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WP 6 presentation

Hydrogeochemical modeling as support tool in control of remediation process

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National workshop in Romania

Rehabilitation of contaminated soil and sites

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Introduction

- **The aim is to improve In-situ chemical oxidation and reduction technologies of contaminated groundwater treatment with regard to time, cost and sustainability**
  - **The strategy: improve monitoring and its interpretation in order to adapt the remediation strategy through:**
  - **on-line and real time monitoring**
  - **modeling for better interpretation of the real time data and definition of site specific feedback instructions**
- **decision-making on further actions**
- **The results of real-time monitoring, periodical sampling and modelling to control the process and to improve the efficiency of the in-situ injection of an oxidant and reductant to the ground**

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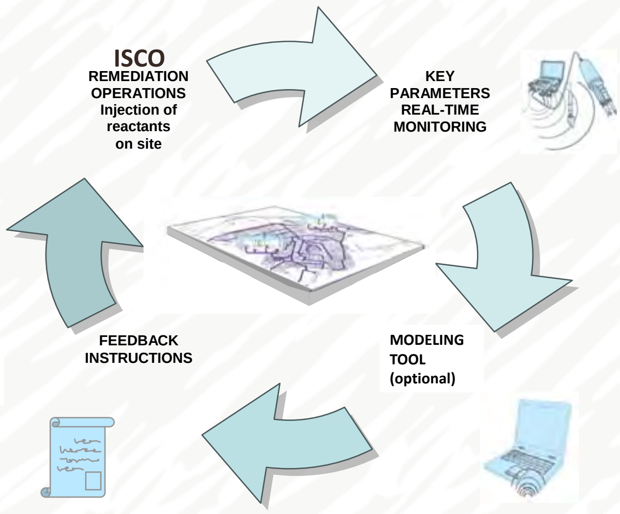
Decision making



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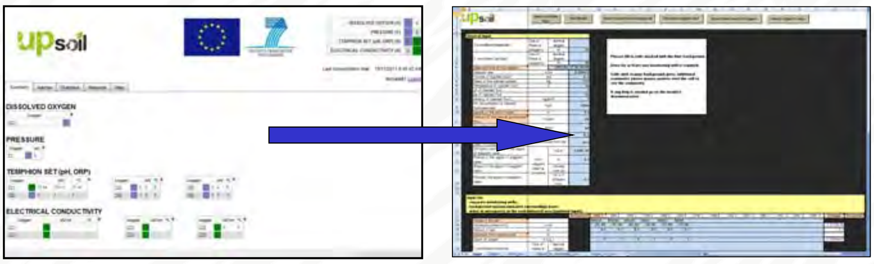
Modelling as suuportive tool

A numerical model has been developed (by IETU) in order to:

- Define an injection strategy
- Predict the remedial effect in time
- Provide a dynamic response => calibrations of model => improved prediction / decision making => optimized remediation

Real-time monitoring data is imported to the model:



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Basic monitoring data

Before injection:

- Installing loggers to porvide on-line data
- Lab tests using material (soil/groundwater) from the site
- Manual monitoring on site
- Definition of "threshold values" and initial feed back instructions

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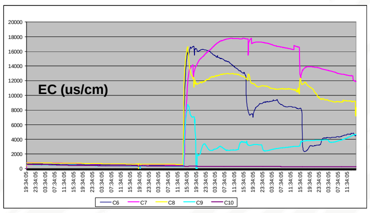
Monitoring data interpretation

Most feasible real-time data measuring include: pH, K, DO, R and T

Parameter	Permanganate	Percarbonate	Persulphate	Fentons	ZVI
pH	≈	↑	↓	↓	↑
T	↑ detectable?	?	↑ detectable?	↑	≈
EC	↑	↑	↑	↑	≈
ORP	↑	↓(<pH ↑)	↑	↑	↓
DO	≈	↑	≈	↑	↓

Changes in the physical parameters for different oxidants and reductants measured bz real time loggers



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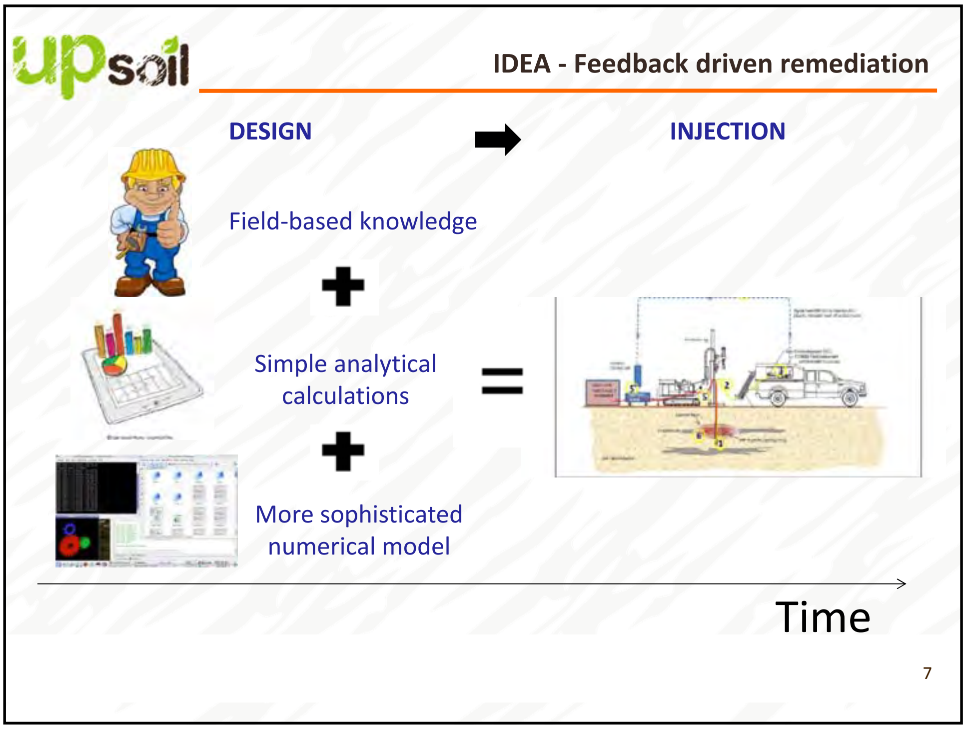
IDEA - Feedback driven remediation
DESIGN
INJECTION
Field-based knowledge
Simple analytical calculations
More sophisticated numerical model
Time
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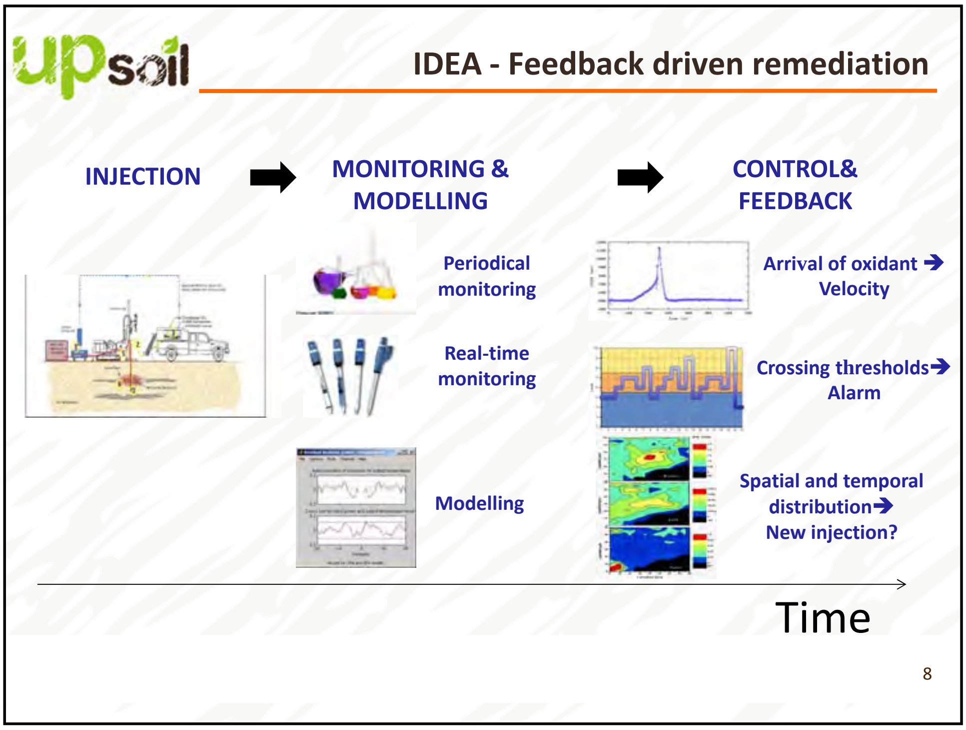
IDEA - Feedback driven remediation
INJECTION
MONITORING & MODELLING
CONTROL& FEEDBACK
Periodical monitoring
Real-time monitoring
Modelling
Arrival of oxidant → Velocity
Crossing thresholds→ Alarm
Spatial and temporal distribution→ New injection?
Time
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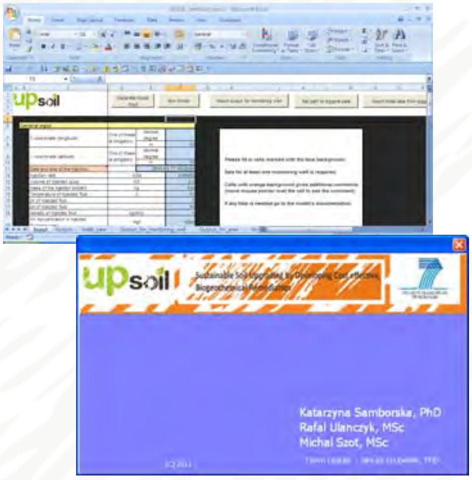
Modeling Tool Requirements



- ✓ Filling necessary data in the spreadsheet named "input" (cells to be filled in are clearly marked)
- ✓ Setting a path to the real-time monitoring data
- ✓ Importing initial conditions based on loggers data
- ✓ Preparing file for geochemical module

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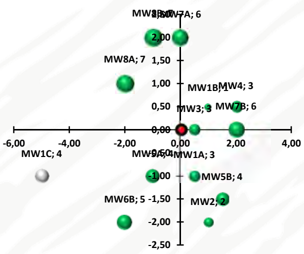
Modeling Tool – Feasibilities

Simple Analytical Calculations Based on Mathematical Expressions

		Well 1
Radius of infuence / Total flow path in model	m	0.901091
Total bulk treatment volume	m3	12.74784
Maximal concentration of oxidant	mg/l	83653.85
Volume of Oxidant	m3	4.461744
Mass of porous media	kg	21671.33
Volume oxidant must be delivered	L	4461.744
Dose of oxidant	mg/Kg	17222.85
Effective porosity, usually 10 to 48% smaller than porosity	[max]	0.315
	[min]	0.182
Pressure		203.8902
Velocity of water for max effective porosity	m/s	0.000154
Velocity of water for min effective porosity	m/s	0.000267
pe of groundwater		1.580366
Time of reaching the ROI for max effective porosity	s	5834.622
Time of reaching the ROI for min effective porosity	s	3371.115
Number of wells for max effective porosity	-	25.49005
Numbers of wells for min effective porosity	-	44.1174



Visualization of Monitoring (Green) and Injection (Red) Wells With The Spherical Image of Screens

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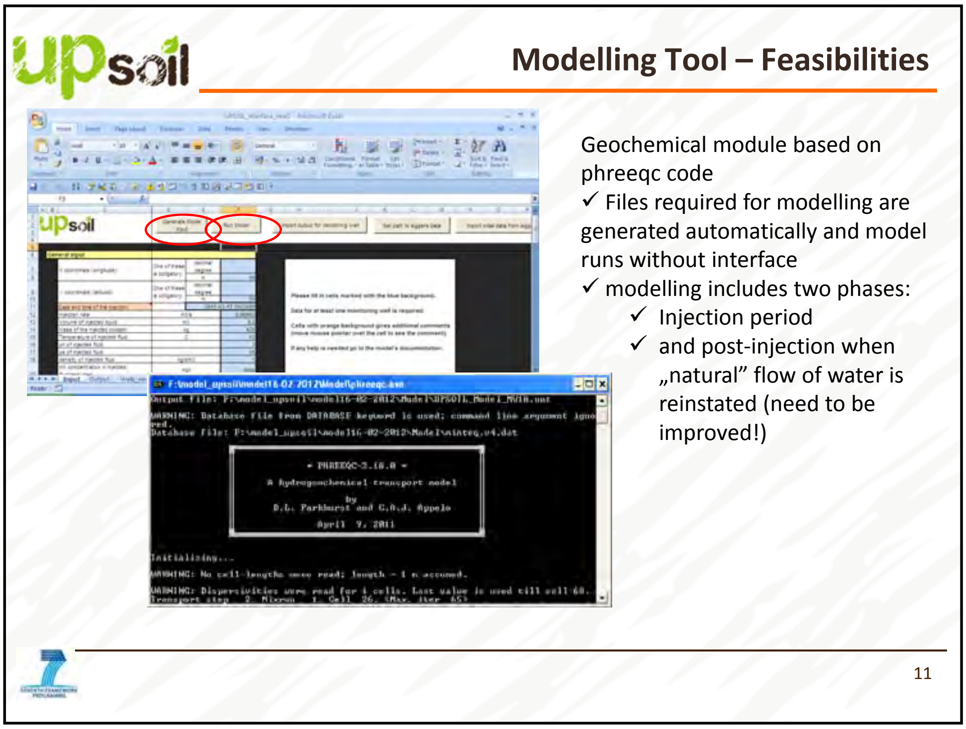
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Modelling Tool – Feasibilities
Geochemical module based on phreeqc code
✓ Files required for modelling are generated automatically and model runs without interface
✓ modelling includes two phases:
✓ Injection period
✓ and post-injection when „natural" flow of water is reinstated (need to be improved!)
PHREEQC-2.18.0
A hydrogeochemical transport model
by
D.L. Parkhurst and C.A.J. Appelo
April 7, 2011
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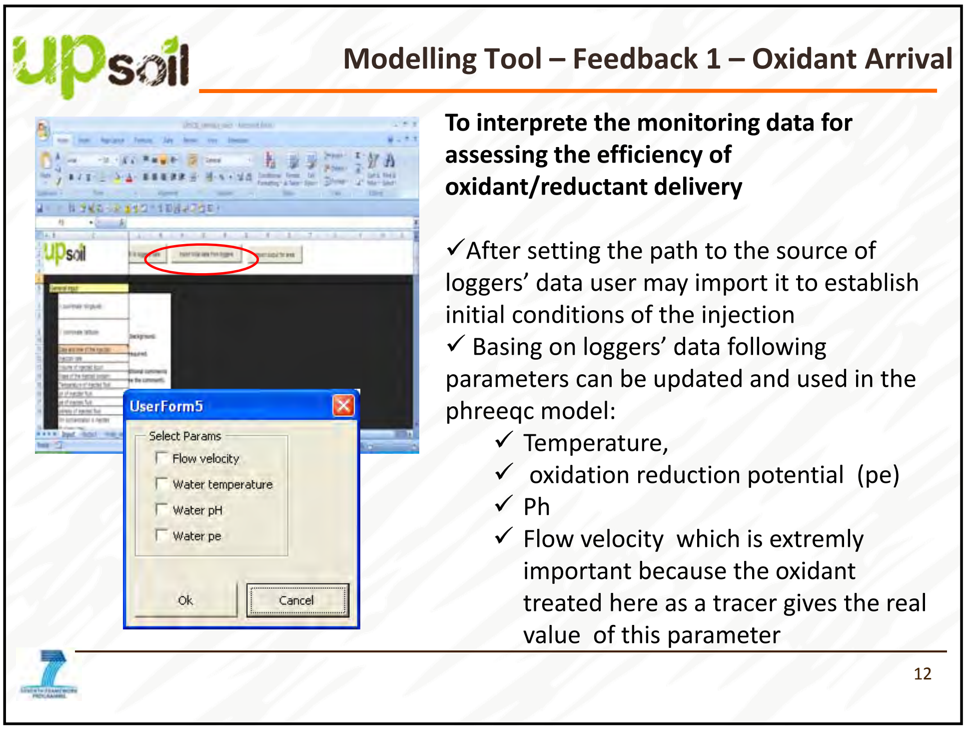
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Modelling Tool – Feedback 1 – Oxidant Arrival
To interprete the monitoring data for assessing the efficiency of oxidant/reductant delivery
✓After setting the path to the source of loggers' data user may import it to establish initial conditions of the injection
✓ Basing on loggers' data following parameters can be updated and used in the phreeqc model:
✓ Temperature,
✓ oxidation reduction potential (pe)
✓ Ph
✓ Flow velocity which is extremly important because the oxidant treated here as a tracer gives the real value of this parameter
UserForm5
Select Params
Flow velocity
Water temperature
Water pH
Water pe
Ok
Cancel
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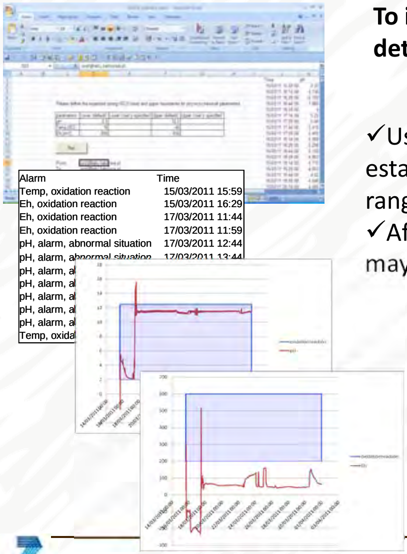
Modelling Tool – Feedback 2 – Alarm



To interprete the monitoring data for detecting unexpected process developments

✓User may incorporate his own data for establishing the oxidation conditions or approve ranges

✓After running this part of the model the user may obtain:

- ✓ 1. Table report with time and the description of the event
- ✓ 2. Charts with the detailed temporal changes in parameters with the highlightning of the oxidation conditions
- ✓ 3. E-mail in case of the alamr situation

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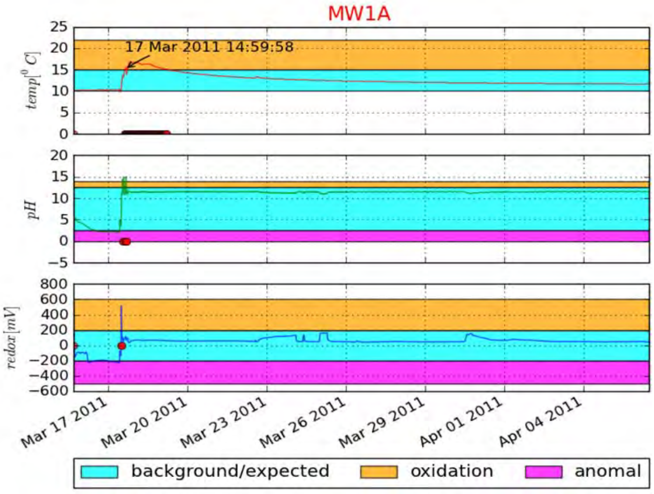
Interpretation of real-time measuring



The Flanders case study real monitoring data analysis

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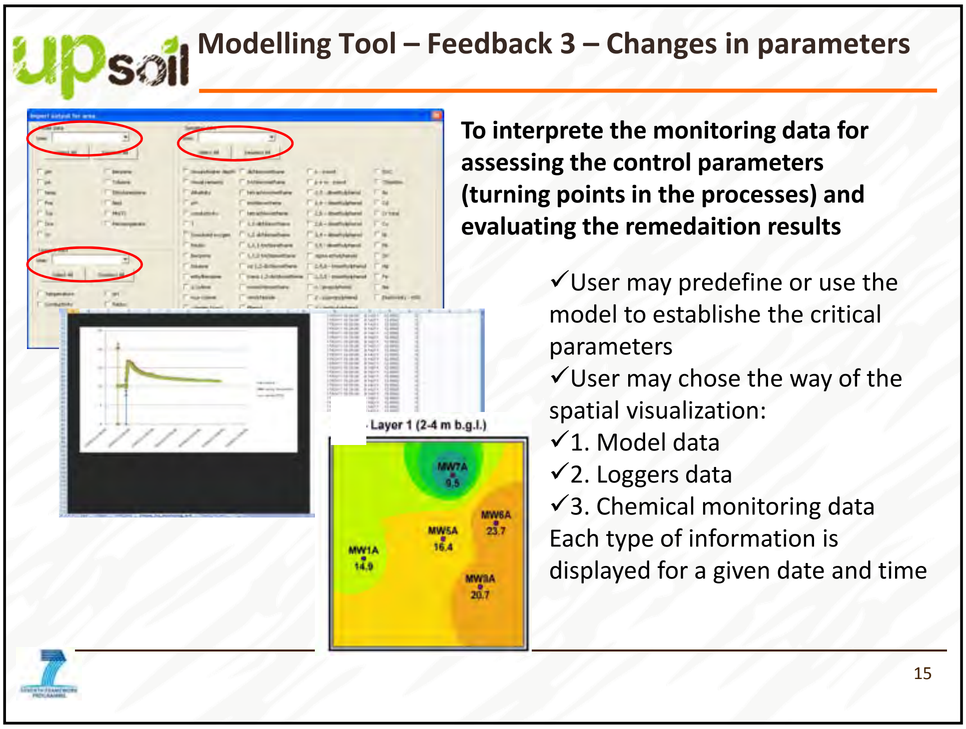
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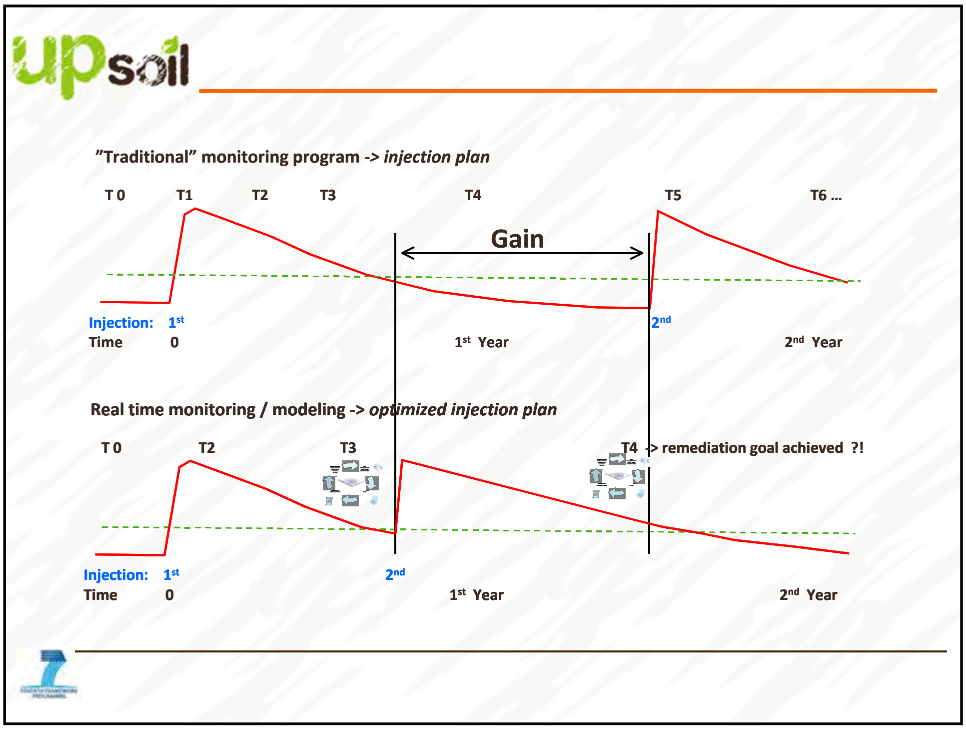
Modelling Tool – Feedback 3 – Changes in parameters
To interprete the monitoring data for assessing the control parameters (turning points in the processes) and evaluating the remedaition results
✓User may predefine or use the model to establishe the critical parameters
✓User may chose the way of the spatial visualization:
✓1. Model data
✓2. Loggers data
✓3. Chemical monitoring data
Each type of information is displayed for a given date and time
Layer 1 (2-4 m b.g.l.)
MW7A
9.5
MW6A
23.7
MW5A
16.4
MW1A
14.9
MW3A
20.7
15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"Traditional" monitoring program -> injection plan
T 0
T1
T2
T3
T4
T5
T6 ...
Gain
Injection: 1st
2nd
Time 0
1st Year
2nd Year
Real time monitoring / modeling -> optimized injection plan
T 0
T2
T3
T4
> remediation goal achieved ?!
Injection: 1st
2nd
Time 0
1st Year
2nd Year

MODELLING TOOL – IMPROVMENT AND FURTHER DEVELOPMENTS

Further developments:

- ✓ Coupling geochemical module and phases (injection and post-injection)
- ✓ Feedback concerning the risk of releasing metals as part of the modelling tool - new freeware phreeplot to estimate physical and chemical conditions which are favorable for leaching of heavy metals
- ✓ Developing predefined contaminat and remediaiton agent specific predefined modeling modules.
- ✓ Incorporating desorption module for modeling release of adsorbed contaminants e.g. hydroccarbons

Improvements:

- ✓ Comparing modelling and monitoring data,
- ✓ Testing the data on different sites but in similar conditions of the injection (permanganate – oxidant, BTEX and CAH) Testing alarm system for real-time collected data

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- Thank you for attention