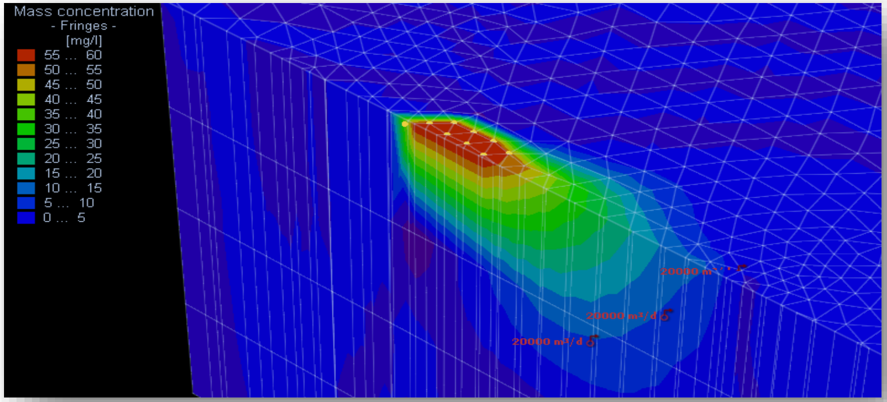

Geostatistics and Numerical Modelling in the characterization of a contaminated site

(#1464)

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Montpellier, France
CORUM CONFERENCE CENTER
43rd IAH congress

Why geostatistics & modelling in contaminated sites?

1. All actions (characterization, containment, remediation, treatments, etc.) are based on the flow field and on the spatial extent of the contamination (i.e. two interpolated datasets);
2. The spatial extent of the contaminant changes in time;
3. Numerical models are often used to support decision making;
4. All numerical model predictions are wrong.

As obvious consequence, it is mandatory to:

- quantify the errors in observations (in space and time);
- assign weight to the observations used in model calibration;
- quantify model predictions uncertainty;

Including this steps in the characterization of a contaminated site can bring to the *Numerically Enhanced Conceptual Model (NECM)* with clear benefits in the decision process.

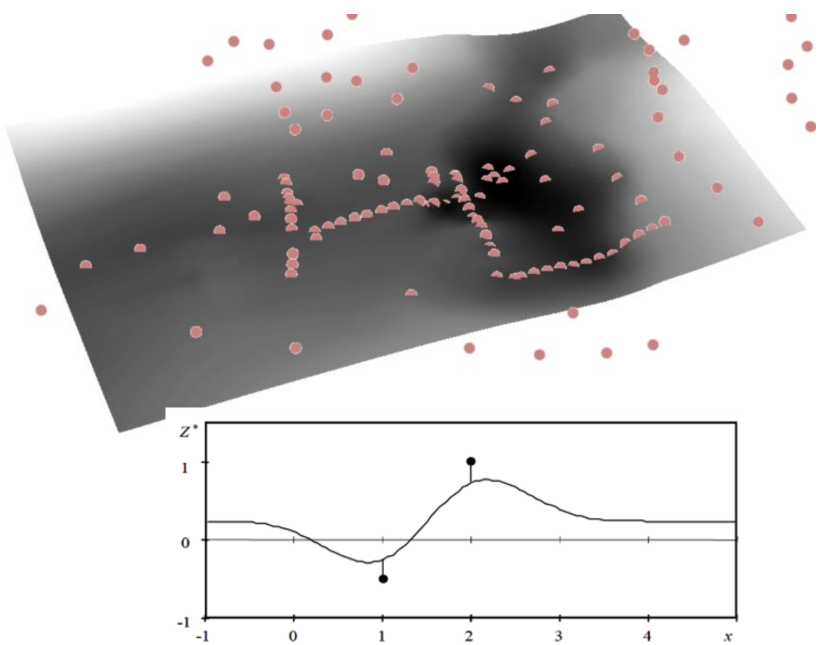
Errors in observations - Geostatistics

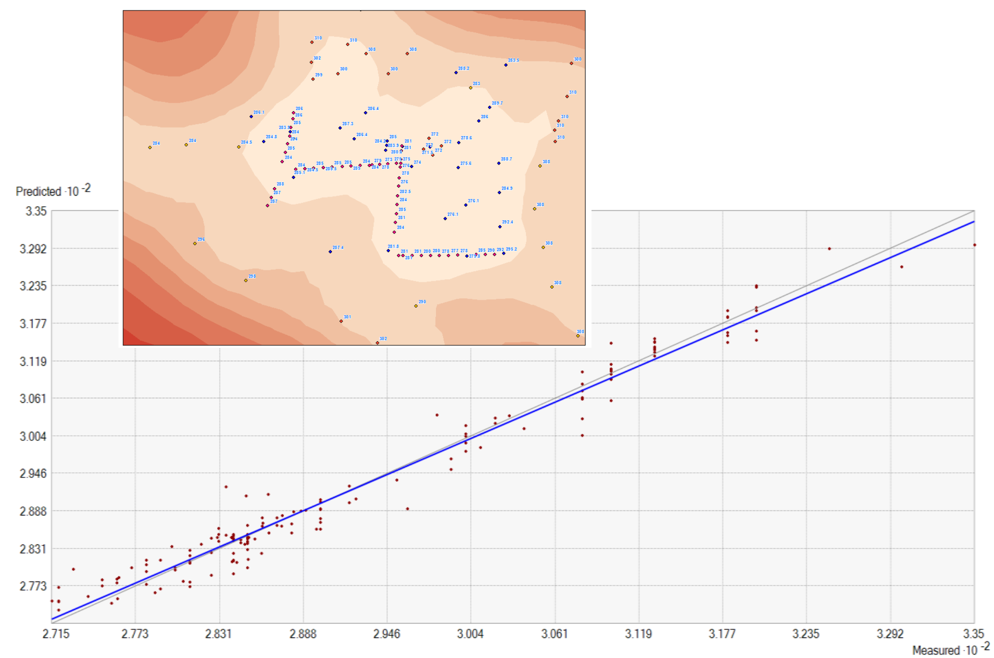
We often give recharge, aquifer bottom and inital heads «for sure», or we say: «we have to keep fixed at least these things…"

But, each recontructed suface has its own RMSE

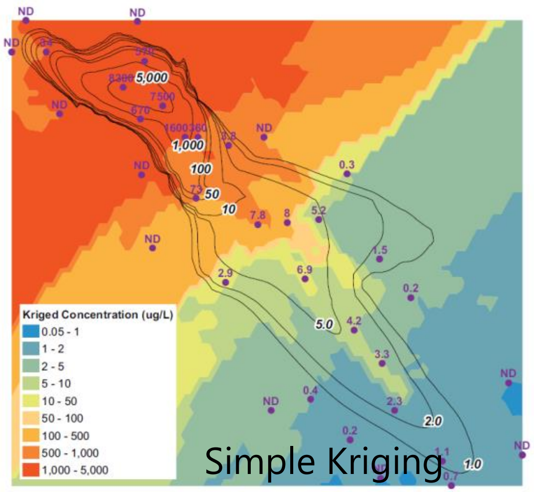
What would be the meaning of a model calibrating observations with an RMSE = 5 m, if the initial head surface presents an RMSE of 10 m?

Given that modelling should support environmental decision making, why should we ignore this aspect?

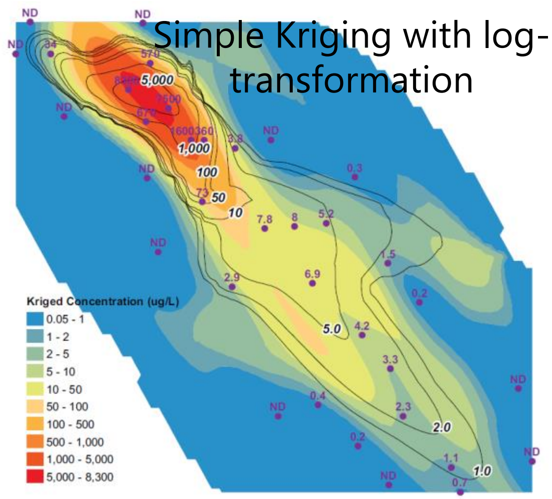




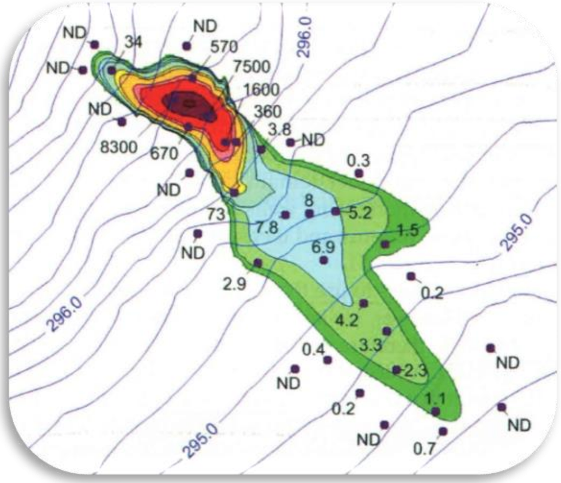
…Shall we give for sure its spatial distribution?

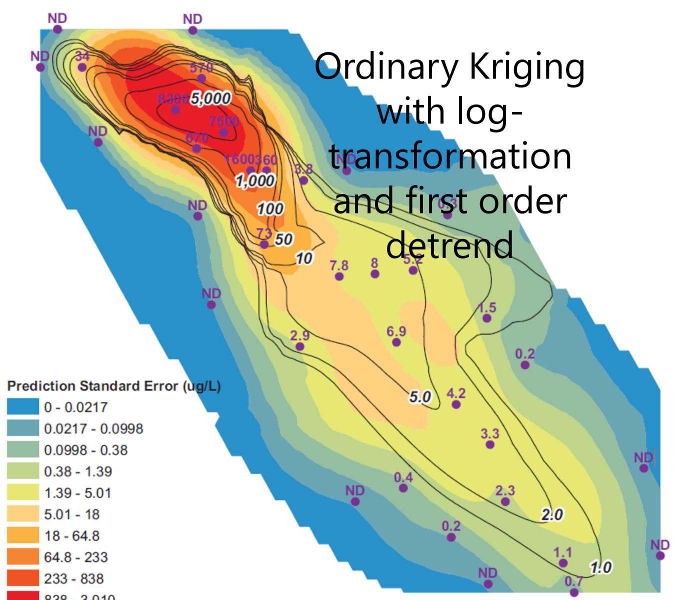


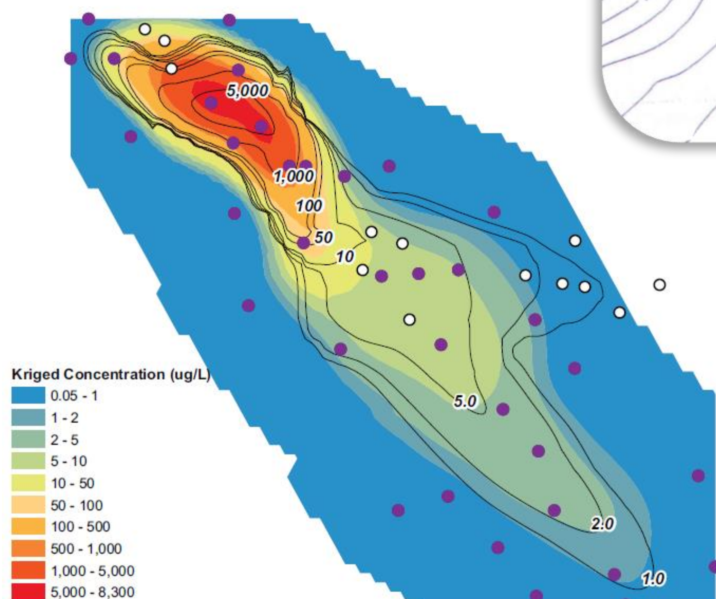
Simple Kriging with log-transformation



Reality (unknown)





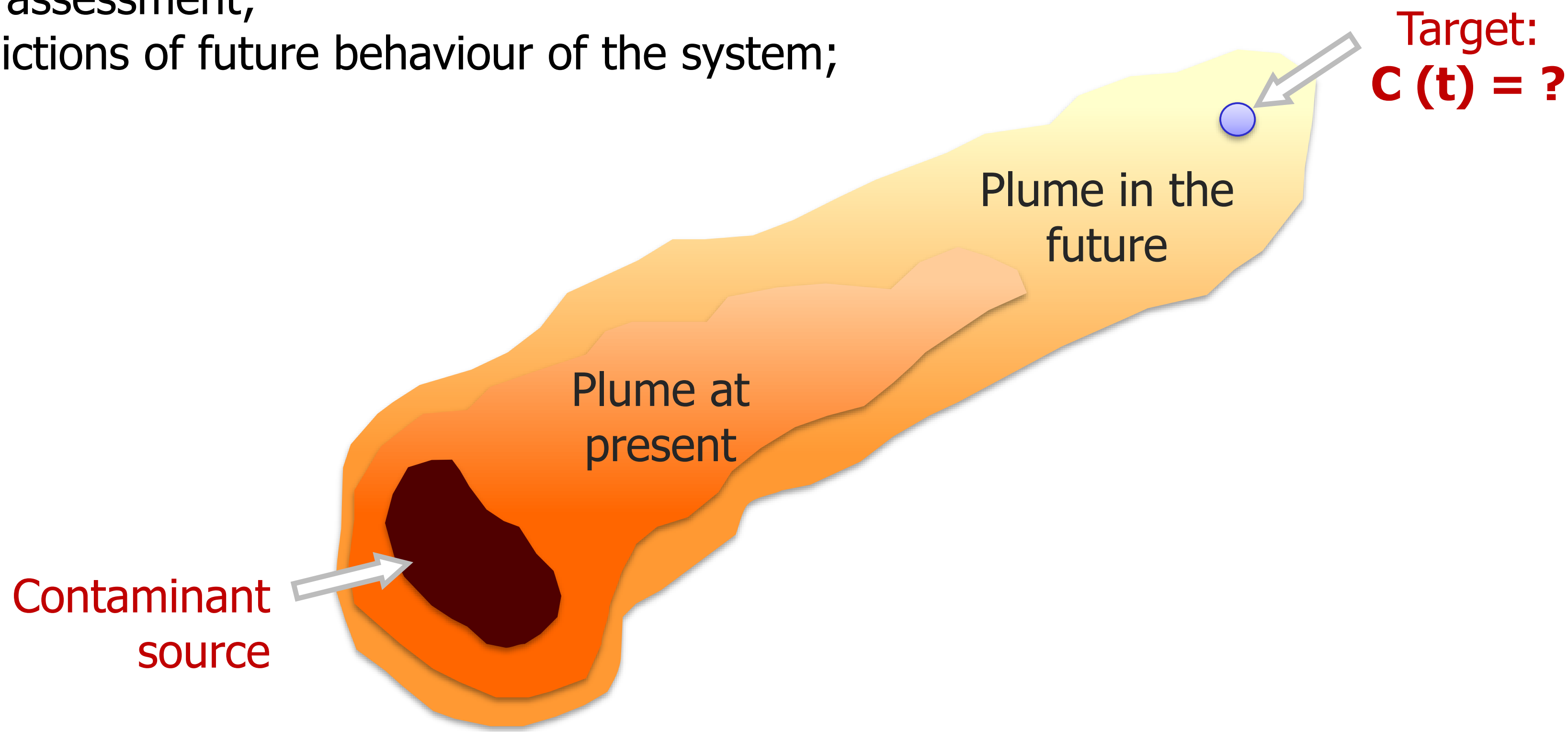


Ordinary Kriging with log-transformation, second order detrend, Co-Kriging with hydraulic heads

(Kresic & Mikszewski, 2013)

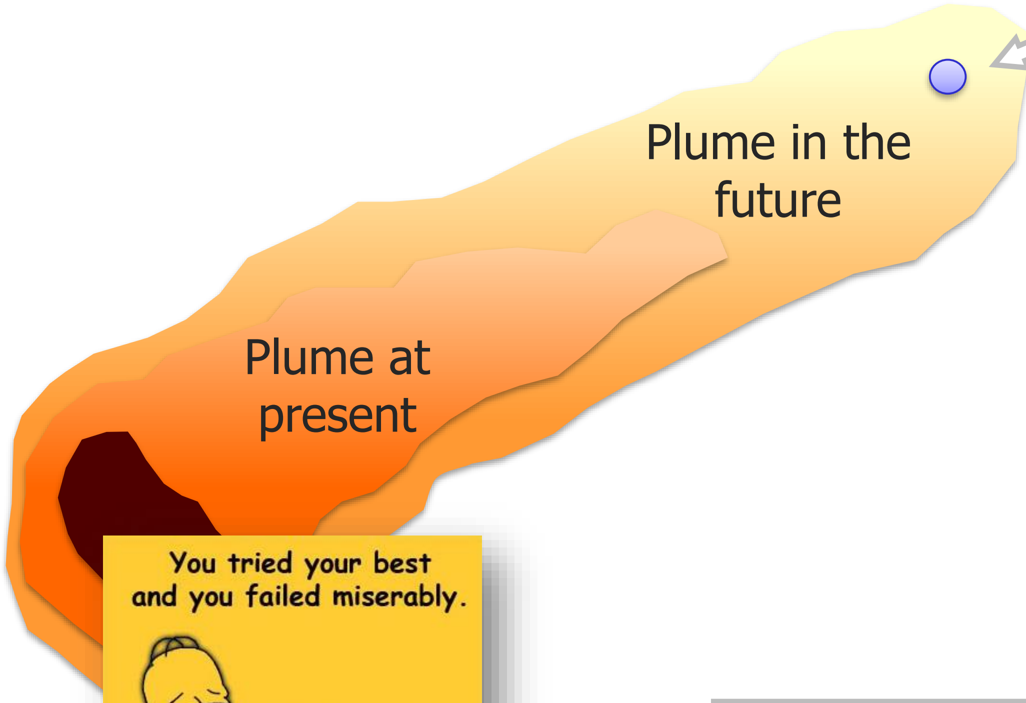
Model Uncertainty - Issues commonly asked to the "magic ball"

- P&T design or evaluation;
- Comparison among different remediation/containment techniques;
- Definition of the potential contamination targets;
- Risk assessment;
- Predictions of future behaviour of the system;
- Etc.



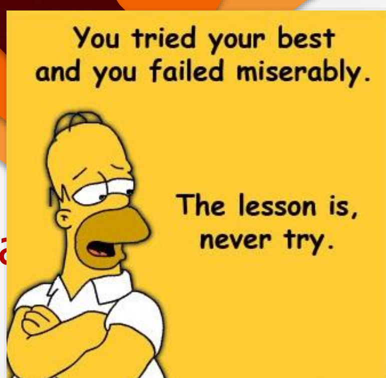
In a few words, model predictions are used in decision making to achieve a wise environmental management.

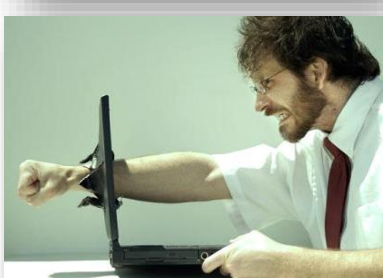
Model Uncertainty - Common answer…



Target:
t = 2 years
C (t) = 82.43 ± 0.24 mg/L

Is this result reliable?
If yes, *how much* reliable is it?





Measurement errors (starting from ground elevation…)	Errors in the preliminary statistical analysis	Errors in spatial distributions of variables
Errors in the conceptual model definition	Errors in the numerical model building	Errors in considering the model outputs as *uniques*

Model Uncertainty – beginning with calibration

Every modeler is aware that his/he model can present a huge number of different solutions equally *well calibrated*.

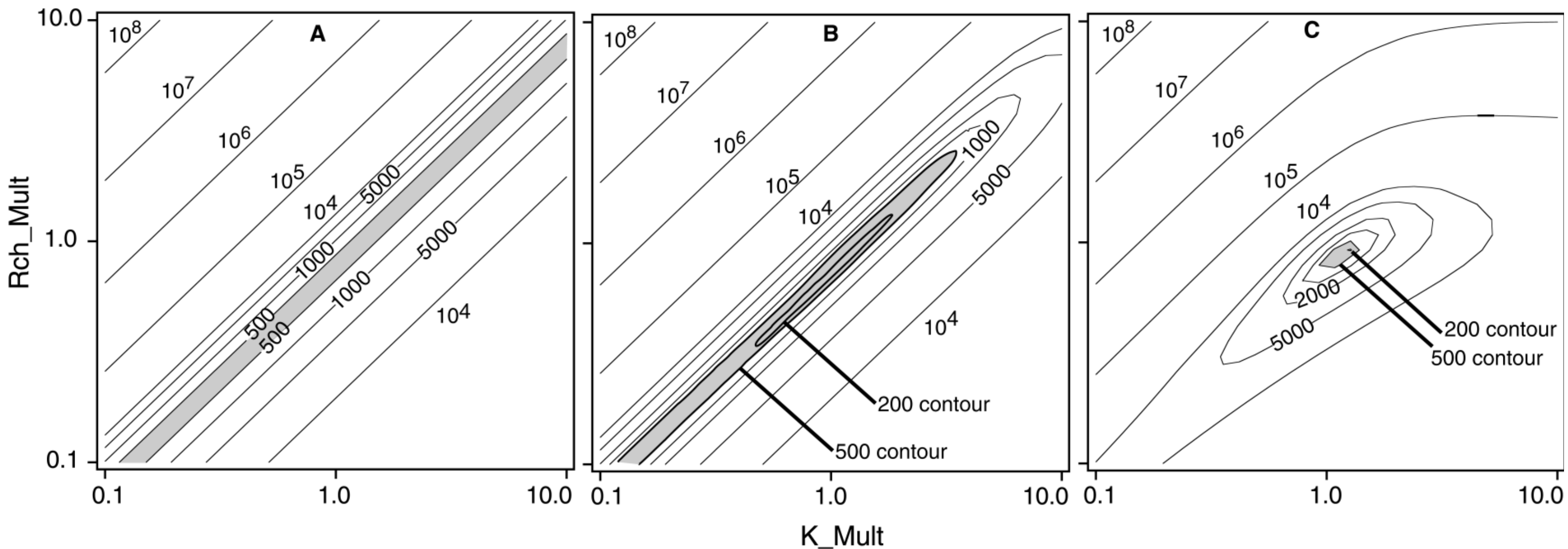
$$\Phi = \sum_{i=1}^{m} (w_i r_i)^2$$

Objective function Φ

r_i = error between observed and simulated *i-th* head;

w_i = weight of the *i-th* head

Φ surfaces, obtained changing 2 combined parameters: Recharge and Hydraulic conductivity



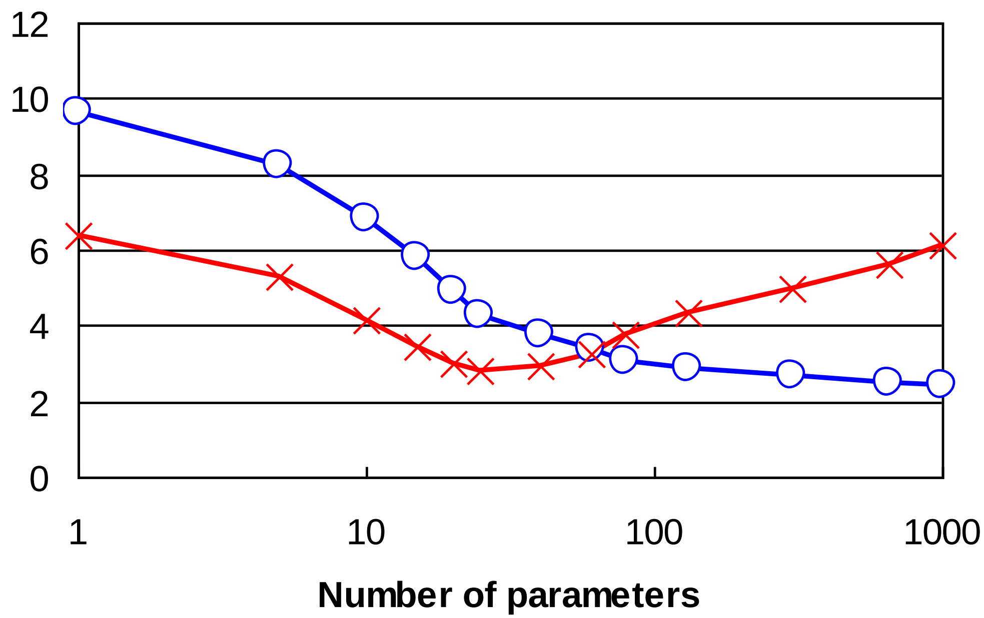
SS calibration over head data: no unique minimum exists; parameter correlation = 1

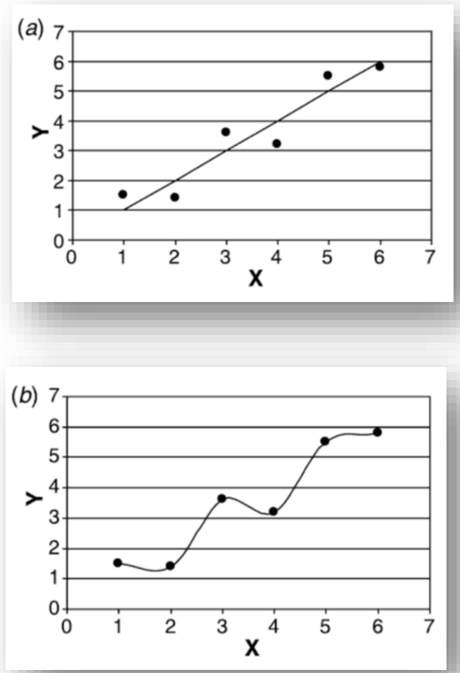
SS calibration over head and flow data, weighted with coeff. of variation = 10%; parameter correlation < 1

SS calibration over head and flow data, weighted with coeff. of variation = 1%; parameter correlation << 1

(Hill and Tiedeman, 2007)

Model Uncertainty – Principle of Parsimony (simplified)





As the number of parameters increases, the error between observed and simulated values decreases, as well as the error in prediction.

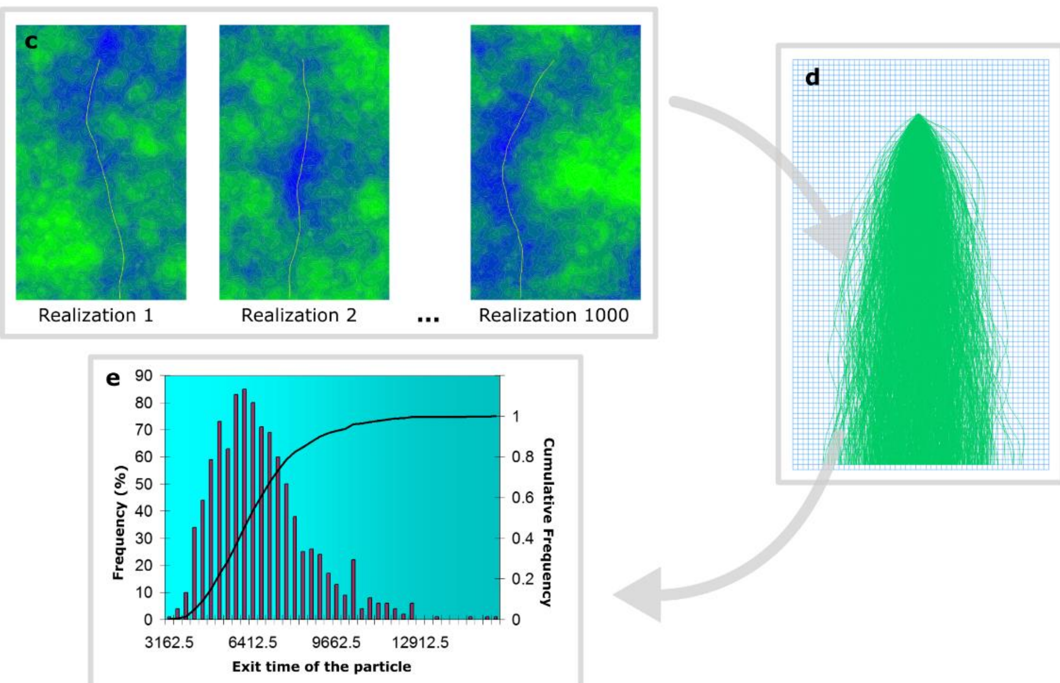
Beyond a certain number parameters, the error between observed and simulated values continues to decrease but <u>prediction error rises</u>, since parameters are no more directly supported by the data (we start fitting the errors).

Model Uncertainty – Highly parametrized methods (simplified)

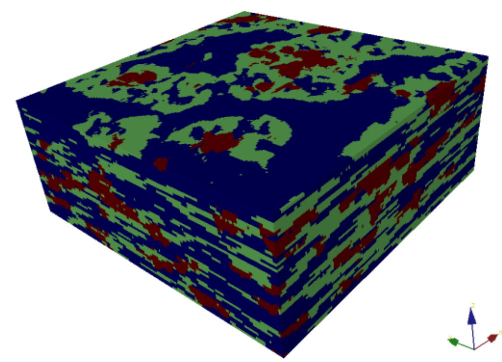
In some cases reality is so heterogenous to be hardly restrained to homogeneous parameter zones. And this is true especially when contamination transport is under study.

Highly-parameterized methods involve the use of *pilot points*. But still, how many *pilot points* can we hope to calibrate?

The level of complexity should be set according to its salience to decision-informative predictions, rather than according to the limited calibration dataset.



Realizations can be based on classical geostatistics distribution or on Multiple Point Simulations (MPS)



(Moore and Doherty, 2005)

An example of NECM

Problem:

- Contaminated site (Chloroform, Benzene, Toluene);
- Main target: River;
- P&T remediation started in 2005;

Question: «What happens if we switch off the P&T?»

First Phase:

- Numerical modelling of the given CM, SS and TS calibration over static heads, pumping tests, river discharges, concentrations of chloroform;

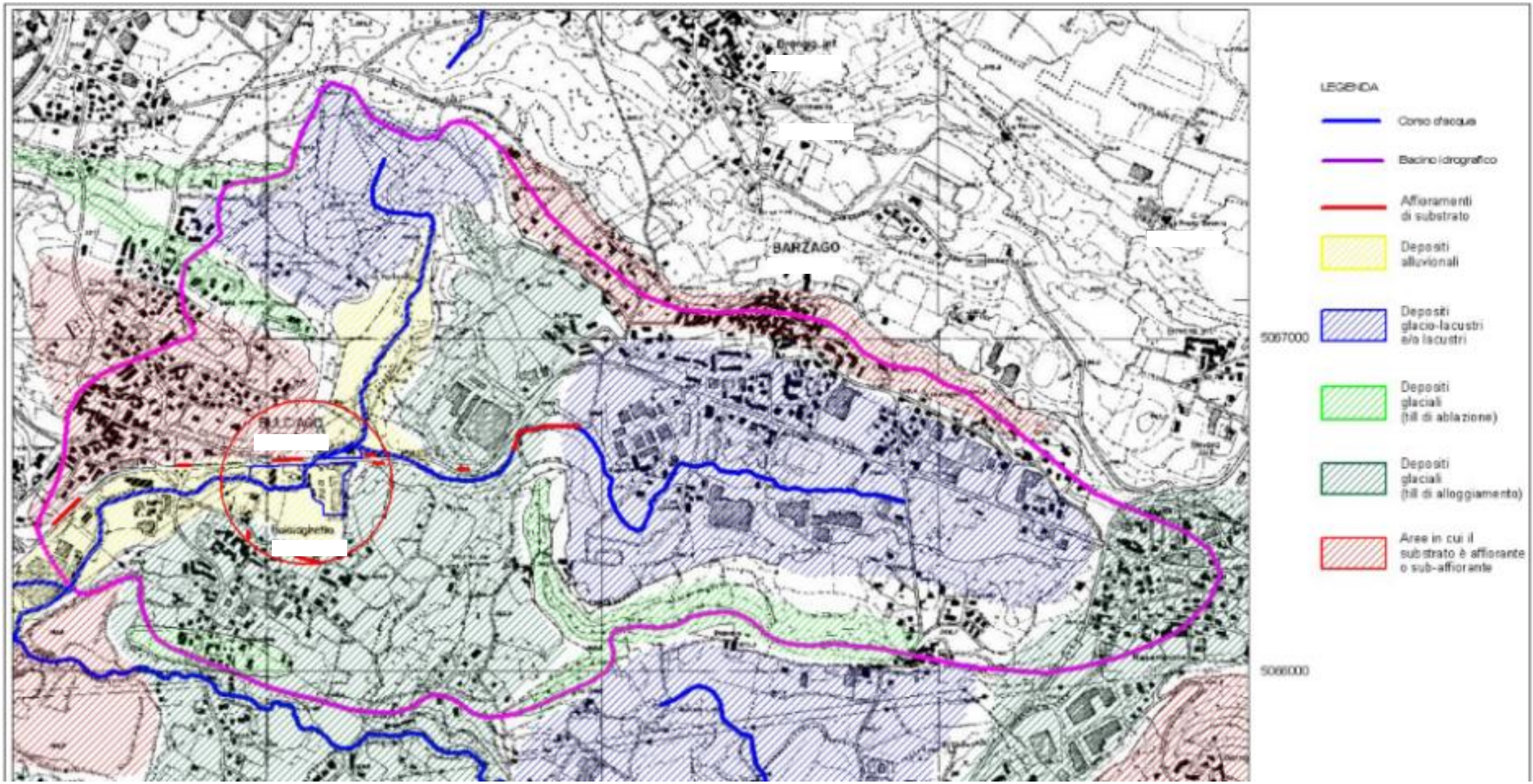
It is not possible to calibrate the observation dataset

Second Phase:

- Complete review/reinterpretation of available spatial and time data;
- linear uncertainty analysis;
- Complete CM redesign – especially parameters with higher influence over prediction uncertainty: **aquifer bottom** and **groundwater-surface water interaction**.

Contaminated site - Geology

Geological settings



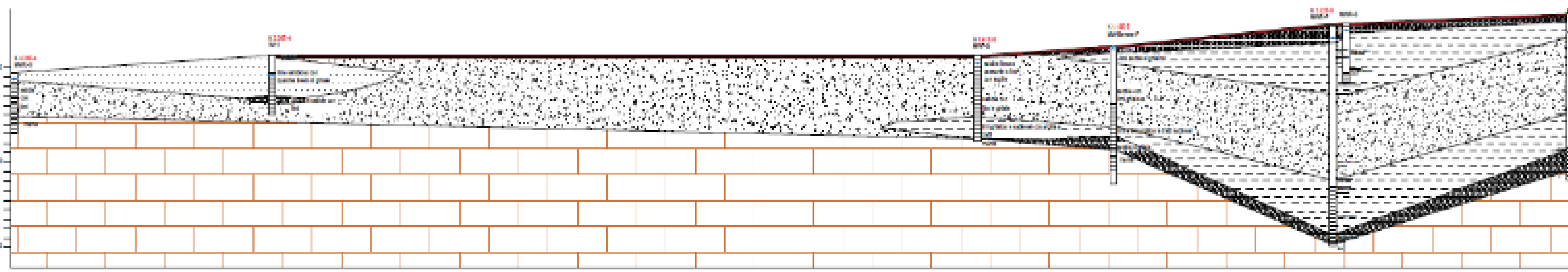
Pleistocene-Holocene fluvio-glacial-lacustrine aquifer, heterogeneous in grain size, unconfined or locally leaky. The aquifer substratum is made up of marly-clayey-silty-calcareous formations (Cretaceous-Eocene).

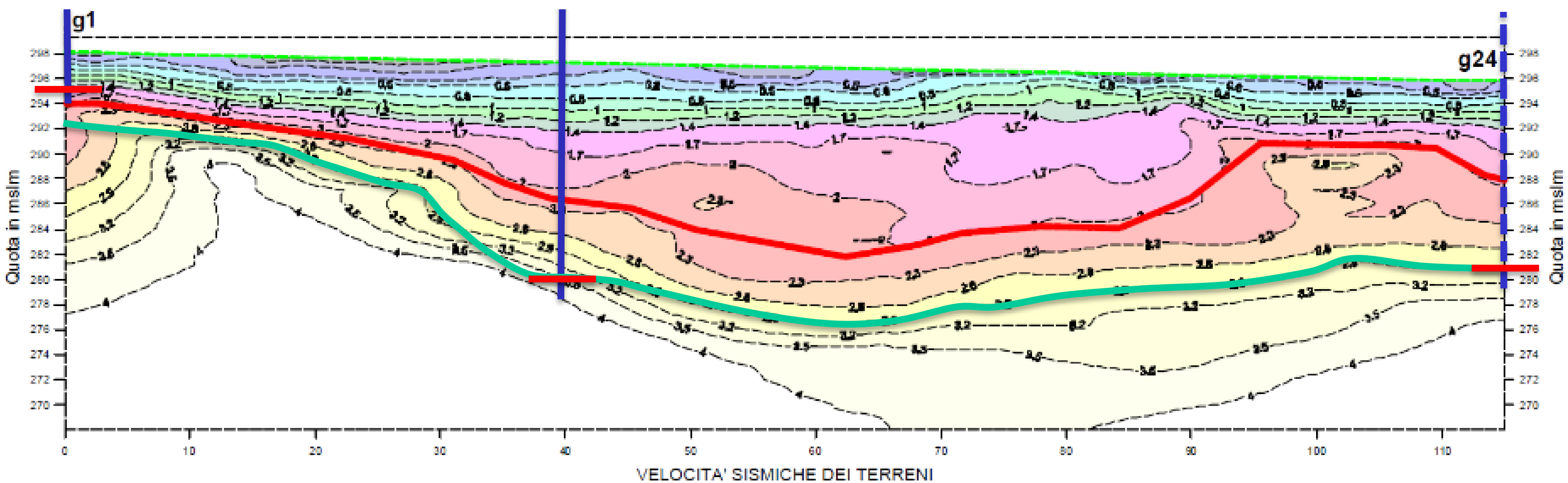
Contaminated site – Aquifer bottom

Geostatistical analysis of:

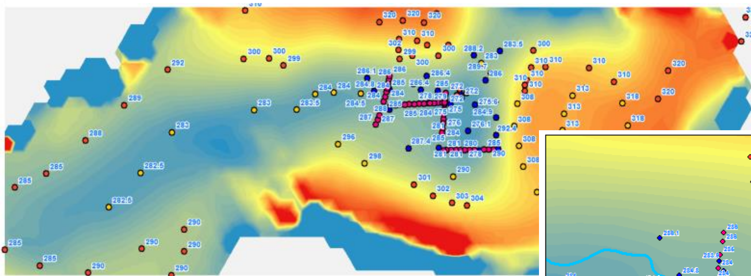
Resistivity survey (reinterpreted) + in site stratigraphic logs + extended area stratigraphic logs+ substratum outcrops

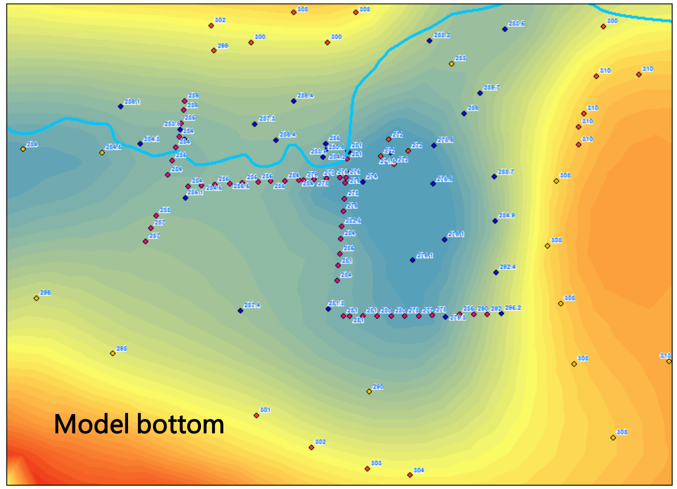
(previously reconstructed only through site boreholes)

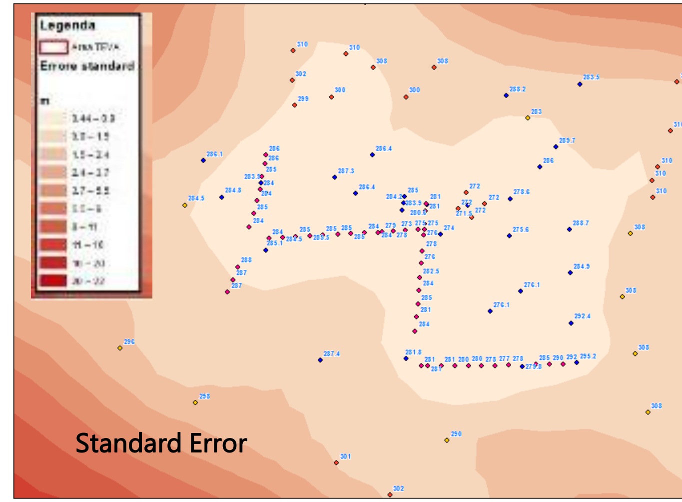


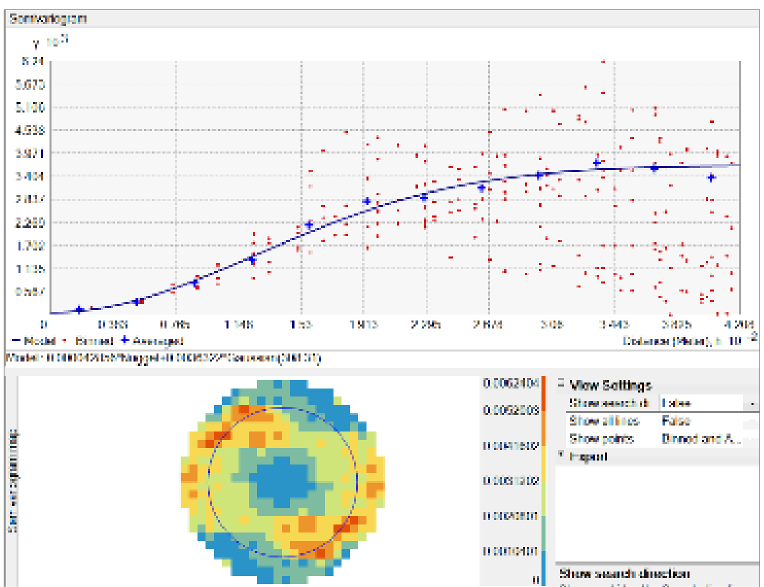


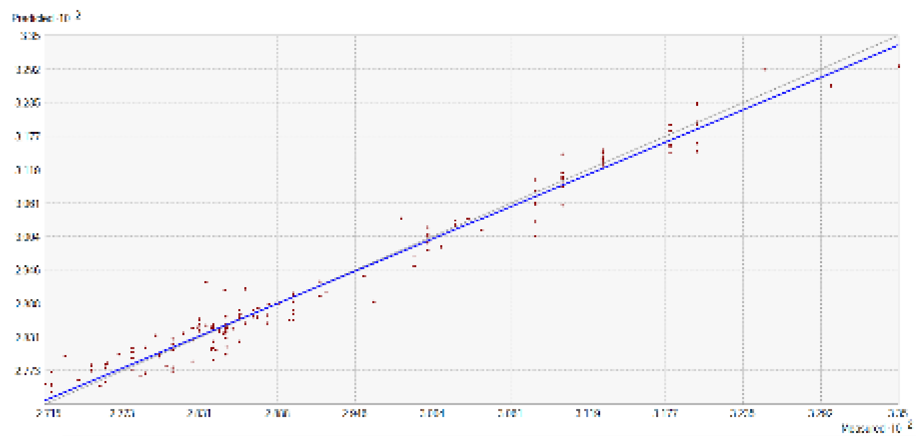
Contaminated site – Aquifer bottom











Results of LOOCV

Prediction Errors	
Samples	156 of 156
Mean	-0.03151056
Root-Mean-Square	2.567203
Mean Standardized	-0.001057841
Root-Mean-Square Standardized	1.093618
Average Standard Error	3.681964

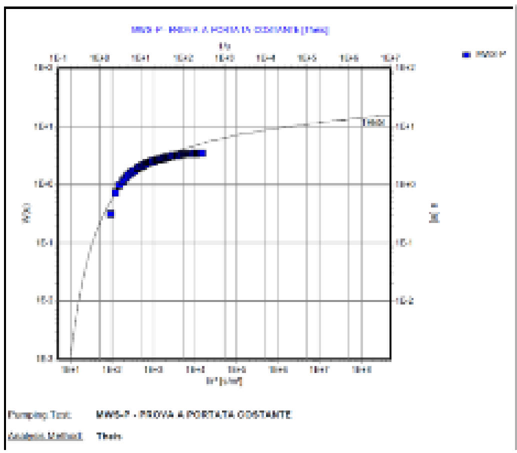
Contaminated site – GW-SW interaction?

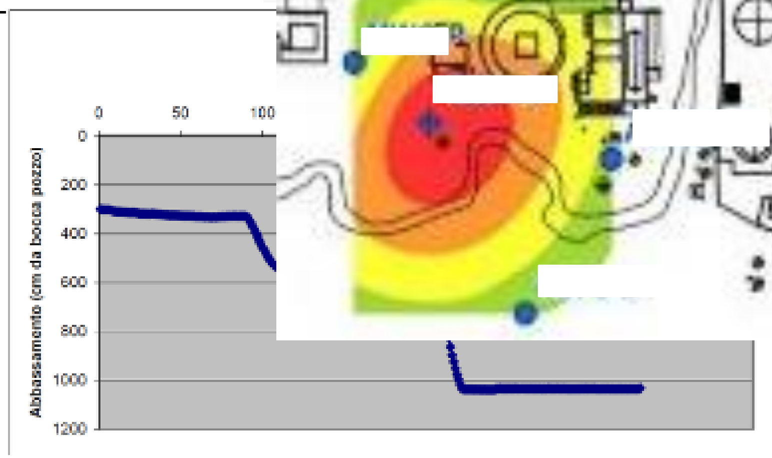
Piezometro	Tipo di prova	N	Media T (m²/s)	Min. T (m²/s)	Max. T (m²/s)	SD T (m²/s)	Media S	Min. S	Max. S	SD S
Profondo	Lunga durata	11	8.88E-04	4.55E-05	6.08E-03	1.75E-03	2.95E-02	1.54E-06	2.84E-01	8.94E-02
	*Media**		*5.46E-04*	*4.99E-04*	*5.94E-04*	*6.70E-05*	*2.72E-04*	*2.03E-04*	*3.41E-04*	*9.78E-05*
Profondo Totale			8.36E-04	4.55E-05	6.08E-03	1.60E-03	2.46E-02	1.54E-06	2.84E-01	8.16E-02
Superficiale	Gradini	5	1.68E-04	3.81E-05	5.00E-04	1.88E-04	3.98E-03	1.78E-03	6.18E-03	3.11E-03
	Lunga durata	70	3.55E-04	2.54E-06	2.05E-03	4.21E-04	1.44E-02	1.02E-06	3.14E-01	4.84E-02
	*Media**		*3.43E-04*	*6.87E-05*	*9.22E-04*	*2.74E-04*	*1.50E-03*	*1.02E-06*	*6.61E-03*	*1.94E-03*
Superficiale Totale		75	3.43E-04	2.54E-06	2.05E-03	3.94E-04	1.18E-02	1.02E-06	3.14E-01	4.34E-02
TOTALE		86	4.07E-04	2.54E-06	6.08E-03	6.88E-04	1.3			

*Valori medi delle prove ritenute più rappresentative (**Tabella 2-1** e Allegato 1).

Tabella 2-2 Valori di trasmissività e coefficiente di immagazzinamento suddivisi

Pumping tests and river

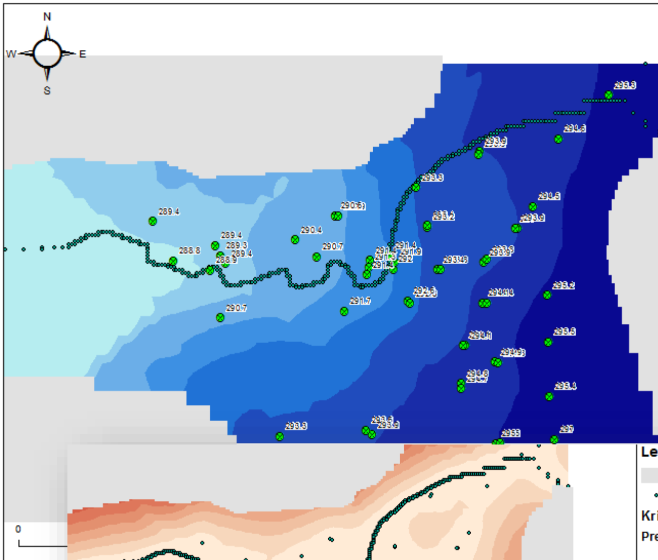




PUNTO DI CAMPIONAMENTO	PORTATA 17/11/05 (l/s)	PORTATA 29/03/06 (l/s)
A	14.1	140.8
B	16.4	136.4
C	22.3	145.9

Discharge increment (C-A): 5-8 L/s

Contaminated site – Flow Model



Initial heads (from measures with no pumpings)

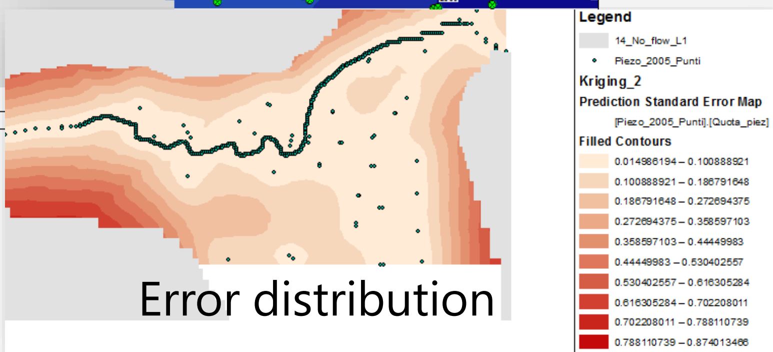
Legenda

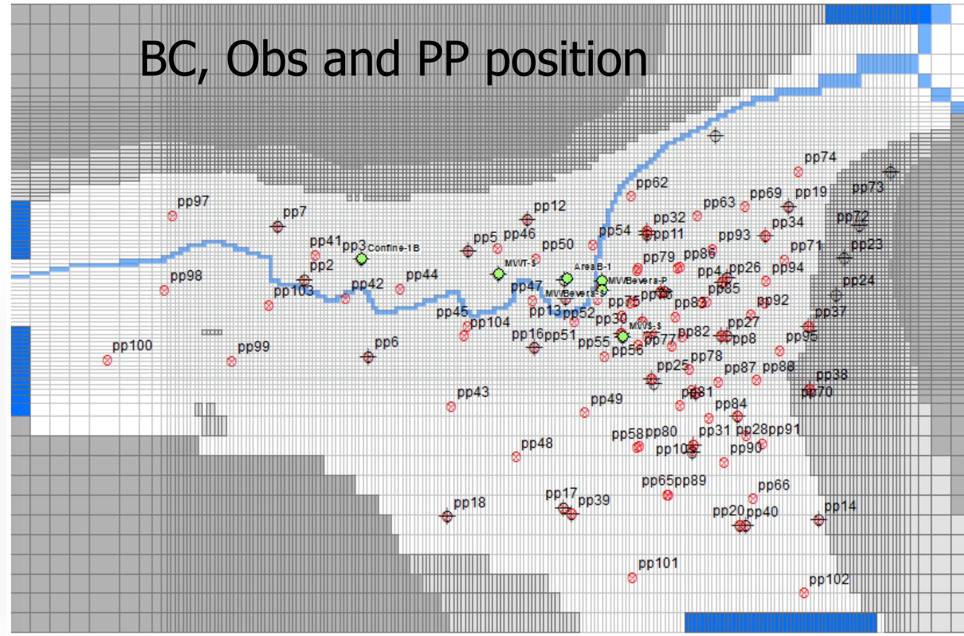
Punti di misura della falda relativi alla campagna di misura di Febbraio 2005

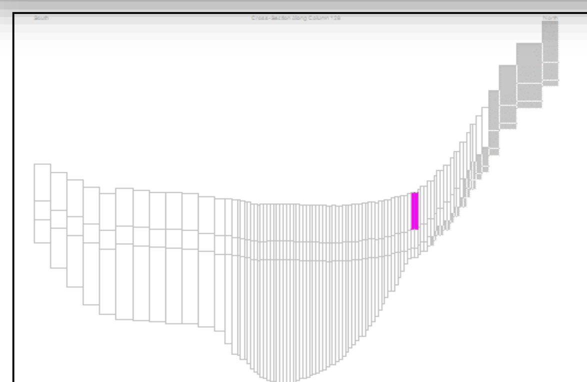
Piezometria acquifero (m s.l.m.) Febbraio 2005

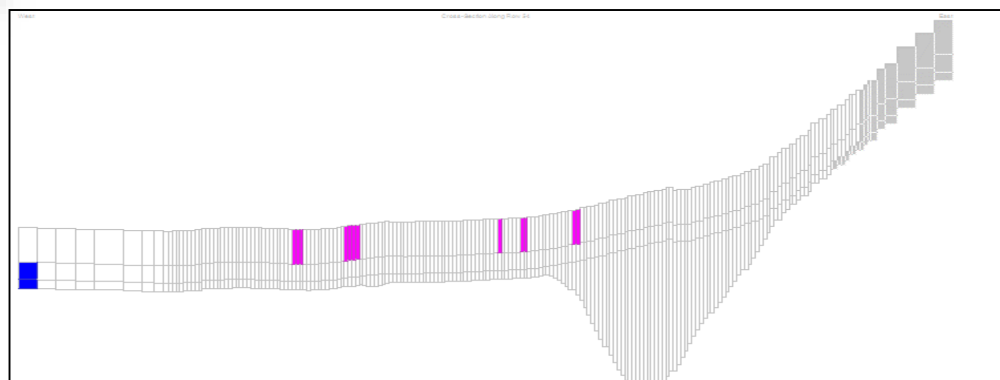
299.63

288.79

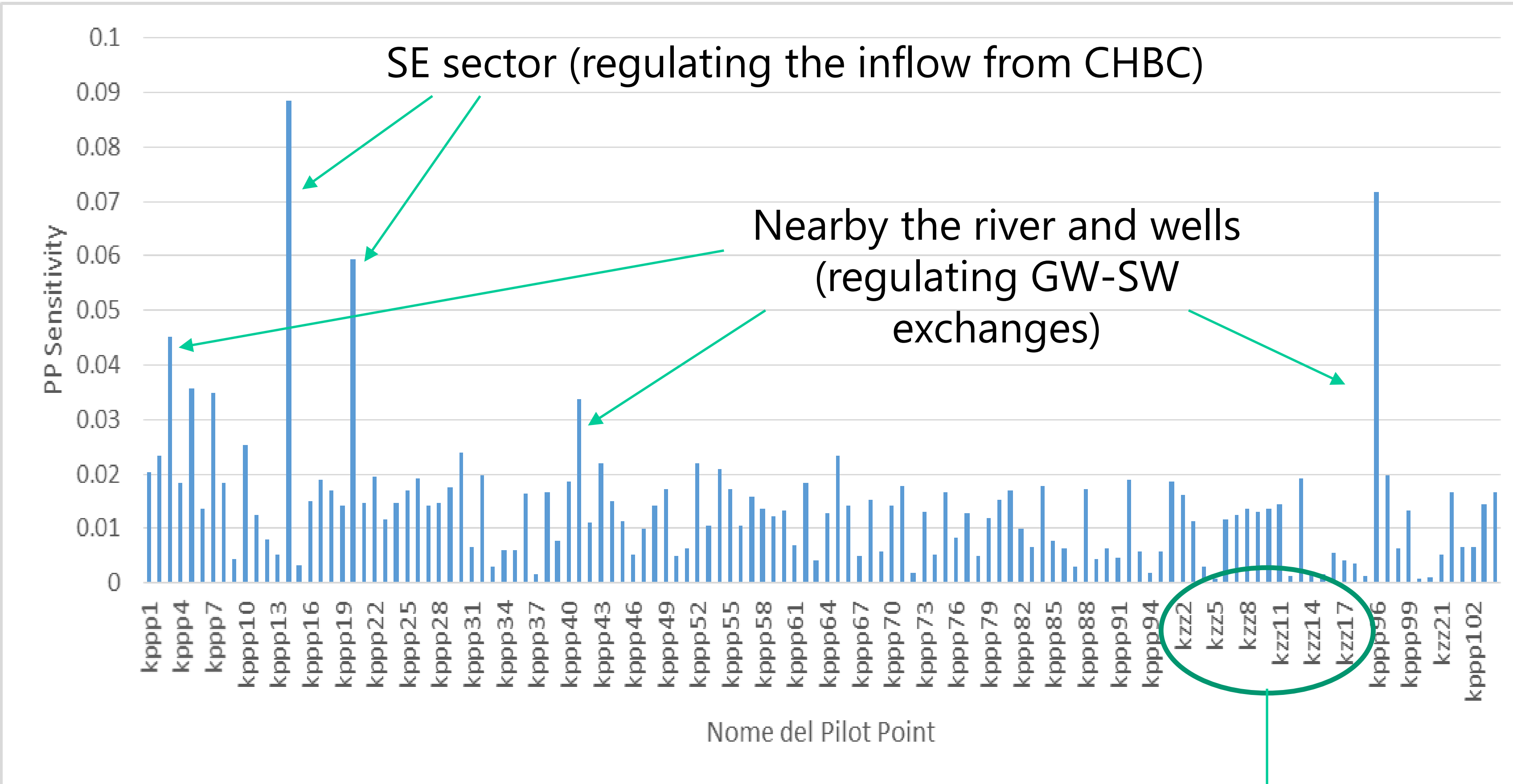








Contaminated site – Flow model – Sensitivity analysis



Relatively low sensitivities of Kz - L2 (usually high when continuous confining units are present)

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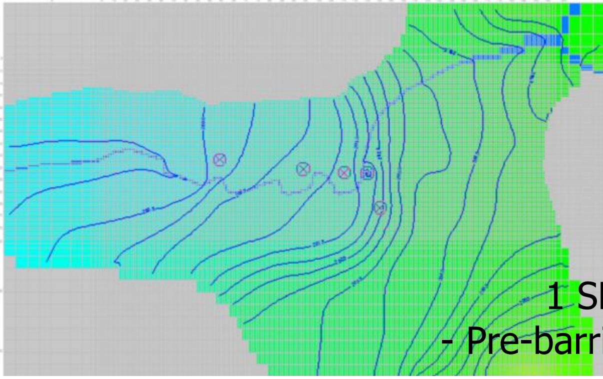
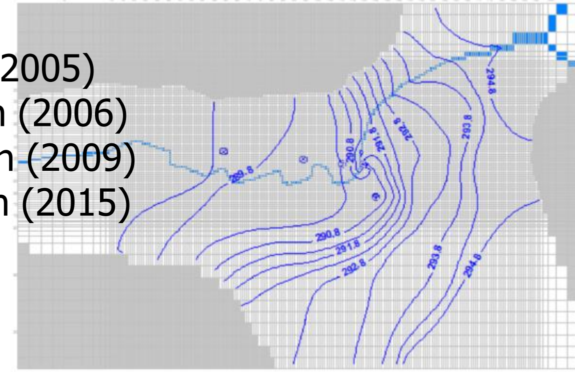
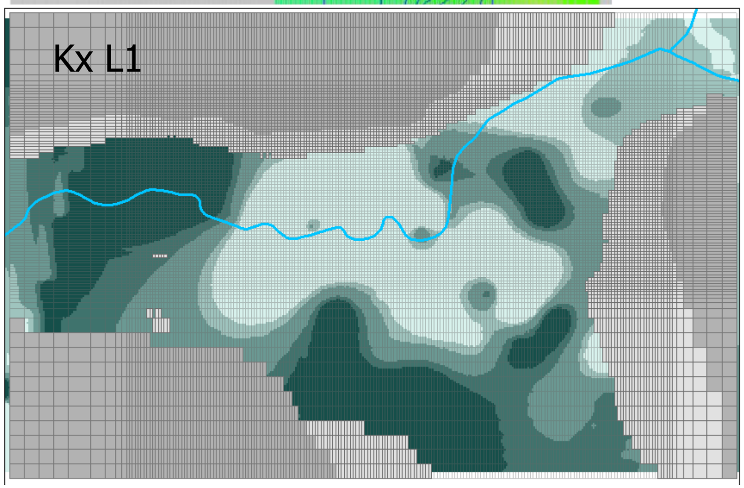
Contaminated site – Flow model – SS Calibrations

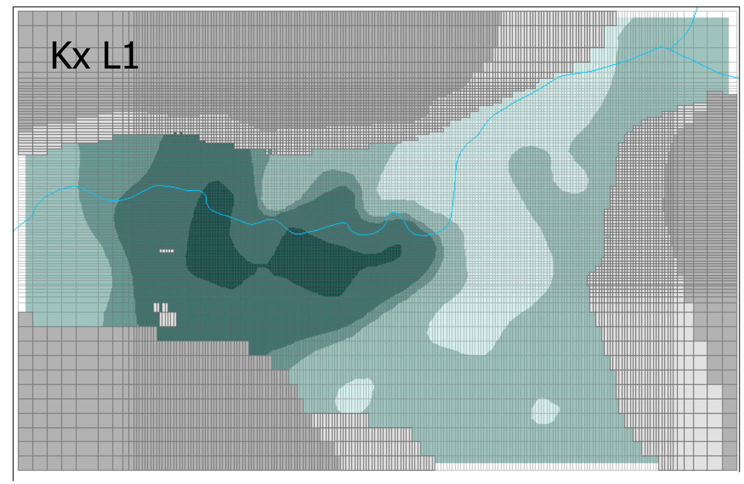


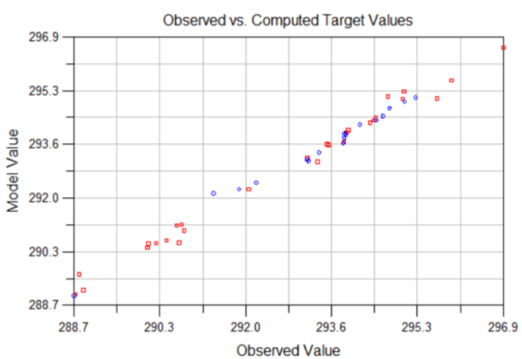
1 SP Steady State
- Pre-barrier conditions (2005)

4 SP Steady State
- Pre-barrier conditions (2005)
- 1st barrier configuration (2006)
- 2nd barrier configuration (2009)
- 3rd barrier configuration (2015)



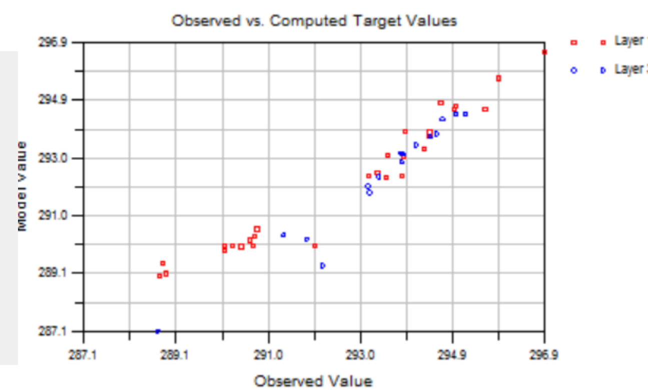




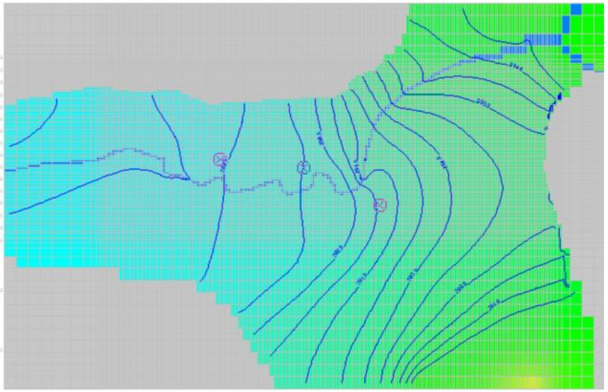


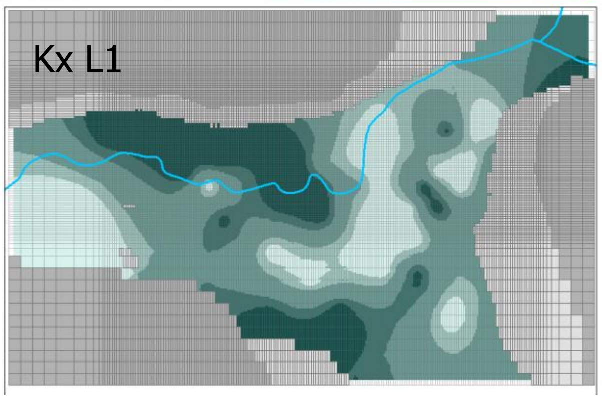
Residual Mean	= -0.09
Residual Standard Dev.	= 0.28
Absolute Residual Mean	= 0.22
Residual Sum of Squares	=3.86e+000
RMS Error	=0.29
Minimum Residual	= -0.86
Maximum Residual	= 0.61
Range of Observations	= 8.20
Scaled Res. Std. Dev.	= 0.034
Scaled Abs. Mean	= 0.027
Scaled RMS	= 0.036
Number of Observations	= 45

Residual Mean	= 0.69
Residual Standard Dev.	= 0.61
Absolute Residual Mean	= 0.75
Residual Sum of Squares	=3.84e+001
RMS Error	=0.92
Minimum Residual	= -0.63
Maximum Residual	= 2.82
Range of Observations	= 8.20
Scaled Res. Std. Dev.	= 0.074
Scaled Abs. Mean	= 0.092
Scaled RMS	= 0.113
Number of Observations	= 45



Contaminated site – Flow model – TS Calibration



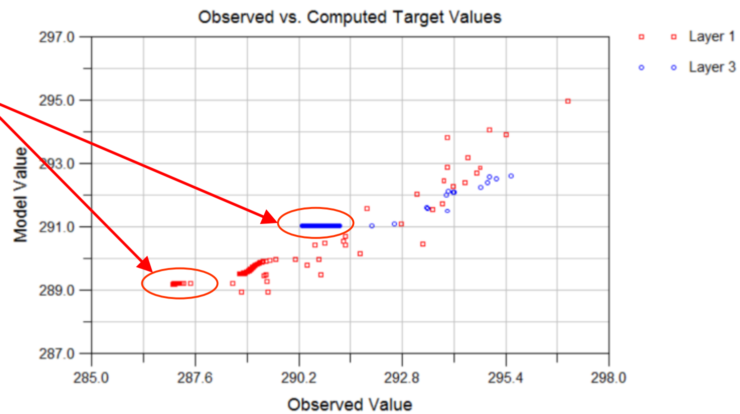


1 SP Steady State + 6 SP Transient State

- SS with active barrier
- 3 different pumping tests

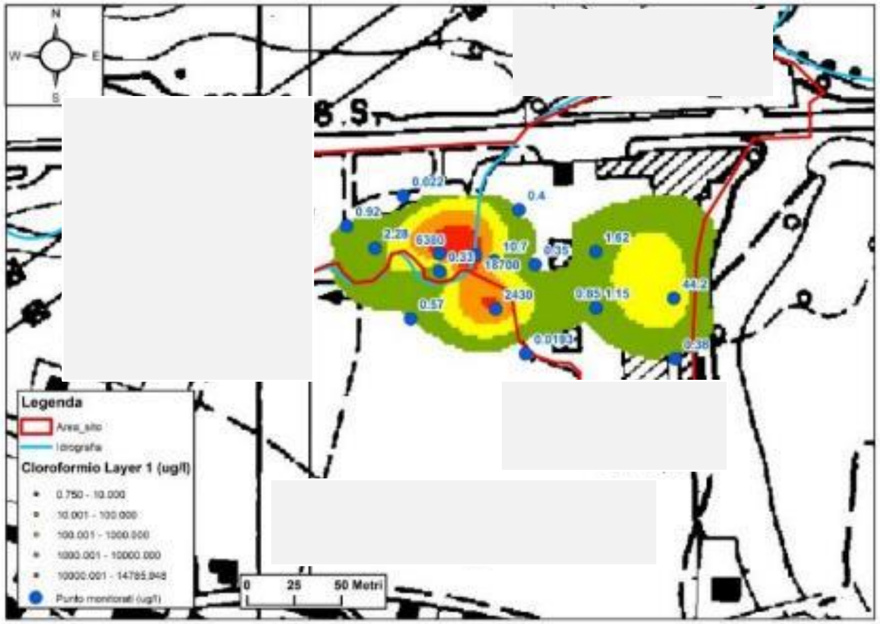
Stress Period	Lenght (s)	Incremental time (s)	Time steps	Pumping well	Flow rate (m^3/s)	Observation points
1	SS	SS	10	-	0	Heads/discharge 02/2005
2	165054	251460	100	BH1	-0.00014	Pz1
3	134676	386136	10	-	0	-
4	46284	432420	100	BH2	-0.00042	Pz2
5	86490	518910	10	-	0	-
6	75300	594210	100	BH3	-0.00032	Pz3
7	86400	680610	10	-	0	-

Pumping tests nearby the river

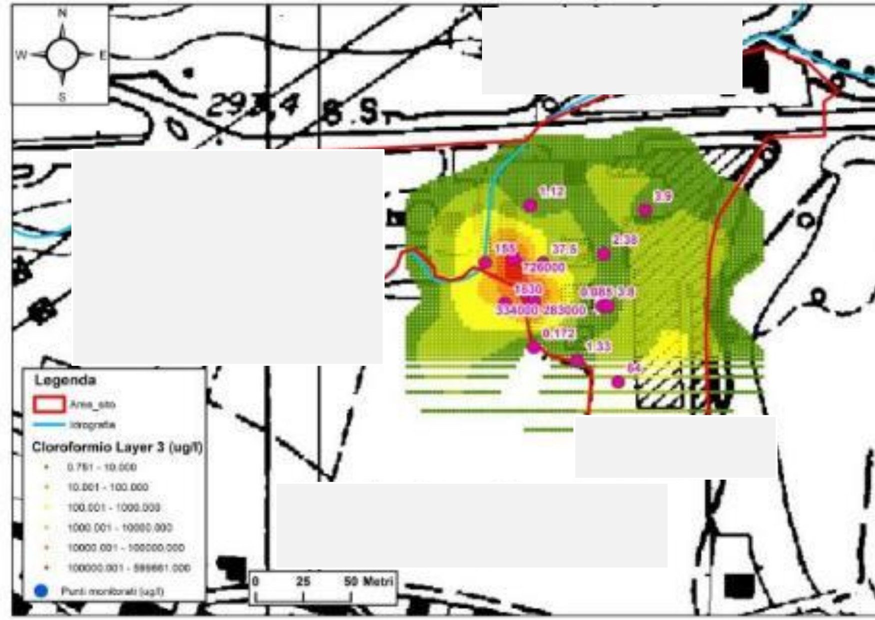


Residual Mean	= -0.60
Residual Standard Dev.	= 0.84
Absolute Residual Mean	= 0.81
Residual Sum of Squares	=8.64e+002
RMS Error	=1.03
Minimum Residual	= -2.18
Maximum Residual	= 2.92
Range of Observations	= 9.92
Scaled Res. Std. Dev.	= 0.084
Scaled Abs. Mean	= 0.081
Scaled RMS	= 0.104
Number of Observations	= 811

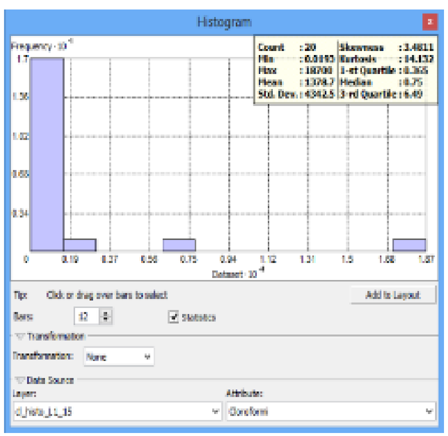
Contaminated site – Transport model



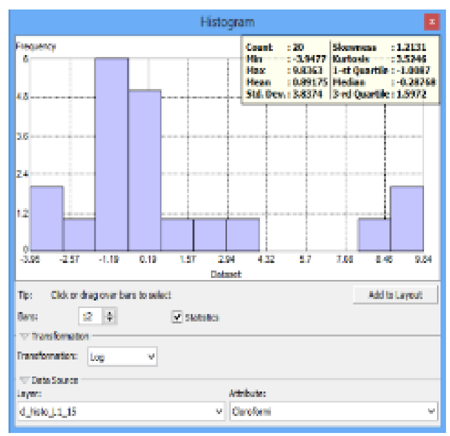
TCM spatial distribution L1



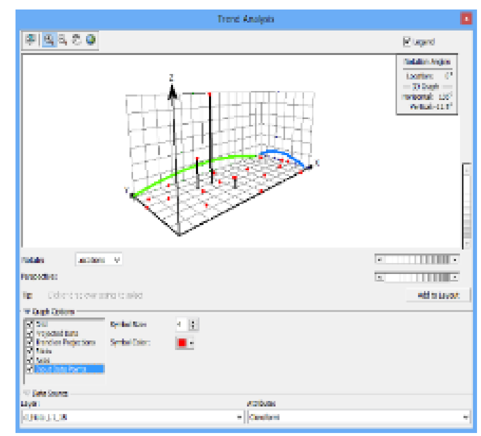
TCM spatial distribution L3



TCM conc histogram



Log of TCM conc

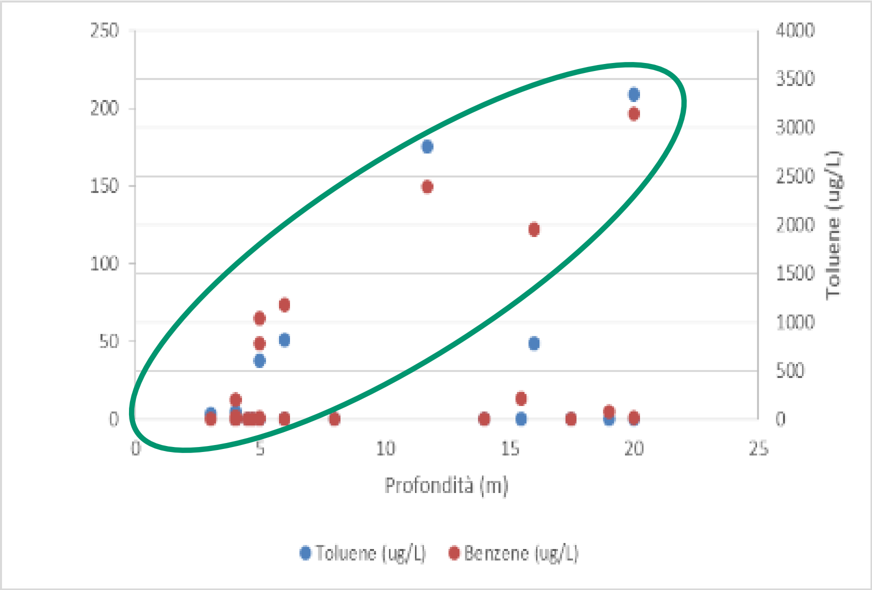


TCM trend analysis

Contaminated site – Transport model

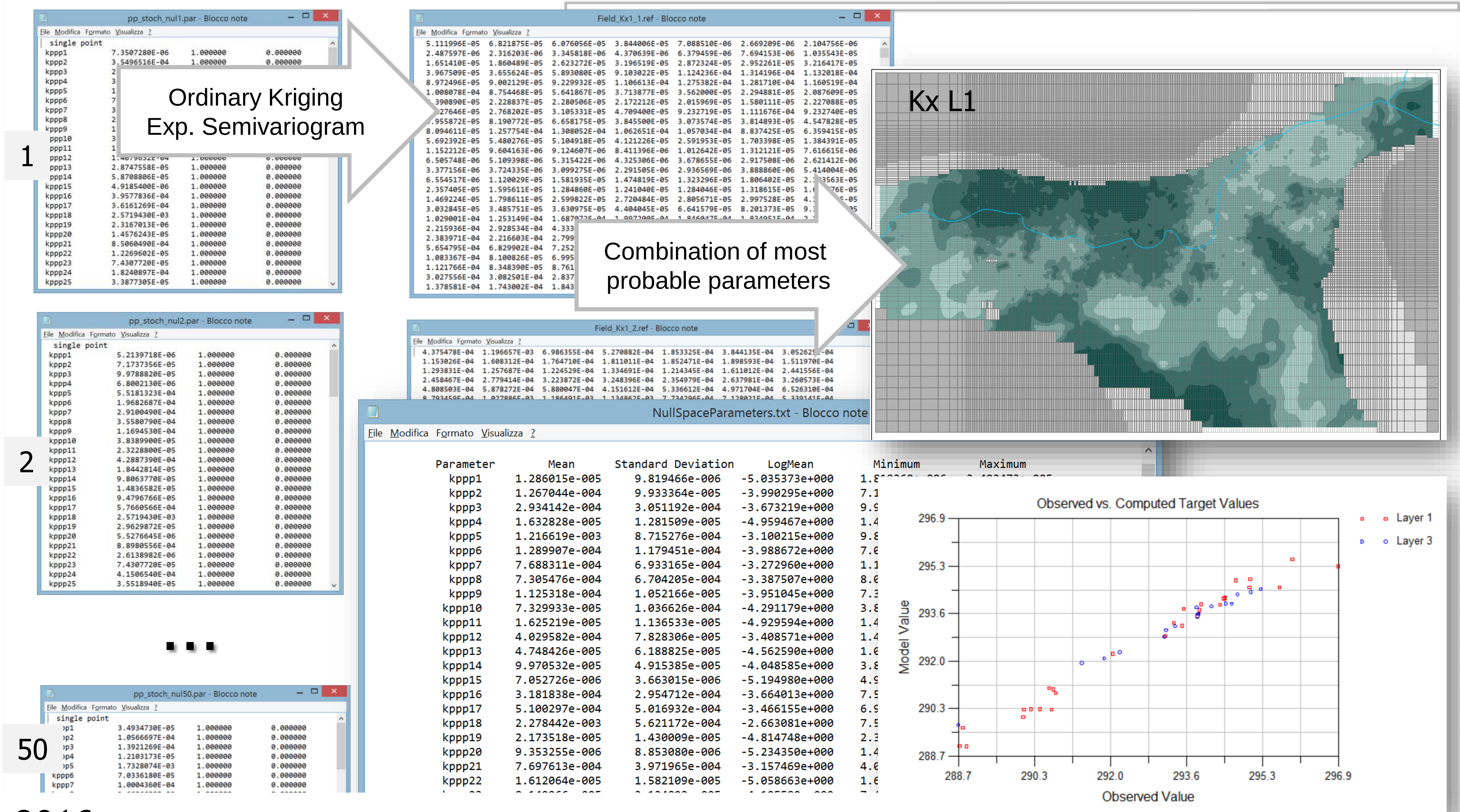
No way to calibrate concentration observations – supposed the presence of a "Diving plume" of Benzene and Toluene, even before the activation of the P&T (2005)

Possible causes:
- Stratigraphic control?
- Bevera River is locally/temporary a loosing stream?
- Existing production pumpings?
- Multicomponent D-NAPL?



Toluene and Benzene concentrations (2005) vs depth

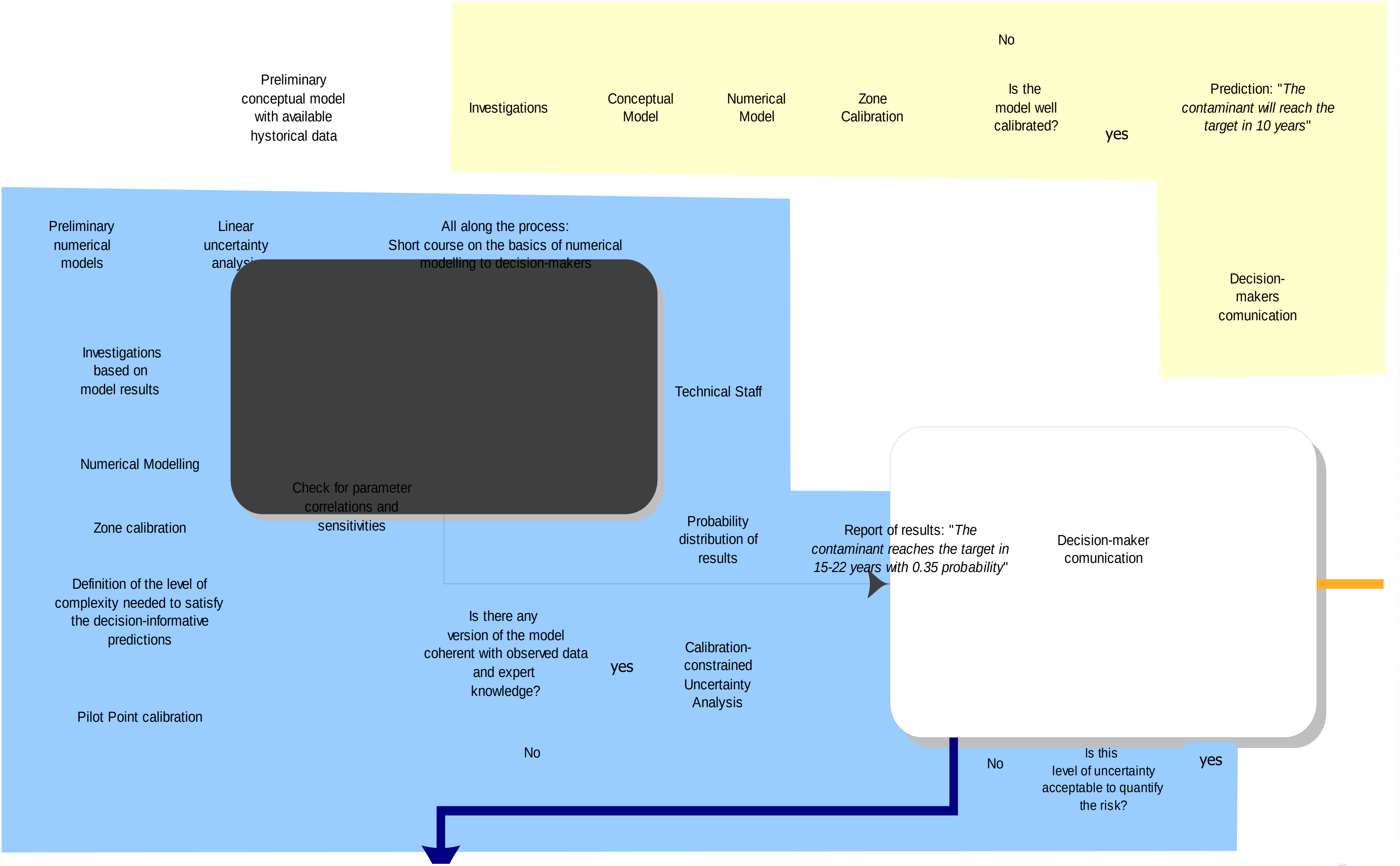
Contaminated site – Transport model – NSMC Calibration (50 realizations)



2016

- 3 new piezometers are drilled in the substratum depression;
- D-NAPL is found;
- New investigations are ongoing on the substratum degree of fracturing…

Remediating groundwater... NECM *vs* one of the widespread workflows



25-29th September 2016
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CORUM CONFERENCE CENTER
43rd IAH congress

Remediating groundwater… Conclusions

- Plume estimation and model constitute often distinct sequential phases: the second phase does not provide information to the first - total uncertainty is not accounted for properly.

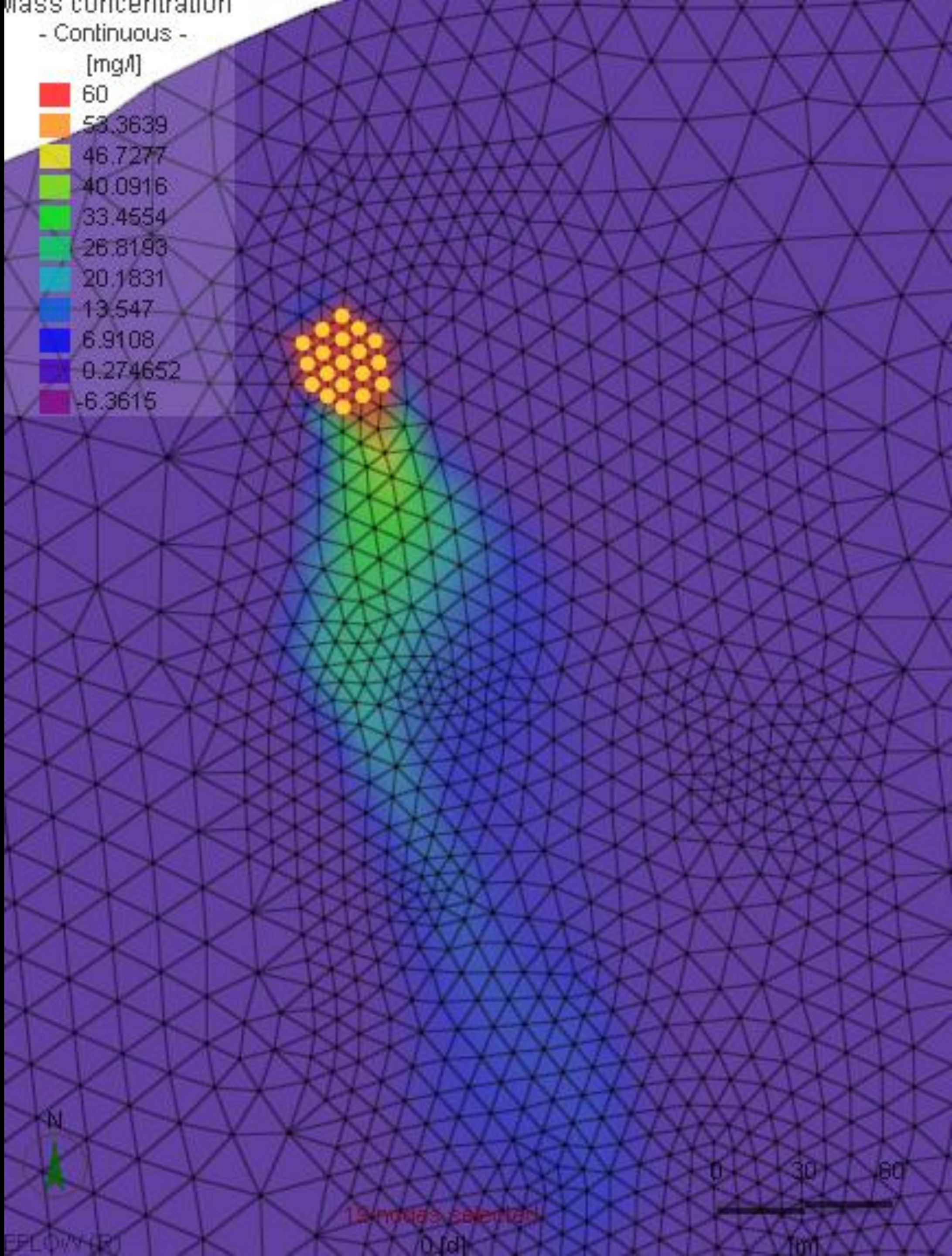
- Combination of the Principle of Parsimony, Highly parametrized inversion and NSMC can support a better understanding of the conceptual model and consequently the decision-making process.

- Modellers are required to understand the system, characterize numerically what they know and what they don't know, and explain to decision makers the risks associated with alternative actions, as these arise from an incomplete knowledge of the complex system which is being managed.

The ideal workflow is a kind of iterative pathway of increasing complexity. It only needs to get more complex when a reduction of uncertainty is required, up to when it won't be able to go further and the *irreducible uncertainty* must be declared. At that point management of the problem will necessarily have to be *adaptive*.

If models can serve these issues, then they will have served the decision-making process well, regardless of the goodness of the fit.

Thank you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