Dispersion with memory in porous media: fractal MIM MODEL

fluxes and dispersion equation for the transport of particles, which can get trapped in some sites of the solid matrix

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organization

1. Motivation
2. Fractional MIM model for diffusion with memory
3. Random walk with IMMOBILIZATION PERIODS and limiting process
4. Non-Fickian flux with memory for such random walks
5. Illustration: comparisons random walks/discretization of Fractional MIM model

1. Motivation

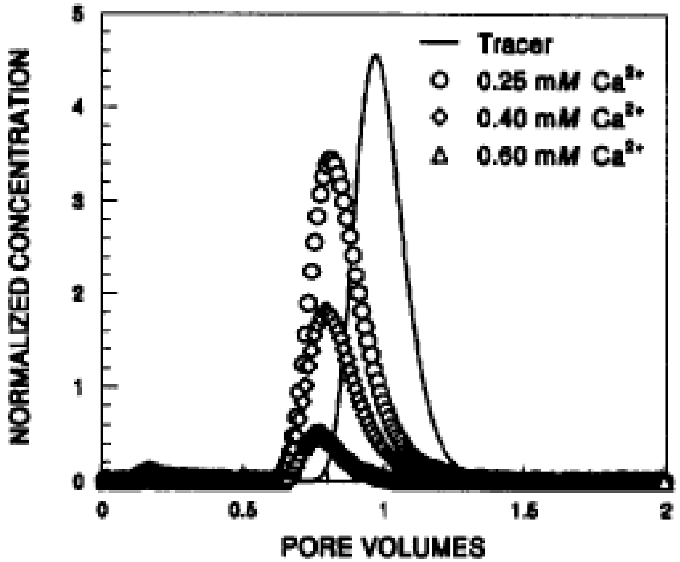
1.a. depending on medium AND tracer a contaminant can spread FASTER or SLOWER than according to ADE with v=Darcy's flow

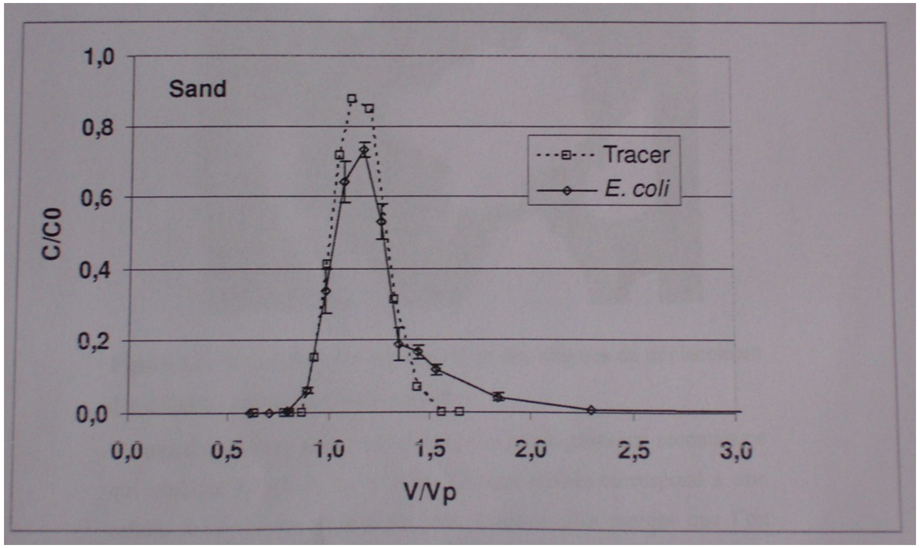
both effects may combine without equilibrating

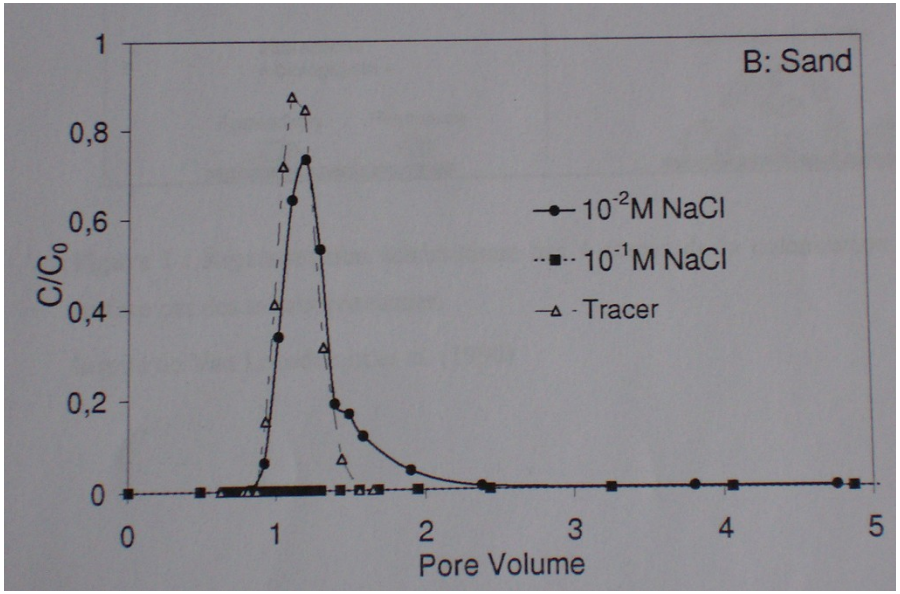
SLOWER is apparently the more significant when tracer=colloid (more especially BACTERIA) and WITH PASSIVE TRACERS in UNSATURATED MEDIA more especially in bounded domains?

1.b. Memory effects, not included in ADE: Breakthrough curves with heavy tails

with bacteria







particles seem to be retained in the medium
then released

2. Fract(ion)al MIM model

2.a Models for diffusion with that memory effects

MIM model

$$\partial_t C(x,t) = (K\Delta - v\nabla)C(x,t) - \beta(C - C_1)$$

$$\partial_t C_1(x,t) = \alpha(C - C_1)$$

$$(\partial_t + \lambda h(t) * \partial_t) C(x,t) = (K\Delta - v\nabla)C(x,t)$$

$$h(t) = e^{-\alpha t}$$

fractional Fokker Planck equation

$$\partial_t^{\gamma} C(x,t) = (K\Delta - v\nabla)C(x,t)$$

2.b Fractional MIM model /fractional diffusion equation

fractional MIM model

$$(Id+\lambda I^{1-\gamma})\partial_t C(x,t)=-\nabla.(K\nabla-v)C(x,t)$$

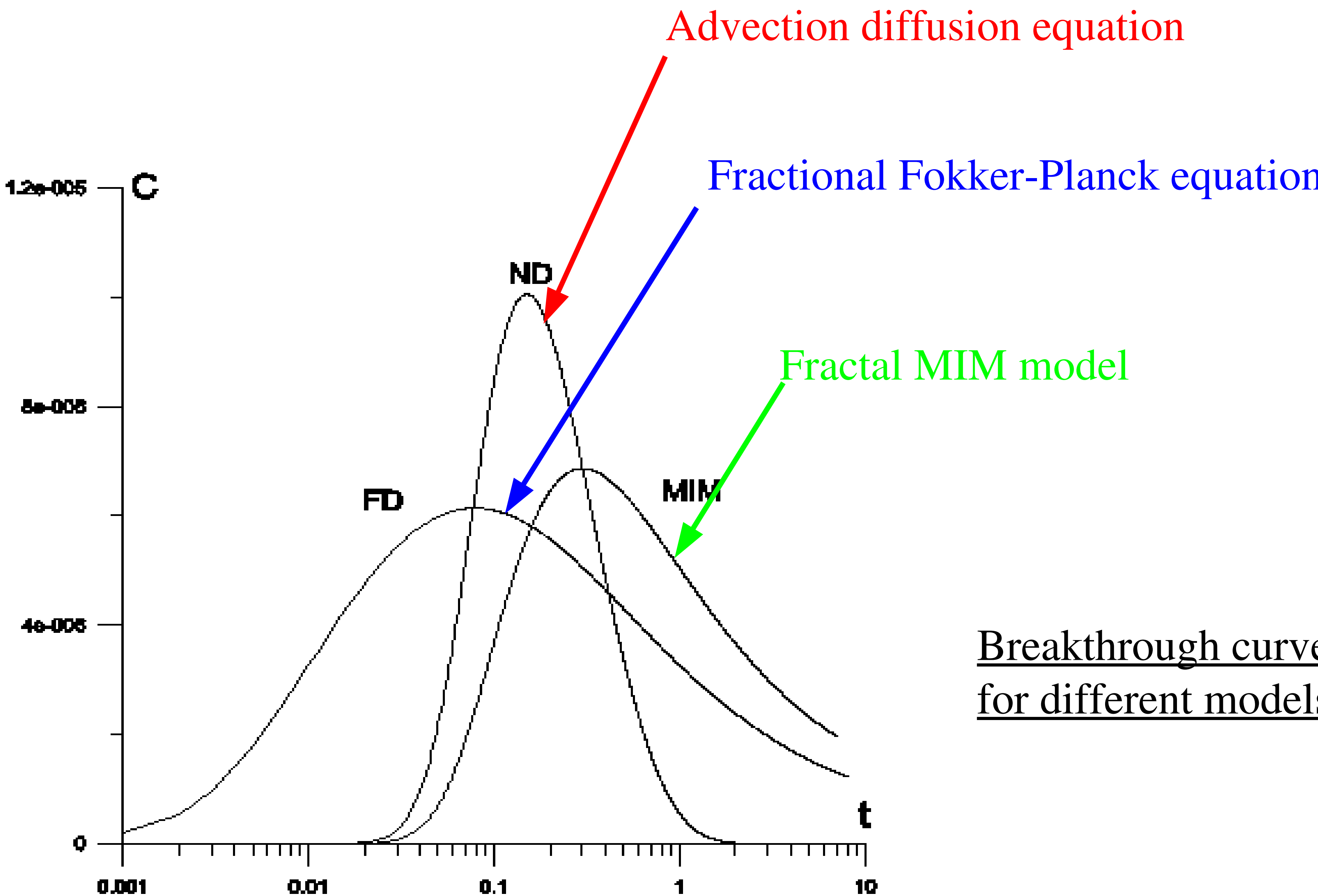
$$I^{\beta}f(t)=\frac{1}{\Gamma(\beta)}\int_0^t (t-t')^{\beta-1}f(t')\,dt'$$

convolution with power kernel

conservative form

$$\partial_t C(x,t)=-\nabla.(K\nabla-v)(Id+\lambda I^{1-\gamma})^{-1}C(x,t)$$

flux



Breakthrough curves for different models

3. Random walks

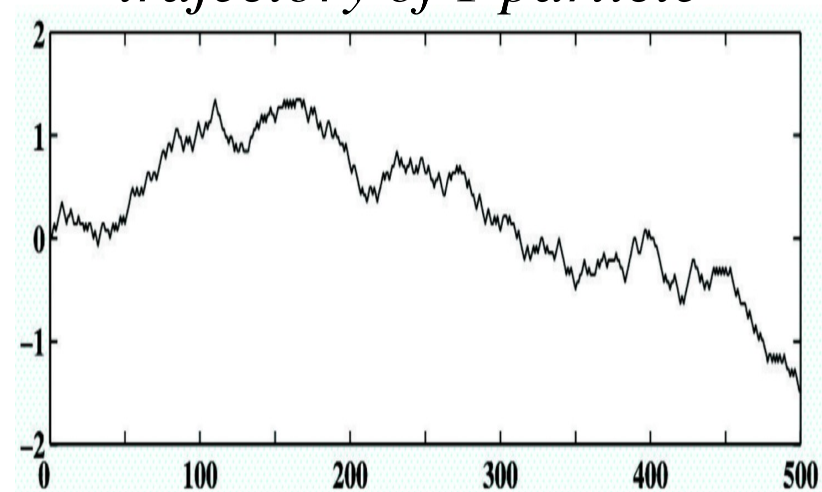
3.a. Brownian motion

For particles performing random jumps after each time step τ
w.r.t. a frame, moving at speed v

successive jumps: independent gaussian random variables,
distributed as $N(0,l)$

$K = l^2/2\tau \qquad l,\tau \longrightarrow 0$

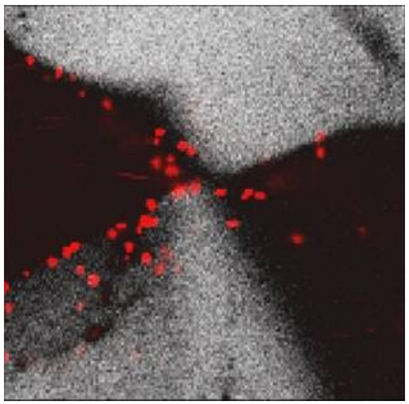
trajectory of 1 particle



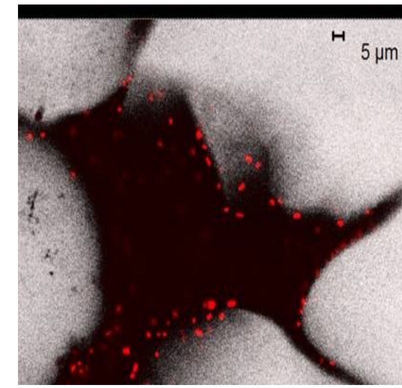
$$\textbf{Flux} = vC(x,t) - K\partial_x C(x,t)$$

Fick's law, Fourier's law, Einstein's reasoning

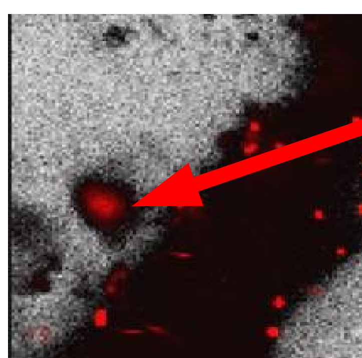
3.b. In some media, certain tracers stick the solid matrix or stay motionless during random periods



bacteria
sand
water



in a column



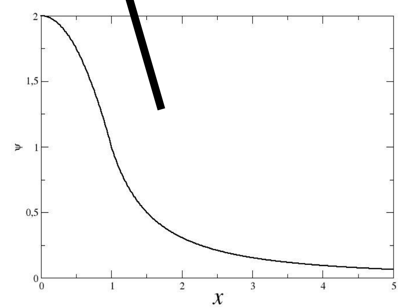
1 bacteria, immobilized in a small cave on a sand grain

4. The flux of walkers which can stick while performing a random walk

4.a. The random walk

Suppose, particles stick the solid matrix of a porous medium, after each time step and each gaussian jump during random sticking periods, of density

$$\psi(t) = \tau^{-1/\gamma} \varphi(t/\tau^{1/\gamma})$$



Laplace transform

$$\tilde{\psi}(s) = 1 - \lambda \tau s^{\gamma} + \ldots$$

2 phases: mobile and sticking

$$C_{tot}(x,t) = C_m(x,t) + C_{imm}(x,t)$$

to be connected with

Flux= $v C_m(x,t) - K \partial_x C_m(x,t)$

4.b. Mobile , immobile, or total population

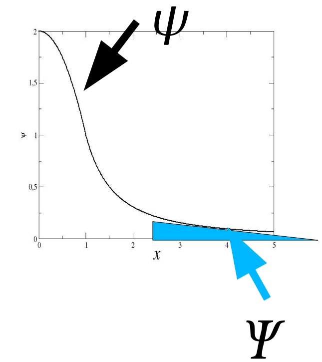
Particles, sticking at x at time t, came from the mobile phase, at time $[t', t'+dt']$

with probability $\frac{dt'}{\tau} C_m(x,t')$

then, sticked there, with (survival) probability $\Psi(t-t') = \int_{t-t'}^{+\infty} \psi(\theta)\, d\theta$

$$C_{imm}(x,t) = \int_0^t C_m(x,t')\, \Psi(t-t')\, \frac{dt'}{\tau}$$

$C_m(x,.) * \Psi$



$$C_{tot}(x,t) = C_m(x,t) + \lambda \frac{\Psi}{\tau} * C_m(x,t)$$

$\longrightarrow I^{1-\gamma} C_m$ *when* $\tau \longrightarrow 0$

$$I^{1-\gamma} f(t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t (t-T)^{-\gamma} f(T)\, dT$$

4.c. A mapping connecting total and mobile concentration, hence giving the flux

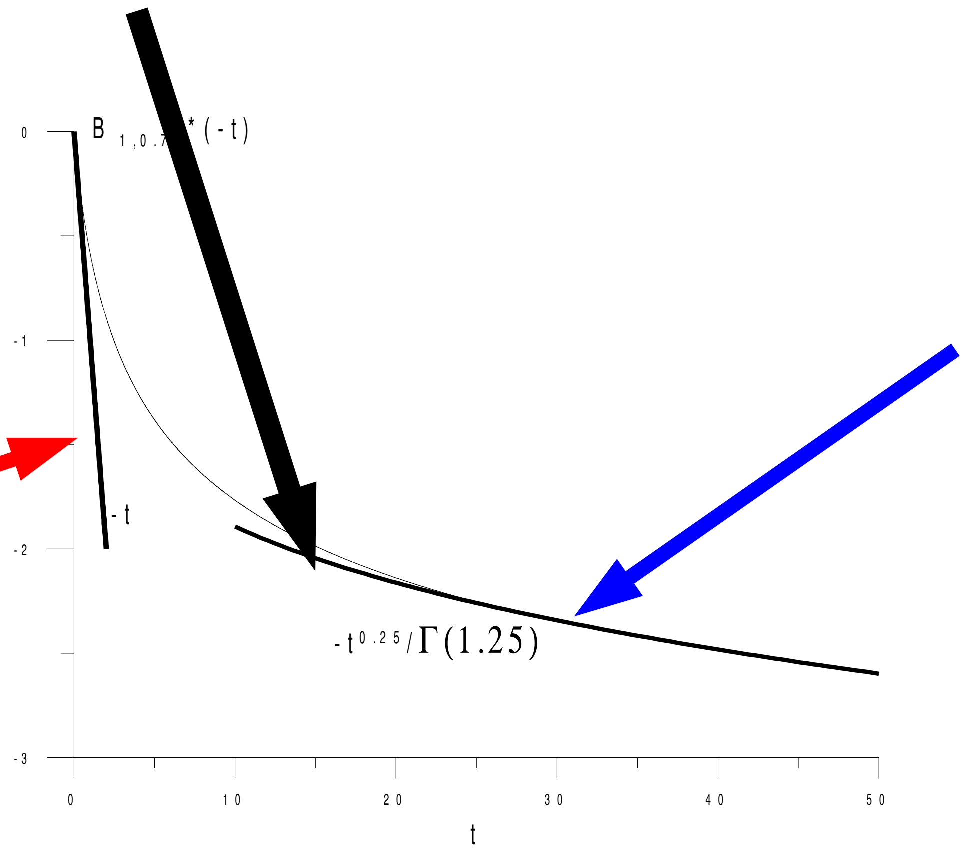
in the limit $\left.\begin{matrix}\tau \\ l\end{matrix}\right\} \rightarrow 0$ *with* $K = l^2/2\tau$

$$C_{tot} = (Id + \lambda I^{1-\gamma}) C_m \quad \longrightarrow \quad C_m = (Id + \lambda I^{1-\gamma})^{-1} C_{tot}$$

Flux= $(v - K\partial_x)(Id + \lambda I^{1-\gamma})^{-1} C_{tot}$

Fick's law for media where particles stick some immobile matrix

the mapping $(Id+\lambda I^{1-\gamma})^{-1}$



early times

Id

$D^{1-\gamma}$

late times

Riemann-Liouville derivative of the order of

$1-\gamma$

with the definition

$$D^{\alpha} f(t)=\partial_t I^{1-\alpha} f(t)$$

4.d. Consequence: Fract(ion)al MIM model with sources

$$\partial_t C(x,t) = -\nabla.(K\nabla - v)(Id + \lambda I^{1-\gamma})^{-1} C(x,t) + r(x,t)$$

source rate

equivalent to

$$(\partial_t + \lambda \partial_t^{\gamma}) C(x,t) = -\nabla.(K\nabla - v) C(x,t) + (Id + \lambda I^{1-\gamma}) r(x,t)$$

when K and v are constant

5. Numerical illustration

constant coefficients

5.a. Schemes for

$$\partial_t C(x,t) = -\nabla.(K\nabla - v)(Id + \lambda I^{1-\gamma})^{-1} C(x,t) + r(x,t)$$

equivalent to

$$(\partial_t + \lambda \partial_t^{\gamma}) C(x,t) = -\nabla.(K\nabla - v) C(x,t) + (Id + \lambda I^{1-\gamma}) r(x,t)$$

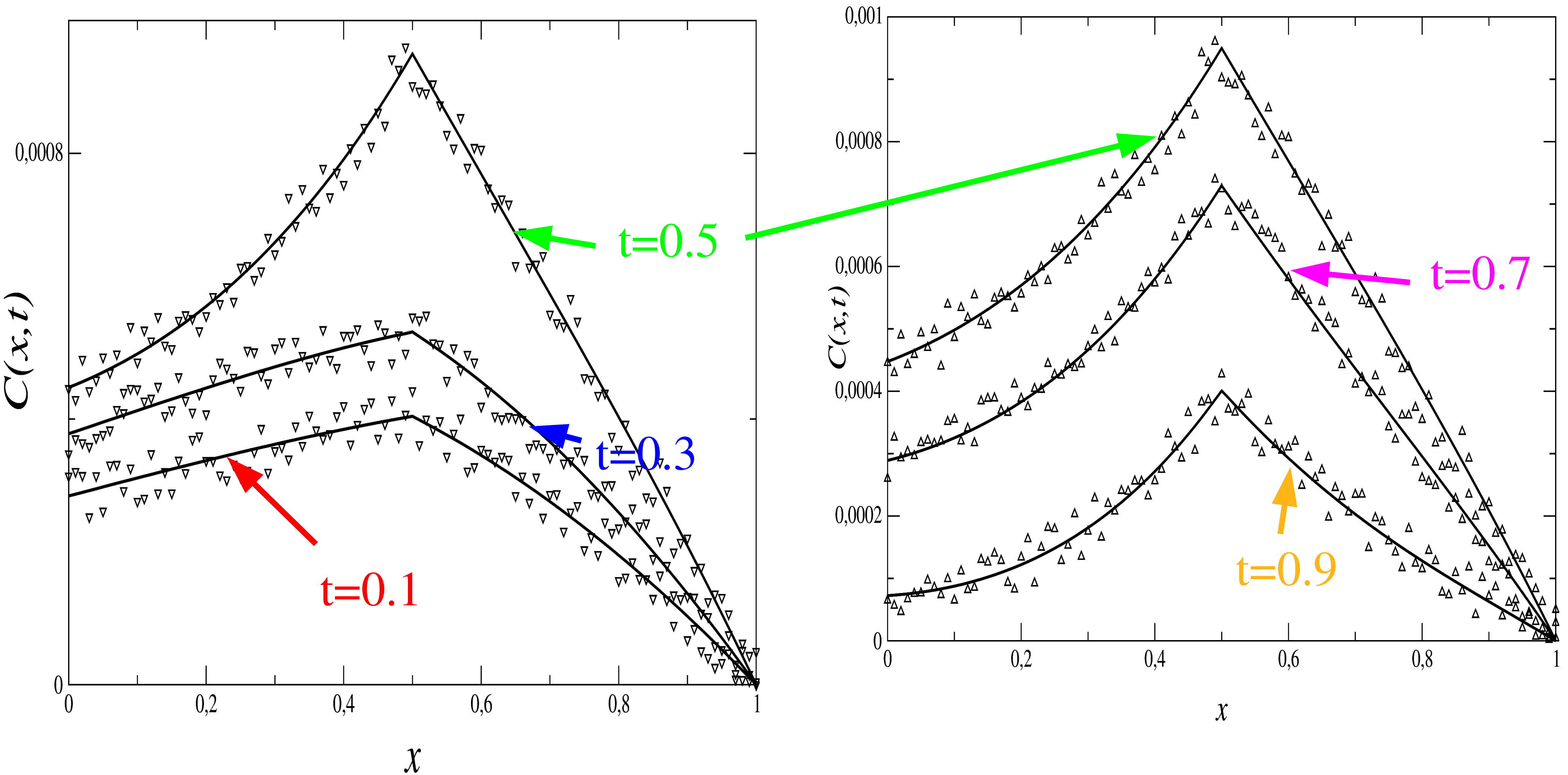
discretize $Id + \lambda I^{1-\gamma}$ then invert

2 interesting schemes:

or

use schemes for Caputo derivative

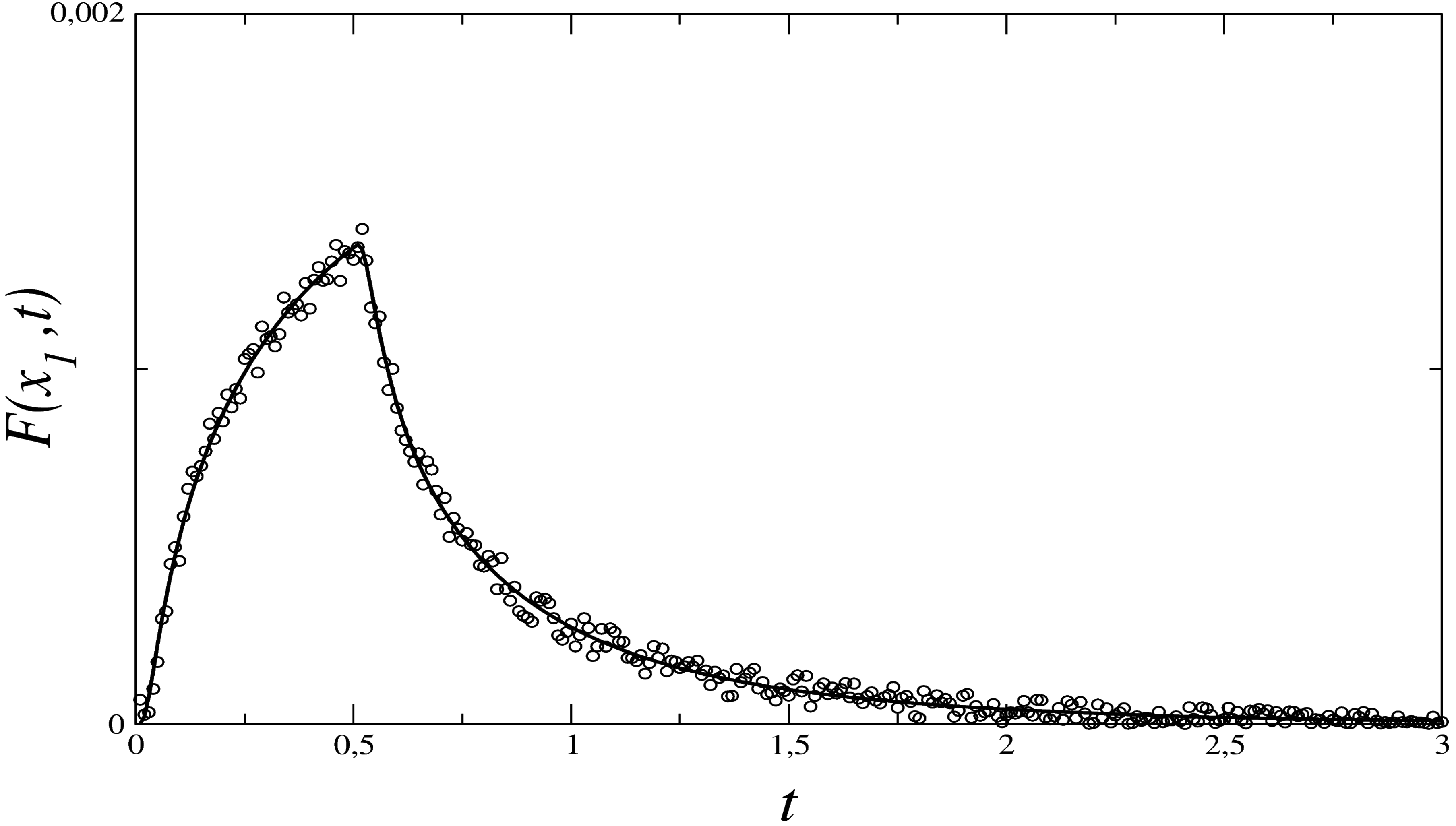
5.b.Comparisons against random walks



constant source at x=0.5 for t between 0 and 0.5

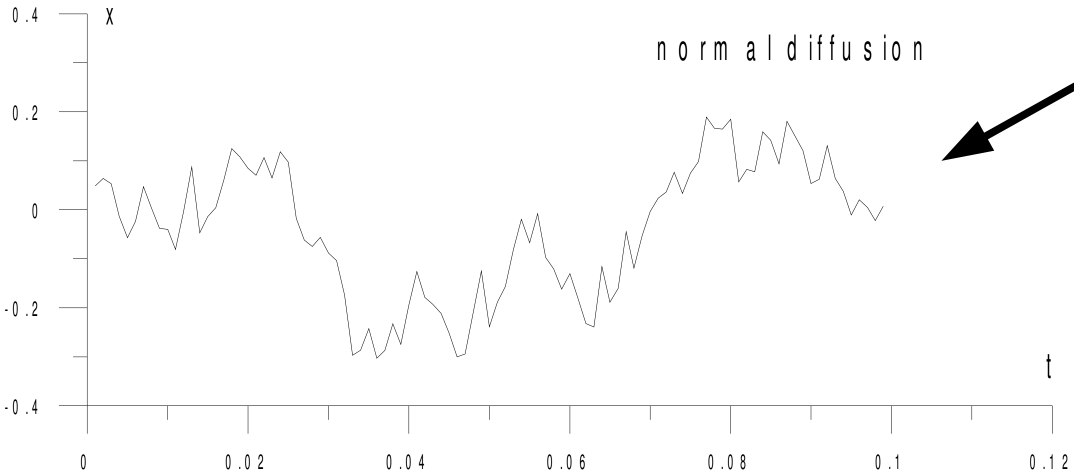
concentration profiles

flux at the outlet



Conclusion

A model for memory effects, coherent with immobilization periods
In terms of fluxes
Numerical discretization
Some parameters are visible in the asymptotic behaviour

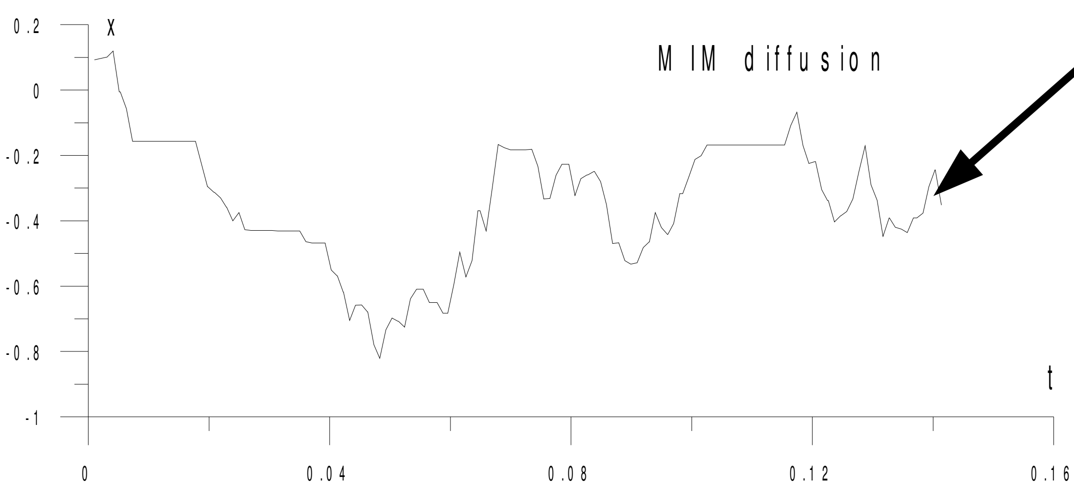


Gaussian jumps, separated by time intervals of duration τ

hydrodynamic limit:

U:Brownian motion

operational time=clock time t



with random immobilizations inserted

hydrodynamic limit:
operational time+
U(operational time)
=clock time t