

Development of Soup Tests for the Risk assessment of NER in Soil. LRI-ECO25

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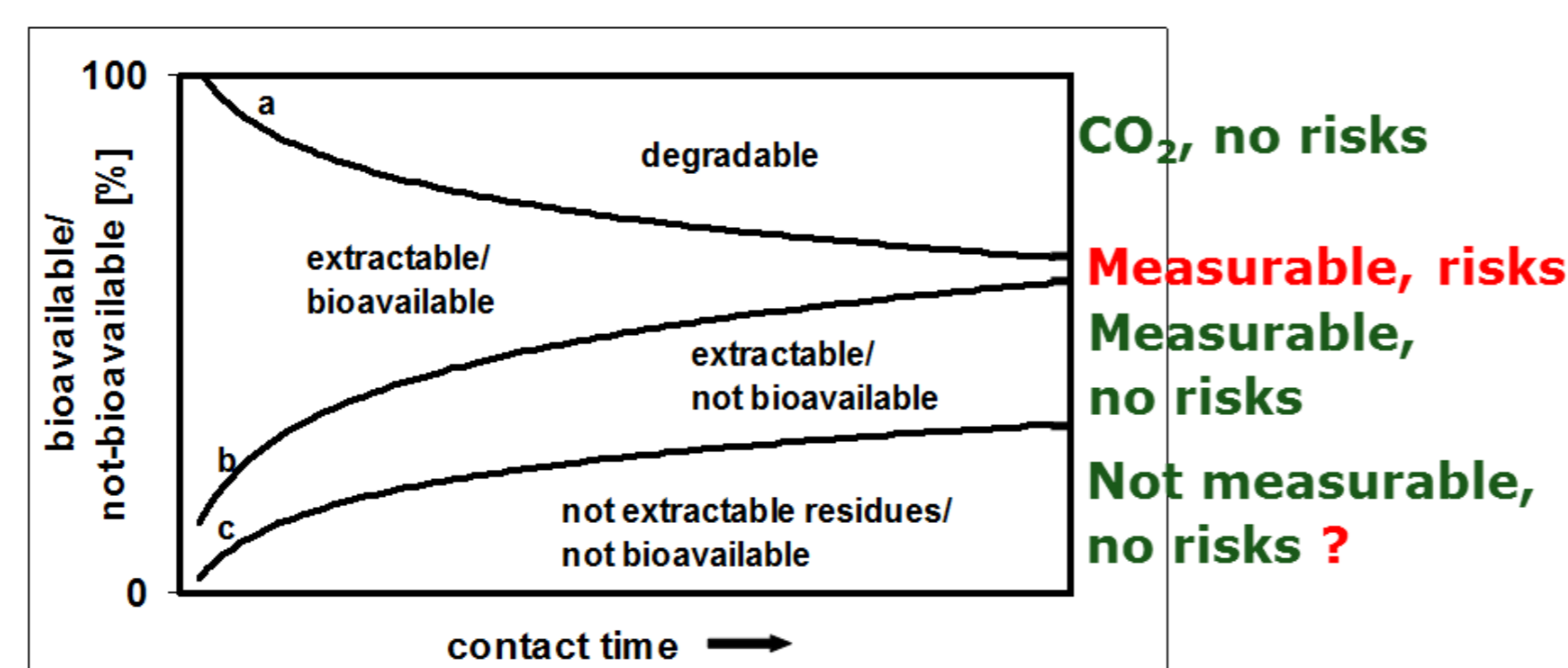
Background

Two ECETOC reports:

- TR 117: Understanding the Relationship between Extraction Technique and Bioavailability.
 - TR 118: Development of interim guidance for the inclusion of non-extractable residues (NER) in the risk assessment of chemicals.
- On the moment NER is considered differently: as a chemical time bomb or as a sustainable detoxification.

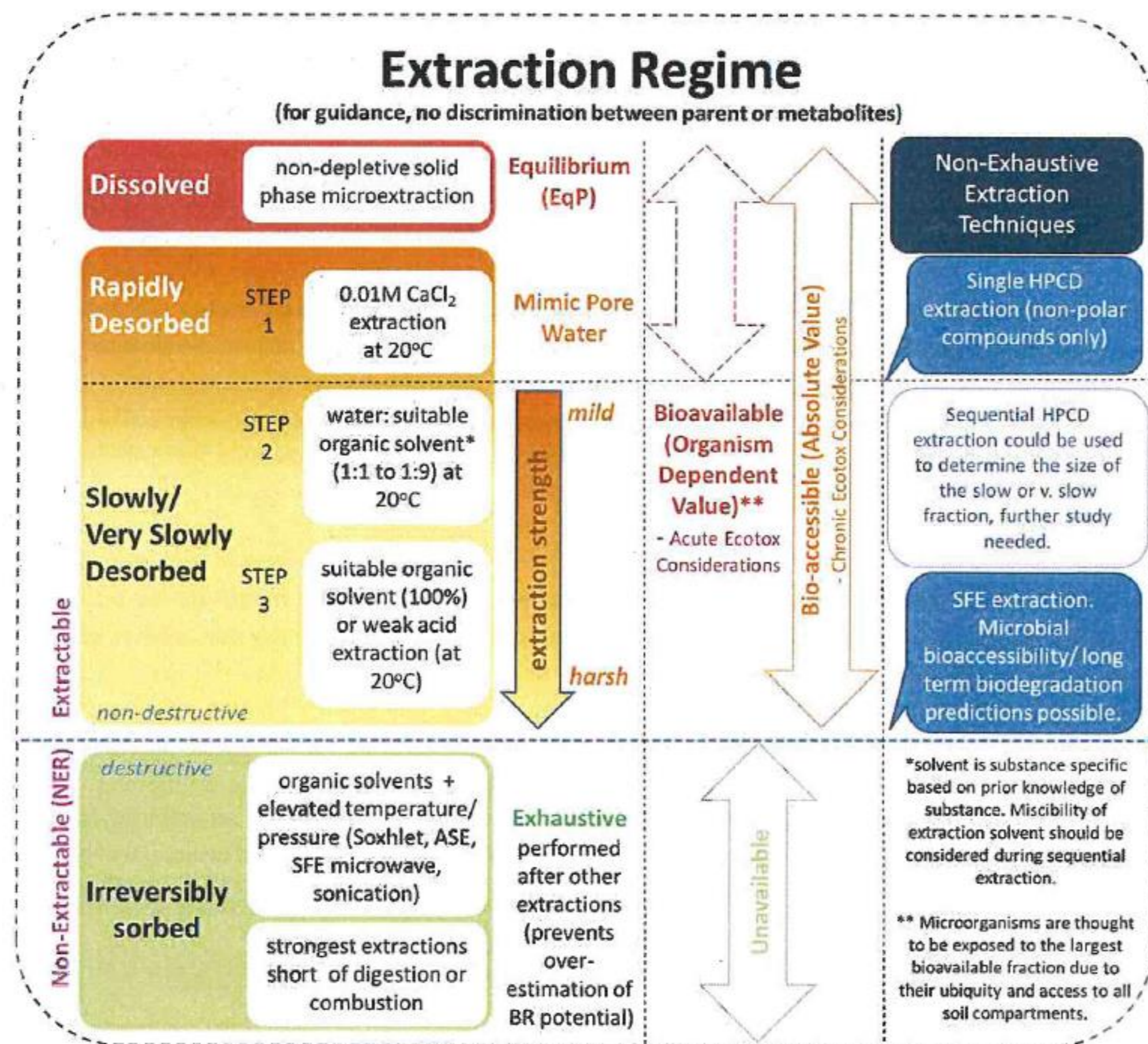
Objective

- Validate the extraction regime of ECOTOC TR 117.
- Develop a "soup test" to assess the toxicity of the different fractions of chemicals.
- provide a clear, mechanistically driven definition to NER and residual toxicity caused by NER.



Conceptual approach

Available extraction techniques are included in Extraction Regime of TR117



In our approach we define the desorption by a sum of three first order decreases as also used by Cornelissen et al, 1997, Harmsen, 2004, ISO17402 and Rhodes et al., 2010).

$$\frac{C_t}{C_0} = F_{rapid} \cdot e^{-k_{rapid} \cdot t} + F_{slow} \cdot e^{-k_{slow} \cdot t} + F_{very\ slow} \cdot e^{-k_{very\ slow} \cdot t}$$

Where:

- C_t = soil sorbed amount (mg/kg d.m.) at time t (y)
- C_0 = soil sorbed amount (mg/kg d.m.) at time 0
- F_{rapid} = fraction of contaminant in rapid desorbing compartment
- F_{slow} = fraction of contaminant in slow desorbing compartment
- $F_{very\ slow}$ = fraction of contaminant in very slow desorbing compartment
- k_{rapid} = rate constant rapid desorption (y^{-1})
- k_{slow} = rate constant slow desorption (y^{-1})
- $k_{very\ slow}$ = rate constant very slow desorption (y^{-1}).

In the mathematical model no non-desorbing fraction is defined. Tenax/cyclodextrine can be used to measure F_{rapid} and F_{slow} .

Using desorption, availability is a matter of time. On geological scale everything will become available if it does not degrade meanwhile. Which part should be considered as non-available?

Fraction	Slurry system (test method)		Unsaturated system (soil)		Method
	Desorption time	Desorption coefficient (year ⁻¹)	Desorption time	Desorption coefficient (year ⁻¹)	
Dissolved	0		0		SPME or SPE, 0.01 M CaCl ₂
Rapidly desorbing	1 day	2600	Weeks to months	>3	HPCD or Tenax 1 day at 20°C (ISO 16751-1)
Slowly desorbing	week	7	Months to years	0.33	HPCD or Tenax during ²⁾ 1 week at 20°C or one day at elevated temperature (60°C)
Very slowly desorbing	Months to year	0.1-0.3	decade	0.03	Exhaustive extraction
Irreversibly sorbed	Years to decades	<0.01	Centuries	<0.001	Organic solvent + destruction of matrix Isotope studies for fraction that cannot be extracted with any method

Selection of chemical

Criteria: (1) occurrence in soil and/or sediment, (2) formation of NER, (3) relevant effect on benthic and/or soil organisms, (4) sufficient analytical accuracy for different extraction methods, (5) known biodegradation and metabolism in soils, (6) variety of chemistry, (7) availability of ¹⁴C radiolabelled compound

1. Trinitrotoluene TNT
2. Cypermethrin
3. Carbendazim
4. Benzo(a)pyrene

- Chemicals can be measured sensitive, using LC/MS.
- Toxicity can be followed using simple bioassays (e.g. microtox, *Daphnia*).
- Earthworm tests are less sensitive (confirmation).
- Suitability of Tenax/cyclodextrine (ongoing).

The way to go

- C14-studies in order to assess partitioning over different fractions of test soil.
- Comparison of C-14 study results to standard chemical analysis of the measurable fractions.
- Measurement of formation speed of NER.
- Use of suitable bioassays to follow toxicity in extracts AND extracted soils.
- Translate the research results in explainable recommendations for regulators.