Tempered fractional model for transient anomalous diffusion

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Abstract

Passive tracers in heterogeneous media experience preasymptotic transport with scale-dependent anomalous diffusion, before eventually converging to the asymptotic diffusion limit. We propose a novel tempered fractional model to capture the slow convergence of sub-diffusion to a diffusion limit for passive tracers in heterogeneous media. Previous research used power-law waiting times to capture the time-nonlocal transport process. Here those waiting times are exponentially tempered, to capture the natural cutoff of retention times. The model is validated against particle concentrations from detailed numerical simulations and field measurements, at various scales and geological environments. Applications to tempered anomalous super-diffusion will also be discussed. In that case, fast particle movements are exponentially cooled, resulting in a transition from fractional advection-dispersion at early time to classical behavior at late time.

Collaborators

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Classical random walk

$$S(t) = Y_1 + \cdots + Y_{[t]}$$

A particle takes a random jump Y_n at time $t = n$. Particle location at time t is a simple random walk $S(t)$ and the scaling limit is a Brownian motion.

$$c^{-1/2} S(ct) \Rightarrow W(t) \approx \underbrace{N(0, \sigma^2 t)} \qquad (c \to \infty)$$

Contract spatial scale

Expand time scale

Normal limit density

Add an advective drift: $L(t) = vt + W(t) \approx N(vt, \sigma^2 t)$

Classical advection and diffusion/dispersion

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2}$$

Fourier transform

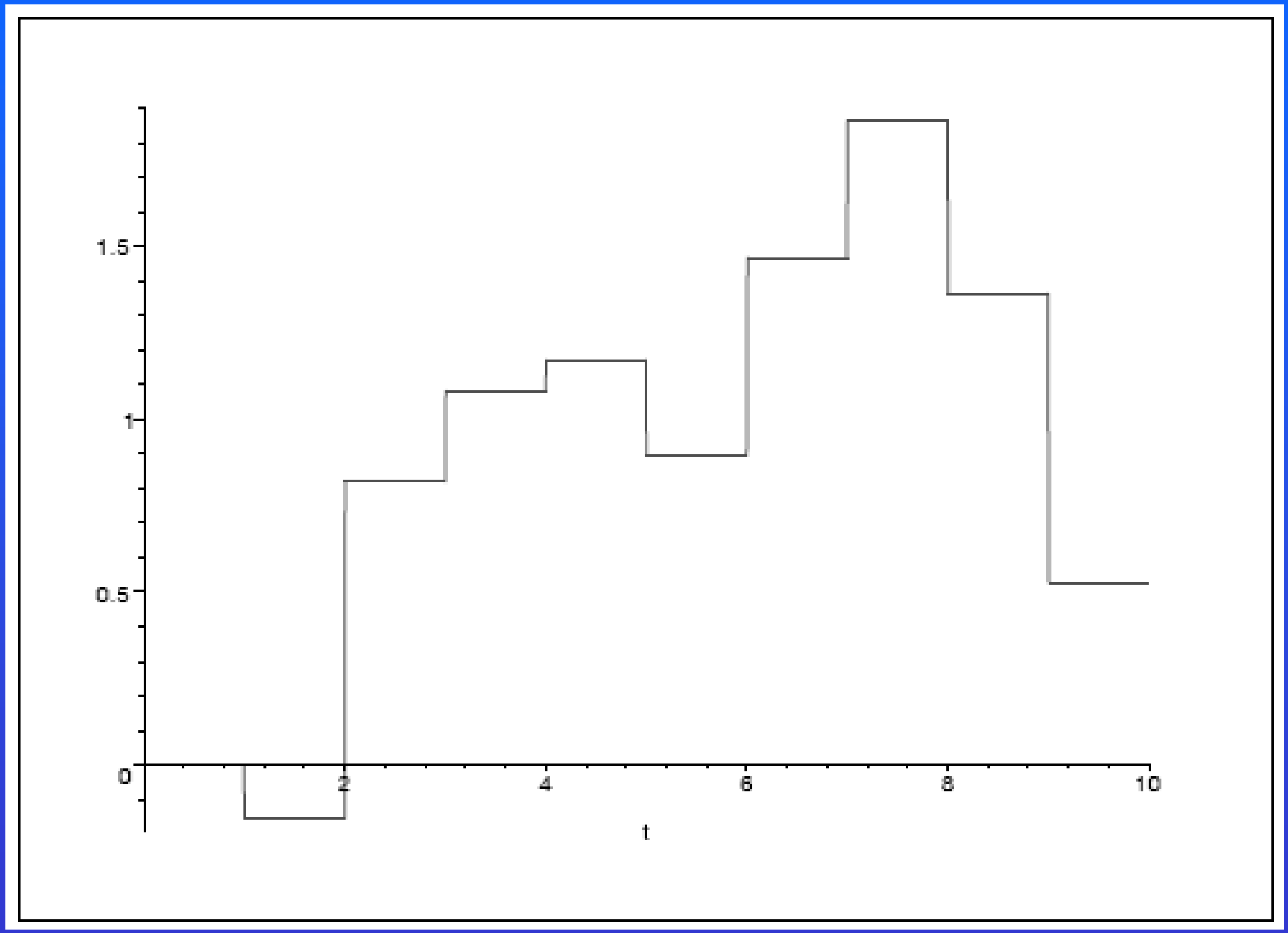
$$\frac{d\hat{C}}{dt} = -v(ik)\hat{C} + D(ik)^2\hat{C}$$

$$\hat{C} = \exp\left(-v(ik)t + D(ik)^2 t\right)$$

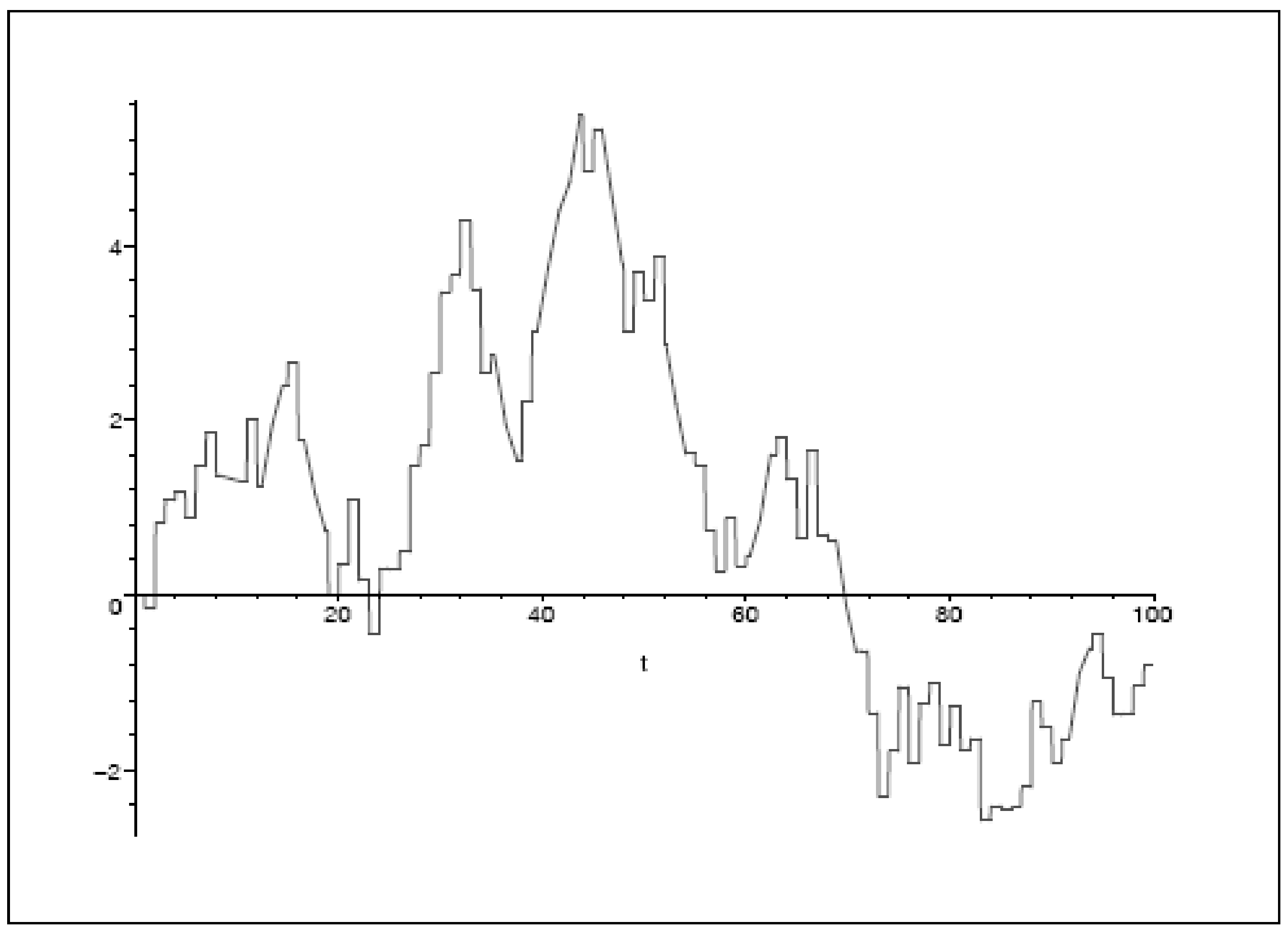
invert

$$C(x,t) = \frac{1}{\sqrt{4\pi D t}}\exp\left(-\frac{(x-vt)^2}{4Dt}\right)$$

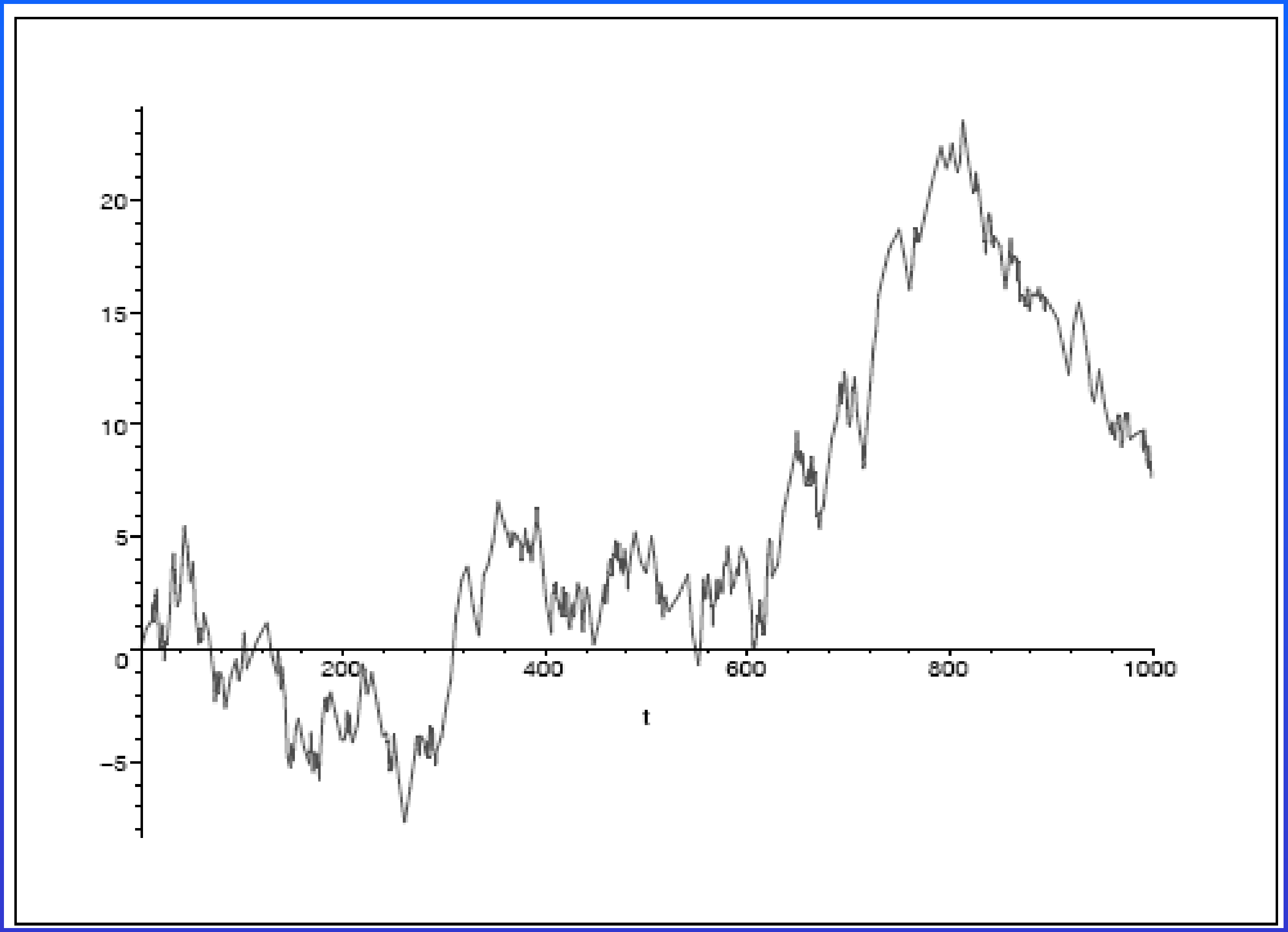
Random walk simulation



Longer time scale



Scaling limit: Brownian motion



Random graph of fractal dimension 1.5 and no jumps.

Heavy tailed particle jumps

For a random walk with heavy tailed particle jumps

$$P(|Y_n| > r) \approx Cr^{-\alpha} \qquad (0 < \alpha < 2)$$

the scaling limit is an α-stable Levy motion

$$c^{-1/\alpha} S(ct) \Rightarrow W(t)$$

leading to a Levy motion with drift

$$L(t) = vt + W(t)$$

Fractional advection-dispersion equation (fADE)

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^{\alpha} C}{\partial x^{\alpha}}$$

Fourier transform

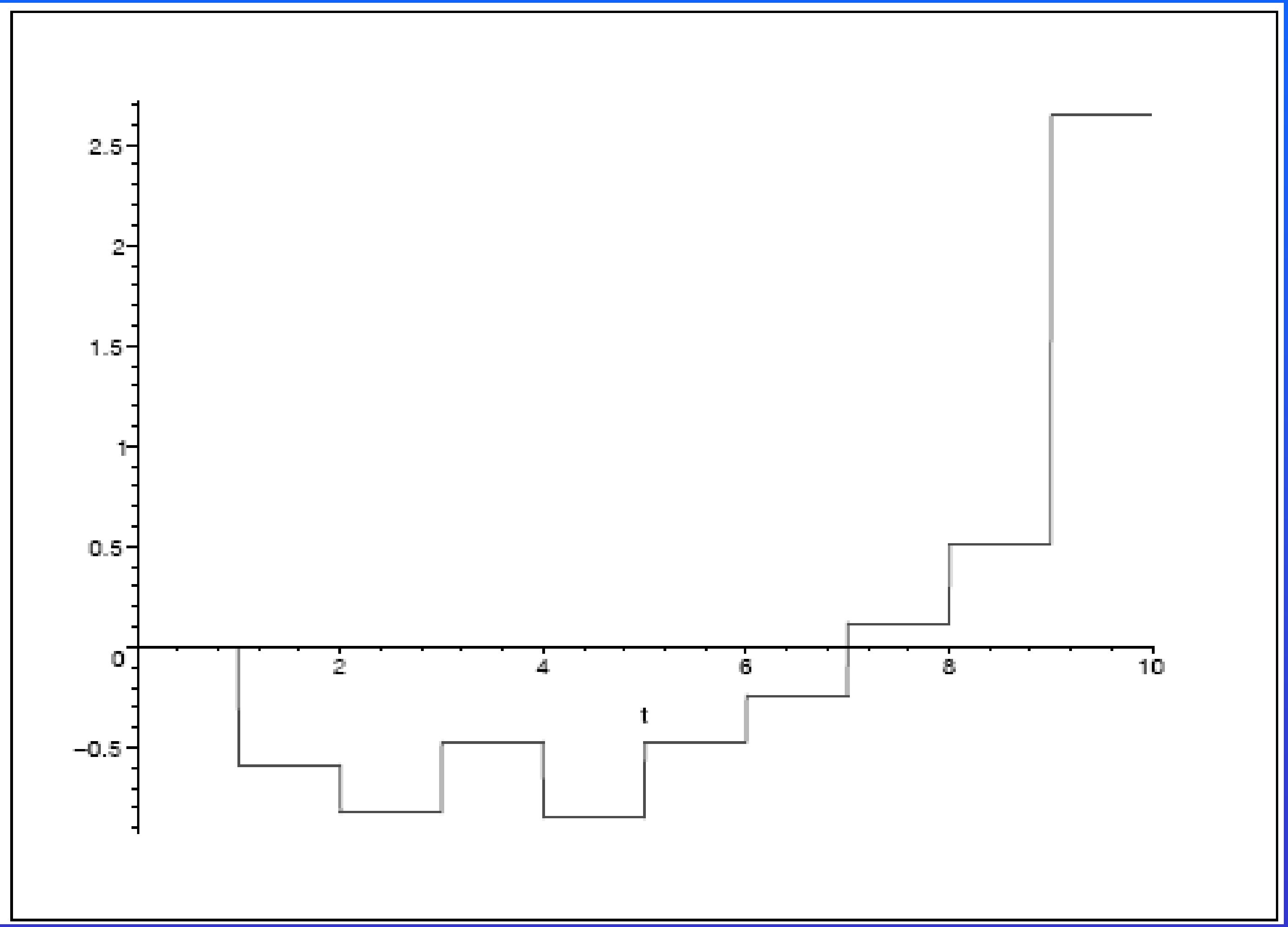
$$\frac{d\hat{C}}{dt} = -v(ik)\hat{C} + D(ik)^{\alpha}\hat{C}$$

$$\hat{C} = \exp\left(-v(ik)t + D(ik)^{\alpha}t\right)$$

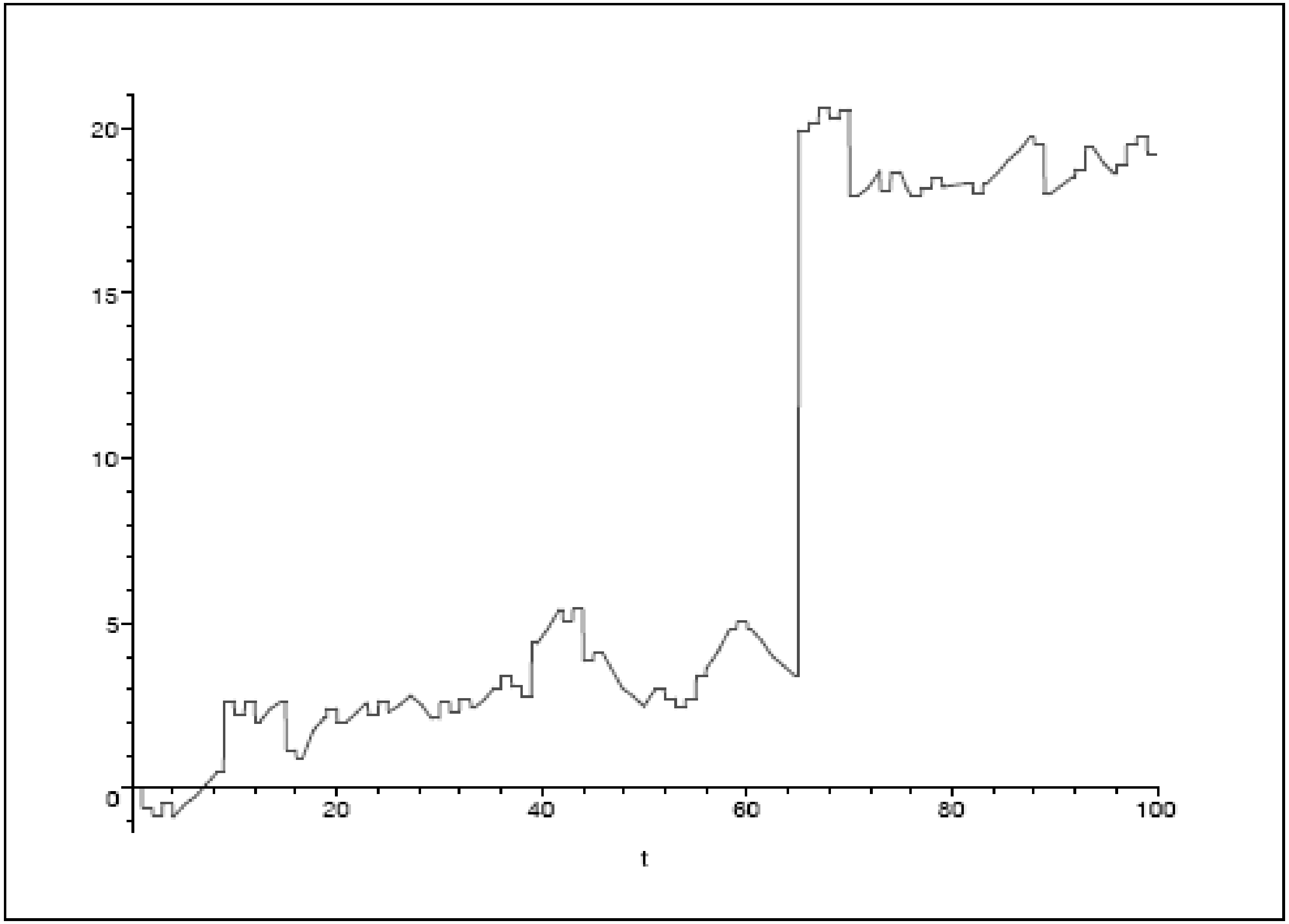
invert

$C(x,t)$ is an α-stable stable density with mean vt

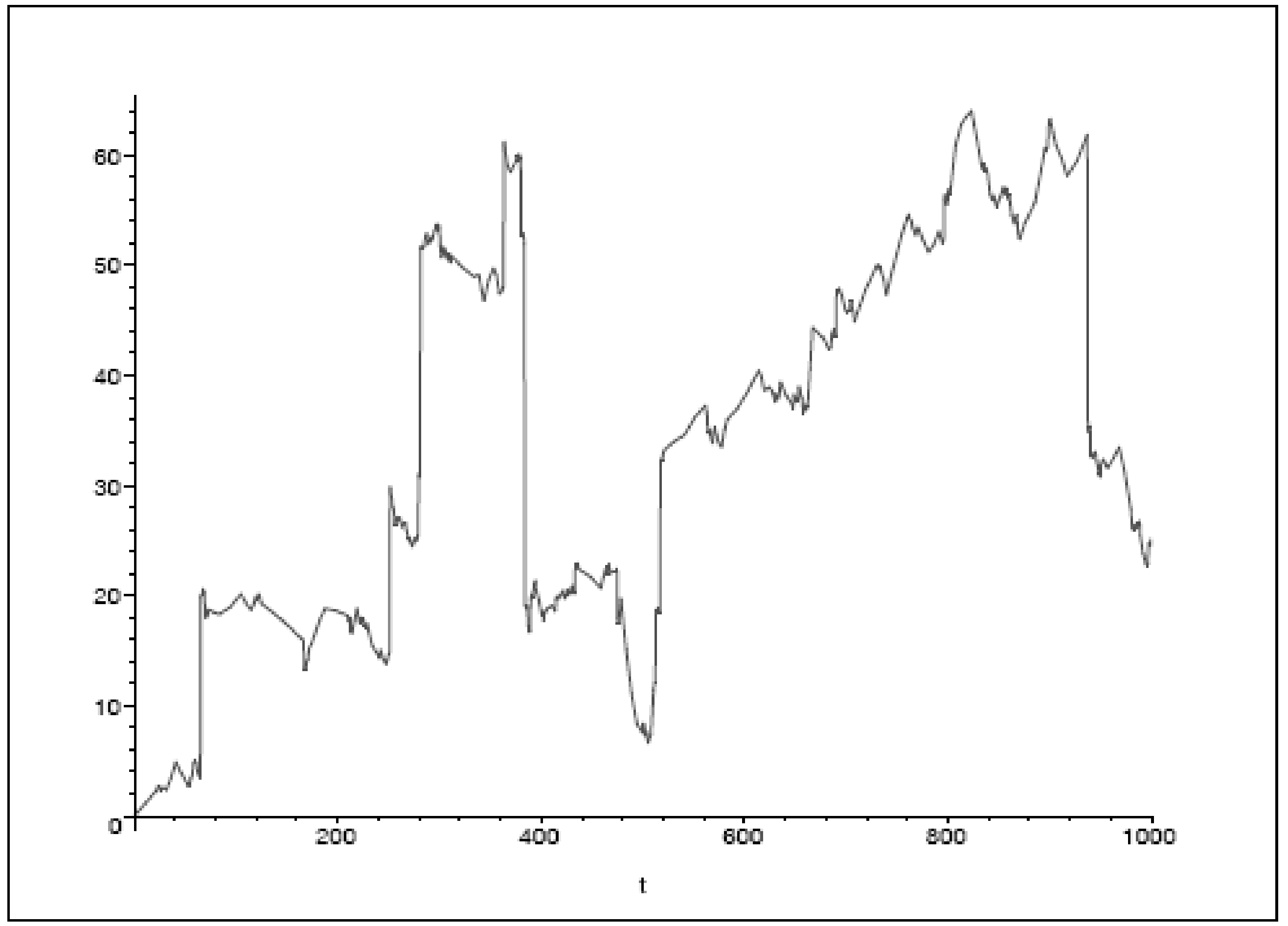
Heavy tailed random walk simulation



Longer time scale

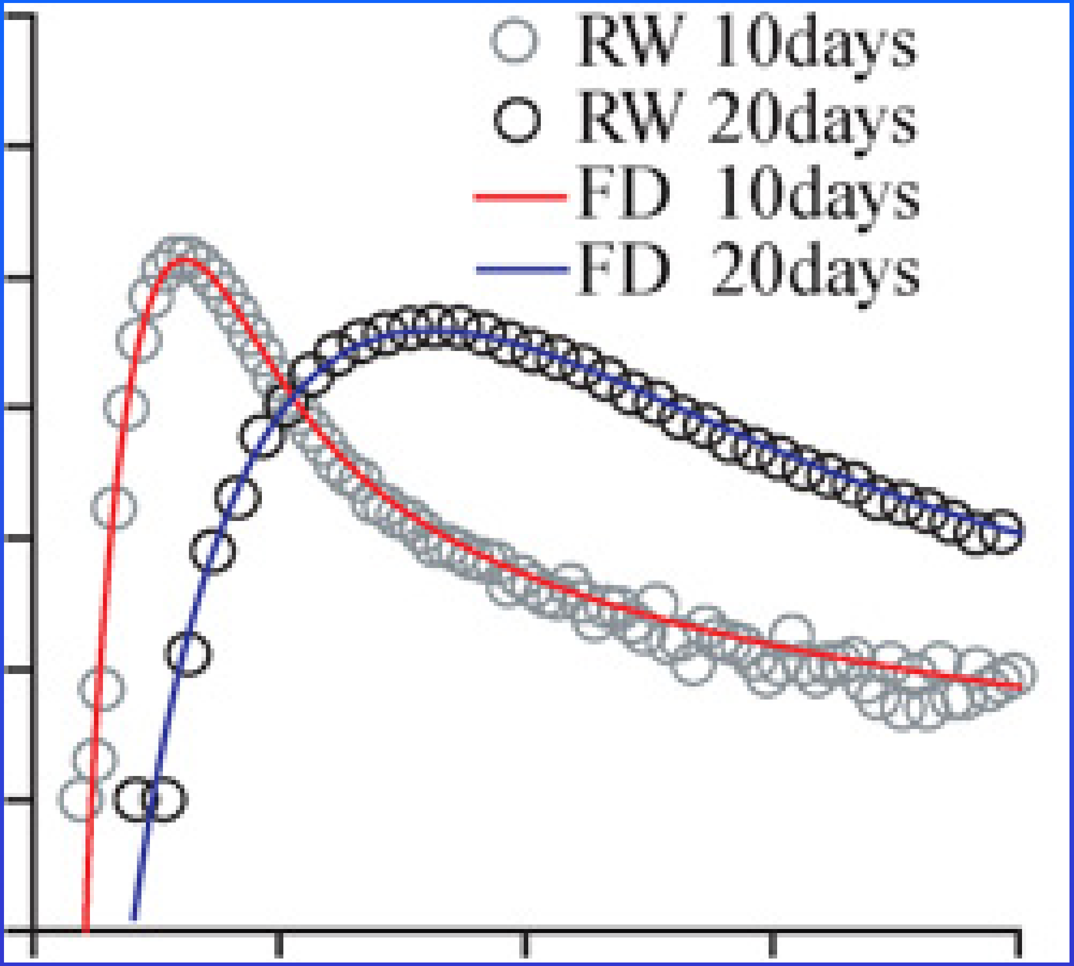


Scaling limit: Stable Levy motion



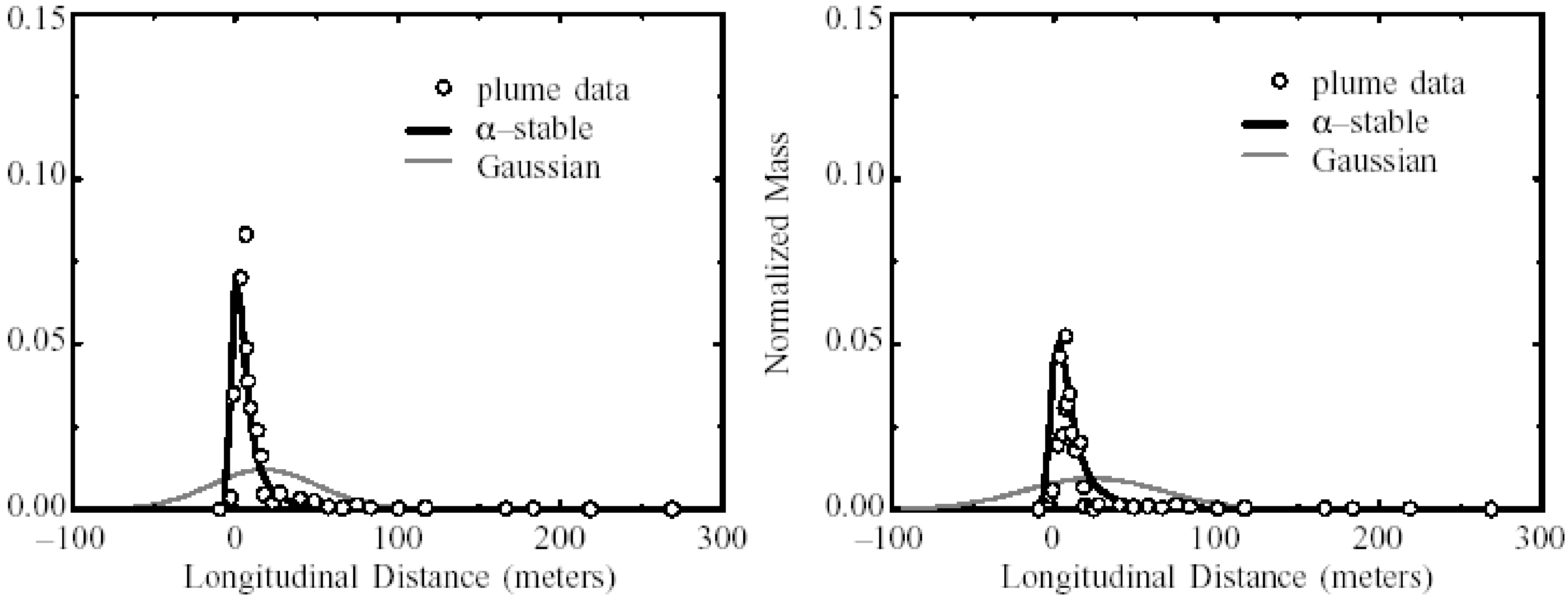
Random graph of fractal dimension 2-1/α includes jumps.

Particle tracking solution (JSP 06)



The stable density has skewness and heavy power law tails.

The MADE tritium plume is skewed (*TIPM* 01)

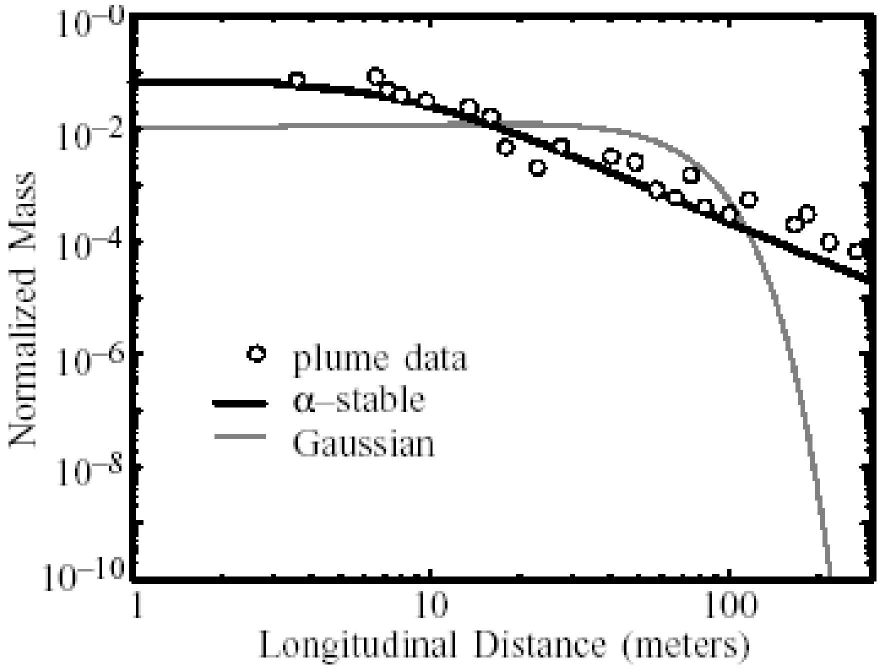


c) Snapshot 3 (day #224)

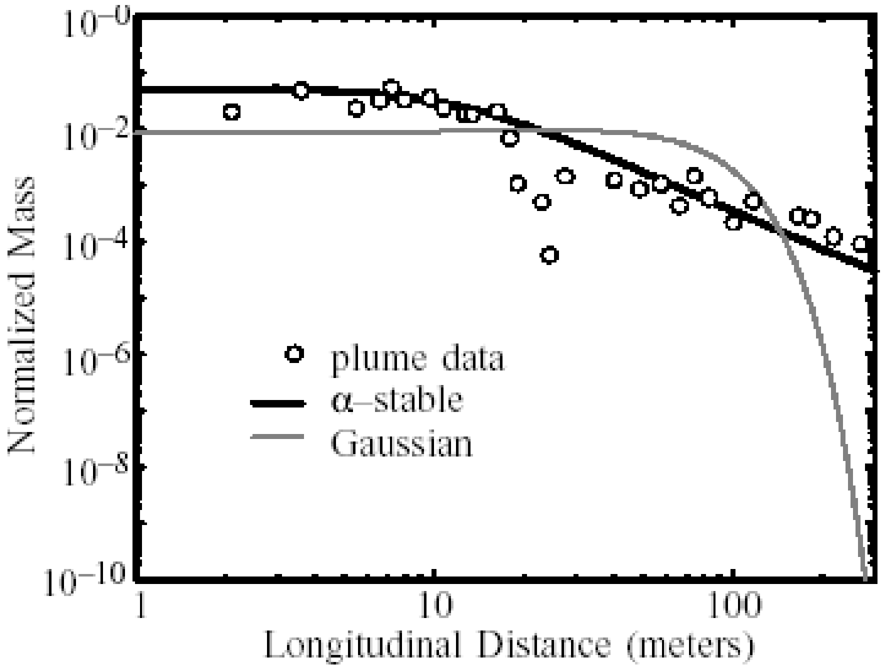
d) Snapshot4 (day #328)

An α-stable stable motion captures the plume skewness and heavy tail.

The MADE plume has a power-law tail (*TIPM* 01)



a) Snapshot 3 (day #224)



b) Snapshot4 (day #328)

The classical Gaussian model seriously underestimates pollution risk.

Heavy tailed waiting times (*JAP* 04)

A particle waits a random time J_n before the nth jump. The nth jump time is

$$T(n) = J_1 + \cdots + J_n$$

and the number of jumps by time t is $N(t) \geq n \longleftrightarrow T(n) \leq t$

For heavy tail waiting times $P(J_n > t) \approx Ct^{-\beta} \quad (0 < \beta < 1)$

$$c^{-1/\beta} T(ct) \Rightarrow P(t) \Longleftrightarrow c^{-\beta} N(ct) \Rightarrow Q(t)$$

Inverse processes have inverse scaling

$$P(ct) \approx c^{1/\beta} P(t) \Longleftrightarrow Q(ct) \approx c^{\beta} Q(t)$$

Continuous time random walks (*AP 04*, *JAP 04*)

Particle location at time *t* follows a CTRW

$$S(N(t)) = Y_1 + \cdots + Y_{N(t)}$$

$$N(ct) \approx c^{\beta} Q(t)$$

$$c^{-1/\alpha} S(ct) \Rightarrow W(t)$$

$$c^{-\beta/\alpha} S(N(ct)) \approx (c^{\beta})^{-\alpha} S(c^{\beta} Q(t)) \Rightarrow W(Q(t))$$

Limit is self-similar $\quad W(Q(ct)) \approx c^{\beta/\alpha} W(Q(t))$

Time-fractional advection-dispersion equation

$$\frac{\partial^\beta C}{\partial t^\beta} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2}$$

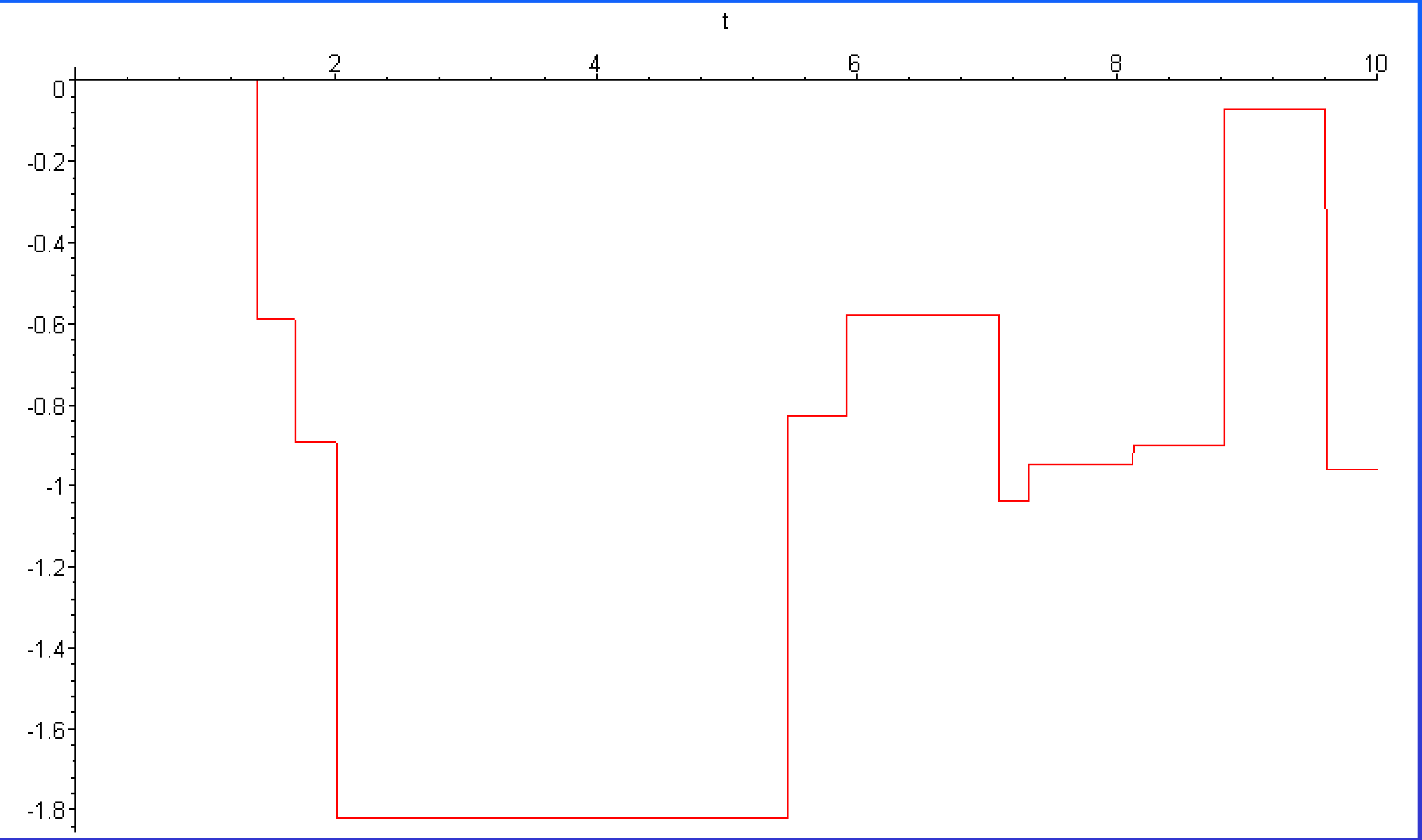
This solution C is the probability density of $W(Q(t))$.

Particle traces are still random fractals.

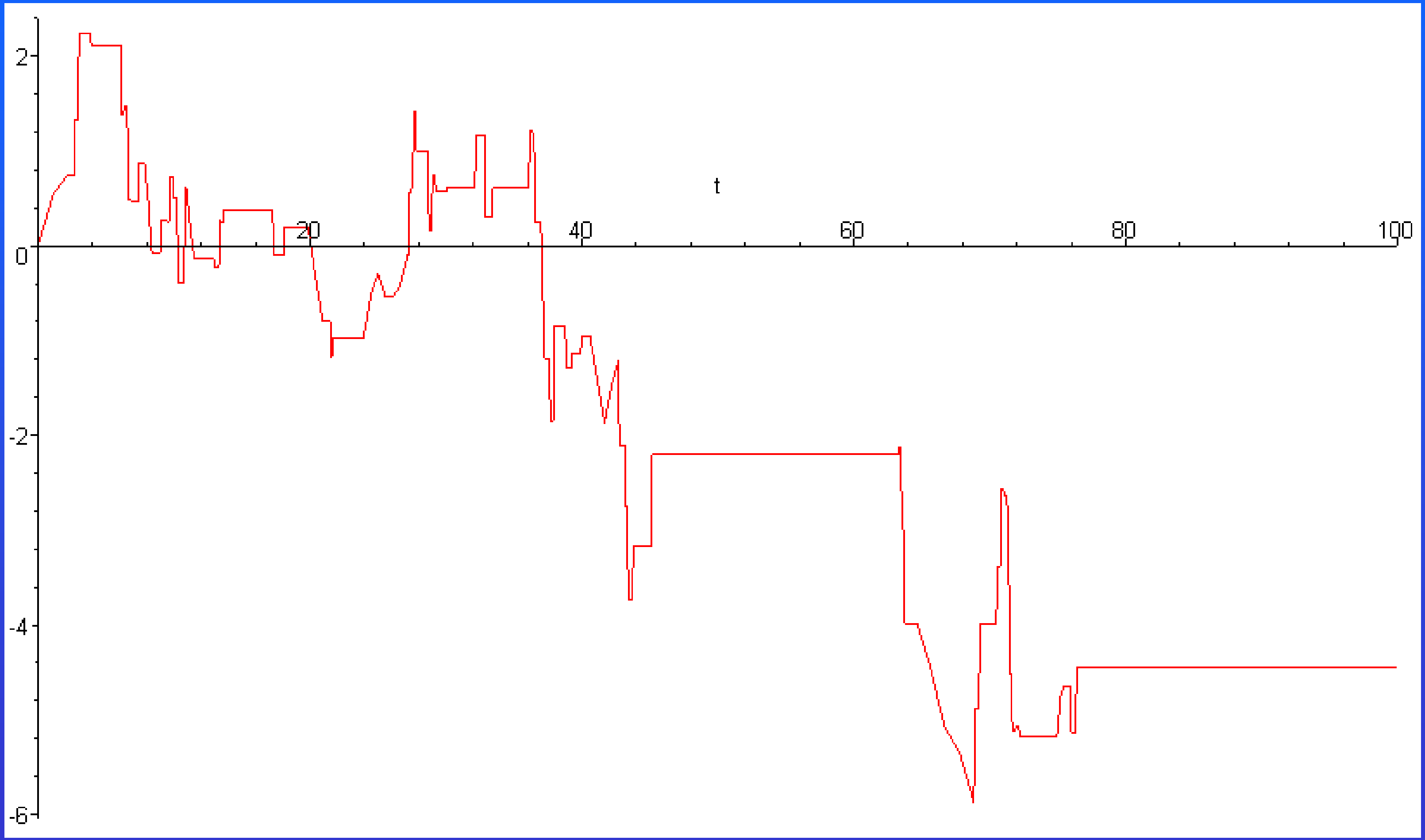
Particle tracking follows $x=W(u)$ and $t=P(u)$.

See Zhang et al. (2006-2008) and Magdziarz et al. (2007).

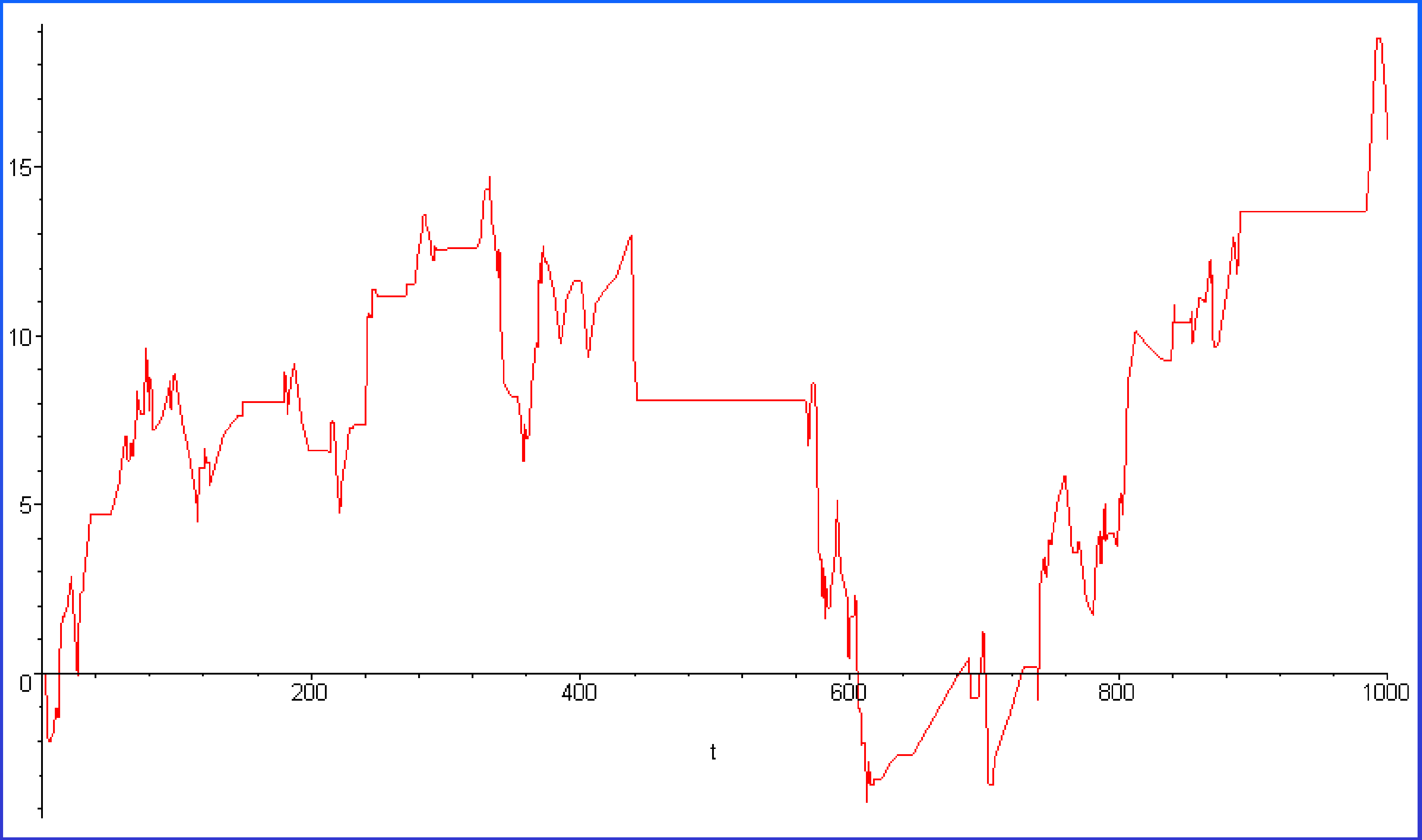
CTRW simulation with heavy tail waiting times



Longer time scale

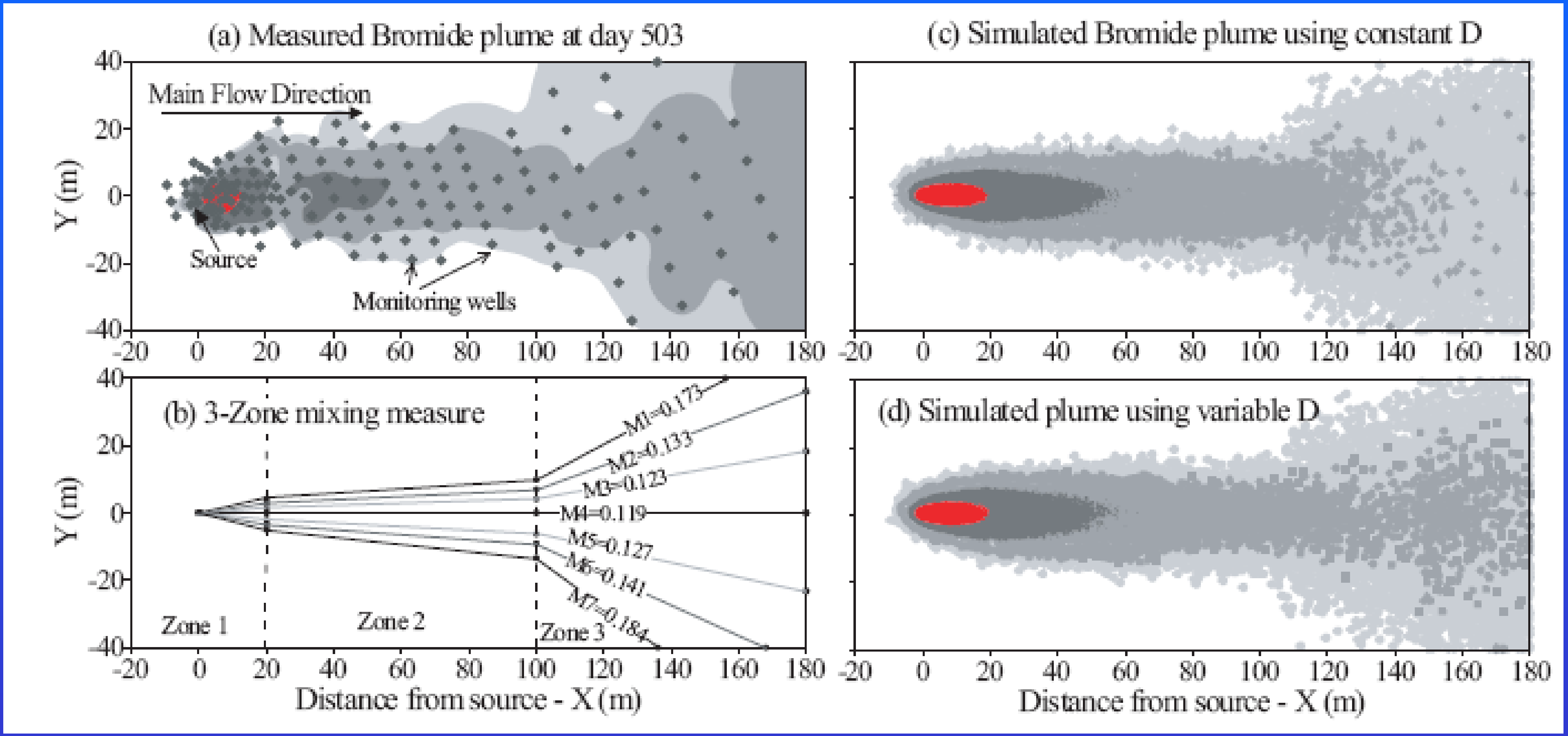


Scaling limit: Subordinated motion



Limit retains long waiting times.

MADE particle tracking solution (PRE 08)



Here β=0.35. Particle tracking solves variable coefficient case.

Coupled space-time derivatives (*AP* 04, *PAMS* 05, PA06)

If waiting times and jumps are dependent random variables, W(t) and Q(t) are coupled, and so are the space and time fractional derivatives.

$$\left(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right)^{\beta} C(x,t) = \frac{t^{-\beta}\delta(x)}{\Gamma(1-\beta)}$$

This example (Shlesinger, Klafter, and Wong *JSP* 1982) assumes

$$P(J > t) = Ct^{-\beta} \qquad (Y \mid J = t) \approx N(0, 2t).$$

Coupled CTRW models have recently been proposed in ground water hydrology [Le Borgne, et al., 2008] and finance [Jurlewicz et al., 2008].

It would be interesting to derive their governing equations!

Transient anomalous sub-diffusion (*GRL 08*)

A particle waits a random time J_n before the nth jump.

Heavy tailed waiting times are tempered stable:

$$P(J_n > t) \approx C t^{-\beta} e^{-\lambda t}$$

Tempering idea originated with Mantegna and Stanley (1994).

Tempered stable process allows elegant mathematics: Rosiński (2007).

Related CTRW model was presented in Dentz et al. (2004).

Tempered anomalous diffusion equation (TADE)

$$\frac{\partial C}{\partial t} + e^{-\lambda t} \frac{\partial^{\beta}}{\partial t^{\beta}}\left(e^{\lambda t} C\right) - \lambda^{\alpha} C = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2}$$

Plume snapshots at early time closely resemble time-fADE.

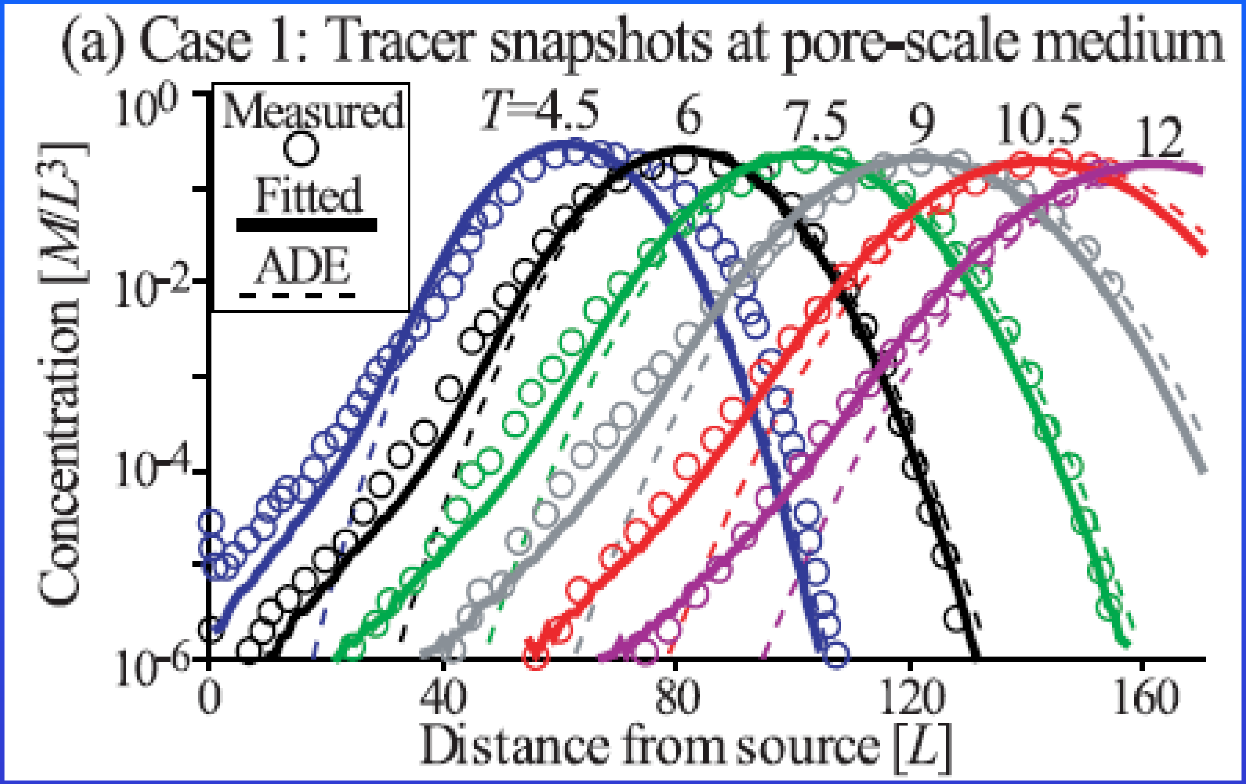
Plume snapshots at late time converge to ADE.

Late-time BTC interpolates between power-law and ADE.

Mobile/immobile and total concentration equations are available.

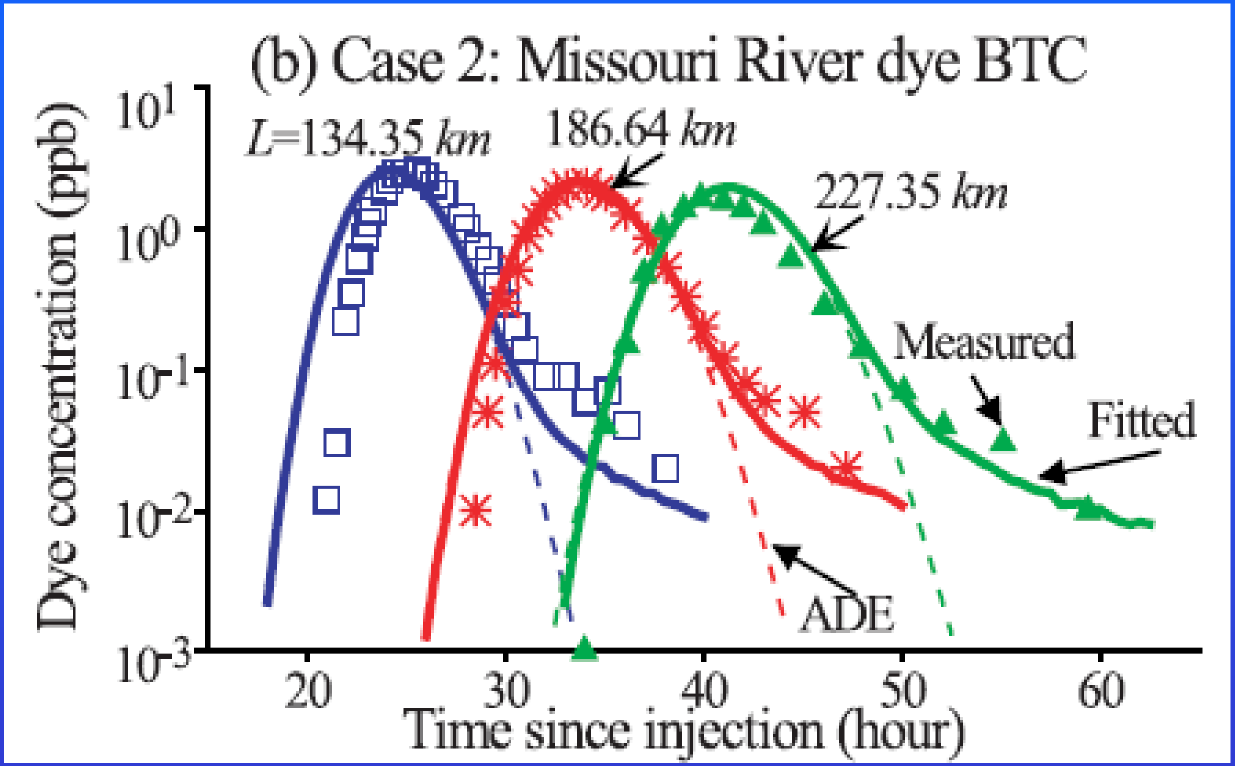
Details are presented in Meerschaert et al. (GRL 2008).

Pore-scale simulations (GRL 08)



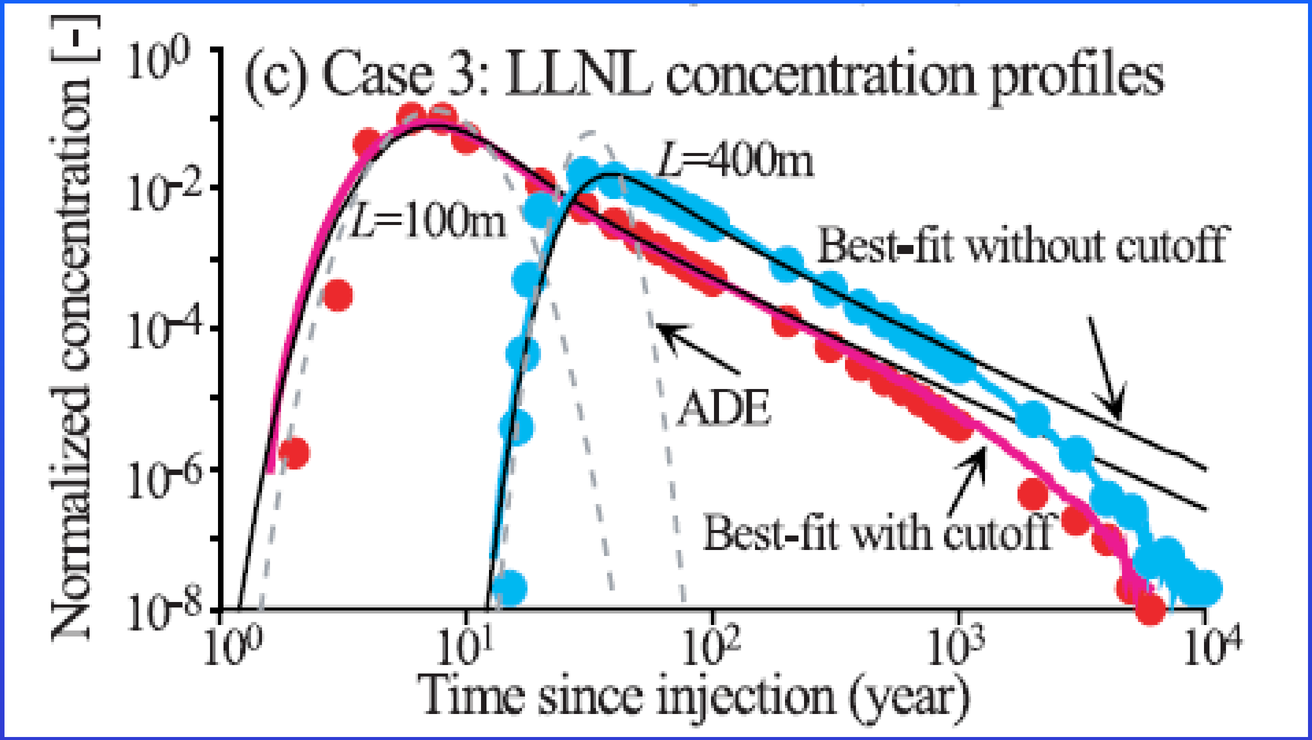
After Zhang and Lv (2007). TADE model with λ=1.0 captures retention near the source.

River flow tracer test (GRL 08)



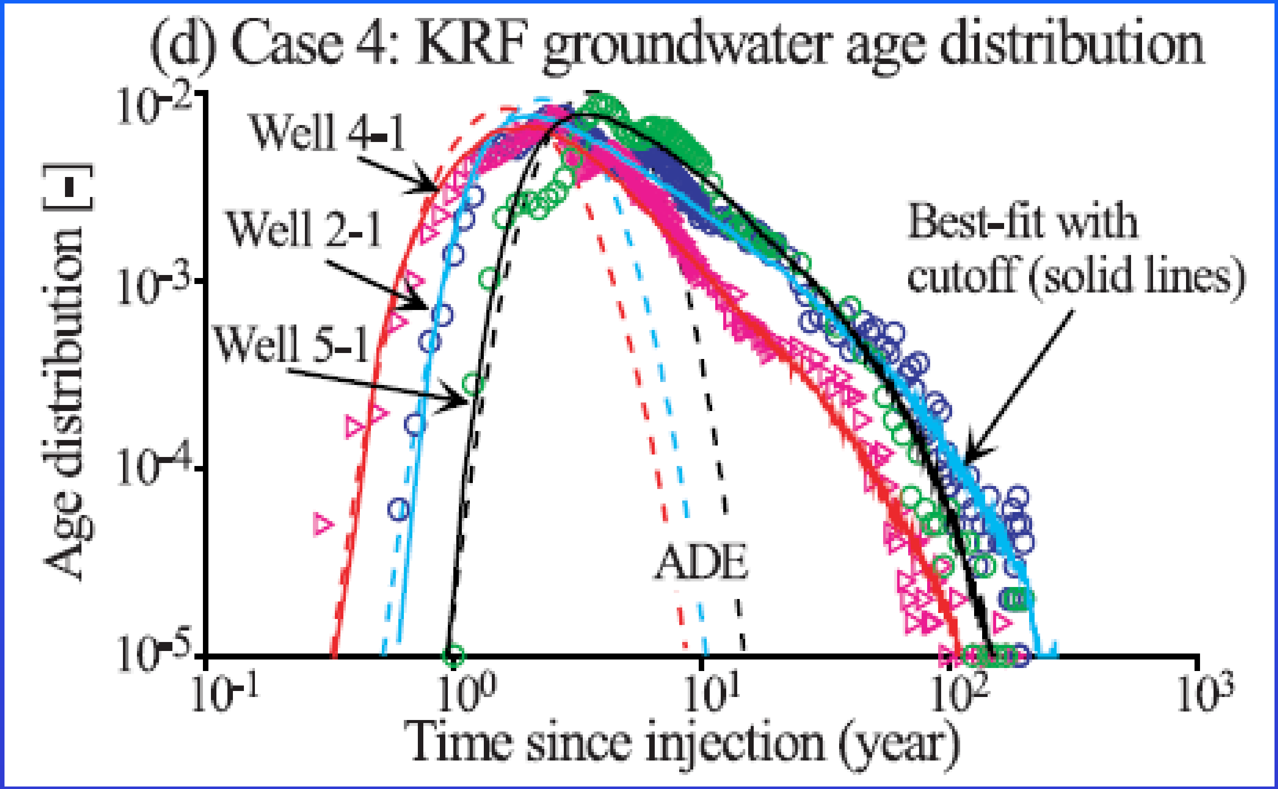
After Deng et al. (2004). TADE model with λ=0.01 captures heavy late tail in the BTC.

Regional scale tracer test (GRL 08)



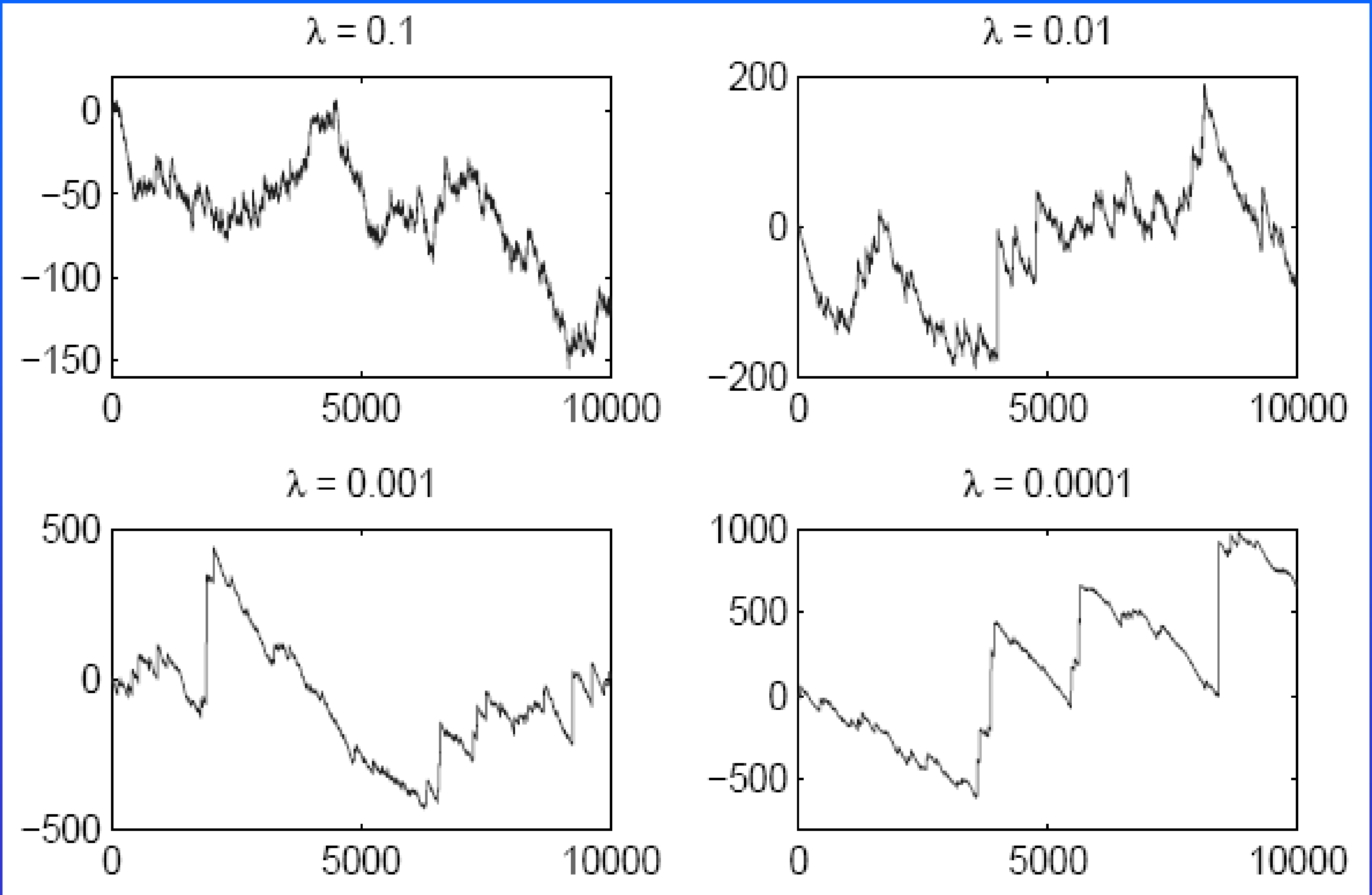
After Zhang et al. (2007). TADE model with λ=0.0006 smoothly interpolates between time-fADE and ADE.

Ground water age distribution (GRL 08)



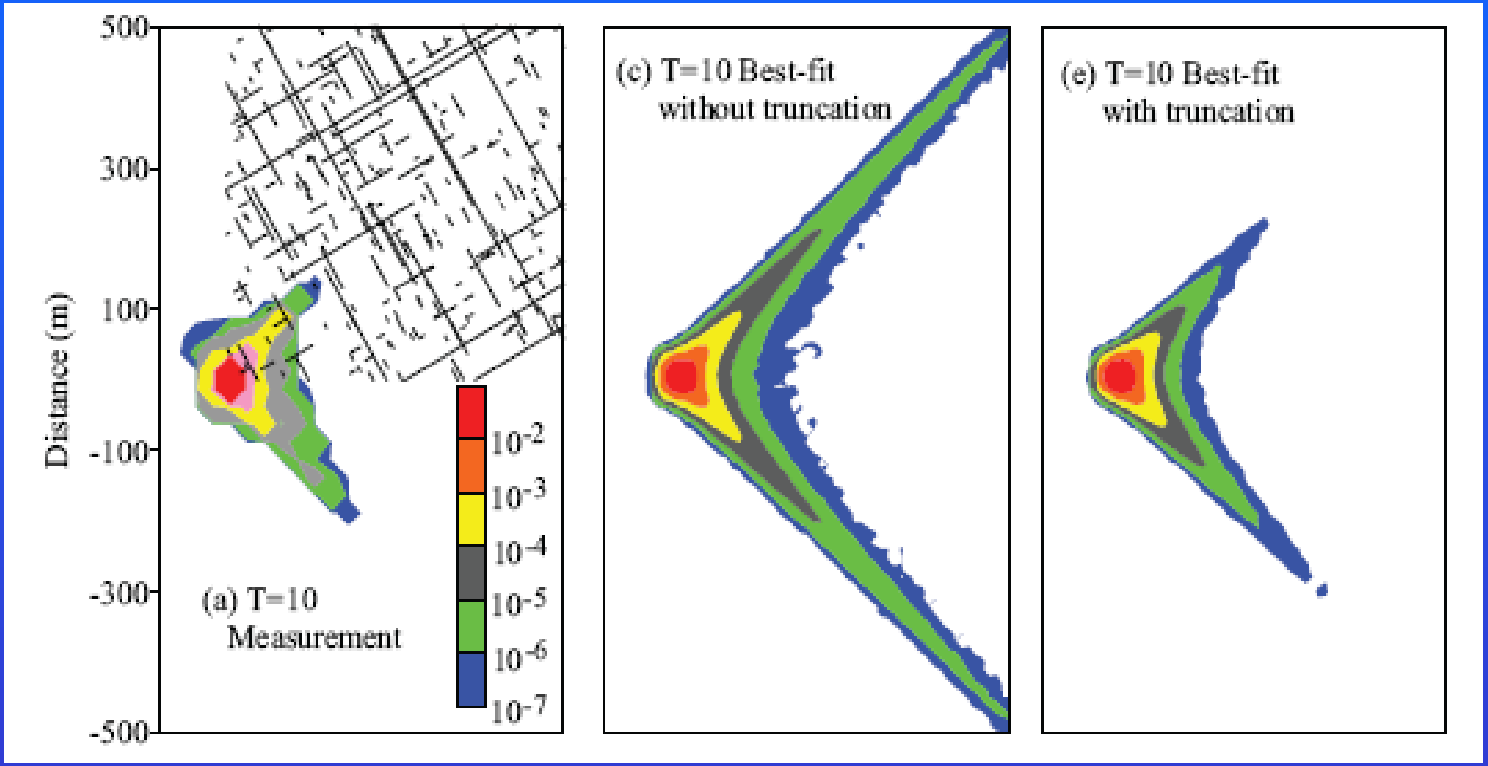
After Weissmann et al. (2002). TADE model with variable λ≈0.01 captures heavy (but not power-law) late time BTC.

Space-TADE (BB&MM 08)



Tempered Lévy flights drive transient super-diffusion.

Simulated fracture flow



After Reeves et al. (2008). Space-TADE gives a more realistic approximation, since power-laws do not extend indefinitely.

Conclusions

- Power laws ⟶ anomalous diffusion ⟶ fADE
- Power law jumps ⟶ fractional in space
- Power law waiting times ⟶ fractional in time
- Intermediate: ADE ⟷ TADE ⟷ fADE
- TADE often gives better fit ☺ than ADE or fADE

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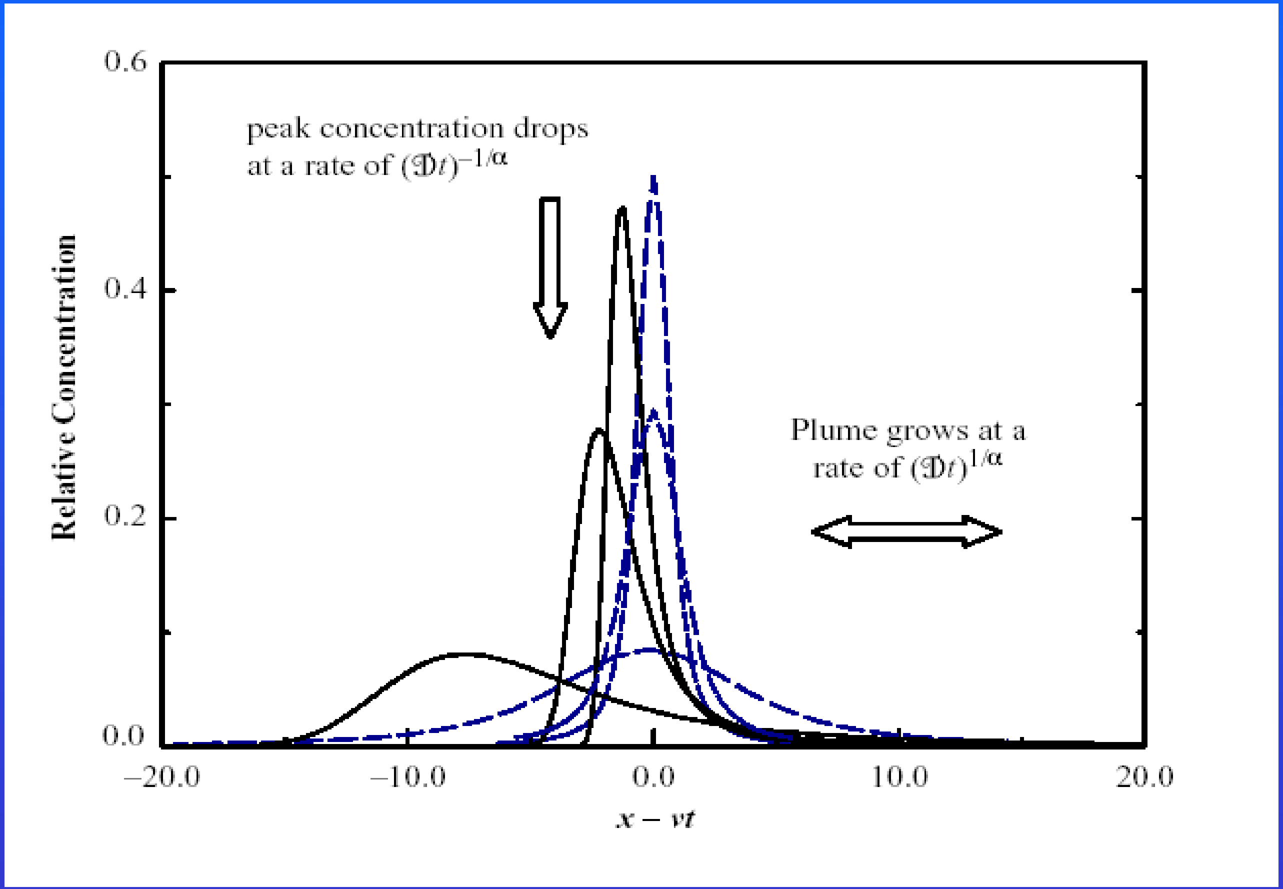
Comparison of normal and stable models



The α-stable stable density has skewness and power-law tails

Fractional derivatives

In the simplest case $0 < \alpha < 1$ the integral

$$\int_0^\infty \left(e^{-iky} - 1\right) \; C\alpha y^{-\alpha-1} dy = -C\Gamma(1-\alpha)(ik)^\alpha$$

Thus the fractional derivative is the inverse FT of

$$\left(\int_0^\infty \left(1 - e^{-iky}\right) \frac{\alpha y^{-\alpha-1} dy}{\Gamma(1-\alpha)} \right) \hat{f}(k)$$

Inverting this FT yields the form (a pseudo-differential operator)

$$\frac{d^\alpha f(x)}{dx^\alpha} = \frac{\alpha}{\Gamma(1-\alpha)} \int_0^\infty \frac{f(x) - f(x-y)}{y} y^{-\alpha} dy$$