1(\Omega)) \times \left[L^2(S; L^2(\Omega; H^1(Y)))\right]^2$, with $(\partial_t U_0^N, \partial_t u^N, \partial_t v^N) \in L^2(S \times \Omega) \times \left[L^2(S \times \Omega \times Y)\right]^2$, such that

$$
\begin{array}{ll}
(i) & (U_0^N, u^N, v^N) \to (U_0, u, v) \text{ weakly in } L^2(S; H^1(\Omega)) \times \left[L^2(S; L^2(\Omega; H^1(Y)))\right]^2 \\
(ii) & (\partial_t U_0^N, \partial_t u^N, \partial_t v^N) \to (\partial_t U_0, \partial_t u, \partial_t v) \text{ weakly in } L^2 \\
(iii) & (U_0^N, u^N, v^N) \to (U_0, u, v) \text{ strongly in } L^2 \\
(iv) & u^N|_{\Gamma_R} \to u|_{\Gamma_R} \text{ strongly in } L^2(S \times \Omega, L^2(\Gamma_R))
\end{array}
$$

Proof of the convergence theorem (sketch)

(i), (ii) result from the energy estimates.
Since

$$||U_0^N||_{L^2(S,H^1(\Omega))} + ||\partial_t U_0^N||_{L^2(S,L^2(\Omega))} \leq c,$$

Lions-Aubin's compactness theorem implies that there exists a subset (again denoted by U_0^N) such that

$$U_0^N \longrightarrow U_0 \text{ strongly in } L^2(S \times \Omega).$$

To get the strong convergences for the cell solutions u^N, v^N, we need the higher regularity with respect to the variable x, i.e.

$$||u^N||_{H^1(\Omega,H^1(Y))} + ||v^N||_{H^1(\Omega,H^1(Y))} \leq c.$$

Moreover, we have that

$$||\partial_t u^N||_{L^2(S\times\Omega\times Y)} + ||\partial_t v^N||_{L^2(S\times\Omega\times Y)} \leq c.$$

Since the embedding

$$H^1(\Omega, H^1(Y)) \hookrightarrow L^2(\Omega, H^\beta(Y))$$

is compact for all $\frac{1}{2} < \beta < 1$, it follows again from Lions-Aubin's compactness theorem that there exist subsequences (again denoted u^N, v^N), such that

$$(u^N, v^N) \longrightarrow (u, v) \text{ strongly in } L^2(S \times L^2(\Omega, H^\beta(Y)),$$

for all $\frac{1}{2} < \beta < 1$. This together with the continuity of the trace operator

$$H^\beta(Y) \hookrightarrow L^2(\Gamma_R), \quad \text{for } \frac{1}{2} < \beta < 1$$

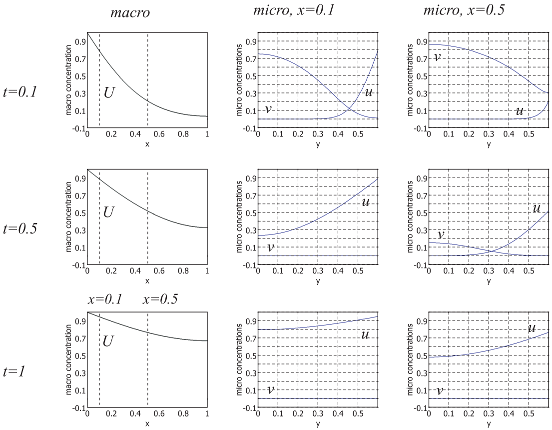
yield the desired convergences.

Key idea for the fast-reaction asymptotics

Get k-independent estimates!

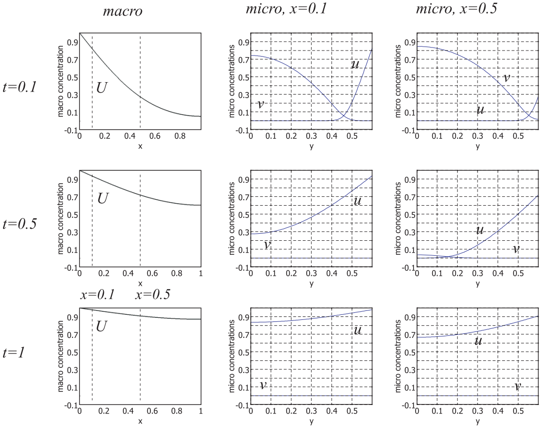
- L^∞-bounds on all concentrations
- energy estimates
- $||\eta(u, v)||_{L^1(S\times\Omega\times Y)} = \mathcal{O}\left(\frac{1}{k}\right)$
- extra two-scale regularity + *assumed* regularity for the micro free boundary
- ...

Concentration profiles in the fast-reaction limit



Solution profiles of the two-scale model at different times ($\boldsymbol{k} = \mathbf{10^3}$). Left columns: Profiles of U. Central and right column: Local cell profiles of u and v at $x = 0.1$ and $x = 0.5$.

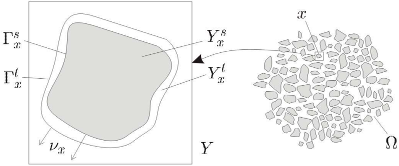
Concentration profiles in the fast-reaction limit



Solution profiles of the two-scale model at different times ($\boldsymbol{k} = \mathbf{10^4}$). Left columns: Profiles of U. Central and right column: Local cell profiles of u and v at $x = 0.1$ and $x = 0.5$.

Open issues

1. Remove the sign condition on the transfer function $b(\cdot)$
2. Any connection between the asymptotics $k \to \infty$ and $t \to \infty$?



3. x-dependent microstructures ...

Related work

- S. Meier, A. Muntean: *A two-scale reaction-diffusion system: Homogenization and fast-reaction limits*. Gakuto Int. Ser. Math. Sci. **32** (2010), 441–459
- A. Muntean, M. Neuss-Radu: *Analysis of a two-scale system for gas-liquid reactions with non-linear Henry-type transfer*. CASA report 09-25, TU Eindhoven, 2009
- T. Fatima, N. Arab, E. Zemskov, A. Muntean: *Homogenization of a reaction-diffusion system modeling sulfate corrosion in locally-periodic perforated domains*. CASA report 09-26, TU Eindhoven, 2009
- S. Meier, A. Muntean: *A two-scale reaction-diffusion system with micro-cell reaction concentrated on a free boundary*. C. R. Mécanique **336**(2008), 481–486
- S. Meier, M. Peter, A. Muntean, M. Böhm, J. Kropp: *A two-scale approach to concrete carbonation* in Proc. Int. RILEM Workshop on Integral Service Life Modeling of Concrete Structures, Guimares, Portugal, 2007, 3–10