Modeling Environmental Pollutants

Lecture 13

Screening Chemicals for Persistence and Long-range Transport Potential

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Christian Bogdal
Model Screening for chemicals with potential for persistence and long-range atmospheric transport

OECD Screening Tool


OECD Screening Tool

Calculated Metrics

Overall Persistence of chemical \(i (P_{OV,i})\)

\[
P_{OV,i} = \frac{M_{i,TOT}}{F_{DEG,i,A} + F_{DEG,i,W} + F_{DEG,i,S}} \quad (d)
\]

Characteristic Travel Distance of \(i (CTD_i)\)

\[
CTD_i = \frac{M_{i,TOT}}{F_{i,E}} \times \frac{M_{i,i}}{M_{i,TOT}} \times v_i \quad (km)
\]

Transport Efficiency \(i (TE_i)\)

\[
TE_i = \frac{F_{i,D}}{F_{i,E}} \times 100\% = \frac{F_{i,D} \times F_{i,A}}{F_{i,E}^2} \times 100\%
\]
OECD Tool: User Interface and Input Data

- Left: databases
- Right: single chemical

Chemical property data required:
- $\log K_{aw}$
- $\log K_{ow}$

Degradation half-lives:
- air
- water
- soil

Available:
OECD Tool: Results

- Left graph: CTD vs. $P_{ov}$
- Right graph: TE vs. $P_{ov}$

With lines for comparison with POP reference chemicals.