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Review of the OECD POV and LRTP Screening Tool 15 years after its release

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Review of the OECD POV and LRTP Screening Tool 15 years after its release

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Paris 2023

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Foreword

The OECD POV and LRTP Screening Tool (hereafter 'the Tool') is software in a spreadsheet format containing multimedia chemical fate models (fugacity-based), which estimate the overall persistence (POV) and long-range transport potential (LRTP) of organic chemicals at a screening level. The Tool is used for comparative assessment of environmental hazard properties of different chemicals. It is specifically designed to help identify potential POPs (Persistent Organic Pollutants) according to persistence and long-range transport metrics.

The Tool has been used widely since the software was published in 2008, particularly for Screening (Annex D) and in the Risk profile (Annex E) in the process of adding new POPs under the Stockholm Convention. The journal article by Wegmann et al. (2009[1]), which describes the software in detail, has been cited regularly for over ten years (a total of over 100 citations). Some of the citing articles have made recommendations to improve the performance of the Tool.

In 2020, the OECD Working Party on Exposure Assessment (WPEA) endorsed its mid-term strategy, which includes the future update of the Tool. In 2021, the WPEA then decided to set up an expert group to review and revise the Tool based on the strategy. The nominated experts are: Qinghong Pu (Australia), Mark Bonnell (Canada), Yoshitaka Imaizumi (Japan), Joost Bakker, Emiel Rorije, and Eric Verbruggen (the Netherlands), Knut Breivik (Norway), Andreas Buser (Switzerland), Ian Doyle and James Lymer (the UK), Jed Costanza the US), Kei Ohno Woodall (the BRS Secretariat), and Martin Scheringer and Matthew MacLeod (OECD nominated experts). The expert group then developed a work plan for the review and update and proceeded with the review, including a survey to gather examples of the application of the Tool application.

The first draft report was prepared and discussed by the experts in January 2023, followed by a review of the WPEA in February–March. It was also circulated to the Persistent Organic Pollutants Review Committee (POPRC) of the Stockholm Convention. The revised report reflecting the comments provided was circulated to the WPEA in May 2023 and then finalised. This report is published under the responsibility of the Chemical and Biotechnology Committee of the OECD.

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Abbreviations

CP	Contamination Potential
CTD	Characteristic Travel Distance
LRTP	Long-Range Transport Potential
OPEs	organophosphate esters
PAHs	Polycyclic Aromatic Hydrocarbons
PBT	persistent, bioaccumulative and toxic
PFASs	per- and polyfluoroalkyl substances
PMOC	Persistent Mobile Organic Compound
POPRC	Persistent Organic Pollutants Review Committee
POPs	Persistent Organic Pollutants
P_{OV}	Overall Persistence
PPP	Plant Protection Product
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
TE	Transfer Efficiency
UNEP	United Nations Environment Programme
VBA	Visual Basic for Applications
VMS	Volatile Methylsiloxanes
vPvB	Very Persistent and Very Bioaccumulative substances
WHO	World Health Organisation
WPEA	Working Party on Exposure Assessment

Executive Summary

The OECD POV and LRTP Screening Tool (hereafter 'the Tool') is software in a spreadsheet format containing multimedia chemical fate models (fugacity-based), which estimate the overall persistence (POV) and long-range transport potential (LRTP) of organic chemicals at a screening level. While the Tool has been used widely since the software was published in 2008, recent scientific developments and emerging pollutants warrant an update of the Tool. This report assesses the continued relevance of the Tool and identifies possible updates to improve the simulation accuracy and usability of the Tool following a citation review, a user survey, simulation accuracy evaluations, and expert discussion.

Through the citation review, we observed that the journal article by Wegmann et al. (2009[1]), which describes the Tool in detail, has been constantly cited, in total, by 125 articles which were published from 2008 to 2022. Each article was reviewed with the view of whether it identified any shortcomings of the Tool and/or made any improvement suggestions and whether it applied the Tool for its study. A good number of application examples were found through the review, although many articles just referred to the Tool as an example of models used in a regulatory context or as the rationale for some input parameter values they adopted. Eleven articles were found to provide some identified shortcomings of the Tool and/or improvement suggestions, including missing environmental pathways and proposed new metrics to assess LRTP instead of Characteristic Travel Distance (CTD) and Transfer Efficiency (TE), currently used in the Tool.

The user survey gathered examples of using the Tool for decision support as well as improvement suggestions. It showed that the Tool is still actively used, particularly for assessing the properties of candidate chemicals under the Stockholm Convention; 15 POPs candidates in total have been examined using the Tool. Several documented shortcomings were also provided through the survey, all of which had already been identified through the citation review. The survey also gathered various improvement suggestions, which were then classified according to the following topics:

- Episodic atmospheric transport and poleward river-based transport in the northern hemisphere
- Particle adsorption, air-particle partitioning
- Parameter value changes
- Ionising substances
- Intermittent precipitation
- Software application/interface changes
- Dataset/database in the Tool
- Input parameter derivation
- Quantitative categorical confidence estimates
- Emissions fractions approach – alternative metrics
- Others

In assessing the limitation and applicability of the tool, we conducted model estimation of CTD/TE and P_{OV} for 19 acknowledged POPs using the Tool. It demonstrates that the P_{OV} and LRTP modelled by the

Tool for these acknowledged POPs generally indicate values above the defined reference lines, which showed a continued relevance of the Tool estimation in terms of POPs identification.

Summing up the results of these activities, we identified the following possible elements for updating the Tool to increase usability, avoid misuse and misinterpretation of the results, and improve simulation accuracy. Some of these elements seem easy to implement and others may need further discussion and work.

Easy to implement

- Add more data sets of reference chemicals
- Adopt intermittent precipitation
- Disclose the VBA code for professional purposes
- Provide manual/guidance, including how to derive the input parameters and interpret the result of confidence estimates, how PhiAir is calculated and the half-life in air is adjusted
- Keep the Excel format but add an option to save estimation reports as PDFs
- Display the calculated log K_{OA} value used to estimate gas-particle partitioning
- Include K_{OA} as an input parameter in addition to K_{OW} and K_{AW}

Further discussion/work needed

- Include the alternative metrics - fractions approach
- Re-define the TE to include:
    - Net deposition rather than Gross deposition
    - Transport in Water
- Develop and include a consensus model to estimate the P_{OV} and LRTP of ionising substances

The final decision on whether/how to adopt each of the elements will be made through further discussion at the Working Party on Exposure Assessment in designing the new version of the Tool.

1 Introduction

Background

The OECD P_{OV} and LRTP Screening Tool (hereafter 'the Tool') is software in a spreadsheet format containing multimedia chemical fate models (fugacity-based), which estimate the overall persistence (P_{OV}) and long-range transport potential (LRTP) of organic chemicals at a screening level. The Tool is used for comparative assessment of environmental hazard properties of different chemicals. It is specifically designed to help identify potential POPs (Persistent Organic Pollutants) according to persistence and long-range transport metrics.

The Tool has its origin at the OECD/UNEP Workshop on the Use of Multimedia Models held in Ottawa, Canada, in 2001 [ENV/JM/MONO(2002)15]. After the workshop, an OECD Expert Group for the Follow-up to the OECD/UNEP Workshop was established. Between 2002 and 2005, the Expert Group developed a consensus model based on existing predictive approaches to environmental persistence and long-range transport. The software has been developed by Switzerland in co-operation with Germany, under the supervision of the OECD Task Force on Environmental Exposure Assessment (TFEEA), and in co-operation with the participants of the OECD/UNEP Training Workshops on Application of Multimedia Models for Identification of POPs held in 2005 and 2006. The software (Version 2.1) was endorsed by the TFEEA in late 2007 and published in April 2008. The updated Version 2.2 was released in April 2009.

The features of the Tool are described as follows;

1. Simple and easy to use

   The Tool has a "Main menu" for entering data, and results are shown in easy-to-read graphical mode, which allows even beginners to utilise it easily.

2. Flexible data management and model setting

   Users can choose chemicals from a database installed in the Tool, or enter data for chemicals of interest, i.e. physical-chemical properties and degradation half-lives. It is possible to transport users' own databases and store them within the Tool. It is also possible to change model settings.

3. Representative of several models

   The model in the Tool was developed as a "consensus model" reflecting features of several existing multimedia fate and transport models.

4. Graphical and numerical output

   The result of a model calculation is shown in both numerical and graphical outputs, such as:

   - Numerical values of P_{OV}, CTD (Characteristic Travel Distance) and TE (Transfer Efficiency) in three emission scenarios to soil, water and air.
   - Plots of CTD and TE vs. P_{OV}.
   - Pie charts showing the fraction of chemicals that are contained in soil, water and air for each scenario.

The Tool has been used widely since the software was published, particularly for Screening (Annex D) and in the Risk profile (Annex E) in the process of adding new POPs under the Stockholm Convention. The journal article by Wegmann et al. (2009[1]), which describes the software in detail, has been cited regularly for over ten years (a total of over 100 citations). Some of the citing articles have made recommendations to improve the performance of the Tool.

In 2020, the OECD Working Party on Exposure Assessment (WPEA) endorsed its mid-term strategy, which includes the future update of the Tool at the 4th meeting of the WPEA. In 2021, the WPEA then decided to set up an expert group to review and revise the Tool based on the strategy at the 5th WPEA meeting.

The expert group discussed and developed the work plan for the review and update described below and then proceeded with the reviewing works, which are summarised in this report.

Work plan

The work plan for the project reviewing and updating the Tool consists of four steps: Review the Tool, Develop an OECD report, Update the software, and Develop a Scientific report. This report is, as Step 2, to summarise the reviewing activities described in Step 1 as well as make recommendations to improve the Tool.

Step 1. Review the Tool

First, the expert group reviewed the Tool by analysing the citing articles, practices of users, and simulation results, which could lead to identifying some possible elements to be updated.

Subtask 1. Review Citing articles

Over 100 scientific articles have cited the Tool sometimes with some recommendations for improvement, e.g., "optional Arctic (PMOC) LRTP setting" (Sühring et al., 2020[2]). This subtask was aimed at identifying the possible revision elements of the Tool through the review of the citing articles. The result is described in Chapter 2.

Subtask 2. Gather user needs

The objective of this subtask was to identify how the Tool had been used as decision support and to gather improvement suggestions from users. This subtask was to be done by input from the expert group as well as the questionnaire sent out to the WPEA and the relevant expert communities in the first half of 2021. The result is described in Chapter 3.

Subtask 3. Assess the Tool limitation and applicability for future revision

This subtask was aimed at identifying the limitations and applicability of the Tool by the results of Subtask 1 and 2, and predicting the P_{OV} and LRTP of the acknowledged POPs, which would result in future revision. The expert group discussed each improvement suggestion gathered from Subtask 1 and 2, including the recent result from the Cefic ECO53 project[1]. The result is described in Chapter 4.

[1] Cefic LRI project ECO 53 - CC-ALT: A chemical categorisation approach for LRTP assessment.

Step 2. Develop an OECD report

The expert group conducted these subtasks and discussed how to derive recommendations for improving the Tool from the results, which were summarised in this report.

Step 3. Update the software

Following the recommendation in the report, the expert group is to develop an updated software of the Tool. The software is to be posted on the OECD website and be free to download.

Step 4. Develop a scientific paper

The expert group is to develop a scientific paper to describe the updated Tool in detail and submit it to a scientific journal.

2 Citation review

The Tool software is described in detail in the journal article by F. Wegmann et al. (2009[1]), Environmental Modeling & Software 24, 228–237, and this article has been cited by many scientific papers, including those which are to apply the Tool in their studies, and even to evaluate the performance of the estimation results conducted by the Tool.

This chapter describes the overview of the citation review results of papers that cite Wegmann et al. (2009[1]), including shortcomings and possible improvements of the Tool indicated by the articles reviewed.

Methodology

Screening Google Scholar[2] for articles citing Wegmann et al. (2009[1]) identified 160 articles. Then the second screening excluded duplicated contents (e.g., journal articles and doctoral thesis), non-English written articles, and articles which are not easy to access (e.g., a book chapter), which resulted in 125 articles for review.

Each article was reviewed in the view of the following three criteria; whether it (i) identified any shortcomings of the Tool and/or made any improvement suggestions, (ii) applied the Tool for its study, but there were no identified shortcomings or improvement suggestions, and (iii) just (briefly) mentioned the Tool, e.g., in its Introduction section.

Results overview

Figure 1 shows the number of reviewed articles citing Wegmann et al. (2009[1]). The total number of citations was found to be still increasing; it was cited the most in the last two years. This result not only assures the continued relevance of the Tool but also implies a higher interest in the Tool from academia in recent years. In addition, it may reflect the outputs of the following projects conducted in parallel with this activity;

- Cefic: Cefic LRI project ECO 53 'CC-ALT: A chemical categorisation approach for LRTP assessment.
- UNEP: Intersessional working group on long-range environmental transport – Consideration of long-range environmental transport when evaluating chemicals proposed for listing under the Stockholm Convention.

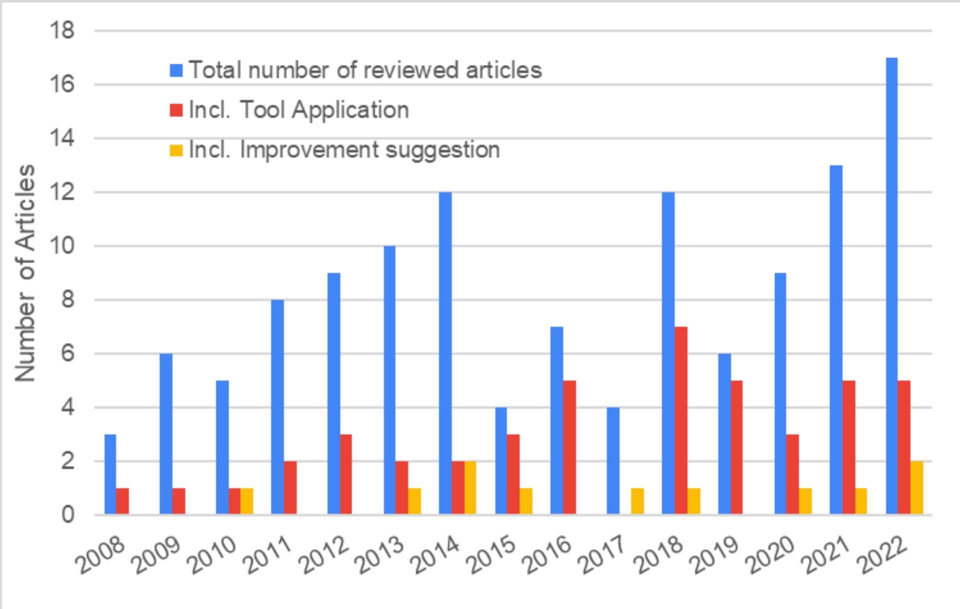
A good number of application examples were found through the review, while many articles just referred to the Tool, such as, in their introduction sections, as an example of models used in a regulatory context and the rationales of some input parameter values they adopted. Eleven articles were found to provide

[2] https://scholar.google.com/

some identified shortcomings of the Tool and/or improvement suggestions that were described in detail in the following section.

The detailed list of reviewed articles is shown in Annex A.

Figure 1. The number of reviewed articles citing Wegmann et al. (2009)



Articles which Identified shortcomings and suggested improvement

1. The precautionary principle and environmental persistence: prioritising the decision-making process (Gouin, 2010[3])

This article demonstrated that chemical partitioning property and environmental persistence information can be effectively combined to provide guidance for regulatory priority setting, and the Tool was used to estimate an overall environmental persistence (P_{OV}), the characteristic travel distance (CTD) and transfer efficiency (TE) for the illustrative substances of concern relating to Stockholm Convention on POPs, REACH, and Canada's Chemical Management Plan.

Gouin (2010[3]) pointed out, in describing the method of estimation by the Tool, that the global parameterisation characterised in the OECD Tool may not reflect the environmental fate of chemicals emitted to other geographic scales, such as regional or country-specific environments.

2. Reliability of environmental fate modelling results for POPs based on various methods of determining the air/water partition coefficient (log K_{AW}) (Odziomek et al., 2013[4])

This article assessed the reliability of environmental fate estimation for POPs by the Tool based on various methods of determining the air/water partition coefficient (log K_{AW}).

It observed that, depending on the method of determination of air–water partition coefficient K_{AW}, there is a statistically significant difference in data values, which largely affected the Tool estimation. It thus highlighted the importance of the K_{AW} deviation method as an input parameter for the Tool estimation.

Specifically, it recommended, to reduce uncertainties, deriving K_{AW} from predicted values of octanol-water and octanol–air partition coefficients rather than calculating K_{AW} from the estimated value of Henry's law constant and then adjusting to ensure its consistency with the other two partition coefficients.

3. A New Metric for Long-Range Transport Potential of Chemicals (Kawai et al., 2014[5])

This article proposed a new metric for LRTP, which they named as *GIF to represent the global average of imported fractions in receptor regions* and evaluate the LRTP and persistence of a wide variety of chlorinated and brominated organic compounds using *GIF* and overall persistence (P_{OV}), respectively, using their global 3D dynamic multimedia model (FATE).

Comparing CTD and TE calculated by the Tool to *GIF* calculated by FATE, a higher rank correlation was observed between GIF and CTD (0.74) than between GIF and TE (0.41), which implied that CTD better represents *GIF* calculated using the 3D dynamic model than does TE. It also noted the potential need for ancillary LRTP assessments using 3D dynamic models with the focus that the highest rank correlation between GIF and CTD was not very high. In addition, the high rank correlation between the P_{OV} values calculated using FATE and the P_{OV} values obtained with the OECD tool was observed (0.93)

4. Comparison of Atmospheric Travel Distances of Several PAHs Calculated by Two Fate and Transport Models (The Tool and ELPOS) with Experimental Values Derived from a Peat Bog Transect (Thuens et al., 2014[6])

This article calculated the CTD of several polycyclic aromatic hydrocarbons (PAHs) and metals using two models, including the Tool. It also tested the performance of the models by comparing the relative ranking of CTDs with the one of experimentally determined travel distances (ETDs).

It indicated that the quality of the Tool estimations would improve with better data on the temperature dependence of the atmospheric degradation half-lives of PAHs and the implementation of this dependence in the Tool since the CTDs of rather volatile compounds are highly sensitive to the half-life in air.

5. A modeling assessment of the physicochemical properties and environmental fate of emerging and novel per- and polyfluoroalkyl substances (Gomis et al., 2015[7])

This study estimated key properties of newly identified fluorinated alternatives using in-silico tools, followed by the estimation of their environmental fate using the derived properties and the Tool, which identified that most of the alternatives were estimated to be similarly persistent and mobile in the environment as the long-chain PFASs.

It indicated that though the Tool was likely sufficient for a preliminary assessment of the environmental fate of fluorinated alternatives (on a global scale), the accuracy of the Tool estimation depended strongly on 1) the consistency and accuracy of input parameters and 2) the environmental processes considered in the model. Particularly, some possibly significant processes that may influence the P_{OV} and LRTP of fluorinated alternatives were found not represented in the Tool, including the possible transfer from the seawater surface to the atmosphere via marine aerosol generation, due to their surfactant-like properties. Since such environmental processes are not included in the OECD Tool, the CTD outputs might be underestimated for some of the fluorinated alternatives.

6. Screening-level exposure-based prioritization to identify potential POPs, vPvBs and planetary boundary threats among Arctic contaminants (Reppas-Chrysovitsinos, Sobek and MacLeod, 2017[8])

This article evaluated 464 individual chemicals mentioned in the Arctic Monitoring and Assessment Programme (AMAP) report according to persistence, bioaccumulation and long-range transport potential and calculated their exposure-based hazard scores for screening-level prioritisation.

It mentioned with citing Gouin (2010[3]) that the Tool might estimate more favourably the deposition of persistent, volatile chemicals over their vertical transfer from troposphere to stratosphere.

7. Environmental fate and exposure models: advances and challenges in 21st century chemical risk assessment (Di Guardo et al., 2018[9])

This article reviewed environmental fate and exposure models focusing on some advancements during the past 25 years as well as remaining challenges, and then proposed the formation of expert groups that compare, discuss and recommend model modifications and updates and help develop practical tools for risk assessment to transfer new scientific developments into the realm of regulatory risk assessment.

The Tool was mentioned as an environmental fate model that was developed explicitly for decision-making purposes and as a good practice to demonstrate how bringing an expert group of modellers together can result in the successful development and adoption of a regulatory modelling tool.

8. Evaluation of the OECD P_{OV} and LRTP screening tool for estimating the long-range transport of organophosphate esters (Sühring et al., 2020[2])

This article evaluated the Tool with respect to the P_{OV} and LRTP estimates that the Tool provides for organophosphate esters (OPEs). It found that the use of default parameter values could significantly underestimate P_{OV} and LRTP values of OPEs and, potentially, other Persistent Mobile Organic Compounds (PMOCs), by not accounting for episodic atmospheric transport and poleward river-based transport in the northern hemisphere.

It thus suggested that the Tool could be modified to include an optional “Arctic (PMOC) LRTP setting” that incorporates episodic atmospheric and river-based transport as well as increased environmental half-lives due to cold temperatures.

9. Application of multimedia models for understanding the environmental behaviour of volatile methylsiloxanes: Fate, transport, and bioaccumulation (Whelan and Kim, 2022[10])

This article reviewed the use of multimedia fate and transport models, including the Tool for understanding the behaviour of volatile methylsiloxanes (VMS). It indicated, citing Xu et al. (2019[11]), that the CTDs of VMS calculated by the Tool may be overestimated, for the empirical CTDs derived from measured concentration data at different latitudes were lower than those predicted by the Tool. It suggested that the actual rates of atmospheric removal may be higher than those assumed in the model.

10. The Emissions Fractions Approach to Assessing the Long-Range Transport Potential of Organic Chemicals (Breivik, McLachlan and Wania, 2022[12])

This article introduced a set of three alternative metrics and implemented them in the Tool's model instead of CTD and TE. The three metrics quantify the extent to which the chemical;

1. reaches a remote region (dispersion, ϕ1);
2. is transferred to surface media in the remote region (transfer, ϕ2), and;
3. accumulates in these surface media (accumulation, ϕ3).

It indicated, in contrast to CTD and TE, the emissions fractions metrics can;

- integrate transport via water and air, enabling comprehensive LRTP assessment;
- provide quantitative mechanistic insight into different phenomena determining LRTP since there is a coherent relationship between the three metrics;
- allow assessment of LRTP with the accumulation metric, ϕ3, in the context of the Stockholm Convention, where the ability of a chemical to elicit adverse effects in surface media is decisive.

It finally concluded that the emission fractions approach has the potential to reduce the risk of false positives/negatives in LRTP assessments.

11. What do we know about the production and release of persistent organic pollutants in the global environment? (Li et al., 2022[13])

This article conducted a literature review to collect and curate quantitative information on the historical global production and multimedia environmental releases of 25 intentionally produced POPs. Preliminary efforts are also made to integrate the production volume information with "hazard" attributes (persistence, bioaccumulation, toxicity, and LRTP) in the evaluation of potential environmental impacts of the 25 POPs.

The persistence and LRTP were characterised using the Tool, but LRTP was evaluated using a new LRTP metric, ϕ3 (Breivik, McLachlan and Wania, 2022[12]), which was implemented in the Tool code from their side.

Summary and Conclusion

The literature review identified not only various application examples of the Tool but also several shortcomings and improvement suggestions. Several articles indicated the importance of the accurate derivation of input parameter values, such as the partition coefficient (Odziomek et al., 2013[4]) and the half-lives (Thuens et al., 2014[6]; Sühring et al., 2020[2]; Whelan and Kim, 2022[10]), to which the simulation result is highly sensitive. Sühring et al., (2020[2]) also suggested an optional Arctic setting, which could reflect the decreased half-lives due to cold temperatures.

Two references pointed out missing environmental pathways in the Tool, which could affect the simulation accuracy. One is the transfer from the seawater surface to the atmosphere via marine aerosol generation in the context of fluorinated alternatives assessment (Gomis et al., 2015[7]). The other is the episodic atmospheric transport and poleward river-based transport in the northern hemisphere (Sühring et al., 2020[2]).

Two articles proposed new metrics to assess LRTP;

- GIF, derived from the more complex (3D dynamic) model, became a good reference to assess the accuracy of the Tool estimation, for example, a high-rank correlation was observed between CTD and GIF (Kawai et al., 2014[5]).
- A set of three metrics based on the emission fraction approach were proposed as an alternative to CTD and TE (Breivik, McLachlan and Wania, 2022[12]). It demonstrated several merits in improving the estimation accuracy of the Tool, which will be further examined in Chapter 4.

Di Guardo et al., (2018[9]) indicated the effectiveness of the formation of expert groups that compare, discuss and recommend model modifications and updates and help develop practical tools for risk assessment to transfer new scientific developments into the realm of regulatory risk assessment, and this reviewing process by the formulated expert group is exactly in line with this recommendation.

3 Application examples and User needs for the updates

Following the work plan, the expert group gathered the Tool application examples as decision support and improvement suggestions from users through a survey. The survey was circulated in March-April 2022 in the WPEA and in other relevant communities, such as the Persistent Organic Pollutants Review Committee (POPRC).

Survey result overview

The expert group prepared six questions as follows:

- Q1: Is the Tool used in your organisation?;
- Q2: If yes, in Q1, what is the context in which it is used?;
- Q3: If yes, in Q1, what kinds of chemical categories (PFAS, BFR, ….) are focused on?;
- Q4: Are there any documented shortcomings of the Tool?;
- Q5: If yes, in Q4, please provide the links to these documents;
- Q6: Provide any recommended improvements keeping in mind the limited time and scope of the expert group.

This online survey was open from the middle of March to the end of April 2022, and 25 completed responses were gathered. The overview responses to each question are described below.

Use examples of the Tool, from the responses to Q1-Q3

Q1 was set for collecting the use/application examples of the Tool. Following the answers to Q1, 10 of 25 answered 'Yes', which means the Tool is used in their organisation, while 13 answered 'No'. Looking at the answers of Q2, the Tool is used, for example, in the context of;

- POPs Review Committee to assess the POP properties of nominated chemicals with (potential) POP properties, i.e. mainly halogenated organics;
- Health risk assessment for pesticides;
- PBT and POP assessments for any chemical with potential long-range transport (probably also applicable for PMTs/vPvM substances);
- Ecological Risk Assessment for all organic substances (however, CTD is also used for eco-prioritisation using another regional scale multimedia model);
- Screening of chemicals for long-range transport, as part of the weight of evidence in the assessment of long-range transport focusing on substances with PBT/vPvB properties or substances with other properties of concern;
- Supporting POP determination for agricultural products, and;
- Assessment of the LRTP of semi-volatile PPP.

The expert group also gathered the Tool application examples in the POPs candidates review under the Stockholm Convention, which were summarised in Table 1.

Table 1. Tool application in evaluating POPs candidates under the Stockholm Convention

Substances	Application stages	Documents
Chlordecone	Annex E Risk profile	UNEP/POPS/POPRC.2/17/Add.2
Hexabromobiphenyl	Annex E Risk profile	UNEP/POPS/POPRC.2/17/Add.3
Hexa- and heptabromodiphenyl ether	Annex E Risk profile	UNEP/POPS/POPRC.3/20/Add.6
Pentachlorobenzene	Annex E Risk profile	UNEP/POPS/POPRC.3/20/Add.7
Alpha hexachlorocyclohexane	Annex E Risk profile	UNEP/POPS/POPRC.3/20/Add.8
Beta hexachlorocyclohexane	Annex E Risk profile	UNEP/POPS/POPRC.3/20/Add.9
Technical endosulfan	Annex E Risk profile	UNEP/POPS/POPRC.5/10/Add.2
Hexachlorobutadiene	Annex E Risk profile	UNEP/POPS/POPRC.8/16/Add.2
Short-chain chlorinated paraffins	Annex E Risk profile	UNEP/POPS/POPRC.11/10/Add.2
Dicofol	Annex E Risk profile	UNEP/POPS/POPRC.12/11/Add.1
Methoxychlor	Annex E Risk profile	UNEP/POPS/POPRC.16/9/Add.1
UV-328	Annex E Risk profile	UNEP/POPS/POPRC.17/13/Add.3
Dechlorane Plus	Annex E Risk profile	UNEP/POPS/POPRC.17/13/Add.2
Chloropyrifos	Annex E draft Risk profile (to be discussed at POPRC-18)	UNEP/POPPS/POPRC.18/4[3]
MCCPs[4]	Annex E draft Risk profile (to be discussed at POPRC-18)	UNEP/POPPS/POPRC.18/5[5]

Shortcomings of the Tool, from the responses to Q4-Q5

This survey also collected suggested shortcomings of the Tool in Q4. 5 of 25 answered that they have documented shortcomings, while the rest were 'No' or 'No answer'.

Three experts provided an article which indicated that the Tool could underestimate P_{OV} and LRTP values of organophosphate esters and, potentially, other Persistent Mobile Organic Compounds (PMOCs), by not accounting for episodic atmospheric transport and poleward river-based transport in the northern hemisphere (Sühring et al., 2020[2]).

Other documented shortcomings in predicting the LRTP of organophosphate esters were also provided. In certain cases, the assessment of POPs candidates, such as chlorpyrifos[6] and methoxychlor[7], showed that the Tool does not simulate the LRTP derived from monitoring results. Zhang et al. (2016[14]) also estimated the LRTP of 94 flame retardants using the Tool and pointed about half of the flame retardants have LRTP potential, which is likely an underestimation.

[3] To be updated after POPRC-18

[4] Chlorinated paraffins with carbon chain lengths in the range C14-17 and chlorination levels at or exceeding 45% chlorine by weight

[5] To be updated after POPRC-18

[6] UNEP/POPS/POPRC.17/5, section 3.3.3

[7] UNEP/POPS/POPRC.16/9/Add.1, para 68

improvement suggestions from the responses to Q6

Seven comments for the improvement suggestions were provided regarding the Q6. In addition, the expert group also discussed possible elements for the improvement of the Tool from the user side. The possible improvement suggested by the survey and the expert group are listed below that are discussed in Chapter 4:

From the survey

- Account for speciation under environmental conditions, i.e. fractions present in the neutral and ionic forms based on pKa and pH in the environmental compartments;
- Extend the approach to include also ionising organic chemicals because numerous substances will be present in their ionic form in the environment depending on their pKa values (i.e., acids, bases, zwitterionic substances);
- Account for intermittent precipitation instead of continuous low rates of precipitation;
- Integrate monitoring data (recent observations and historical time series) that could help improve the accuracy and use of the Tool;
- Move away from Excel to a more modern online tool that provides an option to save reports of calculations as PDFs;
- Be documented in way that demonstrates compliance with OECD standards on documenting the reliability and scientific basis of modelling tools;
- Improve representation of particle-bound transport for (strongly) adsorbing compounds and semi-volatile substances (e.g., implement further gas-particle partitioning approaches; account for Koc values to estimate adsorption to soil particles).
- Display the calculated log Koa value used to estimate gas-particle partitioning (e.g., on the results page below the Kaw and Kow values).
- Add more compounds/chemicals to the data set in Region B (low persistence, high LRTP) and Region C (high persistence, low LRTP) to provide a relative perspective to data for a particular chemical being assessed (This is especially important for the return of results that are bordering these regions);
- Extend parameters to evaluate LRT as recommended in ECETOC ECO 53 project, *A Chemical Categorisation Approach for LRTP Assessment*;

From the expert group

- Allow for a range of wind speeds;
- Develop representative water flow velocity for riverine conditions;
- Adjust for how adsorption of a chemical to solids affects its rate of degradation;
- Incorporate temperature effects on partitioning and half-lives;
- Use K_{OW}, K_{AW}, K_{OA} values input by the user;
- Provide guidance on appropriate half-life estimates for non-degrading substances (i.e., 10,000 or 55,000 hrs);
- Be able to address national program issues as well as global. This means more regional level transport up to the continental level;
- Be able to address water transport via rivers;
- Contain a sediment and vegetation compartment;

- Consider becoming a nested multimedia LRTP model such that local, regional, continental and global scale model environments are contained within the nested scheme;
- Consider providing qualitative categorical “confidence” estimates with predictions based on extremes of physicochemical properties used as inputs;
- Maintain the ability to run a probabilistic model;
- Be able to address ionic substances by allowing alternative partition coefficients (water transport issues);
- Provide fugacity and/or extreme property warnings on input;
- Consider adding a least-squares internal physicochemical consistency method to the model;
- Consider the concept of contamination potential (CP) at various scales in a nested approach;
- Consider mass-fractioning the mode of entry based on partition coefficient information (e.g., use Kaw bins to adjust fraction in air, water, soil given an emission to water or air);

4 Limitations and Applicability of the Tool

The Tool is originally designed for screening the environmental hazard potential of non-ionising organic chemicals whose environmental partitioning can be described by absorptive capacities of environmental media estimated from partitioning between air, water and octanol in the laboratory (Wegmann et al., 2009[1]). The limits of the Tool applicability described in the original report are shown in Box 1.

Box 1. Limits of the Tool applicability

The Tool is a decision support tool, not a decision-making tool. Users must be aware of its aims, assumptions and limitations. Specifically, the Tool is an instrument for screening non-ionising organic chemicals for environmental hazard and for ranking chemicals in terms of long-range transport potential and overall persistence. It should not be used for a concentration-based risk assessment as the emission scenarios used in the Tool are generic. It contains a steady-state, unit-world model with air, water, and soil compartments. The nature of the consensus model included in the Tool implies that only acknowledged and evaluated features have been included the model. The model within the Tool is similar to contemporary multimedia models, however, there are a number of limitations associated with this approach.

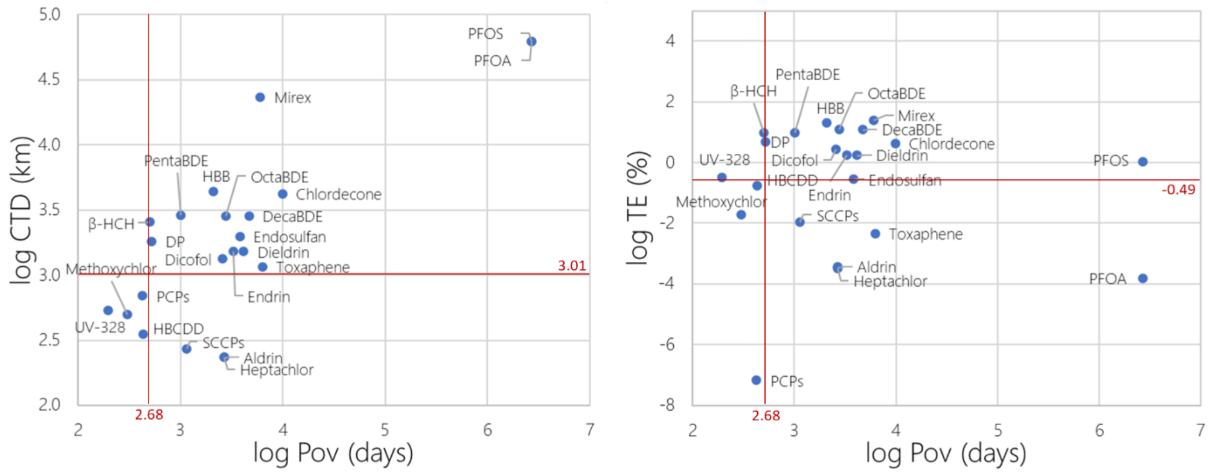
The description of the environment in the Tool does not include site- or time-specific parameterisation and consists only of air, water, and soil. As in all evaluative models of this type, the processes included are simplified. The Tool uses generic, globally averaged values of environmental parameters such as a constant rainfall rate and an averaged aerosol size and deposition velocity.

Hazard assessment with the Tool is only meaningful for specific substance classes. The most important limitation is that the Tool is designed for substances whose environmental partitioning is well described by absorptive capacities in air, water, soil, and particles as described by K_{OW} and K_{AW}. The model cannot be used for acids and bases or metals. The quality of the assessment strongly depends on the quality of the chemical properties used as model input. At the screening-level stage of hazard assessments, these properties may be highly uncertain. The Monte Carlo uncertainty analysis functionality illustrates the impact of uncertainty in chemical properties and helps to prioritise data quality improvement efforts.

Source: (Wegmann et al., 2009[1])

This design has exactly fitted the evaluation of POPs candidates under the Stockholm Convention, and the Tool has been applied in many cases, as shown in Table 1. Figure 2 shows the comparison results of log CTD/log TE versus log P_{OV} for 19 acknowledged POPs using the Tool, which was conducted in Subtask 3. The expert group conducted model estimation of CTD/TE and P_{OV} for 19 acknowledged POPs using the Tool. It demonstrates that the P_{OV} and LRTP modelled by the Tool for these acknowledged POPs generally indicate values above the defined reference lines.

Figure 2. Comparison of log CTD/log TE versus log P_{OV} for 19 acknowledged POPs using the Tool



Note: Model input parameters are the same as used by Li et al (2022[13]). The reference lines for "POP-like" P_{OV} and TE (red lines) were calculated based on selected HCHs, PCBs, DDTs and chlordanes from Breivik et al (2022[12]). We have also included model predictions for methoxychlor (using model input parameters from UNEP/POPS/POPRC.16/INF/16, Table 4), Dechlorane Plus (model input parameters from Sverko et al. 2011), as well as UV-328 (model input parameters from UNEP/POPS/POPRC.17/INF/17, section 2).
Source: provided by the expert group

The expert group also examined the shortcomings and improvement suggestions gathered in Chapters 2 and 3. It was first confirmed as a discussion premise to keep the basic design of the Tool, such as focusing on generic scenarios/situations/conditions, on screening non-ionising organic chemicals, and only on acknowledged and evaluated features as described above.

On the other hand, to meet professional needs, a good option would be that, in keeping the master version, the VBA code is to be published for experts to extend/modify the Tool for their purpose, and in addition, the accompanying manual/guidance on how to expand the function using the code would also be useful.

The expert group discussed each shortcoming and improvement suggestion that is summarised and shown in the next section.

Responses/comments to the improvement suggestions

Episodic atmospheric transport and poleward river-based transport in the northern hemisphere.

Sühring et al. (2020[2]) indicated that the Tool could underestimate P_{OV} and LRTP values of organophosphate esters and, potentially, other Persistent Mobile Organic Compounds (PMOCs), by not accounting for episodic atmospheric transport and poleward river-based transport in the northern hemisphere.

This improvement suggestion, however, is focused on a specific situation, the Canadian arctic environment, which is different from the scope of the Tool and, thus, not to be adopted. It is also noted that the sediment compartment would be an important factor in simulating river-based transport.

Particle-adsorption, air-particle partitioning

Sühring et al. (2020[2]) also indicated in their suggestion that the Tool could underestimate particle-adsorption which may reduce degradation and thereby increase the atmospheric half-life of certain chemicals.

The Tool currently accounts for adsorption to aerosol particles and is reported as PhiAir in Column W in the Database Editor. However, the method of computing PhiAir and how the half-life in air is adjusted are not currently described in the Manual. The experts agreed on the importance of this indication. One option raised by the experts was to put this process, regarded as 'pre-process' in determining the half-life air as an input parameter and out of the scope of the Tool simulation. It could be described in the manual/guidance to be developed, and it then needs to identify what is in the 'pre-process' and what is in the process.

Parameter values changes

There were several suggestions, including by Sühring et al. (2020[2]), about changing the default parameter values, such as wind speed, temperature, and sea depth. The experts confirmed that the Tool uses generic, globally averaged values of environmental parameters and better to keep them in line with its design. However, providing the VBA code could allow expert users to easily modify the Tool adjusted to the specific scenario they are focused on.

Ionising substances

Several suggestions about extending the scope to ionising substances were provided. The experts confirmed that it is technically possible to build a consensus model to estimate the P_{OV} and LRTP of ionising substances, but it would be too much work to be dealt with in this activity.

Intermittent precipitation

Currently, the continuous low rates of precipitation are considered in the Tool setting, but some suggestions were provided for intermittent precipitation to be adopted. It was acknowledged that this discussion occurred in the first development of the Tool, but the concept was rejected at the time for the reason that it was not a consensus model. The experts confirmed that the intermittent precipitation model had reached a 'consensus' over ten years after the first development, which could be adopted in this update.

Software application/interface changes

A comment suggested changing the application from Excel to a more modern online tool that provides an option to save reports of calculations as PDFs. The experts confirmed some advantages of Excel: a commonly used software, particularly by non-experts and easy to handle by them, transparent structure with visible VBA code. Another merit of Excel was pointed out from the government user side of the view that new software sometimes causes a problem in its instalment due to the security of government PCs. In addition, for security reasons, standalone programmes, whether Excel or otherwise, that do not require an internet connection are also preferable for government PCs. On the other hand, the experts confirmed the option to save estimation reports as PDFs is worth considering to increase usability.

Another request for changing the interface was to display the calculated log K_{OA} value used to estimate gas-particle partitioning, e.g., on the results page below the K_{AW} and K_{OW} values, and the experts confirmed it could easily be addressed.

Dataset/database in the Tool

A suggestion provided through the survey to integrate monitoring data (recent observations and historical time series) that could help improve the accuracy and use of the Tool was not supported by the expert for the reason that the Tool is focused on a generic situation, not compared with specific environmental observations.

Another request regarding data in the Tool was to add more data sets of reference chemicals, particularly of low persistence and high LRTP, and high persistence and low LRTP. It was stated that the property data of the specific set of reference chemicals that define the four quadrants should not be open for modification. Another request was that there should be a database that includes all approximately 30 acknowledged POPs. The experts found it reasonable, and the initial step could be to include the new POPs designated after the Tool was released.

How to derive the input parameters

Several suggestions about the derivation of input parameters, such as half-lives and partition-coefficient values, received through the survey were to account for temperature effects, to allow users to input not only K_{OW} and K_{AW} but also K_{OA}, and to include a least-squares internal physicochemical consistency method for adjusting the partition-coefficient values. Also for other physicochemical properties, a more explicit and detailed pre-processing was discussed. This would make it possible to cover various aspects of environmental chemistry that may affect the input values (temperature, conditions of degradation, etc.) and should be addressed, but are not part of the Tool itself. It was also said that input values of physicochemical properties should be checked for internal consistency wherever possible (such as: Koa = Kow/Kaw) and that this should be explained in the revised manual. The experts confirmed that the way to derive the input parameters is to be regarded as 'pre-process' outside the Tool whilst guidance on the appropriate derivation of parameter values could be prepared.

Provide qualitative categorical confidence estimates

A suggestion to consider providing qualitative categorical confidence estimates with predictions based on extremes of physicochemical properties used as inputs was provided through the survey. The experts confirmed that the current Tool provides such information at least partially with warning signals (red, yellow, and green) against extreme properties, while further approaches could be added, e.g., a confidence estimate or statement displayed if important warnings had been missed or ignored.

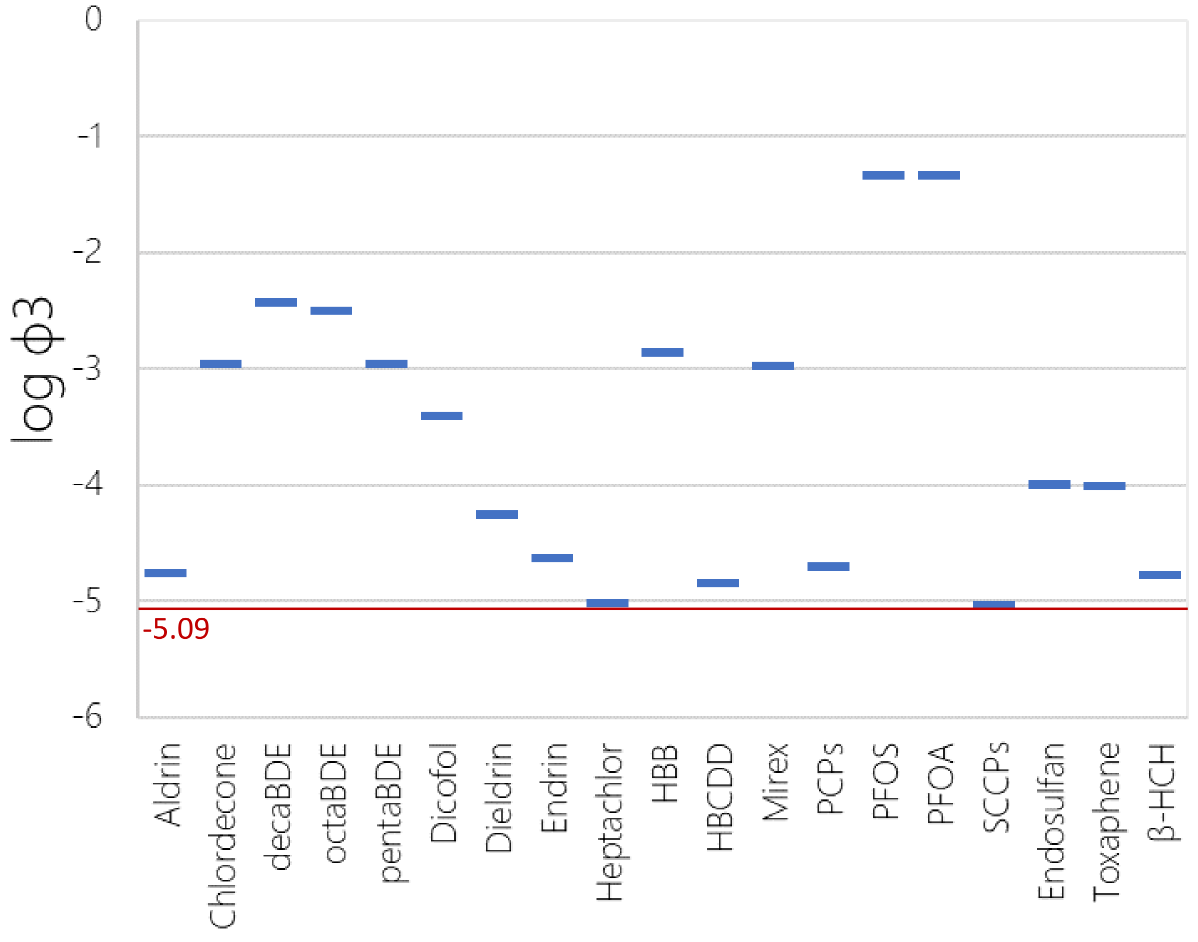
Emissions fractions approach – alternative metrics

Breivik et al. (2022[12]) developed a new method to estimate the LRTP using the three alternative metrics instead of CTD and TE used in the Tool. The three metrics quantify the extent to which the chemical (i) reaches a remote region (dispersion, ϕ1), (ii) is transferred to surface media in the remote region (transfer, ϕ2), and (iii) accumulates in these surface media (accumulation, ϕ3). Some merits of the metrics are indicated to integrate transport via water and air, to provide quantitative mechanistic insight into different phenomena with a coherent relationship between the three metrics, and to allow assessment of LRTP in terms of accumulation in surface media.

The experts discussed whether/how to consider a possible replacement with the alternative metrics. The main concern was how to keep continuity since the current Tool is widely used globally. There was agreement that ϕ2 is superior to TE because it includes reversible deposition. There were differing opinions as to whether ϕ2 is further superior because it also accounts for transfer in water. Some participants argued that ϕ1 is theoretically the same as CTD, while it was also maintained that they are different because the fractions dispersed in air (ϕ1A) and water (ϕ1W) are additive (ϕ1=ϕ1A+ϕ1W), whereas the CTDs for air and water are not. It was also suggested that the current P_{OV}-TE plot can visually cover what ϕ3 represents.

The expert group provided the comparison result of log ϕ3 for acknowledged POPs using the Tool modified by Li et al. (2022[13]). This result shows a better identification of POPs-like substances than those using CTD and TE in Figure 2. A more in-depth analysis was also provided and incorporated into this report as Annex (see Annex B).

Figure 3. Comparison of log φ3 for 19 acknowledged POPs using the Tool



Note: Model input parameters are the same as used by Li et al. (2022[13]). for "POP-like" φ3 (red line) was calculated based on selected HCHs, PCBs, DDTs and chlordanes from Breivik et al. (2022[12]).
Source: provided by the expert group

Others

The experts discussed that the revised manual might have to better explain the emissions used in the Tool. They are not meant to be realistic in any way, i.e. to reflect the actual use pattern of a chemical, but they span the range of emissions only to air, only to water and only to soil, which is what the concept of the Temporal Remote State requires for the best estimate of the persistence in the temporal remote state. This is explained in the paper by Stroebe (2004[15]) and should probably be explained in more detail in the manual.

5 Recommendation for the potential updates of the Tool

Summing up the discussion above, the following updates could be recommended to increase usability, avoid misuse and misinterpretation of the results, and improve simulation accuracy. These elements are classified into the ones that seem easy to implement and the others that need further discussion and work.

Easy to implement

- Add more data sets of reference chemicals (e.g., acknowledged POPs) with CAS RNs
- Add guidance on the domain of applicability in the help file
- Adopt intermittent precipitation
- Disclose the VBA code for professional purposes
- Provide manual/guidance, including how to derive the input parameters and interpret the result of confidence estimates, how PhiAir is calculated and the half-life in air adjusted
- Keep the Excel format but add an option to save estimation reports as PDFs and save the figures as images.
- Display the calculated log K_{OA} value used to estimate gas-particle partitioning
- Include K_{OA} as an input parameter in addition to K_{OW} and K_{AW}

Further discussion/work needed

- Include the alternative metrics - fractions approach
- Re-define the TE to include:
  - Net deposition rather than Gross deposition as done in the fractions approach
  - Transport in water
- Develop and include a consensus model to estimate the P_{OV} and LRTP of ionising substances

The above two, Including the alternative metrics and Redefining the TE, come up mainly triggered by the newly proposed metrics, the fraction approach (Breivik, McLachlan and Wania, 2022[12]). One option had been to replace the current CTD-TE metrics with the set of fraction metrics, but it was not included in the recommendation for considering the importance of keeping the continuity of the Tool, which has been widely used for years. Instead, two recommendations are included; to include the three metrics (dispersion, $\phi 1$, transfer, $\phi 2$, and accumulation, $\phi 3$) as an addition and to re-define TE, one of the current metrics, to improve its weaknesses compared to the alternative metrics. The final decision on whether to adopt both/one of the recommendations will be made through further discussion at the Working Party on Exposure Assessment in designing the new version of the Tool.

Building a consensus model for ionising substances was indicated as technically possible, but it should take much additional time and effort, which requires launching another project dedicated to this topic. The decision on whether to launch it is also left to the Working Party.

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Annex A. List of reviewed literatures

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		Zhao, Ang; Wei, Chao; Xin, Yue; Wang, Xiaoli; Zhu, Qingqing; Xie, Jibing; Ma, Haiyun; Xu, Jianzhong; Wang, Mei;	Pollution Profiles, Influencing Factors, and Source Apportionment of Target and Suspect Organophosphate Esters in Ambient Air: A Case Study in a Typical City of Northern China	2022	Journal of Hazardous Materials	Elsevier
		Ashraf, Maliha; Ahammad, Shaikh Ziauddin; Chakma, Sumedha;	Recent Advances in the Occurrence, Transport, Fate, and Distribution Modeling of Emerging Contaminants A Review	2022	Soil-Water, Agriculture, and Climate Change	Springer
		Aherne, Julian; Yargeau, Viviane; Metcalfe, Chris D;	Compounds of wastewater origin in remote upland lakes in Ireland	2022	Chemosphere	Elsevier
		D'Amico, Marianna; Gambaro, Andrea; Barbante, Carlo; Barbaro, Elena; Caiazzo, Laura; Vecchiato, Marco;	Occurrence of the UV-filter 2-Ethylhexyl 4-methoxycinnimate (EHMC) in Antarctic snow: first results	2022	Microchemical Journal	Elsevier
X		Breivik, Knut; McLachlan, Michael S; Wania, Frank;	The Emissions Fractions Approach to Assessing the Long-Range Transport Potential of Organic Chemicals	2022	Environmental science & technology	ACS Publications
X		Li, Li; Chen, Chengkang; Li, Dingsheng; Breivik, Knut; Abbasi, Golnoush; Li, Yi-Fan;	What do we know about the production and release of persistent organic pollutants in the global environment?	2022	Environmental Science: Advances	Royal Society of Chemistry
		Hahn, Stefan; Klein, Michael; Klein, Judith;	Final Report WP3BFramework on multi-media fate modelling within persistence assessment	2022		
	X	Klein, Judith; Klein, Michael; Hahn, Stefan;	Final Report WP3AModelling Exercises	2022		
	X	Li, Yitao; He, Yuhe; Lam, Chun Ho; Nah, Theodora;	Environmental photochemistry of organic UV filter butyl methoxydibenzoylmethane: Implications for photochemical fate in surface waters	2022	Science of The Total Environment	Elsevier

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
	X	Sala, Serenella; Biganzoli, Fabrizio; Mengual, Esther Sanye; Saouter, Erwan;	Toxicity impacts in the environmental footprint method: calculation principles	2022	The International Journal of Life Cycle Assessment	Springer
		Redman, Aaron D; Bietz, Jens; Davis, John W; Lyon, Delina; Maloney, Erin; Ott, Amelie; Otte, Jens C; Palais, Frédéric; Parsons, John R; Wang, Neil;	Moving persistence assessments into the 21st century: A role for weight-of-evidence and overall persistence	2022	Integrated Environmental Assessment and Management	Wiley Online Library
		Shring, Roxana; Mayer, Philipp; Leonards, Pim; MacLeod, Matthew;	Fate-directed risk assessment of chemical mixtures: a case study for cedarwood essential oil	2022	Environmental Science: Processes & Impacts	Royal Society of Chemistry
		Brunning, Hattie; Sallach, J Brett; Zanchi, Victor; Price, Oliver; Boxall, Alistair;	Toward a Framework for Environmental Fate and Exposure Assessment of Polymers	2022	Environmental Toxicology and Chemistry	Wiley Online Library
	X	Whelan, Michael J; Kim, Jaeshin;	Application of multimedia models for understanding the environmental behavior of volatile methylsiloxanes: Fate, transport, and bioaccumulation	2022	Integrated Environmental Assessment and Management	Wiley Online Library
		KSC Barrett, AL Stuart	Forests effects on the environmental fates of organic pollutants in a tropical watershed	2022	Science of The Total Environment	Elsevier
		P Domercq, A Praetorius, M MacLeod	The Full Multi: An open-source framework for modelling the transport and fate of nano-and microplastics in aquatic systems	2022	Environmental Modelling &	Elsevier
	X	L Zhang, W Xu, W Mi, W Yan, T Guo, F Zhou	Atmospheric deposition, seasonal variation, and long-range transport of organophosphate esters on Yongxing Island, South China Sea	2022	Science of The Total Environment	Elsevier
	X	R Hou, L Lin, H Li, S Liu, X Xu, Y Xu, X Jin, Y Yuan	Occurrence, bioaccumulation, fate, and risk assessment of novel brominated flame retardants (NBFRs) in aquatic environments A critical review	2021	Water Research	Elsevier
	X	K Nishimuta, D Ueno, S Takahashi, M Kuwae	Use of comprehensive target analysis for determination of contaminants of emerging concern in a sediment core collected from Beppu Bay, Japan	2021	Environmental Pollution	Elsevier
		TFM Rodgers, JO Okeme, JM Parnis	Novel Bayesian method to derive final adjusted values of physicochemical properties: Application to 74 compounds	2021	Environmental science & technology	ACS Publications
	X	JJ Feng, XF Sun, EY Zeng	Measurement of octanolair partition coefficients for liquid crystals based on gas chromatography-retention	2021	Chemosphere	Elsevier

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
			time and its implication in predicting long-range transport			
		BL Lin, Y Meng, M Kamo, W Naito	An all-in-one tool for multipurpose ecological risk assessment and management (MeRAM) of chemical substances in aquatic environment	2021	Chemosphere	Elsevier
		K Breivik, S Eckhardt, MS McLachlan	Introducing a nested multimedia fate and transport model for organic contaminants (NEM)	2021	Environmental Science: Processes & Impacts	pubs.rsc.org
		BL Townhill, E Reppas-Chrysovitsinos, R Shring	Pollution in the Arctic Ocean: An overview of multiple pressures and implications for ecosystem services	2021	Ambio	Springer
		AD Redman, J Bietz, JW Davis, D Lyon	Moving persistence assessments into the 21st Century: A role for weight-of-evidence (WoE) and overall persistence (POV)	2021	Integrated Environmental Assessment and Management	Wiley Online Library
		AR Kumar, I Singh, K Ambekar	Occurrence, Distribution, and Fate of Emerging Persistent Organic Pollutants in the Environment	2021	Management of Contaminants of Emerging Concern (CEC) in Environment	Elsevier
	X	JCF Law, Y Huang, CH Chow, TK Lam	Comparative physicochemical properties and toxicity of organic UV filters and their photocatalytic transformation products	2021	Environmental Pollution	Elsevier
X		MJ Whelan, J Kim	Application of multimedia models for understanding the environmental behavior of volatile methylsiloxanes: Fate, transport, and bioaccumulation	2021	Integrated Environmental Assessment and Management	Wiley Online Library
		K Hungerbühler, JM Boucher, C Pereira	Risk Assessment and Management of Chemical Products	2021	Chemical Products and Processes	Springer
	X	M Plaza-Hernández, J Legler, M MacLeod	Integration of production and use information into an exposure-based screening approach to rank chemicals of emerging Arctic concern for potential to be	2021	Emerging Contaminants	Elsevier
		JM Parnis, D Mackay	Multimedia environmental models: the fugacity approach	2020		taylorfrancis.com
		AT Besha, Y Liu, C Fang, DN Bekele	Assessing the interactions between micropollutants and nanoparticles in engineered and natural aquatic environments	2020	Critical Reviews in Environmental Science and Technology	Taylor & Francis
	X	X Zhang, X Sun, R Jiang, EY Zeng	Screening new persistent and bioaccumulative organics in China's inventory of industrial chemicals	2020	Environmental science & technology	ACS Publications
	X	J Zhao, P Wang, C Wang, M Fu, Y	Novel brominated flame retardants in West Antarctic	2020	Science of The Total	Elsevier

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		Li, R Yang	atmosphere (20112018): Temporal trends, sources and chiral signature		Environment	
		JO Okeme, TFM Rodgers, JM Parnis	Gas chromatographic estimation of vapor pressures and octanolair partition coefficients of semivolatile organic compounds of emerging concern	2020	Journal of Chemical & Engineering Data	ACS Publications
X		R Shring, M Scheringer, TFM Rodgers	Evaluation of the OECD P OV and LRTP screening tool for estimating the long-range transport of organophosphate esters	2020	Environmental Science: Processes & Impacts	pubs.rsc.org
		D Mackay, AKD Celsie, JM Parnis	A perspective on the role of fugacity and activity for evaluating the PBT properties of organic chemicals and providing a multi-media synoptic indicator of environmental	2020	Environmental Science: Processes & Impacts	pubs.rsc.org
	X	HJ Lee, JH Kwon	Persistence and bioaccumulation potential of alternative brominated flame retardants	2020	Comprehensive Analytical Chemistry	Elsevier
		Barrett, K. S. C., & Jaward, F. M.	The Potential Influence of Forests and Climate Change on the Environmental Fates of Organic Compounds in Tropical Watersheds.	2020	Current Journal of Applied Science and Technology	
	X	D Muir, X Zhang, CA De Wit, K Vorkamp	Identifying further chemicals of emerging arctic concern based on 'in silico' screening of chemical inventories	2019	Emerging Contaminants	Elsevier
	X	Z Lu, AO De Silva, JF Provencher, ML Mallory	Occurrence of substituted diphenylamine antioxidants and benzotriazole UV stabilizers in Arctic seabirds and seals	2019	Science of The Total Environment	Elsevier
	X	S Xu, N Warner, P Bohlin-Nizzetto, J Durham, D McNett	Long-range transport potential and atmospheric persistence of cyclic volatile methylsiloxanes based on global measurements	2019	Chemosphere	Elsevier
	X	C Rizzi, A Finizio, V Maggi, S Villa	Spatial-temporal analysis and risk characterisation of pesticides in Alpine glacial streams	2019	Environmental Pollution	Elsevier
	X	D Lörchner, W Kraus, R Köppen	Photodegradation of the novel brominated flame retardant 2, 4, 6-Tris-(2, 4, 6-tribromophenoxy)-1, 3, 5-triazine in solvent system: Kinetics, photolysis products and	2019	Chemosphere	Elsevier
		T Junker, A Coors	Compartment-Specific Screening Tools for Persistence: Potential Role and Application in the	2019	Integrated Environmental Assessment and Management	Wiley Online Library

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
			Regulatory Context			
		K Mojsiewicz-Pienkowska, D Krenczkowska	Evolution of consciousness of exposure to siloxanes review of publications	2018	Chemosphere	Elsevier
	X	WJ Hong, H Jia, Y Ding, WL Li, YF Li	Polychlorinated biphenyls (PCBs) and halogenated flame retardants (HFRs) in multi-matrices from an electronic waste (e-waste) recycling site in Northern China	2018	Journal of Material Cycles and Waste Management	Springer
	X	TFM Rodgers, JW Truong, LM Jantunen	Organophosphate ester transport, fate, and emissions in Toronto, Canada, estimated using an updated multimedia urban model	2018	Environmental science & technology	ACS Publications
X		A Di Guardo, T Gouin, M MacLeod	Environmental fate and exposure models: advances and challenges in 21 st century chemical risk assessment	2018	Environmental Science: Processes & Impacts	pubs.rsc.org
	X	JO Okeme, TFM Rodgers, LM Jantunen	Examining the gas-particle partitioning of organophosphate esters: how reliable are air measurements?	2018	Environmental science & technology	ACS Publications
		E Saouter, F Biganzoli, L Ceriani	#VALUE!	2018	European Union Joint Research Centre	researchgate.net
	X	A Gackowska, W Studzinski, E Kudlek	Estimation of physicochemical properties of 2-ethylhexyl-4-methoxycinnamate (EHMC) degradation products and their toxicological evaluation	2018	Environmental Science and Pollution Research	Springer
	X	J Kim, D Mackay, MJ Whelan	Predicted persistence and response times of linear and cyclic volatile methylsiloxanes in global and local environments	2018	Chemosphere	Elsevier
		MA Bonnell, A Zidek, A Griffiths	Fate and exposure modeling in regulatory chemical evaluation: new directions from retrospection	2018	Environmental Science: Processes & Impacts	pubs.rsc.org
		MS McLachlan	Can the Stockholm convention address the spectrum of chemicals currently under regulatory scrutiny? Advocating a more prominent role for modeling in POP	2018	Environmental Science: Processes & Impacts	pubs.rsc.org
	X	E Reppas-Chrysovitsinos, A Sobek	In silico screening-level prioritization of 8468 chemicals produced in OECD countries to identify potential planetary boundary threats	2018	Bulletin of environmental Contamination and Toxicology	Springer
	X	K Yui, T Motoki, H Kato, H Kuramochi	Measurement of vapor pressures and melting properties of five polybrominated aromatic flame retardants	2018	Journal of Chemical & Engineering Data	ACS Publications

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		C Ferrario, A Finizio, S Villa	Legacy and emerging contaminants in meltwater of three Alpine glaciers	2017	Science of the Total Environment	Elsevier
		M Vighi, M Matthies, KR Solomon	Critical assessment of pendimethalin in terms of persistence, bioaccumulation, toxicity, and potential for long-range transport	2017	Journal of Toxicology and Environmental Health	Taylor & Francis
X		E Reppas-Chrysovitsinos, A Sobek, M MacLeod	Screening-level exposure-based prioritization to identify potential POPs, vPvBs and planetary boundary threats among Arctic contaminants	2017	Emerging Contaminants	Elsevier
		RK Göktas, M MacLeod	Hazardous pollutants in the water environment	2017	Hazardous Pollutants in Biological Treatment Systems: Fundamentals and a guide to Experimental Research	books.google.com
		IT Cousins, R Vestergren, Z Wang, M Scheringer	The precautionary principle and chemicals management: The example of perfluoroalkyl acids in groundwater	2016	Environment International	Elsevier
	X	R Suhring, ML Diamond, M Scheringer	Organophosphate esters in Canadian Arctic air: occurrence, levels and trends	2016	Environmental science & technology	ACS Publications
	X	R Suhring, H Wolschke, ML Diamond	Distribution of organophosphate esters between the gas and particle phase model predictions vs measured data	2016	Environmental science & technology	ACS Publications
		Z Wang, IT Cousins, U Berger, K Hungerbühler	Comparative assessment of the environmental hazards of and exposure to perfluoroalkyl phosphonic and phosphinic acids (PFPAs and PFPiAs): current knowledge	2016	Environment International	Elsevier
	X	HJ Lee, JH Kwon	Evaluation of Long-Range Transport Potential of Selected Brominated Flame Retardants with Measured 1-OctanolAir Partition Coefficients	2016	Bulletin of the Korean Chemical Society	Wiley Online Library
	X	LJ Trouborst	Aqueous photolysis of 6: 2 fluorotelomer sulfonamide alkylbetaine	2016	University of Toronto	search.proquest.com
	X	JME Storey, MP Bunce, EM Clarke	Pollutant emissions and environmental assessment of ethyl 3-ethoxybutyrate, a potential renewable fuel	2016	Environmental Science and Pollution Research	Springer
X		MI Gomis, Z Wang, M Scheringer, IT Cousins	A modeling assessment of the physicochemical properties and environmental fate of emerging and novel per-and polyfluoroalkyl substances	2015	Science of The Total Environment	Elsevier
	X	I Liagkouridis, AP Cousins, IT	Physicalchemical properties and evaluative fate	2015	Science of The Total	Elsevier

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		Cousins	modelling of 'emerging' and 'novel' brominated and organophosphorus flame retardants in the indoor and outdoor		Environment	
	X	D Mackay, CE Cowan-Ellsberry	Decamethylcyclopentasiloxane (D5) environmental sources, fate, transport, and routes of exposure	2015	Environmental Toxicology and Chemistry	Wiley Online Library
	X	K Jagiello, T Puzyn	Computational techniques application in environmental exposure assessment	2015	Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment	igi-global.com
		AK Venkatesan, RU Halden	Wastewater treatment plants as chemical observatories to forecast ecological and human health risks of manmade chemicals	2014	Scientific reports	nature.com
		D Mackay, JP Giesy, KR Solomon	Fate in the environment and long-range atmospheric transport of the organophosphorus insecticide, chlorpyrifos and its oxon	2014	Ecological Risk Assessment for Chlorpyrifos in Terrestrial 77 and Aquatic Systems in the United States	library.oapen.org
		D Mackay, DM Hughes, ML Romano	The role of persistence in chemical evaluations	2014	Integrated Environmental Assessment and Management	Wiley Online Library
	X	S Villa, M Vighi, A Finizio	Theoretical and experimental evidences of medium range atmospheric transport processes of polycyclic musk fragrances	2014	Science of the Total Environment	Elsevier
	X	H Kuramochi, H Takigami, M Scheringer	Estimation of physicochemical properties of 52 non-PBDE brominated flame retardants and evaluation of their overall persistence and long-range transport potential	2014	Science of the Total Environment	Elsevier
		JP Giesy, KR Solomon	Evaluation of evidence that the organophosphorus insecticide chlorpyrifos is a potential persistent organic pollutant (POP) or persistent, bioaccumulative, and	2014	Environmental Science Europe	enveurope.springeropen.com
		H Kuramochi, H Takigami, M Scheringer	Measurement of vapor pressures of selected PBDEs, hexabromobenzene, and 1, 2-bis (2, 4, 6-tribromophenoxy) ethane at elevated temperatures	2014	Journal of Chemical & Engineering Data	ACS Publications
X		S Thuens, C Blodau, F Wania, M Radke	Comparison of atmospheric travel distances of several PAHs calculated by two fate and transport models (the Tool and ELPOS) with experimental values derived from	2014	Atmosphere	mdpi.com

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		M Scheringer, A Praetorius, ES Goldberg	Environmental fate and exposure modeling of nanomaterials	2014	Frontiers of nanoscience	Elsevier
X		T Kawai, K Jagiello, A Sosnowska	A new metric for long-range transport potential of chemicals	2014	Environmental science & technology	ACS Publications
		SJ Lim, P Fox	Effects of halogenated aromatics/aliphatics and nitrogen (N)-heterocyclic aromatics on estimating the persistence of future pharmaceutical compounds using a	2014	Science of the total environment	Elsevier
		N Kazantzis, V Kazantzi, EG Christodoulou	Pollutant concentration profile reconstruction using digital soft sensors for biodegradation and exposure assessment in the presence of model uncertainty	2014	Environmental Science and Pollution Research	Springer
		DG Wang, W Norwood, M Alaee, JD Byer, S Brimble	Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment	2013	Chemosphere	Elsevier
	X	S Xu, F Wania	Chemical fate, latitudinal distribution and long-range transport of cyclic volatile methylsiloxanes in the global environment: A modeling assessment	2013	Chemosphere	Elsevier
		A Praetorius, R Arvidsson, S Molander	Facing complexity through informed simplifications: a research agenda for aquatic exposure assessment of nanoparticles	2013	Environmental Science: Processes & Impacts	pubs.rsc.org
		J Klnov, T Harner	The challenge of producing reliable results under highly variable conditions and the role of passive air samplers in the Global Monitoring Plan	2013	TrAC Trends in Analytical Chemistry	Elsevier
		J Kim, DE Powell, L Hughes, D Mackay	Uncertainty analysis using a fugacity-based multimedia mass-balance model: Application of the updated EQC model to decamethylcyclopentasiloxane (D5)	2013	Chemosphere	Elsevier
		SJ Lim, E Jang, SH Lee, BH Yoo, SK Kim	Antibiotic resistance in bacteria isolated from freshwater aquacultures and prediction of the persistence and toxicity of antimicrobials in the aquatic environment	2013	Environmental Science and Health	Taylor & Francis
		M Guo	Life cycle assessment (LCA) of light-weight eco-composites	2013		books.google.com
	X	D Kong, M MacLeod, Z Li, IT Cousins	Effects of input uncertainty and variability on the modelled environmental fate of organic pollutants	2013	Chemosphere	Elsevier

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
			under global climate change scenarios			
X		K Odziomek, A Gajewicz, M Haranczyk	Reliability of environmental fate modeling results for POPs based on various methods of determining the air/water partition coefficient (log KAW)	2013	Atmospheric Environment	Elsevier
		SJ Lim, P Fox	Prediction of the potential fates of future pharmaceutical compounds in indirect potable reuse systems	2013	Science of the total environment	Elsevier
	X	Q Li, J Li, Y Wang, Y Xu, X Pan, G Zhang	Atmospheric short-chain chlorinated paraffins in China, Japan, and South Korea	2012	Environmental science & technology	ACS Publications
		M Scheringer, S Strempel, S Hukari, CA Ng	How many persistent organic pollutants should we expect?	2012	Atmospheric Pollution Research	Elsevier
		AM Buser, M MacLeod, M Scheringer Mark Bonnell, Mark H Russell, Joseph V DePinto, Konrad Hungerbühler	Good modeling practice guidelines for applying multimedia models in chemical assessments	2012	Integrated Environmental Assessment and Management	Wiley Online Library
	X	T Öberg, MS Iqbal	The chemical and environmental property space of REACH chemicals	2012	Chemosphere	Elsevier
	X	EFSA Panel on Contaminants in the Food	Scientific opinion on emerging and novel brominated flame retardants (BFRs) in food	2012	EFSA Journal	Wiley Online Library
		C Zarfl, I Hotopp, N Kehrein, M Matthies	Identification of substances with potential for long-range transport as possible substances of very high concern	2012	Environmental Science and Pollution Research	Springer
		A Hollander, M Hauck, IT Cousins	Assessing the relative importance of spatial variability in emissions versus landscape properties in fate models for environmental exposure assessment of chemicals	2012	Environmental Modeling & Assessment	Springer
		S Gama, D Mackay, JA Arnot	Selecting and designing chemicals: application of a mass balance model of chemical fate, exposure and effects in the environment	2012	Green chemistry	pubs.rsc.org
		S Gama, JA Arnot, D Mackay	Toxic Organic Chemicals	2012	Transport and Fate of Chemicals in the Environment	Springer
		ED Sverko, GT Tomy, EJ Reiner, YF Li	Dechlorane plus and related compounds in the environment: a review	2011	Environmental science & technology	ACS Publications

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
		CH Marvin, GT Tomy, JM Armitage	Hexabromocyclododecane: current understanding of chemistry, environmental fate and toxicology and implications for global management	2011	Environmental science & technology	ACS Publications
		JA Arnot, JM Armitage, LS McCarty, F Wania	Toward a consistent evaluative framework for POP risk characterization	2011	Environmental science & technology	ACS Publications
		C Zarfl, M Scheringer, M Matthies	Screening criteria for long-range transport potential of organic substances in water	2011	Environmental science & technology	ACS Publications
		A Qureshi, M MacLeod	Quantifying uncertainties in the global mass balance of mercury	2011	Global Biogeochemical Cycles	Wiley Online Library
	X	S Sala, D Marinov, D Pennington	Spatial differentiation of chemical removal rates from air in life cycle impact assessment	2011	The International Journal of Life Cycle Assessment	Springer
	X	T Puzyn	On the replacement of empirical parameters in multimedia mass balance models with QSPR data	2011	Journal of hazardous materials	Elsevier
		E Bentzen, M MacLeod, B Hickie	Mixing in the Atmosphere and Surface Waters with Application to Compartment Box Models	2011	Library of Congress Cataloging-in-Publication Data	chemistry-chemists.com
		M MacLeod, M Scheringer, TE McKone	The state of multimedia mass-balance modeling in environmental science and decision-making	2010	Environmental science & technology	ACS Publications
		CW Götz, C Stamm, K Fenner, H Singer	Targeting aquatic microcontaminants for monitoring: exposure categorization and application to the Swiss situation	2010	Environmental Science and Pollution Research	Springer
		K Voigt, R Brueggemann, H Scherb, H Shen	Evaluating the relationship between chemical exposure and cryptorchidism	2010	Environmental Modelling & Software	Elsevier
	X	A Mostrag, T Puzyn, M Haranczyk	Modeling the overall persistence and environmental mobility of sulfur-containing polychlorinated organic compounds	2010	Environmental Science and Pollution Research	Springer
X		T Gouin	The precautionary principle and environmental persistence: prioritizing the decision-making process	2010	environmental science & policy	Elsevier
		M Scheringer	Long-range transport of organic chemicals in the environment	2009	Environmental Toxicology and Chemistry	Wiley Online Library
		M Scheringer, KC Jones, M Matthies	Multimedia partitioning, overall persistence, and long-range transport potential in the context of POPs and PBT chemical assessments	2009	Integrated Environmental Assessment and Management	Wiley Online Library
		J Arnot, L McCarty, J Armitage	An evaluation of hexabromocyclododecane (HBCD) for persistent organic pollutant (POP) properties and	2009	Submitted to UN ECE POP RC	researchgate.net

Shortcoming identification/Improvement suggestion	Application	Authors	Title	Year	Source	Publisher
			the potential for adverse effects in the environment			
		M Matthies, J Klasmeier, A Beyer	Assessing persistence and long-range transport potential of current-use pesticides	2009	Environmental science & technology	ACS Publications
		JA Arnot	Mass balance models for chemical fate, bioaccumulation, exposure and risk assessment	2009	Exposure and Risk Assessment of Chemical Pollution - Contemporary Methodology	Springer
	X	S Becker, CJ Halsall, M MacLeod	Empirical Investigation of the Junge Variability-Lifetime Relationship Using Long-Term Monitoring Data on Polychlorinated Biphenyl Concentrations in Air	2009	Environmental science & technology	ACS Publications
		RK Rosenbaum, TM Bachmann, LS Gold	USEtox the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment	2008	The International Journal of Life Cycle Assessment	Springer
		A Hollander, M Scheringer, V Shatalov	Estimating overall persistence and long-range transport potential of persistent organic pollutants: a comparison of seven multimedia mass balance models and	2008	Journal of Environmental Monitoring	pubs.rsc.org
	X	CW Götz, M Scheringer, M MacLeod	Dependence of persistence and long-range transport potential on gas-particle partitioning in multimedia models	2008	Environmental science & technology	ACS Publications

Annex B. Screening a large set of chemicals for LRTP with the Tool using the existing (CTD, TE) and alternative metrics (emissions fractions φ1-φ3)

Report to the OECD EG on the Tool by Knut Breivik, Michael S. McLachlan and Frank Wania submitted in December 2022

This report was submitted by one of the members of the Expert Group and his collaborators to inform discussions within the Expert Group. Any views expressed herein reflect the authors' perspectives and not those of the Expert Group.

1. Objectives

The objective of the analysis was to assess the implications of the choice of LRTP metrics when screening a large set of chemicals using the Tool. The key motivation was to inform the Expert Group on the differences arising when relying on existing LRTP metrics (CTD, TE) versus an alternative set of three LRTP metrics that we have recently developed, collectively referred to as the Emission Fractions Approach (EFA). Of specific interest was the extent of agreement between the outcome of LRTP assessments based on the current approach [plots of CTD or TE versus P_{OV}] versus the alternative EFA metric φ3 which in addition to dispersion and transfer accounts for accumulation in surface media in a remote region.

2. Methods

The existing LRTP metrics in the Tool are described in Wegmann et al.[1], while the EFA is described in Breivik et al. (2022).[2] As the latter paper was circulated to the members of the EG ahead of the previous meeting, we only reiterate definitions of the EFA metrics here:

φ1: The environmentally dispersed fraction (φ1) expresses the relative potential of a chemical to undergo dispersion by air and water combined.

φ2: The remotely transferred fraction (φ2) expresses the relative extent to which a chemical is net transferred to surface compartments of a remote region, accounting for environmental dispersion in air and water (φ1).

φ3: The remotely accumulated fraction (φ3) expresses the relative extent to which a chemical is accumulating in surface compartments of a remote region, accounting for dispersion (φ1) and transfer (φ2) in air and water.

The three EFA metrics were implemented along with CTD and TE as they are currently formulated in the Level 3 model of the Tool. All environmental input parameters were kept unchanged, except that we modified code to account for the intermittency of precipitation.[2] While this will lead to different numerical results for chemicals subject to wet deposition compared to outputs from the existing version of the Tool, it ensures a consistent approach in the analysis presented herein.

For the analysis we chose an existing curated data set of 12,615 organic chemicals previously published by Arnot et al.,[3] because the required physical-chemical input properties (log K_{AW}, log K_{OW}) and degradation half-lives (air, water and soil) were already available. The data set includes chemicals spanning a wide range of fate properties. Specifically, log K_{AW} varies from -12 to 3 while log K_{OW} spans a range from -4 to 9. Degradation half-lives in air, water and soil (in hours), vary from 4.7E-04 to 1.3E+06, 1.2E+01 to 9.0E+04, and 2.3E+01 to 1.8E+05, respectively.

The reference lines for POP-like LRTP and P_{ov} using any metric, shown in Table A B.1, were calculated using the properties of a set of 14 legacy POPs.[2] Table A B.1 also gives the number and percentage of chemicals out of the 12,615 exceeding each reference line. We have also added the chemical which defines each reference line (i.e., the POP which leads to the lowest value of a metric).

Table A B.1. Reference lines for POP-like behaviour derived on the basis of selected legacy POPs, along with the POP which dictates the reference line. The number of chemicals out of a set of 12,615 organic chemicals exceeding each of these reference lines are included.

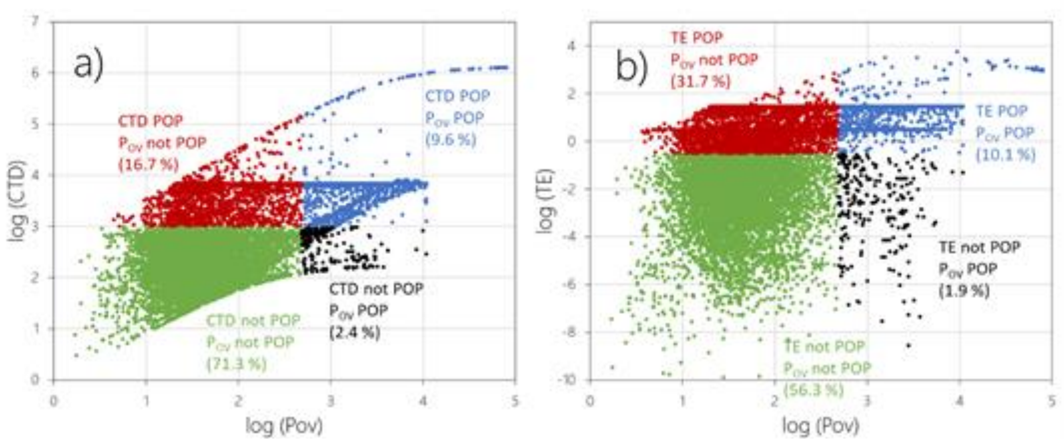
N = 12,615	φ 1	φ 2	φ 3	CTD	TE	P_{OV}
Reference line	7.7E-04	8.4E-05	8.2E-06	1,020	0.32	480
Reference line (log)	−3.1	−4.1	−5.1	3.01	−0.49	2.68
Chemical defining the reference line	*cis*-chlordane	*trans*-chlordane	PCB-28	*cis*-chlordane	*trans*-chlordane	HCB
N ≥ reference line	3,538	5,987	2,982	3,315	5,278	1,511
N ≥ reference line (%)	28.0	47.5	23.6	26.3	41.8	12.0

3. Results

3.1. Existing metrics (LRTP-P_{OV} plots)

Figure A B.1 displays the LRTP-P_{OV} plots, using either CTD (Fig a) or TE (Fig b) as the LRTP metric. The chemicals which fall into each quadrant in these plots are highlighted with differently coloured markers.

Figure A B.1. Plots of LRTP versus P_{OV} from the Tool for 12,615 organic chemicals. The percentages of chemicals falling into each of the four quadrants are included. Chemicals identified as POP-like according to both LRTP and P_{OV} are located in the upper right quadrant (blue markers).



The LRTP assessment based on CTD-P_{OV} (Figure A B.1 a) flags 8,995 out of 12,1615 chemicals (71.3%) as non-POP like (green markers). 305 chemicals (2.4%) will be assessed as not having LRTP according to CTD (i.e., CTD below the reference line in Table A B.1), but POP-like P_{OV} (black markers). 2,109 chemicals (16.7%) will be assessed as having LRTP (CTD) but no POP-like P_{OV}, while 1,206 chemicals (9.6%) will be flagged with POP-like LRTP behaviour and persistence.

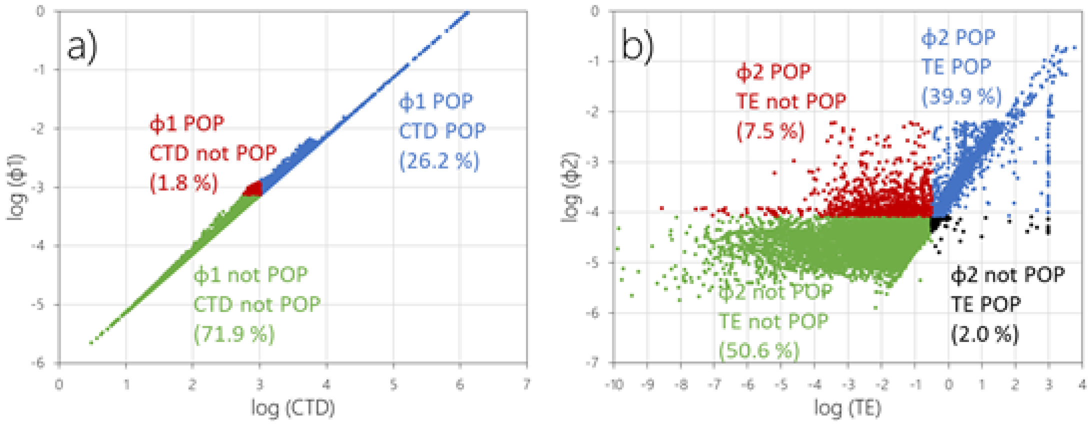
The LRTP assessment relying on TE-P_{OV} (Figure A B.1 b) predicts that (i) 7,099 chemicals (56.3%) are not POP-like, (ii) 238 chemicals (1.9%) do not exceed the reference line for TE, but the reference line for P_{OV}, (iii) 4,005 chemicals (31.7%) are POP-like in terms of TE, but not above the reference line for P_{OV}, and (iv) 1,273 chemicals (10.1%) are POP-like according to both TE and P_{OV}.

1,132 chemicals (9.0%) are flagged as POP-like by both TE and CTD, i.e., fall into the upper right quadrant in both the CTD-P_{OV} plot (Figure a) and TE-P_{OV} plot (Figure b). Another 215 chemicals exceed either the CTD-P_{OV} criteria or the TE-P_{OV} criteria, but not both.

3.2 CTD versus φ1 and TE versus φ2

In Figure A B.2 a), we have plotted the existing as well as the alternative transport-oriented metrics against each other, i.e., CTD versus φ1. Please note that the CTD here is the larger of the CTD in air or water. The existing and alternative transfer-oriented metrics, i.e., TE versus φ2, are compared in Figure A B.2 b).

Figure A B.2. Predictions of dispersion and transfer from the Tool for 12,615 organic chemicals: a) log CTD vs log φ1, and b) log TE versus log φ2.



The CTD_{air} and $\varphi 1_{air}$ convey the same mechanistic information.[2] The same applies to CTD_{water} and $\varphi 1_{water}$.[2] Hence, if the two pairs of transport-oriented metrics are plotted against each other, the plots will show a straight line. The main difference between the two CTDs and φ1, is that $\varphi 1_{air}$ and $\varphi 1_{water}$ are additive, i.e. $\varphi 1 = \varphi 1_{air} + \varphi 1_{water}$, whereas that is not the case for CTD_{water} and CTD_{air}. This explains why in a plot of φ1 against CTD (Figure A B.2 a), a model-predicted φ1 value for a given chemical either falls on or above the 1:1 line. In Figure A B.2 a), 229 chemicals (1.8%) fall into the region highlighted with red markers. These chemicals are above the reference line for φ1, but below the reference line for CTD (Table A B.1). In other words, these are chemicals which only will be classified as having a POP-like transport if combined transport in air and water is considered. While the fraction of chemicals affected may appear small, it clearly indicates the potential for underestimating the total transport in air and water combined, even if CTD_{air} and CTD_{water} are both taken into consideration. We note that two decades ago, Beyer and Matthies[4] had already used model simulations to show that "combined transport in coupled air-ocean systems can accelerate the overall transport into remote regions".

Figure A B.2 b) compares the gross atmospheric transfer to surface media of the remote region (TE) against the net transfer to surface media as a result of both LRAT and LRWT (φ2). The TE accounts for neither dispersion in water and nor the reversibility of atmospheric deposition. Ignoring LRWT leads to a low bias in the TE, whereas ignoring reversible atmospheric deposition leads to TE being biased high. The relatively large fraction of chemicals that is categorized as having POP-like LRTP based on φ2, but not TE (red markers in Figure A B.2 b), *N*=955 or 7.5%) indicates that ignoring LRWT affects a considerably larger number of chemicals than ignoring reversible atmospheric deposition (black markers, 2 %).

For some chemicals, the two biases of the TE may counteract each other. When we isolate the impact of calculating net versus gross deposition by comparing TE with $\varphi 2_A$ (the emission fraction transferred in air which also "ignores" LRWT), a larger number of chemicals falls in the lower right quadrant, i.e. are categorized as POP by TE but not by $\varphi 2_A$ (data not shown). This is because gross atmospheric deposition overestimates atmospheric inputs to surface media of the remote region. A persistent flyer, such as CFC-12 (log TE = ~3, log φ2 = -4), is an example.[2]

In summary, transfer of volatile chemicals can be overestimated in an LRTP assessment based on TE. It can also underestimate the total transfer because it does not allow for transfer with water.

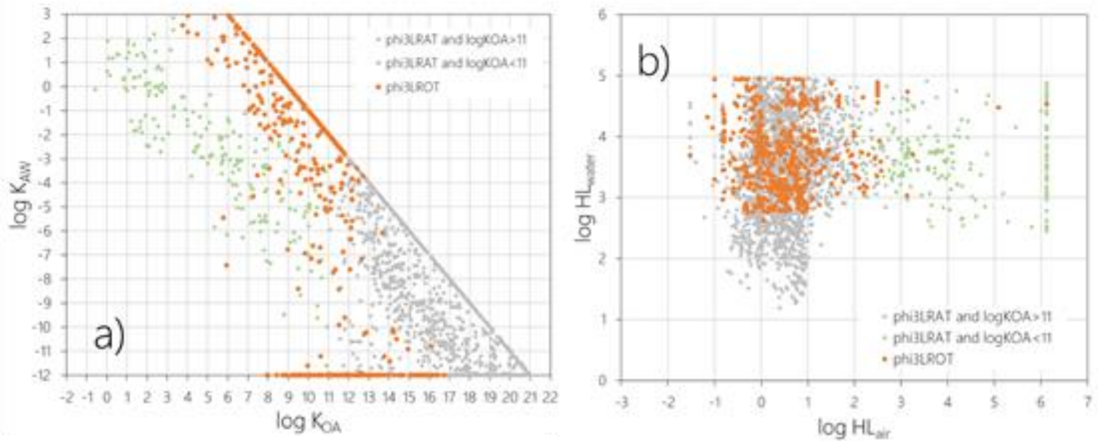
3.3 LRTP-P_{OV} versus accumulation (φ3)

The existing approach to LRTP assessment does not have a metric that seeks to quantify the accumulation of a chemical in a remote region, even though such accumulation is arguably a prerequisite for significant adverse human health and/or environmental effects likely occurring as a result of long-range environmental transport, which is the wording in the Stockholm Convention. To assess whether an LRTP metric and a persistence metric in combination identify chemicals with the potential for accumulation in remote regions, we compare the chemicals categorized as having POP-like LRTP based on a metric directly quantifying remote accumulation (φ3) with the chemicals identified as POP-like in the CTD/P_{OV} and TE/P_{OV} plots in section 3.1 above.

The number of chemicals which are POP-like using the existing approach (CTD-P_{OV}/TE-P_{OV}) is 1,132 or 9.0% (see Section 3.1). In comparison, the total number of chemicals which exceeds the criterion for POP-like accumulation (φ3) is 2,982 or 23.6% (Table A B.1), i.e., more than 2.6 times the number of chemicals fulfilling both LRTP-P_{OV} criteria. Among the 2,982 chemicals in the screening data set which exceed the criterion for POP-like accumulation (φ3), there are 1,402 chemicals which fulfill the criterion for P_{OV} and 1,580 chemicals which do not. In other words, there are many chemicals assessed to have the potential to accumulate in remote regions (based on φ3) without being persistent (i.e., meeting the POV criterion). We conclude that CTD-P_{OV} and/or TE-P_{OV} would underestimate the total number of chemicals that have remote accumulation potential according to φ3.

What then are the combinations of properties that allow a chemical to accumulate in remote regions? In order to elucidate the role LRAT and LRWT play for chemicals with a φ3 above the reference line, we first calculated how many of those chemicals have a $φ3_A$ (the remotely accumulated fraction without dispersion in water) above the reference line value for φ3: 19.5% (N=2,466) of all chemicals were predicted to accumulate in remote surface media as result of LRAT, leaving 4.1% (N=516) which accumulate in remote surface media only when both LRAT and LRWT are accounted for (data not shown). Figure A B.3 displays the partitioning and degradation properties of the chemicals with a φ3 above the reference line using green and grey markers to designate those undergoing LRAT and orange markers to identify the rest of the chemicals which exceed the reference line for φ3 only if both LRAT and LRWT are considered.

Figure A B.3. Diagnostic plots for those chemicals which exceed the reference line for φ3 (N=2,982).



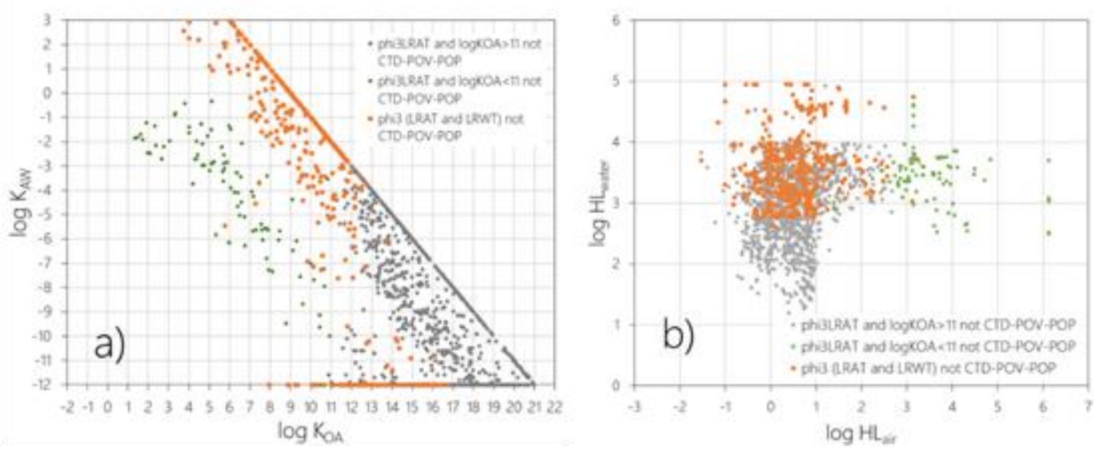
Note: The plot to the left shows results in a chemical space plot, whereas the plot to the right shows the results when plotting degradation half-life in air (hours) versus degradation half-life in water (hours). The colours of the markers identify chemicals which accumulate in surface media in the remote region (i) because of LRAT and with a log K_{OA}>11 (grey), and (ii) because of LRAT and with a log K_{OA}<11 (green). The remaining chemicals only exceed the reference line for φ3 when both LRAT and LRWT are accounted for (orange).

Most chemicals which exceed the criterion for φ3 as result of LRAT have a log K_{OA} above 11 (*N*=2,242 or 17.8%) and therefore are sorbed to atmospheric particles in the Tool. They can undergo LRAT even if their degradation half-life in air is relatively short (Figure A B.3 b); grey markers), because it is assumed that sorption to particles prevents them from undergoing atmospheric degradation reactions. On the other hand, chemicals which exceed the criterion for φ3 as result of LRAT but occur in the atmospheric gas phase, i.e., have a log K_{OA} < 11 (*N*=224 or 1.8%, green markers), need to be persistent in air (log(HL_{air}/h) > 2) (Fig. 3b).

Not surprisingly, the 516 chemicals (4.1%) that only exceed the φ3 reference line when both LRAT and LRWT are accounted for are reasonably persistent in surface media (log(HL_{water}/h) > 2.8, orange markers in Figure A B.3 b). They also have partitioning properties that do not allow for significant evaporation from water, either because they have a low log K_{AW} (approximately below -4) or because they are particle-bound in water (have a log K_{OW} > 6) (orange markers in Figure A B.3 a).

Why does the CTD-P_{OV} and TE-P_{OV} combinations not identify the ability of many of the 2982 chemicals displayed in Figure A B.4 to have a high remote accumulation potential (POP-like according to φ3)? Figure A B.4 is a version of Figure A B.3, which only displays the chemicals (with a φ3 above the reference line) that were not identified by an assessment based on CTD-P_{OV}. A plot showing the compounds not identified by TE-P_{OV} looks rather similar and is therefore not shown. Figure A B.4 indicates that the CTD-P_{OV} combination does not recognize the elevated remote accumulation potential of representatives of all three groups of chemicals: more than half of the involatiles with a log K_{OA} > 11 (N=1,281 out of 2,242 or 10.2% of the screening data set, grey markers), less than half of the chemicals undergoing LRAT in the gas phase (N=103 out of 224; 0.8%, green markers), and most of the chemicals subject to LRWT (N=426 out of 516; 3.4%, orange markers). A comparison of the grey markers between Figure A B.3 b) and Figure A B.4 b) reveals that it is mostly the involatile chemicals that are highly persistent in surface media (with a log(HL_{water}/day) > 4) that are recognized by the CTD-P_{ov} approach as being subject to remote accumulation. A comparison of Figure A B.3 and Figure A B.4 similarly suggests that it is the highly volatile chemicals (green markers in the upper left of Figure A B.3 a) and those that are extremely persistent in air (green markers on the right side of Figure A B.3 b) that the CTD-P_{ov} approach classifies as being subject to remote accumulation.

Figure A B.4. Diagnostic plots for those chemicals which exceed the reference line for φ3, excluding chemicals that are identified as POP-like according to CTD-P_{OV}.



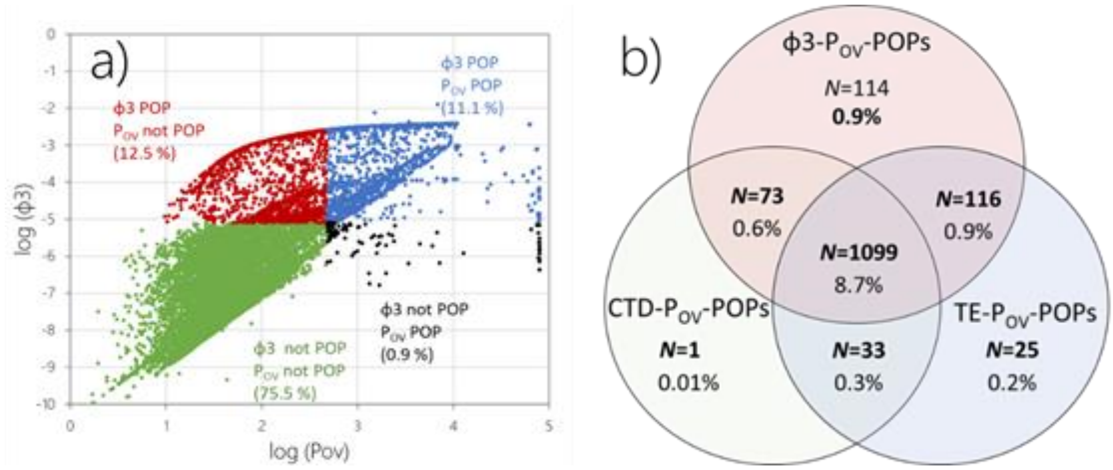
Note: The plot to the left shows results in a chemical partitioning space plot, whereas the plot to the right shows the results when plotting degradation half-life in air (hours) versus degradation half-life in water (hours). The colours of the markers identify chemicals which accumulate in surface media in the remote region (i) because of LRAT and with a log K_{OA}>11 (grey), and (ii) because of LRAT and with a log K_{OA}<11 (green). The remaining chemicals only exceed the reference line for φ3 when both LRAT and LRWT are accounted for (orange).

It is clear that from this analysis that the existing POP-like criteria involving a reference line for P_{OV} (CTD-P_{OV} and/or TE-P_{OV}) do not identify more than half of the chemicals that are subject to dispersion, transfer and accumulation in surface media of the remote region according to the EFA. Figure A B.4 suggests that the explanation for this is not simple. Not accounting for combined air and water transport is one of reasons. Another is that some chemicals have the potential for remote accumulation without meeting the P_{ov} persistence criterion.

4. Identifying chemicals with POP-like LRTP and POP-like persistence using CTD-P_{OV} / TE-Pov versus φ3-Pov

φ3 screens for remote accumulation potential only, but the CTD-P_{ov} (or TE-P_{ov}) combination screens for LRTP and persistence, whereby the P_{ov} metric serves the double purpose of screening for persistence and screening for chemicals dispersed (or transferred) to remote regions, that may or may not accumulate there. A POP identification procedure adopting the emission fraction approach to LRTP assessment likely would also include a persistence assessment, e.g., one based on the P_{ov}. In other words, using an approach analogous to that in the Tool, one could generate φ3-Pov plots which assign each chemical to one of four quadrants. Here φ3 serves as the criterion for LRTP and P_{ov} serves solely as the criterion for persistence. Figure A B.5 a) shows such a plot with the 12,615 chemicals, with the chemicals in the upper right quadrant designating chemicals with POP-like P_{ov} and POP-like LRTP according to φ3. There are 1402 such chemicals (11.1%). Their properties are shown in Figure A B.6 in the appendix.

Figure A B.5. a) Plot of φ3 versus P_{OV}, and b) comparison of the number of chemicals in the screening data set which fall into the category of φ3-P_{OV} POPs versus the number of chemicals which fall into any of the existing POP-categories.



Comparing Figure A B.5 with Figure A B.1 we can determine chemicals that would be classified differently with a φ3-P_{ov} approach and an approach relying on the existing LRTP metrics. From Figure A B.5, we see there are more chemicals (11.1% of the screening data set) that are POP-like according to φ3-P_{OV} in comparison to the existing criteria CTD-P_{OV} (9.6%) and TE-P_{OV} (10.1%) (Figure A B.1). There are in total 1,099 chemicals (8.7%) which are categorized as POP-like according to all criteria (CTD-P_{OV} and TE-P_{OV} and φ3-P_{OV}). This means that there are 303 chemicals (2.4% of the screening data) which are classified as POP-like according to φ3-P_{OV} but not LRTP-P_{OV} (i.e. flagged by both CTD-P_{OV} and TE-P_{OV} as POP-like). From the data in Figure A B.3 b), we can also infer that there are (i) 230 chemicals (1.8% of the screening data set) which are POP-like according to φ3-P_{OV} but not CTD-P_{OV}, and (ii) 187 chemicals (1.5%) which are POP-like according to φ3-P_{OV} but not TE-P_{OV}. Hence, even though the consideration of P_{OV} would eliminate most of the chemicals that a CTD-P_{OV} approach does not recognize as having remote accumulation potential (Figure A B.4), a screening for POP-like LRTP and persistence using φ3 and P_{OV}

would yield different outcomes compared to using CTD or TE. The appendix explores the properties of chemicals that are classified differently (Figure A B.7 to Figure A B.10).

5. Summary

The results presented in this report demonstrate that the existing and alternative LRTP metrics do not convey the same information and do not lead to similar outcomes in LRTP assessments. It is the author's view that the coherent set of metrics of the EFA represents a more mechanistically sound approach to LRTP assessment than the existing metrics. Specifically,

- Assessing dispersion potential with CTD instead of $\varphi 1$ does not account for the possibility of chemicals undergoing combined LRT in air and water.
- Assessing potential for transfer to a remote region with $\varphi 2$, unlike the existing version of TE accounts for (i) the possibility of chemicals being transferred to the remote environment in water, and (ii) accounts for reversible atmospheric deposition.
- Neither the CTD/P_{OV} combination or the TE/P_{OV} combination target potential for accumulation in a remote region.
- Any assessment of the potential for accumulation in a remote region with the CTD/P_{OV} combination instead of $\varphi 3$ will not capture chemicals undergoing LRT (i) without meeting persistence criteria and (ii) in air and water combined.
- Any assessment of the potential for accumulation in a remote region with the TE/P_{OV} combination instead of $\varphi 3$ will not account for chemicals undergoing LRT (i) without meeting persistence criteria and (ii) in water.

There is a possibility for considerable differences in LRTP classifications, dependent on the choice of metrics. The additional consideration of persistence does not eliminate all of these differences in LRTP classifications.

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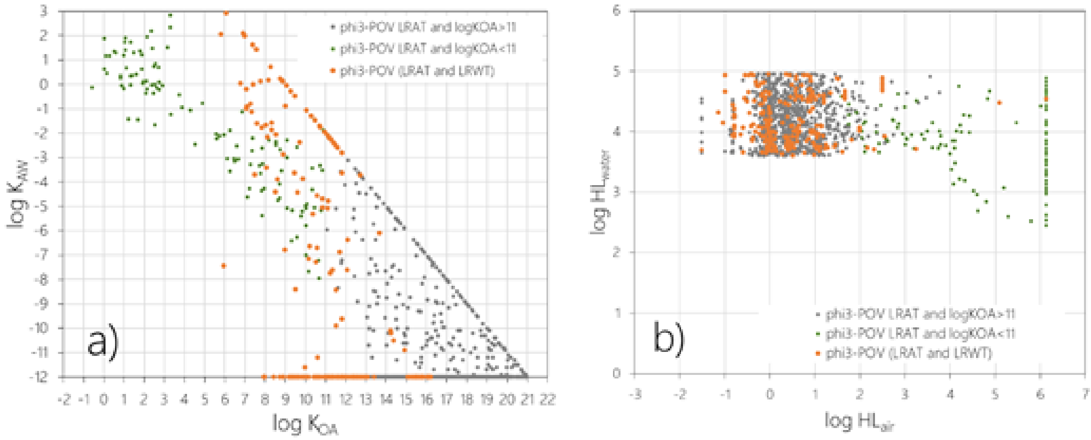
Appendix

Properties of chemicals with POP-like P_{OV} and POP-like φ3

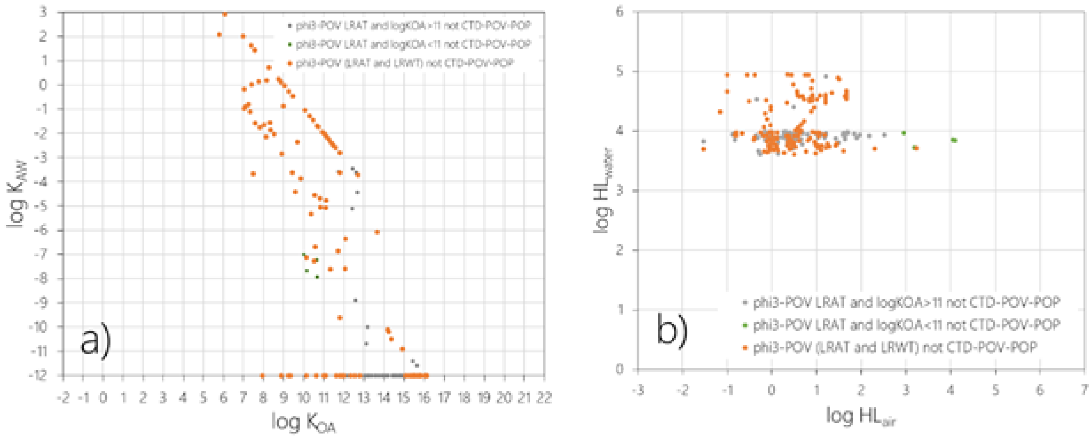
Figure A B.6. Diagnostic plots for those chemicals which exceed the reference lines for φ3-P_{OV} (N=1402; 11.1% in the screening data set).



Note: The plot to the left shows results in a chemical partitioning space plot, whereas the plot to the right shows the results when plotting degradation half-life in air (hours) versus degradation half-life in water (hours). The colours of the markers identify chemicals which accumulate in surface media in the remote region (i) because of LRAT and with a log K_{OA}>11 (grey: 1046; 8.3%), and (ii) because of LRAT and with a log K_{OA}<11 (green: N=125; 1.0%). The remaining chemicals only exceed the reference lines for φ3-P_{OV} when both LRAT and LRWT are accounted for (orange: N=231; 1.8%).

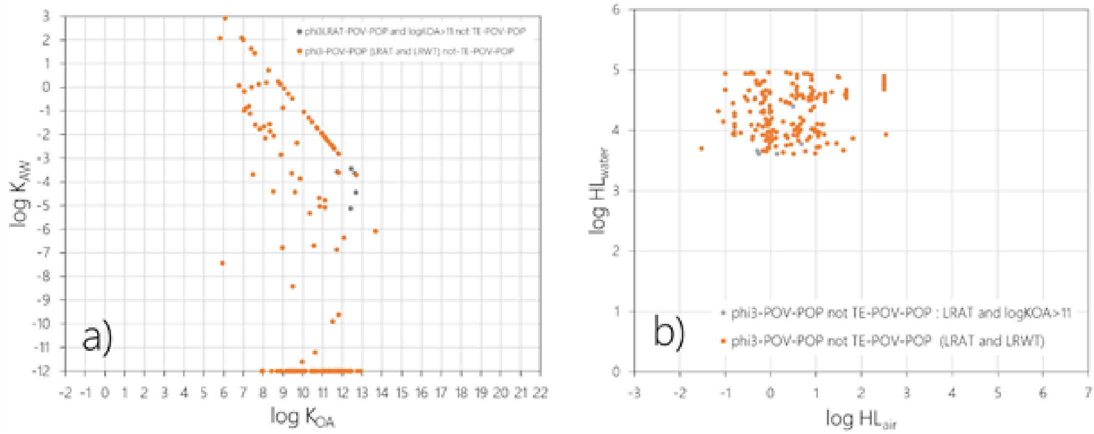
Properties of chemicals not assessed as POPs based on CTD-P_{ov} and TE-P_{ov} criteria.

Figure A B.7. Diagnostic plots for those chemicals which exceed the reference line for φ3-P_{OV}, but not the reference line for CTD-P_{OV} (N=230; 1.8% in the screening data set)



Note: The colours of the markers identify chemicals which accumulate in surface media in the remote region (i) because of LRAT and with a log K_{OA}>11 (grey: N=85; 0.7%), and (ii) because of LRAT and with a log K_{OA}<11 (green: N=4; 0.03%). The remaining chemicals only exceed the reference line for φ3-P_{OV} when both LRAT and LRWT are accounted for (orange: N=141; 1.1%).

Figure A B.8. Diagnostic plots for those chemicals which exceed the reference line for φ3-P_{OV}, but not the reference line for TE-P_{OV} (N=187; 1.5% in the screening date set).



Note: The colours of the markers identify chemicals which accumulate in surface media in the remote region because of LRAT and with a log K_{OA}>11 (grey: N=8; 0.1%). The remaining chemicals only exceed the reference line for φ3-P_{OV} when both LRAT and LRWT are accounted for (orange: N=179; 1.4%).

141 out of the 230 chemicals not assessed as POP-like by CTD-P_{ov} are persistent chemicals for which water is an important transport medium to remote regions. Most of the remainder (85 out of 230) are involatiles (Figure A B.7). Almost all of the chemicals not assessed as POP-like by TE-P_{ov} (179 out of 187) are chemicals for which water transport is important. Most of the involatile chemicals from the CTD-P_{ov} plot (Figure A B.7) do not appear in Figure A B.8.

Properties of chemicals classified as POPs based on CTD-Pov and TE-Pov criteria but not φ3-POV are shown in Figure A B.9 and Figure A B.10.

Figure A B.9. Diagnostic plots for those chemicals which exceed the reference line for CTD-P_{OV}, but not the reference line for φ3-P_{OV} (N=34; 0.3% of the screening data set)

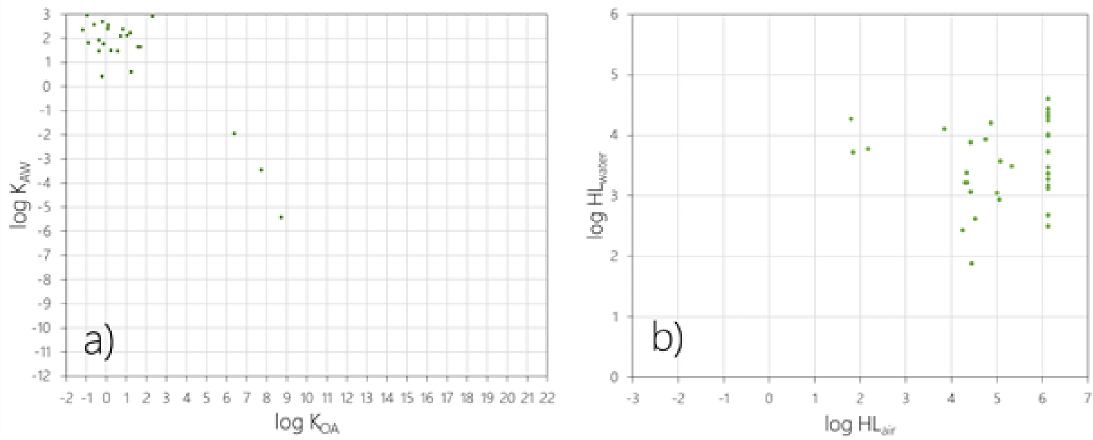
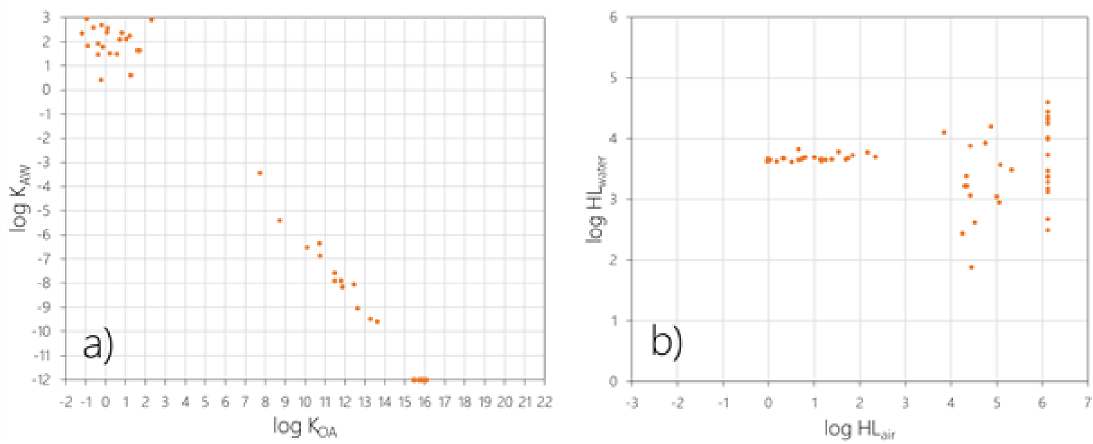


Figure A B.10. Diagnostic plots for those chemicals which exceed the reference line for TE-P_{OV}, but not the reference line for φ3-P_{OV} (N=58; 0.5% in the screening data set).



Chemicals deemed POP-like based on CTD-P_{OV} criteria but not based on φ3-Pov are highly volatile chemicals that are persistent in air (Figure A B.9). The reason for this is likely because CTD does not consider transfer to remote surface media. Chemicals deemed POP-like based on TE-P_{OV} criteria but not based on φ3-P_{OV} also are the volatiles that are persistent in air. Additionally, there is a series of chemicals with a very specific set of properties (log(HLwater/day) = 4.2, a log K_{OW} ~ 4 and a low log K_{AW}).