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Uncertainty and risk evaluation in a truly pluridisciplinary framework, or when you are asked to provide exact solutions with virtually no information and you fail miserably

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A look to the past in hydrogeology

- Early XXth Century: Flow in porous media/well hydraulics. Emphasis: QUANTITY
- Second part of the century: Geochemistry, transport of conservative solutes: Emphasis: QUALITY
- 80's on: Stochastic hydrogeology, modelling
- New stuff every decade: surface/subsurface interactions, coastal aquifer dynamics, geothermal, vadose zone infiltration,...
- multispecies reactive transport, CO2 sequestration, climate change & alternative resources related to integrated water management, risk evaluation, ...

So, we know where we are, but where are we heading to?



Session: Visionary session on the next Hydrological Decade

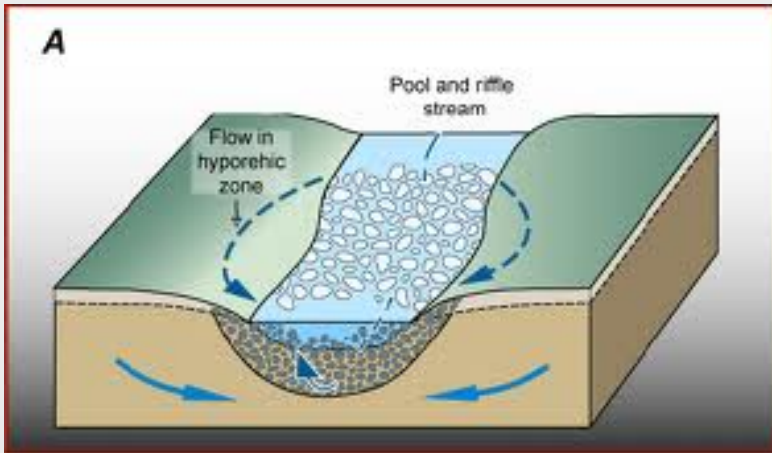
My qualifications: “This is the most stupid idea I have ever heard of. This will definitely be a failure since nobody would be interested in.” a quote by Sanchez-Vila (2009)

... talking about **Twitter**

So, just listen and then do exactly the opposite I will tell you. But at least indulge me taking a look to the following problems



An innocent looking problem



But it combines surface hydrology, hydrogeology, ecology, zoology (vertebrates/invertebrates), biology (bacteria), botany (vegetation), sediment transport,...

But can we work together?: a thought about hydrologists (not bio-, not eco-, not chemo-)

Surface hydrologists consider a nice water cycle where they include runoff, evapotranspiration and something called **losses**

Subsurface hydrologists have a hard time trying to tell students that you do not lose these losses, but rather they are our input and we call them **AQUIFER RECHARGE** (eventually you get to drink them!)



Issues in measurements (both # of points and flow rates)



Surface hydrologists see things!
... and then act accordingly

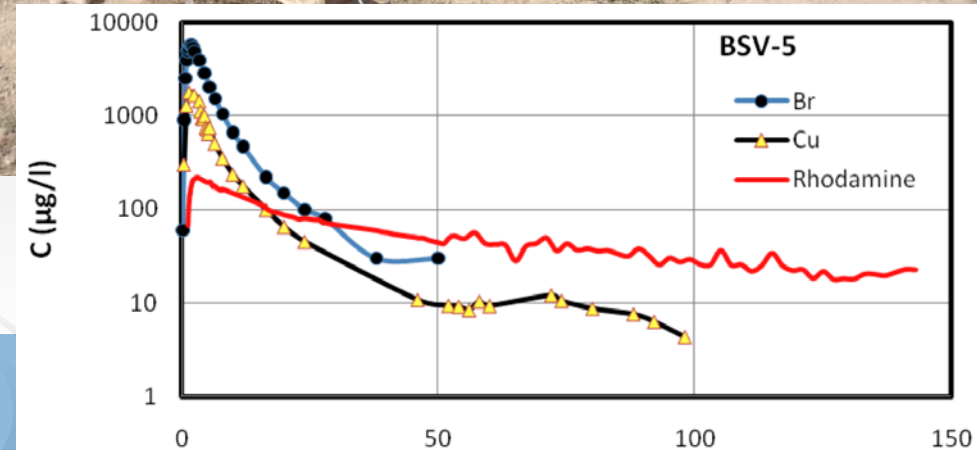


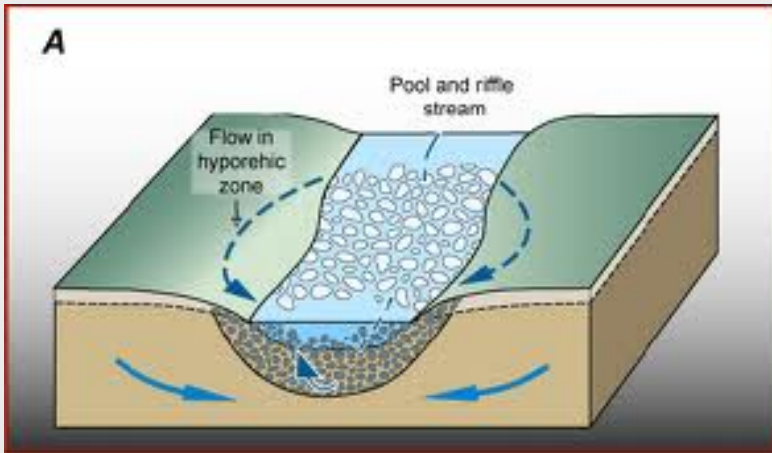
Hydrogeologists do not see anything ... so just guessing?

Scales? Spatial and temporal variability



A tracer test in a river and in an aquifer.
You place a dye and watch it as it moves. You
take pictures!
Or you just record data and then try to interpret



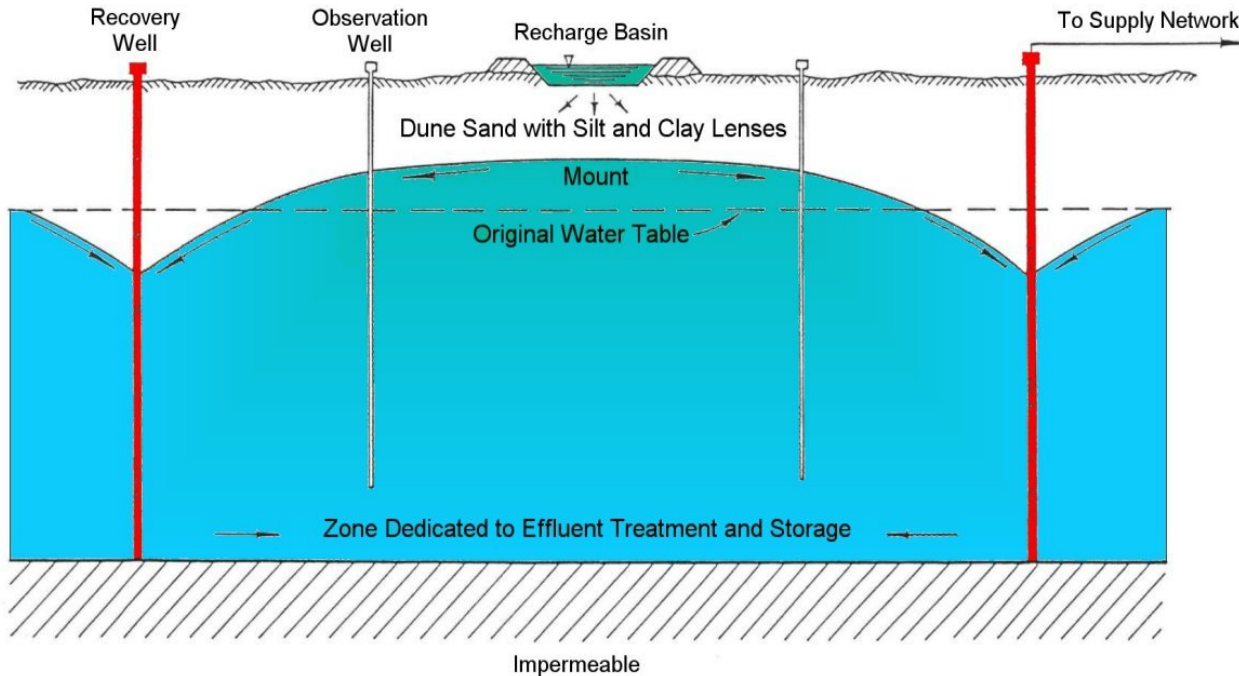


So, back to our innocent looking problem, **what spatial and temporal scales should we consider?** when dealing with exchanges. Reactions take place again at different scales

And more, should we worry about the **presence of fish and existing vegetation** (will this change our problem?)

Another innocent looking problem

Hydro problem, we have water, we pour water, it reaches the aquifer. So simple.

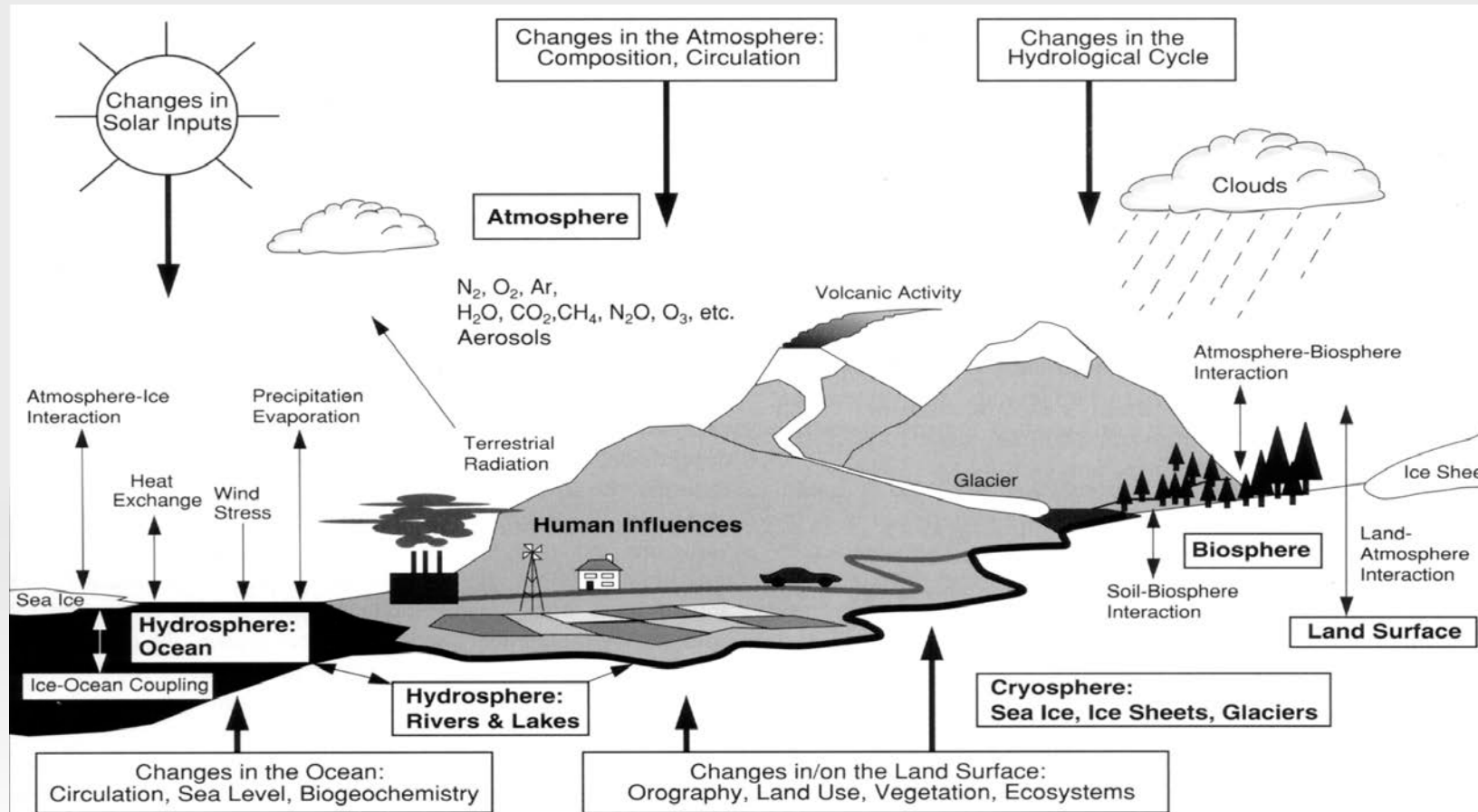


Recharge - Recovery Scheme



BUT it has strong biological and geochemical implications

...and finally nothing innocent about this one



BUZZ WORDS:

Climate

Interactions

Hydro-, bio-, crio-, geo-

C-, N- or P-cycle

Human influences

Last thoughts for discussion

- In short, the really interesting problems can be considered as involving hydro-bio-geo-chemo-thermo-mechanical processes, most of them coupled and non-linear. That is, beautiful complex problems
- But our “clients” want to read results mostly in **economical terms**, and at most, if we are fortunate enough, in ecological or toxicological terms.
- We are expected to come up with solutions, but information is always limited, problems are complex and non-linear and there is huge uncertainty in parameters, processes and scenarios.
- Standard approach: we provide solutions using very sophisticated codes that give one deterministic answer based on some tens (to thousands) of parameters, and we deal with uncertainty by performing some sensitivity analysis.

Envisioning the future

According to IAHR European Congress, four big topics for the future

1. Eco-hydraulics (“eco” badge still sells)
2. Sustainable water resources with emphasis on water quality and emergent pollutants (people take many pills and use lots of personal care products)
3. Extremes and climate change (still a best selling), but with focus on uncertainty evaluation... and how to transmit the concepts/results of uncertainty to decision makers
4. Management of resources in coastal areas (too many people...)

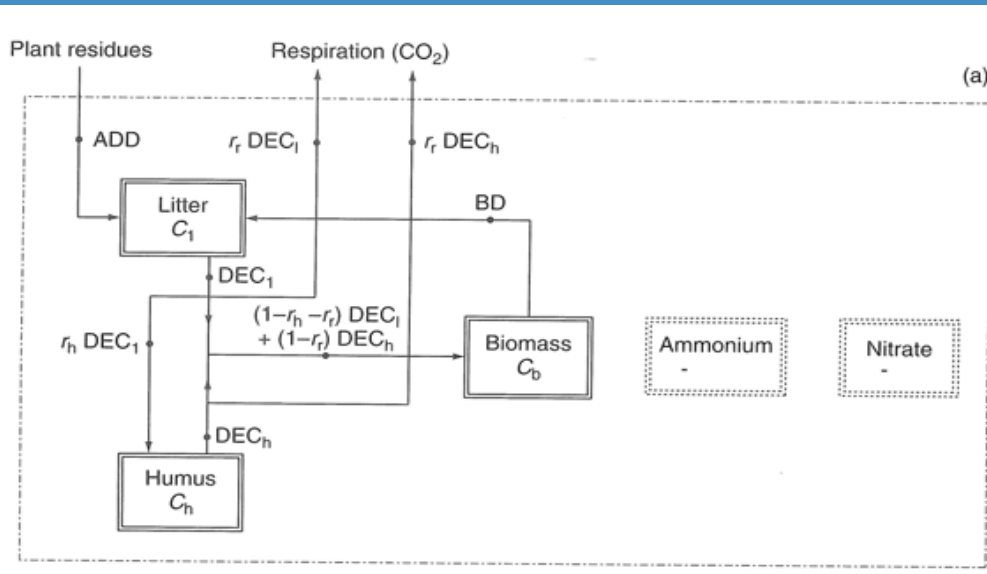
Since it is my talk, let me change the last one

4. Assessment and management of risk to humans (policy is driven by politicians, and they are driven by votes)



1. Ecohydraulics

The simplest problem has an unexpected solution

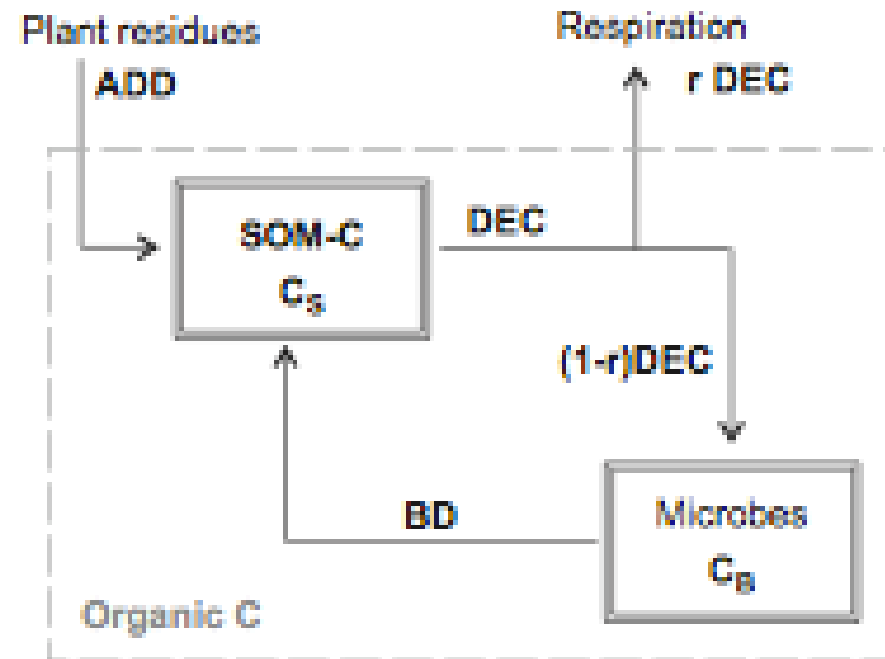


$$\frac{dC_s(t)}{dt} = ADD - DEC' + k_B C_B$$

$$\frac{dC_B(t)}{dt} = (1 - r)DEC' - k_B C_B$$

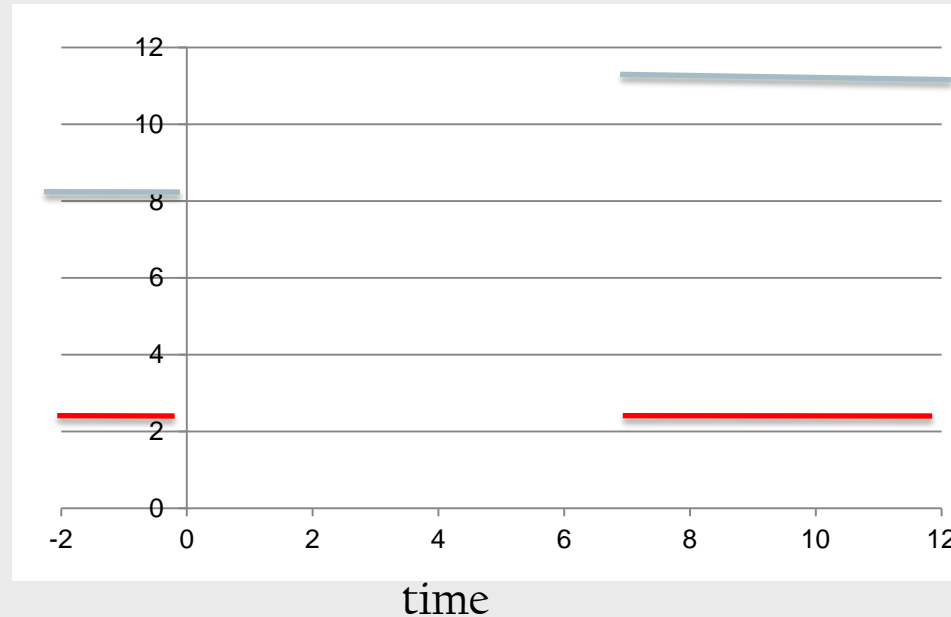
with $DEC' = k_s C_s(t) C_B(t)$,

and k_s a function of soil moisture



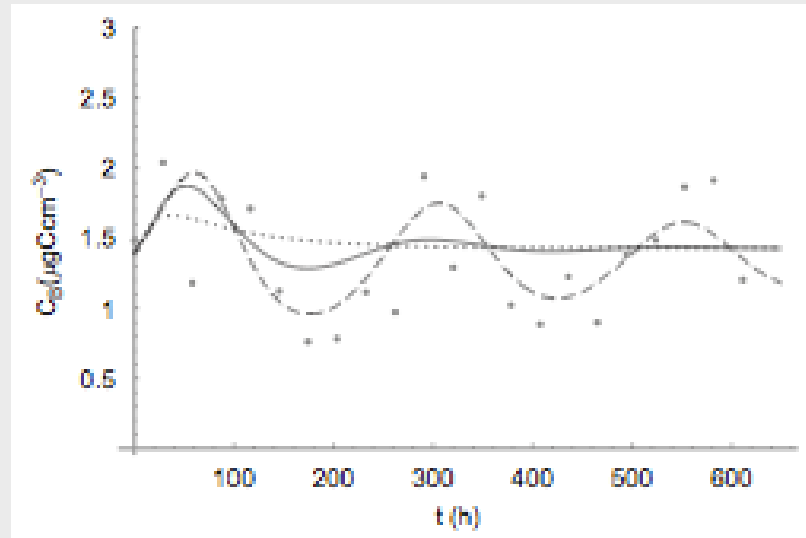
So, a quiz: what would be the solution to?

System originally in equilibrium, and soil moisture is changed (step function). The system will eventually reach a new steady-state. What are the shapes of the concentration functions with time?



Biomass conc

SOM conc

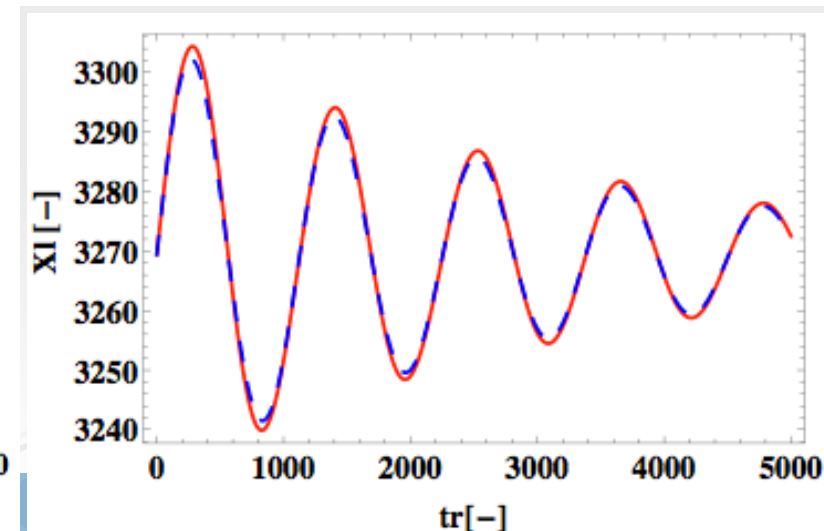
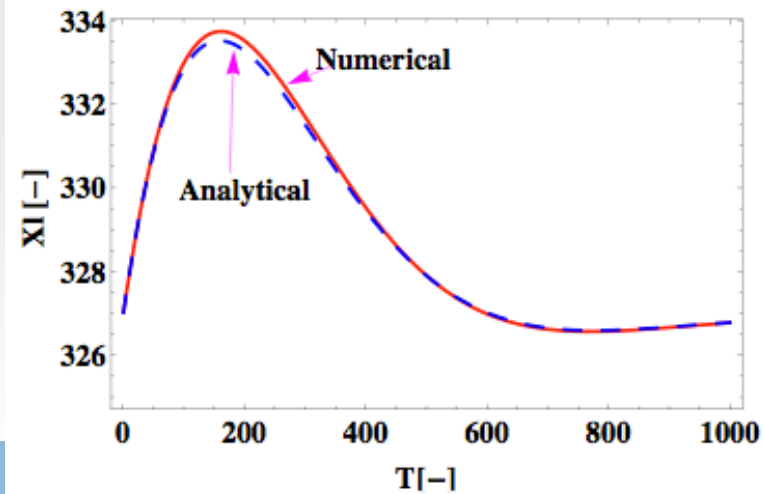
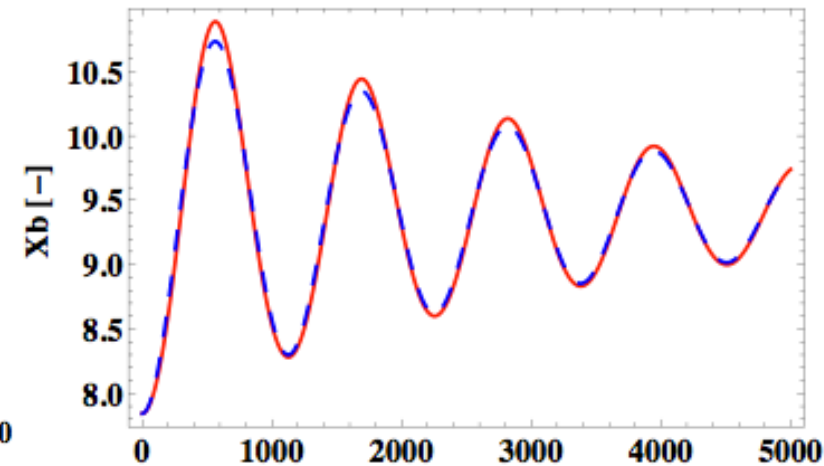
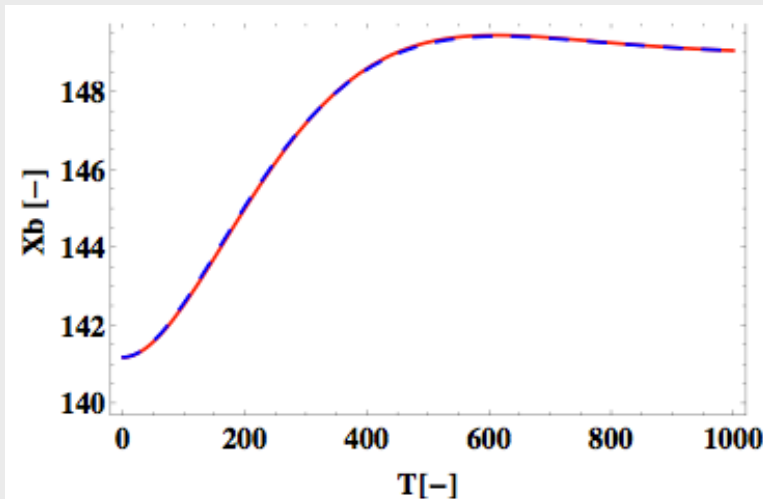


Real solution:
Oscillations might happen!

Manzoni and Porporato (2009)

We have derived the (approximate) closed-form mathematical condition for oscillations to take place. But remember, this is the SIMPLEST problem!

$$0 < ADD < \frac{4k_d^2 r^2}{\varphi f_{\phi}(s)k_b(1-r)}$$



2. Water quality related to reactive transport and emerging pollutants

- Terrible!, we are still fighting about the correct models for transport of conservative solutes, then imagine reactive transport, and new pollutants keep appearing and for these we do not know the reaction laws

Still discussing about incomplete mixing

- Mixing drives reactions.
- Reactions take place in reactors!



Incomplete mixing!



Mixing without reactors?

Mixed, not stirred! (Connery, 1964)

Multispecies Reactive Transport

Mixing of two (or more) waters in perfect geochemical equilibrium (regarding aqueous species, biological species and minerals) produces **local disequilibrium**. Reactions will then take place to re-equilibrate the system (acid/base, redox, precip./dissol.,...)

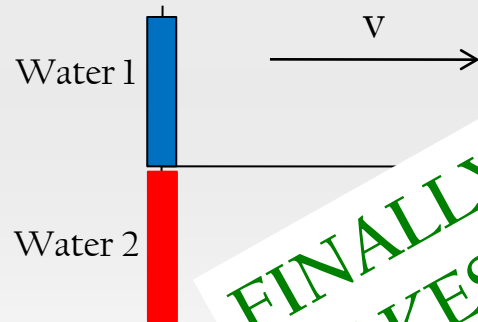
Example not so rare: 19 chemical species and 13 reactions THIS MEANS SOLVING A SYSTEM OF 32 NON-LINEAR PDE's

Coupled flow and reactive transport problem is modeled with **numerical codes**. How to deal with parameter uncertainty here?

Reaction	log <i>K</i>
$\text{CaCl}^+ = \text{Ca}^{2+} + \text{Cl}^-$	0.6938
$\text{CaCl}_{2(\text{aq})} = \text{Ca}^{2+} + 2\text{Cl}^-$	0.6283
$\text{CaHCO}_3^+ = \text{Ca}^{2+} + \text{HCO}_3^-$	-1.0606
$\text{CaOH}^+ + \text{H}^+ = \text{Ca}^{2+} + \text{H}_2\text{O}$	12.9321
$\text{CO}_{2(\text{aq})} + \text{H}_2\text{O} = \text{HCO}_3^- + \text{H}^+$	-6.3636
$\text{CO}_3^{2-} + \text{H}^+ = \text{HCO}_3^-$	10.3524
$\text{OH}^- + \text{H}^+ = \text{H}_2\text{O}$	14.0707
$\text{HCl}_{(\text{aq})} = \text{H}^+ + \text{Cl}^-$	0.6693
$\text{NaCl}_{(\text{aq})} = \text{Na}^+ + \text{Cl}^-$	0.7811
$\text{NaCO}_3^- + \text{H}^+ = \text{Na}^+ + \text{HCO}_3^-$	9.8145
$\text{NaHCO}_{3(\text{aq})} = \text{Na}^+ + \text{HCO}_3^-$	-0.1715
$\text{NaOH}_{(\text{aq})} + \text{H}^+ = \text{Na}^+ + \text{H}_2\text{O}$	14.2479
$\text{CaCO}_{3(\text{s})} + \text{H}^+ = \text{Ca}^{2+} + \text{HCO}_3^-$	1.8789

Problem to study: mixing of two waters

- Water 1 in proportion α ; water 2, $1 - \alpha$ (α is a conservative quantity)
- Mixing takes place BECAUSE of dispersion: NO DISPERSION, NO MIXING!!!

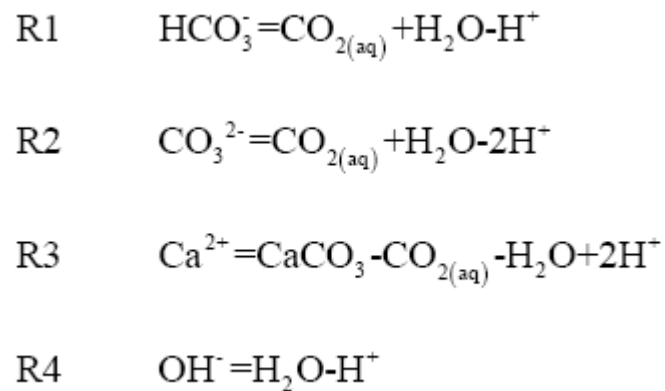


FINALLY SOMETHING THAT
MAKES SENSE!



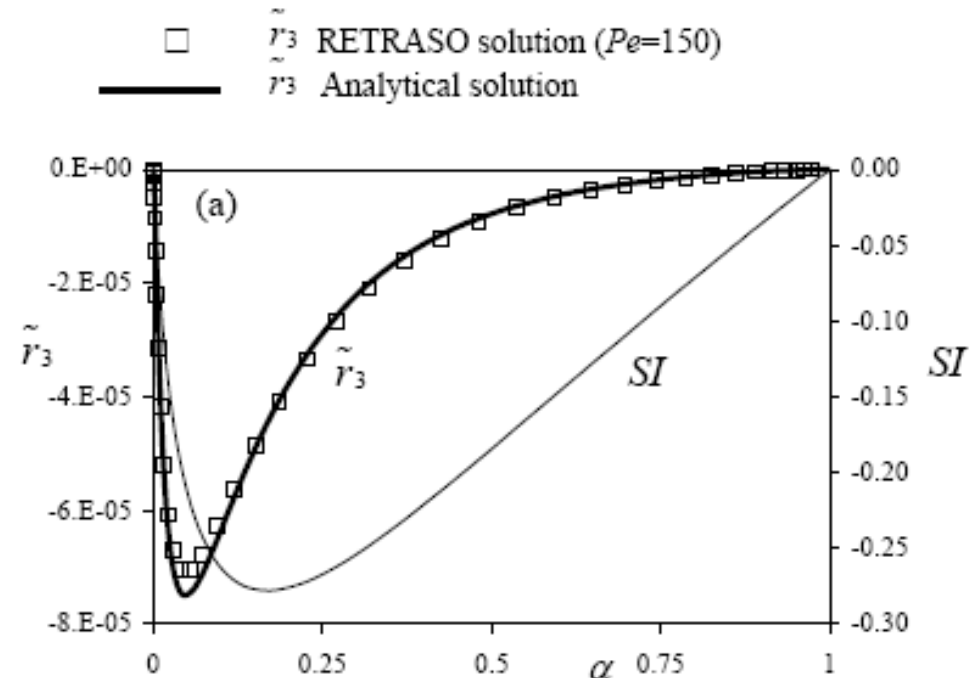
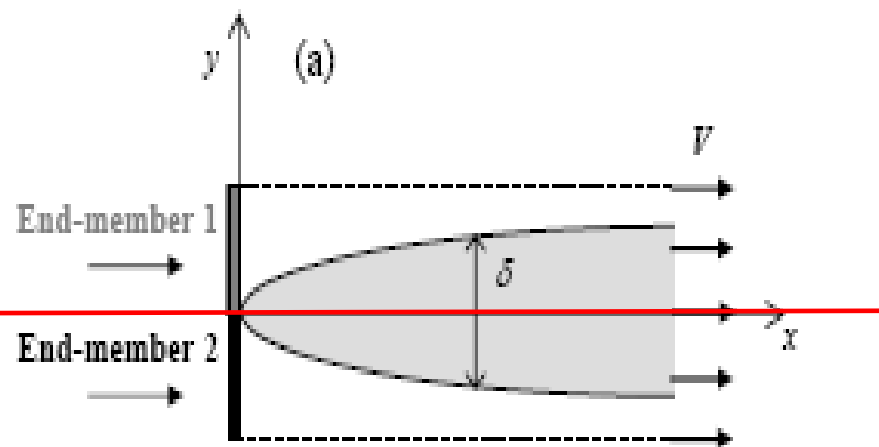
Now same setup mixing fresh and saltwater

- With a geochemical problem involving 8 species (6 aq., 2 ct activity)



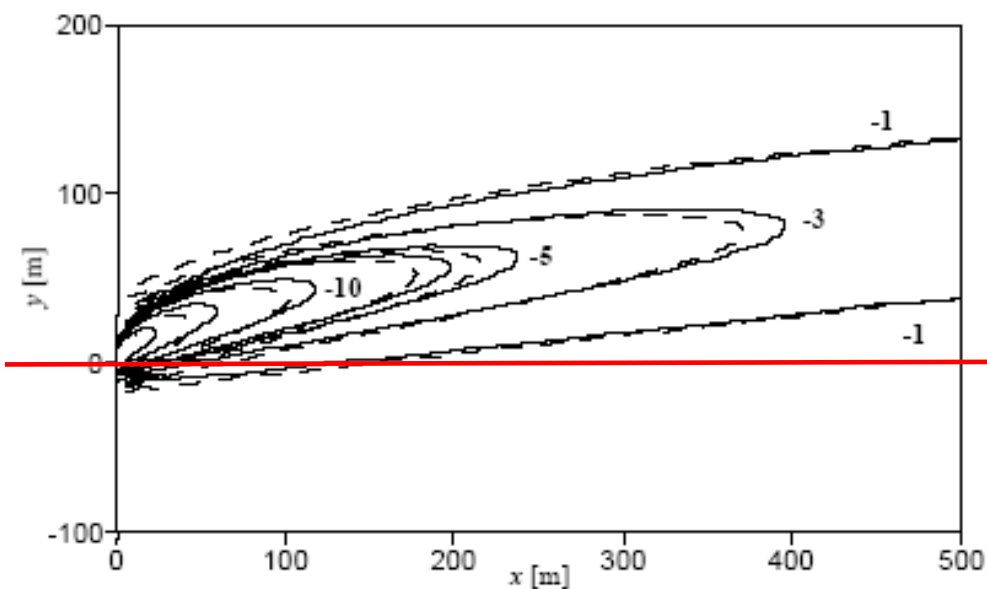
- The full approach would be solving 6 coupled PDE's simultaneously with 4 non-linear identities (huge supercomputer)

- SOLUTION: Solving for mixing proportions based e.g. on Cl content (freshwater – saline water problem). Solve ONE LINEAR PDE
- Then do speciation, which in this case is solving a “simple” 6th order polynomial (pocket calculator/Spread sheet).



— Analytical solution

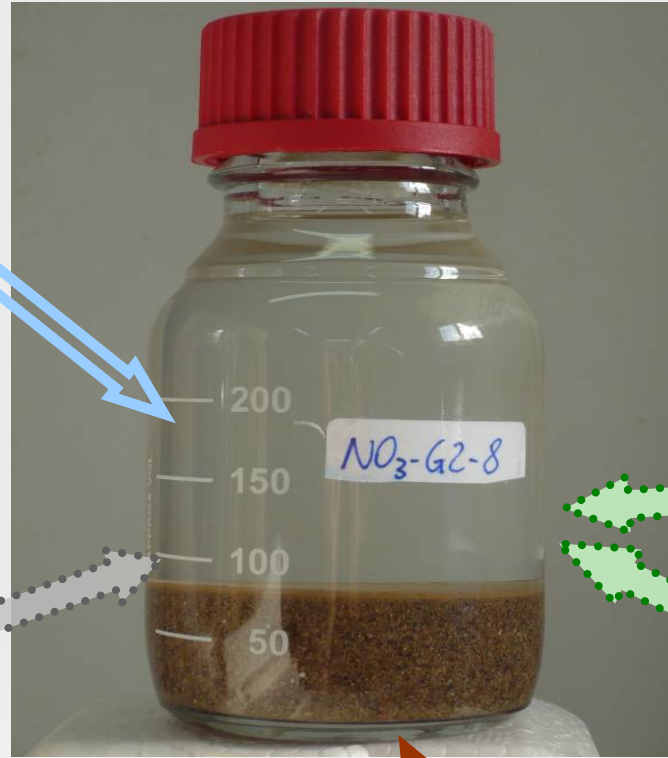
- - - RETRASO solution



But we should also worry about organic chemistry and emerging components

WATER:
240mL
(Synthetic)

Batch experiments under
controlled redox conditions



additional
e⁻ acceptor:
e.g. NO₃

e⁻ donor:

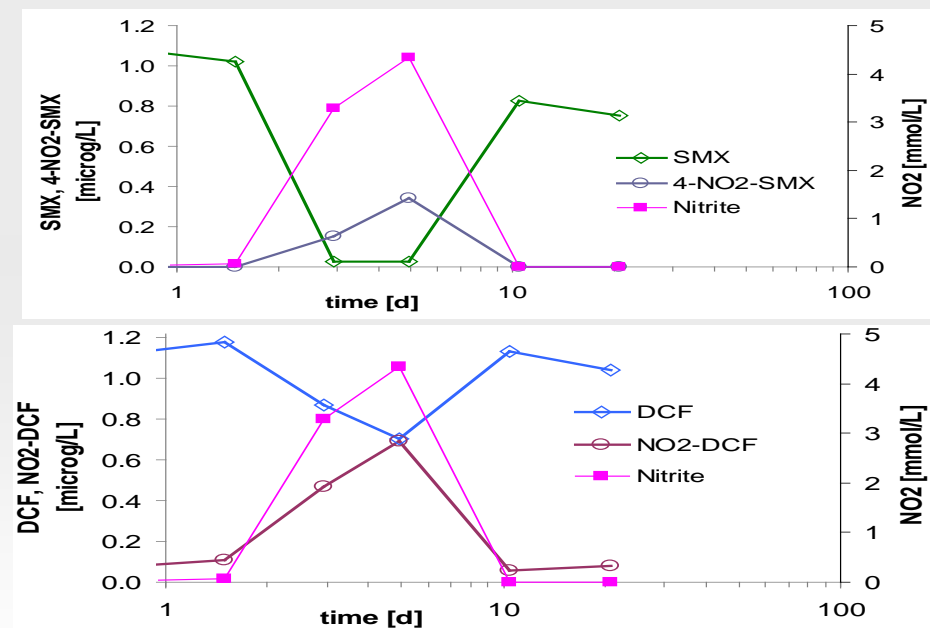
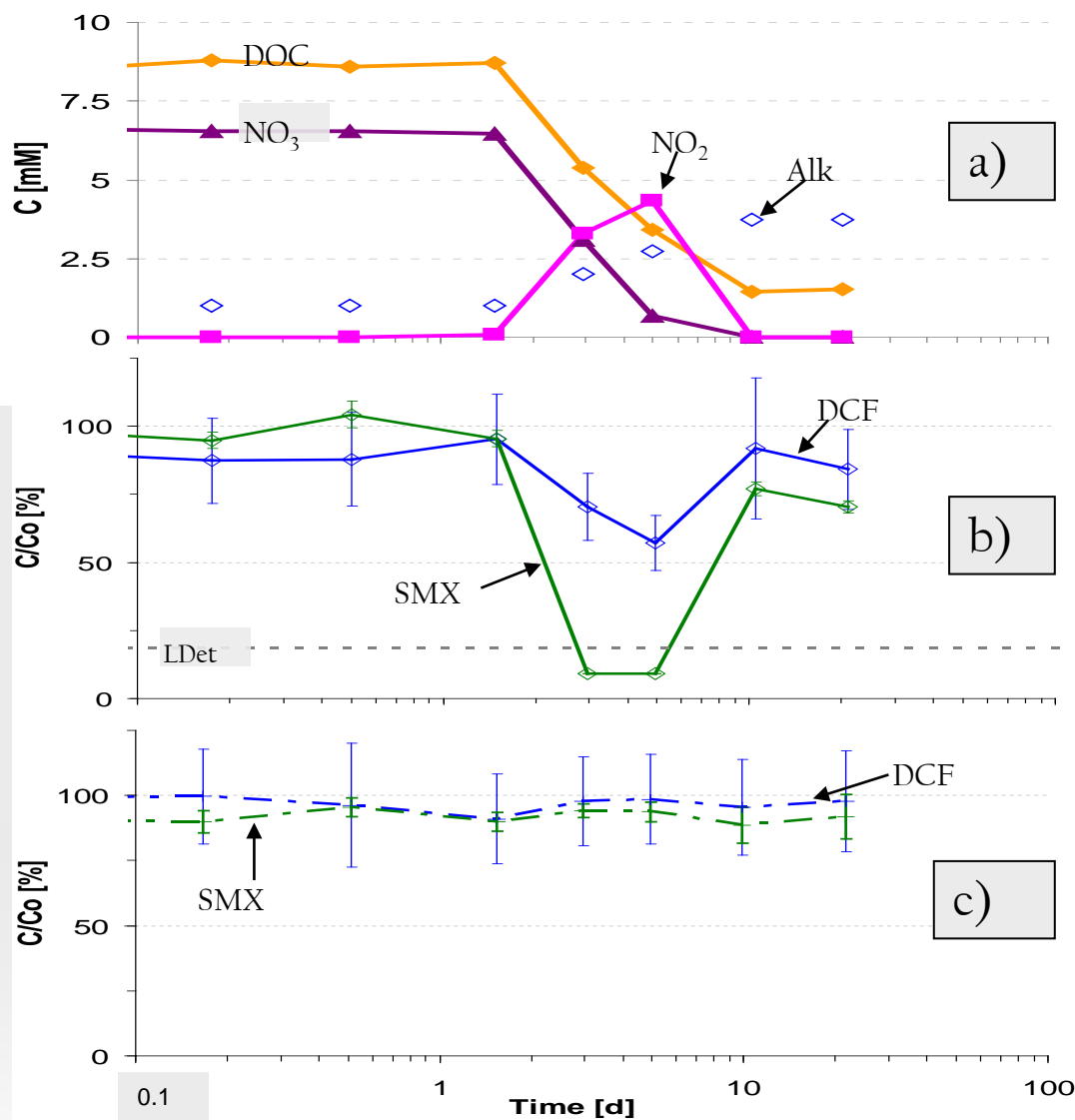
Na-acetate & MeOH
as *easily degradable*
organic substrate

MICROPOLLUTANTS

SOIL: 120g of $d < 1\text{mm}$
(from Test Site)



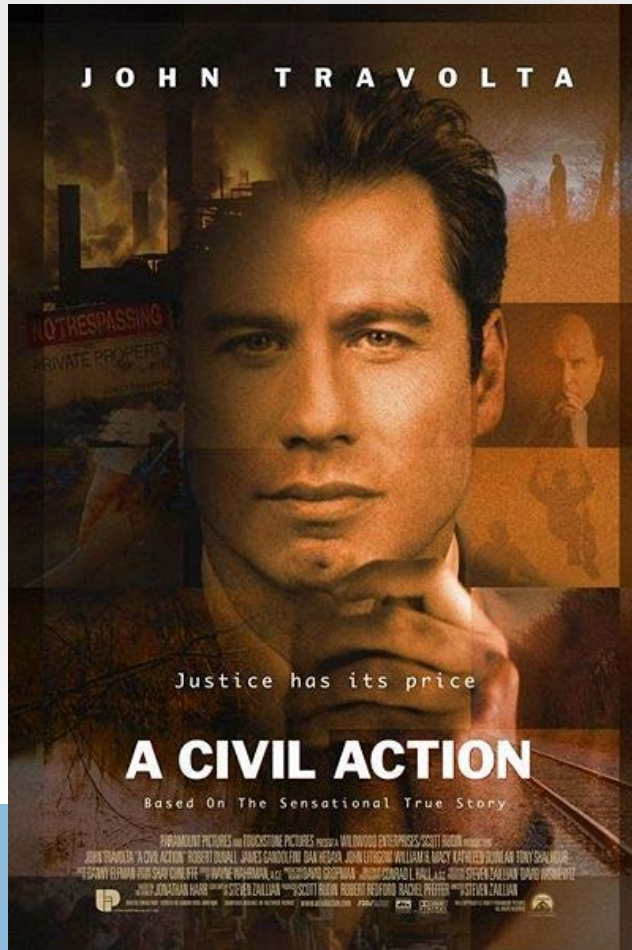
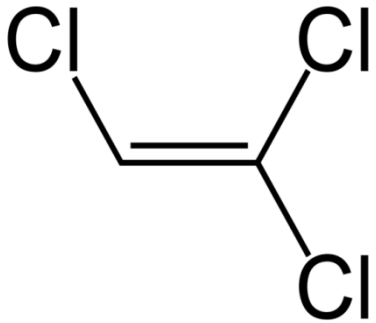
Extremely relevant for
water quality purposes



3. Uncertainty evaluation: Transmitting the concept to lawyers/judges

- Groundwater pollution: when you detect it, it is too late
- Famous case:

Woburn, MA:
Trichloroethylene



PERFECT FOR LAW SUES! The question:
Can you unequivocally assure that pollution
comes from that point?

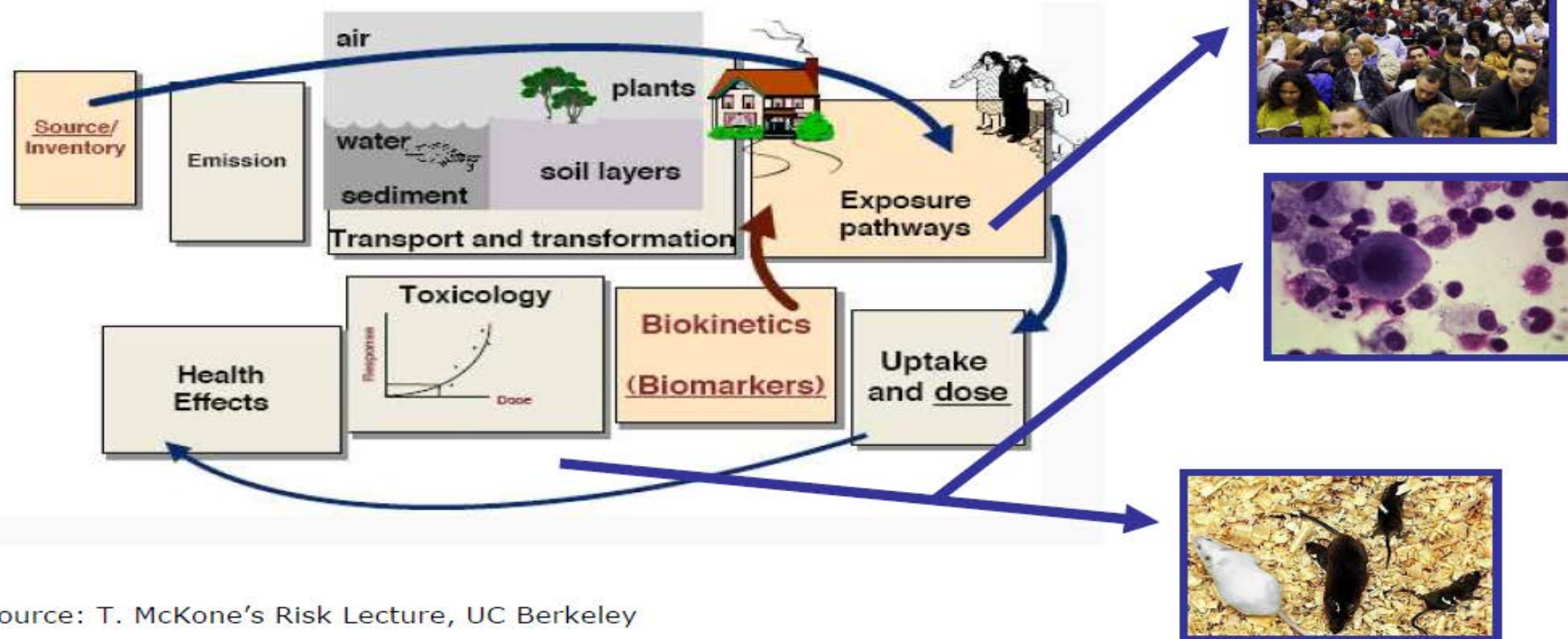
Meaning 100% certainty

You perform a state-of-the-art work and come
up with a zillion Monte Carlo simulations and
you get 98.5% probability. What do you
answer?

**So, no comments on science, but
we need to improve the way we
produce and transmit our results**



4. Risk assessment



Source: T. McKone's Risk Lecture, UC Berkeley

Need Probabilistic Concepts!

Risk: probability of an undesired outcome.

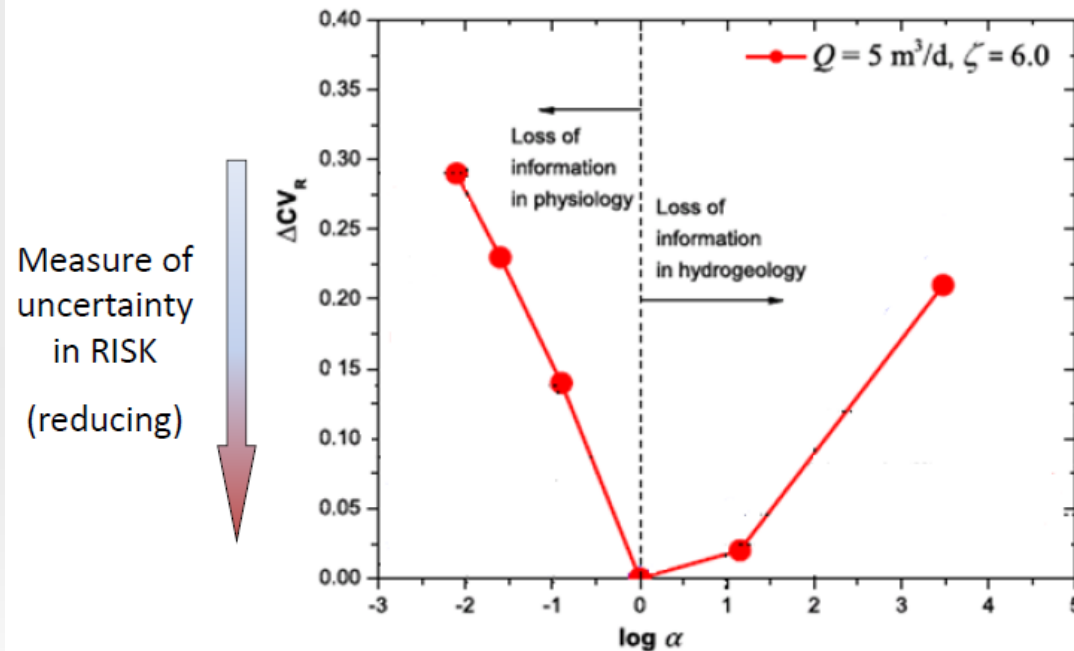
But tell this to a journalist! What they ask you: is there any risk?

The answer to Fukushima problem was: NO WAY, this cannot happen

Risk assessment being so interdisciplinary, where should we place our resources?

Visualization Tool

Comparative Information Yield Curves

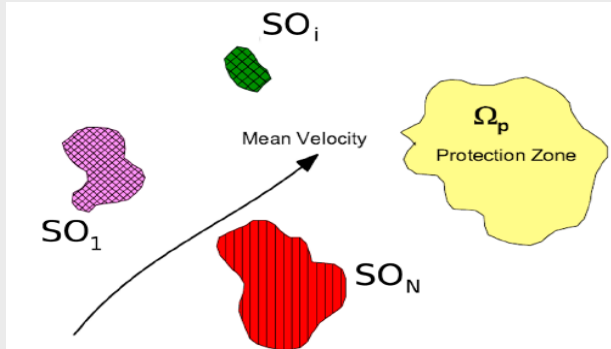


de Barros and Rubin (2008) WRR

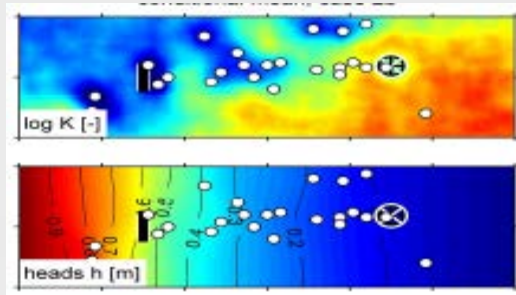
de Barros et al. (2009) WRR

Adding data from physiology while keeping information from hydrogeology fixed

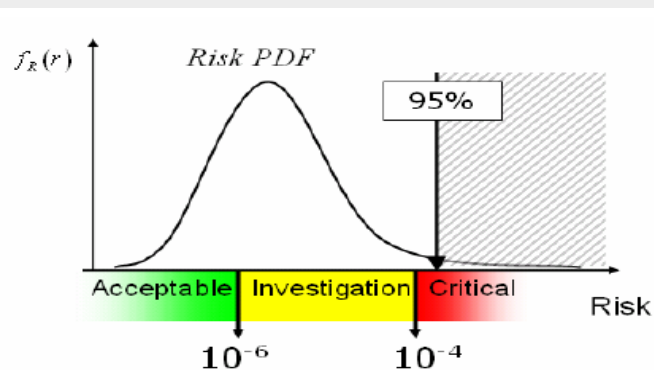
Adding data from hydrogeology while keeping information from physiology fixed



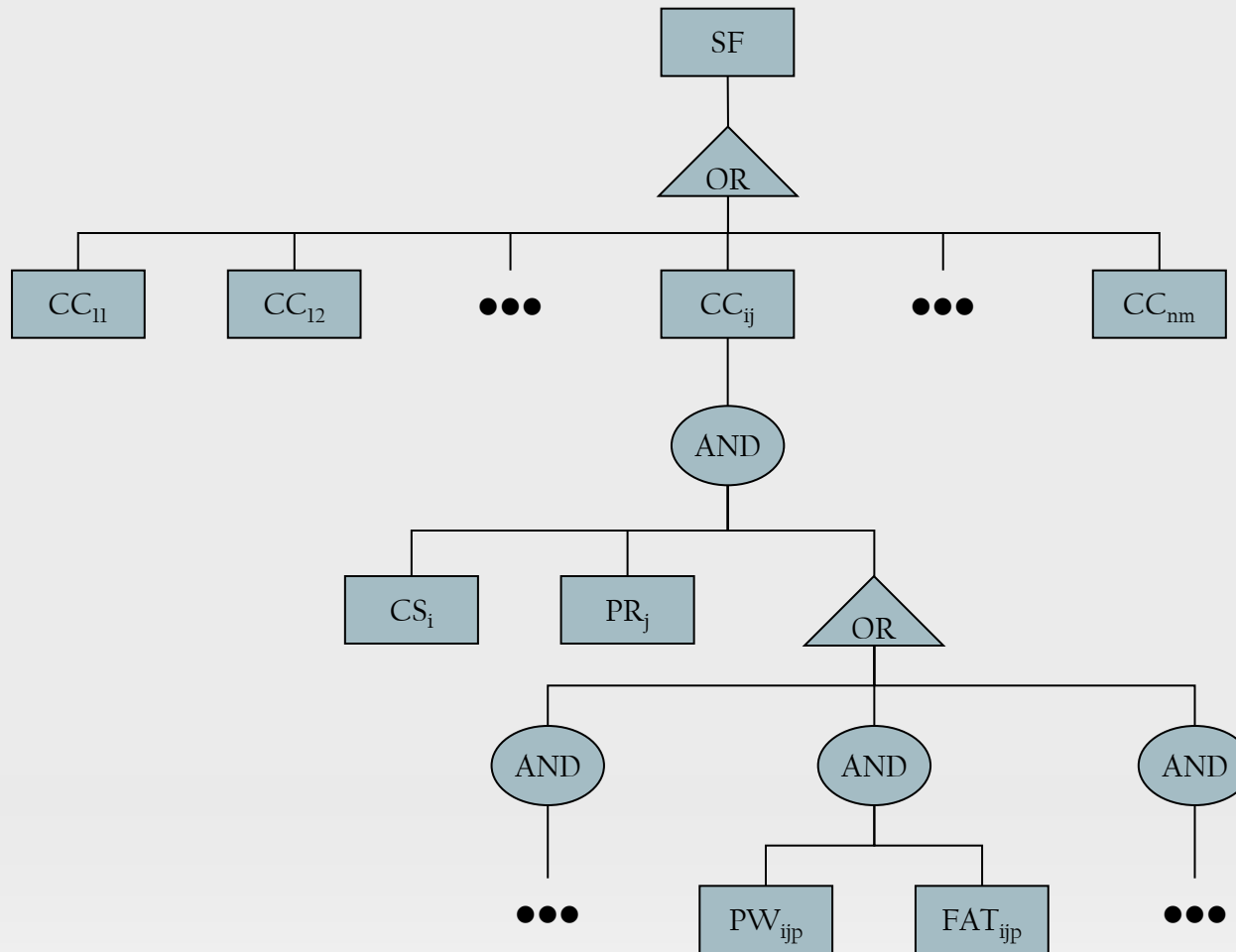
1) Identifying contaminant source releases & environmentally sensitive targets.



2) Data acquisition used to infer modeling parameters! Site characterization.



3) Final task: Estimate human health risk toward decision making! Should a site be remediated or not? Is the exposed population at risk?

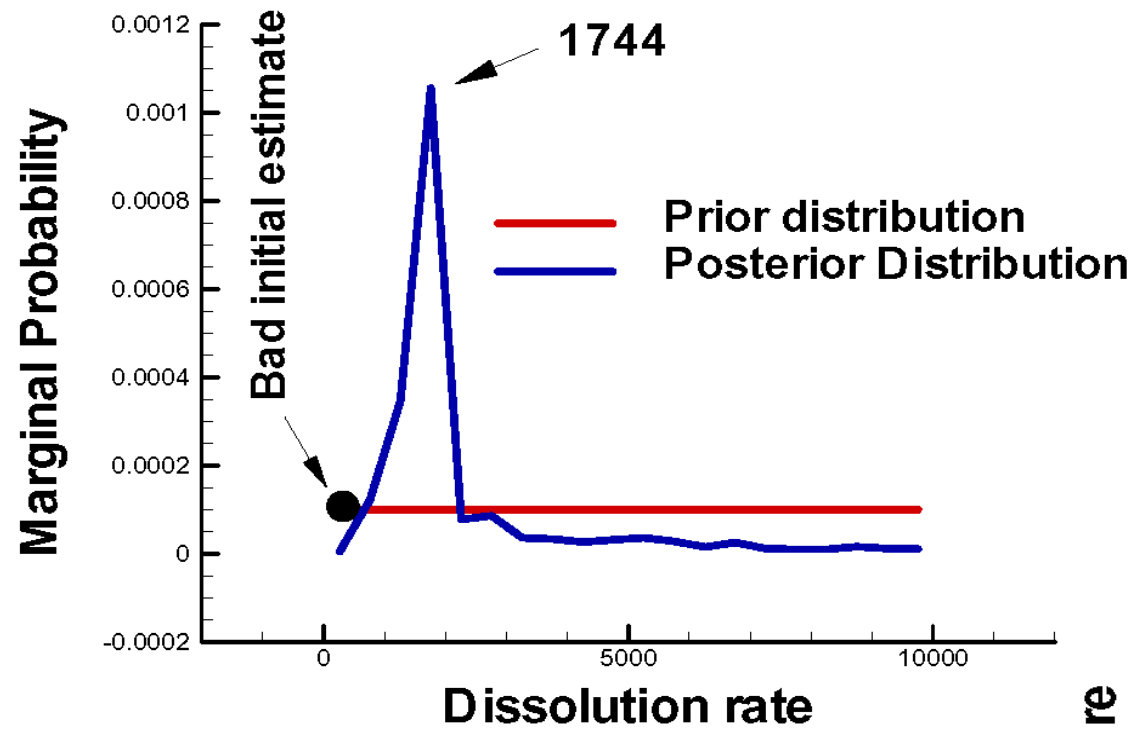


System Failure

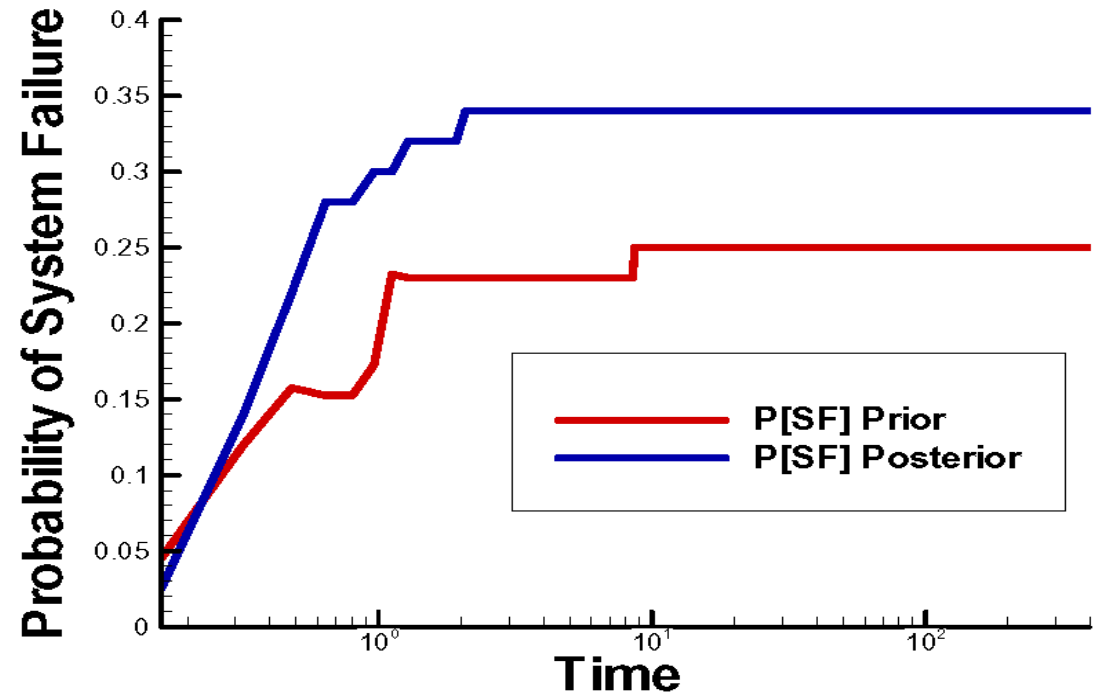
Critical Concentrations

Sources-Receptors

Pathways-Processes



And everything is conditioned to data. It could be done using Bayesian updating



Final remarks

- Ippen (1970) already advocated for the inclusion of complex environmental and social factors when dealing with engineering problems. Add money and we are there
- As engineers we face a daily challenge of solving complex problems and YET provide simple solutions.
- As scientists/researchers we deal with the advancement of science, uncertainty should be treated in a rigorous manner, starting at the small scale, then upscaling, then providing estimates in terms of probabilities
- As professionals living in a real world we need to get **the best of both worlds**. We have to make an effort to convey our clients the problems associated to our job and the impossibility to produce exact results when data is never extensive
- And what about the future? I have shown several interesting problems not yet solved (there are many more). My point is the need to work in pluri- and interdisciplinary problems and beg the audience to spread the word on the need to properly account for complexity and uncertainty when dealing with real problems.