

Software for the Assessment of NAPL Distribution in Aquifer: OREOS

J. Chastanet, S. Kaskassian, J.-M. Côme

Direction Recherche et Développement
19, rue de la Villette
69425 Lyon Cedex 3
Tél. : 04 37 91 20 50 – Fax : 04 37 91 20 69



- Pollution assessment studies always include soil sampling and analysis

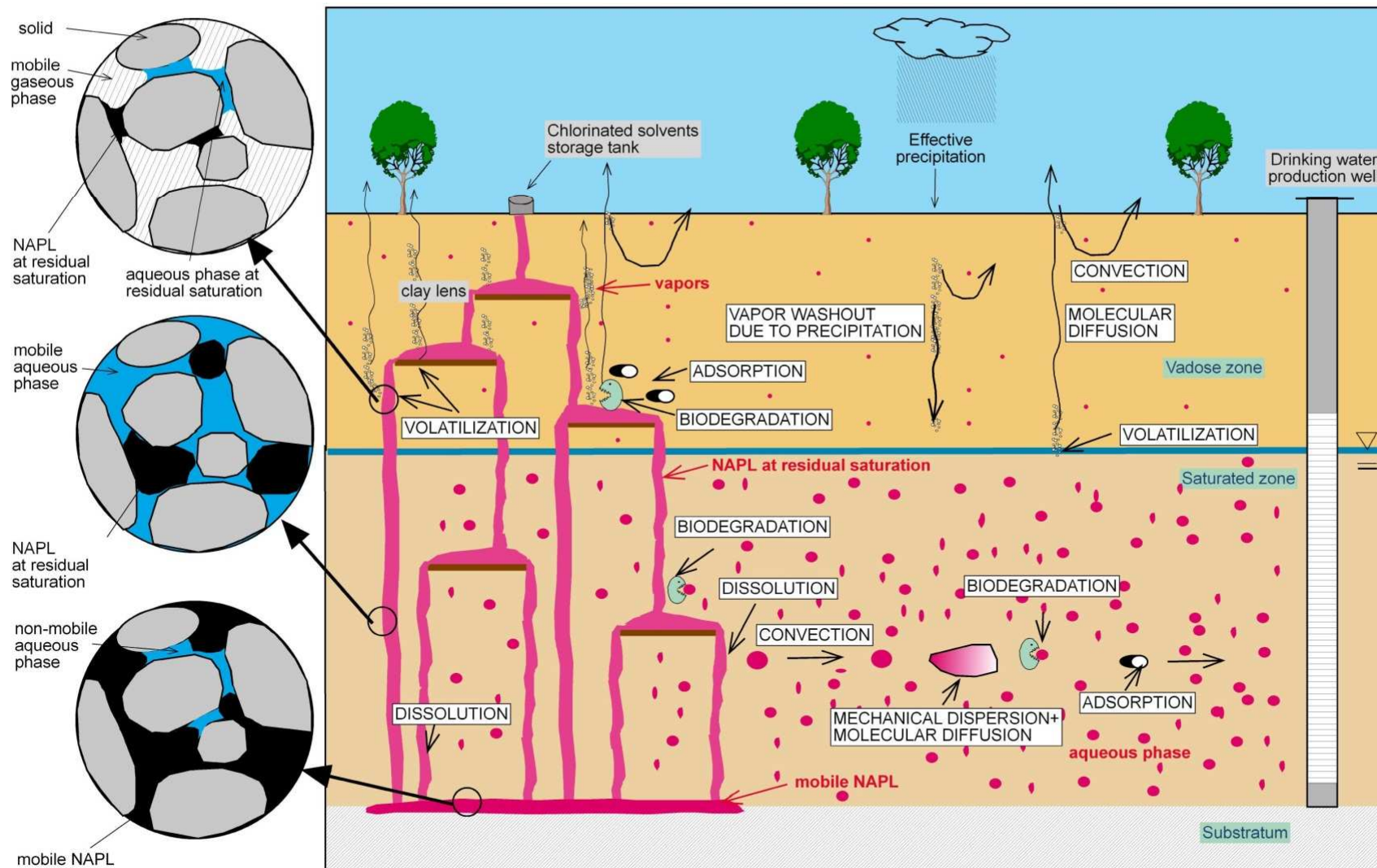


Sample	DW	%	Petroleum Hydrocarbons (mg/kg DW)										Sum
			MeC5-C8	>C8-C10	C10-C12	C12-C16	C16-C20	C20-C24	C24-C28	C28-C32	C32-C36	C36-C40	
SC40	0.5	90	<1,0	<1,0	0.03	0.94	1.80	5.78	10.17	13.05	13.41	9.92	55.1
SC82	0.5	92.3	<1,0	<1,0	0.76	6.36	3.63	7.22	14.40	18.34	18.27	3.72	72.7
SC49	0.7	83.3	<1,0	<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.												

Sample	DW	%	Chlorinated Aliphatic Hydrocarbons (mg/kg DW)														Sum	
			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
SC40	0.5	90	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
SC82	0.5	92.3	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
SC49	0.7	83.3	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
SC91	0.8	66	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
SC47	0.9	63.9	<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
SC60	0.9	92.2	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
SC69	0.		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
SC73	0.		<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
SC48	1.	100	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	
SC40	0.5	90	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	
SC82	0.5	92.3	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	
SC49	0.7	83.3	1.13	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	
SC91	0.8	66	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	
SC47	0.9	63.9	0.050	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	
SC60	0.9	92.2	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	
SC69	0.		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	<1,0	
SC73	0.		52	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	
SC48	1.	100	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	
SC40	0.5	90	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	
SC82	0.5	92.3	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	0.1	
SC49	0.7	83.3	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	
SC91	0.8	66	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	
SC47	0.9	63.9	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	
SC60	0.9	92.2	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	0.0	
SC69	0.		10000	75	2.17	0.56	<0,10	<0,10	<0,020	<0,20	<0,20	<0,10	<0,20	<0,10	<0,050	<2,0	<2,0	
SC73	0.		<0,050	<0,050	<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

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>

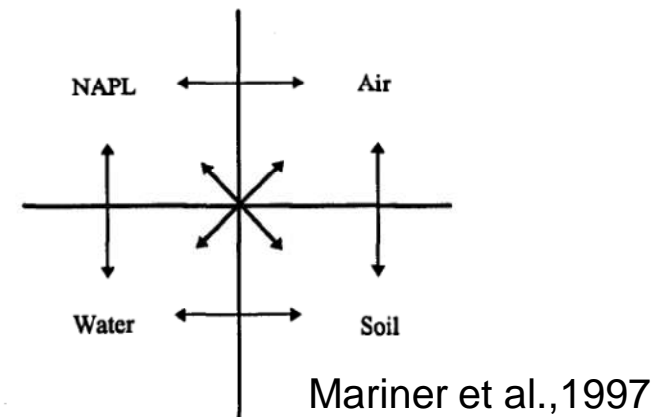
In each soil sample, one may ask ...

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

The **OREOS** software addresses these questions

ORganic contaminant
Evaluation and NAPL
Occurrence assessment in
Soils

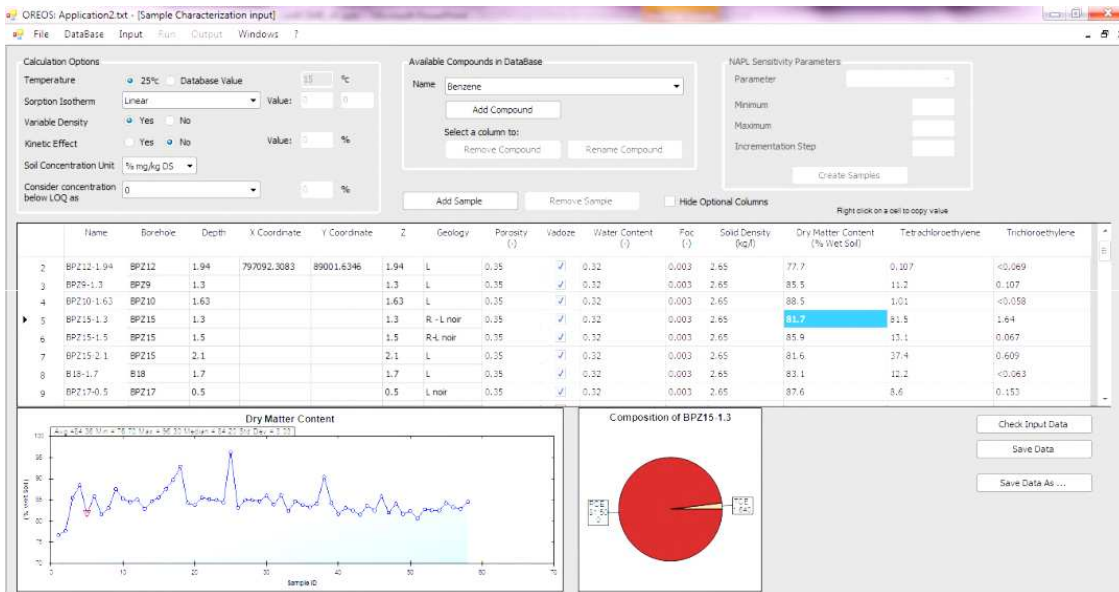
- A set of equations solved by a non linear solver
 - 3 phases (saturated zone) or 4 phases (unsaturated zone) equilibria for multicomponent mixture (Raoult's law ...)
 - Equations of state for each phase (ideal mixture assumption)
 - Mass balances



- 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)

Input - samples characterization and sensitivity analysis



The screenshot shows the 'Input' window of the OREOS software. It features several panels: 'Calculation Options' with radio buttons for '25°C' and 'Database Value', and checkboxes for 'Sorption Isotherm', 'Variable Density', and 'Kinetic Effect'; 'Available Compounds in Database' with a search box for 'Benzene' and 'Add Sample'/'Remove Sample' buttons; 'NAPL Sensitivity Parameters' with input fields for 'Parameter', 'Minimum', 'Maximum', and 'Incrementation Step'; and a main data table with columns for Name, Borehole, Depth, X Coordinate, Y Coordinate, Z, Geology, Porosity, Vadose, Water Content, Porosity, Solid Density, Dry Matter Content, Tetrachloroethylene, and Trichloroethylene. Below the table are two plots: 'Dry Matter Content' (a line graph) and 'Composition of BPZ15 1.3' (a pie chart).

- 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

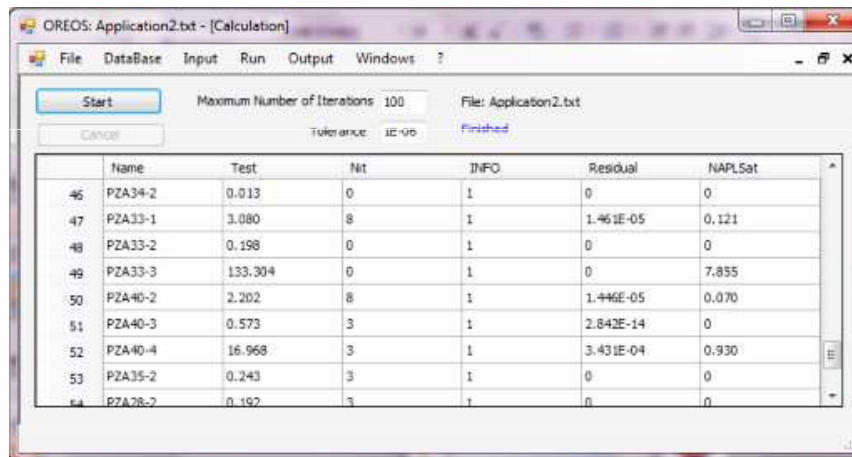
Name	Sporgon	Short name	W CAS	Molecular Formula	Molecular Weight M (g/mol)	Liquid Density		Water Solubility			Vapor pressure						
						d at 25°C	Reference d	S at 25°C (mg/l)	Reference S	Pv at 25°C (Pa)	Reference Pv						
Monoaromatic hydrocarbons																	
Benzene		B	7143-2	C ₆ H ₆	78.11	0.879	[2]	0.185	[2]	1755	[2]	1027.285	[2]	12.680	[2]	12.684	[2]
Biphenyl / Diphenyl (Phenylbenzene)		PhenylB	92-52-4	C ₁₂ H ₁₀	154.2	1.041	[2]	0.109	[2]	7.48	[2]	0.001	[2]	0.004	[2]	0.004	[2]
n-Butylbenzene		n-ButylB	104-51-8	C ₁₀ H ₁₄	134.2	0.859	[2]	0.054	[2]	13.8	[2]	13.300	[2]	0.140	[2]	0.193	[2]
1,2-Dichlorobenzene (Dimethylchlorobenzene)		1,2-DChB	95-50-6	C ₆ H ₄ Cl ₂	147.0	1.303	[2]	0.059	[2]	23.5	[2]	0.290	[2]	0.290	[2]	1.686	[2]
o-Xylene		o-Xyl	98-14-4	C ₈ H ₁₀	106.2	0.885	[2]	0.051	[2]	35.1	[2]	86.395	[2]	1.200	[2]	1.686	[2]
m-Xylene		m-Xyl	107-76-3	C ₈ H ₁₀	106.2	0.885	[2]	0.051	[2]	18.2	[2]	1.024	[2]	0.696	[2]	0.824	[2]
p-Xylene		p-Xyl	98-08-8	C ₈ H ₁₀	106.2	0.869	[2]	0.056	[2]	59	[2]	50.425	[2]	0.590	[2]	0.524	[2]
1-Methyl-4-ethylbenzene (p-Xylene)		1-Methyl-4-ethylB	107-76-3	C ₁₀ H ₁₄	134.2	0.859	[2]	0.054	[2]	23.4	[2]	0.200	[2]	0.277	[2]	0.277	[2]
1-Methyl-2-propylbenzene		1-Methyl-2-propylB	107-76-3	C ₁₀ H ₁₄	134.2	0.870	[2]	0.059	[2]					0.450	[2]	0.620	[2]
1-Methyl-3-propylbenzene		1-Methyl-3-propylB	107-76-3	C ₁₀ H ₁₄	134.2	0.859	[2]	0.054	[2]					0.450	[2]	0.620	[2]
1-Methyl-4-propylbenzene (p-Xylene)		1-Methyl-4-propylB	107-76-3	C ₁₀ H ₁₄	134.2	0.854	[2]	0.054	[2]					0.450	[2]	0.620	[2]
n-Propylbenzene		n-PropylB	103-65-1	C ₉ H ₁₂	120.2	0.880	[2]	0.055	[2]	52.1	[2]	52.482	[2]	0.620	[2]	0.620	[2]
1,2,3-Tetramethylbenzene (Durene)		Durene	69-53-2	C ₁₀ H ₁₄	134.2	0.880	[18]	0.200	[2]	7.34	[2]	7.297	[2]	0.048	[2]	0.072	[2]
1,2,4-Tetramethylbenzene (Pseudooculene)		p-Toluene	95-53-6	C ₁₀ H ₁₄	134.2	0.872	[2]	0.088	[2]	50	[2]	87.447	[2]	0.290	[2]	0.441	[2]
1,3,5-Triethylbenzene		1,3,5-TriEB	618-13-8	C ₁₂ H ₁₈	150.2	0.891	[2]	0.087	[2]	92.5	[2]	89.771	[2]	0.219	[2]	0.258	[2]
1,3,5-Triethylbenzene (Mesitylene)		1,3,5-TriEB	93-87-8	C ₁₂ H ₁₈	150.2	0.881	[2]	0.057	[2]	48.2	[2]	48.825	[2]	0.330	[2]	0.452	[2]
Styrene		Styrene	100-42-5	C ₈ H ₈	104.15	0.900	[2]	0.036	[2]	321.6	[2]	0.700	[2]	0.700	[2]	1.096	[2]
Toluene		Tol	98-06-2	C ₇ H ₈	92.1	0.865	[2]	0.060	[2]	542	[2]	546.500	[2]	3.000	[2]	4.000	[2]
o-Xylene (o-Xylene)		o-Xyl	95-17-6	C ₈ H ₁₀	106.2	0.876	[2]	0.072	[2]	231	[2]	222.488	[2]	0.600	[2]	1.181	[2]
m-Xylene (m-Xylene)		m-Xyl	98-26-3	C ₈ H ₁₀	106.2	0.881	[2]	0.057	[2]	114	[2]	175.448	[2]	1.000	[2]	1.498	[2]
p-Xylene (p-Xylene)		p-Xyl	95-82-3	C ₈ H ₁₀	106.2	0.869	[2]	0.061	[2]	203.7	[2]	203.193	[2]	1.000	[2]	1.579	[2]
Chlorinated hydrocarbons																	
1,1,1-Trichloroethane		1,1,1-TrichloroE	70-133-7	C ₂ HCl ₃	133.4	1.495	[2]	1.405	[2]	150	[2]	150	[2]	2.10	[2]	2.941	[2]
1,1,2-Trichloroethane		1,1,2-TrichloroE	78-08-8	C ₂ HCl ₃	133.4	1.458	[2]	1.450	[2]	160	[2]	160	[2]	9.600	[2]	13.148	[2]
1,1-Dichloroethane		1,1-DichloroE	75-35-4	C ₂ HCl ₂	98.94	1.107	[2]	1.109	[2]	3745	[2]	3745	[2]	80.000	[2]	85.777	[2]
1,1,2-Dichloroethane		1,1,2-DichloroE	78-67-2	C ₂ HCl ₂	98.94	1.283	[2]	1.283	[2]	250	[2]	250	[2]	22.000	[2]	23.700	[2]
Trans-1,2-dichloroethane		1,2-DChE	78-67-2	C ₂ HCl ₂	98.94	1.244	[2]	1.238	[2]	6300	[2]	6300	[2]	44.400	[2]	53.906	[2]
Vinyl Chloride (Chloroethene)		VC	75-04-4	C ₂ HCl	62.5	0.903	[2]	0.894	[2]	2687	[2]	2687	[2]	297.200	[2]	493.488	[2]
Hexachlorobenzene		HexaC	67-72-1	C ₆ Cl ₆	284.74	2.000	[11]	0.000	[2]	0.000	[2]	0.000	[2]	0.000	[2]	0.000	[2]
Pentachlorobenzene		PentaC	76-01-7	C ₆ HCl ₅	202.31	1.675	[2]	1.688	[2]	500	[2]	500	[2]	0.667	[2]	0.666	[2]
1,1,2,2-Tetrachloroethane		1,1,2,2-TetrachloroE	600-20-8	C ₂ Cl ₄	166.85	1.525	[2]	1.527	[2]	1000	[2]	1000	[2]	1.00	[2]	1.24	[2]
1,1,2,2-Tetrachloroethane		1,1,2,2-TetrachloroE	79-59-5	C ₂ Cl ₄	166.85	1.501	[2]	1.497	[2]	2900	[2]	2900	[2]	9.000	[2]	9.944	[2]
1,1,1-Trichloroethane		1,1,1-TrichloroE	71-55-6	C ₂ HCl ₃	133.4	1.73	[2]	1.722	[2]	1000	[2]	1000	[2]	16.000	[2]	20.506	[2]
1,1,2-Trichloroethane		1,1,2-TrichloroE	75-35-4	C ₂ HCl ₃	133.4	1.438	[2]	1.436	[2]	4303	[2]	4303	[2]	3.000	[2]	4.016	[2]
1,1,1-Trichloroethane		1,1,1-TrichloroE	75-35-4	C ₂ HCl ₃	133.4	1.46	[2]	1.46	[2]	2000	[2]	2000	[2]	30.000	[2]	32.264	[2]

- 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

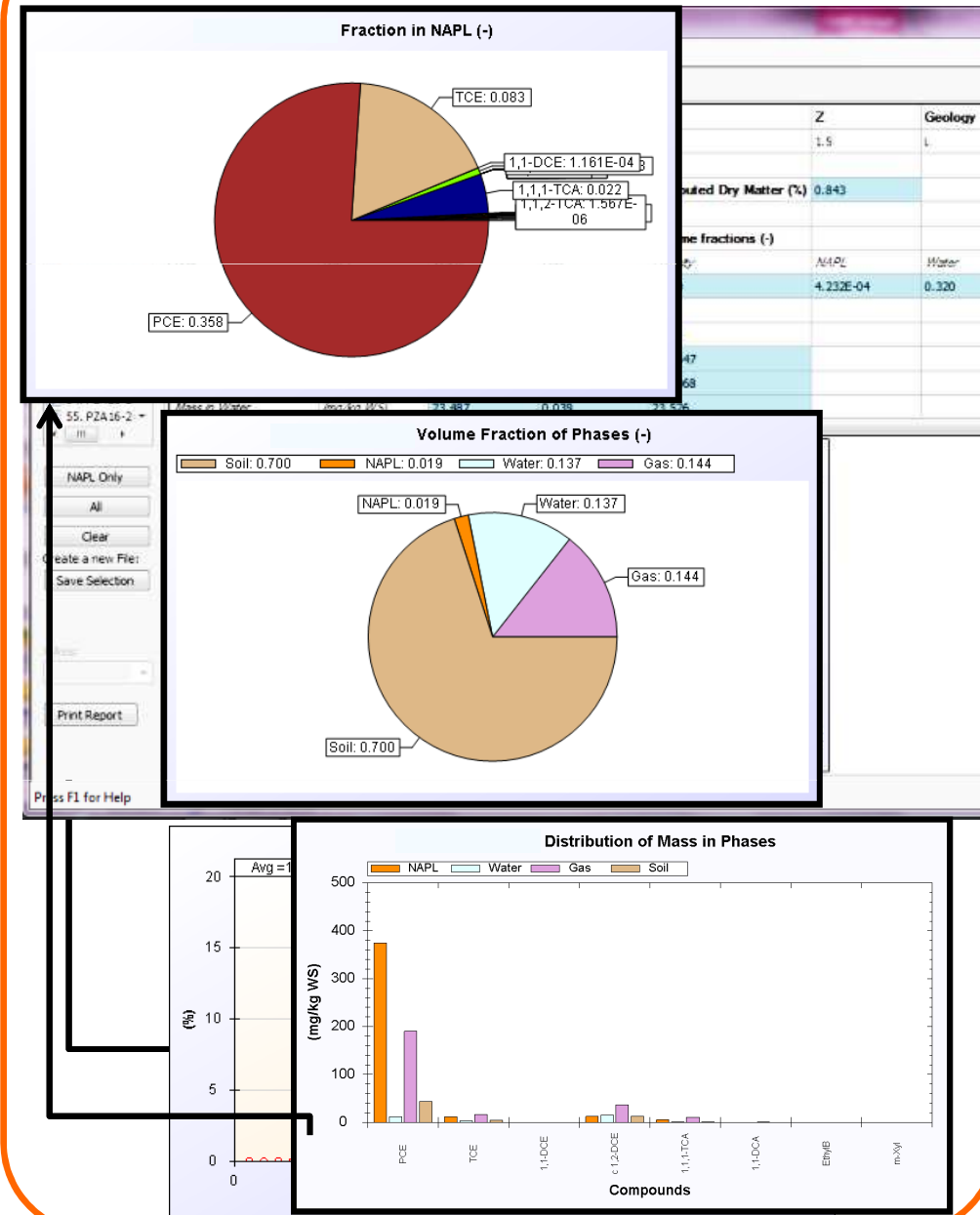
Run window



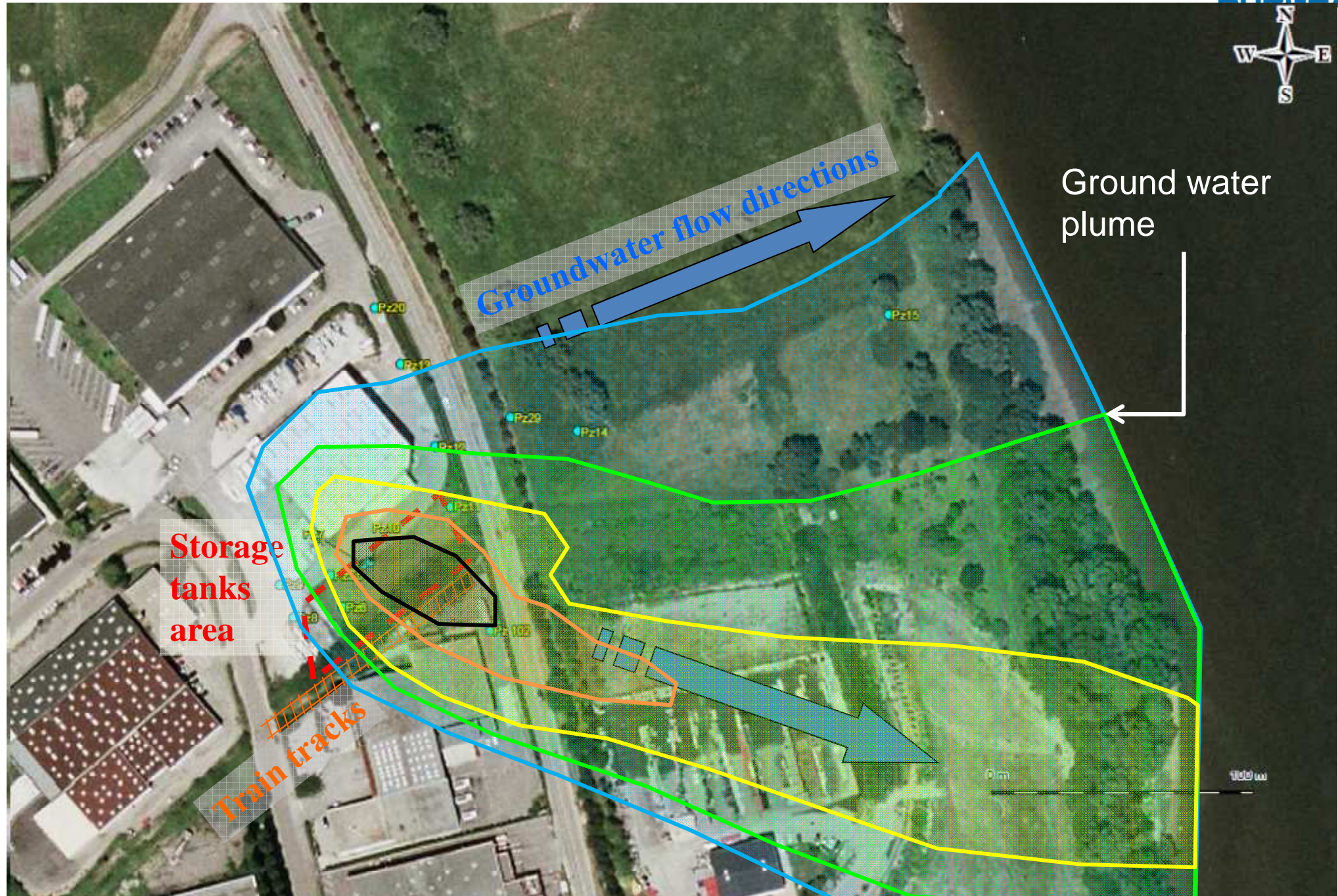
- Numerical parameters: iterations, tolerance ...
- Run report: residual, warnings ...

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

Output window – result and analysis tool



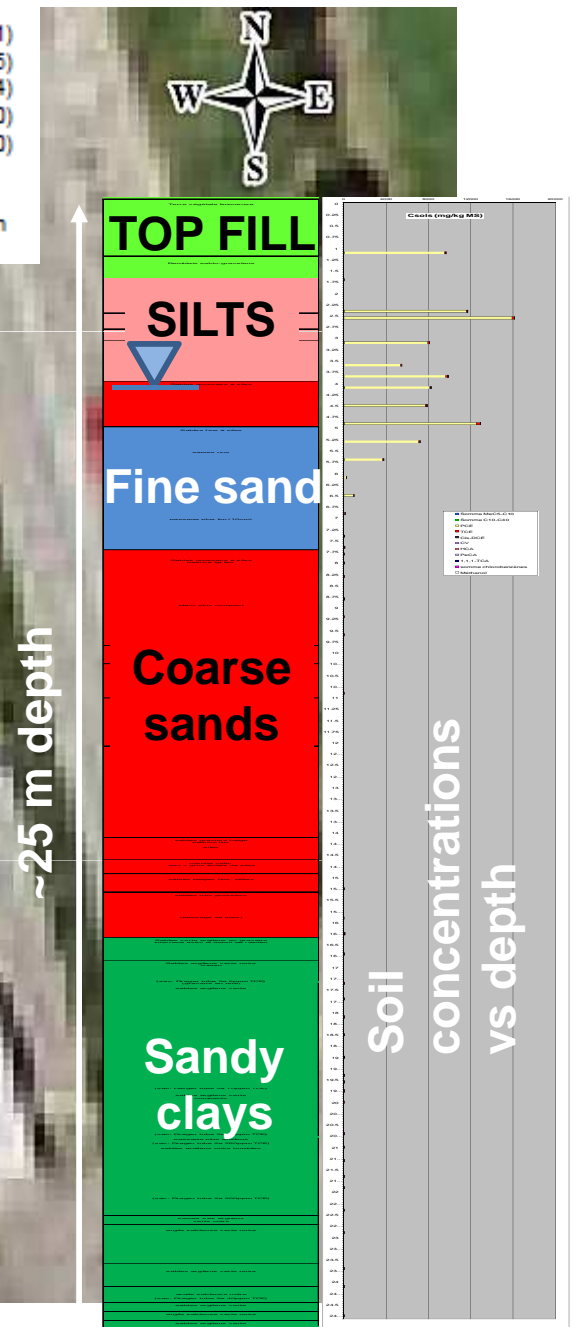
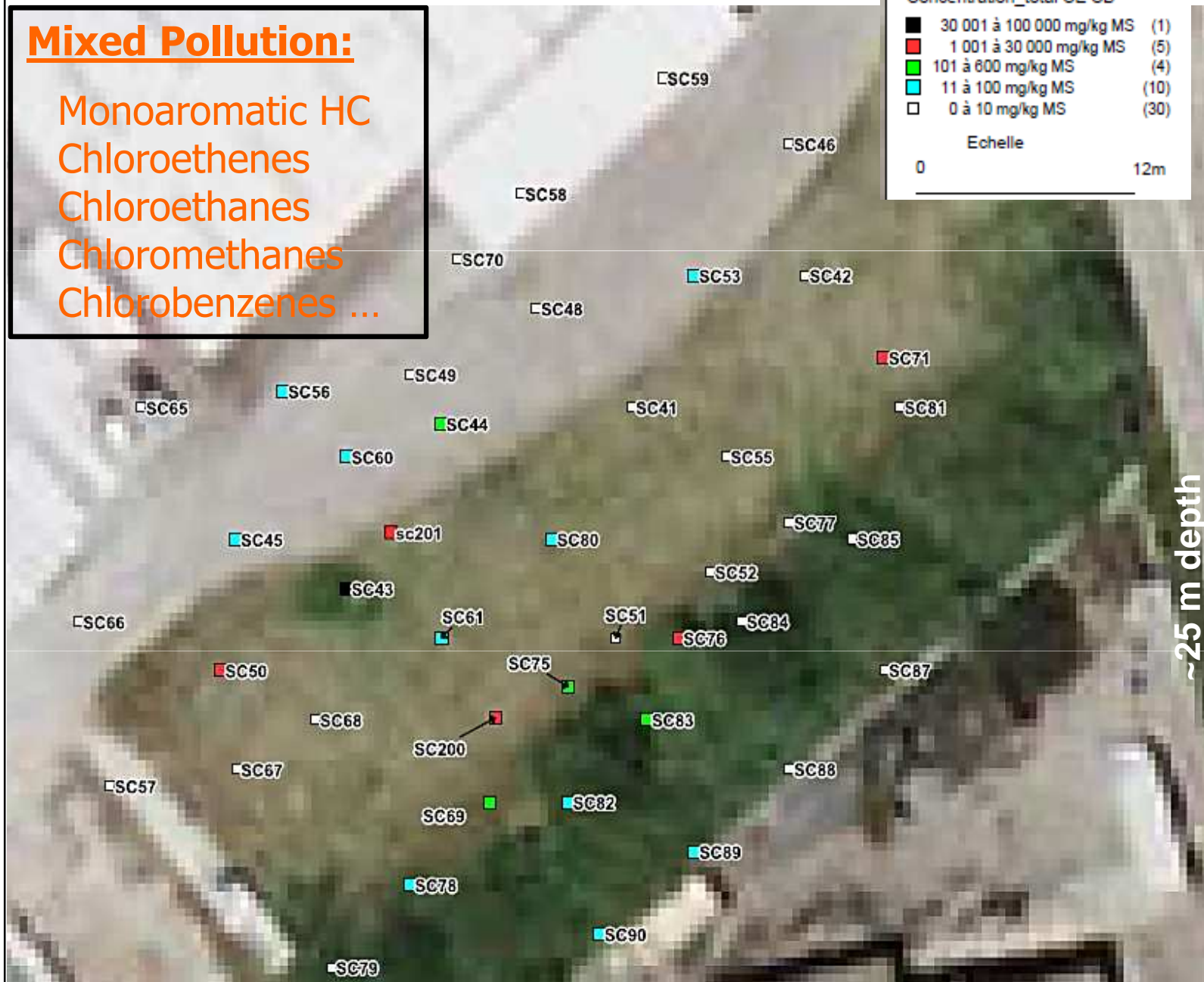
Example: source characterization



Example : soil concentrations analysis

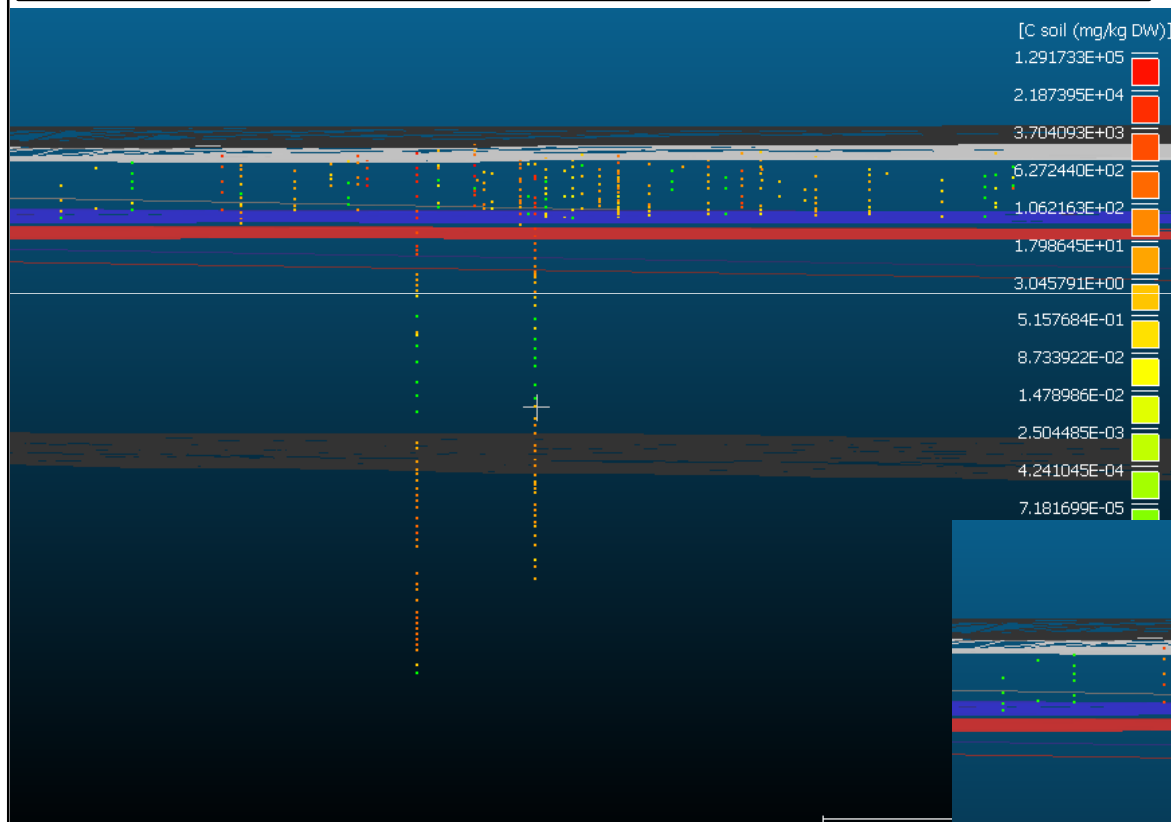
Mixed Pollution:

Monoaromatic HC
 Chloroethenes
 Chloroethanes
 Chloromethanes
 Chlorobenzenes ...

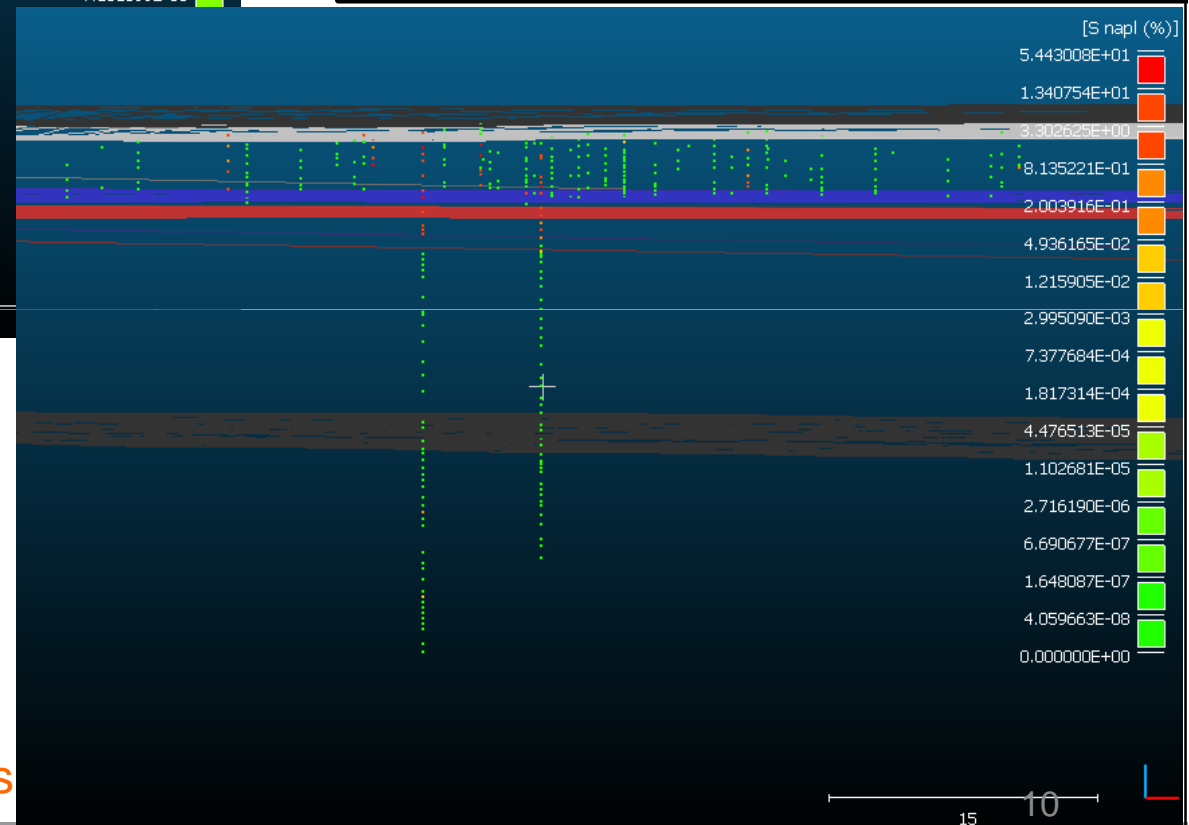


Example : compute NAPL saturations

Soil concentrations (mg/kg DW) - Measured



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

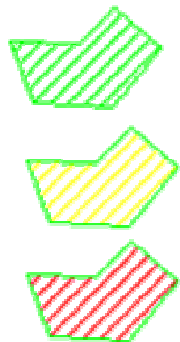


- Csoil from <LQ to 129,173 mg/kg DW
 - Pollution everywhere ?
- 63 samples out of 338 with Csoil <0.1 ppm

- 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

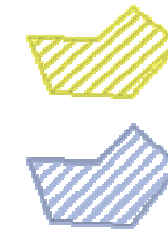


Source zone = NAPL is present

Probable extension = high soil conc.

Sand lense NAPL

Fine sands: 4 to 8 m in depth



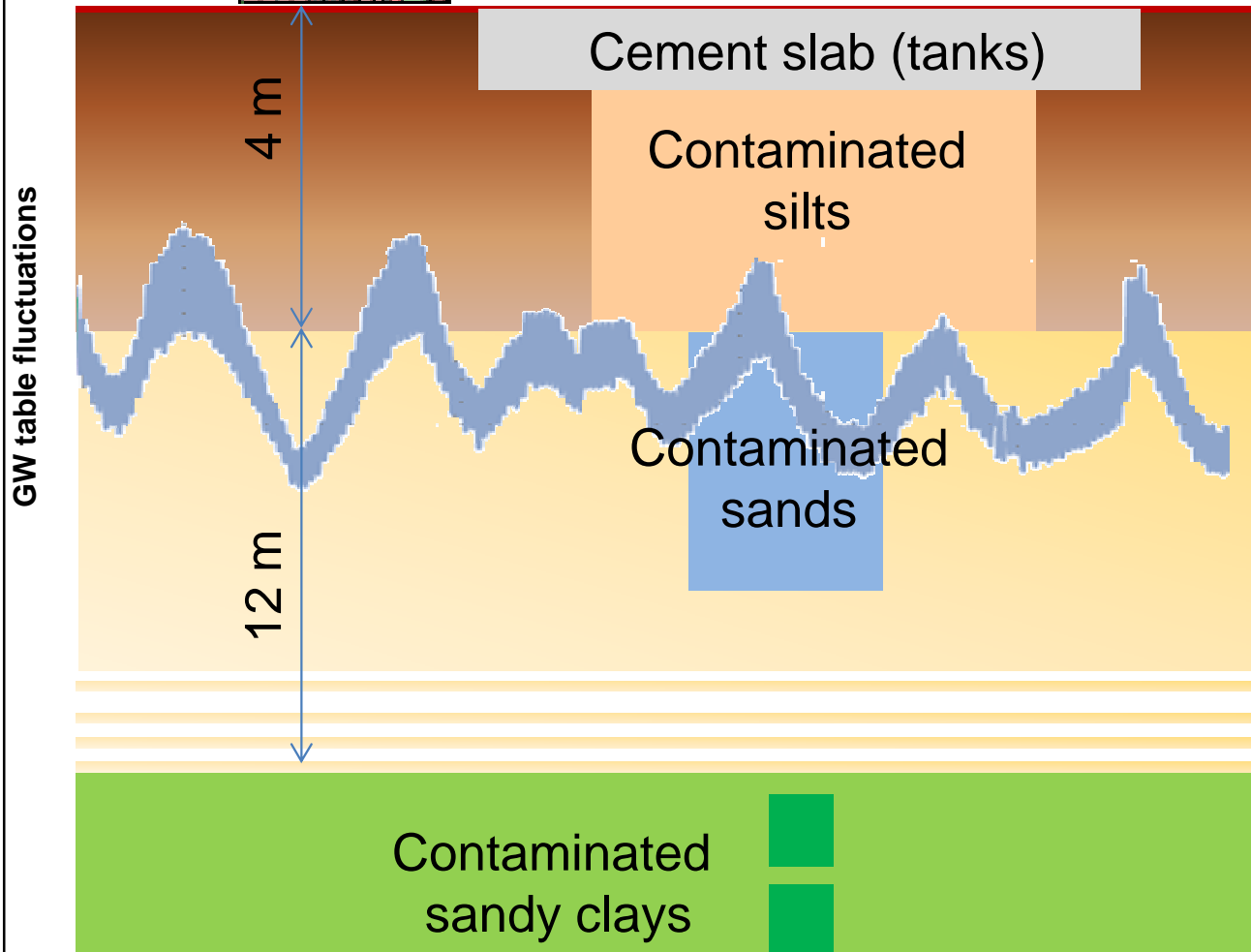
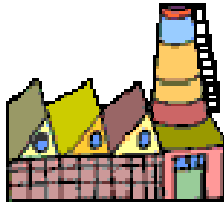
Source zone = NAPL is present

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%



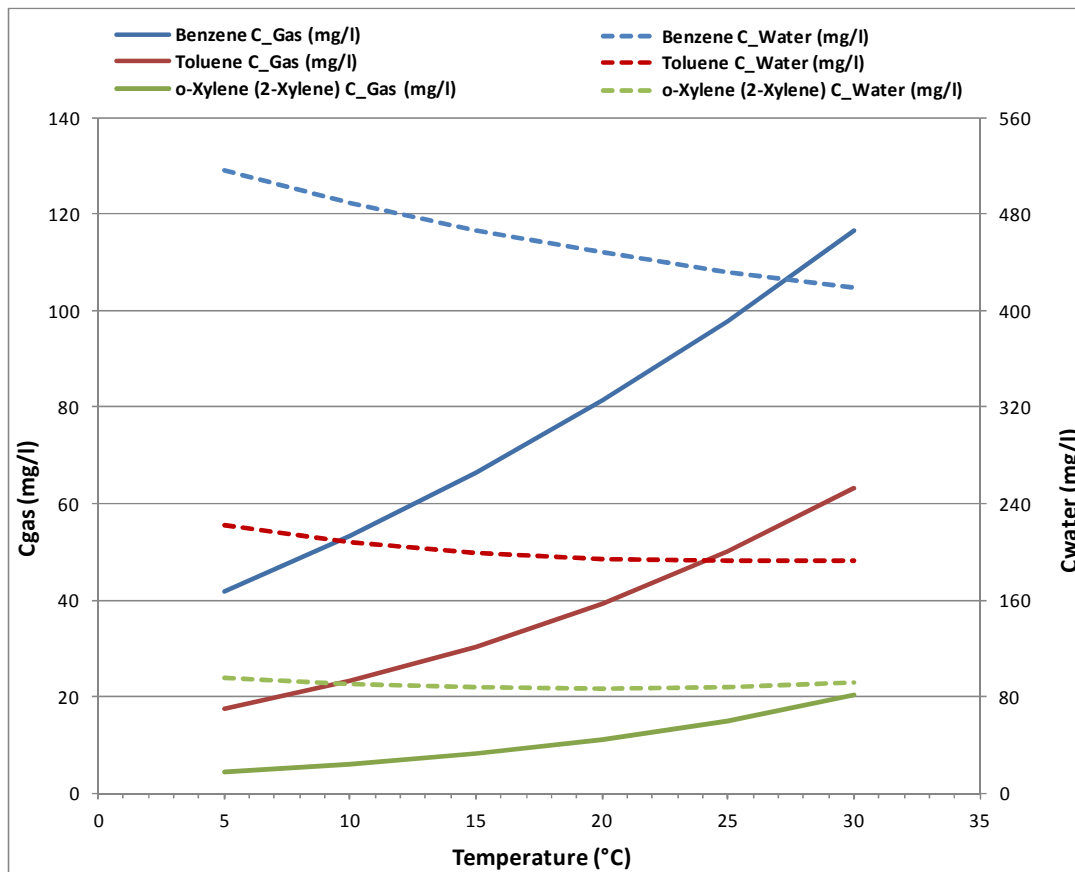
Top fill and Silts :
330 to 410m² contaminated area over a 0.2 to 3.2m depth
CI-VOC: 5 to 20 Tons (240 samples)
 Cutting Oil : 0.9 to 1.9 Tons
 & "Kerosene" : 100 kg (73 samples)
 CI-Benzenes : 360 kg (48 samples)

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

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

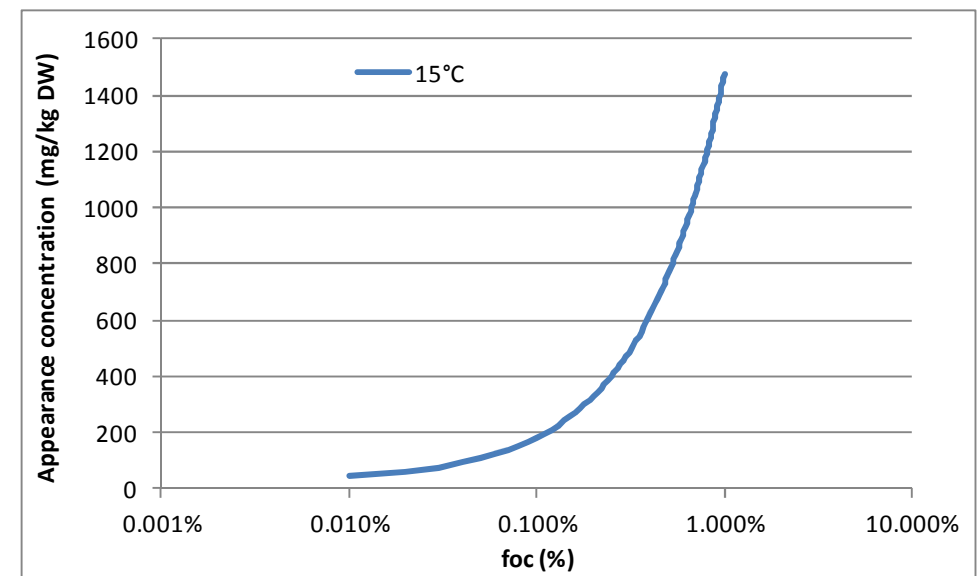
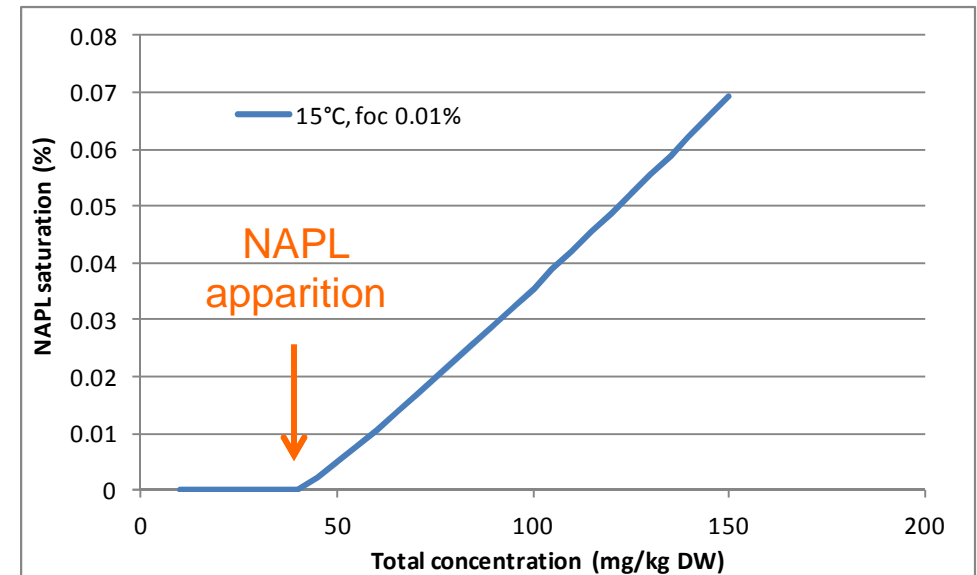
Sensitivity Analysis with OREOS

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



- **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**
 - j.chastanet@burgeap.fr
 - www.burgeap.fr



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