UNIVERSITAT POLITÈCNICA DE CATALUNYA
Department of Civil and Environmental Engineering
Hydrogeology Group GHS (UPC-CSIC)

WE-NEED

POLITECNICO MILANO 1863

universidade de aveiro

WEIZMANN INSTITUTE OF SCIENCE

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Water JPI

A PHYSICALLY-BASED RISK ANALYSIS FRAMEWORK FOR THE SUSTAINABLE USE OF WATER IN THE BOLOGNA AQUIFER

Milan, Italy, June 12th, 2019

Presenting Author: Daniel FERNÀNDEZ-GARCIA (UPC)

Main Co-Authors: Guillem SOLE-MARI (UPC)

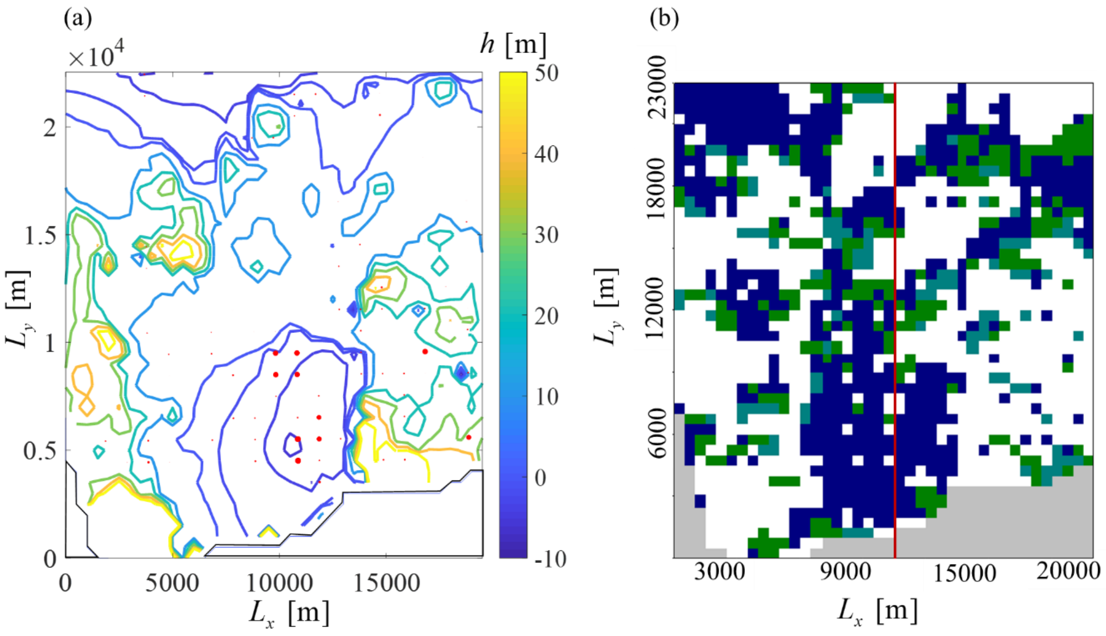
Martina SIENA (Polimi)

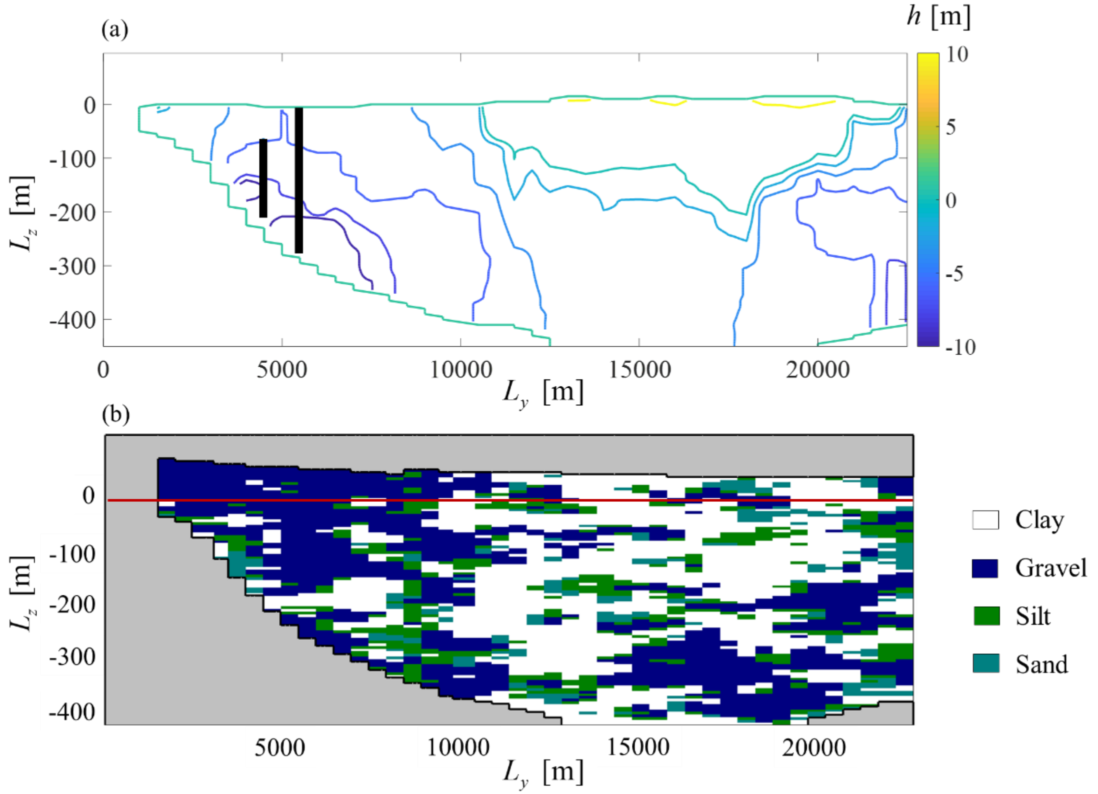
Monica RIVA (Polimi)

TABLE OF CONTENTS

1. INTRODUCTION AND GOALS

Provide a physically-based risk assessment framework for the Bologna aquifer.





1. INTRODUCTION AND GOALS

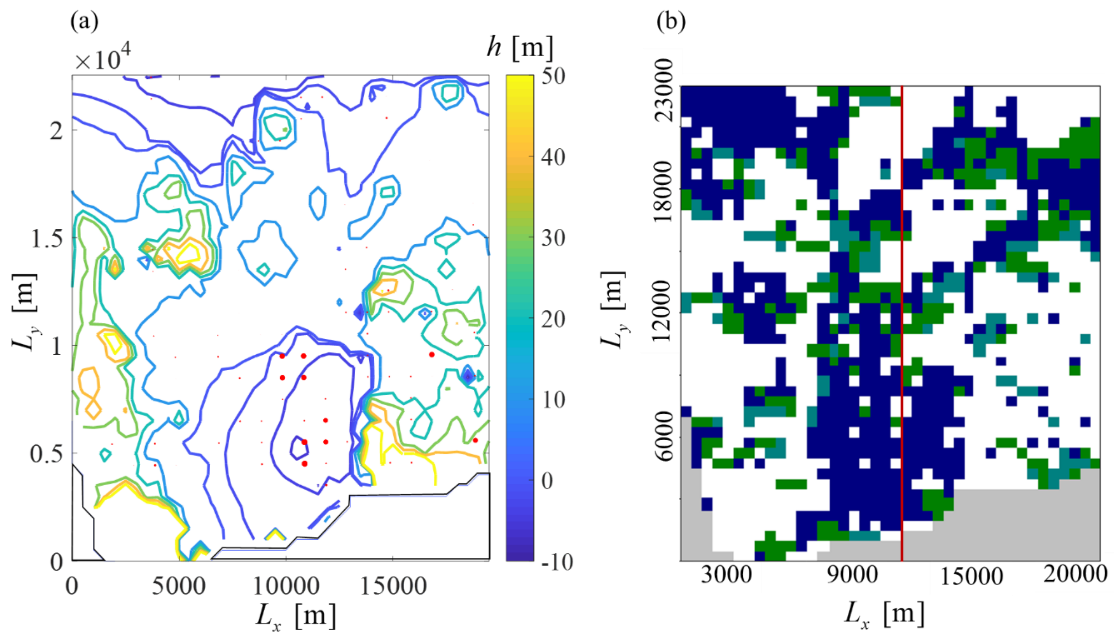
Probabilistic Risk Analysis provides a scientific and legally defensible basis to make decisions under risk

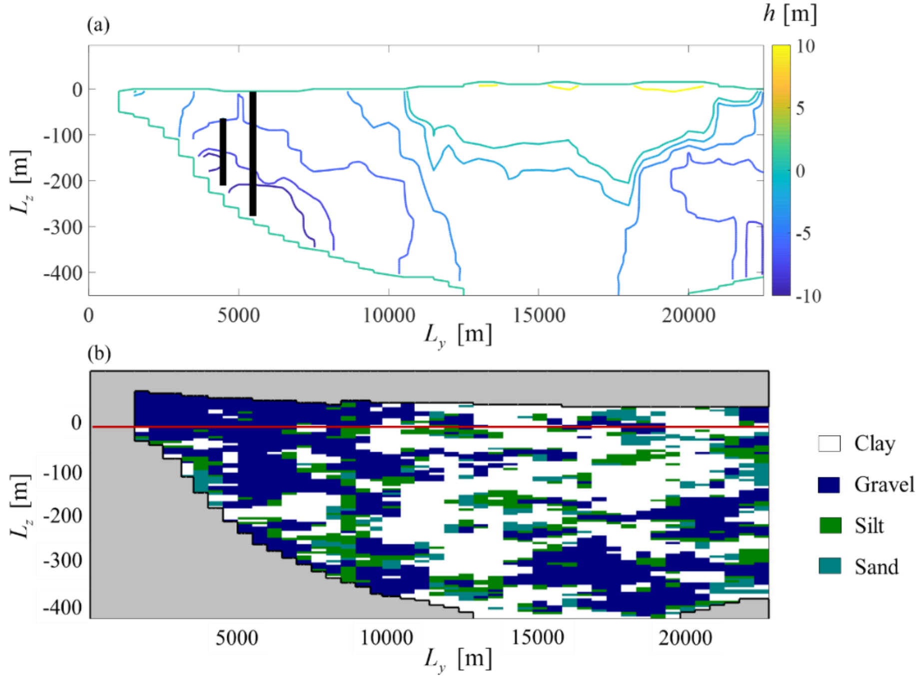
Permits to evaluate the need for protective action at the site

Cost-effective corrective actions:

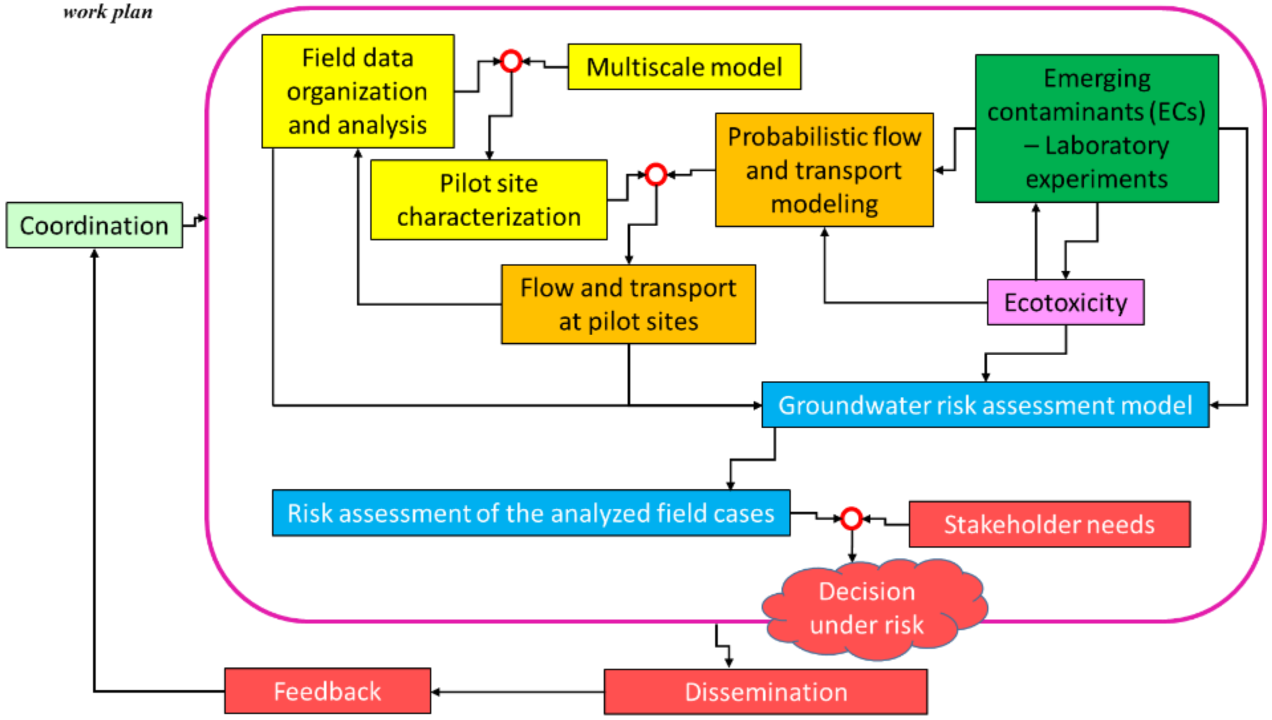
Providing risk-based remediation goals

Focusing corrective actions on the exposure pathways that present the highest risks





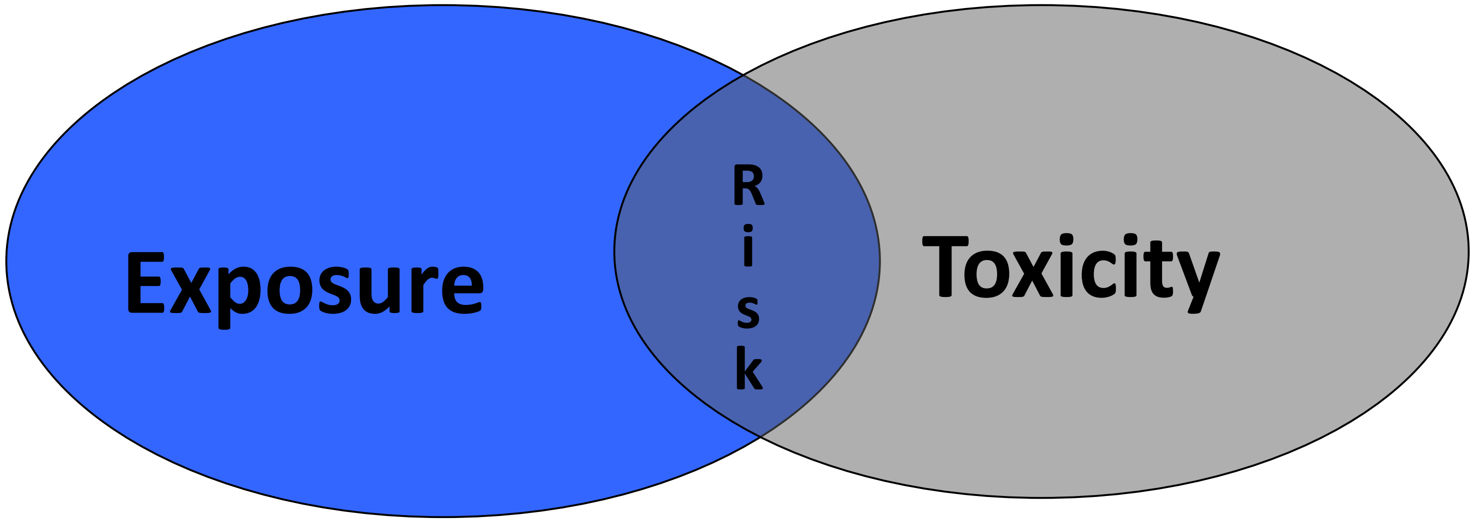
work plan



PRINCIPAL INVESTIGATOR	INSTITUTION	COUNTRY
Monica Riva	**Politecnico di Milano - Polimi**	**Italy**
Brian Berkowitz	Weizmann Institute of Science - Weizmann	Israel
Susana Loureiro	Universidade de Aveiro - UAVR	Portugal
Daniel Fernandez-Garcia	Universitat Politecnica de Catalunya - UPC	Spain

2. RISK ASSESSMENT

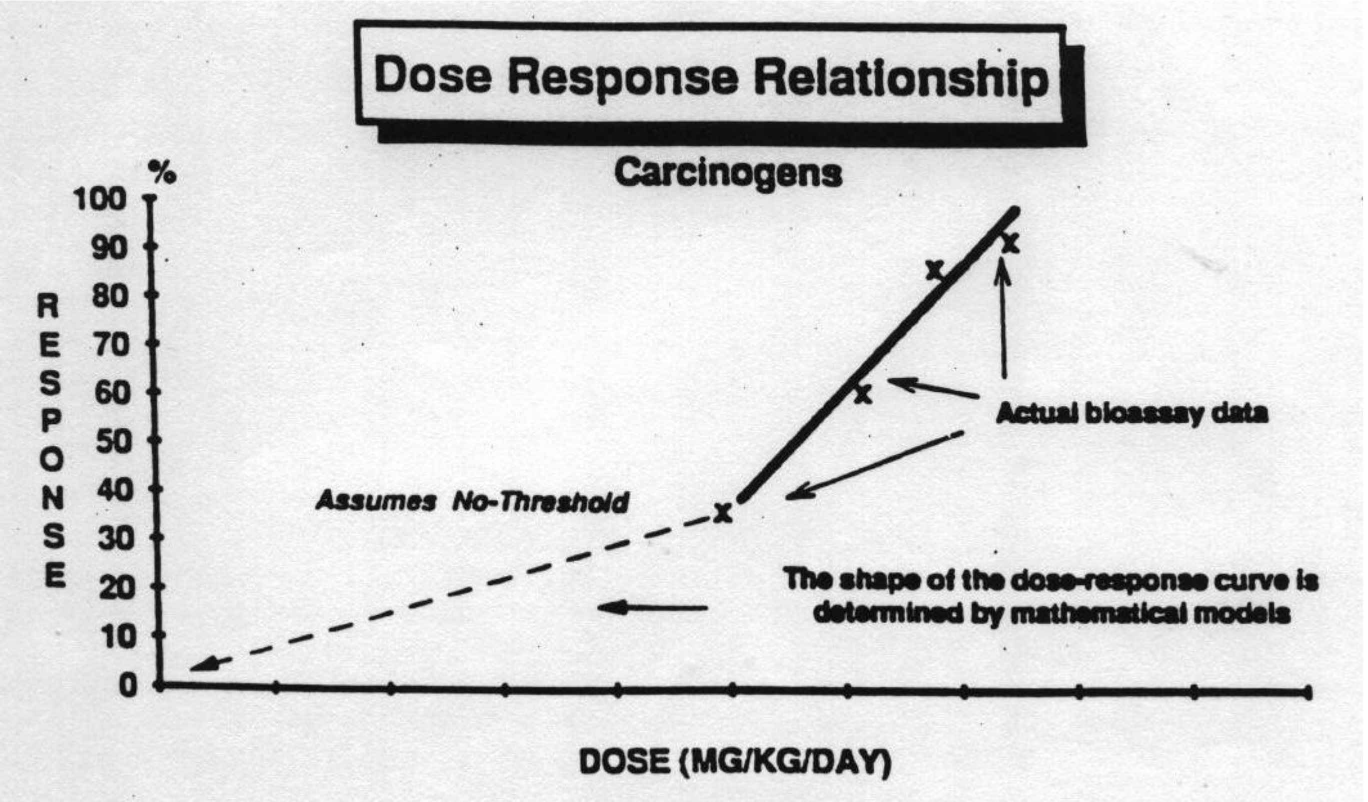
Risk = <u>Probability</u> of suffering harmful effects due to exposure to site related constituents



Provides information and characterizes any potential adverse effects of human exposure

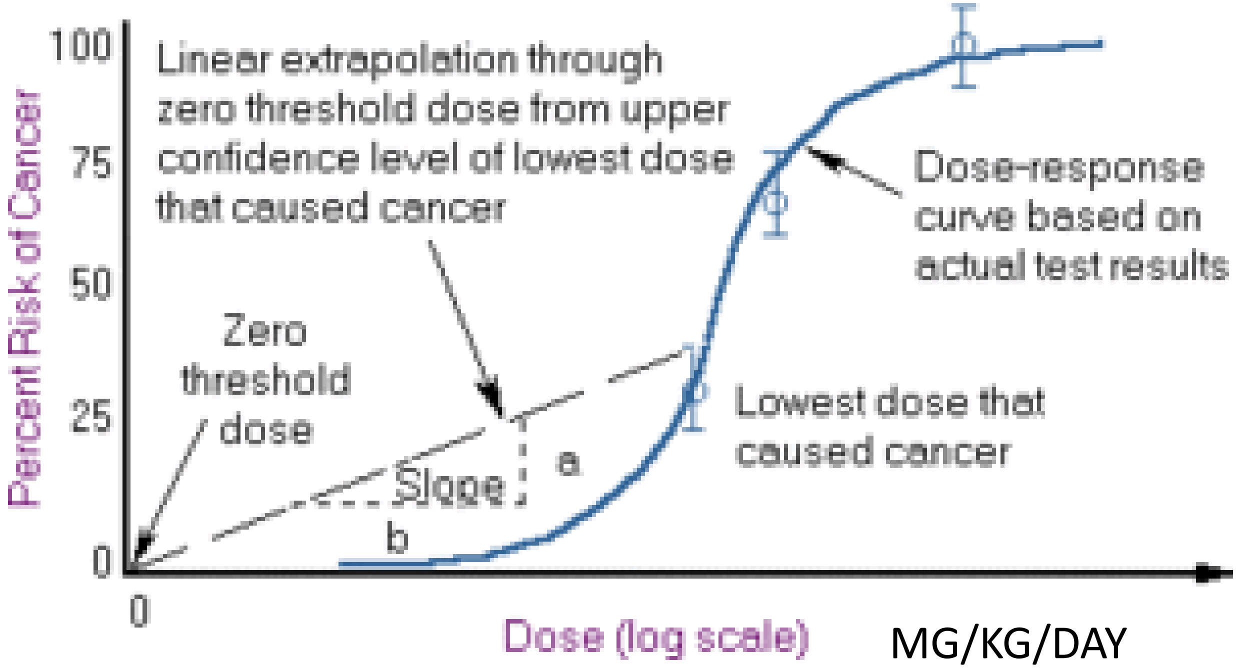
2.1. Dose-response relationship

Mathematical models are used to extrapolate from the high doses used in animal experiments to the low doses to which humans are normally exposed in a chronic setting.



2.2. Measure of toxicity: carcinogenic effects

Linearized Multistage Model (LMS): assumes linear extrapolation with a zero dose threshold from the upper confidence level of the lowest dose that produced cancer in an animal test or in a human epidemiology study.



$$Risk = CSF \times Dose$$

$$CSF = Cancer\ Slope\ Factor$$

2.2. Risk metric

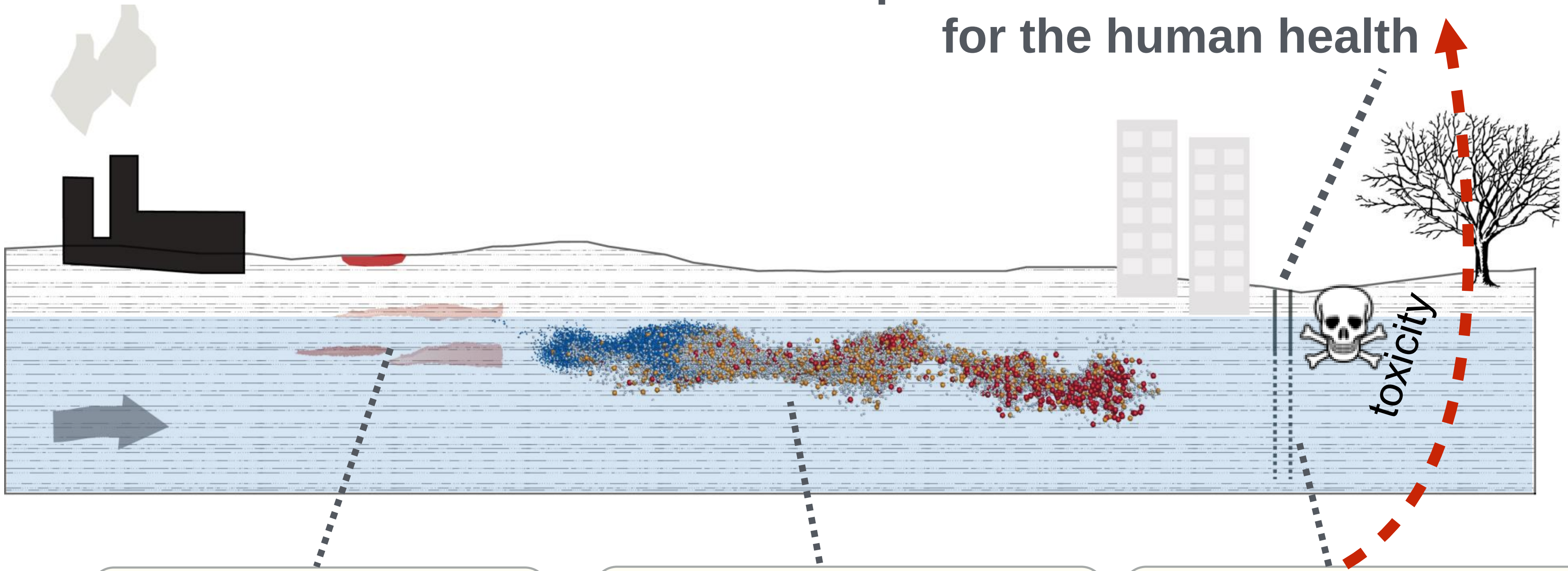
$$\text{Risk} \approx ADD \times CSF$$

Exposure Toxicology

$$\text{ADD=Average Daily Dose (Intake)} = (\text{Chemical Concentration}) \frac{\left(\text{Ingestion Rate}\right)\left(\text{Exposure Duration}\right)\left(\text{Exposure Frequency}\right)}{\left(\text{Body Weight}\right)\left(\text{Averaging Time}\right)} \quad \frac{mg}{Kg \times day}$$

$$\text{ADD} = 1\,\frac{\text{mg}}{\text{L}} \times \left[\frac{2.0\ \text{L}/day}{80\ \text{Kg}}\right] \frac{30\ \text{years} \times 350\ \text{days}/year}{70\ años \times\ 365\ days/year}$$

2.3. Components of a risk model



SOURCE: release of the contaminant

1

PATH: fate and transport of the contaminant

2

EXPOSURE: quantification of the dose

3

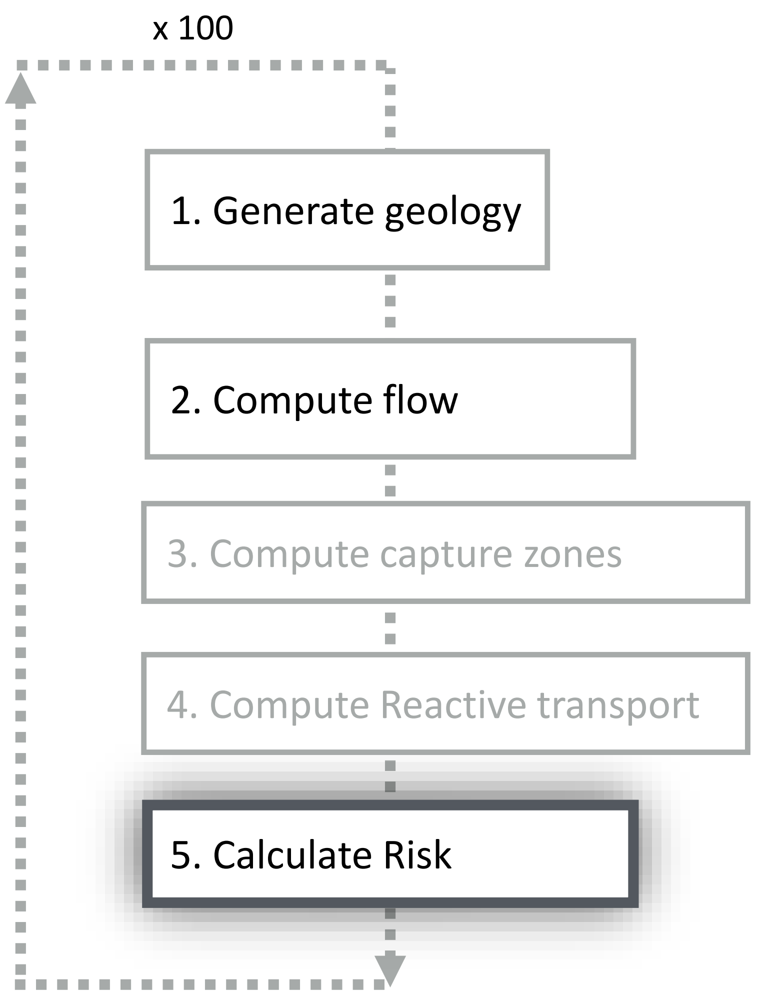
3. PROBABILISTIC T-DEP. CAPTURE ZONES

3.1. Time-related capture probability / capture zones

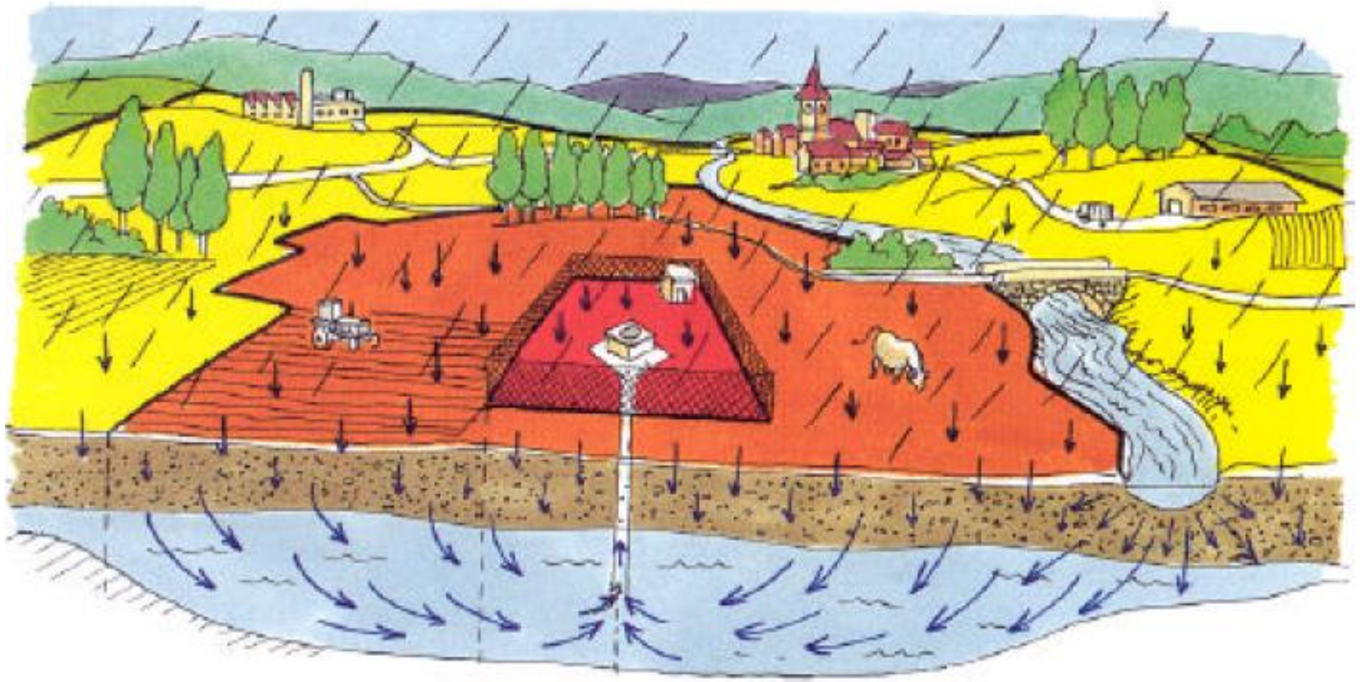
- We run advective transport of particles with initial positions in a uniform lattice covering the whole domain. The simulations run until the particle reaches **a well or the boundary**.

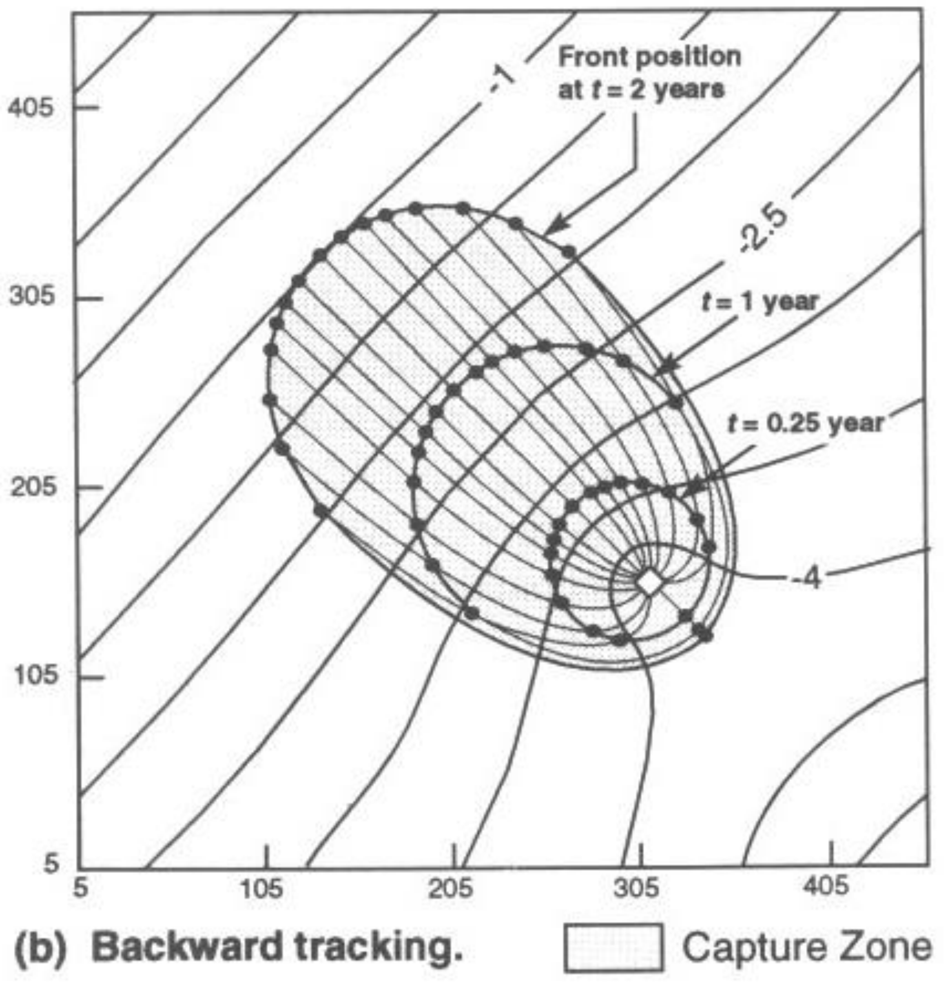
- From the 100 realiz. of the velocity field, we compute the prob. of fluid particles starting at a **given position** in the domain to be extracted by a **given well** over a **given time**.

- We analyze the resulting probabilistic time-dependent capture zones for the **5 most important groups of wells** in terms of yearly production.



3.1. Determining Fluid capture by Pollock's Method

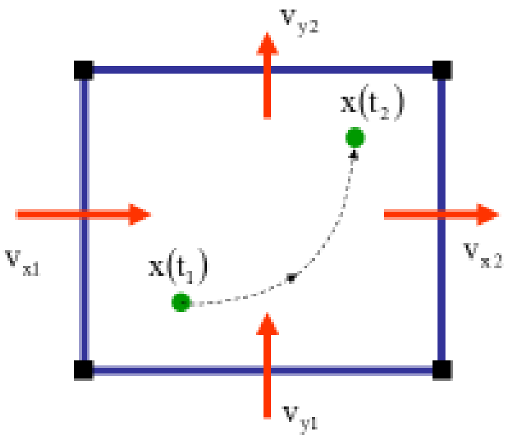




(b) Backward tracking.

3.1. Determining Fluid capture by Pollock’s Method

- **Semi-analytical** method to solve the advective path of a fluid particle.
- Based on **linear interpolation** of velocities between interfaces.
- Interface velocities are obtained from the finite-difference (MODFLOW) solution.



$$\boxed{\frac{dx}{v_x} = dt}$$

$$\frac{1}{A_x}\int_{x(t_1)}^{x(t_2)} \frac{A_x\,dx}{A_x(x - x_1) + v_{x_1}} = \int_{t_1}^{t_2} dt$$

$$\frac{1}{A_x}\ln\left\{\frac{A_x(x(t_2) - x_1) + v_{x_1}}{A_x(x(t_1) - x_1) + v_{x_1}}\right\} = \Delta t$$

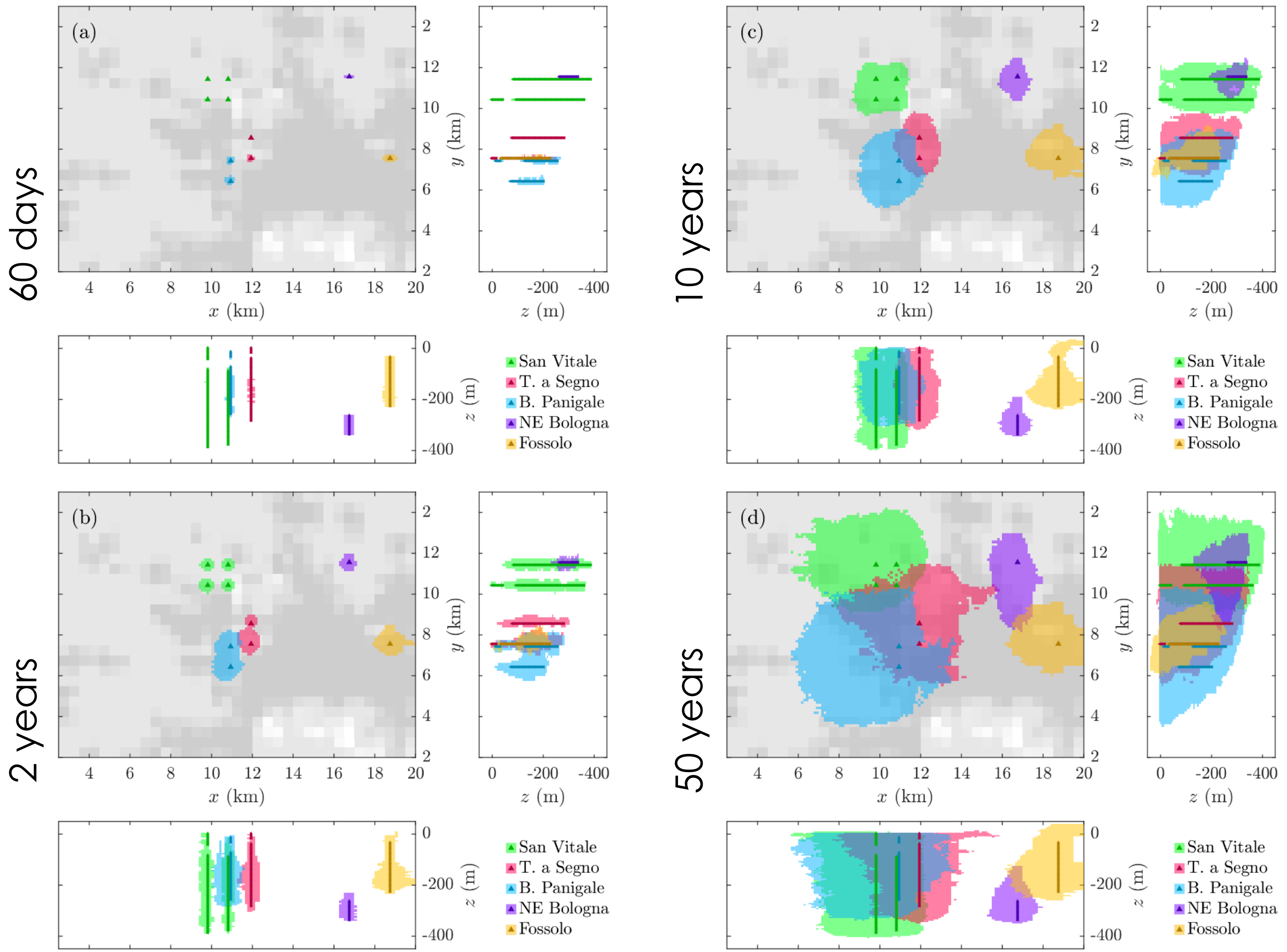
$$A_x = \frac{v_{x_2} - v_{x_1}}{\Delta x}$$

$$\boxed{x(t_2) = x_1 + \frac{1}{A_x}\left[\exp(A_x\Delta t)\cdot v_x(t_1) - v_{x_1}\right]}$$

3. PROBABILISTIC T-DEP. CAPTURE ZONES

3.3. Results

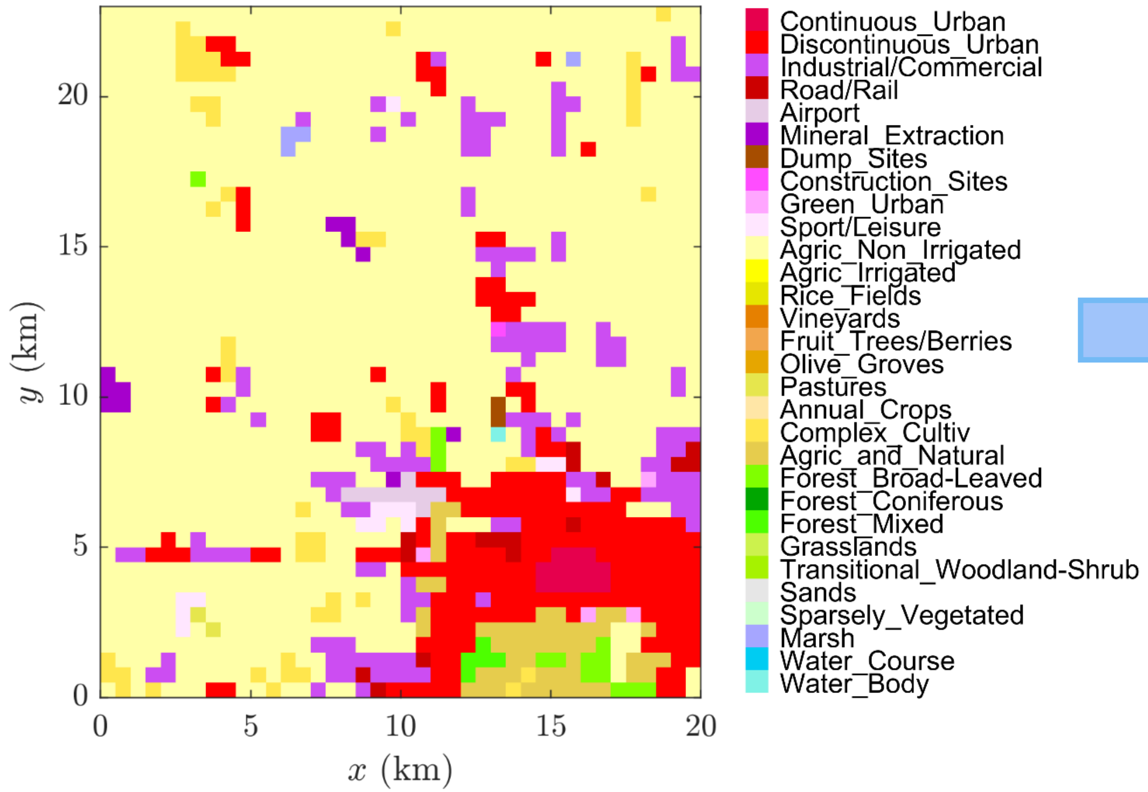
- Areas with capture probability **over 5%**.
- **Borgo Panigale** well field has the largest capture reach.
- **NE Bologna** well does not get any “shallow” water in 50 y.

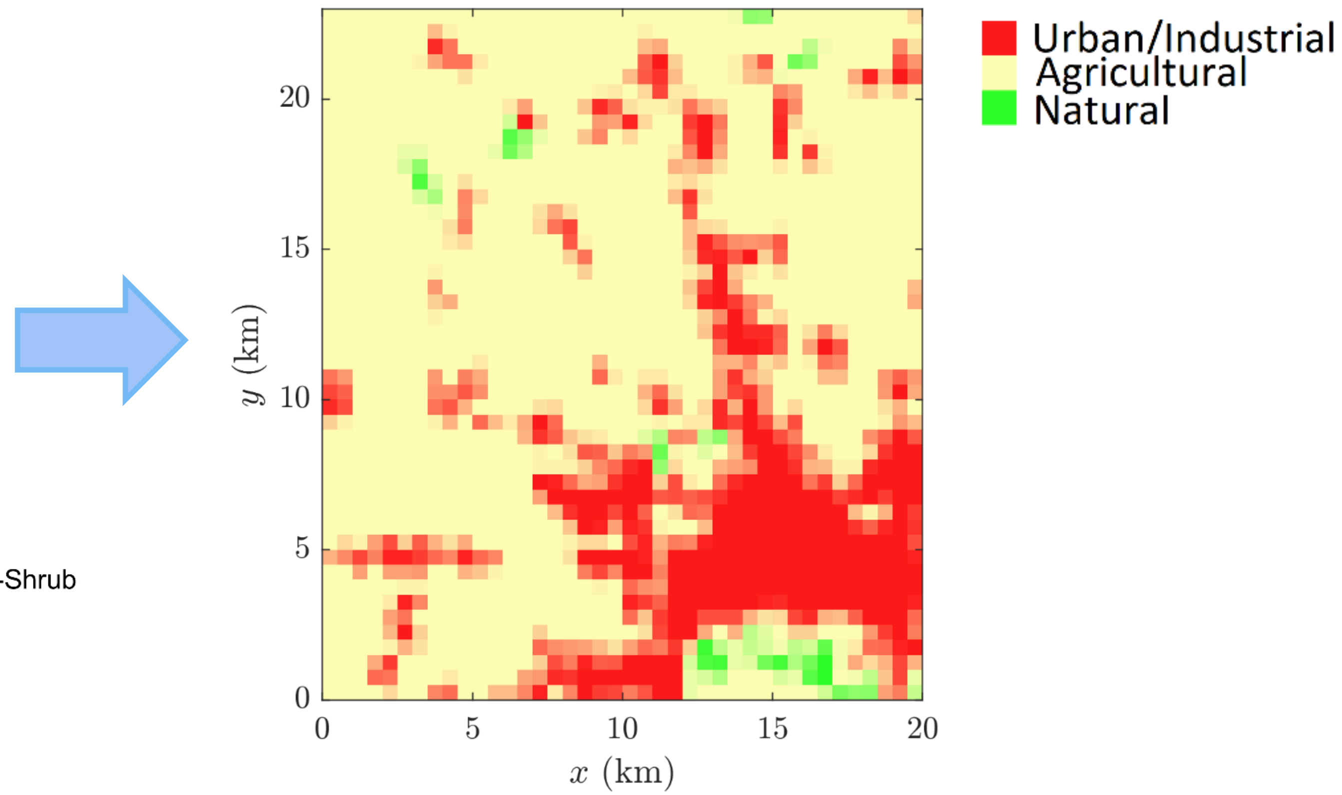


4. CONCENTRATIONS AT WELLS AND RISK

4.1. Land Use

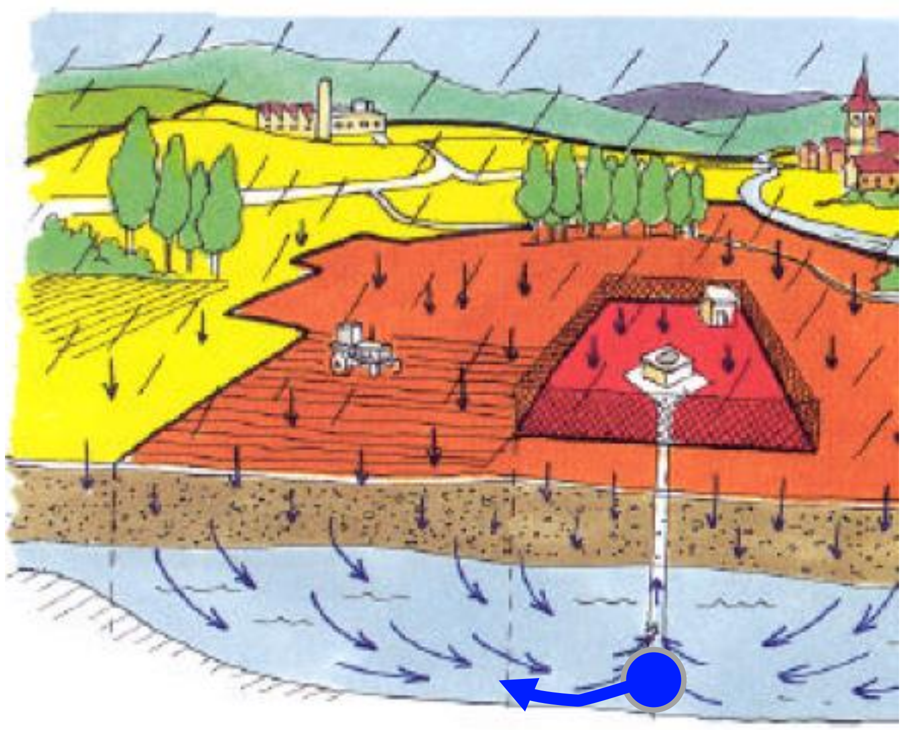
- Corine Land Cover European Land Use database.
- Simplification into 3 categories (**Urban and Industrial**; **Agricultural**; **Natural**).



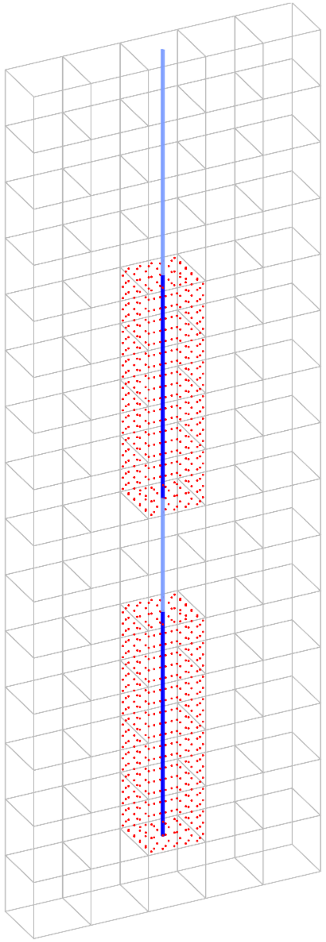


4.2. Numerical approach

- **Backward-in-time** particle tracking from wells (Pollock's method).
- Particle weights proportional to **water flux** towards well at well screen.
- Each particle weight represents participation to total extraction.
- Simulation stops when the particle reaches the **phreatic level** (entry).
- Record: source **land use** and **travel time**.



Backward-in-time

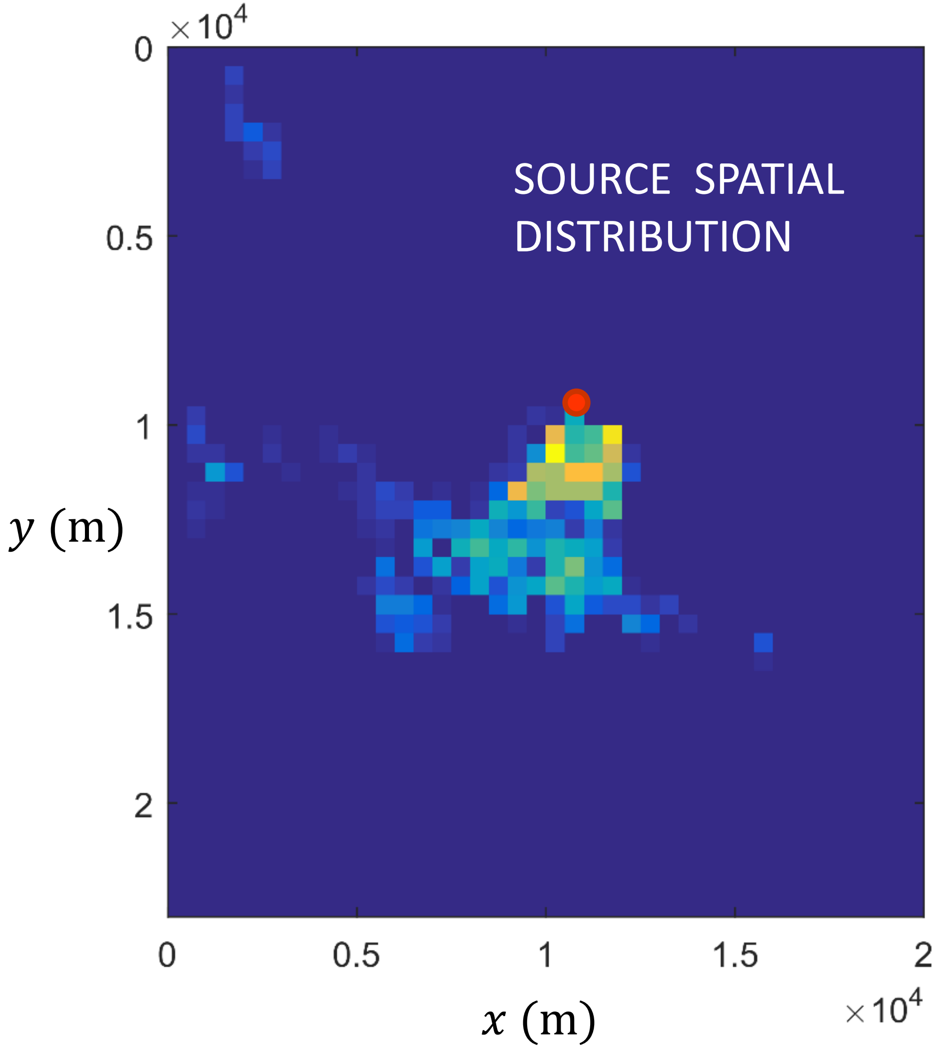


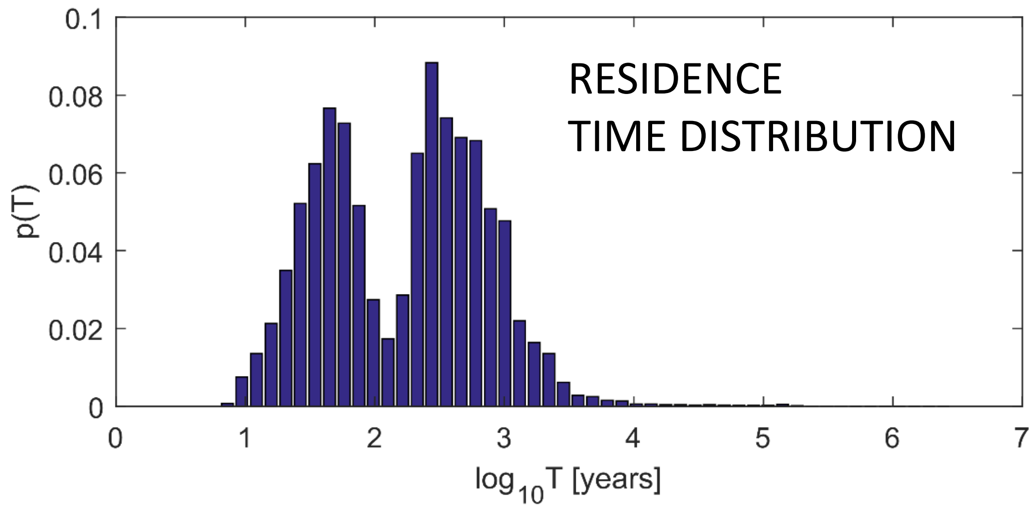
UNIVERSITAT POLITÈCNICA DE CATALUNYA
Department of Civil and Environmental Engineering
Hydrogeology Group GHS (UPC-CSIC)

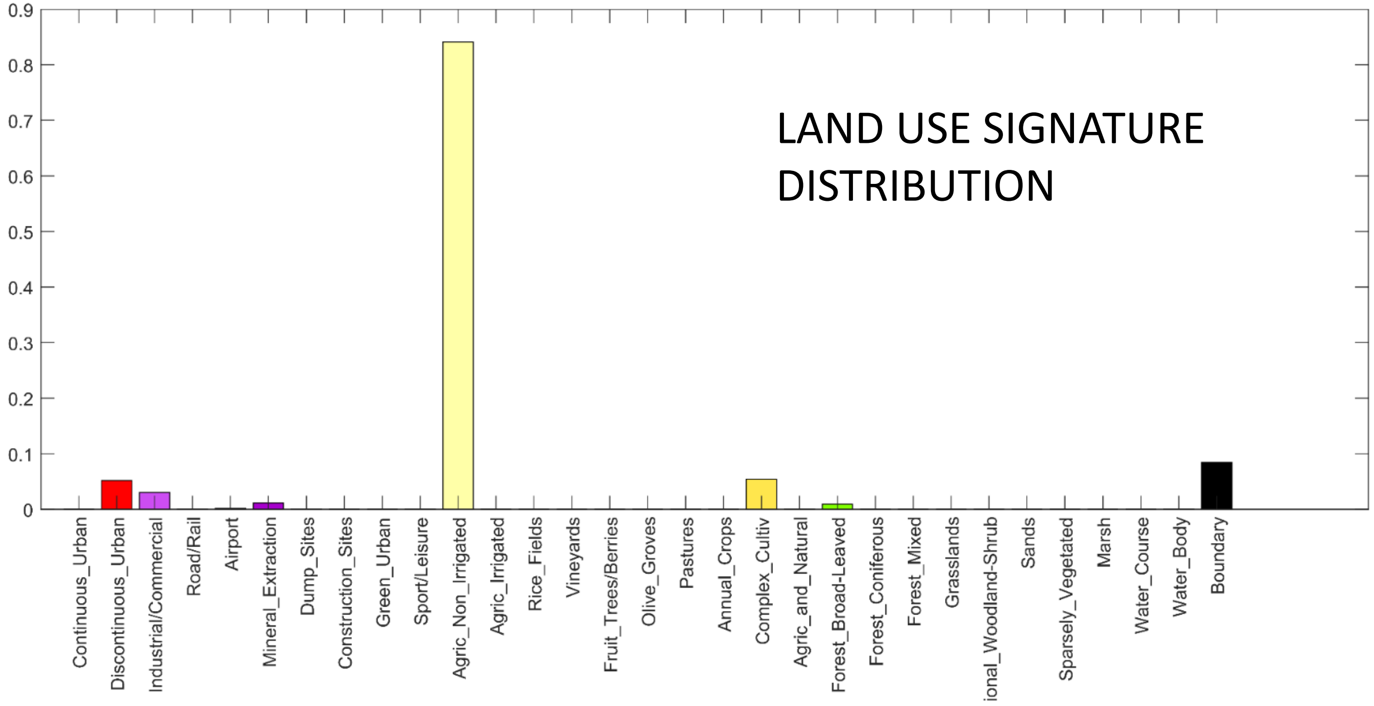
4. CONCENTRATIONS AT WELLS AND RISK

WE-NEED
Water JPI

4.3. Example simulation results (real. 0, well 68)







4.4. Computation of concentrations from particle arrival distributions

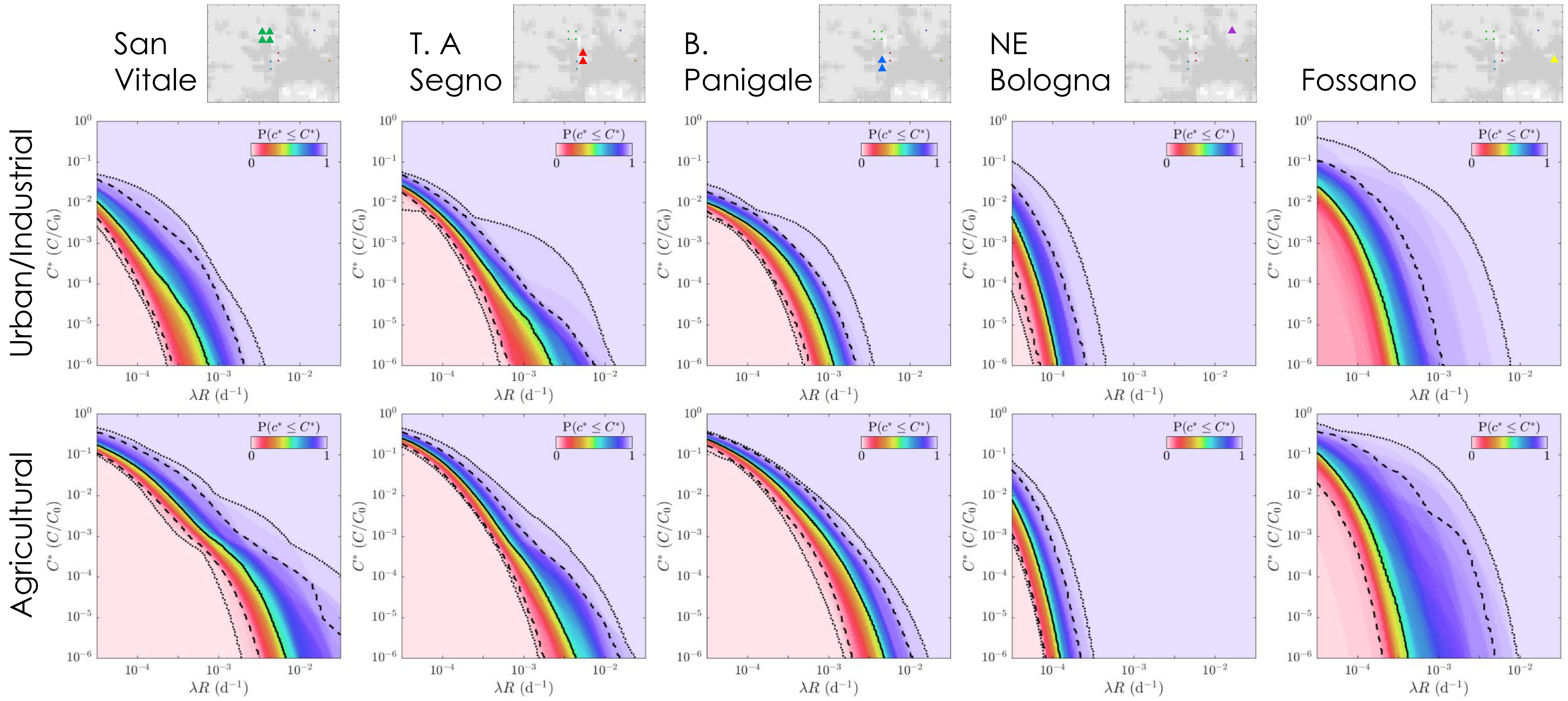
- Simplifying, yet "conservative" **assumptions**:
  - Zero local dispersion (independent **streamtubes**).
  - Input conc. C^0 that is **uniform** over land use type j (e.g. Agriculture) and **constant** in time.
  - Linear **sorption** (retardation factor R) and linear **degradation** (degradation constant λ).
- Then:

$$\mathcal{R}_i C_{i,w}(t) = C_i^0 \sum_{p=1}^{N} \overbrace{m_p^* \, I(\ell_p = j, t \geq R_i T_p)}^{\text{Advection}} \overbrace{\exp(-\lambda_i \mathcal{R}_i T_p)}^{\text{Reaction}} \qquad m_p^* = m_p / \sum_{q=1}^{N} m_q$$

- Maximum expected concentration is $C_{i,w}(\infty)$. Based on the 100 realizations of the velocity field, we compute the **cumulative density function** of $C_{i,w}(\infty)$.

4. CONCENTRATIONS AT WELLS AND RISK

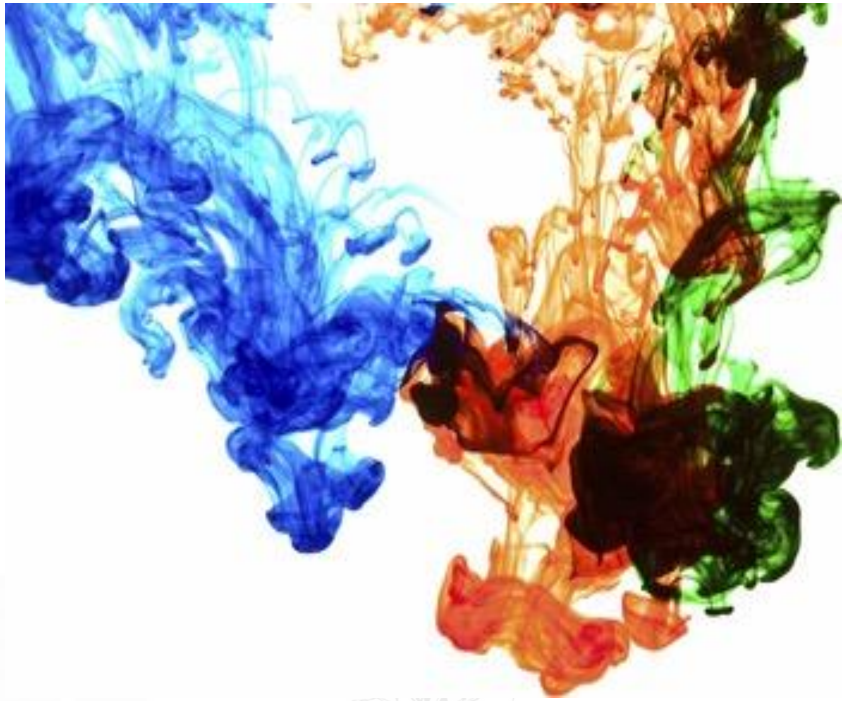
4.5. Concentration cdfs as a function of degradation kinetics (for two different source types)



UNIVERSITAT POLITÈCNICA DE CATALUNYA
Department of Civil and Environmental Engineering
Hydrogeology Group GHS (UPC-CSIC)

Chemical mixtures

Biogeochemical processes



Few examples of degradation related chemical mixtures

radioactive decay

$Pu^{238} \rightarrow U^{234} \rightarrow Th^{230} \rightarrow Ra^{226} \rightarrow Rn^{222} \rightarrow Pb$

$U^{238} \rightarrow U^{234} \rightarrow Th^{230} \rightarrow Ra^{226} \rightarrow Rn^{222} \rightarrow Pb$

reductive dechlorination of chlorinated organic compounds

Tetrachloroethene (PCE) → Dichloroethene (TCE) → Trichloroethene (DCE) → Vinyl chloride (VC)

Carbon tetrachloride → chloroform → dichloromethane → methylene chloride → methane

oxidative pathway of pesticides

Aldicarb → Aldicarb sulfoxide → Aldicarb sulfone

Nitrogen transformation

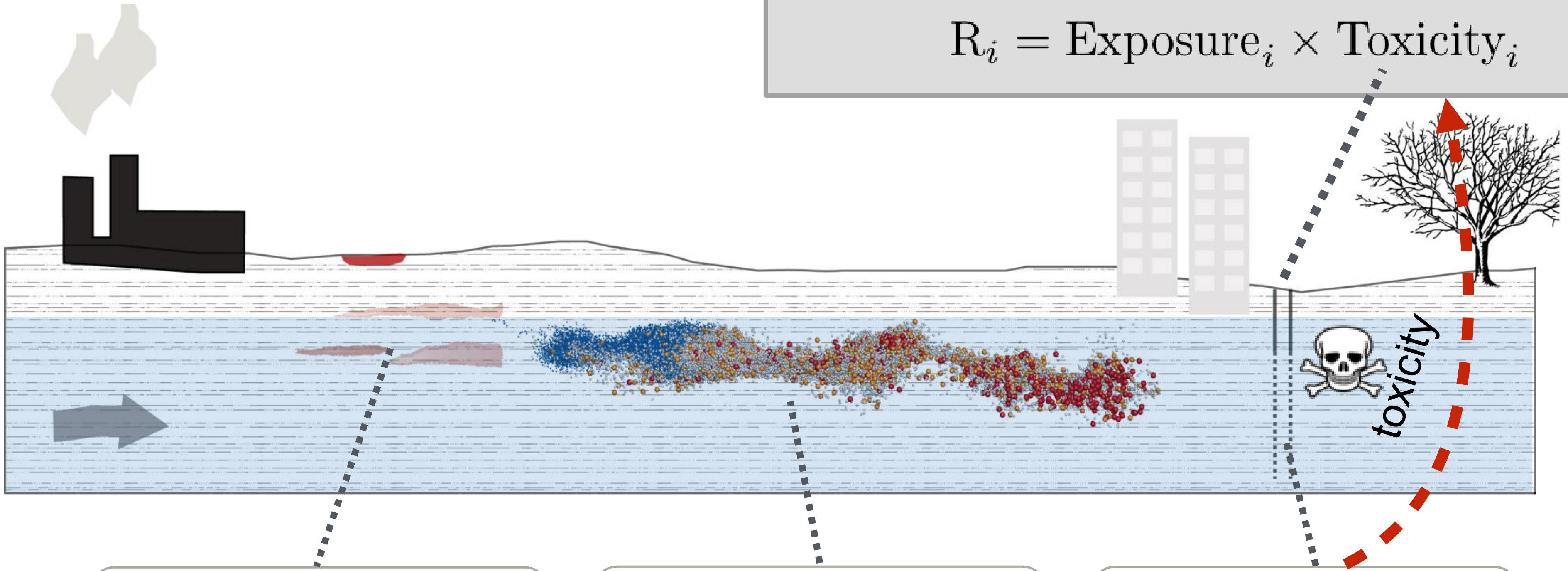
Ammonium (NH_4) → Nitrite (NO_2^-) → Nitrate (NO_3^-)

UNIVERSITAT POLITÈCNICA DE CATALUNYA
Department of Civil and Environmental Engineering
Hydrogeology Group GHS (UPC-CSIC)

Additivity risk model

$$R_T \approx R_{PCE} + R_{TCE} + R_{DCE} + R_{VC}$$

$$R_i = \text{Exposure}_i \times \text{Toxicity}_i$$



release
of the contaminant

1

fate and transport
of the contaminant

2

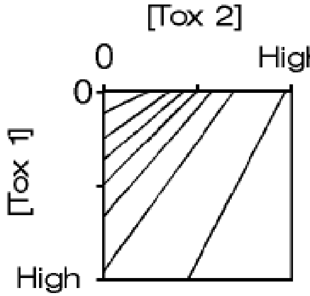
quantification of
the dose

3

4.6. Carcinogenic risk (of a mixture) associated to water consumption

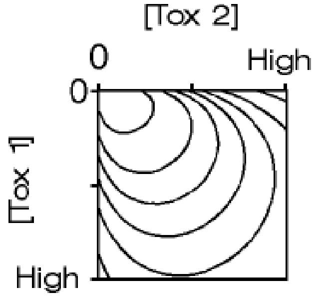
Additivity model

$$R_{CA} = \sum_{i=1}^{N} R_i$$



Synergy/Antagonism

$$R_{SA} = R_{CA} \times \exp\left(-\sum_{i,j} a_{ij}\, Z_i Z_j\right) \qquad Z_i = \frac{R_i}{\sum_{j=1}^{N} R_j}$$



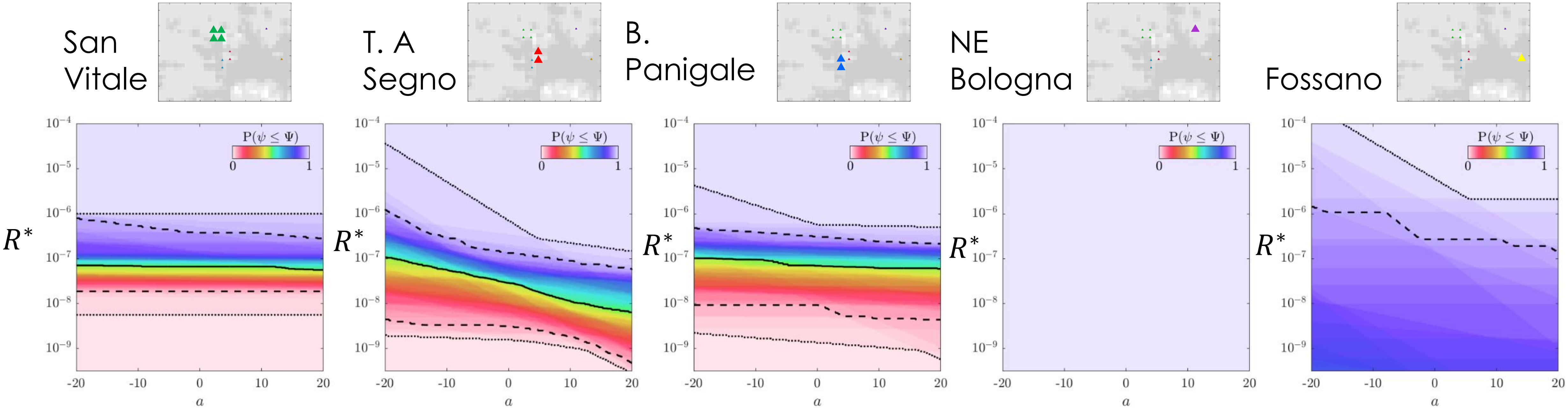
Junker et al. (2005)

Combinations of a mixture can cause a **more severe (synergism)** or a **less severe (antagonism)** effect than calculated from the reference (additivity) risk model

4. CONCENTRATIONS AT WELLS AND RISK

4.7. Risk cdfs for variable chemical synergy parameter a

(for the example of two recalcitrant contaminants, cont. released on urban/industrial and agricultural land, respectively, with identical $c_0 = 0.01\ \mathrm{mg/L}$, and $\lambda\mathcal{R} = 0.001\ \mathrm{d}^{-1}$)



Probability that the total risk R_{SA} is smaller than R^* $P(R_{SA} \leq R^*)$