Nonlinear anomalous diffusion: model and approximate solutions

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Introduction

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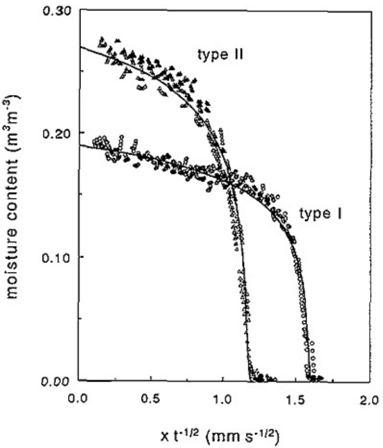
- By $u(x,t)$ we denote the moisture concentration at x at time t.
- We consider the following initial-boundary conditions:

$$u(0,t) = C, \quad u(x,0) = 0.$$

- **Self-similarity** - a characteristic feature of diffusion in our experiment. Moisture concentration $u(x,t)$ can be drawn on a single curve [1]:

$$u(x,t) = U(\eta), \quad \eta = x/\sqrt{t},$$

for $U(0) = C$ i $U(\infty) = 0$.



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- As it turns out and **nobody exactly knows why** but the diffusion not always behaves as we are used to.
- In a number of experiments (ex. [2-4]) the so-called Boltzmann scaling $\eta = x/t^{1/2}$ is not observed.

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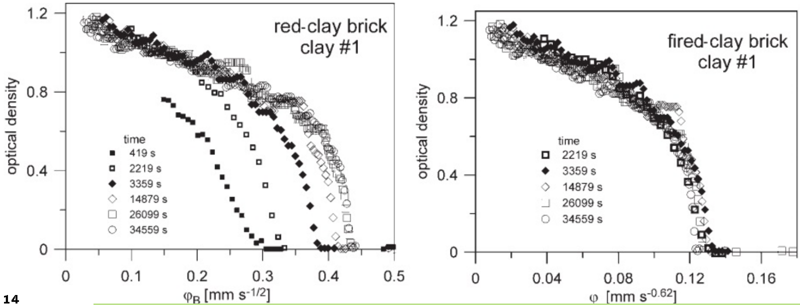
- As it turns out and **nobody exactly knows why** but the diffusion not always behaves as we are used to.
- In a number of experiments (ex. [2-4]) the so-called Boltzmann scaling $\eta = x/t^{1/2}$ is not observed.
- A more appropriate and accurate is the **anomalous diffusion** scaling (Figure from [2])

$$u(x,t) = U(\eta), \quad \eta = x/t^{\alpha/2}, \quad 0 < \alpha < 2.$$



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- In [2,4] the following modification of the constitutive equation has been proposed

$$q = -D(u)\left(\frac{\partial u}{\partial x}\right)^{\frac{1}{\alpha}-1}.$$

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  Result: very complicated equations and average fitting accuracy.
- As it turned out, a more appropriate is to model this phenomenon by an equation with **fractional derivative** (see [5-7])

$$\frac{\partial^\alpha u}{\partial t^\alpha} = \frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right).$$

  We obtain the sought scaling $x/t^{\alpha/2}$ with very small fitting errors.

Fractional derivative!?

- We will be using the following definition of the fractional derivative (α is not necessarily a fraction).
- **The Riemann-Liouville fractional derivative** of order α with respect to time is defined by the formula

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_0^t (t-s)^{n-\alpha-1} u(x,s) ds,$$

  where $n = [\alpha] + 1$.
- This derivative has all the properties that can be expected by a generalization of derivation, for ex.

$$\frac{d^\alpha}{dx^\alpha} x^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)} x^{\beta-\alpha}$$

  for $\beta > -1$. Additionally, it reduces to the ordinary derivative for $\alpha \to k$, $k \in \mathbb{Z}$.

Our problem: can we say something analytical about the nonlinear anomalous diffusion?

- All the previous results concerning anomalous diffusion in porous media consist mainly of numerical solutions of the fractional differential equations (which is far from trivial!).
- We have managed to find some approximations of the solutions of the nonlinear anomalous diffusion equation. These approximations have a very simple, analytical form.

[8] **Ł.Płociniczak, H.Okrasińska-Płociniczak**, *Approximate self-similar solutions to a nonlinear diffusion equation with time-fractional derivative*, Physica D 261 (2013), 85–91

[9] **Ł.Płociniczak**, *Approximation of the Erdelyi-Kober fractional operator with application to the time-fractional porous medium equation*, SIAM Journal of Applied Mathematics, under review

Overview of our method

- Model: anomalous diffusion equation with diffusivity $D(u) = D_0 u^m$ (in nondimensional form)

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \frac{\partial}{\partial x}\left(u^m(x,t)\frac{\partial u}{\partial x}(x,t)\right), \quad 0 < \alpha < 1,$$

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  with initial-boundary conditions $u(0,t) = 1$, $u(x,0) = 0$. **Remark:** With these conditions it does not matter whether we use R-L or Caputo version of the fractional derivative.
- We seek for a self-similar solution $u(x,t) = U(\eta)$, where $\eta = x/t^{\alpha/2}$. We obtain an ordinary integro-differential equation

$$\frac{d}{d\eta}\left(U^m(\eta)\frac{d}{d\eta}U(\eta)\right) = \left[(1-\alpha) - \frac{\alpha}{2}\eta\frac{d}{d\eta}\right] I^{0,1-\alpha}_{-\frac{2}{\alpha}} U(\eta),$$

  with $U(0) = 1$ and $U(\infty) = 0$, where the integral operator is of the **Erdelyi-Kober** type

$$I^{a,b}_c U(\eta) := \frac{1}{\Gamma(b)}\int_0^1 (1-z)^{b-1} z^a U(\eta z^{\frac{1}{c}}) dz.$$

Overview of our method cont'd

- Theorem

  For analytic U and $a > -1$, $b > 0$, $c > 0$ we have the following representation

$$I_c^{a,b} U(\eta) = \sum_{k=0}^{\infty} \lambda_k U^{(k)}(\eta) \frac{\eta^k}{k!},$$

where $\lambda_k = \sum_{j=0}^{k} \binom{k}{j} (-1)^{k-j} \frac{\Gamma\left(a+\frac{j}{c}+1\right)}{\Gamma\left(a+b+\frac{j}{c}+1\right)}$.

Moreover, we have an asymptotic expansion when $k \to \infty$

$$\lambda_k \sim (-1)^k \frac{c}{\Gamma(b)} \sum_{n=0}^{\infty} \binom{b-1}{n} (-1)^n \Gamma\left(c(a+n+1)\right) \left(\frac{1}{k}\right)^{c(a+n+1)}.$$

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- The series converges very fast, especially for η close to 0. **Let us use it!**

Overview of our method cont'd

- If it happens that U is not analytic, we can hope that the first terms in the expansion of the $E-K$ operator will give us a decent approximation.
- Let us use it for our main equation. We obtain

$$(U^m U')' = \frac{1}{\Gamma(1-\alpha)} U - \left(\frac{\alpha}{2}\lambda_0 - \lambda_1\right) \eta U',$$

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- Being lead by physical intuition and previous results on the classical case we can expect that there exists such η^* for which $U(\eta) = 0$ for $\eta \geq \eta^*$.
- Now, our conditions transform into $U(0) = 1$ and $U(\eta^*) = 0$.
- **Problem:** we do not know η^* which gives us a **free boundary problem**.

Overview of our method cont'd

- To proceed we use an idea introduced in [10]. We make a substitution

$$U(\eta) = \left(m(\eta^*)^2 y(z)\right)^{\frac{1}{m}}, \quad z = 1 - \frac{\eta}{\eta^*}.$$

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- Now, the equation is

$$\frac{1}{m} y'^2 + y y'' = \frac{1}{\Gamma(1-\alpha)} y + \frac{1}{m}\left(\frac{\alpha}{2}\lambda_0 - \lambda_1\right)(1-z)y'.$$

with **initial** conditions $y(0) = 0$ and $y'(0) = \frac{\alpha}{2}\lambda_0 - \lambda_1$.

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  with **initial** conditions $y(0) = 0$ and $y'(0) = \frac{\alpha}{2}\lambda_0 - \lambda_1$.
- The condition for the derivative is obtained from the structure of equation.
- When we know y we can very easily obtain the front position: $\eta^* = 1/\sqrt{my(1)}$.
- As it turns out, the Taylor series for y converges very quickly.

Overview of our method cont'd

- When we take a few first terms in the Taylor series for $y(z) = \sum_{i=1}^{\infty} a_i z^i$ we obtain (in original variables)

$$U_1(\eta) = (1 - \eta/\eta_1^*)^{\frac{1}{m}}$$
$$U_2(\eta) = ((1 - \eta/\eta_2^*)(1 - m a_2 \eta_2^* \eta))^{\frac{1}{m}},$$

  where a_i can be determined, for ex. $a_1 = y'(0) = \frac{\alpha}{2}\lambda_0 - \lambda_1$. The rest a_i are much complicated.

- Additionally, we can calculate the cumulative moisture intake

$$I_i(t) := \int_0^\infty u_i(x,t)dx = \int_0^\infty U_i\left(\frac{x}{t^{\frac{\alpha}{2}}}\right)dx = t^{\frac{\alpha}{2}} \int_0^{\eta^*} U_i(\eta)d\eta.$$

  We have

$$I_1(t) = \frac{m}{m+1}\eta_1^* t^{\frac{\alpha}{2}},$$
$$I_2(t) = \frac{m}{m+1}\eta_2^* \, {}_2F_1\left(-\frac{1}{m}, 1; 2 + \frac{1}{m}; \frac{a_2}{a_1 + a_2}\right) t^{\frac{\alpha}{2}}.$$

Numerical results

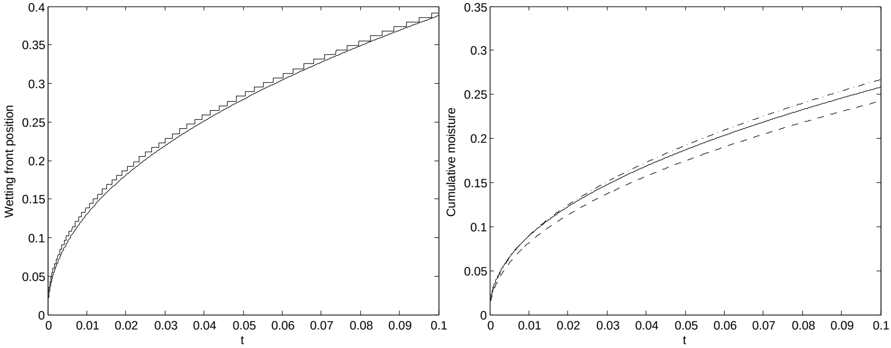

Figure : On the left: front position $\eta^*(t)$ (zig-zag) and its approximation $\eta_3^*(t) = \eta_3^* t^{\alpha/2}$ (smooth line). On the right: cumulative moisture (solid line) and approximations I_1 (dashed line) i I_2 (dot-dashed line). Here, $\alpha = 0.95$ and $m = 2$.

Numerical results cont'd

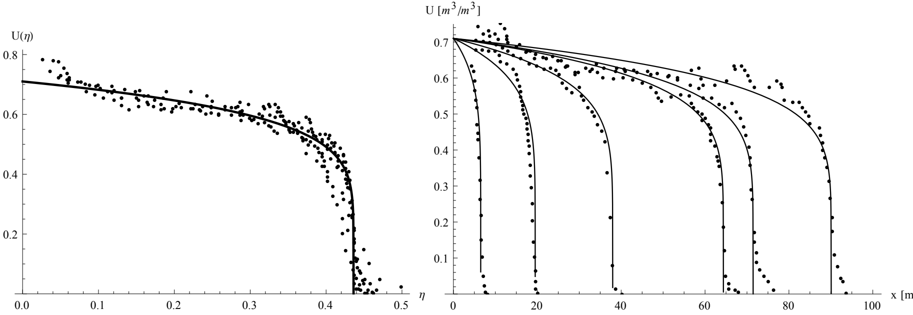

Figure : Fitting U_3 with experimental data from [2]. On the left: a self-similar profile; an the right: time evolution. Here $\alpha = 0.855$, $C = 0.71$ m^3/m^3, $m = 6.98$, $D_0 = 5.36$ mm/s$^{0.855}$.

Bibliografia

1. L. Pel, K. Kopinga, G. Bertram and G. Lang, *Water absorption in a fired-clay brick observed by NMR scanning*, J. Phys. D.: Appl. Phys. 28 (1995) 675–680.
2. Abd El-Ghany, El Abd and J.J. Milczarek, *Neutron radiography study of water absorption in porous building materials: anomalous diffusion analysis*, J. Phys. D.: Appl. Phys. 37 (2004) 2305–2313.
3. S.C. Taylor, W.D. Hoff, M.A. Wilson and K.M. Green, *Anomalous water transport properties of Portland and blended cement-based materials*, J. Mater. Sci. Lett. 18 (1999) 1925–27.
4. M.Kuntz and P.Lavallee, *Experimental evidence and theoretical analysis of anomalous diffusion during water infiltration in porous building materials*, J. Phys. D: Appl. Phys. 34 (2001), 2547-2554
5. E. Gerolymatou, I.Vardoulakis and R.Hilfer, *Modelling infiltration by means of a nonlinear fractional diffusion model*, J. Phys. D: Appl. Phys. 39 (2006), 4104–4110.
6. D.N. Gerasimov, V.A. Kondratieva and O.A. Sinkevich, *An anomalous non-self-similar infiltration and fractional diffusion equation*, Physica D 239 (2010) 1593–1597.
7. Y. Pachepsky, D. Timlin and W. Rawls, *Generalized Richard's equation to simulate water transport in unsaturated soils*, J. Hydrol. (2003) 2723–13
8. J.R. King, Approximate solutions to a nonlinear diffusion equation, Journal of Engineering Mathematics 22: 53-72 (1988)
9. **Ł.Płociniczak, H.Okrasińska-Płociniczak**, Approximate self-similar solutions to a nonlinear diffusion equation with time-fractional derivative, Physica D 261 (2013), 85–91
10. **Ł.Płociniczak**, Approximation of the Erdelyi-Kober fractional operator with application to the time-fractional porous medium equation, SIAM Journal of Applied Mathematics, under review