Assessment of persistence and mobility of REACH-registered chemicals – The influence of input parameters, evaluation criteria and concepts

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Introduction

Anthropogenic chemicals that are environmentally stable and highly polar (mobile in water) have the potential to break through natural and technical barriers in the aquatic environment and thus threaten the quality of our raw water resources (Reemtsma et al., 2016). Such substances are called **persistent (P)** and **mobile (M)** organic chemicals **(PMOCs)**.

In order to identify PMOCs among the wealth of anthropogenic chemicals it is of vital scientific and regulatory interest to predict and assess P and M of substances in commerce. P and M can be assessed based on degradation test results and chemical property data, respectively, which are available from the open or grey literature, either experimentally derived or based on QSAR modeling.

Conclusions

- Assessment of intrinsic substance properties depends on the evaluation approach, criteria and data sources. This is more pronounced for P than for M.
- Experimental data should preferably be used in chemical assessments. For QSARs the application domain is important to consider (e.g. for ionic chemicals).
- Large data gaps exist for experimental property data as well as test results. The REACH registration process should be sharpened to help close the data gaps.
- All approaches deliver valuable results in terms of identifying chemicals for scientific scrutiny.
- In order to use assessment approaches in the regulatory context, a well-defined, harmonized and validated approach is necessary.

Methods

A total of 167 industrial chemicals (registered under REACH) that were suspected to be PMOCs were initially chosen for this study. Three different approaches were used to assess the intrinsic substance properties P and M of the target chemicals based on different evaluation criteria. A traffic-light color scheme was used to classify the results:

- **Red**: Assessment with available information that the chemical possesses the intrinsic substance property
- **Yellow**: Indication by available information that the chemical possesses the intrinsic substance property
- **Green**: Assessment with available information that the chemical does not possess the intrinsic substance property

Approaches, evaluation criteria and data sources

Kalberlah approach (Criteria by Kalberlah et al. (2014); data sources and interpretation of data with respect to the criteria by the present study)

Criteria
- P: An environmental half-life >40 d in freshwater (red)
- M: Water solubility >150 µg/L and log K_{oc} <4.5 in the pH range 6-8 (red)

Data sources
Manually collected data from
- Public dossiers on the ECHA website
- Chemical safety reports obtained from the German Environment Agency
- Scientific literature
- QSARs

PROMOTE approach (Arp et al., submitted; translation of the results by Arp et al. into the color scheme by the present study)

Criteria
- P: An environmental half-life >60 d in freshwater (red); >40 d but <60 d (yellow)
- M: log K_{oc} <2 or water solubility >1 g/L (red); log K_{oc} <3 but >2 or water solubility >50 mg/L but <1 g/L (yellow)

Data sources
Predominantly automatically retrievable data from
- Public dossiers on the ECHA website
- Scientific literature
- QSARs

Present approach

Criteria
- P: An environmental half-life >40 d in freshwater (red)
- M: log K_{oc} <3.5 or water solubility >50 mg/L (red); log K_{oc} <5 but >3.5 and water solubility >0.15 mg/L but <50 mg/L (yellow)

Data sources
Same as for Kalberlah approach

Results and Discussion

Of the 167 target chemicals 15 were eliminated because either P or M could not be assessed by at least one of the approaches, leaving a total of 152 assessed substances

Assessment results of the individual approaches

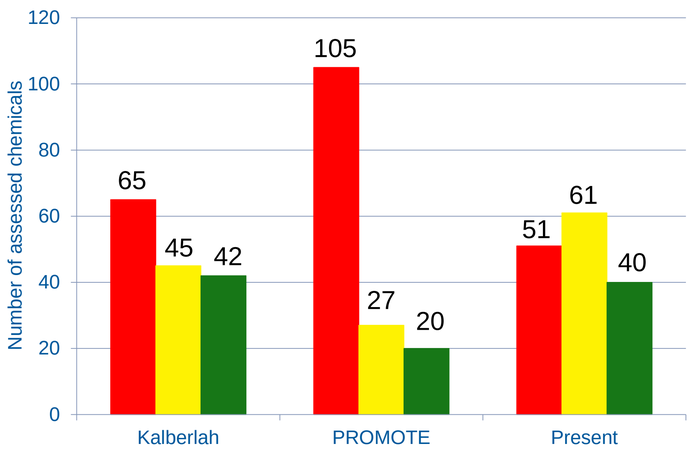

Fig. 1. Summarized results of P evaluation

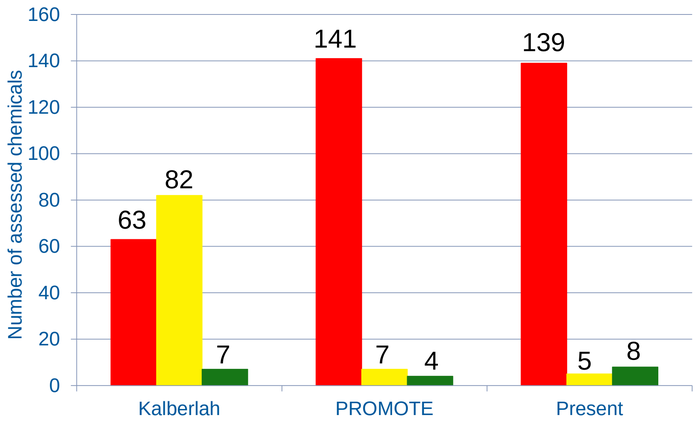

Fig. 2. Summarized results of M evaluation

Persistence

- Relatively large differences between the results of the different assessment approaches (Fig. 1, see also Fig. 3)
- Main reasons for the differences:
  - Use of different test results
  - Interpretation of degradation test results with respect to the criterion (half-life in freshwater)
  - Use of experimental vs. QSAR data

Mobility

- Good comparability of results between PROMOTE and Present approaches (Fig. 2)
- Main difference: yellow in Kalberlah vs. red in the other approaches
  - Based on different interpretation (red or yellow) of QSAR data for ionic and ionizable compounds outside the application domain

Comparison of assessment results

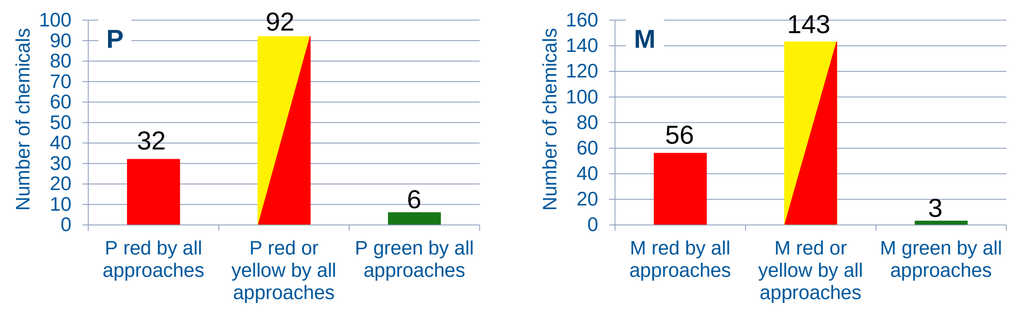

Fig. 3. Comparison of the results of P and M for all approaches

- Only 32 chemicals were assessed P red by all approaches (Fig. 3) vs. up to 105 chemicals in the individual approaches (Fig. 1). For P green these numbers are 6/42, for M red 56/141 (Fig. 2) and for M green 3/8
- For both P and M there were chemicals that were assessed with red in one approach and green in another (results not shown)

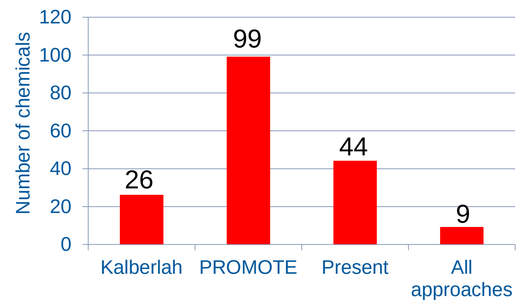

Fig. 4. Chemicals assessed red for both P and M

- In the individual approaches up to 99 chemicals were assessed as PMOCs (P and M red, Fig. 4)
- Only 9 of the target substances were assessed as PMOCs by all approaches (Fig. 4)

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References
Arp, H.P.H., et al. (submitted) Ranking REACH registered neutral, ionizable and ionic organic chemicals based on their aquatic persistency and mobility.
Kalberlah, F., et al. (2014) Guidance for the precautionary protection of raw water destined for drinking water extraction from contaminants regulated under REACH. Project (UFOPLAN) FKZ 371265416. Umweltbundesamt, Dessau.
Reemtsma, T., et al. (2016) Mind the Gap: Persistent and Mobile Organic Compounds – Water Contaminants That Slip Through, *Environ. Sci. Technol.*, 2016, 50: 10308-10315