Modelling of CECs

Screening for possible CECs with a potential for adverse affects in remote regions due to LRAT (Aarhus) / LRET (Stockholm) using the Emissions Fractions Approach

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CECs in the context of CLRTAP?

Aarhus Protocol on POPs, Article 1: Definitions

7. POPs are organic substances that: (a) possess toxic characteristics; (b) are persistent; c) bioaccumulate; (d) are prone to LRAT and deposition; and (e) are likely to cause significant adverse human health or environmental effects near to and distant from their sources.

9. "Emission" means the release of a substance from a point or diffuse source into the atmosphere.

Aarhus Protocol on POPs, Article 2: Objective

The objective of the present Protocol is to control, reduce or eliminate discharges, emissions and losses of POPs.

Aarhus Protocol on POPs, Article 8: Research, development and monitoring

The Parties shall encourage research, development, monitoring and cooperation related, but not limited, to
(a) Emissions, LRT and deposition levels and their modelling, [...], the elaboration of procedures for harmonizing relevant methodologies.

CECs in the context of CLRTAP

Aarhus Protocol on POPs, Article 14: Amendments

1. Any Party may propose amendments to the presented Protocol
6 (a): The proposer shall provide the Executive Body (EB) with the information specified in EB decision 1998/2, including any amendments thereto:

Submission of a Risk Profile

a) Potential for LRAT, vapor pressure < 1,000 Pa, atmospheric half-life > 2 days; and
b) Toxicity: Potential to adversely affect human health and/or the environment; and
c) Persistence: Evidence half-lives: Water > 2 months, or Soil > 6 months, or Sediments > 6 months (alternatively, evidence that the substance is otherwise sufficiently persistent to be of concern)
d) Bioaccumulation: BCF/BAF > 5,000 or log K_{OW} > 5; or high toxicity

My interpretation: CECs are chemicals (typically not regulated) that may have a potential to cause adverse human health or environmental effects in remote regions due to LRAT and atmospheric deposition.

EB decision 1998/2 (EB.AIR/WG.5/52, Annex II) on information to be submitted for adding substances [...]

Stockholm Convention on POPs

Global treaty to protect human health and the environment from POPs, incl. remote areas such as the Arctic. (Not control, reduce or eliminate discharges, emissions and losses of POPs - Aarhus)

Nomination process:

a) Screening criteria (Annex D)

Persistence, Bioaccumulation, Toxicity, Long-range environmental transport potential (LRTP) and atmospheric half-life > 2 days

b) Draft risk profile (Annex E)

"the purpose is to evaluate whether the chemical is likely, as a result of its LRET, to lead to significant adverse human health and/or environmental effects, such that global action is warranted."

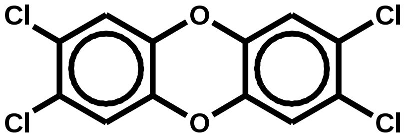
The tiered screening in the SC is built on the premise that a chemical needs to fulfill the four criteria in order to fulfil the ultimate listing

What is required for a chemical to elicit adverse effects due to LRAT / LRET?

Deposition (Aarhus) / Transfer (Stockholm) to remote regions and accumulation (inhalation in the remote areas is not the main concern)

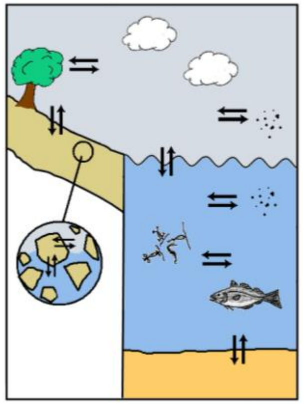
The OECD Tool (Wegmann et al 2009)

Model input:



Chemical Data

Chemical Emissions



Environmental Data

The OECD P_{OV} and LRTP Screening Tool ("The Tool") for assessing chemicals for persistence (P) and long-range transport potential (LRTP)

Model

Model equations reflecting mechanistic knowledge (consensus)

Model output:

- 2 LTRP metrics
- Overall persistence

Chemical data

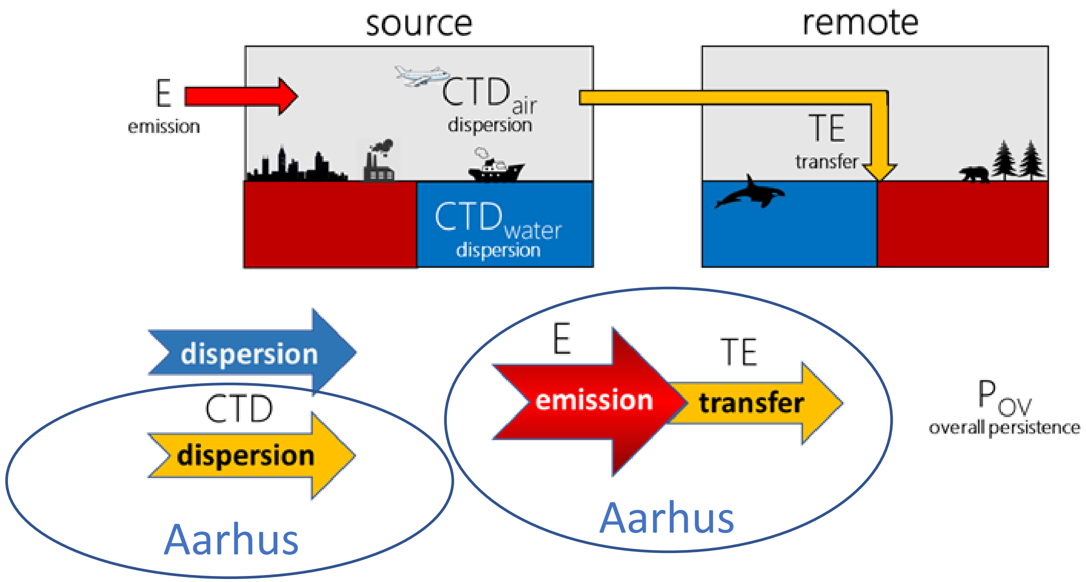
- Log K_{OW}, log K_{AW}
- Degradation half-lives in air, water and soil

Emission scenarios (for each chemical)

- 100% to air, 100% to water, 100% to soil

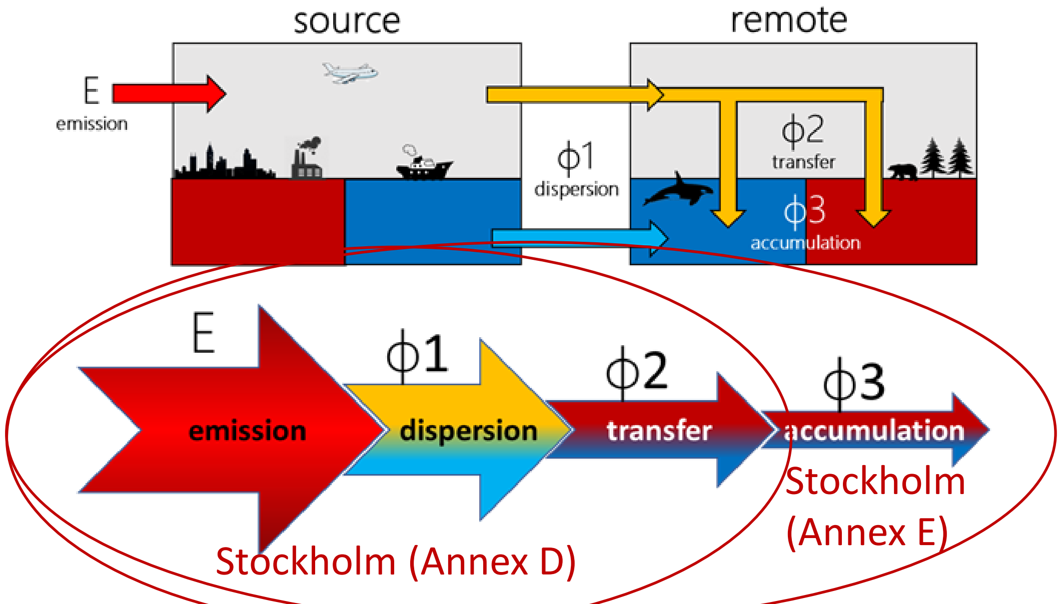
The OECD Tool (Wegmann et al 2009)

a) CTD, TE and P_{OV}



- Screens for "POP-like" LRTP-P_{OV} (hazard)
- TE: LRAT only ("Aarhus protocol")
- No integrated treatment of LRT via air and water and TE>100% (no rev. dep.)
- Metrics are not coherent
- No target-oriented metric (accumulation)

b) EFA (ϕ1, ϕ2, ϕ3)



- Net atmospheric deposition
- LRAT and LRWT are additive
- Metrics are coherent and multiplicative
- Allows distinction between transfer to versus accumulation in remote surface media

(requires a MM with surface compartments)

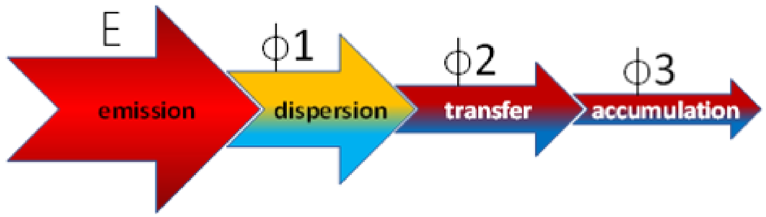
Breivik et al 2022 Environ. Sci Technol 56: 11983-11990

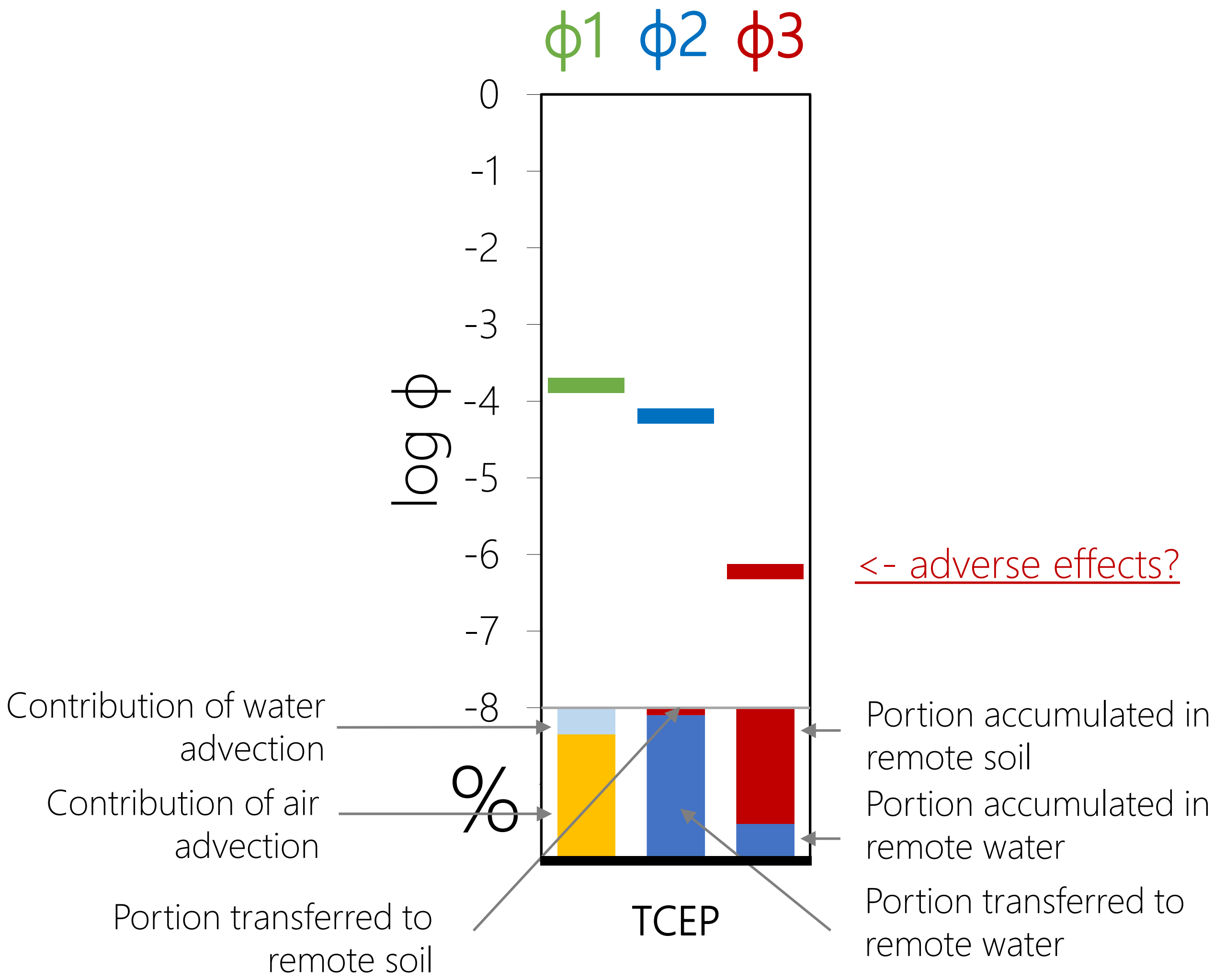
The emission fractions approach to LRTP assessment

Illustration of the approach:
TCEP
100% emissions to air

Fraction of emissions which is:

- Dispersed (LRAT+LRWT) [ϕ1]
- Transferred to remote surface [ϕ2]
- Accumulated in remote surface [ϕ3]





Breivik/McLachlan/Wania (2022)

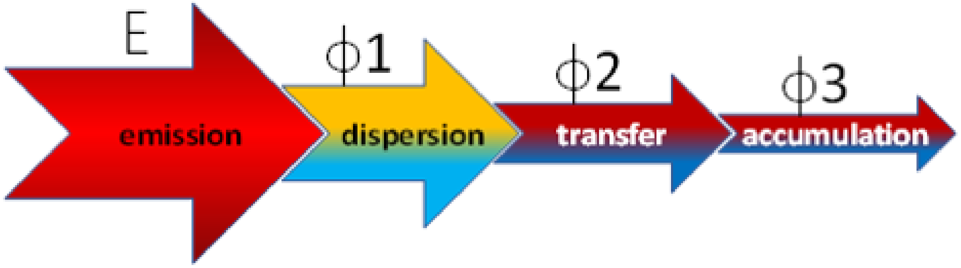
ϕ3

The emission fractions approach to LRTP assessment

Illustration of the approach:
Chemical report by emission scenario

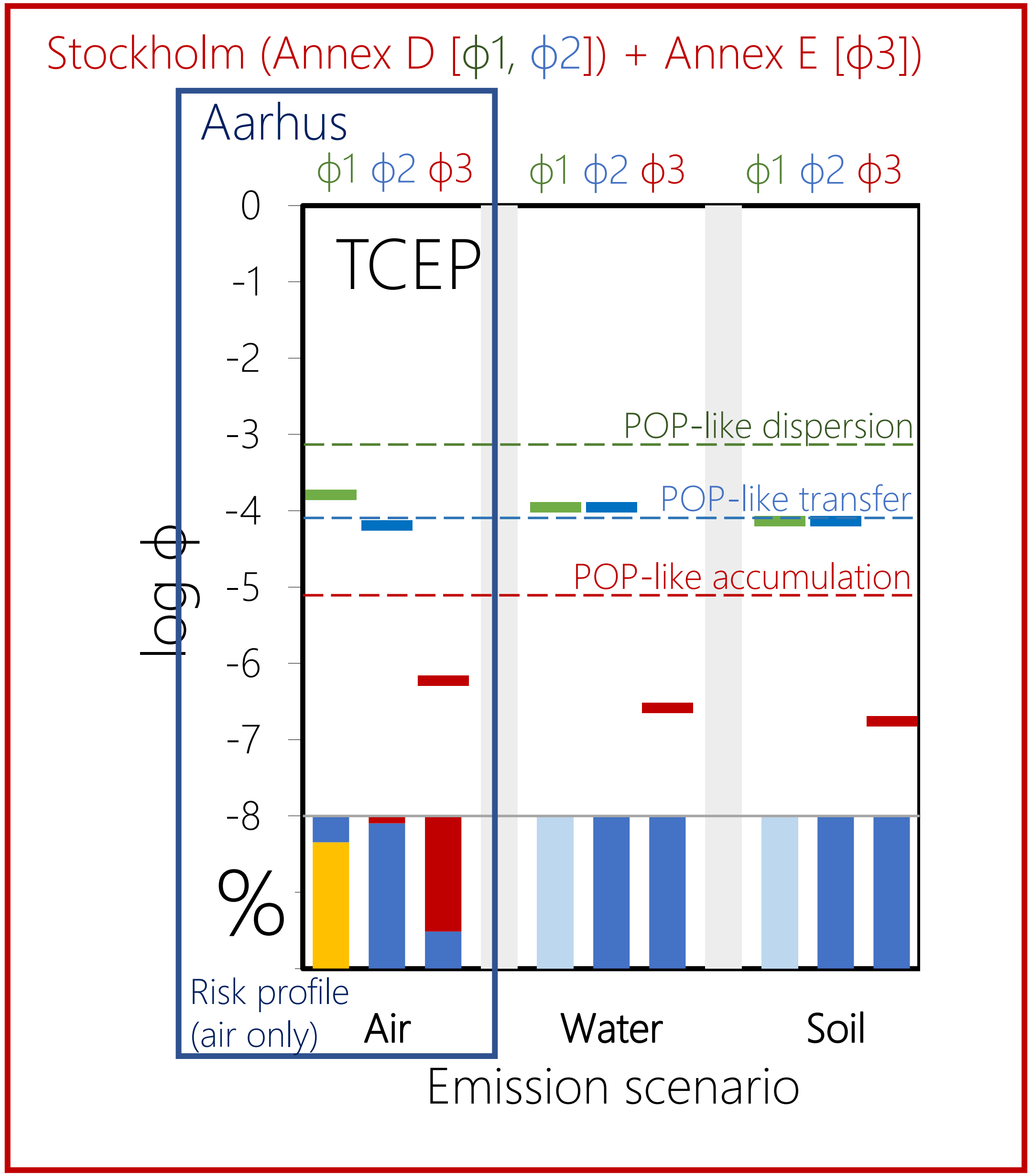
Opportunities for benchmarking *)

- - - - - - POP-like dispersion
- - - - - - POP-like transfer
- - - - - - POP-like accumulation



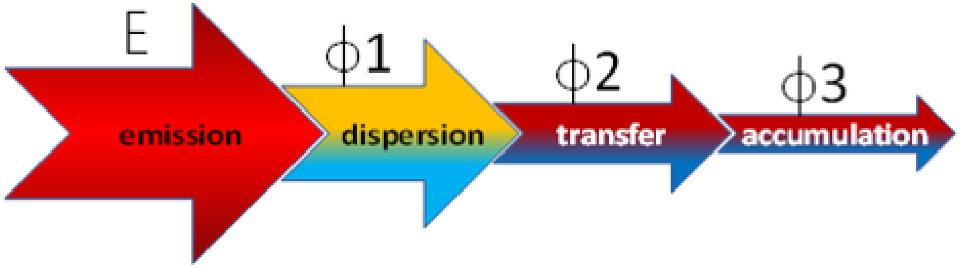
Thresholds: not a scientific question but a political one and likely dependent on policy context (Aarhus vs SC)

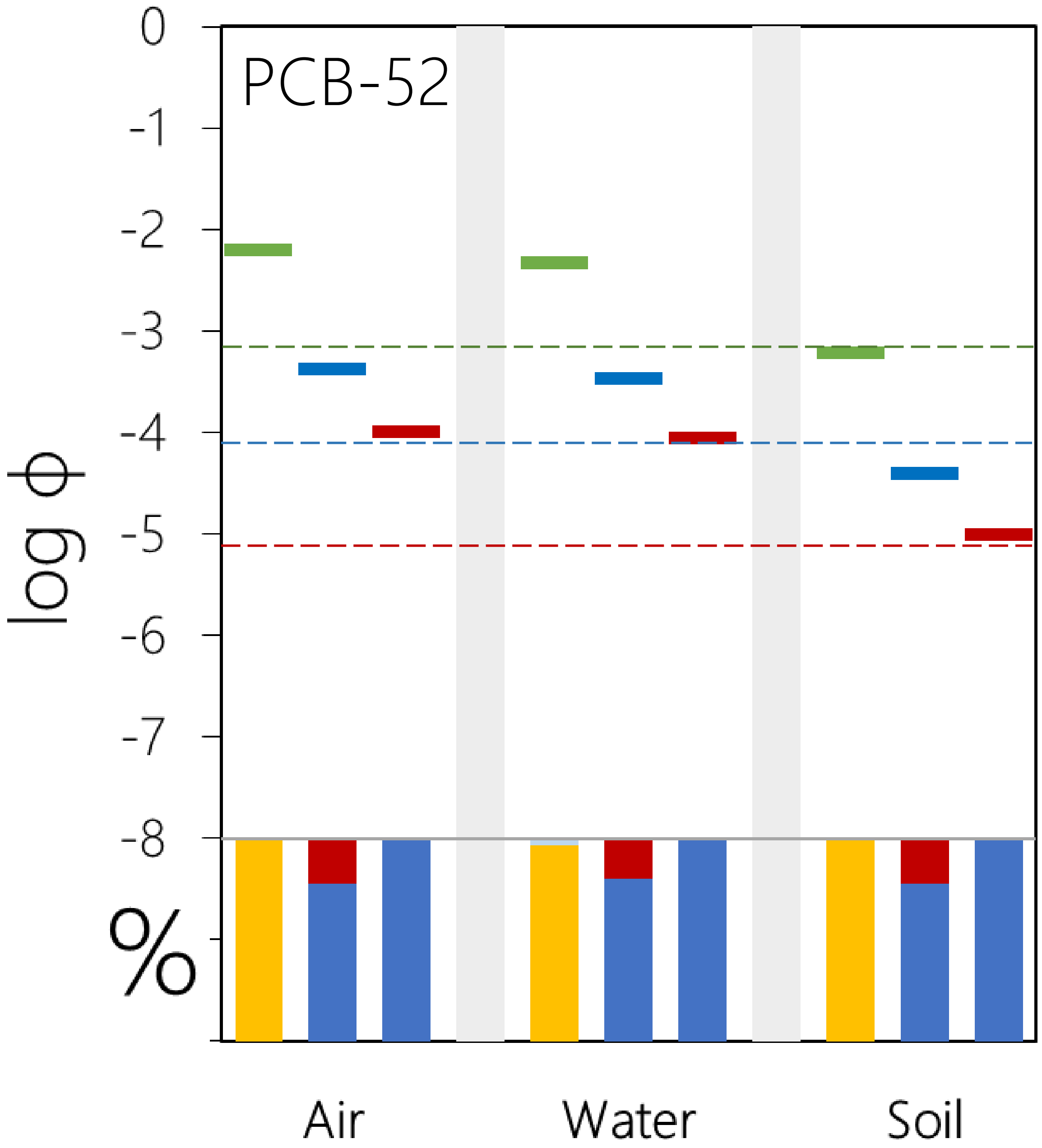
Breivik/McLachlan/Wania (2022)



Some Examples

POP-like dispersion
POP-like transfer
POP-like accumulation





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POP-like transfer
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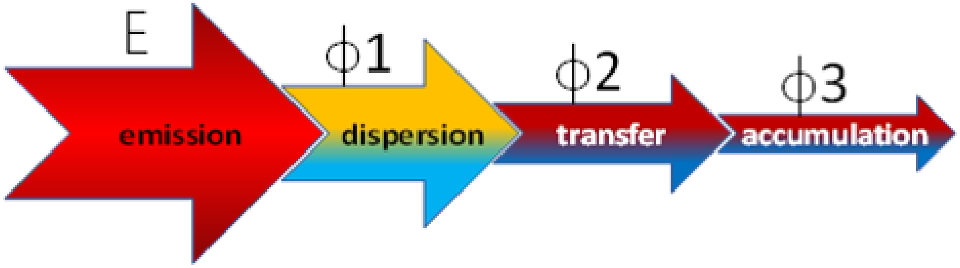
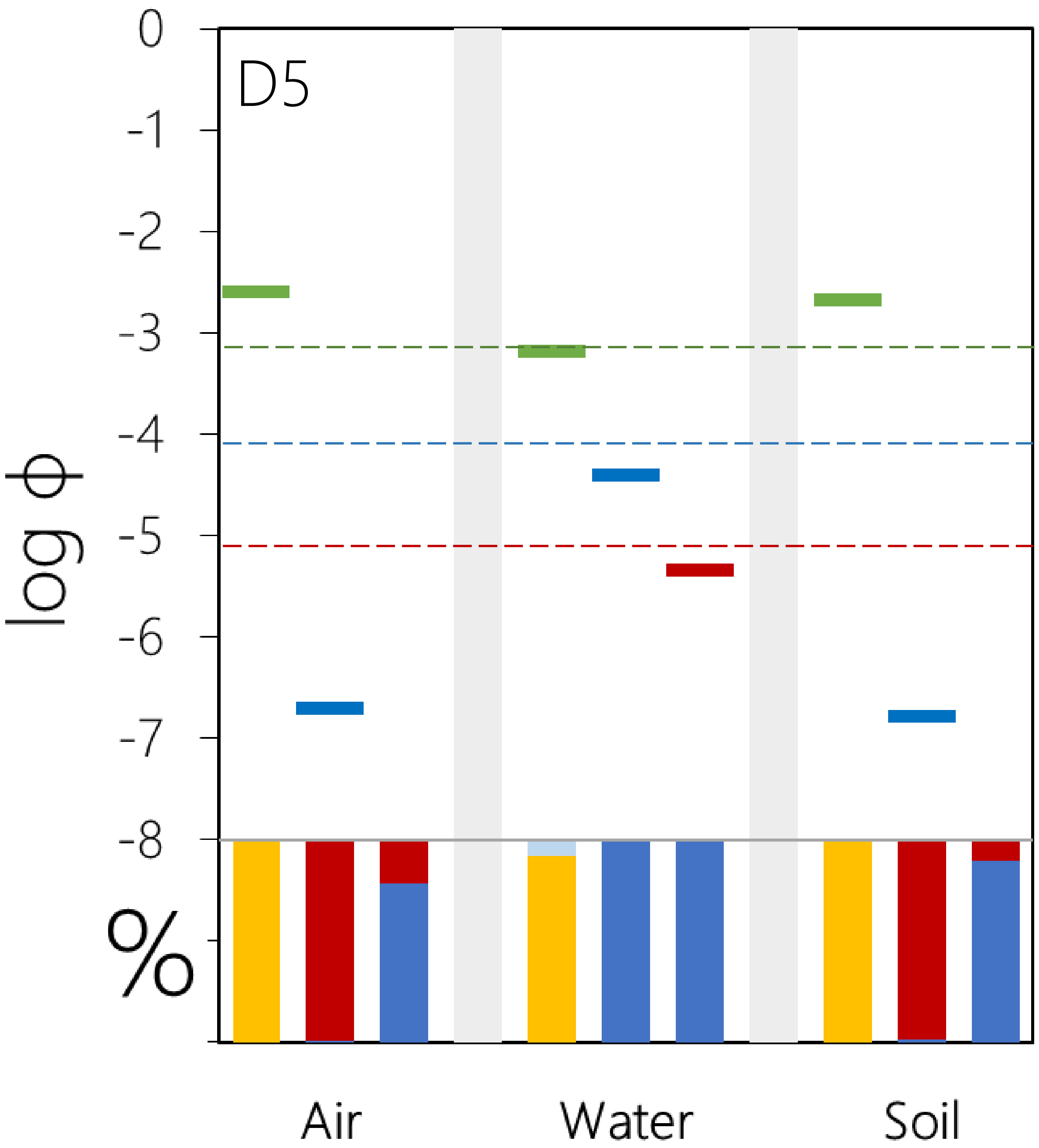
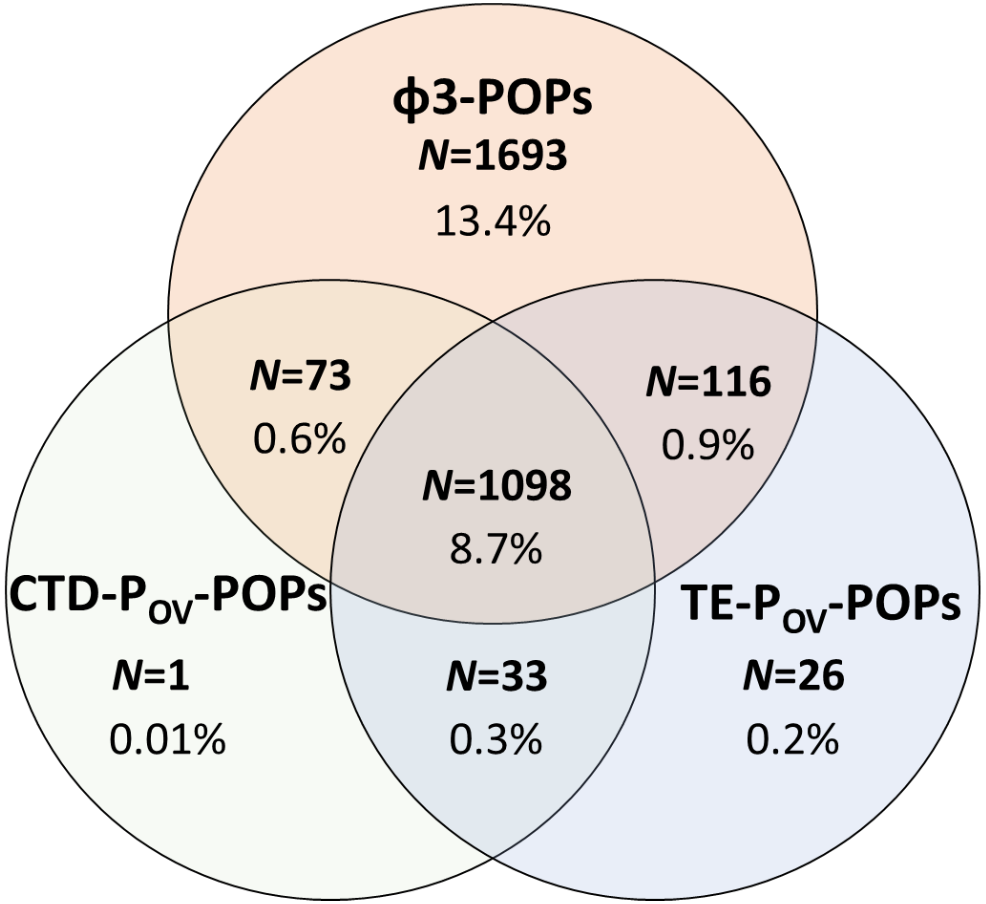




The OECD Tool with existing and EFA metrics
(non-regulatory screening of 12,615 HPVs)



The EFA classifies a larger number of HPVs as having the potential for accumulation in remote regions than is classified as POP-like by the existing method recommended by the OECD (CTD/TE-P_{OV}).

Breivik K, McLachlan MS, and Wania F. 2023. **Added value of the emissions fractions approach when assessing a chemical's potential for adverse effects as a result of long-range transport.** Environ. Sci. Advances. 2. 1360 DOI: 10.1039/d3va00189j

Implications for LRTP assessments

The EFA identifies chemicals capable of accumulating in remote regions without fulfilling the criterion for persistence.
Using simpler metrics (such as half-life criteria, P_{OV}, and LRTP-P_{OV} combinations) in a hazard-based assessment according to Annex D is problematic as it may prematurely screen out many of the chemicals with potential for adverse effects as a result of LRET.

The SC is not targeting chemicals that meet formal criteria of P, B, LRTP, and T (Annex D). These criteria rather are meant to aid in the task of identifying chemicals that are to lead to significant adverse human health and/or environmental effects (Annex E).

The remote accumulation fraction of the EFA is the LRATP/LRTP assessment metric most suited for the risk assessment stage (Annex E of the SC).

-> CECs with a potential to accumulate may deserve attention (CLRTAP/SC).

Stockholm Convention POP Recommendation Committee (POPRC-19): FAO Headquarters, Rome, 9-13 October 2023