Software for the Assessment of NAPL Distribution in Aquifer: OREOS

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Framework

- Pollution assessment studies always include soil sampling and analysis

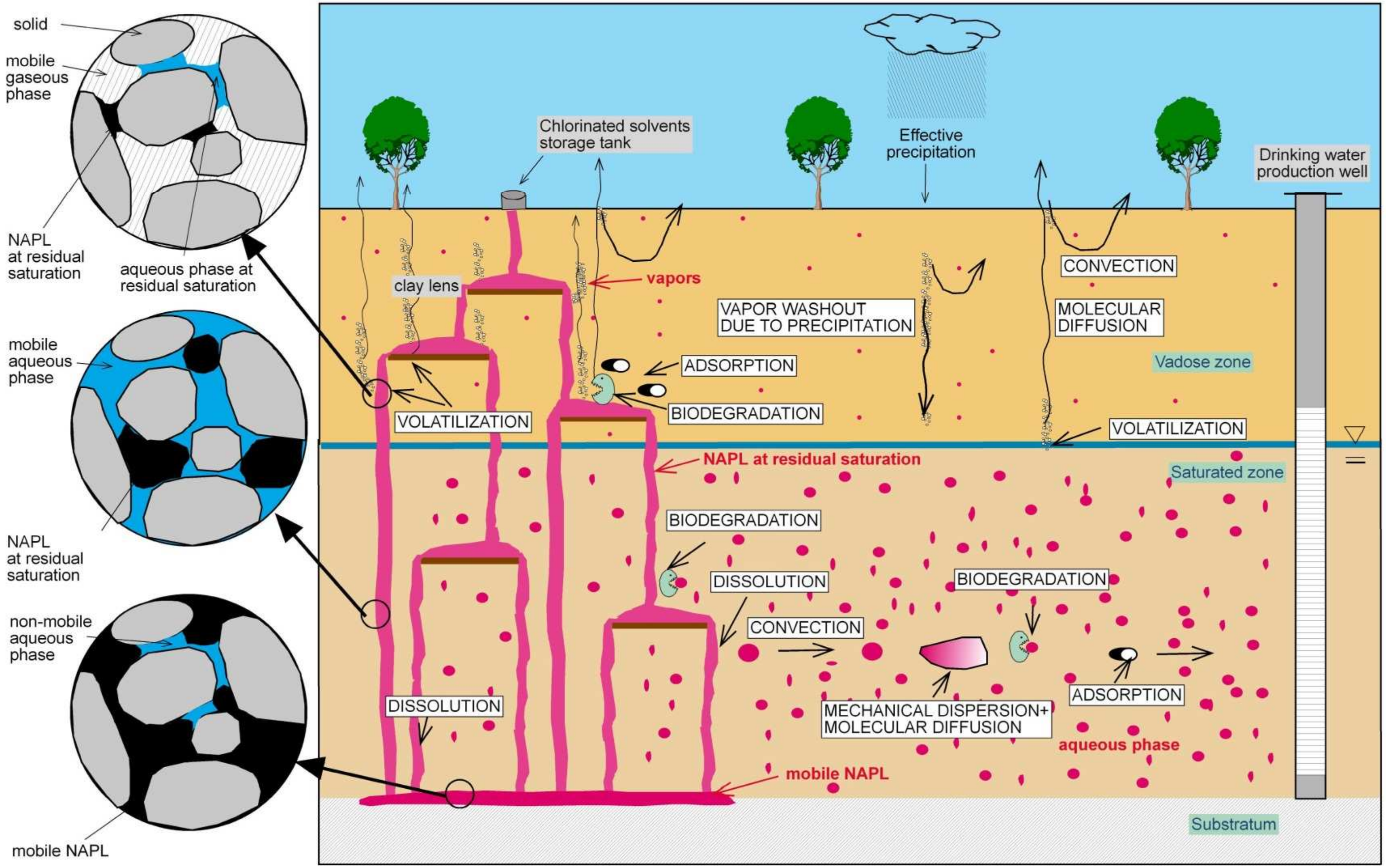
Sample		DW	Petroleum Hydrocarbons (mg/kg DW)										
		%	MeC5-C8	>C8-C10	C10-C12	C12-C16	C16-C20	C20-C24	C24-C28	C28-C32	C32-C36	C36-C40	**Sum**
SC40	0.5	90	<1,0	<1,0	0.03	0.94	1.80	5.78	10.17	13.05	13.41	9.92	55.1
SC82	0.5	92.3	<1,0	<1,0	0.76	6.36	3.63	7.22	14.40	18.34	18.27	3.72	72.7
SC49	0.7	83.3	<1,0	<1,0	0.26	1.51	4.95	10.67	15.62	20.06	21.59	16.34	91.0
SC91	0.8	66	<1,1	<1,1	1.24	1.43	3.59	7.10	8.61	11.60	9.71	4.42	47.7
SC47	0.9	63.9	<1,0	<1,0	2.53	3.71	5.70	8.49	12.49	19.56	26.67	7.74	86.9
SC60	0.9	92.2	<1,0	<1,0	17.35	38.07	34.78	38.57	73.06	79.81	73.89	61.47	417.0
SC69	0.												
SC73	0.												
SC48	1.												

Chlorinated Aliphatic Hydrocarbons (mg/kg DW)															
PCE	TCE	Cis-DCE	1,1-DCE	Trans-DCE	CV	HCA	PeCA	1,1,1,2-PCA	1,1,2,2-PCA	1,1,1-TCA	1,1,2-TCA	1,1-DCA	1,2-DCA	CA	**Sum**
48.9	11.1	0.33	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	60.3
20	0.477	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	20.5
0.808	0.242	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	1.1
3.43	<0,050	<0,10	<0,10	<0,10	<0,022	<0,23	<0,23	<0,10	<0,23	<0,10	<0,23	<0,10	<0,050	<2,3	3.4
<0,050	<0,050	<0,10	<0,10	<0,10	0.115	<0,24	<0,24	<0,10	<0,24	<0,10	<0,24	0.22	<0,050	<2,4	0.3
3000	119	1.59	<0,10	<0,10	0.053	<0,20	<0,20	<0,10	<0,20	0.55	<0,20	<0,10	<0,050	<2,0	3121.2
6.43	0.088	<0,10	<0,10	<0,10	<0,021	<0,21	<0,21	<0,10	<0,21	<0,10	<0,21	<0,10	<0,050	<2,1	6.5
<0,051	<0,051	<0,10	<0,10	<0,10	<0,025	<0.25	<0.25	<0.10	<0.25	<0.10	<0.25	<0.10	<0.051	<2.5	0.0
[illegible]	,050	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	<2,0
[illegible]	46	0.84	<0,10	<0,10	0.035	0.49	<0,20	<0,10	<0,20	2.69	<0,20	<0,10	<0,050	<2,0	30355.7
[illegible]	157	<0,15	<0,15	<0,15	<0,038	<0,38	<0,38	<0,10	<0,38	<0,15	<0,38	<0,15	<0,076	<3,8	2.6
[illegible]	.13	21.1	<0,10	0.11	2.03	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	44.5
[illegible]	321	0.22	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	11.8
[illegible]	,050	0.24	<0,10	<0,10	0.068	<0,22	<0,22	<0,10	<0,22	<0,10	<0,22	<0,10	<0,050	<2,2	0.3
[illegible]	06	<83,9	<0,10	<0,10	<0,021	<0,21	<0,21	<0,10	<0,21	1.38	<0,21	<0,10	<0,050	<2,1	2497.4
[illegible]	,788	<1,58	<1,58	<1,58	<0,394	<3,94	<3,94	<0,79	<3,94	<1,58	<3,94	<1,58	<0,788	<39,4	<LQ
[illegible]	252	8.22	<0,10	0.15	<0,021	4.21	<0,21	<0,10	0.7	<0,10	<0,21	<0,10	<0,050	<2,1	1087.3
[illegible]	0,05	<0,10	<0,10	<0,10	<0,02	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,05	<2,0	<2,0
[illegible]	063	0.14	<0,10	<0,10	<0,021	<0,21	<0,21	<0,10	<0,21	<0,10	<0,21	<0,10	<0,050	<2,1	0.3
[illegible]	,050	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	0.1
[illegible]	400	1580	4.52	1.41	78.3	<0,47	<0,47	<0,10	<0,47	80.8	<0,47	6.3	<0,094	<4,7	9281.3
[illegible]	115	85.2	<0,10	<0,10	0.041	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	0.15	<0,050	<2,0	86.2
[illegible]	334	0.17	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	23.9
[illegible]	,050	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	0.0
[illegible]	175	2.17	0.56	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0
<0,050	<0,050	<0,10	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	<2,0

- But, how does one interpret (read) these results ?
  - in the absence of reference concentrations
  - in a risk based site management framework
  - for source delineation and NAPL quantity estimation

Behavior of organic contaminants in soils

Migration and fate of chlorinated solvents in the subsurface



Natural attenuation of chlorinated solvents in aquifers, technical guide, MACOH R&D Project (2001-2006), ADEME

http://www2.ademe.fr/servlet/KBaseShow?sort=-1&cid=96&m=3&catid=10143

In each soil sample, one may ask …

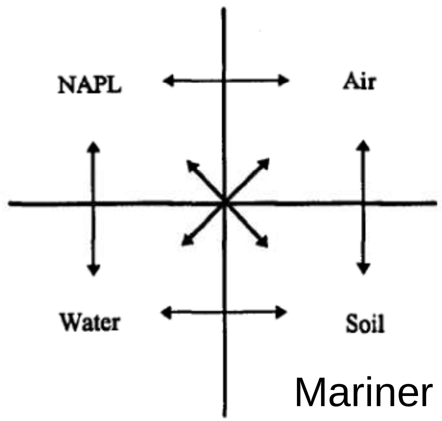
- Is NAPL present ?
- If so, how much (i.e. NAPL saturation) ?
- If so, is the NAPL mobile (Snapl > Sor) ?
- How do contaminants distribute in soil phases (NAPL, water, gas, solid) ?
- What is the composition of each phase ?

The **OREOS** software adresses these questions

ORganic contaminant
Evaluation and NAPL
Occurrence assessment in
Soils

Theoretical background

- A set of equations solved by a non linear solver
  - 3 phases (saturated zone) or 4 phases (unsaturated zone) equilibria for multicomponent mixture (Raoult's law …)
  - Equations of state for each phase (ideal mixture assumption)
  - Mass balances



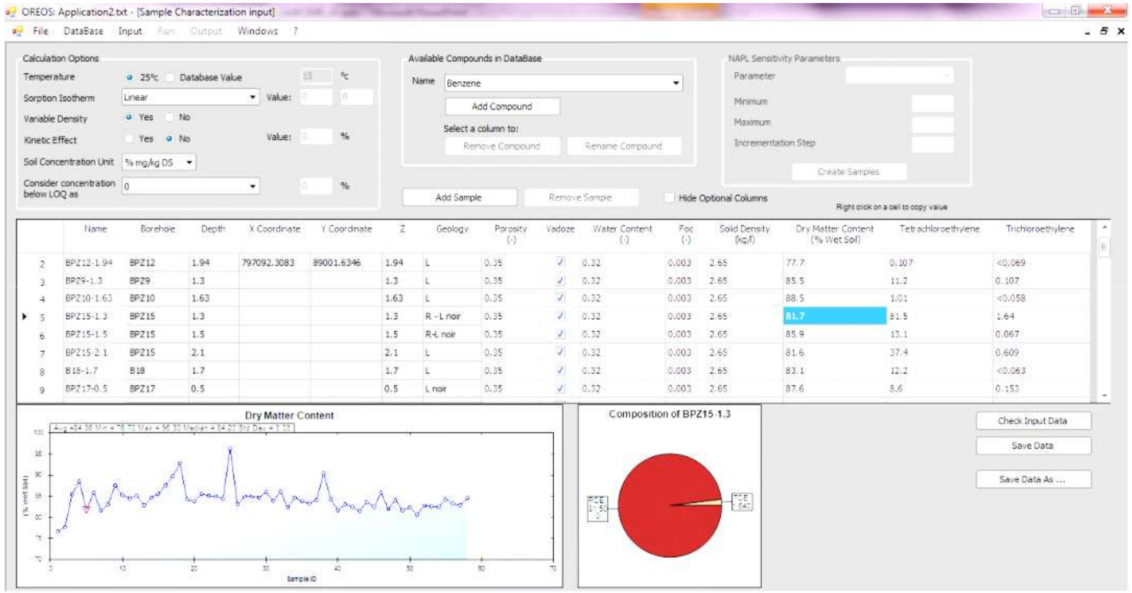
Mariner et al.,1997

- Two specific features
  - Temperature effect on contaminants physico-chemical parameters
  - Kinetic effect due to heterogeneities of soil properties and pollution spatial distribution

Software architecture (1)

BURGEAP

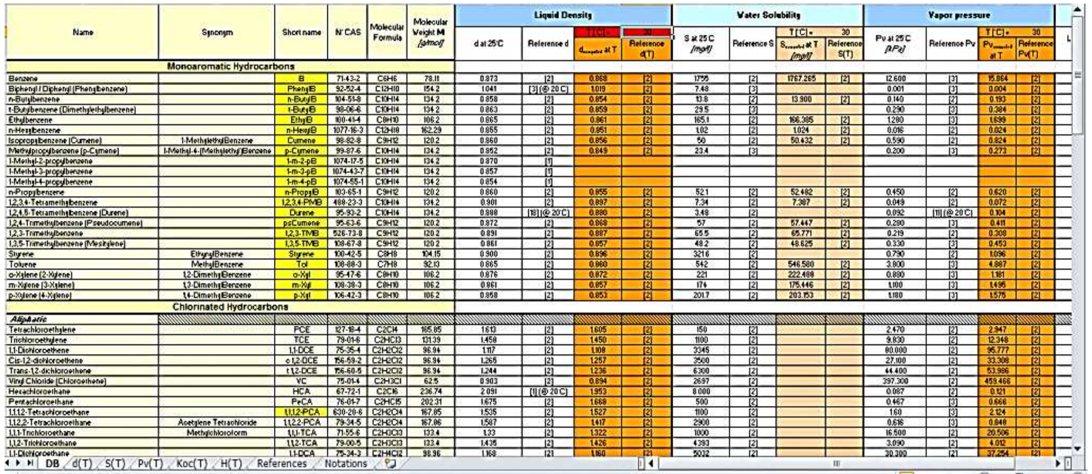
Input - samples characterization and sensitivity analysis



- Data preparation through an interface
- Contaminant concentrations & soil properties
- Import/export input data from/to a spreadsheet
- Treat many (>1000) samples simultaneously
- Statistical analysis over samples

+

Database of physico-chemical parameters



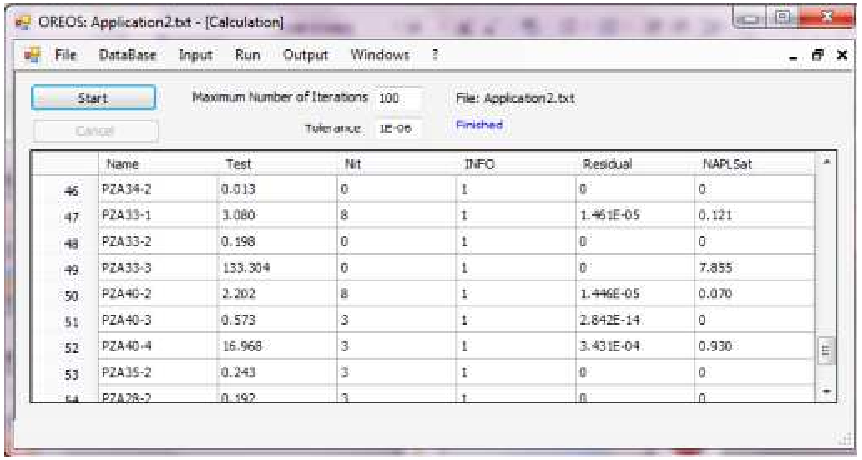
- Database of 137 components (monoaromatic hydrocarbons, chlorinated hydrocarbons, TPH, alkanes, PAH, MTBE …)
- Molecular Weight, Density, Solubility, Vapor Pressure, Henry constant, Koc
- Temperature correlations for most components
- Open format to allow modifications and appendings

Software architecture (2)

Sample Input + Component Database

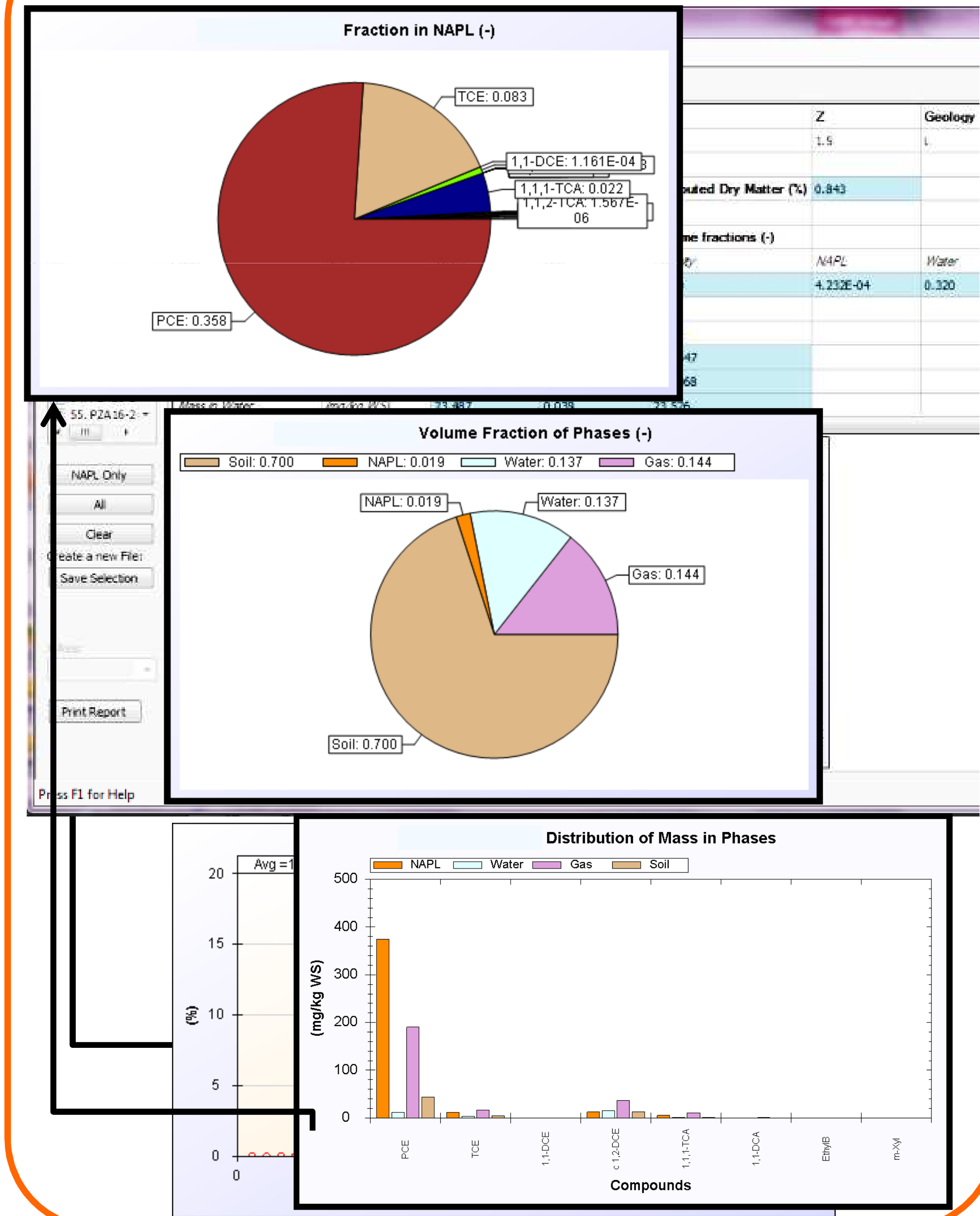
↓

Run window



- **Numerical parameters: iterations, tolerance …**
- **Run report: residual, warnings …**

Ouput window – result and analysis tool



- **Table of results**
- **Statistical analysis**
- **Visualisation of results with graphics and pie charts**
- **Export to a spreadsheet**

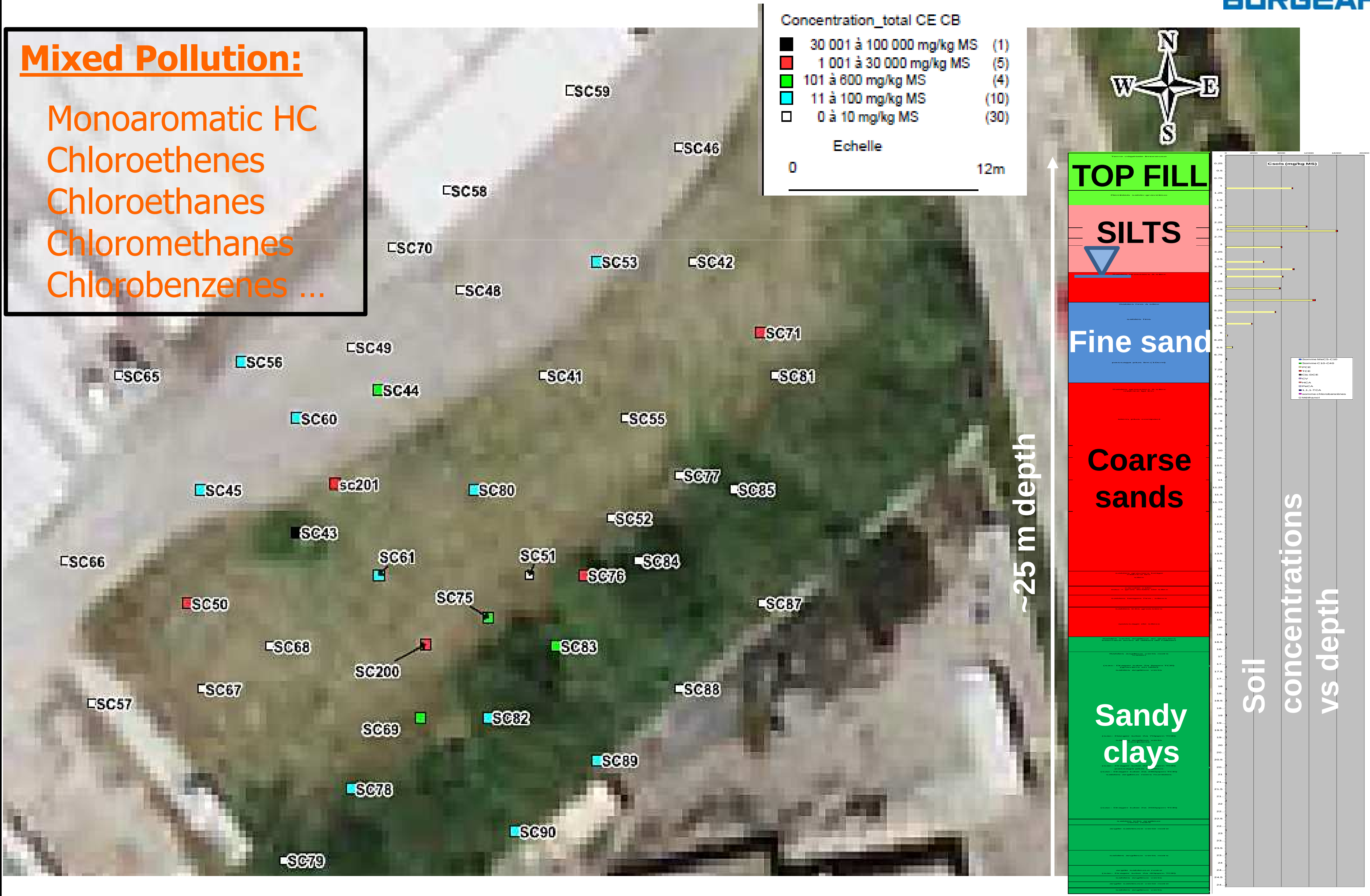
Example: source characterization

Example : soil concentrations analysis

BURGEAP

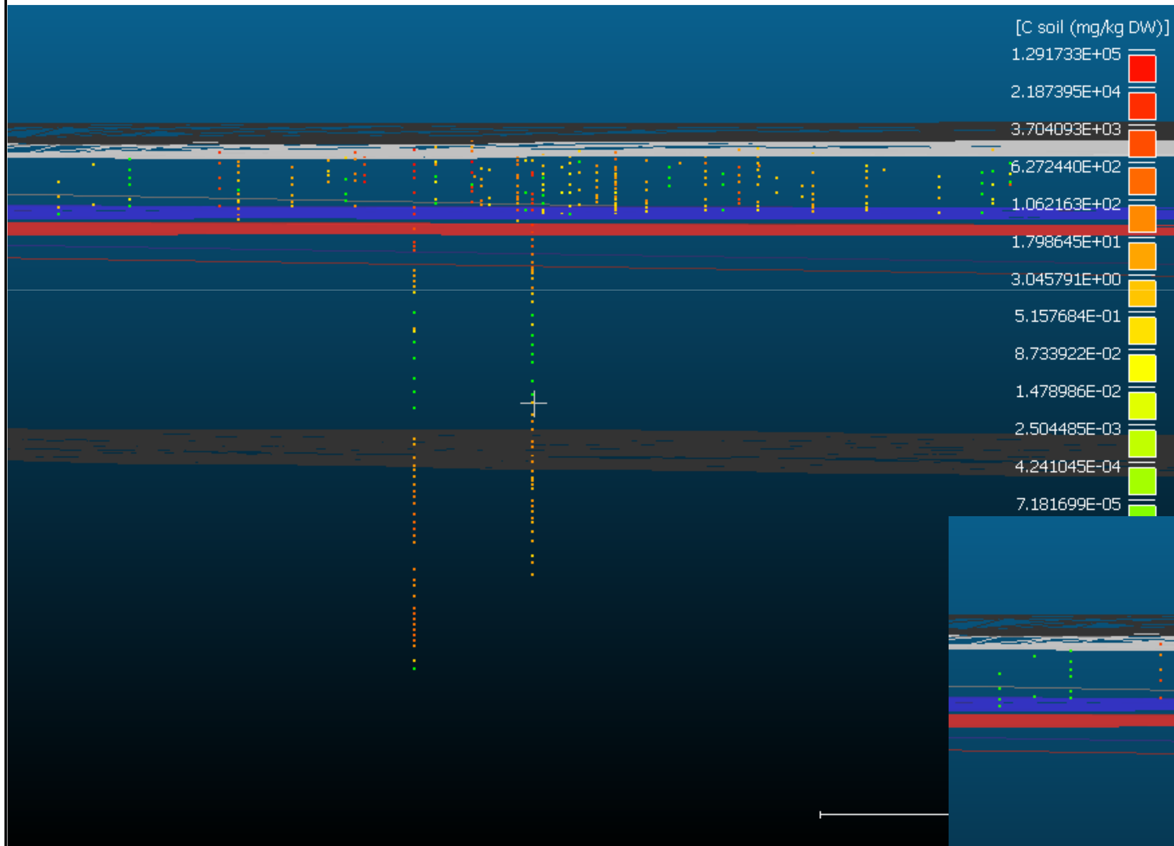
Mixed Pollution:

Monoaromatic HC
Chloroethenes
Chloroethanes
Chloromethanes
Chlorobenzenes …



Example : compute NAPL saturations

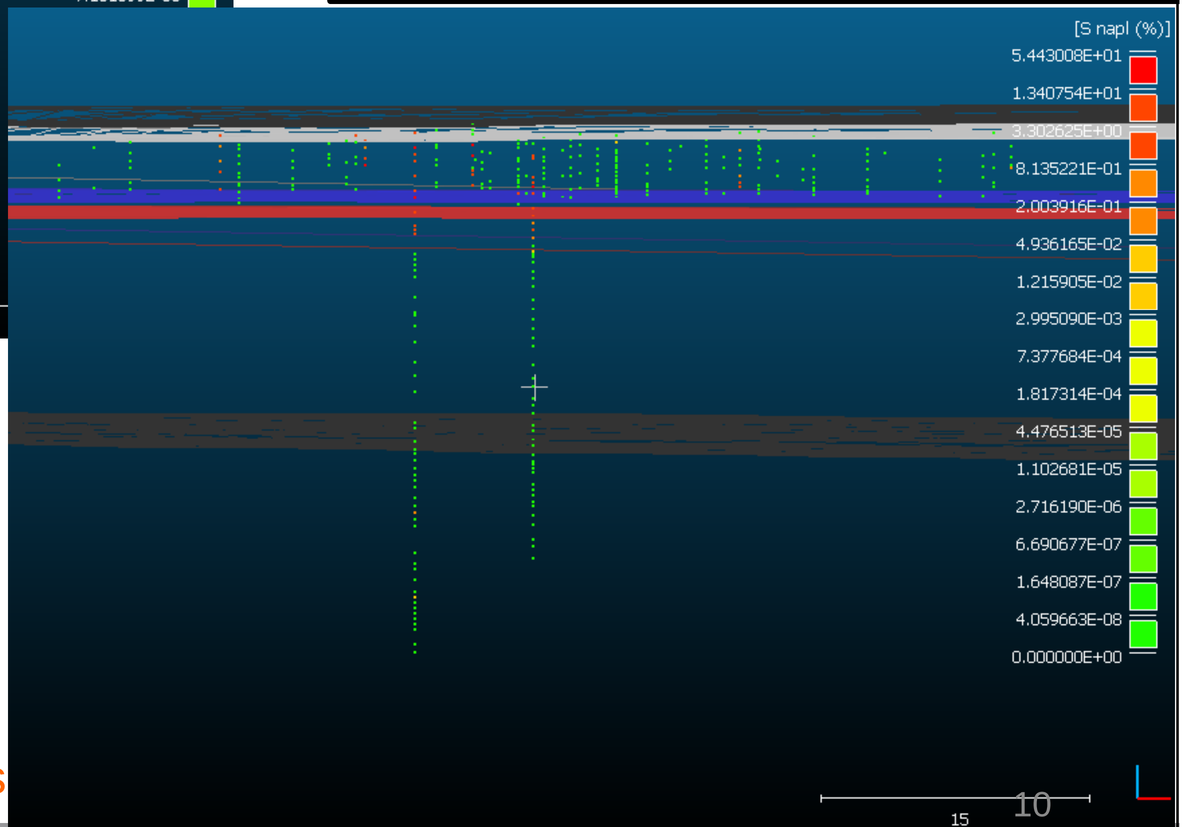
Soil concentrations (mg/kg DW) - Measured



– Csoil from <LQ to 129,173 mg/kg DW
– Pollution everywhere ?

63 samples out of 338 with Csoil <0.1 ppm

NAPL saturations (%) - Computed with OREOS from soil concentration analysis



– Snapl from 0 to 54.4%
– Source zone can be delineated where Snapl > 0, i.e. 49 samples

Example: source 3D delineation

Top fill & silts: 0 to 4 m in depth

Source zone = NALP is present

Probable extension = high soil conc.

Sand lense NAPL

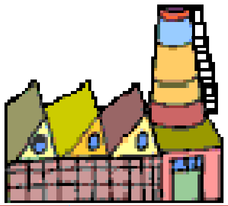
Fine sands: 4 to 8 m in depth

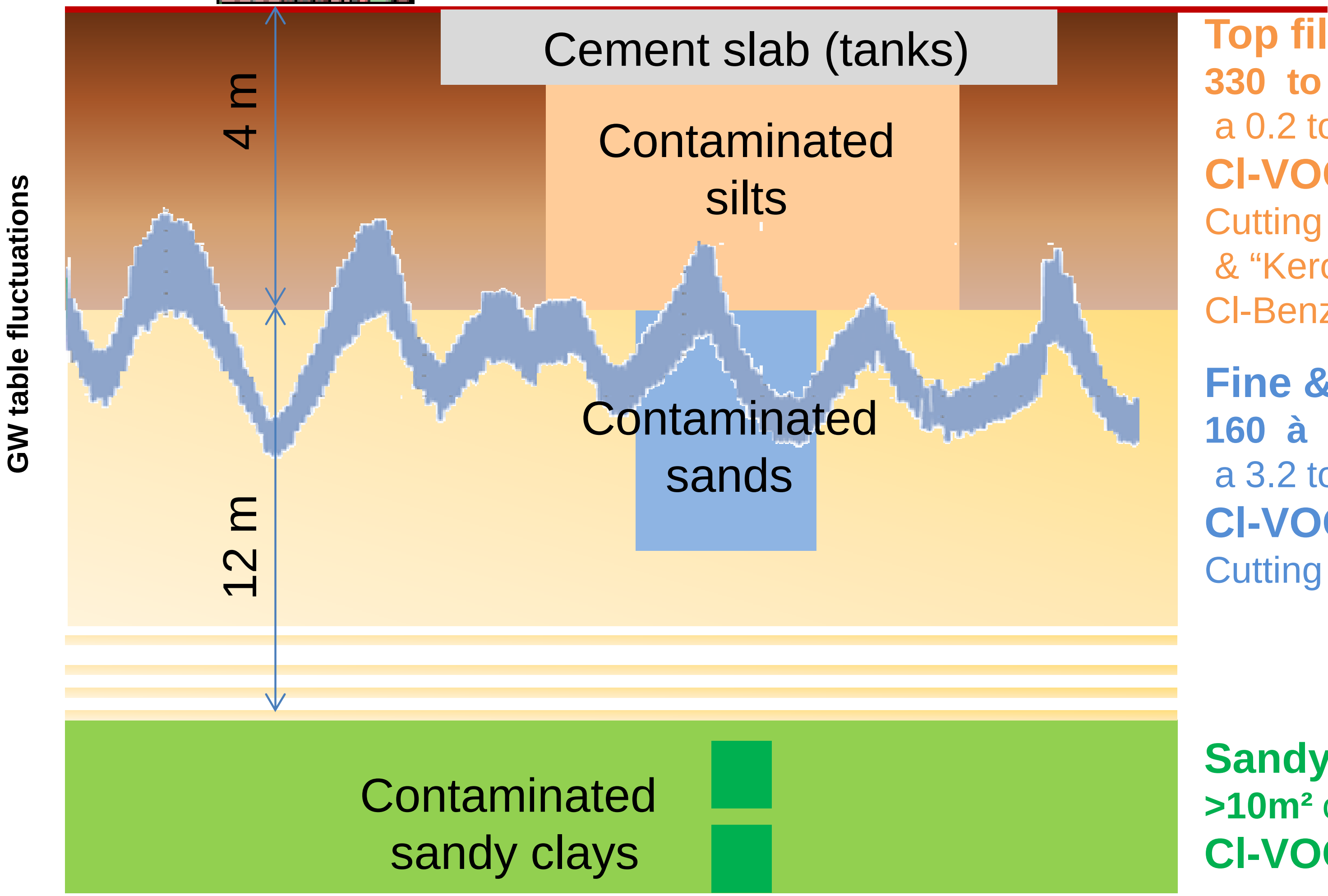
Source zone = NALP is present

Probable extension = high soil conc.

Example: source quantification

	Napl Saturation			Napl composition (molar fraction)			
	min	avrg	max	PCE	TCE	DCE	CV
SILTS	0,2%	3,6%	22,2%	91,6%	7,8%	0,6%	0,0%
SANDS	1,2%	6,8%	19,1%	97,0%	2,9%	0,1%	0,0%
CLAYS	0,1%	0,2%	0,3%	11,6%	83,9%	4,4%	0,0%





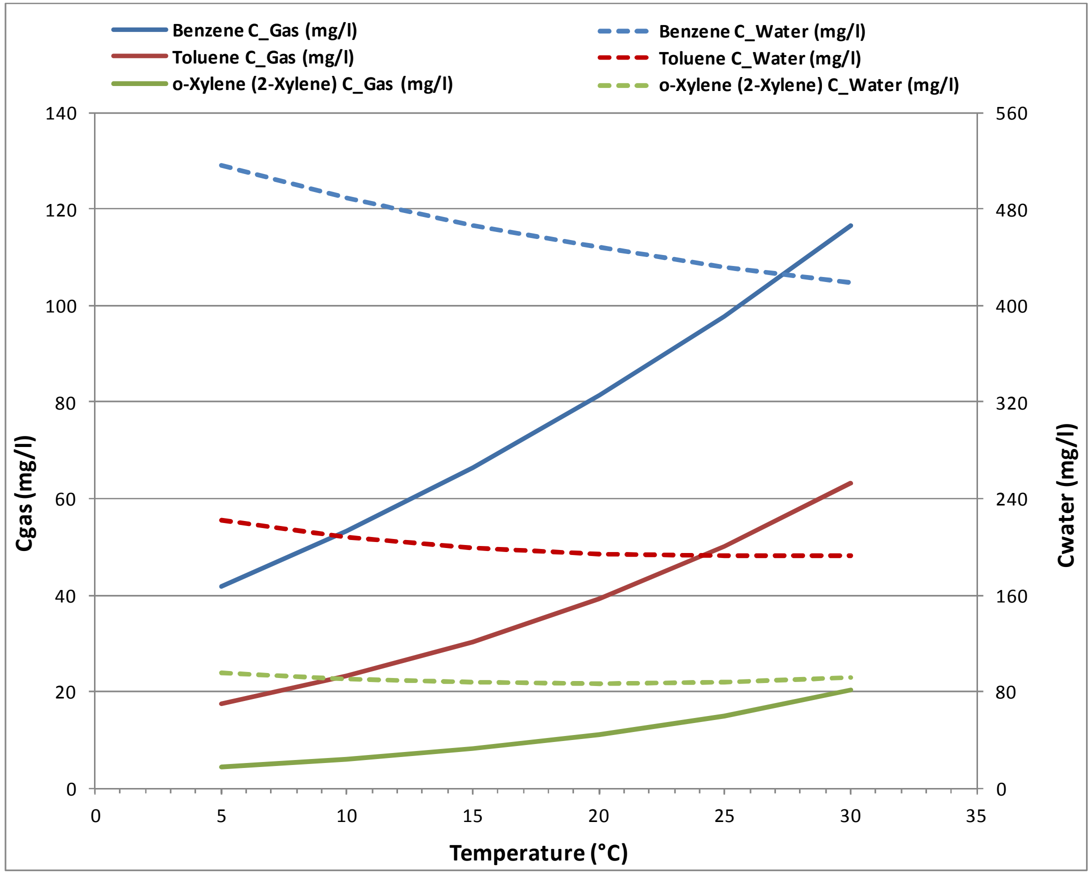
Top fill and Silts :
330 to 410m² contaminated area over a 0.2 to 3.2m depth
Cl-VOC: 5 to 20 Tons (240 samples)
Cutting Oil : 0.9 to 1.9 Tons
& "Kerosene" : 100 kg (73 samples)
Cl-Benzenes : 360 kg (48 samples)

Fine & medium sands :
160 à 320m² contaminated area over a 3.2 to 4.7m depth
Cl-VOC : 2 to 7 Tons (93 samples)
Cutting Oil : 1 to 2 Tons (52 samples)

Sandy clay :
>10m² contaminated over 7m depth
Cl-VOC > 50 kg (48 samples)

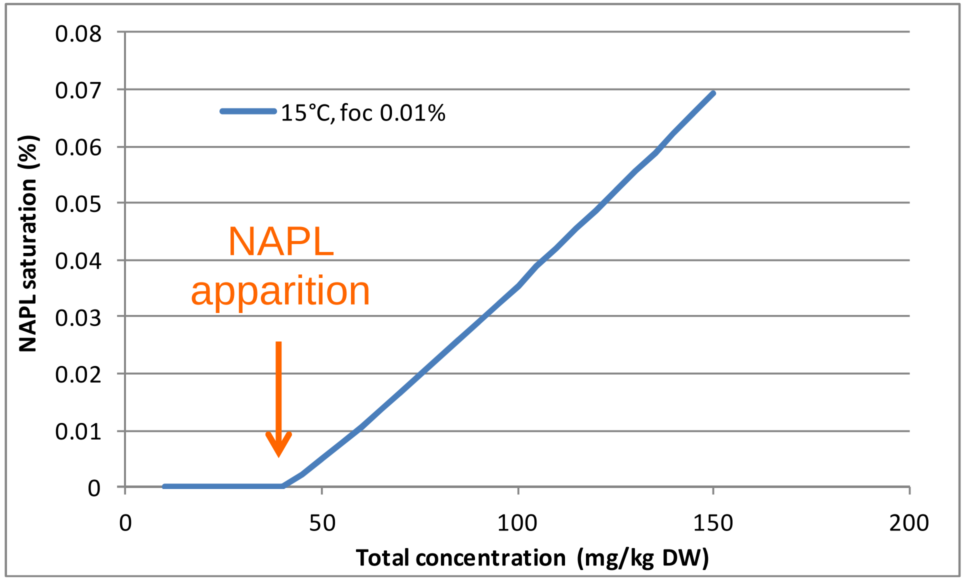
Sensitivity Analysis with OREOS

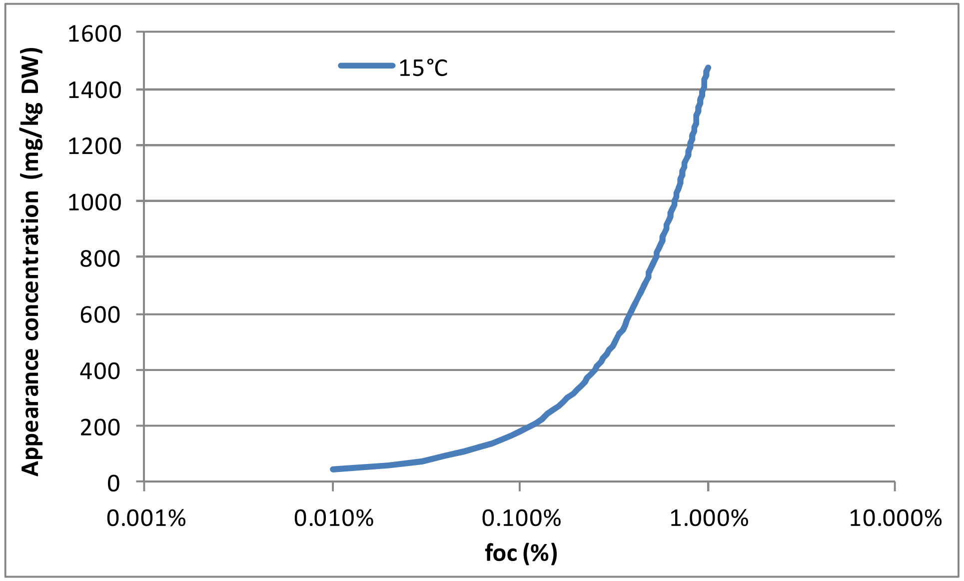
1. Impact of temperature variations on Cw and Cgas



- Benzene / Toluene / o-Xylene = 33% each
- $\theta = 30\%$, $\theta_w = 7.5\%$, *foc* = 0.01%

2. NAPL apparition related to soil *foc*





Conclusions

- **OREOS** is a valuable tool in order to
  - Delineate and quantify Source Zones (NAPL presence)
  - Evaluate contaminant transfers to soil water and gas
  - Assess uncertainty on numerous soil parameters
- It features
  - A fully opened database of contaminant properties (>130 species)
  - A strong theoretical background allowing fast computations
  - An user friendly interface allowing large input files (>1000 samples x dozens of contaminants)
- Contact us at
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  - www.burgeap.fr

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