Geometry controlled dispersion in periodic channels

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How to characterize the dispersion of small particles in channels ?

1. **Introduction : dispersion in confined media**
2. **The Fick-Jabobs approximation : study of narrow channels**
3. **Different regimes of dispersion : narrow to wide channels**
4. **Special case of narrow discontinuous channels**
5. **Conclusion**

1 Introduction : dispersion in confined media

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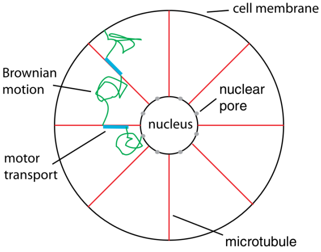
Some examples of dispersion in confined media 1

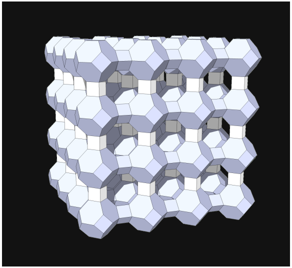
- How fast does a cloud of tracer particles disperse in heterogeneous media ?
- Active field of research.

biological cells



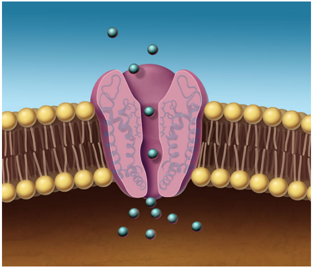
Bressloff and Newby, RMP (2013)

zeolites



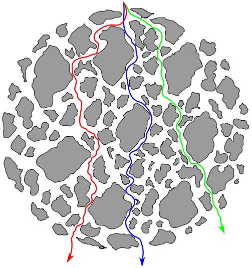
Karger and Ruthven (1992)

ion channels



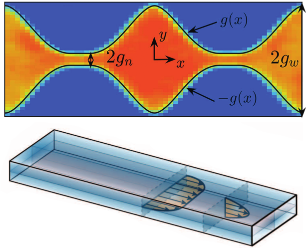
Some examples of dispersion in confined media 2

contaminant spreading in porous media



Leitmann and Franosch, PRL (2017)

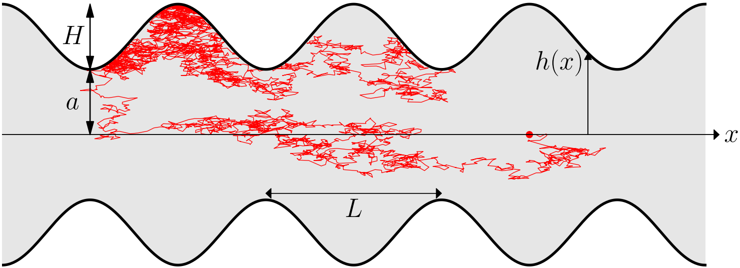
microfluidic devices



Yang *et al.*, PNAS (2017)

Aminian *et al.*, Science (2016)

The dispersion in symmetric two-dimensional periodic channels



- Periodicity of the channel : $\boldsymbol{L}$.
- Height of the channel : $\boldsymbol{h(x) = a\zeta(x)}$, where a is the minimum height.
- We define $\boldsymbol{\varepsilon = a/L}$ and $\boldsymbol{\xi = H/a}$, where H is the variation of height.
- Microscopic, homogeneous and isotropic, diffusivity $\boldsymbol{D_0}$. What global dispersion appears at long time ?
- Long-time effective diffusivity along the channel : $\boldsymbol{D_e} = \lim_{t\to\infty} \frac{\overline{x^2(t)}}{2t}$.

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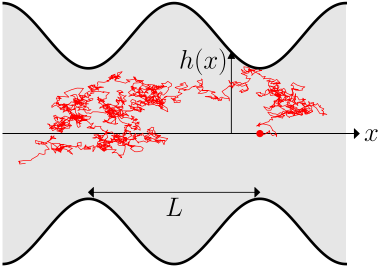
Famous traditional approach : reduction to one-dimensional problem



- narrow regions = entropic barriers
- wide regions = entropic traps
- Entropic trapping of particles
- Slowing down of dispersion

$$D_e \leq D_0$$

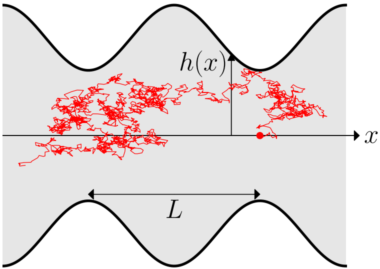
- Marginal stationary probability $p_s^*(x) \propto h(x) \propto \exp[-\beta\varphi(x)]$
- Effective potential $-\beta\varphi(x) = \ln h(x)$
- Long-time effective diffusivity

$$\frac{D_e}{D_0} = \frac{1}{\langle \exp(-\beta\varphi) \rangle \langle \exp(\beta\varphi) \rangle} = \frac{1}{\langle h \rangle \langle h^{-1} \rangle} \leq 1 \text{ [Jensen's inequality]}$$

- Spatial average

$$\langle h \rangle = \frac{1}{L} \int_0^L dx \; h(x)$$

Fick-Jacobs' one-dimensional equation



- Effective one-dimensional potential

$$-\beta\varphi(x) = \ln h(x)$$

- Effective one-dimensional diffusivity

$$D(x) = D_0\left(1 - \frac{1}{3}h'(x)^2 + \cdots\right)$$

- Modified Fick-Jacobs' equation

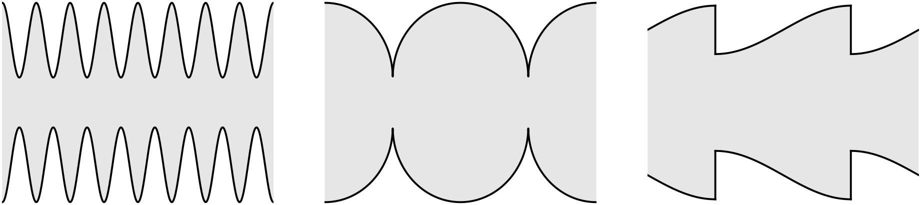
$$\frac{\partial p^*}{\partial t} = \frac{\partial}{\partial x}D(x)\left[\frac{\partial p^*}{\partial x} + \beta\varphi'(x)p^*\right]$$

- Long-time effective diffusivity

$$D_e = \frac{1}{\langle h\rangle\langle D^{-1}h^{-1}\rangle}$$

Limits of Fick-Jacobs improvements

- The FJ approximation is valid for slowly varying channels ($h'(x) \ll 1$).
- The effective one-dimensional process is clearly non Markovian, the definition of an effective diffusivity $D(x)$ is not valid.
- What happens for wide channels ($\varepsilon \gg 1$) ? the intermediate range of ε ? sharp-neck channels ? discontinuous channels ? ($h'(x) = \infty$)



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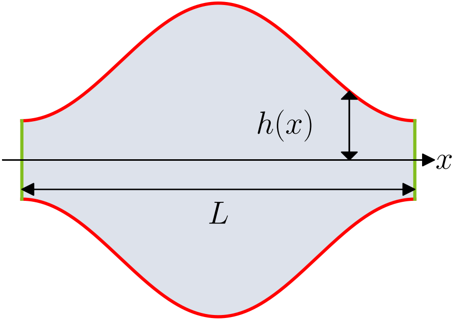
Starting point : Exact formula of D_e, non relying on 1d-reduction

- Explicit equation for the long-time effective diffusivity

$$\frac{D_e}{D_0} = 1 - \frac{1}{\langle h \rangle} \int_0^L dx\ h'(x)\ f(x, h(x))$$

- Partial differential equations for the auxilliary function $f(x, y)$



$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$

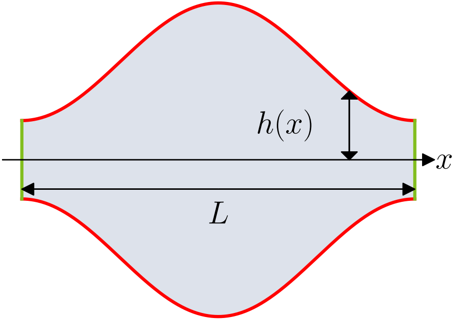
$$h'(x)\ \frac{\partial f}{\partial x}\bigg|_{y=h(x)} - \frac{\partial f}{\partial y}\bigg|_{y=h(x)} = h'(x)$$

$$f(x+L, y) = f(x, y)$$

Guérin and Dean, PRE (2015)

Simplifications using complex analysis

- Auxilliary function f as an analytic function $w(z = x + iy)$



$$f(x,y) = \frac{1}{2}[w(x+iy) + w(x-iy)] \\ = \mathrm{Re}\, w(x+iy)$$

$$\mathrm{Im}\, w(x + ih(x)) = h(x) - C$$

$$w(z+L) = w(z)$$

- Long-time effective diffusivity

$$\frac{D_e}{D_0} = \frac{C}{\langle h \rangle}$$

Back to the Fick Jacobs approximation when $\varepsilon \ll 1$

- Corrections up to $\mathcal{O}(\varepsilon^6)$:

$$\frac{D_e}{D_0} = \frac{C_0 - \varepsilon^2 C_2 + \varepsilon^4 C_4 - \varepsilon^6 C_6}{\langle \zeta \rangle}$$

- The expression of C_i are given by

$$C_0 = \langle \zeta^{-1} \rangle^{-1}$$

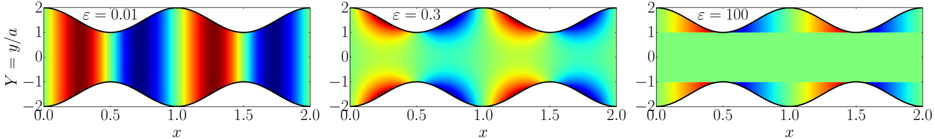
$$C_2 = \frac{\langle \zeta'^2 / \zeta \rangle}{3 \langle \zeta^{-1} \rangle^2}$$

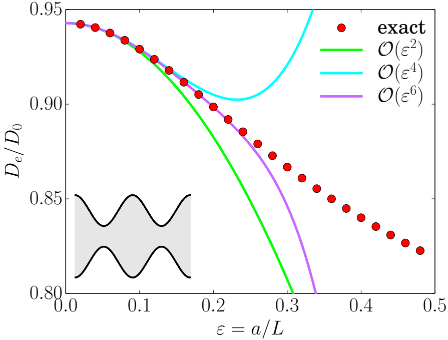
$$C_4 = \frac{\langle \zeta'^2 / \zeta \rangle^2}{9 \langle \zeta^{-1} \rangle^3} + \frac{4 \langle \zeta'^4 / \zeta \rangle + \langle \zeta''^2 \zeta \rangle}{45 \langle \zeta^{-1} \rangle^2}$$

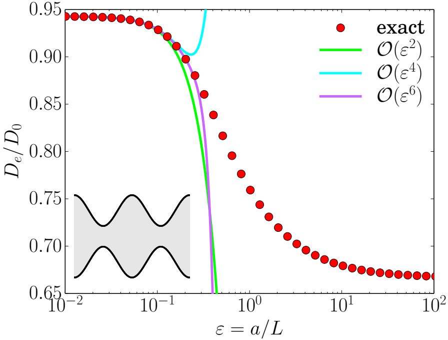
$$C_6 = \frac{\langle \zeta'^2 / \zeta \rangle^3}{9 \langle \zeta^{-1} \rangle^4} + \frac{8 \langle \zeta'^4 / \zeta \rangle + 2 \langle \zeta''^2 \zeta \rangle}{45 \langle \zeta^{-1} \rangle^3} \frac{\langle \zeta'^2 / \zeta \rangle^2}{3} + \cdots$$

$$\cdots + \frac{44 \langle \zeta'^6 / \zeta \rangle + 5 \langle \zeta^2 \zeta''^3 \rangle + 45 \langle \zeta'^3 \zeta''^2 \rangle + 2 \langle \zeta^3 \zeta'''^2 \rangle}{945 \langle \zeta^{-1} \rangle^2}$$

Numerical results : validity of the perturbative expansion

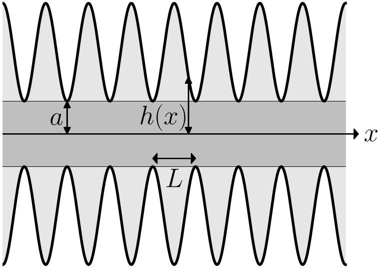






- Improvements of D_e at each order.
- What happens for wide channels ($\varepsilon \gg 1$) ?

Entropic trapping of particles in wide channels



- Particles trapped in regions $|y| > a$

$$\overline{x^2(t)} \geq 2D_0 t'$$

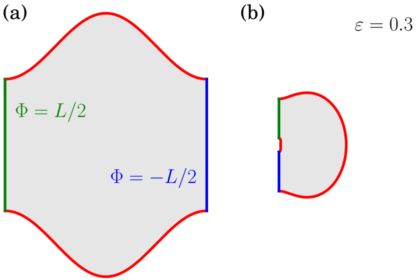
- t' is the time spend in $|y| < a$ region.

- The long-time effective diffusivity is bounded

$$1 \geq \frac{D_e}{D_0} \geq \frac{t'}{t} = \frac{a}{\langle h \rangle}$$

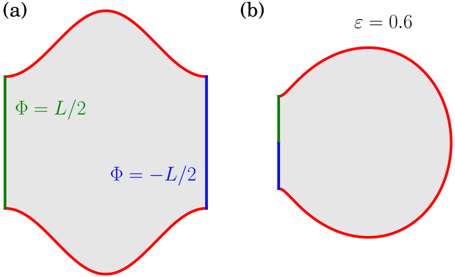
- For $a \gg L$, the lower bound becomes exact.
- Presence of a boundary layer at $y = a$.

Finding the finite corrections in the wide channel regime



- Conformal mapping $G(z) = \exp[-i\pi(z - ia)]$

Finding the finite corrections in the wide channel regime



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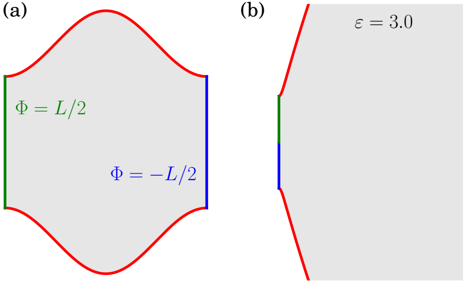

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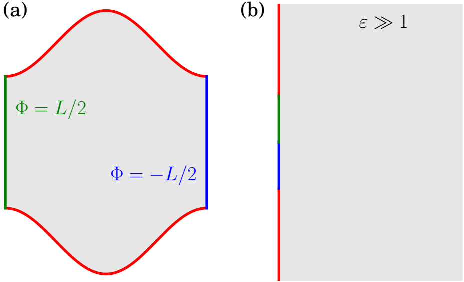


- Conformal mapping $G(z) = \exp[-i\pi(z - ia)]$
- Long-time effective diffusivity, with a correction $\mathcal{O}(1/\varepsilon)$

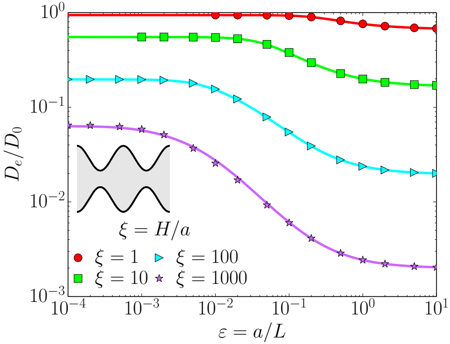
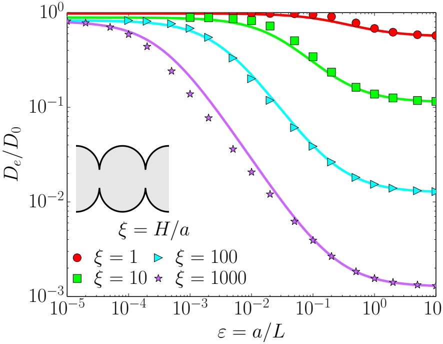
$$\frac{D_e}{D_0} = \frac{a}{\langle h \rangle}\left(1 + \frac{\ln 2}{\pi\varepsilon}\right)$$

- Identification of a universal constant $\ln 2/\pi$.

Intermediate regime of dispersion

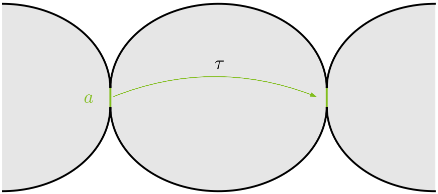
- Padé approximant with $\varepsilon \ll 1$ and $\varepsilon \gg 1$ expansions

$$\frac{D_e}{D_0} = \frac{1}{\langle h \rangle \langle h^{-1} \rangle} \frac{1 + a_1\varepsilon + a_2\varepsilon^2 + \cdots}{1 + b_1\varepsilon + b_2\varepsilon^2 + \cdots}$$

- The Padé approximant fit well the numerical data for smooth channels.
- What happens in the large-ξ limit, in presence of small openings ?

Narrow escape regime for small openings

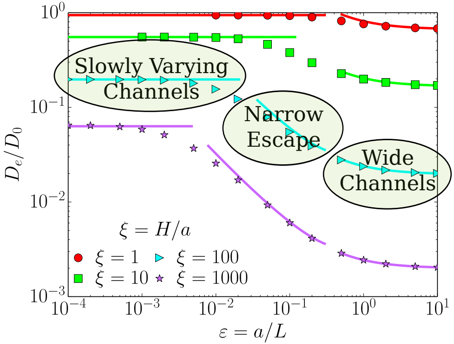


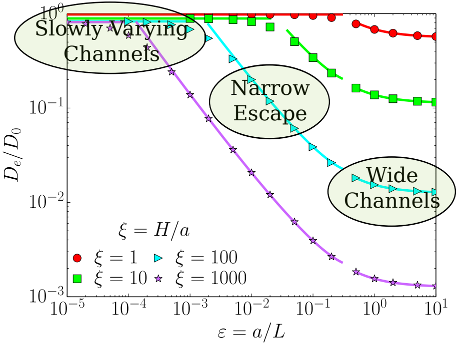
- τ : FPT to reach a small opening
- Long-time effective diffusivity

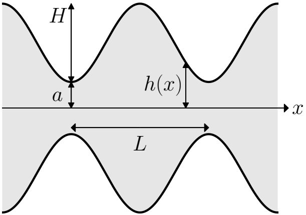
$$\frac{D_e}{D_0} = \frac{L^2}{2D_0\tau} = \frac{L}{\langle h \rangle} \frac{\pi}{2\ln(K/\varepsilon)}$$

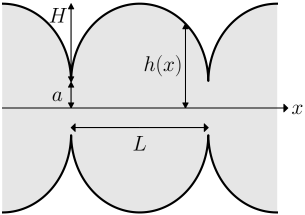
- Expression valid for $\varepsilon \ll 1$ and $\xi \gg 1$.

Classification of dispersion regimes









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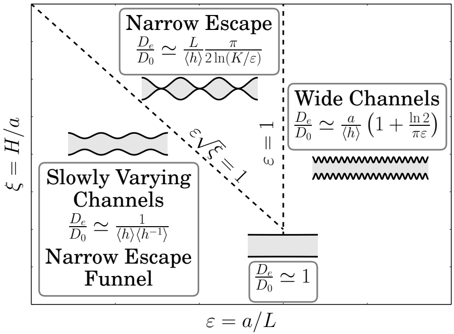

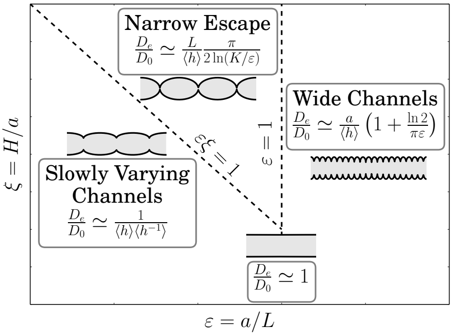

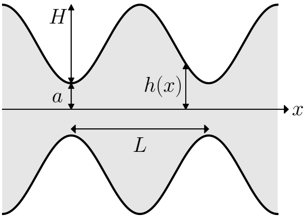

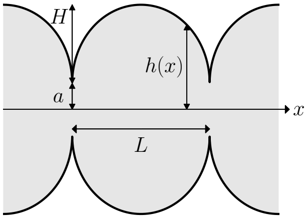

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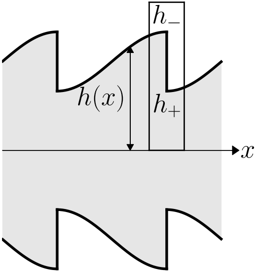
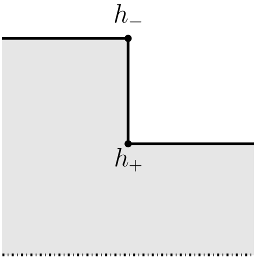
Failure of perturbation theory ($h'(x) = \infty$)



- Discontinuity at $x = 0$. Perturbative solution valid at $x \neq 0$.
- Boundary layer at the discontinuity.

Failure of perturbation theory ($h'(x) = \infty$)



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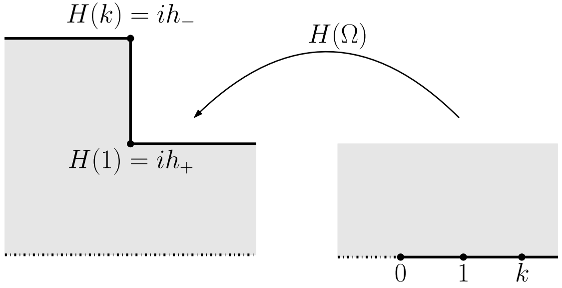
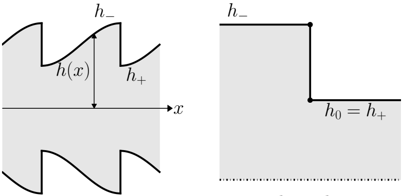


- Discontinuity at $x = 0$. Perturbative solution valid at $x \neq 0$.
- Boundary layer at the discontinuity.
- Conformal mapping $z = H(\Omega)$ via a Schwarz-Christoffel transformation.
- Long-time effective diffusivity, with a correction $\mathcal{O}(\varepsilon)$ instead of $\mathcal{O}(\varepsilon^2)$!

$$\frac{D_e}{D_0} = \frac{1}{\langle h \rangle \langle h^{-1} \rangle} \left(1 - \frac{\varepsilon}{\pi \langle \zeta^{-1} \rangle} \sum_i \gamma(\nu_i) \right)$$

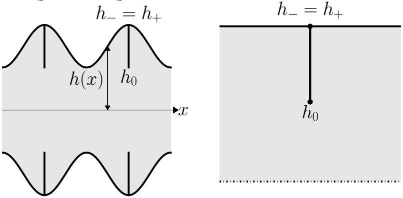
- The discontinuity plays the role of a local trap.

Three kinds of discontinuities



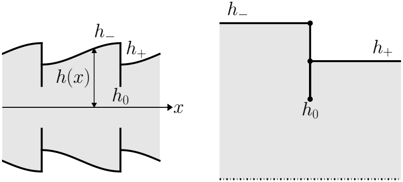
$$\gamma(\nu) = \frac{1+\nu^2}{\nu} \ln \frac{1+\nu}{1-\nu} - 2 \ln \frac{4\nu}{1-\nu^2}$$

$$\nu = h_+/h_- \leq 1$$



$$\gamma(\nu) = -4 \ln \sin \frac{\pi\nu}{2}$$

$$\nu = h_0/h_- \leq 1$$



$$\gamma(\nu, \tilde{\nu}) = \frac{1+(\nu\tilde{\nu})^2}{\nu\tilde{\nu}} \ln \frac{\nu+\tilde{\nu}}{\nu-\tilde{\nu}} - 2 \ln \frac{4\nu\tilde{\nu}}{\nu^2-\tilde{\nu}^2}$$

ν and $\tilde{\nu}$ functions of h_0/h_- and h_0/h_+.

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What we have characterized

- Exact PDEs to get the effective diffusivity, simplified by the use of complex analysis in two dimensions through a compact formalism.
- Fick-Jacobs approximation revisited and wide channels limit characterized by a universal constant.
- Classification of all regimes of dispersion for periodic smooth-neck and sharp-neck channels.
- Discontinuities associated to an effective local trapping.
- The dispersion of particles is controlled by the geometry of the channel.

Geometry controlled dispersion in periodic corrugated channels, EPL **118**, 40004 (2017).

Dispersion in two dimensional channels - the Fick-Jacobs approximation revisited, J. Stat. Mech. (2017), 123205.

Dispersion in two dimensional periodic channels with discontinuous profiles, in preparation.

What is the next step ?

- What happens with a longitudinal force ? In presence of hydrodynamics flows for example.
- What happens with a normal force ? In presence of gravity for example.
- How to characterize the dispersion in moving channels $h(x,t)$? For biological systems for example.
- Is the complex analysis possible in 3-dimensions ?

Thank you for your attention !