DIFFUSION IN HYDROGELOGY

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DIFFUSION FUNDAMENTALS II

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OUTLINE

- WHAT IS HYDROGEOLOGY?
- OCCURRENCE OF THE DIFFUSION EQUATION
- CHALLENGES IN HYDROGEOLOGY

- PUMPING TESTS
- USE OF TRACERS
- MEASUREMENTS OF DIFFUSION

- MODELLING: DOUBLE POROSITY & LAPLACE TRANSFORMS

- KEY POINTS
- PLEASE 'LET ME KNOW…'

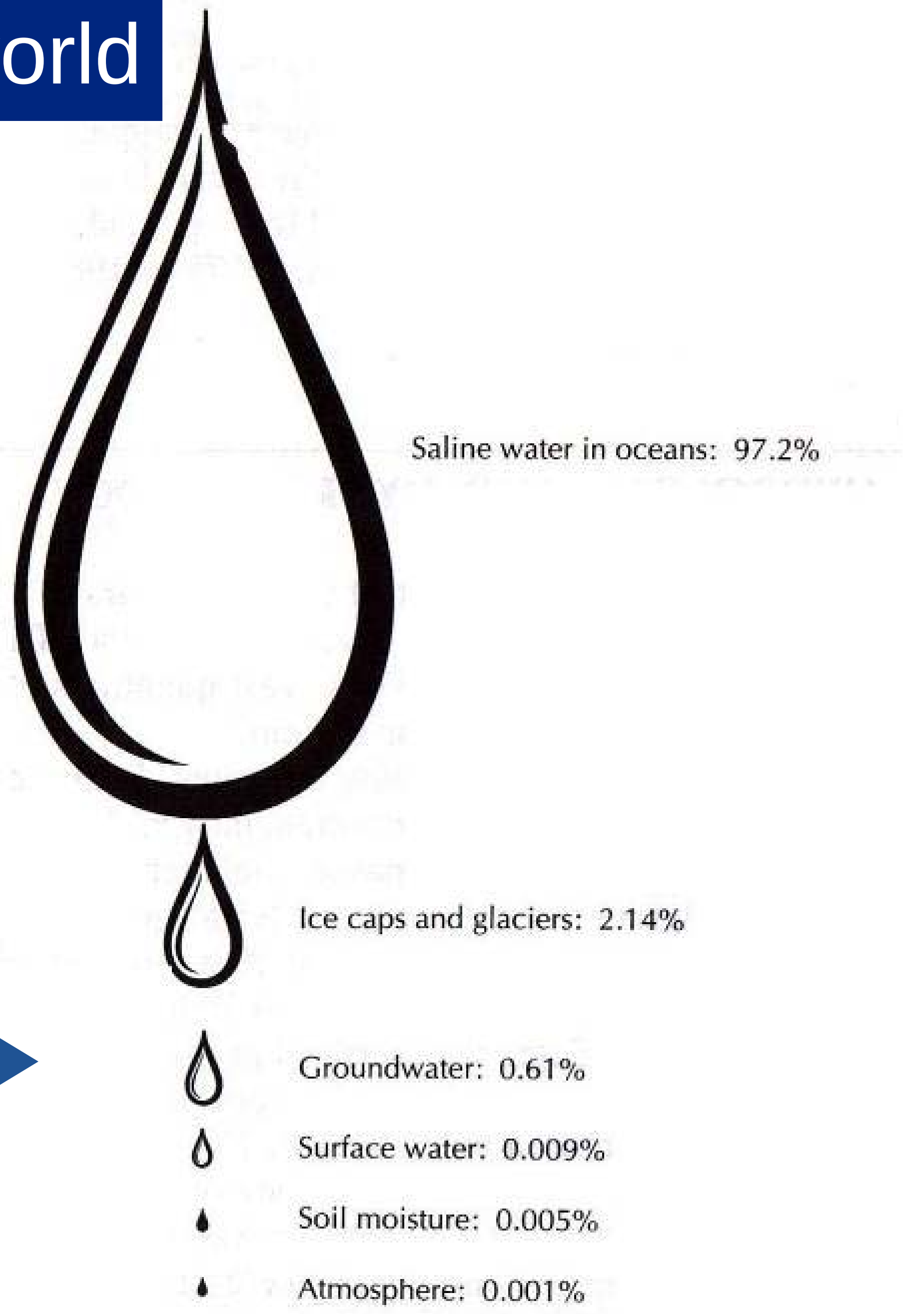
HYDROGEOLOGY

ONE DEFINITION: Hydrogeology is the study of groundwater (water below the ground surface) and its qualities: flow, amount, speed, direction, sustainability, extraction or replenishment capabilities.

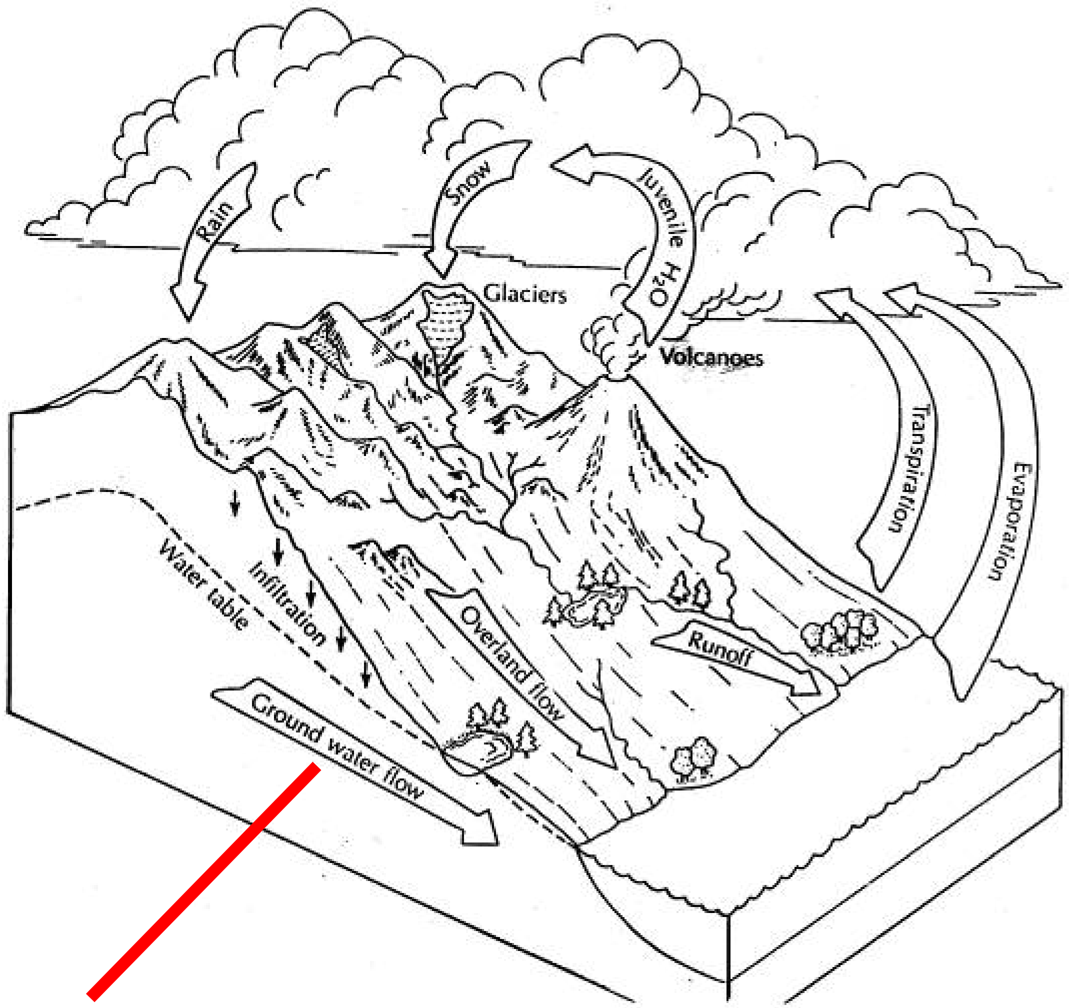
- Water resources: quantity and quality
- Geotechnics (mining, dams, dewatering, slope stability,…)
- Flooding
- Environmental preservation (e.g. streams, wetlands)
- Decontamination (e.g. soils and water)
- Waste disposal (e.g. radwaste and landfill)
- Geothermal energy
- Oil and gas extraction
- CO_2 sequestration

Water volumes: world

98% of liquid fresh water
is Groundwater



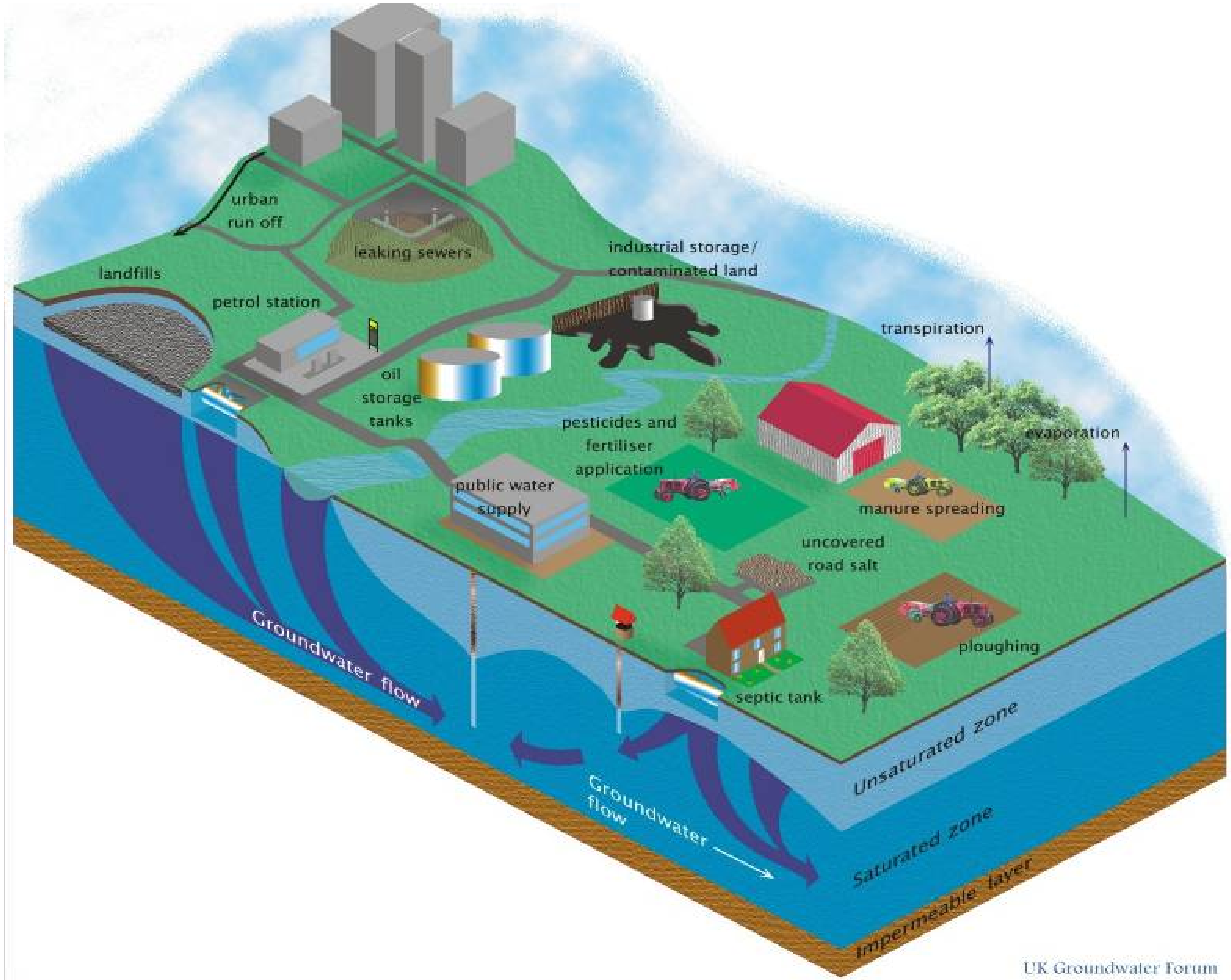
Hydrologic Cycle



Fetter, 1994

GROUNDWATER

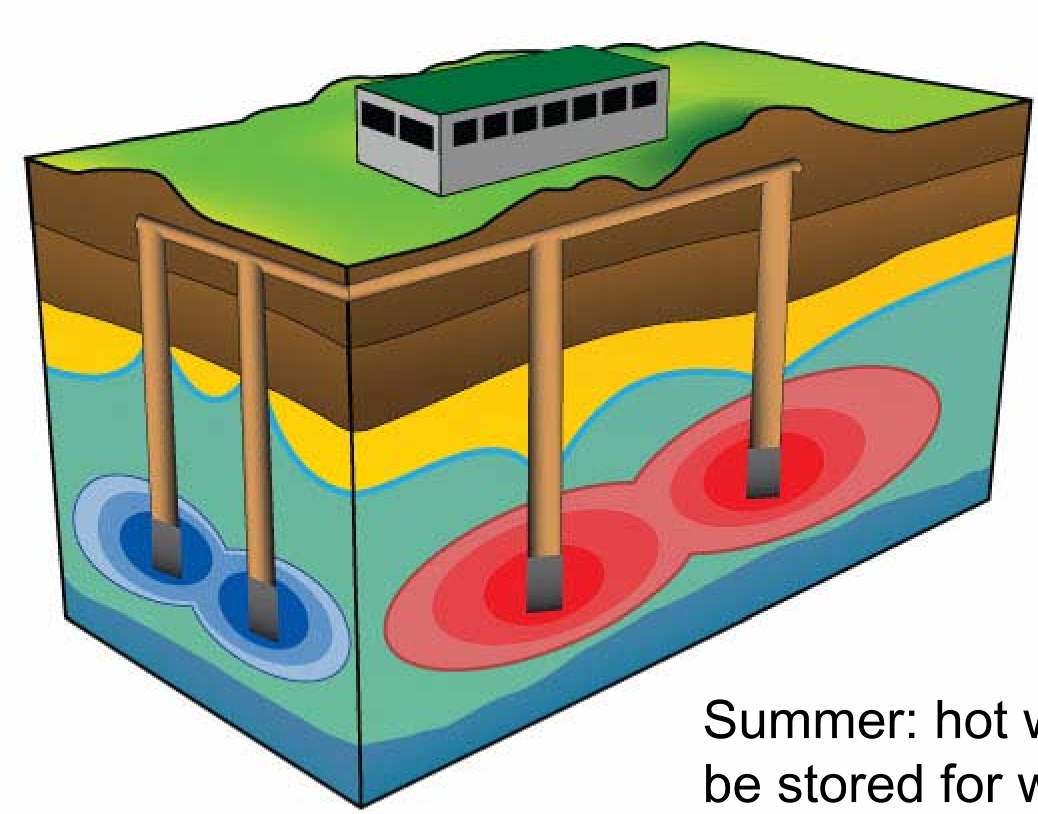
Hazards to water quality



Diffusion Equations

- Heat: Fourier’s law
- Solute (e.g. pollutants): Fick’s laws
- Flow: Darcy’s law

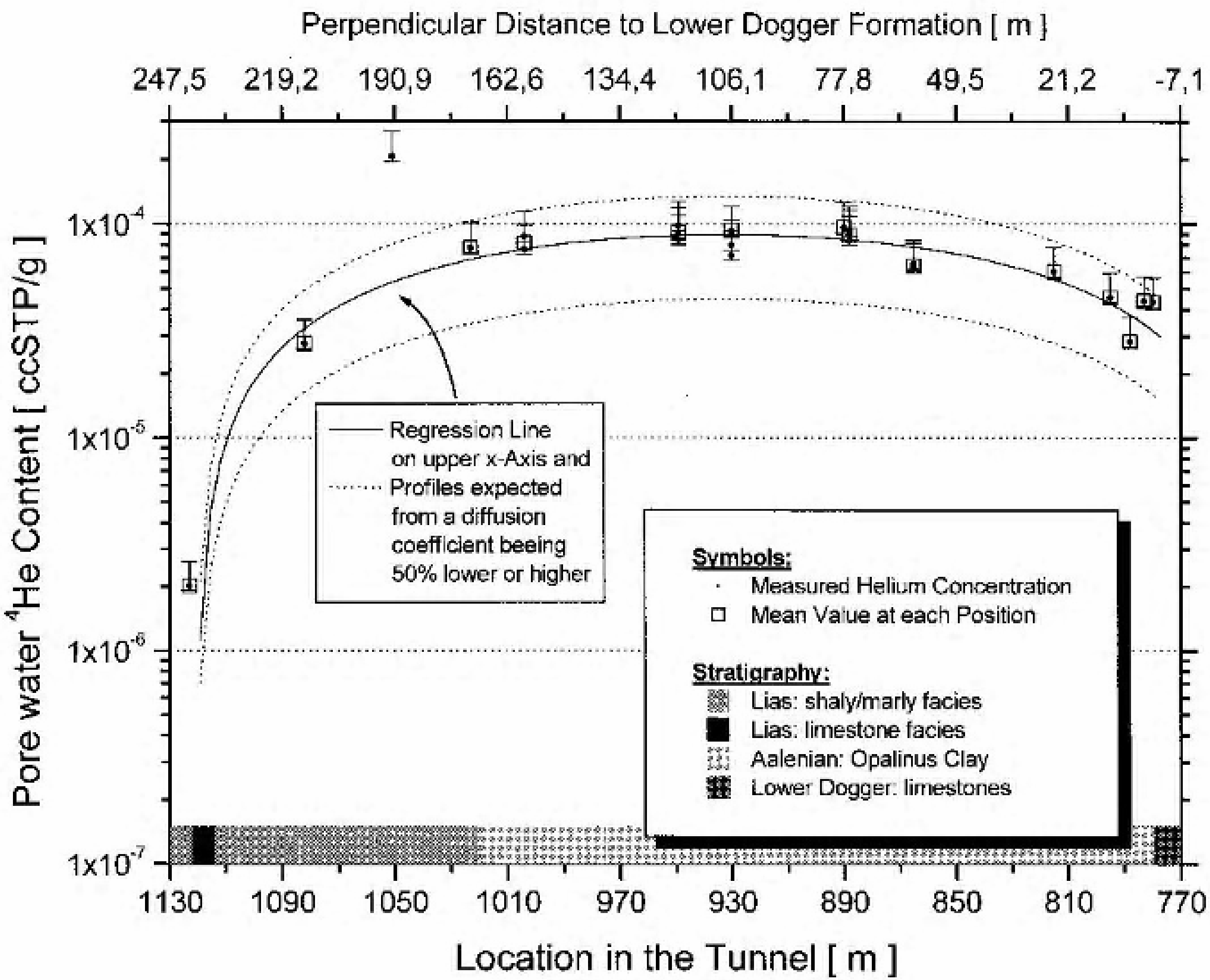
BRIEF MENTION OF ‘HEAT’



Summer: hot water can be stored for winter heating. Winter: cool water can be stored for summer cooling.

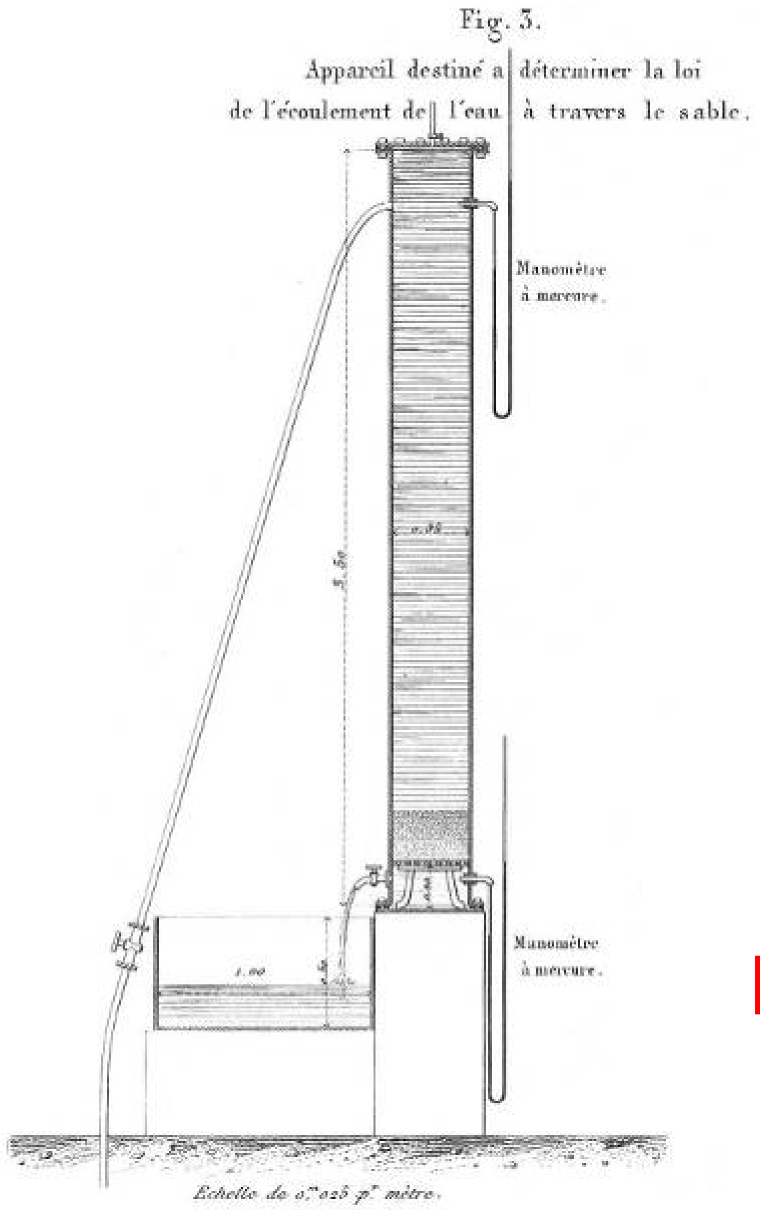
MOLECULAR DIFFUSION: Long times

Mont Terri underground rock laboratory in Switzerland



Observed diffusion profile for helium in a clay formation with a fitted diffusion (with production) model. A D value of about 3×10^{-11} m^2/s over a distance of about 250 m gives a characteristic time of 10 to 50 Ma.

DARCYS LAW: Darcy's Experiment



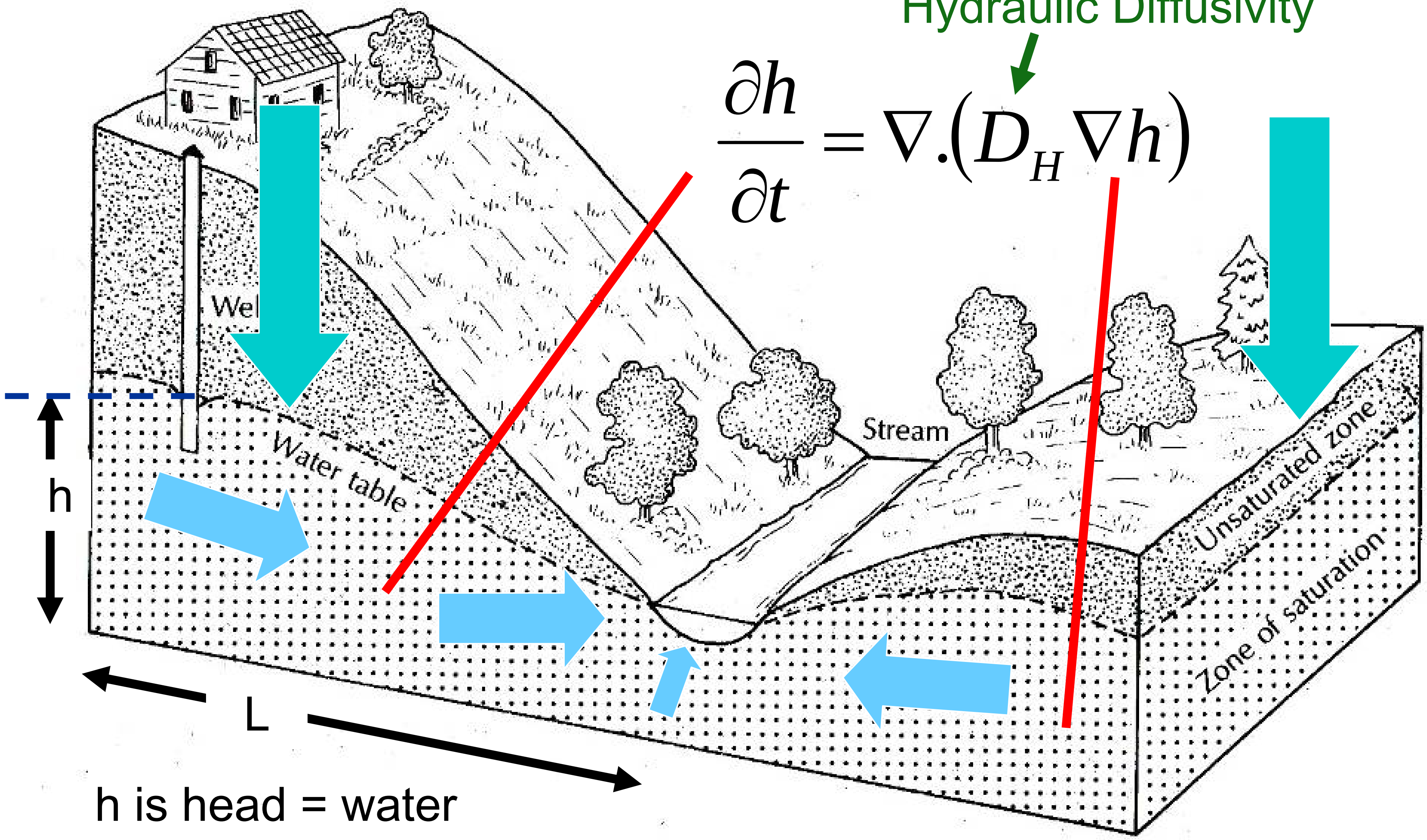
Henry Darcy, 1856. Détermination des lois d'écoulement de l'eau à travers le sable. Les Fontaines Publiques de la Ville de Dijon, Paris, Victor Dalmont, pp.590 - 594

Darcy's Law:

Flow rate=
K×Area ×Head Gradient

K='hydraulic conductivity'
Or 'permeability'

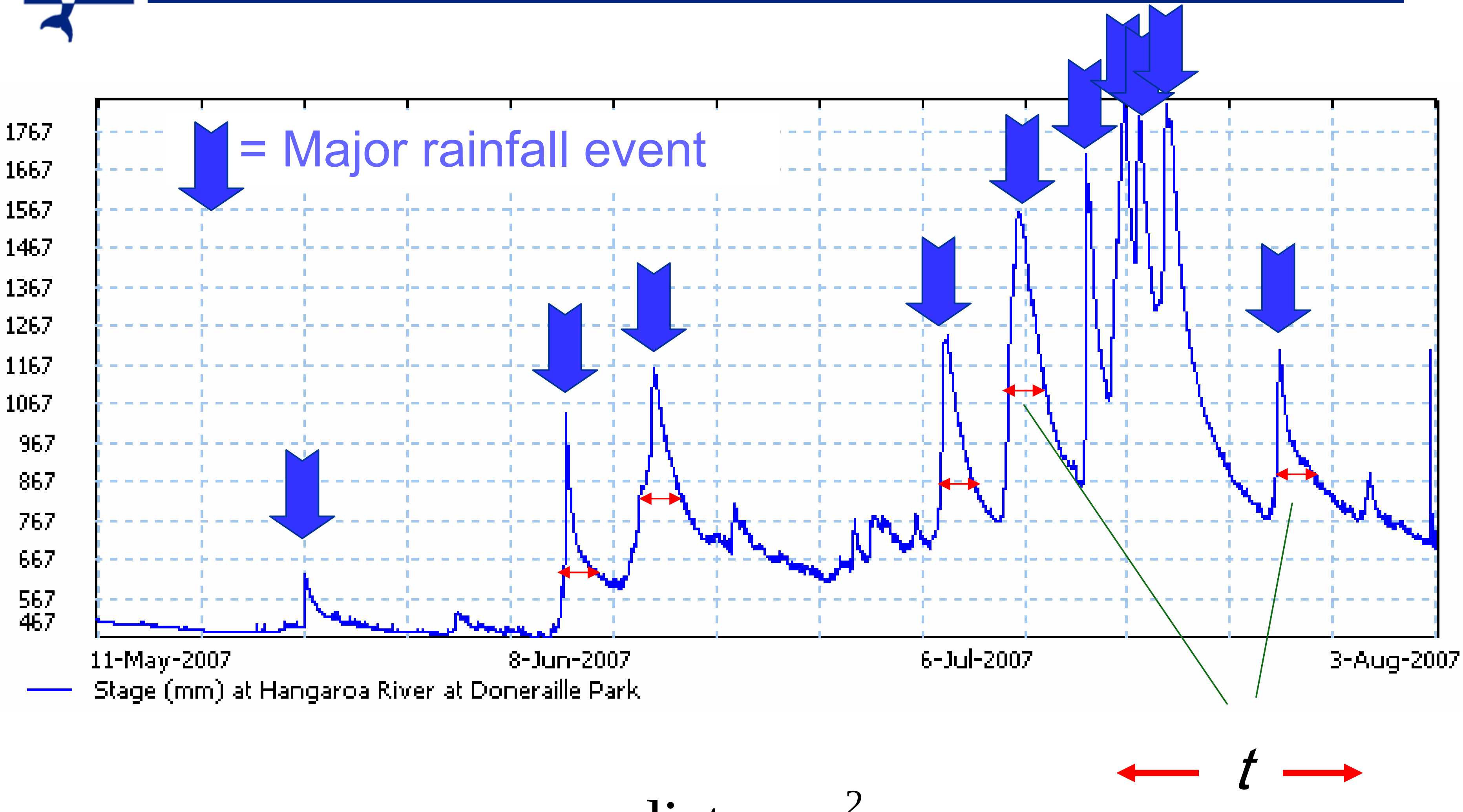
Why do rivers flow when it is dry?



$$\frac{\partial h}{\partial t} = \nabla.\left(D_H \nabla h\right)$$

h is head = water level in wells

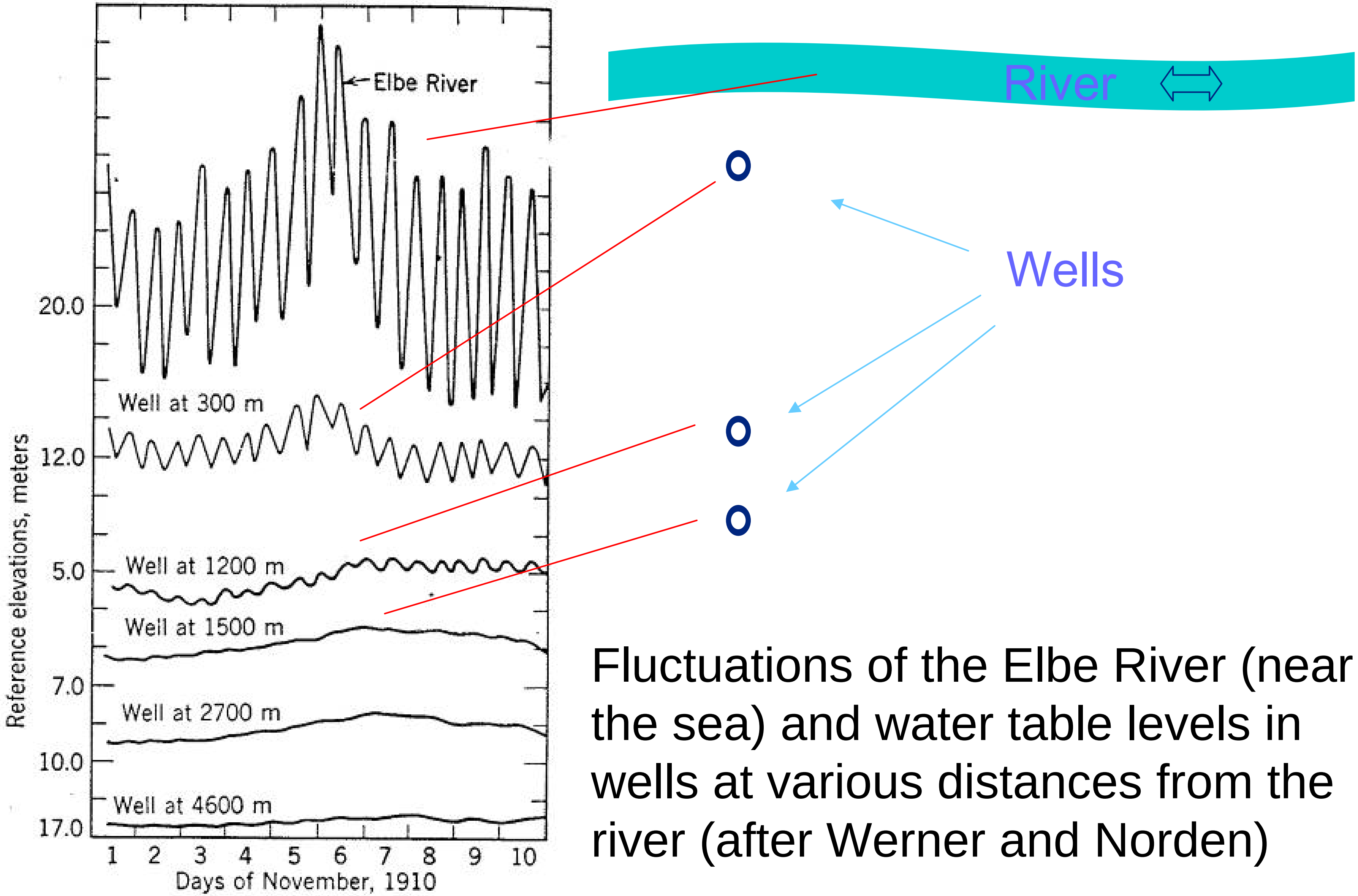
Why do rivers flow when it is dry?



$$\text{time constant} = \frac{\text{distance}^2}{\text{hydraulic diffusivity}}$$

$$t \approx \frac{L^2}{D_H}$$

NATURAL FLUCTUATIONS:
Verification of 'Fick's Second Law'



Fluctuations of the Elbe River (near the sea) and water table levels in wells at various distances from the river (after Werner and Norden)

Solution of the diffusion equation:

$$h(x,t) = H_{MSL} + H_0 \exp\left(-x\sqrt{\frac{\pi}{TD_H}}\right)\sin\left(\frac{2\pi}{T}\left(t - t_{shift}\right)\right)$$

i.e. exponentially decaying with time (phase) shift of

$$t_{shift} = x\sqrt{\frac{T}{4\pi D_H}}$$

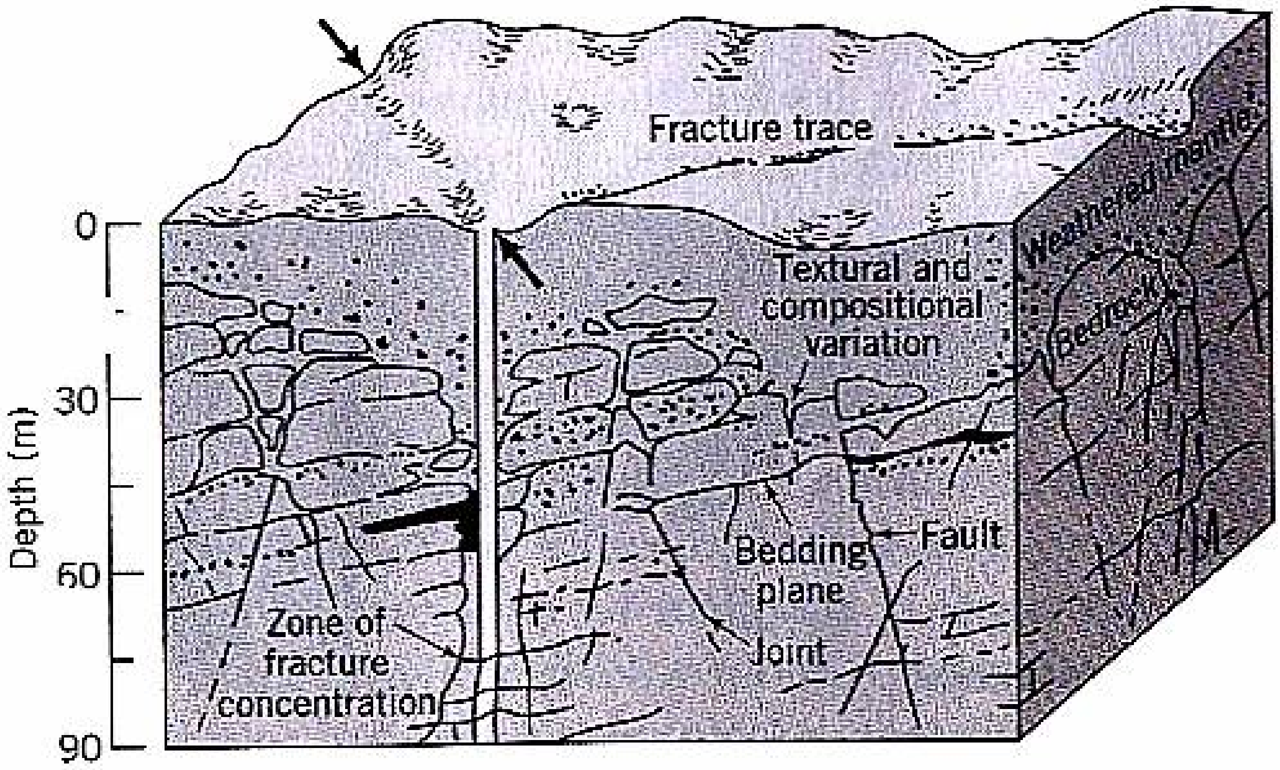
Both the amplitude and time shift depend are determined by the 'hydraulic diffusivity', D_H.

Validates Hydraulic "Fick's Second Law")

CHALLENGES

- HETEROGENEITY
- INACCESSIBILITY

HETEROGENEITY

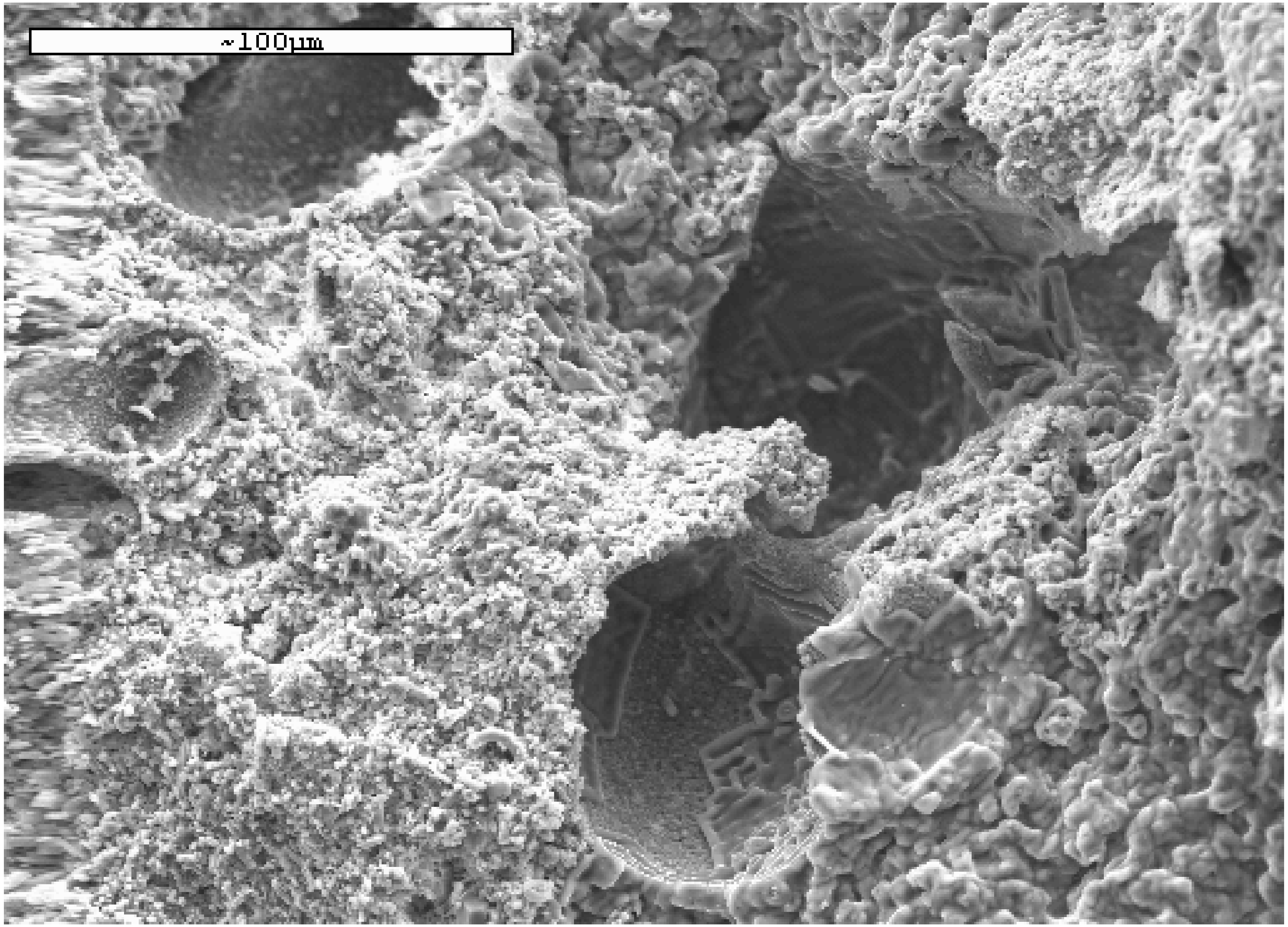


HETEROGENEITY

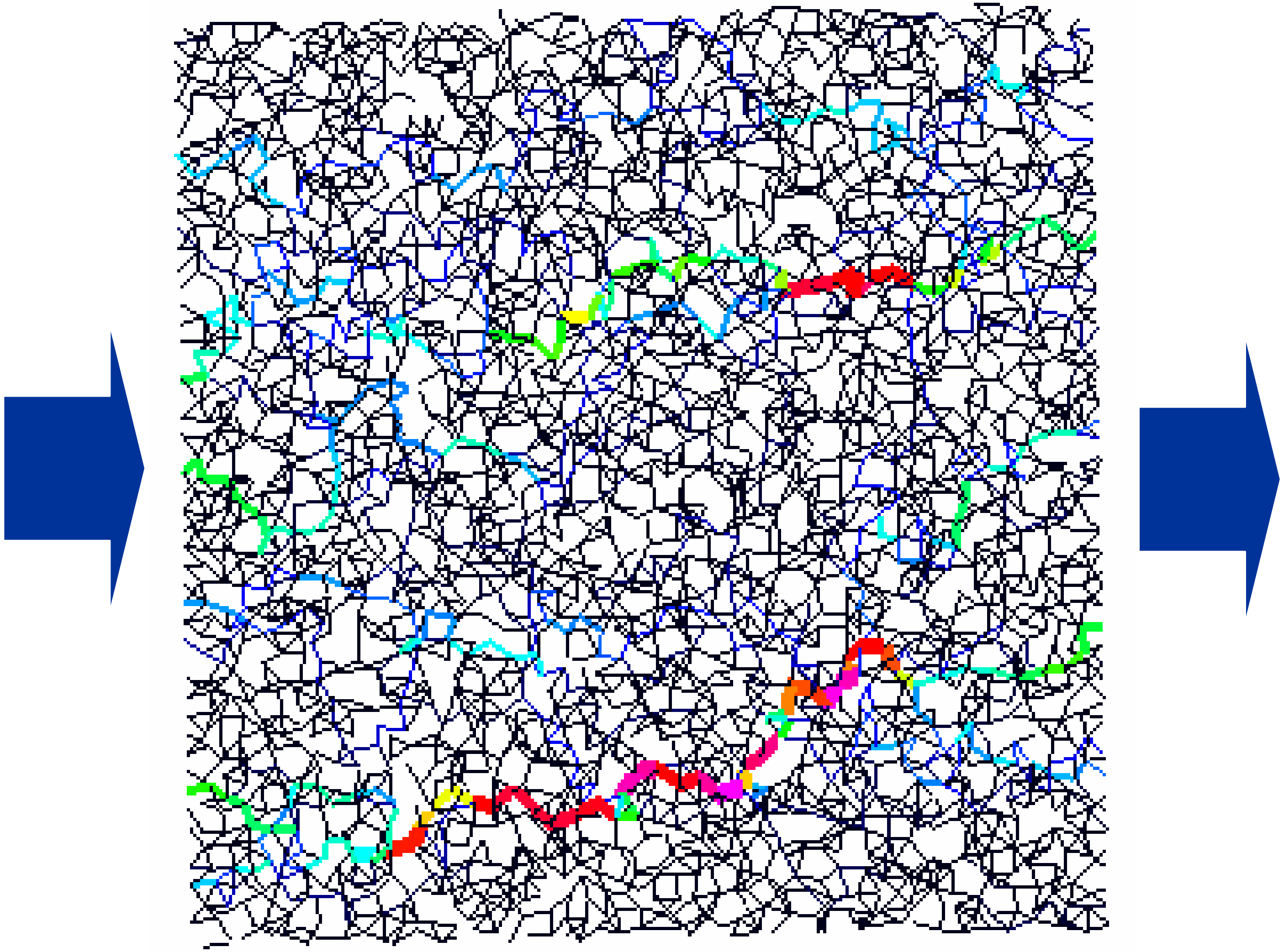
Fractrure apertures range over several orders of magnitude and flow rate is proportional to the cube of the aperture.

Heterogeneity: Anthropogenic

HETEROGENEITY: Microscopic



HETEROGENEITY: Self-Organisation

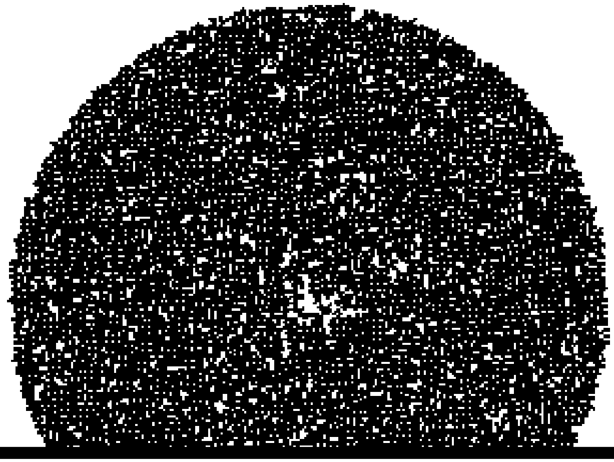


HETEROGENEITY ➔ CHANNEL FLOW ➔ 'DEAD' ZONES

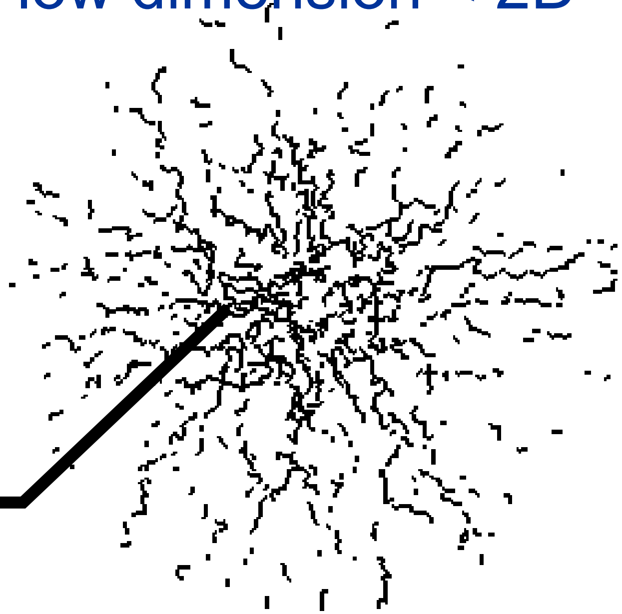
HETEROGENEITY: Flow dimension?

FORCED FLOW TO CENTRAL POINT

Heterogeneous 2D system → Flow dimension < 2D



Similar to experiment described by Charles Nicholson: ‘probe molecules’ to brain.



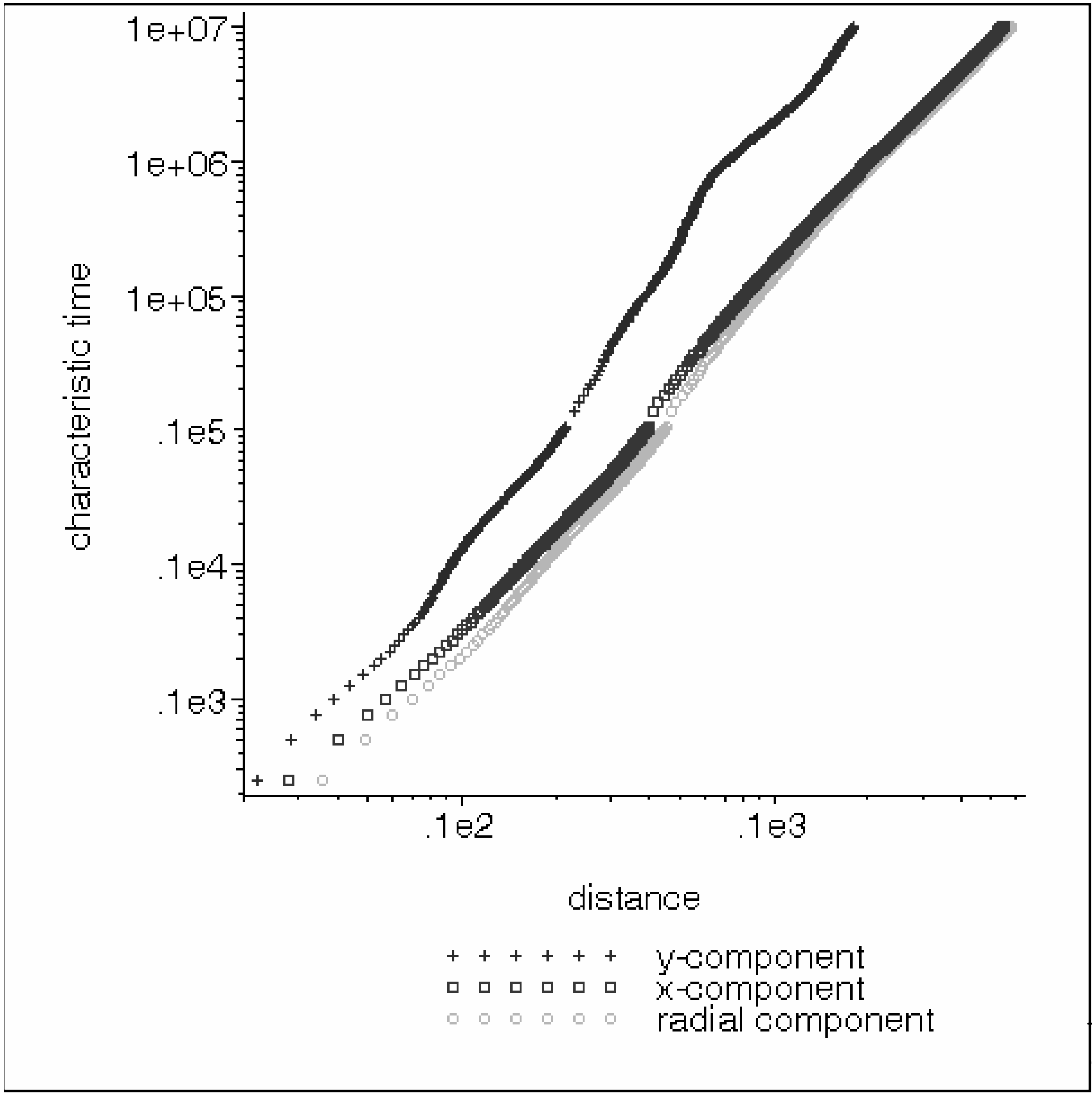
Major flow paths

Barker (1988) “Flow dimension should be treated as an empirical value which may be non-integer”

Flow Dimensions: a problem

- Following 1988 paper many measurements in fractured rock indicate flow to a well typically has a dimension of 1.4 to 1.7.
- But how do we use that value in a regional groundwater model? That is, how do we get H(x,y,z,t) rather than H(r,t).
- Perhaps flow on a fractal.

Random walk on a fractal: work by Shaun Sellers



19,683×19,683 lattice

For each fixed origin, we created an ensemble of walkers (typically 30,000-50,000 particles) with total time steps ranging from 1 million to 100 million.

Power law depends on time and start point and direction.

SO

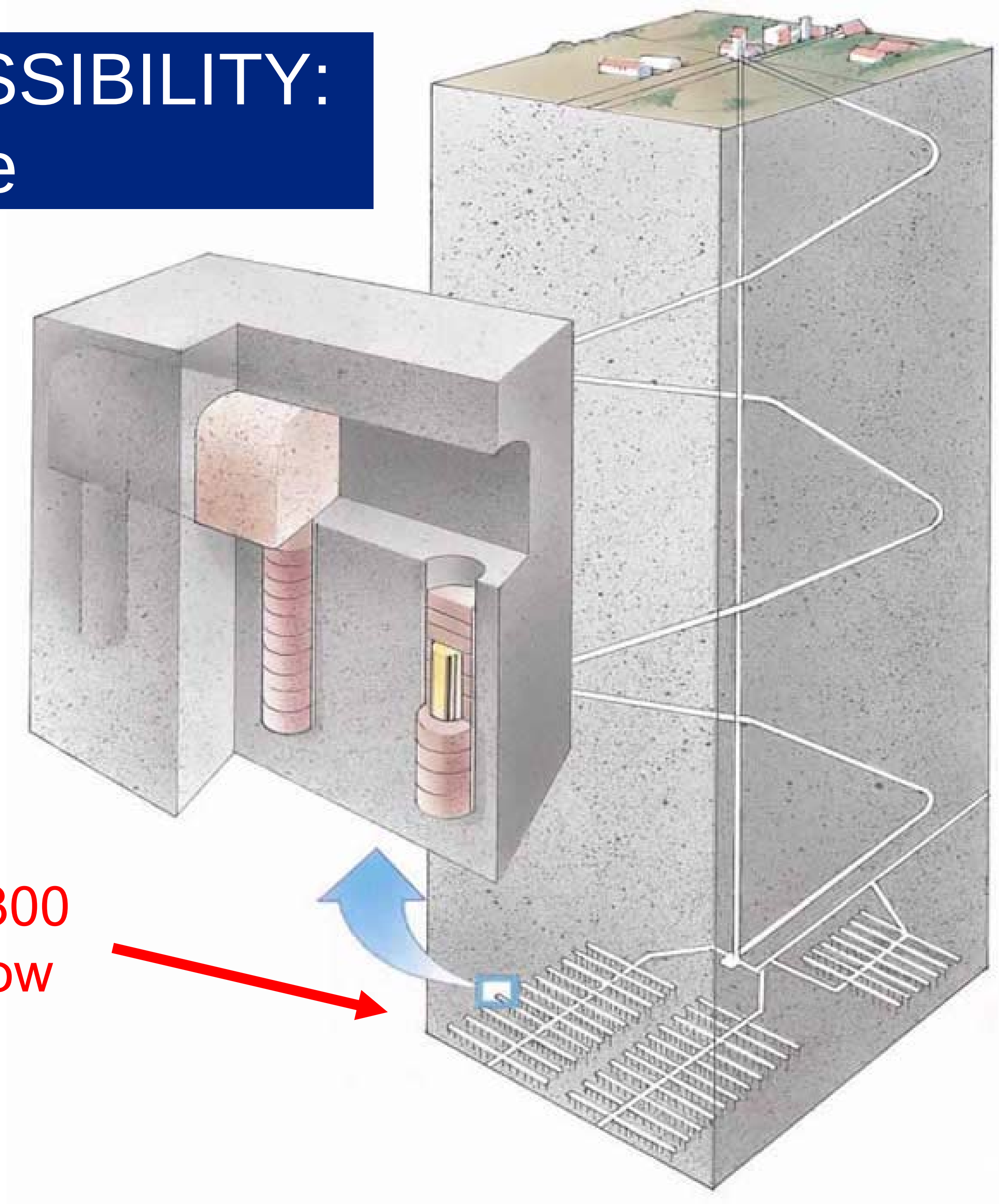
None of the proposed equations such as that below work well.

$$\frac{\partial}{\partial t} H(r,t) = \frac{D_0}{r^{d_f - 1}} \frac{\partial}{\partial r}\left(r^{d_f - d_w + 1} \frac{\partial}{\partial r} H(r,t) \right)$$

INACCESSIBILITY of subsurface

DATA?

INACCESSIBILITY: Radwaste



Target depth of repository typically 300 to 2000 metres below ground level

PUMPING TESTS:
Radial flow to a pumped well

- Probably the most important field technique in hydrogeology.

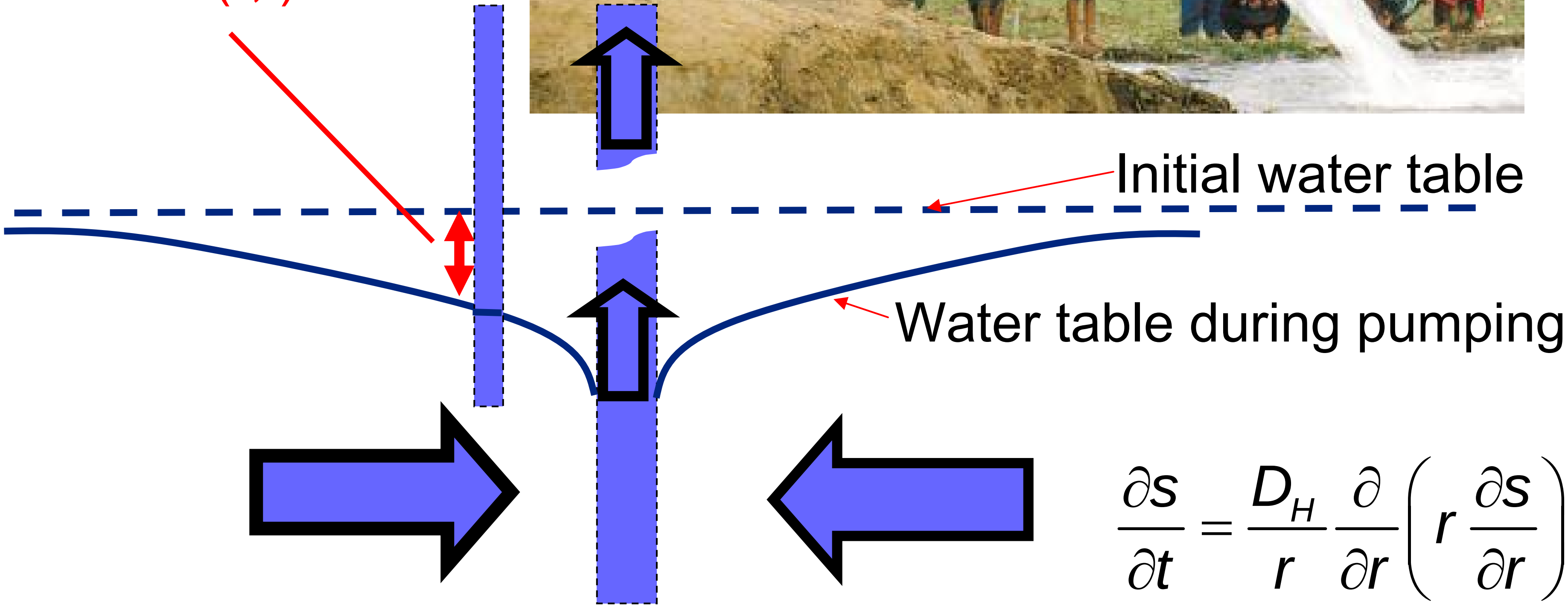
- Determines the permeability and diffusivity.

- Heterogeneity? Radial diffusion averages properties. HOW EXACTLY? – IS THIS KNOWN IN OTHER FIELDS?

A major tool: the pumping test

We measure the drop in water table as a function of time:

s(r,t)



$$\frac{\partial s}{\partial t} = \frac{D_H}{r}\frac{\partial}{\partial r}\left(r\frac{\partial s}{\partial r}\right)$$

A large-diameter ‘dug’ well

Deepening a large-diameter well

A rectangular ‘well’

TRACER TESTS

USED TO DETERMINE:

- Flow paths (connection)
- Velocities (arrival times, protection)
- Flow and transport properties

Tracers in Hydrogeology

- Particles: e.g. Lycopodium spores, Microspheres
- Microbiological: e.g. Phage, Bacterial spores
- Inorganic salts: e.g. Cl, Li
- Fluorescent dyes: e.g. Rhodamine WT, Rhodamine B, Fluorescein
- Fluorocarbons: e.g. SF6, freon (CFC-12)
- Isotopes: e.g. Br-82, Cl-36, I, Tritiated water, Deuterated water

Historical Tracers

- ~330 BC Alexander the Great: Sinking River Rhigadanus:

  TRACER=Two Dead Horses

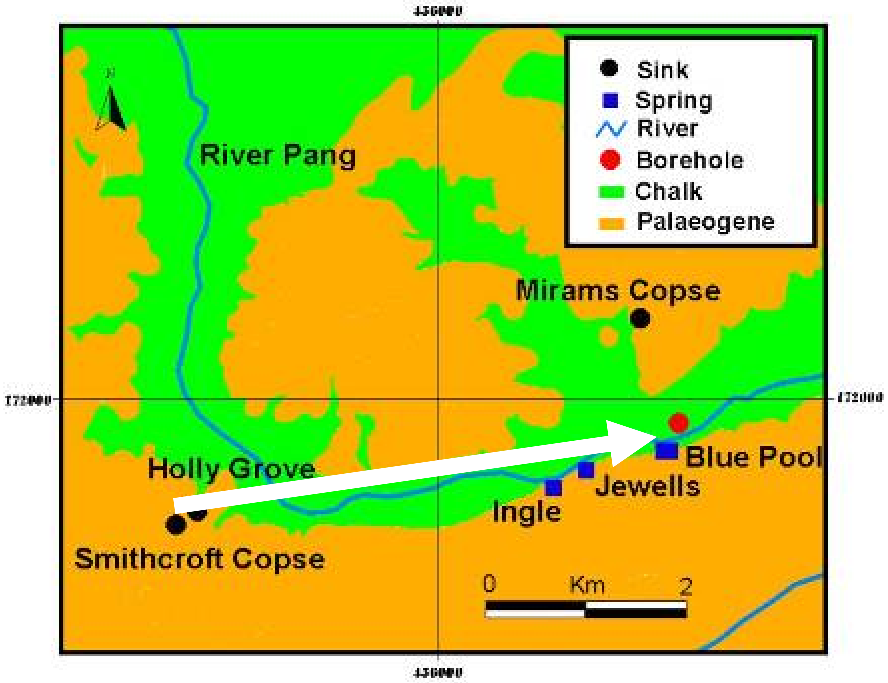
- ~10 AD Tetrach Philippus: Source of the Jordan: TRACER=Chaff

- 1901 Pernod Factory at Pontarlier: River Doube: TRACER=Absinthe (Accident)

TRACERS IN HYDROGEOLOGY

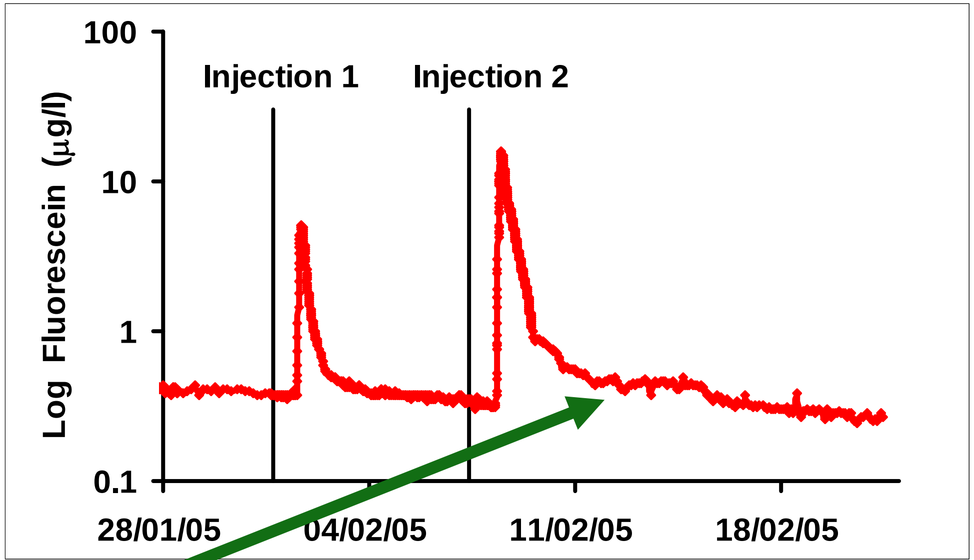
Will I ever see any of this again anywhere?

Success – This time



Results of tracer test over 4 km.

Velocity ≈ 5 km/day



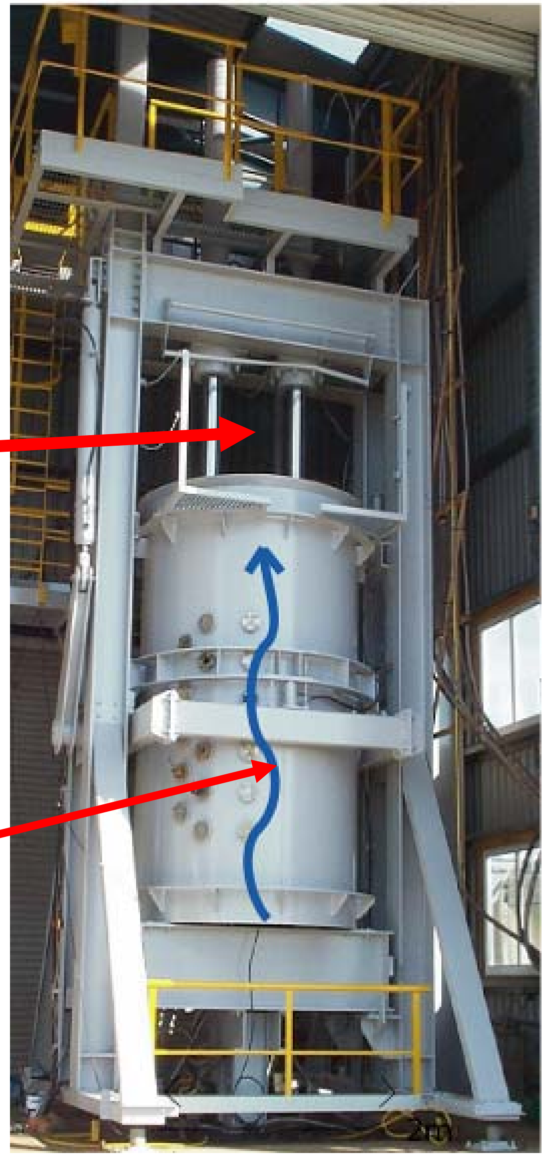
Long tail is charcteristic of 'double-porosity' behaviour (later)

Laboratory: Closed system

CURRENT TEST AT PITSEA

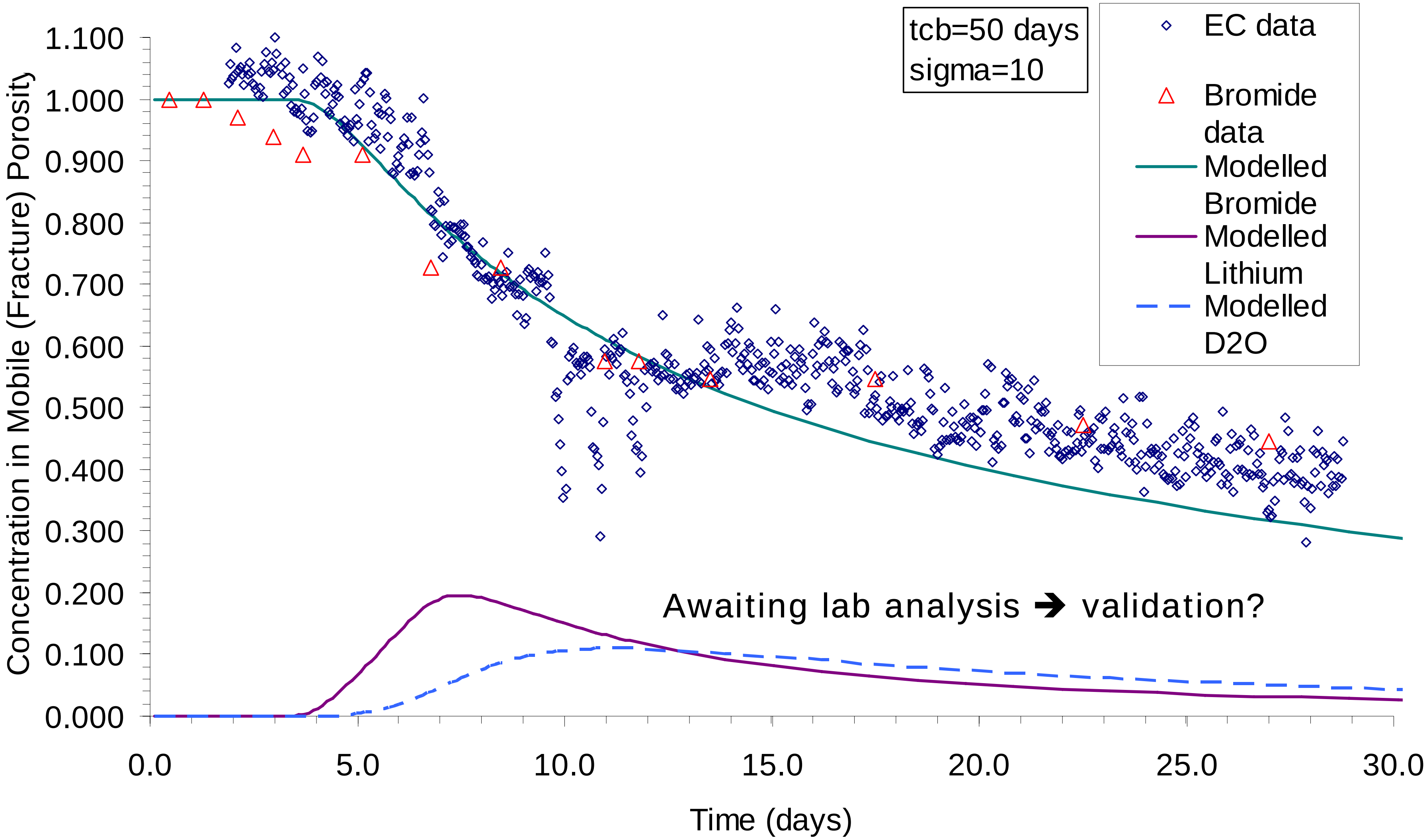
- University of Southampton Waste Research Cell. Diameter = 2m.
- Waste is compressed to represent a particular depth in a landfill.

Currently performing a tracer test



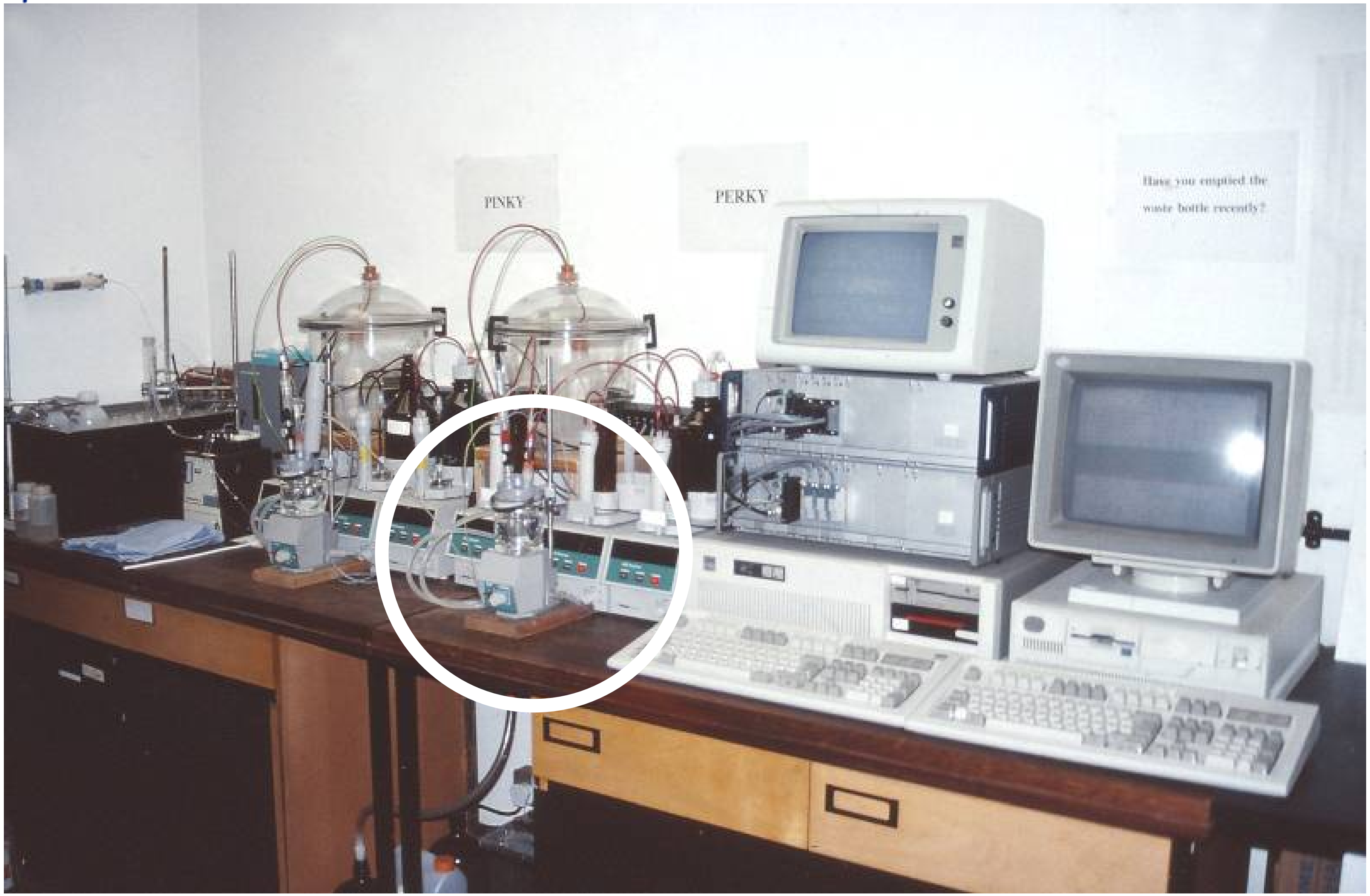
Dilution of the Pitsea brew…

Results so far…

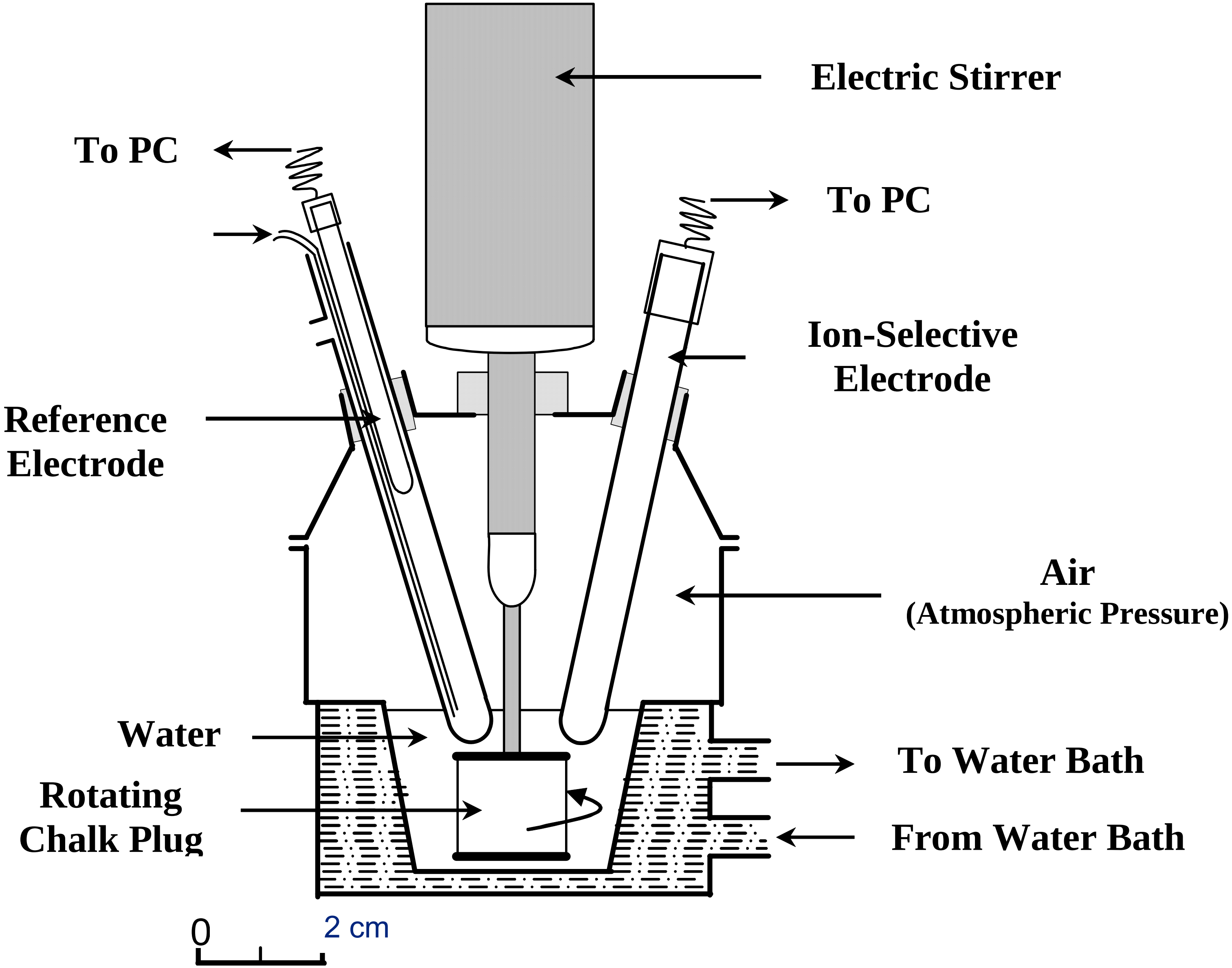


SOME DIFFUSION MEASURMENTS

Rapid measurement of D

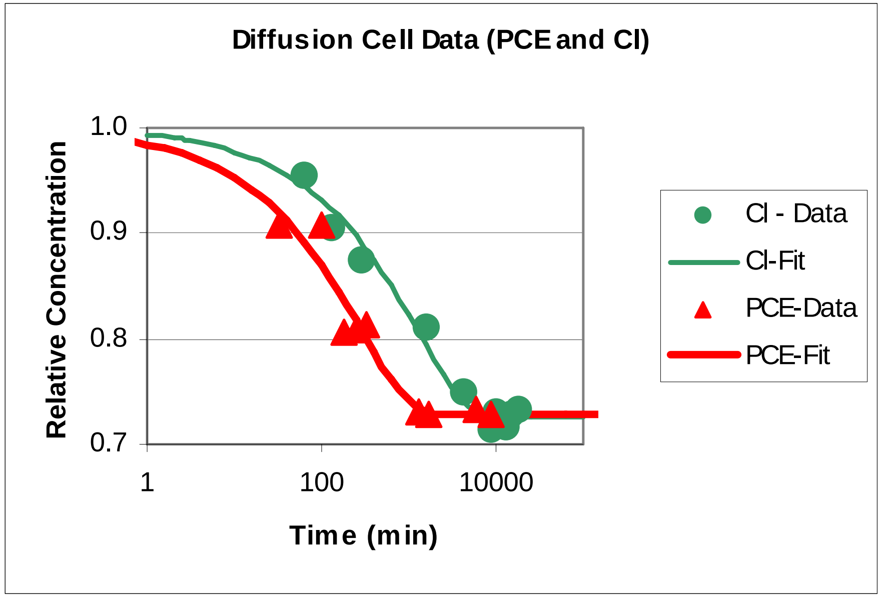


Measuring D for Cl in a 1-inch chalk plug



Help! – an anomaly

Diffusion cell data.
Annular concentrations show a lag of chloride behind PCE (anomalously) indicating that the latter is diffusing faster.
The asymptotic values give the same porosity, in agreement with the known value, indicating negligible retardation.



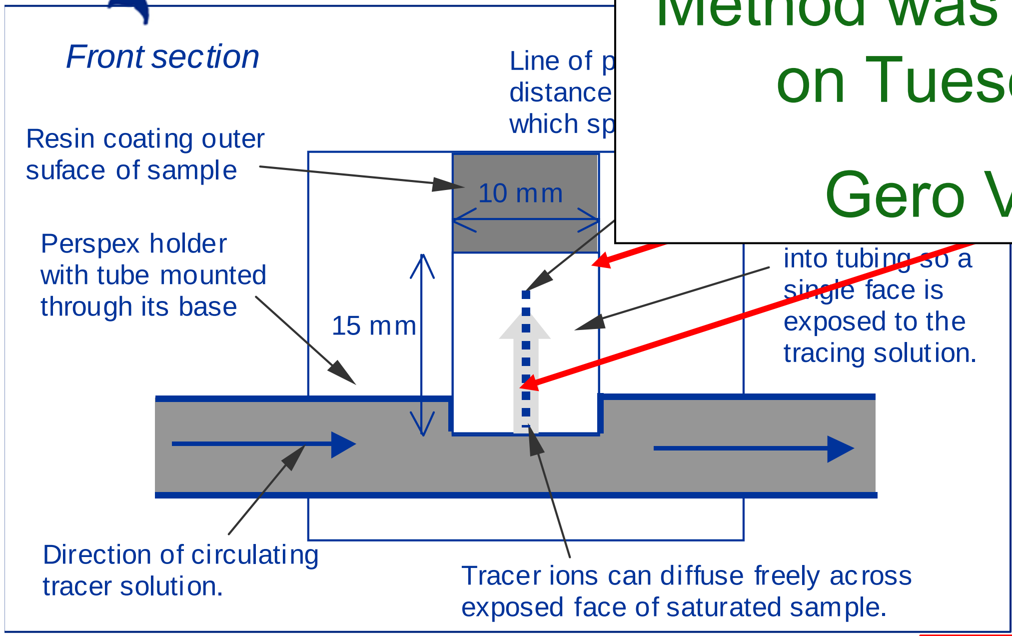
PCE:-

UPAC name: trichloroethene
Molecular formula: C_2HCl_3
Molar mass: 131.39 g mol^{-1}

Tomographic X-ray fluorescence (TXRF)

Method was introduced on Tuesday by

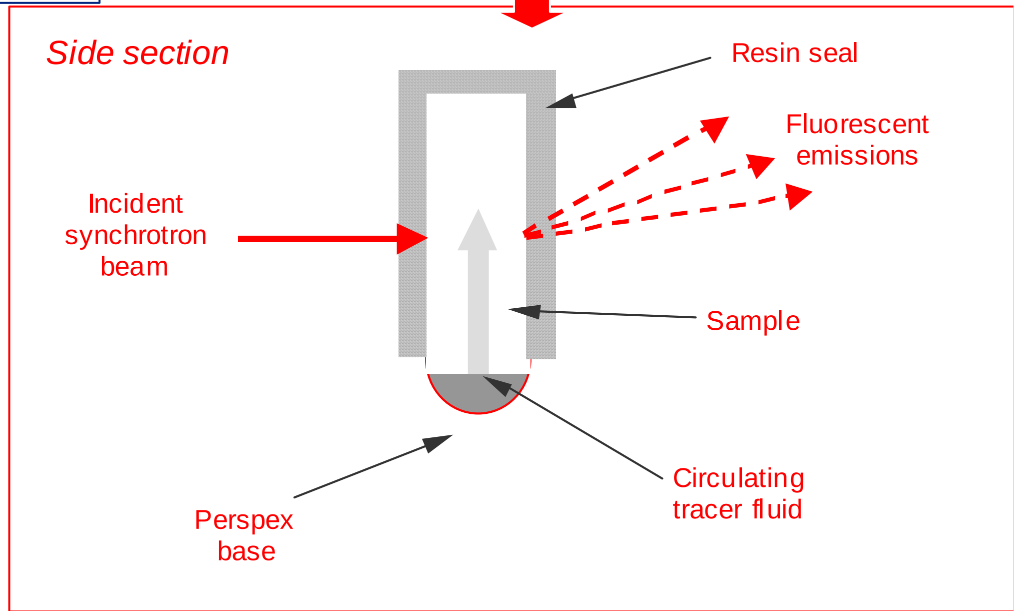
Gero Vogel



lk sample

usion from
circulating water

X-ray measurements



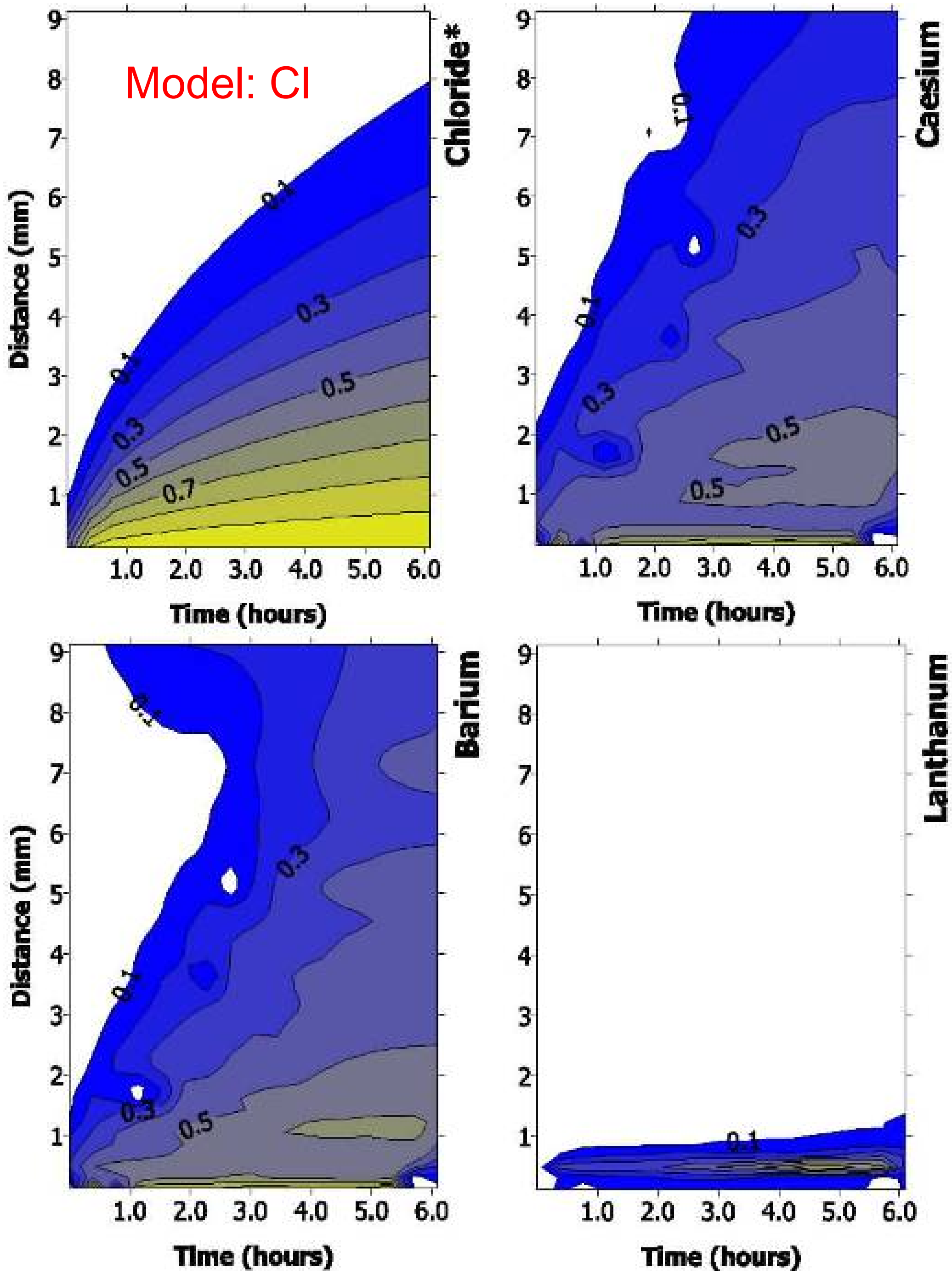
M. Betson, Barker, J.A., Barnes, P. & Atkinson, T.C. (2005) Use of Synchrotron Tomographic Techniques in the Assessment of Diffusion Parameters for Solute Transport in Groundwater Flow. Transport In Porous Media, 60(2): 217–223.

Results

Relative concentrations versus time.
(Vertical line.)

C obtained from tracer-ion X-ray fluorescence intensities

Sample: Chalk
Scan Height: 9mm



MODELLING

MAINLY:-

- DOUBLE-POROSITY

- TWO FUNCTIONS CHARACTERIZING GEOMETRY

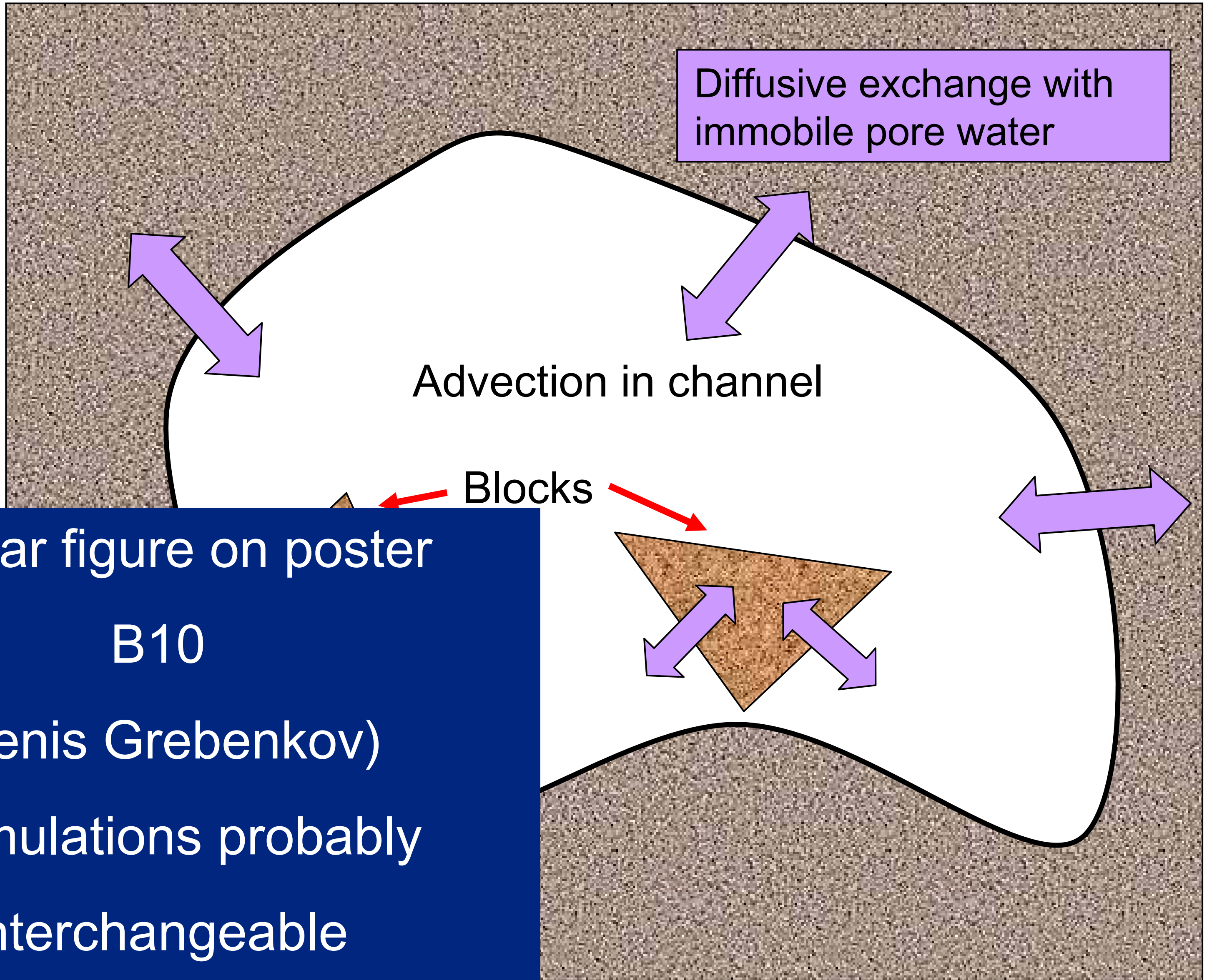
- LAPLACE TRANSFORM SOLUTIONS

A ‘Double-Porosity’ Medium

DP Model: flow in ‘fractures’ diffusion into ‘matrix’

Usually: Fractures and matrix co-exist: 6-D model.

Transport through a channel in a porous medium filled with porous blocks



Similar figure on poster

B10

(Denis Grebenkov)

Formulations probably

interchangeable

Transport through channel – contd.

Laplace transform solution for output concentration:

$$\bar{c}(x,p) = \int_0^\infty e^{-pt} c(x,t)\,dt$$

$$= \bar{c}(0,p)\exp\left\{-pt_a\left[1 + \sigma \mathrm{B}\left(\sqrt{pt_{cb}}\right) + \rho \mathrm{C}\left(\sqrt{pt_{cc}}\right)\right]\right\}$$

Focus on the B() and C() functions

Similarly: LT solution for pumping from a well in a double-porosity rock.

$$\frac{\pi T}{Q}\bar{s}_w(r,t) = \frac{1}{p\left[t_c p + \mathrm{C}(\mu)\right]}$$

C() represents the well shape, normally a circle.

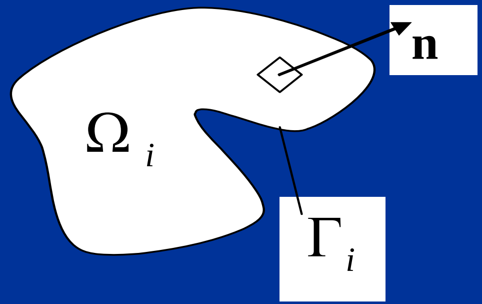
where

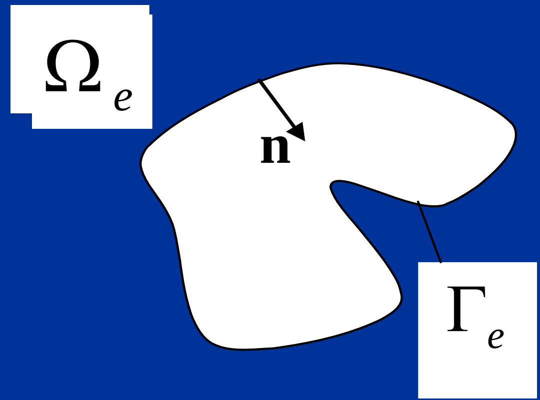
$$\mu^2 = t_w p\left[1 + \sigma \mathrm{B}(\sqrt{t_a p})\right]$$

B() represents the 'block shape'

Here the diffusion is 'hydraulic': both in the fractures and the rock matrix blocks.

Definitions of B(x) and C(x)





$$B(\zeta) = \frac{\beta}{\zeta^2}\left\langle \frac{\partial \psi}{\partial n} \right\rangle_{\Gamma_i} = \langle \psi \rangle_{\Omega_i}$$

$$C(\zeta) = \frac{\alpha}{\zeta^2}\left\langle \frac{\partial \psi}{\partial n} \right\rangle_{\Gamma_e}$$

$$\beta^2 \nabla^2 \psi = \zeta^2 \psi \text{ in } \Omega_i$$

$$\psi = 1 \text{ on } \Gamma_i$$

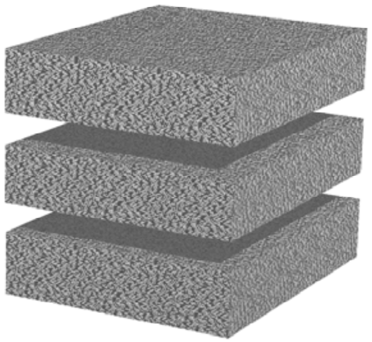
$$\alpha^2 \nabla^2 \psi = \zeta^2 \psi \text{ in } \Omega_e$$

$$\psi = 1 \text{ on } \Gamma_e$$

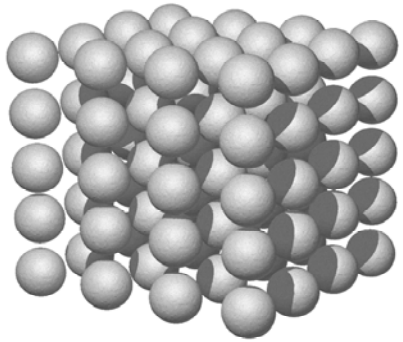
In the time domain obtain solution as sum of exponentials.

Familiar? Probably discovered in may fields?

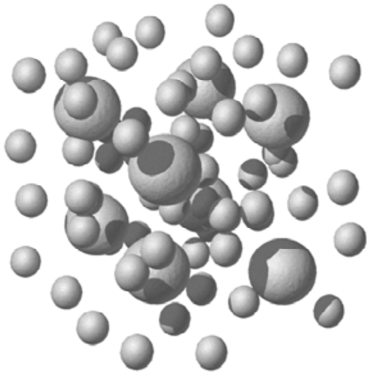
Typical block geometries



SLABS



SPHERES



MIXTURES

An atypical 'block geometry'

Charles Nicholson
Suggested a variety of novel geometries.

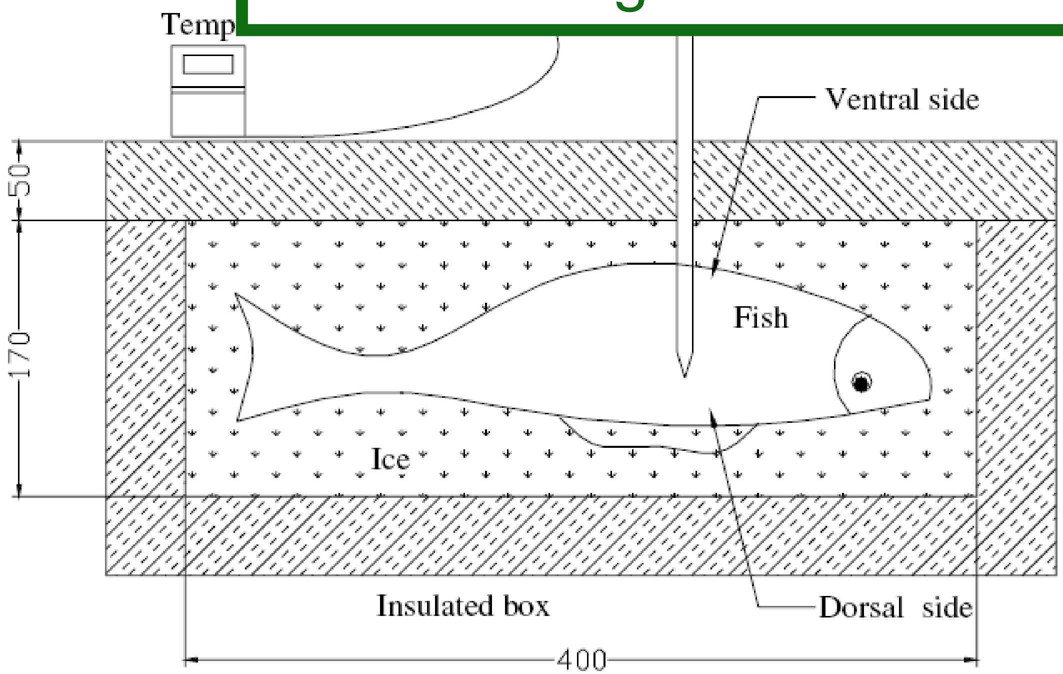


Fig. 1. Schematic diagram of experimental arrangement of fish (*L. rohita*) cooling with ice; all dimension in mm.

ment of
atical model
for cooling the fish with ice
Journal of Food Engineering 71 (2005) 324–329

Some Block-Geometry Functions

Also known as 'shape factors' and 'effectiveness

OTHER NAME

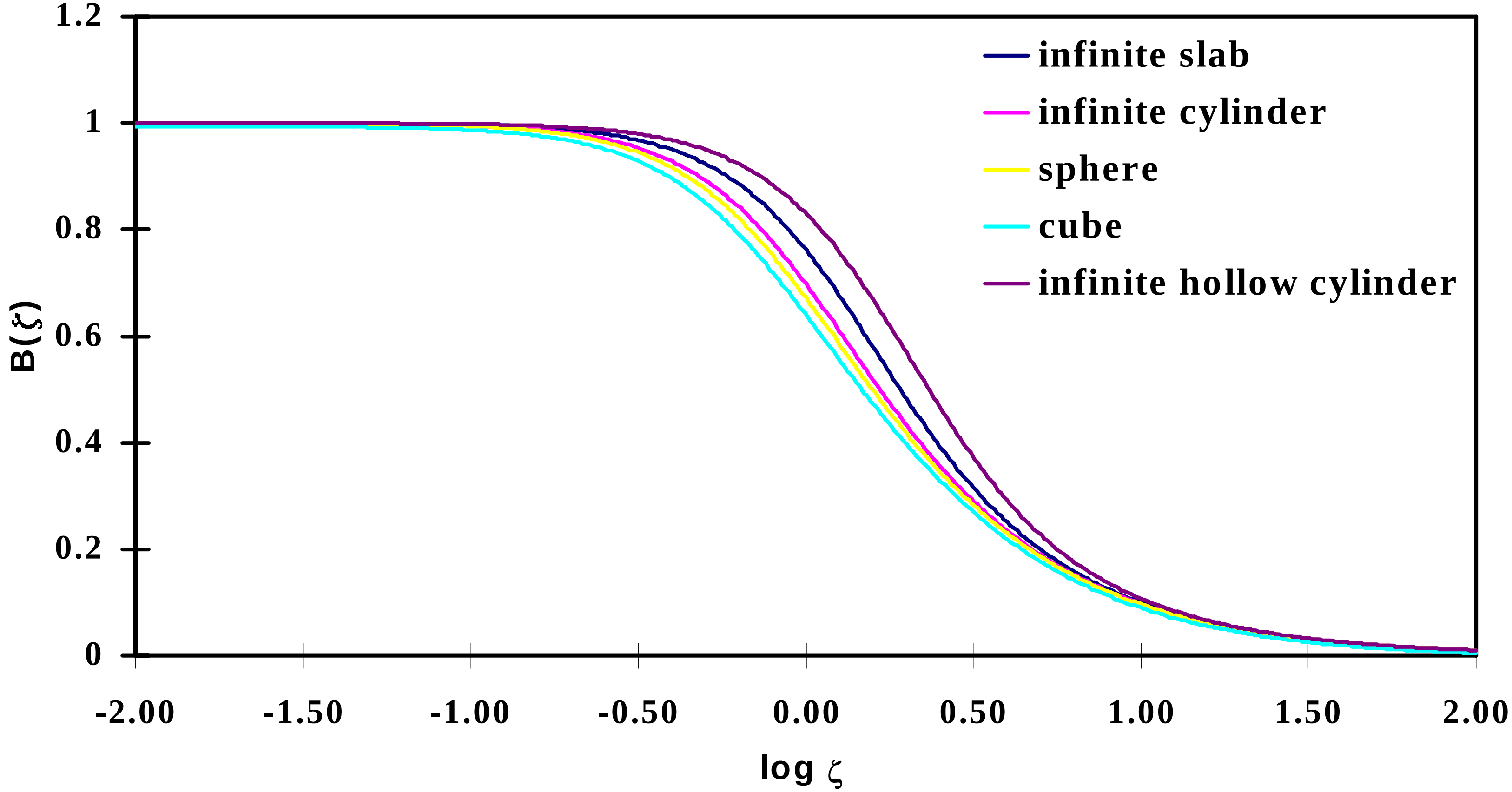
Appears in
B26
(Traytak & Traytak)
which uses spherical
geometry.
Could be generalized
to B()

GEOMETRY	BGF, B(x)	
Slab	(tanh x)/x	
Cylinder (infinite)	$I_1(2x)/x\ I_0(2x)$	
Sphere	$(\coth 3x)/x - 1/3x^2$	
n-D Sphere	$I_{n/2}(nx)/x\ I_{n/2-1}(nx)$	Radius / n

b=Bock volume/Block area

First-order exchange $\propto k(c_f - c_m)$, $B(x)=k/(k+x^2)$ **BEST k or k's?**

Block Geometry Functions, B(x)



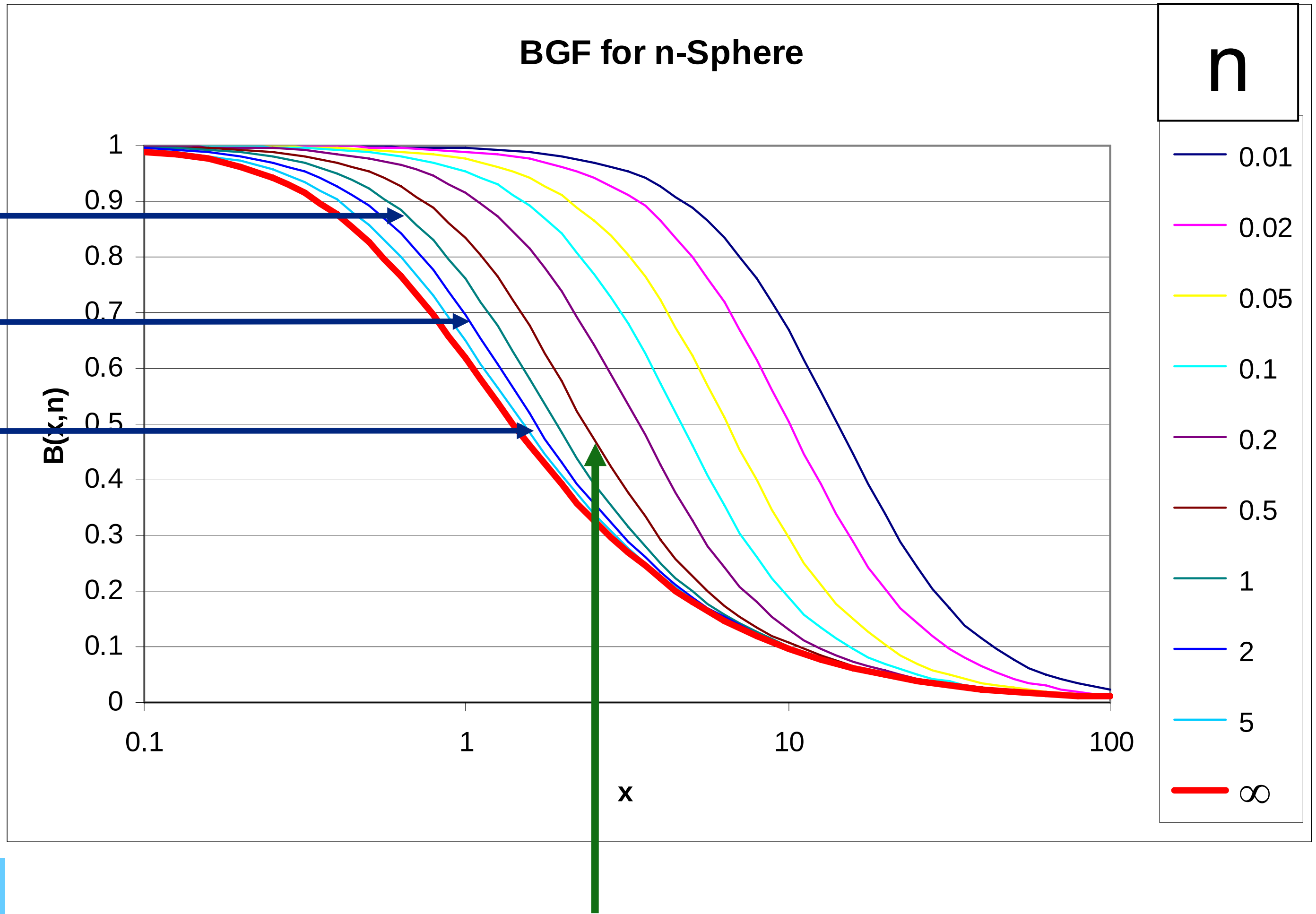
Similar when ‘distance scale’ = volume/contact area.

B(x) for 'spheres' of various dimensions

1D: Slab

2D: Cylinder

3D: Sphere



$$B(x,n) = \frac{I_{n/2}(2x)}{xI_{n/2-1}(2x)}$$

$$B(x,\infty) = \frac{2}{1+\sqrt{1+4x^2}}$$

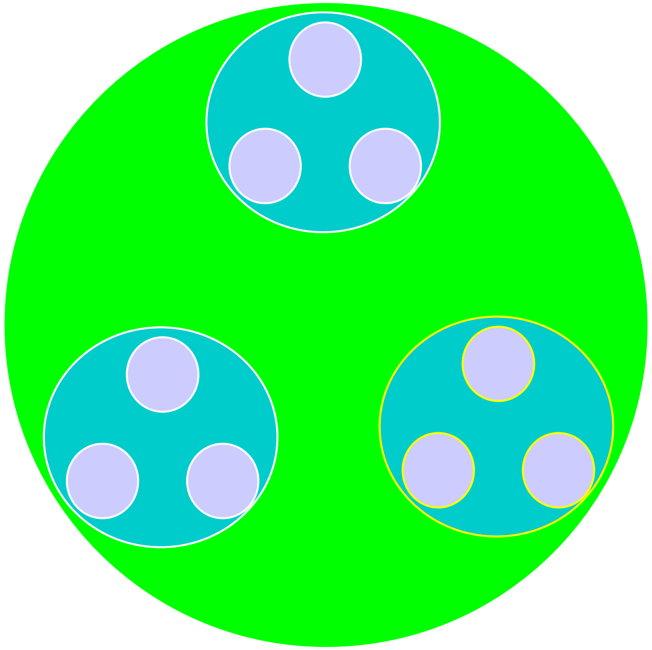
What does a sphere of dimension ½ look like?

Hierarchical-Porosity Block

C11

(Wehring et al.)

Also has a hierarchical geometry



$$\mu^2 = t_w p \beta_N$$

$$\beta_0 = 1$$

$$\beta_n = 1 + \sigma_n \beta_{n-1} \mathrm{B}_n\left(\sqrt{p t_n \beta_{n-1}}\right) \qquad 1 \le n \le N$$

Mixtures of Blocks: Candidate for empirical B() functions

$$B(x) = \sum_{i=1}^{N_s} \int_0^{\infty} p_i(\beta)\, B_i\left(\frac{x\beta}{b}\right) d\beta$$

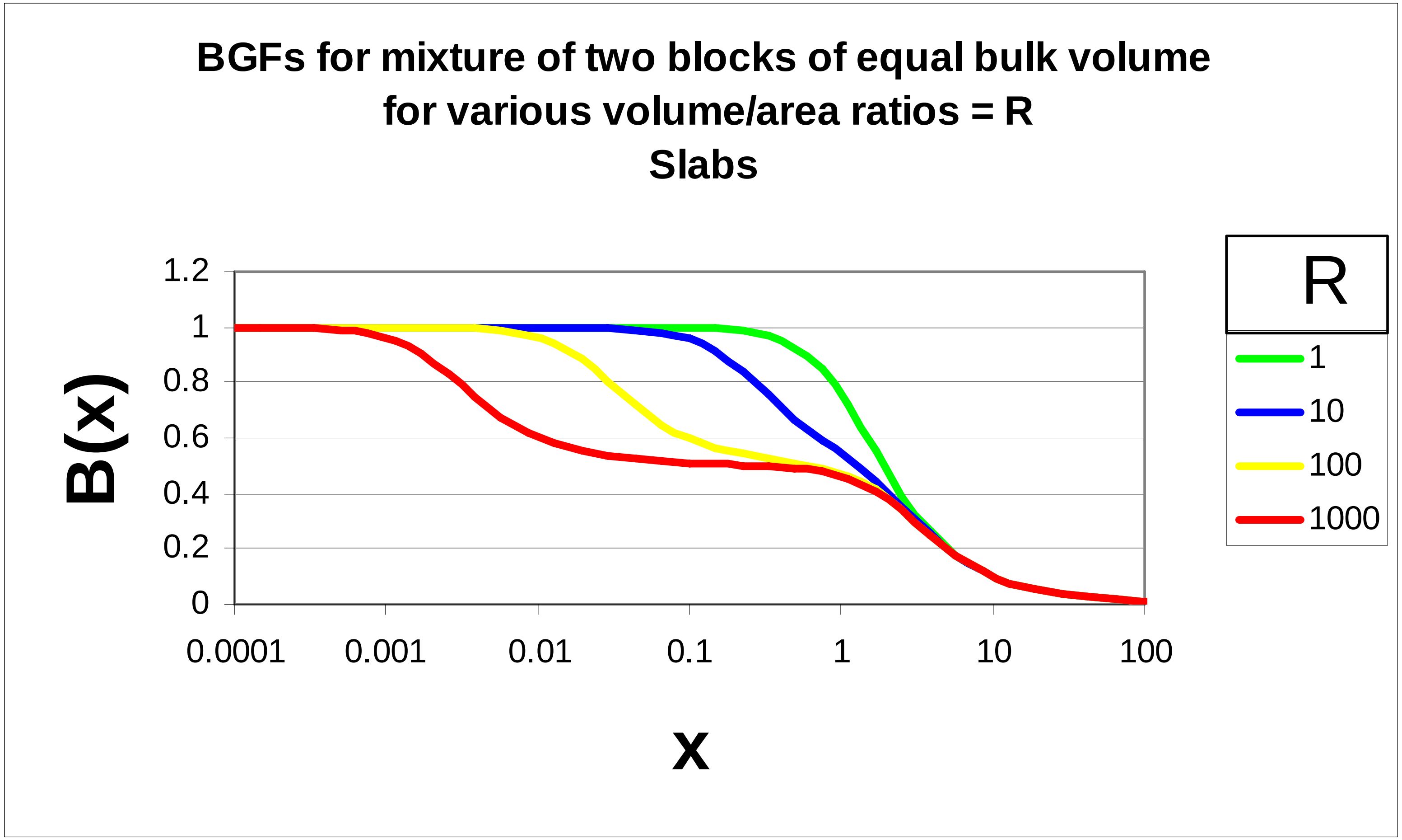
where

$$\frac{1}{b} = \sum_{i=1}^{N_s} \int_0^{\infty} \frac{p_i(\beta)}{\beta} d\beta$$

and $p_i(\beta)\, d\beta$ is the proportion by volume of blocks of shape *i* (i=1,...,N_s) in the size (volume to area) range β to $\beta + d\beta$.

Motivation: Extreme heterogeneity especially in waste.

BGF's for Mixtures of Blocks



Examples of the 'C' function

Sheet: $\mathrm{C}(\zeta) = 1/\zeta$

Circle: $\mathrm{C}(\zeta) = 2\zeta \mathrm{K}_1(\zeta)/\mathrm{K}_0(\zeta)$

Ellipse: $$C(\zeta) = -\frac{4\pi}{\zeta^2}\sum_n \left[A_0^{(2n)}(q)\right]^2 \frac{Fek'_{2n}(\xi_0,-q)}{Fek_{2n}(\xi_0,-q)}$$

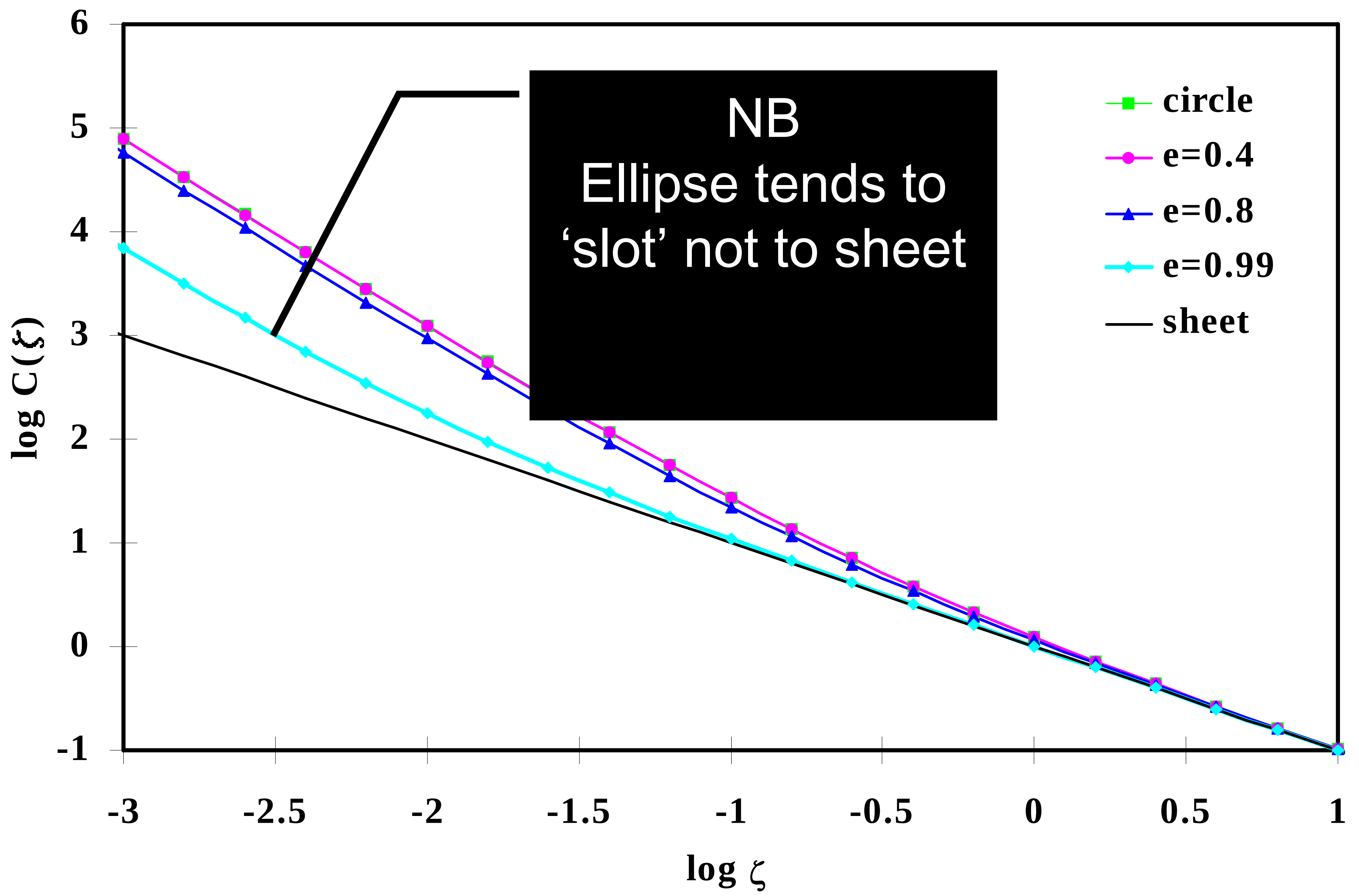
where $\cosh\xi_0 = 1/e, \quad \sinh\xi_0 = e/\sqrt{1-e^2},$

and $$q = \left(\frac{\zeta e}{8E(e)}\right)^2$$

These are the ONLY analytical results I have. OTHERS?

Examples of C(): the Channel Geometry Function

e= eccentricity of elliptical channels



Laplace Transform Solutions

- Reminder of the Laplace transform
- In praise of LT solutions
- Numerical inversion

The Laplace Transform (LT)

$$\bar{f}(p) = \int_0^\infty e^{-pt} f(t)\,dt$$

Examples

$f(t)$ ⟺	$\bar{f}(p)$
1	1/p
t	$1/p^2$
δ(t)	1
exp(-kt)	1/(p-k)
erfc(a/√4t)	exp(-a √p)

Key operational property

$$\frac{\partial f(t)}{\partial t} \Leftrightarrow p\bar{f}(s) - f(0)$$

so

$$\frac{\partial c}{\partial t} = D\nabla^2 c \Leftrightarrow p\bar{c} - c(0) = D\nabla^2 \bar{c}$$

Basis of ‘hybrid’ LT-FD and LT-FE methods.

In praise of LT solutions

- Simple to obtain and relatively simple compared with time-dependent solutions, which are often not obtainable.
- Asymptotic behaviour readily derived
- Convolutions simplified $\int_0^t f(\tau)g(t-\tau)d\tau \Leftrightarrow \bar{f}(p)\bar{g}(p)$
- Easy to obtain integrals (e.g. for mass balance)

$$\int_0^t f(\tau)d\tau \Leftrightarrow \bar{f}(p)/p$$

- Moments readily obtained

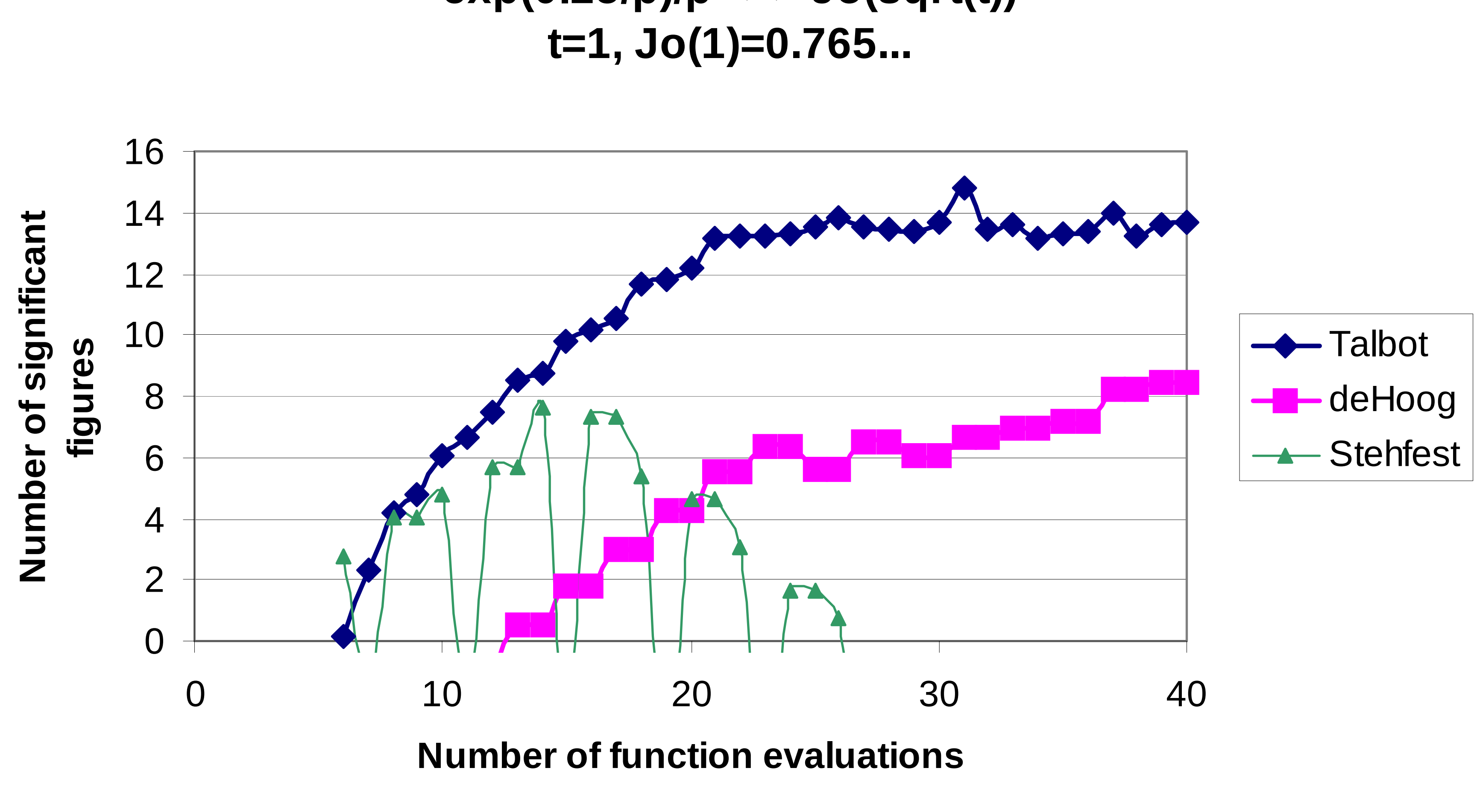
$$E(t^N) = \int_0^\infty t^N f(t)dt = \lim_{p\to 0}\left[(-1)^N \frac{\partial^N \bar{f}}{\partial p^N}\right]$$

- Numerical inversion is not difficult and allows accurate evaluation at short and long times. (No propagation of errors.)

Numerical inversion of Laplace Transform: 3 methods

$$\int_0^\infty e^{-pt} J_0\left(\sqrt{t}\right) dt = \frac{1}{p} e^{\frac{1}{4p}}$$

Discrete form of the inverse Laplace transform used by Asmund Ukkenberg and his colleagues in two 'unnumbered' posters.



Quick and easy LT inversion

The ‘Stehfest’ algorithm coded for 16 function evaluations in VBA (within Excel)

- Function Stehfest16(tau As Double) As Double
- ' Stehfest Algorithm coded by JAB for N=16 (Vs is exact)
- Dim i As Integer, rt As Double, Vs As Variant, Sum As Double, p As Double
- Vs = Array(-1 / 2520#, 5377 / 2520#, -33061 / 60#, 6030029 / 180#, -7313986 / 9#, 302285513 / 30#, -3295862234# / 45#, 106803784103# / 315, -147355535079# / 140, 27108159943# / 12, -101991059533# / 30, 35824504617# / 10, -77744822441# / 30, 36811494863# / 30, -2399141888# / 7, 299892736# / 7)
- rt = 0.693147137704615 / tau
- Sum = 0#
- For i = 1 To 16
-   p = i * rt
-   Sum = Sum + Vs(i - 1) * **Exp(-0.25 / p) / p**
- Next i
- Stehfest16 = rt * Sum
- End Function

$$\int_0^\infty e^{-pt} J_0\left(\sqrt{t}\right) dt = \frac{1}{p} e^{\frac{1}{4p}}$$

KEY POINTS

- HYDROGEOLOGY – WIDE VARIETY OF DIFFUSION PROBLEMS. (I HAD TO LEAVE OUT A LOT!)
- GEOLOGICAL TIMES ARE LONG (E.G. RADWASTE)
- CHALLENGES: HETEROGENEITY AND INACCESSIBILITY
- IMPORTANT TOOLS: PUMPING TESTS & TRACER TESTS
- CHARACTERIZATION OF DIFFUSION TO BLOCKS AND CHANNELS BY B() AND C().
- THE LAPLACE TRANSFORM AND ITS NUMERICAL INVERSION

PLEASE LET ME KNOW ABOUT RELATED WORK, ESPECIALLY…

- How to use non-integer radial-flow dimension in a 3D (x,y,z) model.
- Averaging by radial diffusion in heterogeneous media.
- ‘Blocks’ in the shape of spheres of non-integer dimension. Meaningful?
- Empirical B() functions (c.f. effectiveness factors). And from empirical B() to geometry?
- Is the C() function for channels used elsewhere? Analytical results (e.g. slot)?
- Hybrid LT-FD or LT-FE methods. (Early papers?)
- Asymptotic methods? (Important in waste flushing.)
- Could PCE diffuse faster than chloride?

END

Thank you for your attention.

My sincere thanks to the organisers for their invitation.