On the homogenization of a system of parabolic PDEs modeling mass transfer in heterogeneous catalysis

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Heterogeneous Catalysis

Catalysis

Hastens chemical reactions by lowering the activation energy through alternative mechanisms/pathways

- *Homogeneous*, e.g., acid-catalyzed reactions
- *Heterogeneous*, e.g., use of solid catalysts in liquid solutions

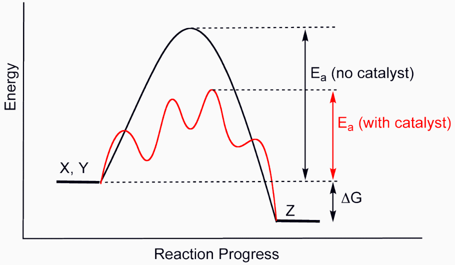

Figure 1: Potential energy diagram for $X + Y \rightarrow Z$

Heterogeneous Catalysis

- Catalyst is of a di erent phase than reactants or products

Figure 2: Model for heterogeneous catalysis

Related literature

- Hornung and Jäger (1991): Stokes equations coupled with reaction-diffusion-advection-adsorption equations, reaction occurs on the surface of the catalyst
- Gahn, Neuss-Radu, Knaber (2016): reaction-diffusion systems in two-component porous media with nonlinear flux conditions
- Gahn, Neuss-Radu, Pop (2021): reaction-diffusion-advection equation in evolving microdomains

Problem Formulation

Model

- Catalysts are uniform and have smooth boundary
- Catalysts are not fixed, i.e., they move together with the fluid
- Movement of fluid and catalyst is assumed to be *known* a priori
- At time $t = 0$, the catalysts are arranged periodically
- Moving domain is described by a diffeomorphism that assumed to be as smooth as necessary, e.g., smooth enough to justify change of variables, necessary regularity of coefficients in PDEs, etc.

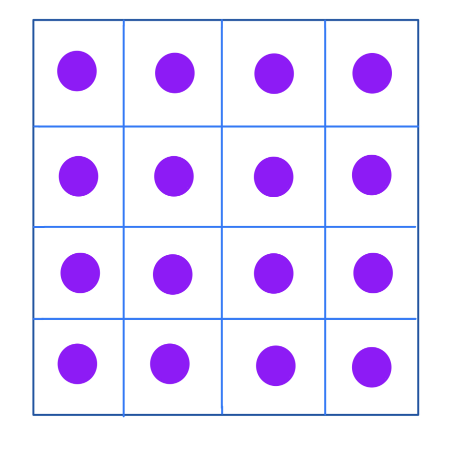

Figure 3: Model of a reactor with catalyst particles at time t=0

Model

$$
\begin{aligned}
\partial_t v_\varepsilon - D_F \Delta v_\varepsilon + u_\varepsilon \cdot \nabla v_\varepsilon &= 0; && \text{in } F_\varepsilon(t)\\
\partial_n v_\varepsilon &= 0; && \text{on } \partial\Omega\\
D_F \partial_n v_\varepsilon &= D_S \partial_n w_\varepsilon; && \text{on } \Gamma_\varepsilon(t)\\
D_F \partial_n v_\varepsilon + {}_\varepsilon (v_\varepsilon - w_\varepsilon) &= 0; && \text{on } \Gamma_\varepsilon(t)\\
\partial_t w_\varepsilon - D_S \Delta w_\varepsilon + r w_\varepsilon &= 0; && \text{in } S_\varepsilon(t)\\
v_\varepsilon(0) &= v_{\varepsilon;0}; && \text{in } F_\varepsilon(0)\\
w_\varepsilon(0) &= w_{\varepsilon;0}; && \text{in } S_\varepsilon(0)
\end{aligned}
$$

Fixed domain problem

The diffeomorphism between the $\Omega(t)$ to $\Omega(0)$, is obtained by solving:

$$
\begin{aligned}
\partial_t X_\varepsilon(t;y) &= b_\varepsilon(t; X_\varepsilon(t;y)), && t \in (0;T) \\
X_\varepsilon(0;y) &= y, && y \in \Omega;
\end{aligned}
$$

where b_ε is:

- equal to the solid velocities in $S_\varepsilon(t)$
- equal to $\mathbf{0}$ outside a neighborhood of $S_{\varepsilon;i}(t)$
- smooth and divergence-free

$$
\begin{aligned}
b_\varepsilon(t;x) := \varphi_\varepsilon(t;x) \sum_i \left(h'_{\varepsilon;i}(t) + M_{\varepsilon;i}(t)(x - h_{\varepsilon;i}(t)) \right) \\
- \sum_i B^{\varepsilon}_{K_i(t)} \left(\nabla\varphi_\varepsilon(t;\cdot) \cdot \left(h'_{\varepsilon;i}(t) + M_{\varepsilon;i}(t)(\cdot - h_{\varepsilon;i}(t)) \right) \right)(x).
\end{aligned}
$$

Roughly, X_ε is

- the identity *away* from the solid catalysts
- a rigid transformation in the solid domain
- a smooth-volume preserving *"glue"* in between

Remark

Observe that, one can instead use the *known* velocity, u_ε, to construct the mapping, i.e., we solve

$$\partial_t X_\varepsilon(t;y) = u_\varepsilon(t; X_\varepsilon(t;y)), \qquad t \in (0,T)$$
$$X_\varepsilon(0;y) = y, \qquad y \in \Omega.$$

However, to guarantee that X_ε has the necessary regularity, requires that u_ε must also be regular. We found it more reasonable to assume that the solid velocities instead satisfy this.

Using the diffeomorphsim, we can map the problem to a fixed domain.

$$
\begin{aligned}
\partial_t v_\varepsilon - \operatorname{div}(A_F^\varepsilon \nabla v_\varepsilon) + U_\varepsilon^1 \cdot \nabla v_\varepsilon &= 0, && (0,T) \times F_\varepsilon \\
A_F^\varepsilon \nabla v_\varepsilon \cdot n &= 0, && (0,T) \times \partial\Omega \\
A_F^\varepsilon \nabla v_\varepsilon \cdot n &= A_S^\varepsilon \nabla w_\varepsilon \cdot n, && (0,T) \times \Gamma_\varepsilon \\
A_F^\varepsilon \nabla v_\varepsilon \cdot n + \alpha_\varepsilon (v_\varepsilon - w_\varepsilon) &= 0, && (0,T) \times \Gamma_\varepsilon \\
\partial_t w_\varepsilon - \operatorname{div}(A_S^\varepsilon \nabla w_\varepsilon) - U_\varepsilon^2 \cdot \nabla w_\varepsilon + \nabla w_\varepsilon &= 0, && (0,T) \times S_\varepsilon \\
v_\varepsilon(0) &= v_{\varepsilon;0}, && \text{in } F_\varepsilon \\
w_\varepsilon(0) &= w_{\varepsilon;0}, && \text{in } S_\varepsilon;
\end{aligned}
$$

where

$$
\begin{aligned}
A_F^\varepsilon(t,x) &:= D_F \nabla X_\varepsilon^{-1}(t,x) \nabla X_\varepsilon^{-T}(t,x) J_{F_\varepsilon}(x); \\
A_S^\varepsilon(t,x) &:= D_S \nabla X_\varepsilon^{-1}(t,x) \nabla X_\varepsilon^{-T}(t,x) J_{S_\varepsilon}(x) \\
U_\varepsilon^1 &:= (\nabla X_\varepsilon)^{-1} (u_\varepsilon \circ X_\varepsilon - \partial_t X_\varepsilon) \\
U_\varepsilon^2 &:= (\nabla X_\varepsilon)^{-1} \partial_t X_\varepsilon
\end{aligned}
$$

We say that $(v_\varepsilon; w_\varepsilon)$ are weak solutions to the fixed domain problem if, for every test function $(\varphi; \psi)$, we have

$$\int_0^T \int_{F_\varepsilon} \left(\partial_t v_\varepsilon + U_\varepsilon^1 \cdot \nabla v_\varepsilon\right) \varphi + \int_0^T \int_{S_\varepsilon} \left(\partial_t w_\varepsilon - U_\varepsilon^2 \cdot \nabla w_\varepsilon\right) \psi$$

$$+ \int_0^T \int_{F_\varepsilon} A_F^\varepsilon \nabla v_\varepsilon \cdot \nabla \varphi + \int_0^T \int_{S_\varepsilon} A_S^\varepsilon \nabla w_\varepsilon \cdot \nabla \psi + \int_0^T \int_{S_\varepsilon} \nabla w_\varepsilon$$

$$= \int_0^T \int_{\Gamma_\varepsilon} \varepsilon (w_\varepsilon - v_\varepsilon)(\varphi - \psi);$$

and $v_\varepsilon(0) = v_{\varepsilon;0}$ and $v_\varepsilon(0) = v_{\varepsilon;0}$.

We have the following result:

Proposition

Let $(v_\varepsilon; w_\varepsilon)$ be the weak solutions of the fixed domain problem. Then if X_ε has sufficient regularity, the functions $\tilde{v}_\varepsilon := v_\varepsilon \circ X_\varepsilon$ and $\tilde{w}_\varepsilon := w \circ X_\varepsilon$ are solutions to our problem in the noncylindrical domain.

Remark
Note that it is important that the time derivatives of the solutions are in L_x^2 rather than in the dual of a Sobolev space. This allows us to do a straightforward change of variables between the fixed and moving domains.

Well-posedness

To establish existence, we construct approximate solutions by solving successively a sequence of steady-state problems.

Indeed, we let $N \in \mathbb{N}$ and $k := \frac{T}{N}$. We set $v_\varepsilon^0 := v_{\varepsilon,0}$ and $w_\varepsilon^0 := w_{\varepsilon,0}$. We then solve:

$$
\begin{aligned}
\frac{v_\varepsilon^m - v_\varepsilon^{m-1}}{k} - \operatorname{div}\left(A_F^{\varepsilon,m} \nabla v_\varepsilon^m\right) + U_\varepsilon^{1,m} \cdot \nabla v_\varepsilon^m &= 0, && \text{in } F_\varepsilon\\
A_F^{\varepsilon,m} \nabla v_\varepsilon^m \cdot n &= 0, && \text{on } \partial\Omega\\
A_F^{\varepsilon,m} \nabla v_\varepsilon^m \cdot n &= A_S^{\varepsilon,m} \nabla w_\varepsilon^m \cdot n, && \text{on } \Gamma_\varepsilon\\
A_F^{\varepsilon,m} \nabla v_\varepsilon^m \cdot n + \varepsilon (v_\varepsilon^m - w_\varepsilon^m) &= 0, && \text{on } \Gamma_\varepsilon\\
\frac{w_\varepsilon^m - w_\varepsilon^{m-1}}{k} - \operatorname{div}\left(A_S^{\varepsilon} \nabla w_\varepsilon^m\right) - U_\varepsilon^{2,m} \cdot \nabla w_\varepsilon^m + r w_\varepsilon^m &= 0, && \text{in } S_\varepsilon,
\end{aligned}
$$

where

$$A_F^{\varepsilon,m}(x) := A_F^\varepsilon(mk, x), \quad A_S^{\varepsilon,m}(x) := A_S^\varepsilon(mk, x),$$

and

$$U_\varepsilon^{i,m} := \frac{1}{k}\int_{(m-1)k}^{mk} U_\varepsilon^i \, dt, \quad i = 1, 2.$$

The approximate solutions are then defined as:

$$v_{\varepsilon,k}(t,x) := \sum_{m=1}^{N} v_\varepsilon^m(x)\,\chi_{[(m-1)k,mk)}(t)$$

$$w_{\varepsilon,k}(t,x) := \sum_{m=1}^{N} w_\varepsilon^m(x)\,\chi_{[(m-1)k,mk)}(t)$$

$$v_{\varepsilon,k}(t,x) := \sum_{m=1}^{N} \left(v_\varepsilon^{m-1}(x) + \frac{v_\varepsilon^m(x) - v_\varepsilon^{m-1}(x)}{k}(t - mk) \right) \chi_{[(m-1)k,mk)}(t)$$

$$w_{\varepsilon,k}(t,x) := \sum_{m=1}^{N} \left(w_\varepsilon^{m-1}(x) + \frac{w_\varepsilon^m(x) - w_\varepsilon^{m-1}(x)}{k}(t - mk) \right) \chi_{[(m-1)k,mk)}(t)$$

From estimates on the approximate solutions, we have that, up to a subsequence, the following convergences hold:

$$
\begin{aligned}
v_{\varepsilon;k} &\rightharpoonup v_\varepsilon; && \text{wk} \quad L^2\left(0;T;H^1(F_\varepsilon)\right)\\
w_{\varepsilon;k} &\rightharpoonup w_\varepsilon; && \text{wk} \quad L^2\left(0;T;H^1(S_\varepsilon)\right)\\
\partial_t v_{\varepsilon;k} &\rightharpoonup \partial_t v_\varepsilon; && \text{wk} \quad L^2\left(0;T;H^1(F_\varepsilon)\right)\\
\partial_t w_{\varepsilon;k} &\rightharpoonup \partial_t w_\varepsilon; && \text{wk} \quad L^2\left(0;T;H^1(S_\varepsilon)\right) :
\end{aligned}
$$

One can then show that $(v_\varepsilon; w_\varepsilon)$ are our desired solution. Indeed, we have

Theorem

There exists a unique weak solution $(v_\varepsilon; w_\varepsilon)$ to the fixed domain problem.

As mentioned previously, in order to have the correspondence between fixed and moving domain solutions, we need the time derivatives to be in L^2_x. Indeed, we have shown

Theorem

Suppose that $(v_{\varepsilon;0}; w_{\varepsilon;0}) \in H^1(F_\varepsilon) \times H^1(S_\varepsilon)$. Then $\partial_t v_\varepsilon \in L^2\left(0;T;H^1(F_\varepsilon)\right)$ and $\partial_t v_\varepsilon \in L^2\left(0;T;H^1(F_\varepsilon)\right)$.

Remark

Uniqueness and stability follow from the estimates.

Homogenization

Motivation

- Heterogeneous behavior can be very complex.
- Is it possible if there is a simpler model that solutions tend to?

Figure 4: Illustration of xed bed and uidized bed reactors

Suppose A is a bounded Y-periodic function, $f \in L^2(\Omega)$. Consider,

$$
\begin{aligned}
-\operatorname{div}\left(A\left(\tfrac{x}{\varepsilon}\right)\nabla u_\varepsilon\right) &= f, \quad \text{in } \Omega \\
u_\varepsilon &= 0, \quad \text{on } \partial\Omega
\end{aligned}
$$

Its weak formulation is given by:

$$
\int_\Omega A\left(\frac{x}{\varepsilon}\right)\nabla u_\varepsilon(x)\cdot\nabla\varphi(x)\,dx = \int_\Omega f(x)\varphi(x)\,dx,
$$

for all $\varphi \in H^1_0(\Omega)$.

Classical example

We know that

$$u_\varepsilon \rightharpoonup u_0 \quad \text{weakly in } H^1(\Omega)$$

$$A\left(\frac{x}{\varepsilon}\right) := A_\varepsilon \rightharpoonup M_Y(A) \quad \text{weakly in } L^2(\Omega)$$

However, it is not true that

$$A_\varepsilon \nabla u_\varepsilon \rightharpoonup M_Y(A) \nabla u_0 \quad \text{weakly in } L^2(\Omega) \ .$$

In fact, u_0 is the unique weak solution of

$$-\operatorname{div}(A_0 \nabla u_0) = f \, ; \quad \text{in } \Omega$$
$$u_0 = 0 \, ; \quad \text{on } \partial\Omega \, ;$$

where $a_0^{ij} = \sum_{k=1}^{N} |Y|^{-1} \int_Y \left(a^{ij} - a^{ik} \partial_{y_k} \chi_j \right) dy$ and χ_j's are solutions to a unit cell problem.

Definition

Let Ω and Y be bounded open sets in $\mathbb{R}^n$, and $T > 0$. A sequence $\{u_\varepsilon\}$ in $L^2((0;T)\times\Omega)$ is said to two-scale converge to a limit $u \in L^2((0;T)\times\Omega\times Y)$ if

$$\lim_{\varepsilon\to 0}\int_0^T\int_\Omega u_\varepsilon(t;x)\,\psi\left(t;x;\frac{x}{\varepsilon}\right)dx\,dt = \frac{1}{|Y|}\int_0^T\int_\Omega\int_Y u(t;x;y)\,\psi(t;x;y)\,dy\,dx\,dt;$$

for all $\psi \in L^2((0;T)\times\Omega;\, C_{per}(Y))$.

Proposition

1. Every bounded sequence $\{u_\varepsilon\}$ in $L^2((0,T)\times\Omega)$ has a two-scale convergent subsequence.
2. Let $\{u_\varepsilon\}$ be a bounded sequence in $L^2\left((0,T);H^1(\Omega)\right)$. Then there exists $u_0 \in L^2\left((0,T);H^1(\Omega)\right)$ and $u_1 \in L^2\left((0,T)\times\Omega;H^1_{per}(Y)\right)$ and a subsequence, still denoted by u_ε, such that

$$u_\varepsilon \to u_0 \qquad \text{in the two-scale sense},$$
$$\nabla u_\varepsilon \to \nabla_x u_0 + \nabla_y u_1 \qquad \text{in the two-scale sense}.$$

De nition

Let f u g be a sequence such that u 2 $L^2((0;T)$) for each > 0. We say that u converges in the two-scale sense on the surface to a limit u_0 2 $L^2((0;T)$) if

$$\lim_{\,!\,0} \int_0^T \int u(t;x) \quad t;x;\frac{x}{} \; dS_x \, dt = \int_0^T \int \int u_0(t;x;y) \; (t;x;y) \, dS_y \, dx \, dt;$$

for all 2 $L^2((0;T)$; $C_{per}($)).

Proposition

Let $\{ u \}$ be a sequence of functions such that $u \in L^2((0;T)\quad)$ for each > 0. Suppose $\sqrt{\;}\;\|u\|_{L^2((0;T)\quad)} \quad C$ for some constant $C > 0$, independent of . Then a subsequence exists that converges in the two-scale sense on .

Theorem

Let v be the uid solution and v be its zero extension. Then, there exist $v^0 \in L^2(0,T;H^1( ))$ and $v^1 \in L^2((0,T) \; ; H^1_{per}(Y))$ such that, up to a subsequence, the following holds

$$v \to v^0 1_{Y_F} \qquad \text{in the two-scale sense}$$

$$\overline{\nabla v} \to \nabla_x v^0 + \nabla_y v^1 \qquad \text{in the two-scale sense}$$

$$v| \to v^0 \qquad \text{strongly in the two-scale sense on}$$

$$\partial_t v \rightharpoonup |Y_F| \partial_t v^0 \qquad \text{weakly in } L^2(0,T;H^1( ) \quad)$$

Theorem

Let w be the solid solution and w be its zero extension. Then, there exists $w^0 \in L^2((0;T) \quad)$ such that, up to a subsequence, the following holds

$$w \to Y_S w^0 \qquad \text{strongly in the two-scale sense}$$

$$\overline{\nabla w} \to 0 \qquad \text{in the two-scale sense}$$

$$w| \to w^0 \qquad \text{strongly in the two-scale sense on}$$

$$\partial_t w \rightharpoonup |Y_S| \partial_t w^0 \qquad \text{weakly in } L^2(0;T;\ H^1(\ ) \quad)$$

Key points

We make the assumption

$$\int_0^T \int \left| A^{F(\varepsilon/S)}(t,x) - A_0^{F(\varepsilon/S)}\left(t,x,\frac{x}{\varepsilon}\right) \right|^2 dx\,dt \to 0, \quad \text{as } \varepsilon \to 0;$$

This is crucial because two-scale convergence requires the use of special test functions.

In the classical example, periodicity and boundedness assumptions on the coefficient matrix allow us to use directly two-scale convergence to take limits.

As a demonstration of the use of this assumption, we have

$$\int_0^T \int_{F^\varepsilon} A^F_\varepsilon(t,x)\nabla v_\varepsilon(t,x) \cdot \nabla(\varphi_\varepsilon(x))\,\psi(t)\,dx\,dt$$

$$= \int_0^T \int_{F^\varepsilon} \overline{\nabla v_\varepsilon}\; A_0^F\left(t,x,\frac{x}{\varepsilon}\right) \nabla(\varphi_\varepsilon(x))\,\psi(t)\,\chi_{Y_F}\left(\frac{x}{\varepsilon}\right) dx\,dt$$

$$+ \int_0^T \int_{F^\varepsilon} \overline{\nabla v_\varepsilon} \left(A_\varepsilon^F(t,x) - A_0^F\left(t,x,\frac{x}{\varepsilon}\right)\right) \nabla(\varphi_\varepsilon(x))\,\psi(t)\,\chi_{Y_F}\left(\frac{x}{\varepsilon}\right) dx\,dt$$

$$\xrightarrow{\varepsilon \to 0} \int_0^T \int_{\Omega} \int_{Y_F} A_0^F(t,x,y)\left(\nabla_x v^0(t,x) + \nabla_y v^1(t,x,y)\right) \cdot \left(\nabla\varphi(x) + \nabla_y \varphi^1(x,y)\right)\psi(t)\,dy\,dx\,dt.$$

Key points

Another key point is, because Y_S is compactly contained in Y, one can show that

$$\overline{\nabla w_\varepsilon} \to 0 \quad \text{in the two-scale sense.}$$

This, then leads us to conclude that the limit function w^0 solves an ODE.

Key points

We summarize these results, together with the results for the fluid solution in the following theorem:

Theorem

v^0, v^1, and w^0 are the the unique weak solutions of

$$\operatorname{div}_y \left(A_F^0(t;x;y) \left(\nabla_x v^0(t;x) + \nabla_y v^1(t;x;y) \right) \right) = 0; \quad \text{in } (0;T) \qquad Y$$

$$|Y_F|\, \partial_t v^0 \quad \operatorname{div}_x \int_{Y_F} A_F^0(t;x;y) \left(\nabla_x v^0(t;x) + \nabla_y v^1(t;x;y) \right) dy$$

$$= |\;| \quad v^0(t;x) \quad w^0(t;x) \quad \text{in } (0;T)$$

$$\partial_t w^0 + \nabla w^0(t;x) = \frac{|\;|}{|Y_S|} \quad w^0(t;x) \quad v^0(t;x) \quad \text{in } (0;T)$$

We also have a corrector result.

Theorem

The following holds:

$$\int_0^T\int_{F_\varepsilon} |v_\varepsilon - v_0|^2 + \int_0^T\int_{S_\varepsilon} |w_\varepsilon - w_0|^2 + \int_0^T\int_F \left|\nabla v_\varepsilon(t,x) - \nabla v_0(t,x) - \nabla_y v^1\left(t,x,\frac{x}{\varepsilon}\right)\right|^2 \to 0, \quad \text{as } \varepsilon \to 0.$$

- Note that the Sobolev compactness theorem does not hold for $v_\varepsilon, w_\varepsilon$ since they are not in $H^1(\Omega)$.
- Alternatives:
  - Sobolev extensions (Gahn, Neuss-Radu, Knaber 2016), (Cioranescu, Saint Jean Paulin 1979)
  - Extensions of the Rellich theorem in perforated domains (Allaire, Murat 1993)
- In our result, we used the fact that $(v_\varepsilon; w_\varepsilon)$ are solutions to a PDE to give us the strong convergence.

error products of two-scale convergent sequences

terms that go to zero

+ terms that are asymptotically nonpositive

Examples

We consider the case when the solid velocities satisfy $\|U_{S,\varepsilon}\|_\infty \leq \varepsilon^\alpha$ for some $\alpha > 1$.

In this case, one can show that $\|b_\varepsilon\|_\infty \leq \varepsilon^\alpha$ and $\|\nabla b_\varepsilon\|_\infty \leq \varepsilon^{\alpha-1}$.

Thus,

$$\nabla X_\varepsilon(t;y) = e^{\int_0^t \nabla b_\varepsilon(s;X_\varepsilon(s;y))\,ds}.$$

And hence,

$$\nabla X_\varepsilon \to I, \quad \text{in } L^\infty((0,T)\times\Omega).$$

.

The limit problem then reads as

$$
\begin{aligned}
&\mathrm{div}_y \left(\nabla_x v^0(t,x) + \nabla_y v^1(t,x,y) \right) = 0, \quad \text{in } (0,T) \times Y_F \\
&|Y_F|\, \partial_t v^0 - \mathrm{div}_x \int_{Y_F} D_F \left(\nabla_x v^0(t,x) + \nabla_y v^1(t,x,y) \right) dy \\
&\qquad = -|\ |\left(v^0(t,x) - w^0(t,x) \right) \quad \text{in } (0,T) \\
&\partial_t w^0 + r w^0(t,x) = \frac{|\ |}{|Y_S|} \left(w^0(t,x) - v^0(t,x) \right) \quad \text{in } (0,T)
\end{aligned}
$$

We consider the case a similar case as previously but now with = 1 and the solid velocities are assumed to be periodic in space, i.e., the motion is the same for each cell but are not necessarily periodic in time.

In this case, one can show that

$$b_\varepsilon(t;x) = \varepsilon b\left(t;\frac{x}{\varepsilon}\right)$$

$$X_\varepsilon(t;x) = \varepsilon X\left(t;\frac{x}{\varepsilon}\right);$$

where b is the extension of the solid velocity in the unit cell to the whole cell and X is the diffeomorphism obtained from b.

So that the coefficient matrices satisfy

$$A^F_\varepsilon(t,x) = A^0_F\left(t,\frac{x}{\varepsilon}\right) := D_F 1_{Y_F}\left(\frac{x}{\varepsilon}\right)(\nabla X)^{-T}\left(t,\frac{x}{\varepsilon}\right)(\nabla X)^{-1}\left(t,\frac{x}{\varepsilon}\right)$$

$$A^S_\varepsilon(t,x) = A^0_S\left(t,\frac{x}{\varepsilon}\right) := D_S 1_{Y_S}\left(\frac{x}{\varepsilon}\right)(\nabla X)^{-T}\left(t,\frac{x}{\varepsilon}\right)(\nabla X)^{-1}\left(t,\frac{x}{\varepsilon}\right):$$

. Here, the limit problem reads as

$$-\mathrm{div}_y\left(A^0_F(t,y)\left(\nabla_x v^0(t,x) + \nabla_y v^1(t,x,y)\right)\right) = 0, \quad \text{in } (0,T)\times\Omega\times Y_F$$

$$|Y_F|\,\partial_t v^0 - \mathrm{div}_x\left(\int_{Y_F} A^0_F(t,y)\left(\nabla_x v^0(t,x) + \nabla_y v^1(t,x,y)\right)dy\right) = |\Gamma|\left(v^0(t,x) - w^0(t,x)\right) \quad \text{in } (0,T)\times\Omega$$

$$\partial_t w^0 + r w^0(t,x) = \frac{|\Gamma|}{|Y_S|}\left(w^0(t,x) - v^0(t,x)\right) \quad \text{in } (0,T)\times\Omega:$$

Note that A^0_F is not the identity matrix since ∇X is not an orthogonal matrix nor the identity matrix.

Future Work

Future work

Figure 5: Model for heterogeneous catalysis

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