National Institute for Public Health
and the Environment
*Ministry of Health, Welfare and Sport*

# Screening for PMT

## How to identify PMTs

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# Criteria or screening values

- Criteria
  - Criteria facilitate prospective risk assessment
  - Criteria require amendment of REACH legislation
  - Mobility criterion has no defined endpoint

- Screening values
  - Screening values could be lower tier
    - log $K_{oc}$ in M assessment comparable to log $K_{ow}$ in B assessment

- Purpose: Suitable for SVHC (e.g. 57f) or general risk assessment?
  - SVHC is case-by-case assessment
    - Field data
    - Mostly retrospective assessment

# Developments of alternatives for OECD 305

- *In vitro* metabolism for fish
  - OECD guidelines and guidance document completed in 2018
    - BCFs more uncertain than BCFs from dietary exposure or minimised test
      - Additional step: Extrapolation from *in vitro* to overall *in vivo* degradation rate
- Bioaccumulation test with *Hyalella azteca*
  - CEFIC-LRI ECO 40 (Fraunhofer)
  - Invertebrate test
  - Aqueous bioconcentration tesy
  - *In vivo* test
  - Comparable to fish
  - Differences in metabolism (e.g. BaP)

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# Persistence

- Persistence criteria for PBT could be applicable
  - Includes screening criteria
  - Little discussion

- Inherent property of PMT: mobile
  - Low sorption
  - High solubility

- Relevant compartment is water
    - › Preferred simulation test is OECD 309

# Persistence crtieria

- Persistence criteria for surface water defined as:
  - P:
    - Degradation half-life in freshwater >40 d
    - Degradation half-life in marine water >60 d
  - vP:
    - Degradation half-life in fresh and marine water >60 d
- Persistence criteria for soil and sediment defined as:
  - P:
    - Degradation half-life in soil and freshwater sediment>120 d
    - Degradation half-life in marine water sediment>180 d
  - vP:
    - Degradation half-life in soil fresh and marine water sediment >180 d

# Mobility

- Endpoint for mobility is not clear

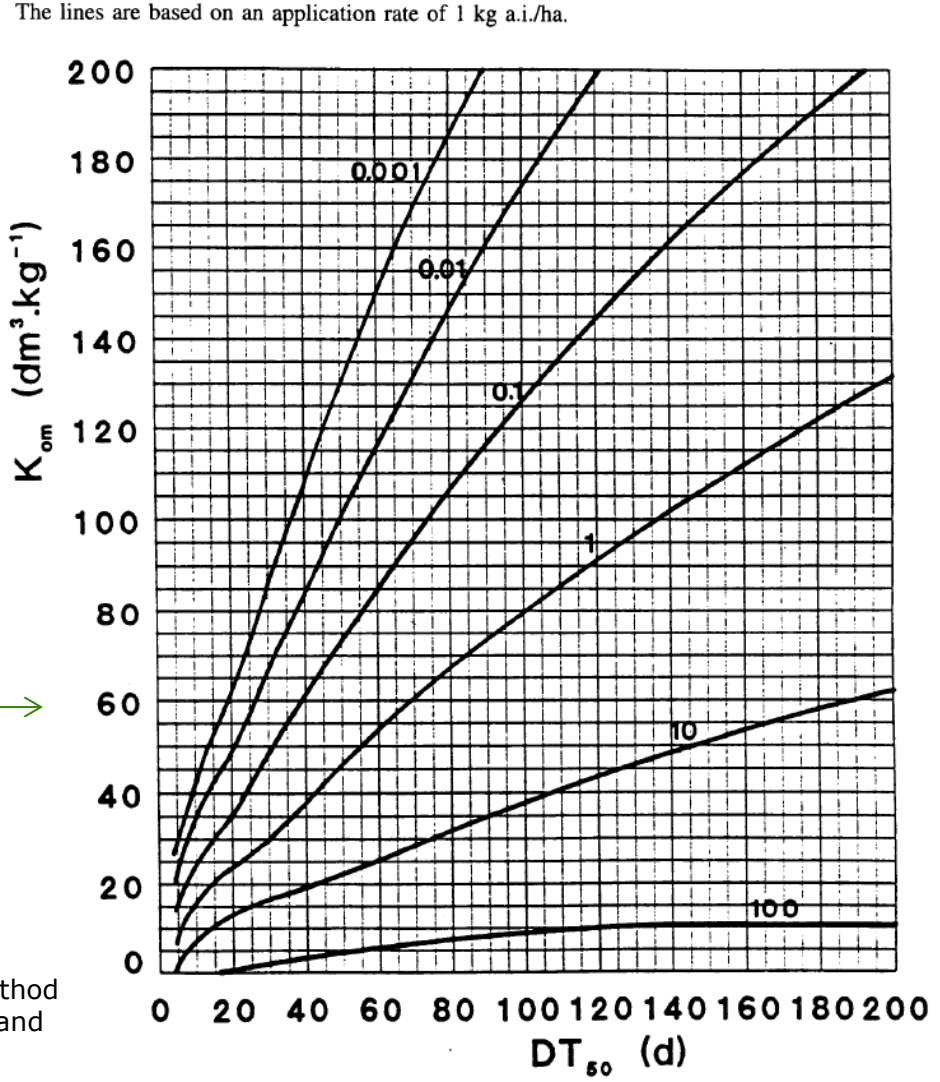
- Mobile substances are characterised by
  - Low adsorption potential ($K_{oc}/K_d$)
  - High water solubility

- Other parameters: e.g. volatility

- What would be discriminating values for log $K_{oc}/K_d$ or solubility?
  - UBA proposal:
    - M: S ≥0.15 mg/L and log $K_{oc}/D_{oc}$ ≤ 4.0
    - vM: S ≥0.15 mg/L and log $K_{oc}/D_{oc}$ ≤ 3.0
      - At 12 °C and worst-case of pH 4-9

# Mobility on its own?

- Mobility and persistence in isolation?
  - Less persistent, highly mobile
  - Very persistent, less mobile
- Combination is used elsewhere:
  - Acceptable application rates for pesticide authorisation

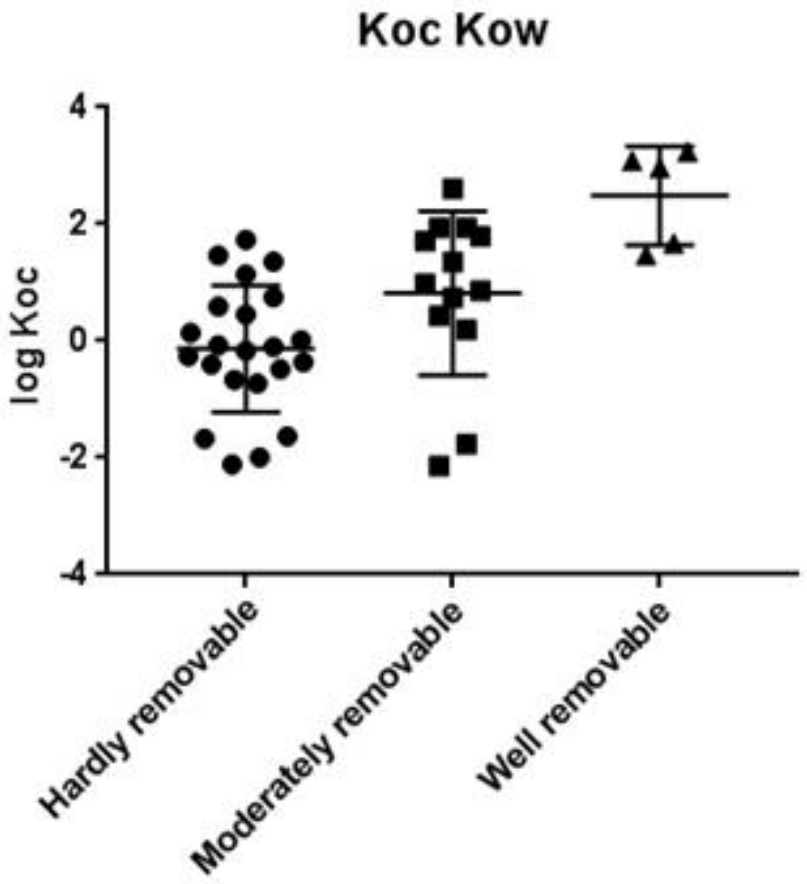



  - Leaching index

DI Gustafson. 1989. Groundwater ubiquity score: A simple method for assessing pesticide leachability. Environmental Toxicology and Chemistry 8(4):339 – 357.

# Mobility and drinking water treatment

- Substances problematic in drinking water preparation
  - All substances:
    - Maximum log $K_{oc}$ ≈ 3
  - Hardly removable:
    - Maximum log $K_{oc}$ ≈ 2



# Screening mobility

- Mobility criteria by DE are not very selective
  - EPIWIN QSAR calculcations
    - 69% M, 54% vM
    - For comparison, 13% B, 7% vB

- Alternative: M log $K_{oc}$ ≤ 3.0, vM log $K_{oc}$ ≤ 2.0,
  - EPIWIN QSAR calculcations
    - 54% M, 32% vM
  - Similar fractions PM/vPvM as PB/vPvB
    - Persistence less correlated with mobility than with bioaccumulation

# Toxicity

- Values for toxicity least discussed
- For T in PBT:
  - NOEC or EC10 for marine or freshwater organisms <10 µg/L
  - Classified as as carcinogenic (category 1A or 1B)
  - Classified as germ cell mutagenic (category 1A or 1B)
  - Classified as toxic for reproduction (category 1A, 1B, or 2)
  - Other chronic toxicity, classified as STOT RE (category 1 or 2)
- DE proposal: additional criteria
  - Classified as as carcinogenic (category 2)
  - Classified as germ cell mutagenic (category 2)
  - Effects on lactation, endocrine disruption
  - Derived-No-Adverse-Effect-Level (DNEL) ≤ 9 µg/kg/d
    - (oral, long term, general population)

# Toxicity remarks

- Bioaccumulation
  - Lipophilicity -> bioaccumulation -> more toxic
  - Toxicity is related to bioaccumulation
- Mobility
  - Hydrophilicity -> mobility -> less toxic
  - Toxicity is inversely related to mobility

- Higher NOEC or EC10 for marine or freshwater organisms?

- Criteria based on intrinsic toxicity?
  - Body burden

# Conclusions

- PMT can be a useful concept

- Two possibilities: criteria or screening values
  - Case-by-case?
  - Prospective or retrospective

- Current criteria/screening values are at the moment tentative
  - P criteria OK
  - Mobility and toxicity need more discussion
  - Combination of mobility and persistence?