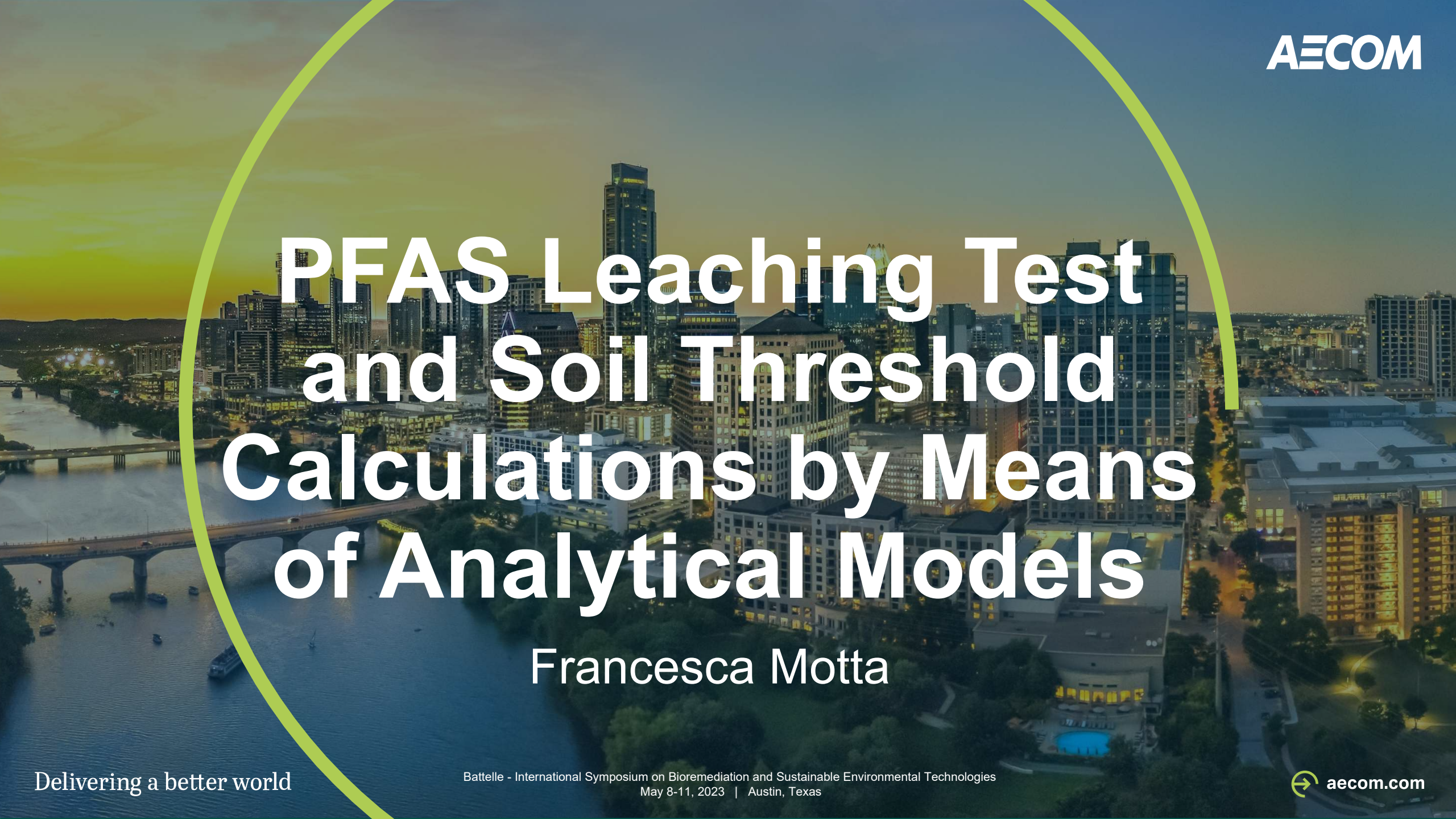

PFAS Leaching Test and Soil Threshold Calculations by Means of Analytical Models

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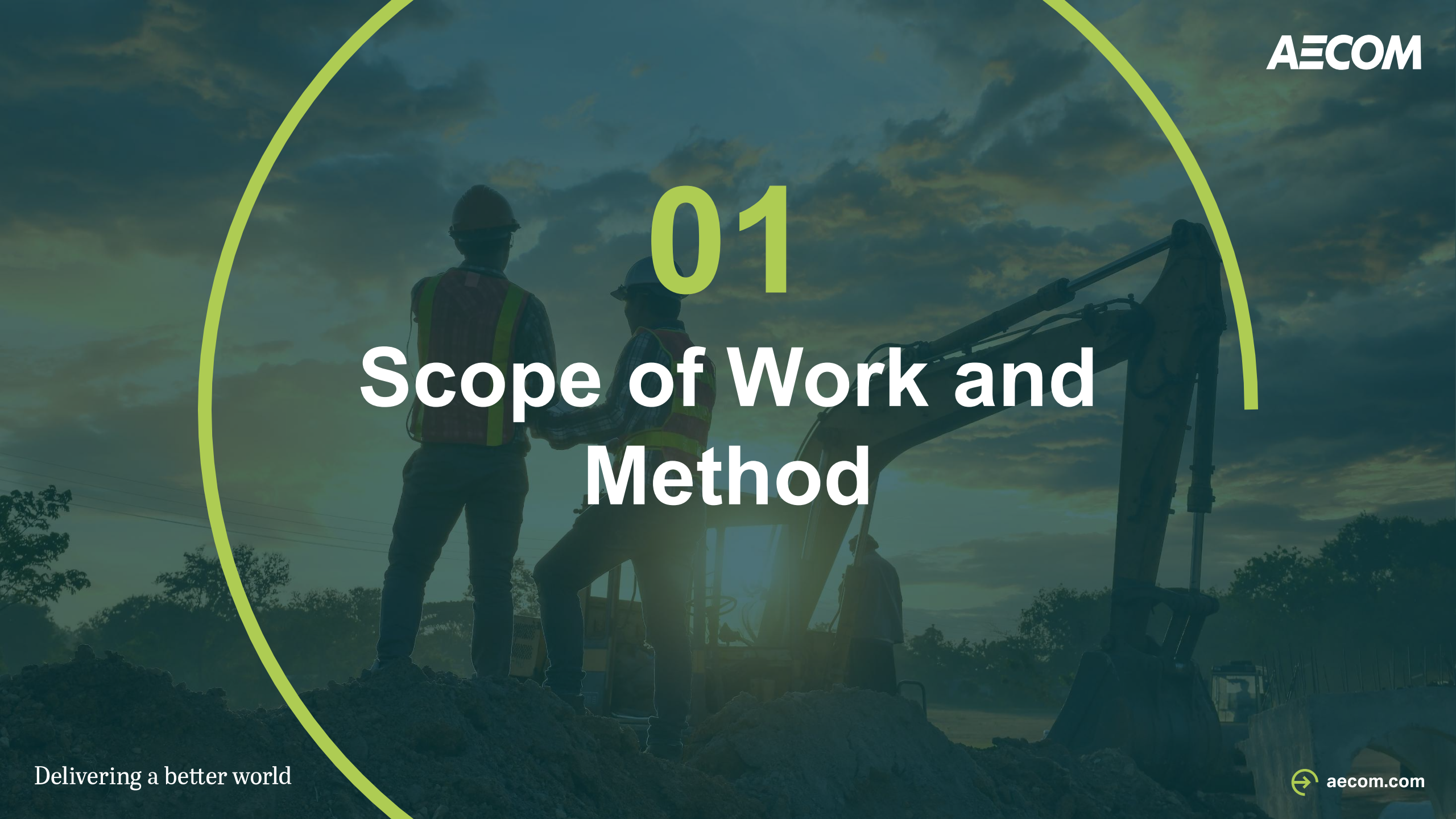
Agenda

01 Scope of Work & Method

02 Leaching test results and modelling approach

03 Validation



01

Scope of Work and Method

Scope of Work

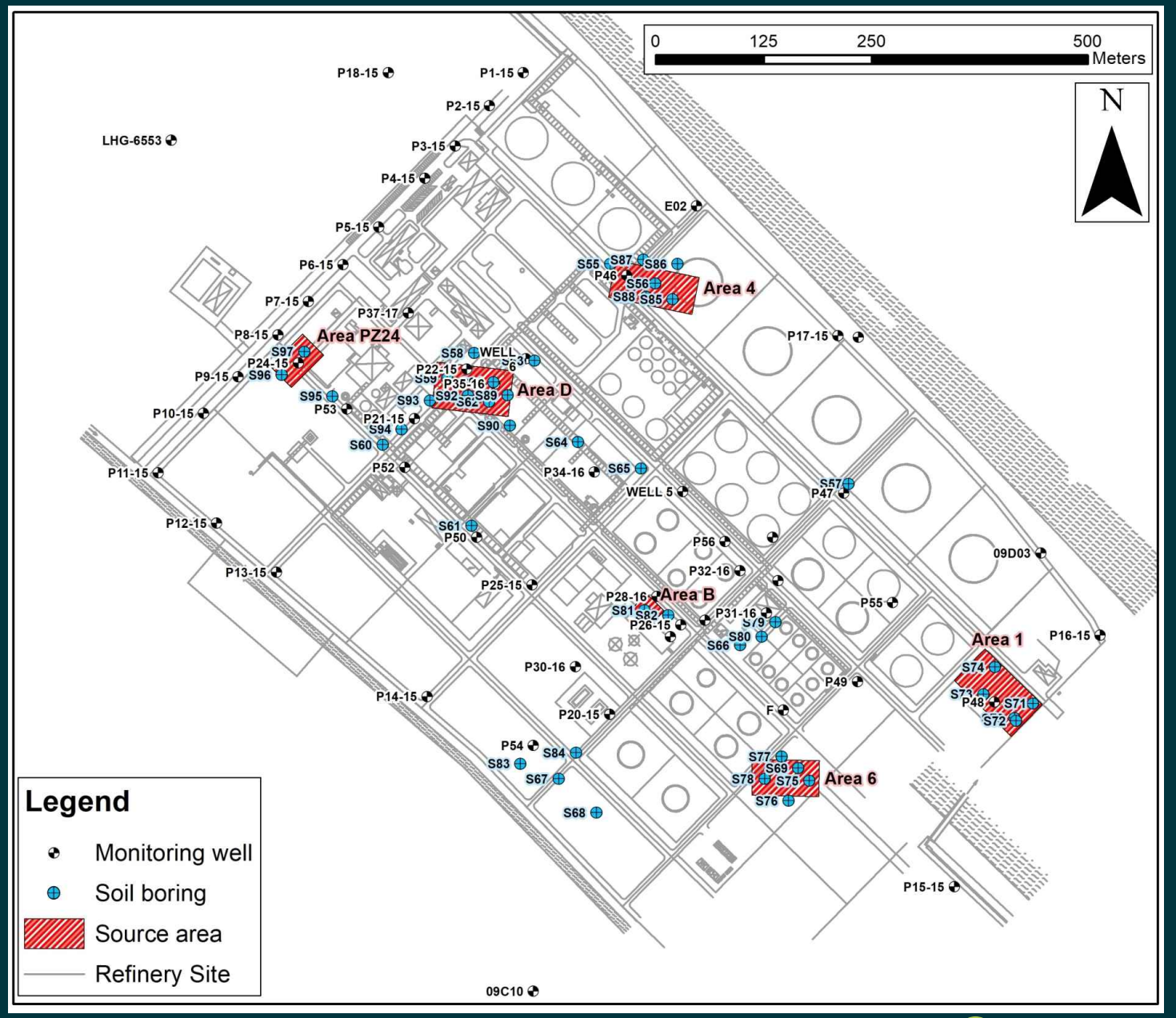
Background: No remediation guideline values in soil for PFAS are defined in Switzerland; values for managing soil off-site disposal are available - OLED values and 2022-05-01 draft guideline based on toxicity equivalent factors

Objective: deriving site specific soil clean up levels in order to achieve downgradient water quality standard (at the site boundary)

Water quality value for PFAS is 50ng/L TEQ (draft guideline based on toxicity equivalent factors)

Method

- Application of Leaching Environmental Assessment Framework (LEAF), developed by the US Environmental Protection Agency (EPA), including laboratory column tests (which better represent the infiltration process through the unsaturated part of the soil), and the static test with different S/L at 3 test source areas (Area 1, Area 6, Area PZ24)
- Collection of soil samples for site –specific properties and soil analyses

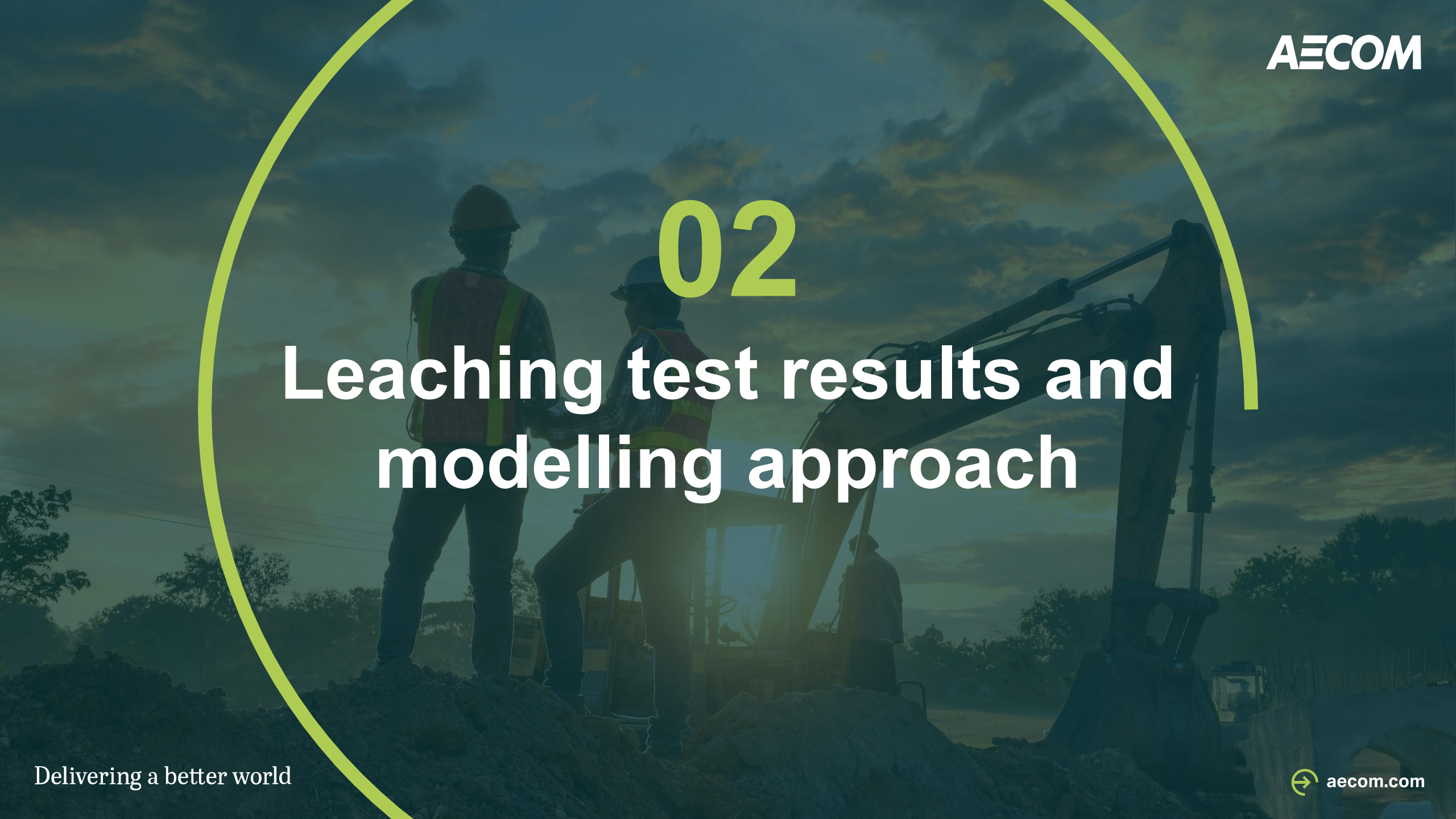


Leaching test

Figure 1. Column equipment for dinamic leaching test.

- EPA method 1314 : column tests (which better represent the infiltration process through the unsaturated part of the soil), production of eluates by dynamic leaching, starting from soil samples, by liquid-solid partitioning, as a function of the time-varying L/S ratio.

- EPA method 1316: production of eluates, starting from soil samples, by liquid-solid partitioning, according to the variation of the L/S ratio. The method in question is used to monitor the quantity of inorganic and organic non-volatile substances PFAS contained in soil samples.

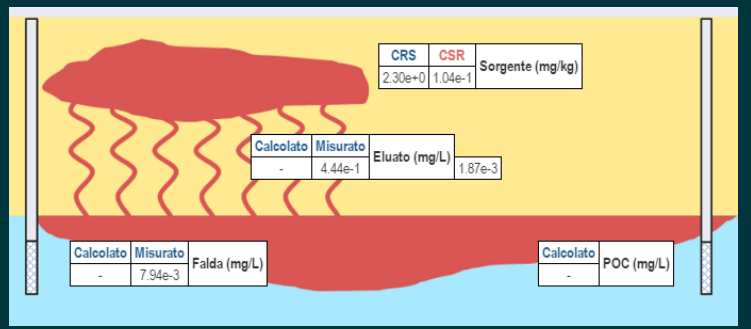


02

Leaching test results and modelling approach

Leaching test results and modelling approach

- Analysis of leaching test results, with identification of the most significant constituent of the mixture (PFOS)
- Calculation of site-specific partition coefficient
- Application of unsaturated transport model to groundwater and calibration with groundwater quality at monitoring well located below the source area
- Application of the migration pathway transport analytical model to the Point of Compliance (POC) at the site downgradient boundary
- Validation of the modelled concentration at the POC with the numerical model calibrated in 2021 for Area 1.
- Validation of the site-specific PFOS Log koc value with other experimental values reported in the literature
- Calculation of target concentrations in the source area both in the leachate and in soil (dry matter) with site specific partitioning coefficient



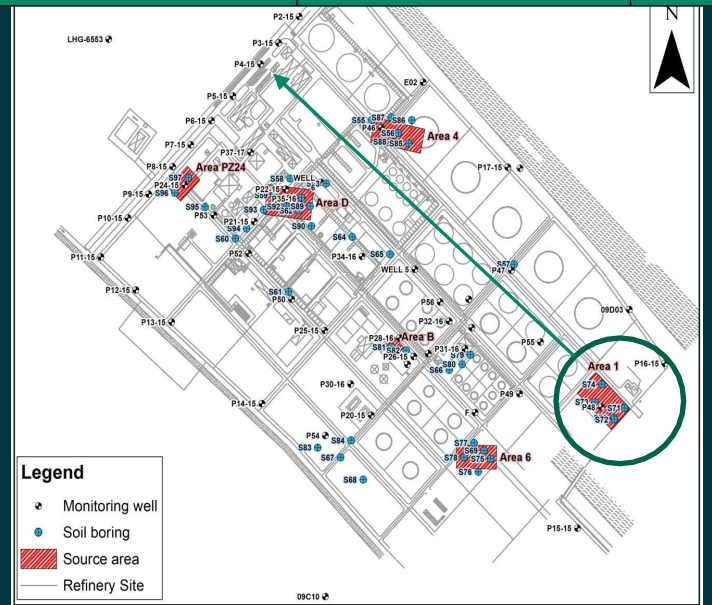
Assumptions

- All the mass of PFOS was estimated to be present in the layer with maximum concentrations detected in the leachate test done with 2:1 L/S
- Site-specific values of soil (foc, particle size distribution) and site-specific infiltration rates were used to model leaching from unsaturated to saturated zone
- Site-specific saturated zone properties correspond to values used in the calibrated numerical model with the exception of dispersivity

Area 1

	Concentration in soil mg/kg	Concentration in soil mg/kg	Leaching test 2:1 mg/l	Leaching test - Dynamic - EPA 1314 sum of concentrations T1÷T9 mg/l	Leaching test - Static - EPA 1316 maximum concentration T1÷T5 mg/l	GW concentration POC=0 mg/l			GW concentration POC>0 mg/l			
	S74 (0-1 m) - raw material	S113 (0-1 m)	S74 (0-1 m)	S113 (0-1 m)	S113 (0-1 m)	P-48			P-3			
	May-21	Aug-22	May-21	Aug-22	Aug-22	10/2/2020	5/27/2021	3/28/2022	1/22/2020	9/30/2020	5/27/2021	3/29/2022
PFBA	0.00056	<0,00093	0.00023	0.001238	0.0012	0.00011	0.00043	0.00014	0.000032	0.000037	0.00004	0.000046
PFBS	0.000036	0.00116	0.000017	0.002278	0.00199	0.000022	0.000021	0.0000061	0.000017	0.00002	0.0000094	0.0000059
PFHpA	0.0017	0.0044	0.00072	0.014884	0.008	0.000064	0.0011	0.00018	0.000044	0.000051	0.000074	0.000067
PFHxA	0.0038	0.0034	0.00077	0.009026	0.0072	0.00018	0.00086	0.00031	0.000078	0.00012	0.000085	0.00012
PFHxS	0.0122	0.045	0.0036	0.21234	0.095	0.00016	0.0015	0.00024	0.00014	0.00027	0.0002	0.00024
PFNA	0.004	0.00212	0.00049	0.004163	0.00147	0.000007	0.000051	0.000015	0.0000013	<0,00001	0.0000017	0.0000024
PFOA	0.034	0.045	0.016	0.19803	0.101	0.00009	0.0029	0.00015	0.00011	0.00018	0.00016	0.00019
PFOS	2	2.3	0.69	3.0872	0.444	0.0004	0.0094	0.00085	0.0003	0.00043	0.00049	0.00064
PFPeA	0.00146	0.00208	0.00075	0.004231	0.0038	0.00029	0.0012	0.00052	0.0001	0.00015	0.00014	0.00017

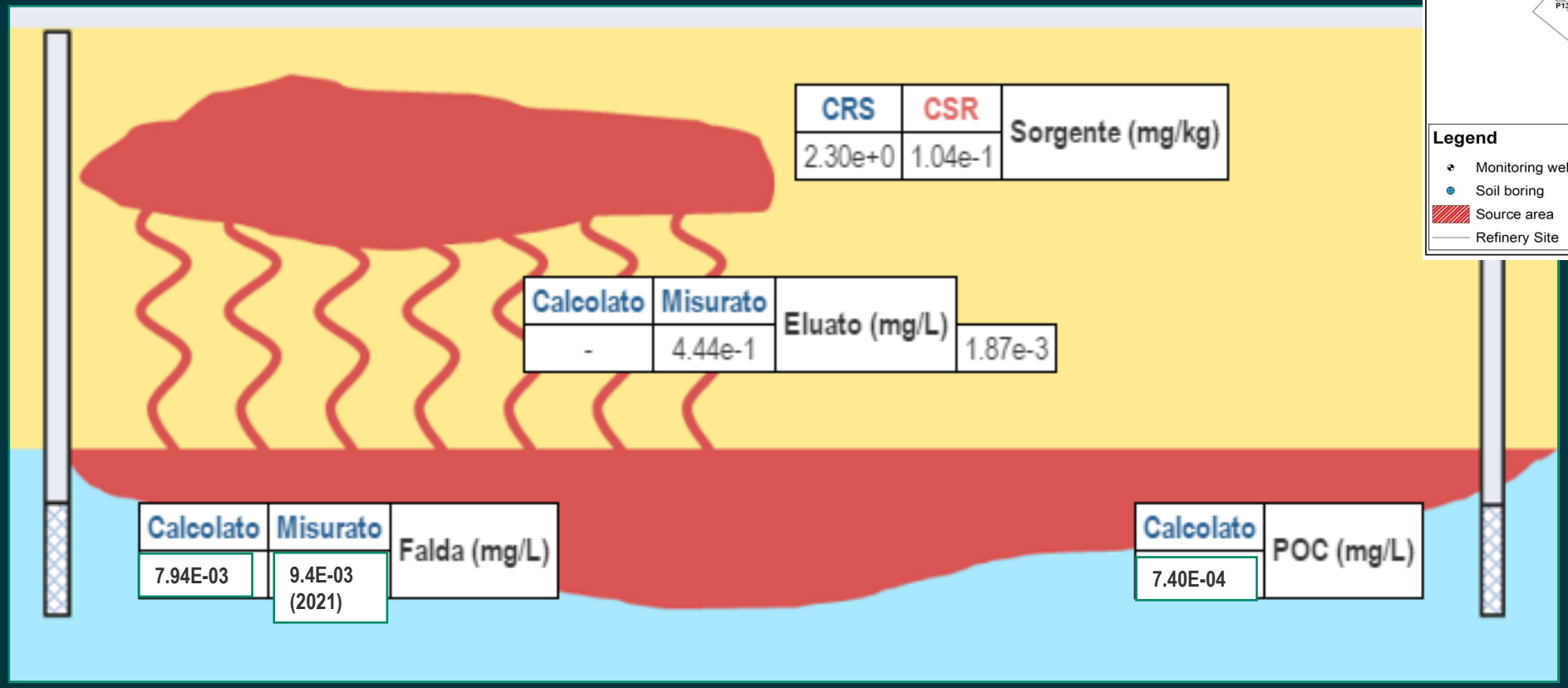
7.94E-03

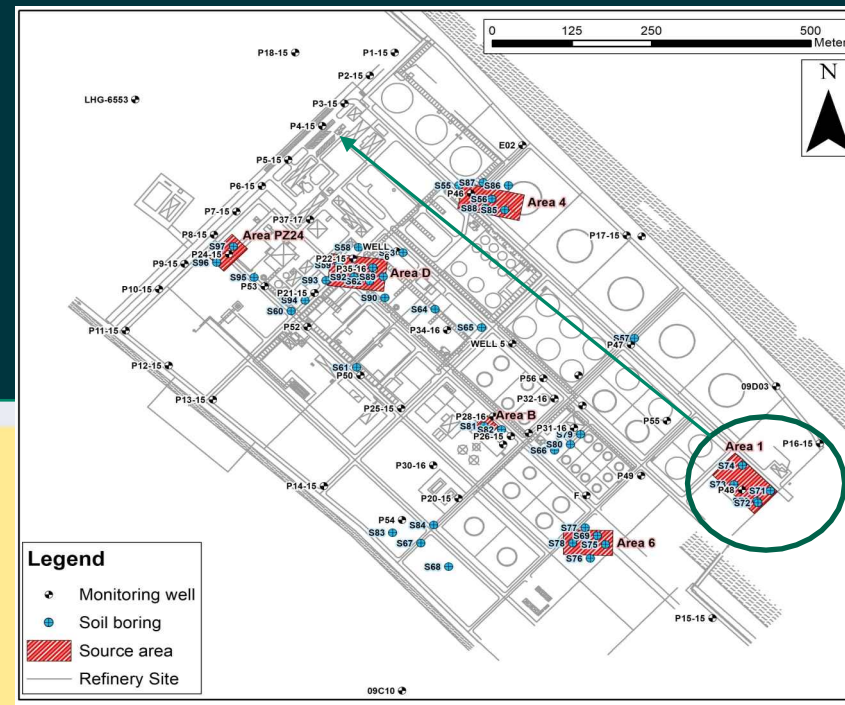


Area 1

Area 1.xlsx

- EPA 1316





Area 1

- EPA 1316

Static test EPA 1316

Concentrazione al POE - Percorso Eluato da Suolo Superficiale	concentrazione eluato	concentrazione attesa in falda	
Contaminante	Suolo superficiale	Cgw on-site	Cgw off-site
	mg/L	mg/L	mg/L
PFBA (User)	1.20E-03	2.15E-05	2.00E-06
PFBS (User)	1.99E-03	3.56E-05	3.32E-06
PFHpA (User)	8.00E-03	1.43E-04	1.33E-05
PFHxA (User)	7.20E-03	1.29E-04	1.20E-05
PFHxS (User)	9.50E-02	**1.70E-03**	1.58E-04
PFNA (User)	1.47E-03	2.63E-05	2.45E-06
PFOA (User)	1.01E-01	**1.81E-03**	1.68E-04
PFOS (User)	4.44E-01	**7.94E-03**	7.40E-04
PFPeA (User)	3.80E-03	6.79E-05	6.33E-06

Dynamic test EPA 1314

Concentrazione al POE - Percorso Eluato da Suolo Superficiale	concentrazione eluato	concentrazione attesa in falda	
Contaminante	Suolo superficiale	Cgw on-site	Cgw off-site
	mg/L	mg/L	mg/L
PFBA (User)	1.24E-03	2.21E-05	2.06E-06
PFBS (User)	2.28E-03	4.07E-05	3.80E-06
PFHpA (User)	1.49E-02	2.66E-04	2.48E-05
PFHxA (User)	9.03E-03	1.61E-04	1.50E-05
PFHxS (User)	2.12E-01	3.80E-03	3.54E-04
PFNA (User)	4.16E-03	7.44E-05	6.94E-06
PFOA (User)	1.98E-01	3.54E-03	3.30E-04
PFOS (User)	3.09E+00	5.52E-02	5.14E-03
PFPeA (User)	4.23E-03	7.56E-05	7.05E-06

Leaching test 2:1

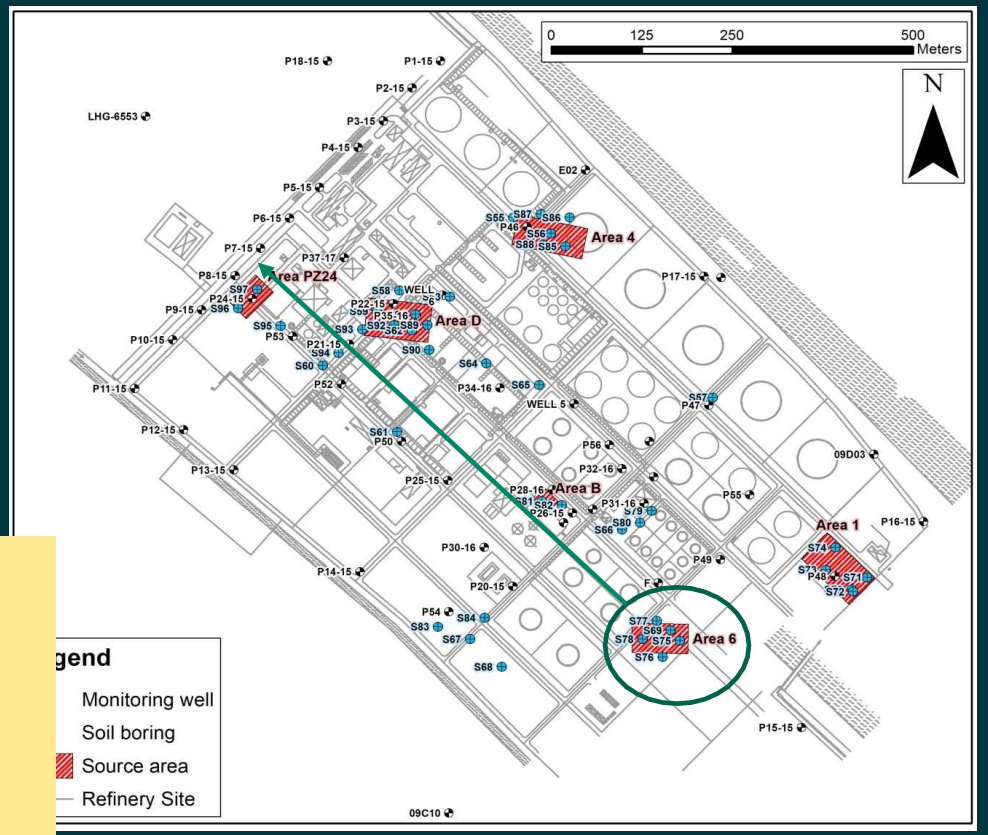
Concentrazione al POE - Percorso Eluato da Suolo Superficiale	concentrazione eluato	concentrazione attesa in falda	
Contaminante	Suolo superficiale	Cgw on-site	Cgw off-site
	mg/L	mg/L	mg/L
PFBA (User)	2.30E-04	4.11E-06	3.83E-07
PFBS (User)	1.70E-05	3.04E-07	2.83E-08
PFHpA (User)	7.20E-04	1.29E-05	1.20E-06
PFHxA (User)	7.70E-04	1.38E-05	1.28E-06
PFHxS (User)	3.60E-03	6.44E-05	6.00E-06
PFNA (User)	4.90E-04	8.76E-06	8.16E-07
PFOA (User)	1.60E-02	2.86E-04	2.67E-05
PFOS (User)	6.90E-01	1.23E-02	1.15E-03
PFPeA (User)	7.50E-04	1.34E-05	1.25E-06

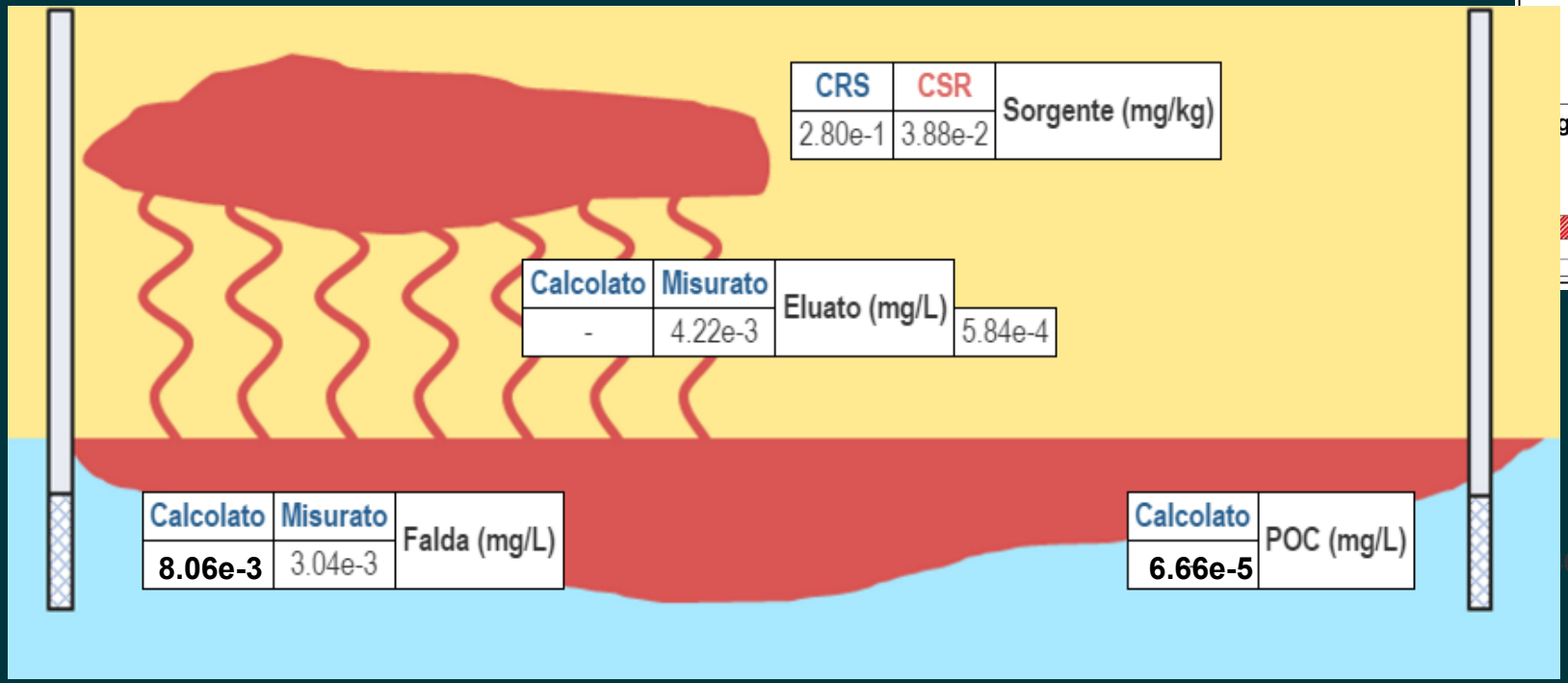
	GW concentration POC=0 mg/l			
	P-48			
	10/2/2020	5/27/2021	3/28/2022	Average
PFBA	1.10E-04	4.30E-04	1.40E-04	2.27E-04
PFBS	2.20E-05	2.10E-05	6.10E-06	1.64E-05
PFHpA	6.40E-05	1.10E-03	1.80E-04	4.48E-04
PFHxA	**1.80E-04**	**8.60E-04**	**3.10E-04**	4.50E-04
PFHxS	1.60E-04	1.50E-03	2.40E-04	6.33E-04
PFNA	7.00E-06	5.10E-05	1.50E-05	2.43E-05
PFOA	9.00E-05	2.90E-03	1.50E-04	1.05E-03
PFOS	**4.00E-04**	**9.40E-03**	**8.50E-04**	3.55E-03
PFPeA	2.90E-04	1.20E-03	5.20E-04	6.70E-04

Concentrazione al POE - Percorso Eluato da Suolo Superficiale	concentrazione eluato	concentrazione attesa in falda	
Contaminante	Suolo superficiale	Cgw on-site	Cgw off-site
	mg/L	mg/L	mg/L
PFBA (User)	1.20E-03	2.15E-05	2.00E-06
PFBS (User)	1.99E-03	3.56E-05	3.32E-06
PFHpA (User)	8.00E-03	1.43E-04	1.33E-05
PFHxA (User)	7.20E-03	1.29E-04	1.20E-05
PFHxS (User)	9.50E-02	1.70E-03	1.58E-04
PFNA (User)	1.47E-03	2.63E-05	2.45E-06
PFOA (User)	1.01E-01	1.81E-03	1.68E-04
PFOS (User)	4.44E-01	7.94E-03	7.40E-04
PFPeA (User)	3.80E-03	6.79E-05	6.33E-06

Area 6

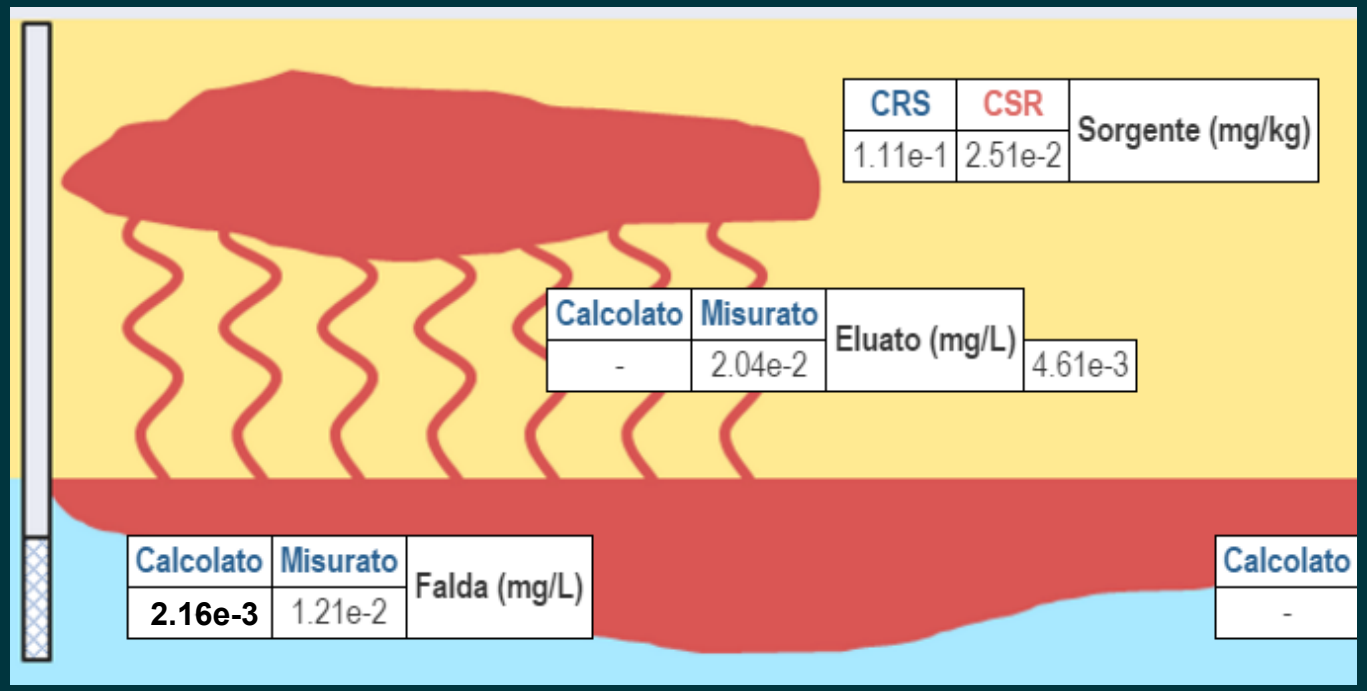
- Area 6.xlsx
  - EPA 1314
  - P28-16, located at approximately 150 m from source

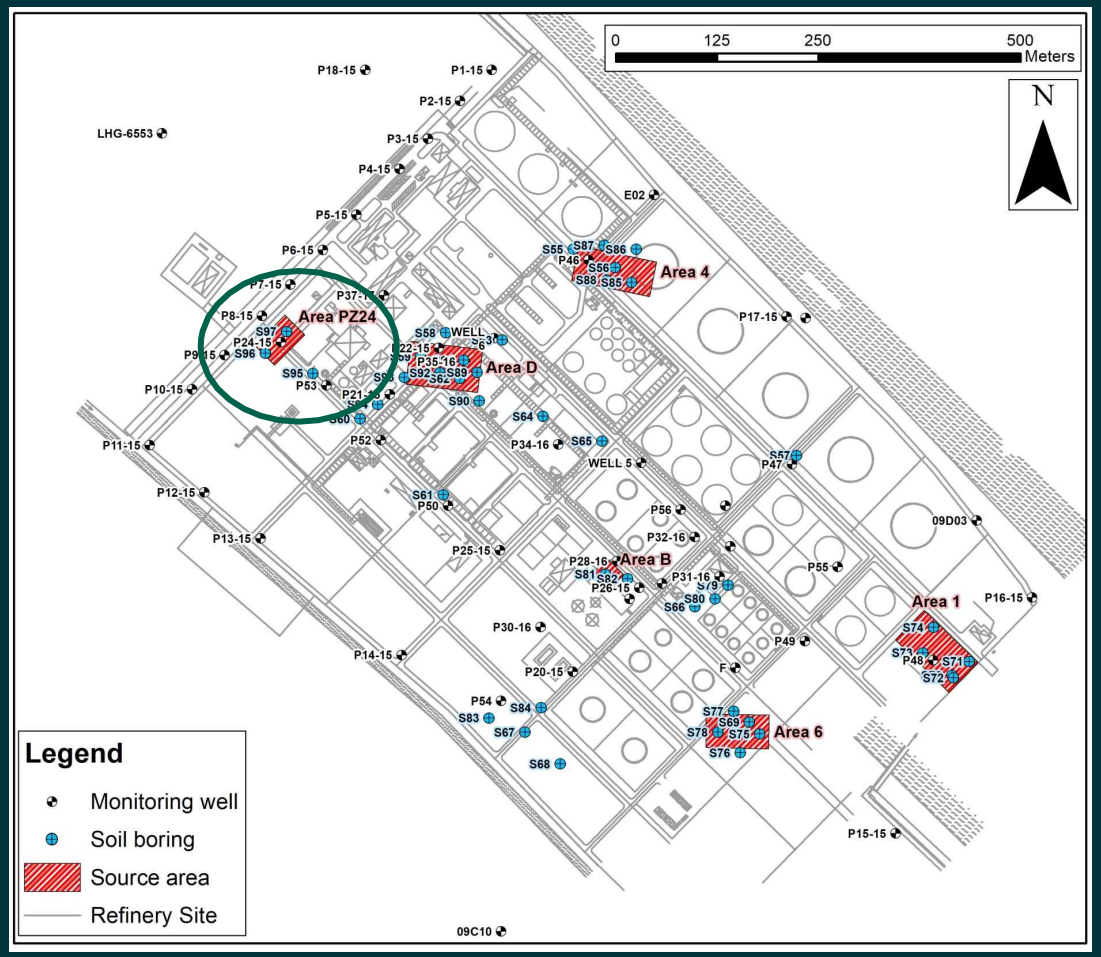




Area PZ24

- Area PZ24.xlsx
  - EPA 1314
  - POC = site downgradient boundary, likely getting impact from other sources located upgradient





03

Validation

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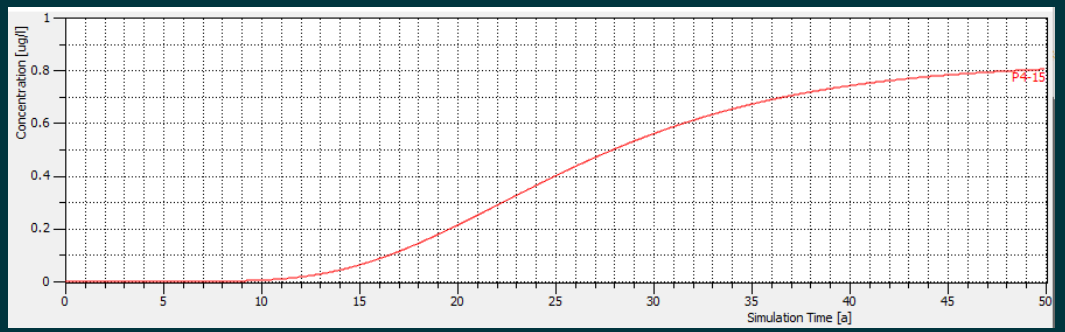
Validation of the modelled concentration at the POC with the numerical model calibrated in 2021 for Area 1

- The concentration of PFOS modelled at the POC was validated with the use of a finite elements numerical model (Feeflow® code), calibrated with 2021 groundwater concentrations
- **50** years simulation time
- Area 1 PFOS mass-flux (2nd-kind) BC as from calibrated 2021 numerical model (i.e. 1.7E-04 g/m^2/d), corresponding to a flux deriving from leachate concentration of 0.444 **mg/l (leachate test EPA 1316 results)**
- Numerical model simulated PFOS concentrations at POC of **8.0E-04 mg/l**
- Analytical model simulated PFOS concentrations at POC of **7.4E-04 mg/l**
- Average measured (Jan and Oct 2020, May 2021) PFOS concentration at POC of **6.7E-04 mg/l**

POC simulated PFOS concentrations



Validation of the site–specific Log Koc value for PFOS - Area 1

$$K_{ws} = \frac{C_{sol}}{C_{tot}} = \frac{\rho_s}{\left(K_d \cdot \rho_s + \theta_w + H \cdot \theta_a\right)}$$

$$K_d = K_{oc} \times f_{oc}$$

$$koc = \frac{\rho s - kws\theta w - kwsH\theta a}{\rho s * kws * foc}$$

INPUT	
Csol (mg/l):	0.444
Ctot (mg/kg)	2.3
ρs (g/cm3)	1.7
θw (-)	0.288
θa (-)	0.057
H (-)	1.81E-05
foc (-)	0.01052

OUTPUT	
Kws	0.193043
Kd	5.01E+00
Koc	4.76E+02
log K_{oc}	2.7

Table 1
Published distribution coefficients derived from laboratory sorption experiments ($\log K_d$, $\log K_{OC}$).

Sample	$\log K_d$ ($\log$l kg^{-1})	$\log K_{OC}$	References
PFOS			
Five sediments with C_{org} of 0.56–9.66%, dithionite–citrate–bicarbonate extractable iron of 116–1025 μmol/g	–	2.7	Higgins and Luthy (2006)
Ottawa sand standard	2.81	–	Johnson et al. (2007)
Kaolinite	5.31	2.4	Johnson et al. (2007)
Goethite	7.88	–	Johnson et al. (2007)
High iron sand standard	8.90	–	Johnson et al. (2007)
Lake Michigan sediment	7.52	2.4–2.6	Johnson et al. (2007)
Clay	18.3	2.8	3 M corp. cited in Johnson et al. (2007)
Clay loam	9.72	2.6	3 M corp. cited in Johnson et al. (2007)
Sandy loam	35.3	3.1	3 M corp. cited in Johnson et al. (2007)
River sediment	7.42	2.8	3 M corp. cited in Johnson et al. (2007)
Water treatment sludge	120	2.5	3 M corp. cited in Johnson et al. (2007)
Paddy soil (0.91% C_{org}) at c(water) = 5.0 μg l^{-1}	–	3.3	Chen et al. (2009)
Crude oil spiked to soil	–	4.2–4.4	Chen et al. (2009)
Oil-derived black carbon (diesel soot), c(water) = 5–50 μg l^{-1} at pH = 5.05	–	3.0–3.1	Chen et al. (2009)
Aquifer sediment Washington County, USA (t = 0)	0.1	2.5	Ferrey et al. (2009)
Aquifer sediment Washington County (t = 574 d)	−0.7	2.8	Ferrey et al. (2009)
Taihu Lake	–	2.9 ± 0.6	Yang et al. (2011)
Sediment 1	1.2	4.7	Ahrens et al. (2011)
Sediment 2	1.2	3.0	Ahrens et al. (2011)
Sediment 3	1.9	3.8	Ahrens et al. (2011)
Average PFOS ($\log$l kg^{-1})		3.0	
Standard deviation PFOS ($\log$l kg^{-1})		0.7	
Coefficient of variation PFOS (%)		21	
Median PFOS ($\log$l kg^{-1})		2.8	

Conclusions and limitations

- Leaching test results performed with EPA Method 1314 and 1316 could be used to define site specific soil target concentrations to reach acceptable concentrations in groundwater at the site downgradient boundary

- Significant differences in leaching test results conducted with 2:1 L/S with results obtained from EPA 1314 and 1316 were recorded in Area 1. For Area 6 and PZ24 results of EPA 1314 and 2:1 L/S were similar. Consequently, site-specific target values could be derived based on 2:1 L/S leaching test also for other source areas

- The work has been performed only on 3 source areas; additional validation of the method applied may be required

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