Organisation for Economic Co-operation and Development

ENV/CBC/MONO(2026)24

Unclassified English - Or. English

16 July 2026

ENVIRONMENT DIRECTORATE
CHEMICALS AND BIOTECHNOLOGY COMMITTEE

**Cancels & replaces the same document of 9 July 2026**

# Manual for the OECD Overall Persistence (Pov) and Long-range Transport Potential (LRTP) Screening Tool (version 3.0)

**OECD Series on Testing and Assessment, No. 444**

E-mail: ehscont@oecd.org

JT03590716

This work was approved and declassified by the Chemicals and Biotechnology Committee on 16/06/2026.

**Please cite this publication as:**

OECD (2026), *Manual for the OECD Overall Persistence (Pov) and Long-range Transport Potential (LRTP) Screening Tool (version 3.0)*, OECD Series on Testing and Assessment, No. 444, OECD Environment, Health and Safety, Paris, Environment, Health and Safety, Paris, https://one.oecd.org/document/ENV/CBC/MONO(2026)24/en/pdf.

**Contact us**

**OECD Environment Directorate,**
**Environment, Health and Safety Division**
**2 rue André-Pascal**
**75775 Paris Cedex 16**
**France**

**E-mail: ehscont@oecd.org**

# About the OECD

The Organisation for Economic Co-operation and Development (OECD) is an intergovernmental organisation in which representatives of 38 countries in North and South America, Europe and the Asia and Pacific region, as well as the European Union, meet to co-ordinate and harmonise policies, discuss issues of mutual concern, and work together to respond to international problems. Most of the OECD's work is carried out by more than 200 specialised committees and working groups composed of member country delegates. Observers from several Partner countries and from interested international organisations attend many of the OECD's workshops and other meetings. Committees and working groups are served by the OECD Secretariat, located in Paris, France, which is organised into directorates and divisions.

The Environment, Health and Safety Division publishes free-of-charge documents in twelve different series: **Testing and Assessment**; **Good Laboratory Practice and Compliance Monitoring**; **Pesticides**; **Biocides**; **Risk Management**; **Harmonisation of Regulatory Oversight in Biotechnology**; **Safety of Novel Foods and Feeds; Chemical Accidents; Pollutant Release and Transfer Registers; Emission Scenario Documents; Safety of Manufactured Nanomaterials;** and **Adverse Outcome Pathways.** More information about the Environment, Health and Safety Programme and EHS publications is available on the OECD's World Wide Web site (https://www.oecd.org/en/topics/chemical-safety-and-biosafety.html).

This publication was developed in the IOMC context. The contents do not necessarily reflect the views or stated policies of individual IOMC Participating Organizations.

The Inter-Organisation Programme for the Sound Management of Chemicals (IOMC) was established in 1995 following recommendations made by the 1992 UN Conference on Environment and Development to strengthen co-operation and increase international co-ordination in the field of chemical safety. The Participating Organisations are FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank, Basel, Rotterdam and Stockholm Conventions and OECD. The purpose of the IOMC is to promote co-ordination of the policies and activities pursued by the Participating Organisations, jointly or separately, to achieve the sound management of chemicals in relation to human health and the environment.

# Disclaimer

This manual and accompanying software titled the OECD Overall Persistence ($P_{OV}$) and Long-range Transport Potential (LRTP) Screening Tool ("the Tool") are updates to what was originally produced by ETH Zürich (Martin Scheringer, Matthew MacLeod, and Fabio Wegmann), under contract with the OECD, and under the supervision of the Working Party on Exposure Assessment.

The OECD is pleased to allow those who may choose to download and copy the Tool for their personal, non-commercial and industrial scientific research purposes, provided no profit is derived from its use (the "Permitted Use"). No other use of the Tool is authorised without prior written permission from the OECD.

All legal rights, obligations, and limitations applicable to the Tool are set out exclusively in the End User License Agreement. Users should refer to the EULA for the complete and governing legal terms.

Information contained in the Tool or results generated by the Tool do not imply the expression of any opinion whatsoever on the part of the OECD Secretariat concerning the legal status of any country or of its authorities.

If Users want to share comments or corrections, please send an e-mail to the OECD Environment, Health and Safety Division (ehscont@oecd.org) with a copy to the developers (thetool@chem.ethz.ch).

### *Version History*

*The OECD $P_{OV}$ and LRTP Screening Tool v2.x is the follow-up version of the software POPorNot 1.0 that was distributed at the OECD/UNEP Workshop on Application of Multimedia Models for Identification of Persistent Organic Pollutants, ETH Zürich, August 30–31, 2005. Version 2.2 fixed a bug introduced by changes in Excel 2007.*

*Release Dates: v2.1: May 2008, v2.2: April 2009; v3.0: July 2026*

# Acknowledgements

The OECD would like to thank the members of the OECD Expert Group who contributed to the development and updating of version 3.0 of the OECD Overall Persistence ($P_{OV}$) and Long-range Transport Potential (LRTP) Screening Tool. Their scientific expertise in multimedia fate modelling, exposure assessment and software development has been essential to improving the Tool.

The Organisation also acknowledges the efforts of the project coordinators, technical contributors and reviewers from participating institutions who supported the preparation of the updated User Manual. In particular, the OECD wishes to thank Liisa Toose and Jon Arnot (ARC Arnot Research and Consulting Inc.), Knut Breivik (Norwegian Institute for Air Research, NILU), Andreas Buser (Swiss Federal Office for the Environment, FOEN), and Michael Beking (Environment and Climate Change Canada, ECCC).

The OECD further gratefully recognises the financial support provided by the Swiss Federal Office for the Environment (FOEN), the German Federal Environmental Agency (UBA), Environment and Climate Change Canada (ECCC) and the Research Council of Norway, which made this work possible.

# Foreword

The OECD Overall Persistence ($P_{OV}$) and Long-range Transport Potential (LRTP) Screening Tool (hereafter 'the Tool') is a macro-driven Microsoft Excel™-based software package containing multimedia chemical fate models, which estimate the overall persistence ($P_{OV}$) and long-range transport potential (LRTP) of organic chemicals for screening level assessment. The Tool is used to support comparative assessment of the environmental hazard properties of different chemicals. It is specifically designed to help identify potential Persistent Organic Pollutants (POPs) according to persistence and long-range transport metrics.

The Tool is regarded as a consensus model and is used in risk assessment world-wide for chemical fate. Since the Tool was published in 2008, it has been applied widely by both OECD member and non-member countries, particularly for the Screening and in Risk profile stages in the process of adding new POPs under the Stockholm Convention. The journal article by Wegmann et al. (2009), 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 offered recommendations for improving the Tool's performance.

In 2020, the OECD Working Party on Exposure Assessment (WPEA) endorsed its mid-term strategy, which included the update of the Tool. In 2021, the WPEA established an expert group, which developed a work plan and began its review, including launching a survey to collect examples of the Tool application. The survey provided both case examples of decision-support use and suggestions for improvement. Based on these inputs, the review report was prepared, and the Review of the OECD $P_{OV}$ and LRTP Screening Tool 15 years after its release (ENV/CBC/MONO(2023)36) was published in 2023.

This document serves as a user manual to the Tool, providing a concise, updated description of the Tool's functions, explaining how to select the calculation method, where to input parameters and select model options, a description of each button/field, and how to operate the databases and export results. Simultaneously, several scientific recommendations from the Review were implemented within the Tool, including the implementation of the emission fractions approach (EFA), intermittent precipitation calculations, updated reference chemical databases, and user interface enhancements. A separate journal article describing the scientific updates in greater detail is in preparation. The manual and updated Excel-based software were circulated to the WPEA in March 2026 and then finalised.

These updates to the Tool provided a long-needed science refresh, enhancing the understanding and predictive power of chemical fate and transport in air as well as water. However, additional issues identified in the Review were not addressed in this round of updates, such as the consideration of modelling approaches for ionising chemicals. These issues, and the long-term maintenance of the Tool, will be further considered and discussed among OECD Expert Group members.

The document and updated Excel-based software is to be posted on the OECD website and be free to download on the OECD website. This document is published under the responsibility of the Chemicals and Biotechnology Committee.

# Table of contents

## FIGURES



## TABLES

# Abbreviations

| | |
|---|---|
| BDE | Brominated Diphenyl Ethers |
| $CCl_4$ | Carbon tetrachloride |
| CTD | Characteristic Travel Distance |
| EFA | Emission Fractions Approach |
| GIF | Global average of Imported Fractions in receptor regions |
| HBCD | Hexabromocyclododecane |
| HCBD | Hexachlorobutadiene |
| HCB | Hexachlorobenzene |
| HCH | Hexachlorocyclohexane |
| LRTP | Long-Range Transport Potential |
| MCCPs | Medium-Chain Chlorinated Paraffins |
| PBT | Persistent, Bioaccumulative and Toxic |
| PCBs | Polychlorinated Biphenyls |
| PCNs | Polychlorinated Naphthalenes |
| POPs | Persistent Organic Pollutants |
| *P*ov | Overall Persistence |
| UNEP | United Nations Environment Programme |
| SCCPs | Short-Chain Chlorinated Paraffins |
| VBA | Visual Basic for Applications |
| WPEA | Working Party on Exposure Assessment |

# 1 Introduction

This document provides a short description of the OECD $P_{OV}$ and LRTP Screening Tool software ("the Tool"), the input data required and the results that are produced. A full description of the multimedia mass balance model incorporated in the Tool and its scientific and technical background can be found in the publication by Wegmann et al. (2009). A full description of the Emission Fractions Approach (EFA) concepts can be found in Breivik et al. (2022) and a comparison of the "new" EFA metrics to the "traditional" $P_{OV}$ and Characteristic Travel Distance (*CTD*) metrics are in OECD (2023) and in Breivik et al. (2023).

The purpose of the OECD $P_{OV}$ and LRTP Screening Tool is to estimate overall environmental persistence ($P_{OV}$) and long-range transport potential (LRTP) of organic chemicals at a screening level, and to provide context for making comparative assessments of environmental hazard properties of different chemicals. The Tool requires estimated degradation half-lives in soil, water and air, and at least two of three partition coefficients between air and water, octanol and water, or octanol and air as chemical-specific input parameters. From these inputs the Tool calculates metrics of $P_{OV}$ and LRTP from a generic multimedia chemical fate model and provides a graphical presentation of the results.

This document is divided into three sections. Section 1 is an introduction to the Tool software and contains instructions for performing different types of calculations and customizing the presentation of results. Section 2 provides guidance for interpreting results from the Tool, including definitions of the $P_{OV}$ and LRTP metrics. Section 3 presents a brief history of the Tool that describes its development and relationship to other multimedia chemical fate models, as well as a summary of the main updates in version 3.0. Before using the Tool, the user should carefully read the license agreement at the end of this document.

# 2 How to Run the Tool

## General Information

The Tool consists of five main components, which include: a level III multimedia fate and transport model; a graphical representation of the model results; various pages of numerical model output; a list of databases for the analysis of larger sets of chemicals; and a preferences page for changes of model settings. The software including these five components is called The OECD $P_{OV}$ and LRTP Screening Tool.

The Tool is a Microsoft Excel™ file with included Visual Basic for Applications (VBA) in Windows code. The program code and input and output data are integrated with the spreadsheet functions of Excel. This combination facilitates easy data transfer from the users' databases to the Tool and vice versa. The Tool also includes flexible data management features that allow the users to store their substance data within the Tool.

The Tool is a cross-platform Excel file that runs on both Windows and Macintosh computers. Operating system and software requirements are Excel 2002 or higher on a Windows PC, or Excel 2004 for Macintosh on Mac OS X 10.3 or higher. Importantly the version of Excel must support VBA; therefore, the Tool does not work with Excel 2008 for Macintosh. Version 3.0 was updated using Excel for Microsoft 365 MSO 64-bit.

## Opening the Software and Running the Tool for a Single Chemical

To run the Tool, the Excel Workbook needs to be opened. Because the Tool makes use of the VBA macro language, the user may be asked to enable macros when the Tool workbook file is opened. Without macros enabled, the Tool will not function. If the user has all macros disabled, the Tool displays a page describing how the required macros can be enabled. Depending on the security settings within Excel, the user may not be asked when opening the Tool.

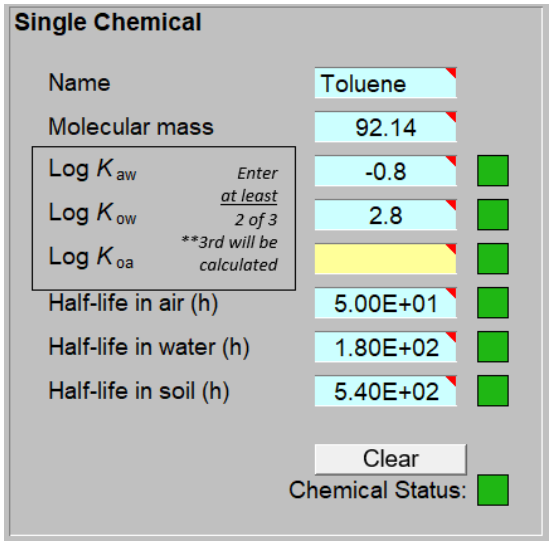
When macros are enabled, launching the Tool workbook file will take the user to the "**Main Menu"** page which consists of two panels. The "Databases" panel on the left contains a listbox of databases of input data, i.e. chemical properties, for different sets of chemicals. These databases can be modified by the user and can be used to calculate $P_{OV}$ and LRTP for large sets of chemicals (up to several thousands), see below.

## Single Chemical $P_{OV}$ and LRTP Screening

The "Single Chemical" panel on the right of the "**Main Menu**" page (Sheet "**MAIN**") contains cells in which chemical properties of a compound can be entered, see Figure 2.1. When values are entered, a green color code to the right of each cell indicates that the entered values are appropriate as inputs to the Tool and are within the expected numerical range. Two types of warnings are possible if the value entered is suspect, or invalid. A yellow color indicates the value may be in error because it is outside of the expected

range for that input parameter, but that calculations are still possible, and a red color indicates that calculations are not possible with the entered value. The domain of applicability of the model (showing a green color) includes log $K_{AW}$ −11 to 2, log $K_{OW}$ −1 to 10, log $K_{OA}$ −3 to 21 and half-lives of $1\times10^{-4}$ to $1\times10^{10}$ hours. Values outside these ranges should be interpreted with caution. Two of three partition coefficients are required to run the model. The third will be calculated if it is left blank. If the user enters all three partition coefficients, then the values are checked for thermodynamic consistency. If there is an inconsistency, a warning is shown asking the user if the log $K_{OA}$ should be automatically recalculated to balance with the other partition coefficients, if the model should be run with the values as they are entered, or if the model should be stopped for the user to update the partition coefficients manually.

**Figure 2.1. Input cells into which chemical properties of a single chemical are entered on the "Main Menu" page.**




Short descriptions of each input parameter can be viewed by hovering the cursor over the small red tab in the upper-right corner of each input cell. The color code next to "Chemical Status" indicates whether the single chemical screening is possible (green or yellow) or not (red).

When no database is selected, by clicking on the "**Deselect**" button (as desired) and valid data are provided for a single chemical, clicking the "**Calculate**" button under the two panels leads to the "**Graphical Results**" page (Sheet "**Results**") that shows the results for the single chemical in two plots of LRTP versus $P_{OV}$. The $P_{OV}$ metric shown on the x-axis is the same in both plots: the overall residence time of the chemical in the entire model system. In the plot on the left, the LRTP metric is the characteristic travel distance (*CTD*, in km). *CTD* indicates the distance from a point source at which the chemical's concentration has dropped to 37% of its initial concentration. In the plot on the right, the LRTP metric is the remotely transferred fraction ($\phi 2$, unitless) that estimates the net fraction of emitted chemical that is transferred to surface media after transport away from the region of release. The input parameters and the numerical results of the single chemical investigated are shown in the panel underneath the left $P_{OV}$-LRTP plot.

More detailed presentations of the results for the single chemical can be obtained by clicking the "**Classic Details**" or "**EFA Details**" buttons, which lead to a page with a detailed listing of all model results based on previous versions of the Tool ("Classic") or relating to the EFA analysis for the chemical selected (see below for a description of the contents of these pages). To navigate back to the "**Main Menu**" page, use the buttons provided on the top of each page.

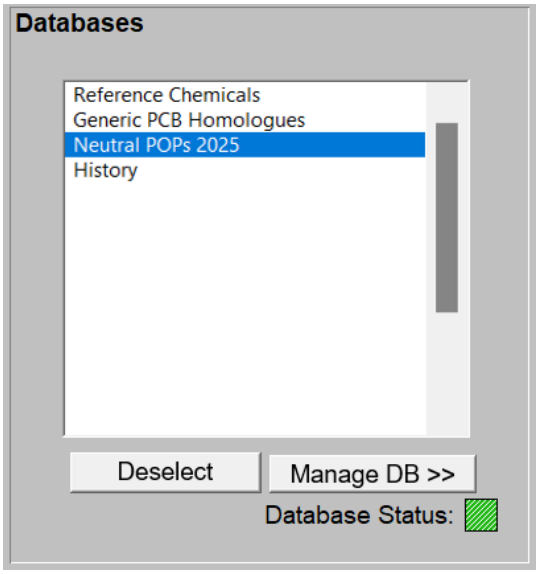
An additional option that is provided on the "**Main Menu**" page for a single chemical is a Monte Carlo calculation based on uncertainty ranges of the chemical's properties. See the Subsection below on "Monte Carlo Uncertainty Analysis" for a description of this option.

Finally, the Tool allows for simultaneous analysis of a single chemical and a database containing a set of additional chemicals. This is useful for evaluating a particular chemical in comparison to a certain selection of other chemicals. To do this, the user must enter single chemical properties in the panel on the right-hand side and to select a database in the panel on the left-hand side (see below) before clicking the "**Calculate**" button.

## Using Databases

The panel on the left-hand side of the "**Main Menu**" page contains a list of available databases, see Figure 2.2. There are four databases included in the distribution version of the Tool. Users can create additional custom databases of chemicals of interest. The four databases included in the Tool are named "Reference Chemicals", "Generic PCB Homologues", "Neutral POPs 2025" and "History". The first contains 270 entries representing 10 organic compounds; this database is described in more detail below in the Subsection on "Comparison of Model Results to Results for Reference Compounds" in Section 3. The second database contains property data describing 10 generic PCBs with the number of chlorines ranging from one to ten. The third database, "Neutral POPs 2025" was created in 2025 and includes neutral organic POPs that have been added to the Stockholm Convention between 2009 and 2023. The "History" database stores properties and results for all compounds that are entered as single chemicals on the "**Main Menu"** page.

### Figure 2.2. Database list on the "Main Menu" page.

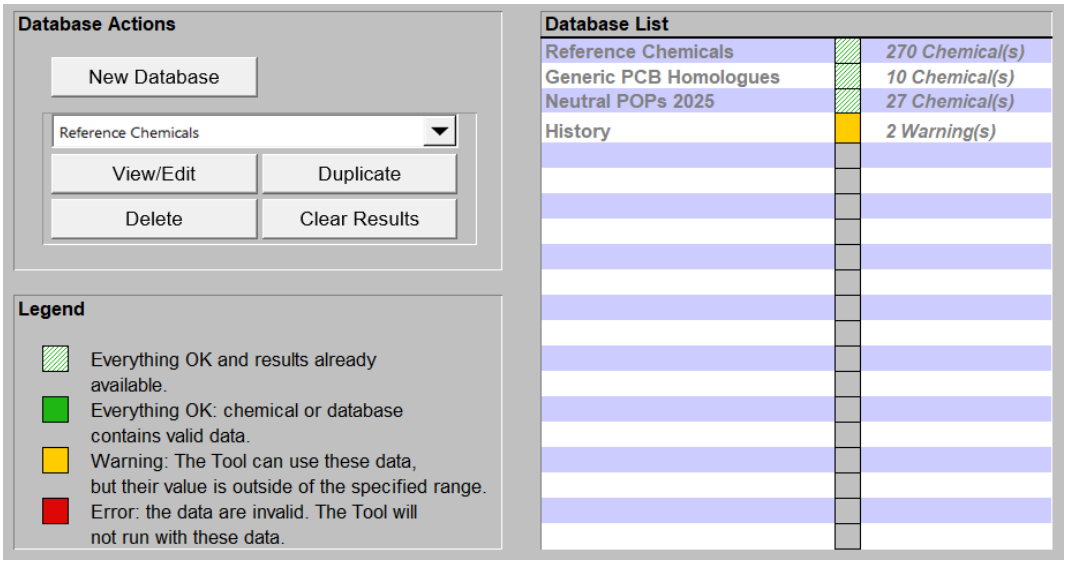



There are two main options for using chemical databases available on the "**Main Menu**" page. The first is to select a database and calculate results for all chemicals contained in this database by clicking the "**Calculate**" button. On the "**Graphical Results**" page, all chemicals in the database are then displayed in the two $P_{OV}$-LRTP plots; in addition, they are listed in the panel underneath the plot on the right-hand side. Any individual chemical can be selected by either highlighting its symbol in one of the two plots or by selecting it from the list in this panel. A chemical is highlighted in the plot by clicking once on its symbol, thereby selecting the data series. After a short pause, a second click on the chemical's symbol is needed to highlight the specific chemical (this is different from a double-click). If a chemical is selected from the

list, the size of its symbol is increased in both plots; on Windows computers, the symbol also changes its color. Chemical properties and $P_{OV}$ and LRTP results for the chemical selected are given in the panel on the left and can be analyzed in more detail by clicking the "**Classic Details**" or "**EFA Details**" buttons, which then leads to a page containing detailed results for the chemical selected.

The second option for working with databases from the "**Main Menu**" page is to click the "**Manage DB**" button, which leads to a new page that is labeled **Database Management** (Sheet "Management DB"). The panel in the top left corner of this page contains a pull-down menu for selecting a database and buttons for manipulating databases, see Figure 2.3.

**Figure 2.3. Database actions and database list as shown on the "Database Management" page.**




Databases can be created, duplicated, deleted, viewed and edited. Click on the "**View/Edit**" button to view and edit the database selected with the pull-down menu. Each database is stored on a separate worksheet within the Tool workbook file, with the name, molecular weight and the six chemical properties required by the model as columns of input data (purple column headings). To generate results for the database, all three partition coefficients must be listed. Model results are displayed in columns I to X (light green headings). Columns I to K contain the main results for $P_{OV}$, *CTD*, $\phi 2$, see Section 2 below for the selection of these three values. In columns L to W, all results for $P_{OV}$, *CTD*, and $\phi 2$ are given for the three release scenarios (emission to air, water and soil separately). For emissions to air, only the *CTD* in air is calculated; the same applies to water. The output –999 indicates that other combinations (e.g. *CTD* in air for release to water) are not calculated by the model and these columns (N, Q, U and V) are hidden. The chemical's fraction in air that is bound to aerosol particles, f Particle-bound in Air, is displayed in column X. By clicking on the "**Toggle Classic/EFA Results**" button, the classic results in columns I to X are hidden/shown and EFA results in columns Y to AK are shown/hidden. The EFA results are structured as the maximum $\phi$ 1, $\phi$ 2 and $\phi$ 3 (columns Y to AA) as well as the total values for each emission scenario (columns AB to AJ). The chemical's fraction in air that is bound to aerosol particles, f Particle-bound in Air, is displayed with the EFA results again in column AK. Additional EFA and TE results are shown in hidden columns AN to EA. Finally, the cells in "NotValid?" (column AL) shows either "Error", "Warning" or <<blank>> when the "**Check Results**" button is clicked.

The name of the database can be changed by selecting the database in the pull-down menu on the "**Database Management**" page, clicking the "**View/Edit**" button and changing the entry in cell B3.

In each database, the chemicals can be sorted according to any column of data (drop-down menu “Sort by”). Filters can be activated and deactivated by the “**Filters On/Off**” button. The filters allow sub-sets of data to be selected and screened in any data column (see Excel help for detailed instructions on using the filters feature).

Changes made within the databases are saved as soon as the Tool workbook file is saved because all databases are stored within that file. As an important consequence, whenever the Tool workbook file is passed on to another user, all databases are passed on as well. It is possible to delete some databases and to clear the History database (see description of the “**Preferences**” page below) beforehand.

In databases for which results have been calculated in an earlier model run, these results can be deleted by clicking the “**Clear Results**” button on the “**Database Management**” page. This also changes the color code to the right of the selected database in the database list from white-green to green. If existing results have been deleted, new model results are calculated when the Tool is run for this database (select database and click “**Calculate**” button on “**Main Manu**” page). If existing results are not deleted with the “**Clear Results**” button, they are kept in the database; in this case, the Tool does not perform new calculations but directly displays the existing results if the “**Calculate**” button is clicked.

## Presentation of Detailed Model Results

The results from the multimedia mass balance model employed in the Tool are presented if either the “**Classic Details**” or “**EFA Details**” button on the “**Graphical Results**” page is clicked for a selected chemical.

### *“Classic Details”*

Clicking the “**Classic Details**” button on the “**Graphical Results**” page leads to a new page that contains a full list of model output for the selected chemical, based upon the output provided in earlier versions of the Tool (Ver.2.1 and 2.2), with some modifications as described here. In the box to the right of the chemical’s name, the numerical values of $P_{OV}$, *CTD* and $\phi 2$ displayed on the “**Graphical Results**” page are given. Further to the right, all $P_{OV}$, *CTD* and $\phi 2$ values obtained for the three emissions scenarios (to air, water and soil) are listed. The two *CTD* versus $P_{OV}$ plots from the “**Graphical Results**” page are shown. Additionally, any notes specific to the calculation including “v3.0 always considers intermittent rainfall, whereas previous versions only consider constant rainfall” and notes about which, (if any) partition coefficient was calculated. The user could add additional text here before printing the single pdf, though any additions are not saved or transferred. At the bottom of the output, three pie charts show the chemical fractions that are contained in soil, water and air in the three emission scenarios.

In addition to these primary model results, the page displays a table with properties of the model compartments (bulk compartment properties and sub-compartment properties) and a second table with all mass fluxes calculated by the model (degrading reactions, physical removal, and inter-compartment exchange). Using these additional outputs, the users can identify processes that dominate the calculated fate of a particular chemical.

The user may choose to print the main section (columns A to J) as a pdf by clicking on the “**Print PDF**” button.

### *“EFA Details”*

Clicking the “**EFA Details**” button on the “**Graphical Results**” page leads to a new page that contains a full list of model output for the selected chemical, using the EFA detailed in Breivik et al. (2022). In the box to the right of the chemical’s name, the maximum numerical values of the total dispersed fraction ($\phi 1$), the

total remotely transferred fraction ($\phi 2$) and the total remotely accumulated fraction ($\phi 3$) are given. Further to the right, all $\phi 1$, $\phi 2$ and $\phi 3$ values obtained for the three emissions scenarios (to air, water and soil) are listed. A summary table of the EFA output for chemical dispersed by, transferred to and accumulated in each medium under each emissions scenario is shown. To the right of this table, a figure summarizing the data in the table is shown (as in Breivik et al. 2022). Below the table is a section where notes regarding the calculation of the results are shown.

In addition to these primary model results, the page displays a table with properties of the model compartments (bulk compartment properties and sub-compartment properties) and a second table with all mass fluxes calculated by the model (degrading reactions, physical removal, and inter-compartment exchange), $\phi 1$, $\phi 2$ and $\phi 3$ results for each emission scenario is shown. Using these additional outputs, the users can identify processes that dominate the calculated fate of a particular chemical.

The user may choose to print the main section (columns A to J) as a pdf by clicking on the "**Print PDF**" button.

## Monte Carlo Uncertainty Analysis

The Tool software provides a simple sensitivity and uncertainty analysis of results for the single chemical if the "**Include Monte Carlo Analysis for Single Chemical**" box is checked on the "**Main Menu**" page. Six cells are displayed in which default dispersion factors for the six chemical properties are presented and can be changed by the user; every value greater than 1 is possible. For the Monte Carlo calculations, log-normal distributions are assumed for all six chemical properties; this assumption cannot be changed by the user. The property values entered in the single-chemical panel are used as geometric mean values of these log-normal distributions; the geometric mean multiplied and divided by the dispersion factor spans the range containing 95% of the values of the distribution. When the Monte Carlo option is checked, by default the model results are calculated for a set of 100 random realizations of the original chemical (the number of Monte Carlo realizations, *n*, can be changed on the "**Preferences**" page). In the graphical results plot, all *n* realizations are shown, which can make the plot somewhat difficult to interpret if the Monte Carlo set size is larger than 100 realizations.

When the Monte Carlo option is selected, the "**Graphical Results**" page contains two unique buttons in the panel "Select a chemical" underneath the plot of $\phi 2$ versus $P_{OV}$. These buttons are labelled "**MC data**" and "**MC analysis**". "**MC data**" leads to a page containing the chemical properties and model results for all *n* chemical realizations used in the present Monte Carlo run. If another run is performed, they are overwritten by data for new chemical realizations. Therefore, if the users want to keep a particular set of chemical realizations with their properties and model results, they should copy and paste the data to a different page or workbook before performing a new Monte Carlo run.

The "**MC analysis**" button leads to an analysis of the Monte Carlo results that shows the contribution of the uncertainty ranges of the six chemical properties to the uncertainty of the model results. First, there are three panels with graphical results for the contribution to variance, *CTV*, for $P_{OV}$, *CTD*, and $\phi 2$. For each of these three metrics (denoted by *y*), the Spearman rank correlation coefficient between the metric *y* and every individual input parameter (denoted by *x*) is calculated (denoted by $r_{xy}$), see Morgan and Henrion (1990, p. 208). The rank correlation coefficient expresses how similar the rank order of the *n* results for the metric *y* and the *n* corresponding values of the input parameter *x* are. The contribution to variance shown in the plots is then $CTV = r_{xy}^2 / \sum_x r_{xy}^2$ for all input parameters, *x*. In addition, there are 18 "relationship charts" in which for every metric ($P_{OV}$, *CTD*, and $\phi 2$) the results of the *n* Monte Carlo runs are plotted against every input parameter.

## Changing Model Settings

The "**Preferences**" page can be accessed by clicking the "**Preferences**" button on the "**Main Menu**" page. It contains six panels where parameter values used by default in the Tool can be changed by the user. The first panel (top left) contains the upper and lower limits of the input parameters that define the range of appropriate chemical property values. By default, the model provides a warning but still performs the calculation if parameter values lie outside these limits. This setting can be changed to less restrictive (remove check of input data validity so no warning is shown if input values are outside limits) or more restrictive (add checkmark to "Treat warnings as errors" so no calculation is undertaken if input values are outside limits).

In the second panel (bottom left), criteria lines to be shown in the plot of the model results on the "**Graphical Results**" page can be defined. By default, no lines are shown. If the box "Draw criteria lines in results charts" is checked, lines are drawn at $P_{OV}$ = 195 days, *CTD* = 5097 km, and, though not used in graphical output, *TE* = 2.2476 is included as a legacy parameter. Additionally, if this box is checked, EFA limits are drawn on the "**EFA Details**" plot using the default values set here as, $\phi 1 = 2.44\times10^{-3}$, $\phi 2 = 8.95\times10^{-5}$ and $\phi 3 = 5.72\times10^{-6}$. These values are the minimum modelled values for reference chemicals that are known as persistent organic chemicals. These threshold values are specific to the environmental parameterization used in the Tool v3.0 and users may obtain different values using other models; see Section 3 below for a more detailed description of the use of reference chemicals. Users can replace these numbers with other values at which lines for $P_{OV}$, *CTD* and $\phi 2$ shall be drawn on the LRTP versus $P_{OV}$ plots on the "**Graphical Results**" and "**Classic Details**" output pages as well as the EFA plot on "**EFA Details**" output page.

In the third panel (top right), the function of the History database can be modified. By default, every single chemical for which the model is run is included in the History database, even if the same name is used in different runs. Users can switch off the History feature or can select the option that chemicals with the same name are not individually recorded. The History database can be cleared by clicking on the "**Clear History**" button.

The fourth panel (centre) enables the user to "reset" the workbook to prepare it for distribution by clicking the "**Set for Distribution**" button.

The two panels in the bottom right contain the settings for the Monte Carlo uncertainty analysis. In the panel to the right, the default values of the dispersion factors that are used to define the log-normal distributions of the chemical properties are defined. Default values are 10 for half-lives and 5 for partition coefficients. Note that these are generic values that should be replaced by more specific values whenever possible. For many chemicals, partition coefficients and environmental half-lives are uncertain or poorly known (Pontolillo and Eganhouse 2001, MacLeod et al. 2002, Schenker et al. 2005). In these cases, determination of mean values and dispersion factors requires careful evaluation of the property data in the literature and publicly accessible databases including (but not limited to) EAS-E Suite (2025), CompTox Dashboard (USEPA, 2025) and ECHA CHEM (Glüge et al. 2023). The generic dispersion factors provided with this model only serve as a substitute for chemical-specific and data-based dispersion factors. Whenever possible, they should be replaced by more reliable values.

In addition to the dispersion factors, the "**Preferences**" page contains the number of chemical realizations that is used in a Monte Carlo run (cell for "Monte Carlo set size"). The default value of the set size is 100. In principle, the set size should be so large that the results of successive Monte Carlo runs (i.e. the distributions of the model output in terms of mean and standard deviation) are stable. "Stable" means that the results are not significantly changed if the set size is further increased. In many cases, more than 100 realizations would be required to obtain stable results. If the users want to perform a methodologically sound Monte Carlo calculation, they need to evaluate the stability of the results and to increase the set size accordingly. See Morgan and Henrion (1990), Cullen and Frey (1999) for more information on uncertainty analysis and Monte Carlo calculations.

## Overview of Buttons for Navigation between Pages of the Tool

### *Main Menu*

| | |
|---|---|
| Button "**Help**" | Leads to the **Help and Additional Information** page. |
| Button "**Preferences**" | Leads to the **Preferences** page, where you can customize various features of the Tool. |
| Button "**Manage DB>>**" | Leads to the **Database Management** page, where you can view, edit, copy, sort, filter, or delete databases containing substance properties, or create new ones. |
| Button "**Deselect**" | Deselects a database selected from the list on the left. If a database is selected, it will be evaluated when the "Calculate" button is clicked. |
| Button "**Calculate**" | Runs the Tool and displays the Graphical Results page. |
| Button "**Clear**" | Deletes values from input cells for Single Chemical properties. |
| Checkbox "**Include Monte Carlo Analysis for Single Chemical**" | Displays cells in which dispersion factors for the Single Chemical can be entered; with this option selected, Monte Carlo results are displayed in the graphical results plots. |
| Button "**Reset**" | Only visible if the Monte Carlo option is selected. Returns dispersion factors back to default values. |

### *Database Management*

| | |
|---|---|
| Button "**<< Main Menu**" | Returns to the Main Menu page. |
| Button "**New Database**" | Prepares a new database page, asks for its name and presents an empty database sheet into which substance properties can be entered. |
| Button "**View/Edit**" | Applies to the database selected from the pull-down menu. Opens the database worksheet so that its entries can be viewed and the database can be edited. |
| Button "**Delete**" | Applies to the database selected from the pull-down menu. Deletes the database from the file after confirmation. |
| Button "**Duplicate**" | Applies to the database selected from the pull-down menu. Duplicates the database and asks for a name of the copy. |

| | |
|---|---|
| Button "**Clear Results**" | Applies to the database selected from the pull-down menu. Deletes existing results from the database and changes the database's color code from white-green to green. Without this, existing results for the chemicals in the selected database will not be re-calculated by pushing the "Calculate" button but will be displayed without any change. |

### *Database Editor*

| | |
|---|---|
| Button "**<< Return**" | Returns to the Database Management page. |
| Button "**Check Validity**" | Checks the substance properties and presents the result in a dialog box. Substance rows with warnings are marked yellow, rows with errors are marked red. |
| Button "**<< Main Menu**" | Returns to the Main Menu page. |
| Pull-down menu "**Sort by**:" | Allows the user to select sorting criteria from all input parameters, results and the problem indicator (see "Check"). |
| Button "**Filters On/Off**" | Displays a subset of the database that fulfills your criteria. See Excel Autofilter help documentation for further details. |
| Button "**Print Table**" | Prints the database from columns A to Y to PDF with all columns appearing across a landscape-oriented page. |
| Button "**Toggle Classic/EFA Results**" | Toggles showing columns I:X (Classic Results) or Y:AK (EFA Results). |

### *Graphical Results*

| | |
|---|---|
| Button "**<< Main Menu**" | Returns to the Main Menu page. |
| Button "**Classic Details**" | Shows detailed results for the highlighted compound. |
| Button "**EFA Details**" | Shows detailed EFA results for the highlighted compound |
| Button "**Single Chemical**" | Highlights the single chemical in the two plots. This button is only visible if a single chemical run has been performed. If a Monte Carlo screening has been carried out, this button highlights the chemical realization whose substance parameters are equal to the median values. |

| | |
|---|---|
| Button "**MC data**" | Leads to the Database Editor page for the Monte Carlo set. This button appears only when the Monte Carlo option is selected. |
| Button "**MC analysis**" | Leads to the page that shows the contributions to variance and the relationship charts. This button appears only if the Monte Carlo option is selected. |
| Button "**Create Report for all Database Results**" | Prompts the user to select either Classic or EFA results to report. Creates a PDF file including the tabular database inputs/results as well as a single detailed output sheet for each chemical in the database. This button is only visible if the Tool is run when a database is selected on Main Menu. |

### *Preferences*

| | |
|---|---|
| Button "**<< Main Menu**" | Returns to the Main Menu page. |
| Button "**Reset to Default**" | Restores the default values in the panels the button is located in. |
| Button "**Clear History**" | Clears the history of single chemical runs. This may be needed before the Tool is passed on to another user. |
| Button "**Set for Distribution**" | Opens the sheet that displays the warning about disabled macros. Note that the databases (including the History) are not deleted or modified by this button. |

### *OECD $P_{OV}$ & LRTP Screening Tool v3.0 (Classic Details) / OECD Emissions Fractions Screening Tool v3.0 (EFA Details)*

| | |
|---|---|
| Button "**Print PDF**" | Prints detailed output sheet to a single-page PDF |
| Button "**<< Result Summary**" | Returns to the Graphical Results page |
| Button "**<< Main Menu**" | Returns to the Main Menu page. |

# 3 Interpretation of Model Results

## Multimedia Fate and Transport Model Used

The geometry of the multimedia model used in the Tool reflects the global land-to-water surface ratio (30% land and 70% ocean water); long-range transport occurs in both air and ocean water, which have flow velocities of 4 m/s and 0.02 m/s, respectively. Properties of the media volumes and sub-compartments (e.g. atmospheric aerosols) are given on the page titled "**OECD *P*ov & LRTP Screening Tool v3.0**" with detailed model results for a single chemical ("**Classic Details**" button on the "**Graphical Results**" page). A detailed description of all model parameters is given by Wegmann et al. (2009).

For each chemical, the model is run three times: for an emission of 100 mol/hour to air, water, and soil. In every run, $P_{OV}$, $\phi 2$ are determined; *CTD* is calculated in water for release to water and in air for release to air. This leads to three values for $P_{OV}$ and $\phi 2$ and two values for *CTD*; all these results are displayed in columns G to J and rows 3 to 5 of the page with detailed model results ("**Classic Details**" button on the "**Graphical Results**" page). Finally, the $P_{OV}$, *CTD* and $\phi 2$ values shown in the plots on the "**Graphical Results**" page are derived by selecting the highest values of $P_{OV}$, *CTD*, and $\phi 2$ from the results obtained for all three emission scenarios. This approach is motivated by two considerations: First, most chemicals are mainly transported in the air and exhibit their highest *CTD* and $\phi 2$ values in air. However, the lower the chemical's Henry's law constant is, the more important transport in water becomes and for relatively water-soluble compounds, *CTD*s and $\phi 2$s in water might be observed that are even higher than those in air. To include this effect of transport in water, the higher of the two *CTD* or $\phi 2$ values is selected. The *CTD* value is a good approximation of the transport distance in the "spatial remote state" (Stroebe et al. 2004a), in which the effect of coupled transport in both mobile media, air and water, is fully visible. Coupled transport means that the chemical is exchanged between water and air while it is transported in both media.

A similar consideration holds for $P_{OV}$. Depending on a chemical's half-lives and partition coefficients, there is a situation in which the chemical's degradation takes place in all media at the same rate. This situation is called the "temporal remote state" (Stroebe et al. 2004b). An explicit calculation of the temporal remote state is not included in the Tool; however, Stroebe et al. (2004b) have shown that the persistence in the temporal remote state can be well approximated by the highest persistence that is obtained for releases to air, water, and soil. Therefore, the highest $P_{OV}$ value is selected from the results for the three emission scenarios.

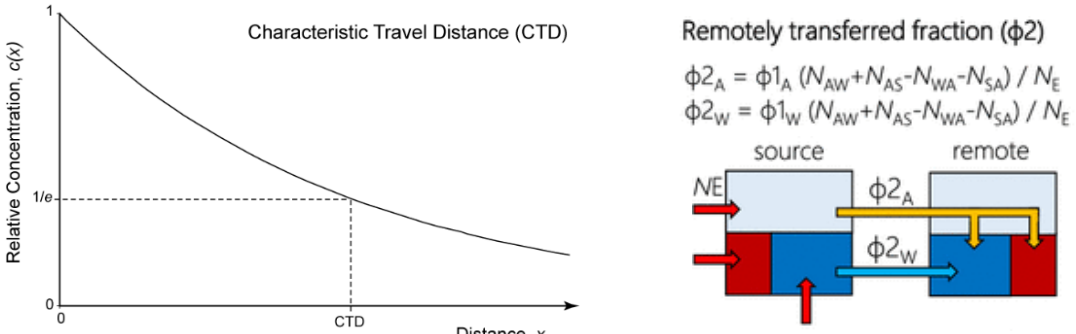
## LRTP Metrics

The primary output of the model is presented in two plots of an LRTP metric (characteristic travel distance, *CTD*, and remotely transferred fraction, $\phi 2$) versus overall persistence, $P_{OV}$. This type of plot, which was introduced by Scheringer (1997), makes it possible to compare a set of chemicals in two dimensions of hazard indicators, LRTP and $P_{OV}$. For both $P_{OV}$ and LRTP several metrics have been proposed in the scientific literature. LRTP metrics include the Spatial Range, *R*, (Scheringer 1996, 1997), the Characteristic Travel Distance, *CTD*, (Bennett et al. 1998, Beyer et al. 2000), the Characteristic Box Length (Hertwich and McKone 2001), the Mobility Ratio (van de Meent 2005), the Arctic Contamination Potential (Wania

2003), the Great Lakes Transfer Efficiency (MacLeod and Mackay 2004), Distance Residence Time (Mackay and Reid, 2008) Global average of Imported Fractions in receptor regions (GIF) (Kawai et al. 2014) and Emissions Fractions Approach (EFA) by Breivik et al. 2022 and others; see Scheringer (2002) for an overview of some of the early LRTP metrics and Scheringer et al. (2009) for the use of these metrics in the context of PBT chemical assessments.

LRTP metrics can be grouped in transport-oriented and target-oriented metrics (Fenner et al. 2005). Transport-oriented LRTP metrics characterize the shape of a curve of concentration as a function of place, $c(x)$, see Figure 3.1. A curve that extends over a larger distance leads to higher values of transport-oriented LRTP metrics. Target-oriented metrics, on the other hand, specify the fraction of the mass released to the model system that reaches a particular target region, e.g. the Arctic, and is deposited to (or contained in) the surface media, water and soil, in this region. To receive a high score with a target-oriented LRTP metric, a chemical needs to be transported to the selected target and to have a strong deposition mass flux and low loss mass flux.

### Figure 3.1. Transport-oriented and target-oriented LRTP metrics in comparison.




from Breivik et al., (2022)

Studies comparing transport-oriented metrics of LRTP have been conducted (Scheringer et al. (2001), Beyer et al. (2001), Scheringer (2002, chapter 6), and Stroebe et al (2004a)). In general, different transport-oriented metrics provide similar results when chemicals are prioritized relative to each other. The Characteristic Travel Distance (*CTD*) has been selected to describe the output of the Tool because it is based on a well-known metric (the point at which a function has decreased to $1/e \approx 37\%$ of its initial value); the *CTD* is given in units of km. *CTD* results are shown in the graph on the left-hand side on the "**Graphical Results**" page.

In addition to the *CTD*, the Tool calculates a target-oriented LRTP metric called the remotely transferred fraction ($\phi 2$). The remotely transferred fraction is calculated to quantify to what extent a chemical can reach surface media in remote regions following transport in air and water combined. Both fluxes must be expressed in the same units on a mass basis (eg, kg/year) or on a mole basis (eg. moles/hour). Remotely transferred, $\phi 2$, results are shown in the graph on the right on the "**Graphical Results**" page; the $\phi 2$ is given as the fraction of emission flux that is transferred (deposited less re-volatilized) to the soil and water of a hypothetical region adjacent to the region receiving emissions.

## *P*OV Metrics

*P*OV metrics described in the scientific literature are, among others, the residence time at steady state (Mackay and Paterson 1981), the equivalence width (Scheringer 1996), and the temporal remote state persistence (Stroebe et al. 2004b). A first important aspect of all *P*OV metrics is that they combine estimates of single-media half-lives with the multi-media partitioning of a chemical. Current legislation such as the

Stockholm Convention on Persistent Organic Pollutants (UNEP 2004) relies only on the single-media half-lives as persistence criteria. $P_{OV}$ metrics provide a somewhat different perspective because they consider the environmental media a chemical is likely to partition to and weigh the single-media half-lives with the chemical's fractions in the individual media (Webster et al. 1998).

The $P_{OV}$ metric calculated by the Tool is the residence time at steady state attributable to degradation processes. It is calculated as the total mass of chemical in the model system (kg) divided by the degradation flux from all model compartments (kg/day). The residence time is easy to calculate with steady-state models but has the disadvantage that it depends heavily on the release scenario. For example, if a chemical has a very short half-life in air and longer half-lives in water and soil, release to air will lead to a lower residence time than release to water or soil.

As mentioned above, it is also possible to calculate the persistence in the temporal remote state (Stroebe et al. 2004b); this metric is independent of the release scenario. The temporal remote state is the period of time in which the slowest degradation reaction and the rate of mobilization from the compartment with the slowest degradation reaction determine the loss of the chemical from the model system (after an initial pulse release). For many chemicals, this is degradation in the soil, and this is the case independent of the initial release pattern. The release pattern only determines how long it takes for the system to reach the temporal remote state: if the chemical is released to the soil, the system reaches the temporal remote state quickly; if the chemical is released to the other media, it takes a longer period to change the chemical's initial mass distribution so that it corresponds to the temporal remote state. The temporal remote state persistence is not a steady-state quantity but requires a dynamic model. However, as mentioned above, the temporal remote state persistence can be well approximated by using a steady-state model, releasing the chemical to the compartments air, water, and soil separately, and taking the highest steady-state residence time that is obtained with these three release scenarios. This is the approach employed in the Tool; the $P_{OV}$ results are given in days.[1]

## Emissions Fractions Approach (EFA) Metrics

In the Tool v3.0, additional LRTP metrics including the dispersed ($\phi 1$), transferred ($\phi 2$) and remotely accumulated ($\phi 3$) fractions of emissions are calculated. The EFA is described in detail in Breivik et al. (2023), and the various metrics are summarized in Table 3.1.

### Table 3.1. Definition of three metrics of the emission fractions approach.

| Metric | Definition |
|---|---|
| $\phi 1$ | The environmentally dispersed fraction ($\phi 1$) quantifies the relative extent to which a chemical can reach remote regions. |
| $\phi 2$ | The remotely transferred fraction ($\phi 2$) expresses to what relative extent a chemical can reach surface media in remote regions |

[1] Although the three releases to air, water, and soil individually may not reflect the actual release pattern of a chemical, the persistence obtained with the temporal remote state approach is not a purely hypothetical value. It reflects the time scale of degradation of the most long-lived reservoir of the chemical in the environment. In the long-term, this time scale becomes relevant for any initial release pattern. The initial release pattern only determines how long it takes until this time scale of slowest degradation becomes relevant once the emissions of the chemical have ceased.

| | |
|---|---|
| $\phi 3$ | The remotely accumulated fraction ($\phi 3$) assesses the fraction of the chemical's emission that is accumulating in the surface media of remote regions. |

Note: Each metric is a fraction of the total emissions as well as a fraction of the preceding metric.
Source: This table appears in Breivik et al. (2023).

The EFA metrics reflect transport, transfer and accumulation of chemical to remote regions, and are intrinsically related to each other. Viewed together on the "**EFA Details**" summary output, the user can gain insight into the mode and LRTP for an individual chemical. When results are viewed in tabular format or as a series of summary outputs in the generated pdf report, the relative hazards posed for all chemicals within a database can easily be discerned.

## Comparison of Model Results to Results for Reference Chemicals

So far, no absolute criteria for classifying chemicals as compounds with high or low $P_{OV}$ and LRTP have been established (in contrast to criteria for single-media half-lives such as two months in water used in the Stockholm Convention). In principle, similar criteria could be defined for $P_{OV}$ and LRTP as well.

In the absence of agreed upon regulatory criteria for identifying POP-like or non-POP-like chemicals based on $P_{OV}$ and LRTP, the OECD Expert Groups proposed making comparative assessments based on a set of substances selected as reference compounds. $P_{OV}$ and LRTP results for the reference substances can then be used to provide comparative context for other chemicals. Klasmeier et al. (2006) have described this approach in detail. They propose 10 reference chemicals, six chemicals with high environmental half-lives and empirically known transport to remote regions (PCBs 28, 101, 180; hexachlorobenzene; α-hexachlorocyclohexane; and carbon tetrachloride; called "POP-like") and four chemicals with low half-lives and less pronounced (or no) occurrence at remote locations (p-cresol, atrazine, biphenyl, aldrin); the properties of these 10 chemicals are contained in the database "Reference Chemicals" that is included in the Tool. Using the model results for the reference chemicals, Klasmeier et al. (2006) defined four areas in the plot of LRTP versus $P_{OV}$, see Figure 2.1 in Klasmeier et al. (2006). The $P_{OV}$ value of the POP-like reference chemical with the lowest $P_{OV}$ result defines the boundary between high and low $P_{OV}$; the LRTP value of the POP-like reference chemical with the lowest LRTP result defines the boundary between high and low LRTP. This approach has been applied using the Tool to derive $P_{OV}$ and LRTP boundaries that can be used as reference points in screening chemicals. The $P_{OV}$ boundary is 195 days ($P_{OV}$ of α-HCH) and the LRTP boundaries are 5097 km (*CTD* of PCB-28) and $8.95\times10^{-5}$ ($\phi 2$ of PCB-28). To display these boundaries in the plots on the "**Graphical Results**" page, one must select the option "Draw criteria lines in result charts" on the "**Preferences**" page. It is also possible to enter new, user-defined values as $P_{OV}$ and LRTP reference criteria.

Klasmeier et al. (2006) also investigated the influence of uncertainty in the chemical properties of the 10 reference compounds. To this end, they defined uncertainty ranges of partition coefficients and environmental half-lives and determined $P_{OV}$ and LRTP values for all combinations of half-lives and partition coefficients. The database "Reference chemicals" in the OECD model contains all 270 realizations obtained by creating all possible combinations of high and low property values.

Webster et al. (1998) and Klasmeier et al. (2006) have pointed out that it is possible to create combinations of chemical properties which would receive different classifications if evaluated according to single-media half-life criteria and $P_{OV}$/LRTP criteria from multimedia models. Accordingly, the Tool provides a useful additional perspective in the evaluation of potential new POPs: it makes it possible to complement the classification of potential POPs based on the criteria in Annex D of the Stockholm Convention (UNEP 2004) by a classification based on $P_{OV}$ and LRTP criteria employed in the Tool.

# 4 Model Background

The Tool is based on a comparison and evaluation of several multimedia fate and transport models that had its origin at an OECD/UNEP Workshop on *The Use of Multimedia Models for Estimating Overall Environmental Persistence and Long-Range Transport in the Context of PBT/POPs Assessment* that was held in Ottawa, Canada, in October 2001 (OECD 2002). Recommendations from the workshop included that

- "guidance for users on model applicability and fitness for purposes" should be provided;
- model intercomparison studies should be performed; and
- "a core set of multimedia models should be available and accessible at no cost to the public" (OECD 2002, p. 27).

After the workshop, an *OECD Expert Group for the Follow-up to the OECD/UNEP Workshop on Multimedia Models* was established. From 2002 to 2005, the members of this expert group worked on several tasks: (i) they developed a guidance document on *The Use of Multimedia Models for Estimating Overall Environmental Persistence and Long-Range Transport* (OECD 2004), (ii) they performed an extensive comparison of different existing multimedia fate and transport models (Fenner et al. 2005); (iii) they evaluated in what way POP-like reference compounds can be used to identify possible new POPs (Klasmeier et al. 2006); and (iv) they developed, based on broad experience in developing and applying different multimedia models, the model included in the Tool.

The different models compared by the OECD expert group have different structure and background but have all been used for $P_{OV}$ and LRTP calculations. The comparison of these models (Fenner et al. 2005) demonstrated that the models yield similar results if a set of chemicals is ranked according to $P_{OV}$ and LRTP. Certain differences observed for specific chemicals could be explained by characteristic differences in the models' geometry and process description. For these reasons, the expert group decided that a consensus model reflecting features from various individual research models would be helpful to make the technique of using multimedia models available for a broader audience.

Wegmann et al. (2009) compared the multimedia model contained in the Tool with existing multimedia models in the same way that was used in the comparison study by Fenner et al. (2005); they also provide a description and discussion of all model features.

A report titled "*Review of the OECD $P_{OV}$ and LRTP Screening Tool 15 years after its release"* was issued in 2023 by the OECD Chemicals and Biotechnology Committee as part of a four-step plan to update the Tool (OECD, 2023). These steps include i) review citing articles, gather user needs and assess limitations of the current version; ii) develop the report with recommendations for updates; iii) update the software; iv) develop a scientific paper. The report summarizes the suggestions made in the literature review and by the expert group. It concludes with a list of several updates to the Tool, of which the following have been included in the Tool v3.0:

1. Added a new database of POPs called "**Neutral POPs 2025**" which are neutral POPs that have been added to the Stockholm Convention since 2009.
2. Added guidance on the domain of applicability in this user manual.

3. Adopted intermittent precipitation as per Jolliet and Hauschild (2005) and MacLeod et al., (2010) into the model calculations.
4. The VBA code of the Tool v3.0 is provided for professional purposes.
5. Provided an updated manual/guidance, including how to derive the input parameters and interpret the result of confidence estimates.
6. Added an option to save “Classic” and “EFA” summary reports as PDFs.
7. Added the option to enter a Log $K_{OA}$ value in addition to Log $K_{AW}$ and Log $K_{OW}$. Entry to two partition coefficients is mandatory; the third will be calculated if left blank. Add Log $K_{OA}$ (indicated as entered or calculated) as an output.
8. Included calculation and output of alternative metrics – the Emission Fractions Approach.

# References


Bennett, D.H., McKone, T.E., Matthies, M., Kastenberg, W.E. (1998) General Formulation of Characteristic Travel Distance for Semivolatile Organic Chemicals in a Multi-Media Environment, *Environmental Science & Technology* **32**, 4023–4030. https://doi.org/10.1021/es980328g.

Beyer, A., Mackay, D., Matthies, M., Wania, F., Webster, E. (2000) Assessing Long-Range Transport Potential of Persistent Organic Pollutants, *Environmental Science & Technology* **34**, 699–703. https://doi.org/10.1021/es990207w.

Beyer, A., Scheringer, M., Schulze, C., Matthies, M. (2001) Comparing Representations of the Environmental Spatial Scale of Organic Chemicals, *Environmental Toxicology & Chemistry* **19**, 922–927. https://doi.org/10.1002/etc.5620200430.

Breivik, K., McLachlan, M.S., Wania, F. (2022). The Emissions Fractions Approach to Assessing the Long-Range Transport Potential of Organic Chemicals. *Environmental Science & Technology*. **56**, 11983–11990. https://doi.org/10.1021/acs.est.2c03047.

Breivik K., McLachlan, M.S., Wania, F. (2023). Added Value of the Emissions Fractions Approach when Assessing a Chemical's Potential for Adverse Effects as a Result of Long-Range Transport. *Environmental Science: Advances* **2**, 1360–1371. https://doi.org/10.1039/d3va00189j.

Cullen, A.C., Frey, H.C. (1999) *Probabilistic Techniques in Exposure Assessment*. Plenum Press, New York and London. https://link.springer.com/book/9780306459566.

EAS-E Suite (Ver.0.981 - BETA, release September, 2025). www.eas-e-suite.com. Developed by ARC Arnot Research and Consulting Inc., Toronto, ON, Canada.

Fenner, K., Scheringer, M., MacLeod, M., Matthies, M., McKone, T.E., Stroebe, M., Beyer, A., Bonnell, M., Le Gall, A.C., Klasmeier, J., Mackay, D., Pennington, D.W., Scharenberg, B., Wania, F. (2005) Comparing Estimates of Persistence and Long-Range Transport Potential among Multimedia Models, *Environmental Science & Technology* **39**, 1932–1942. https://doi.org/10.1021/es048917b.

Glüge, J., Scheringer, M. 2023. Evaluation of Physicochemical Property Data in the ECHA Database. *Journal of Physical and Chemical Reference Data* **52,** 043101. https://doi.org/10.1063/5.0153030.

Hertwich, E.G., McKone, T.E. (2001) Pollutant-Specific Scale of Multimedia Models and Its Implications for the Potential Dose, *Environmental Science & Technology* **35**, 142–148. https://doi.org/10.1021/es9911061.

Jolliet, O., Hauschild, M. 2005. Modelling the influence of intermittent rain events on long term fate and transport of organic air pollutants. *Environmental Science & Technology*. **39**, 4513–4522. https://doi.org/10.1021/es049913+.

Kawai, T., Jagiello, K., Sosnowska, A., Odziomek, K., Gajewicz, A., Handoh, I.C., Puzyn, T., Suzuki, N. (2014), A New Metric for Long-Range Transport Potential of Chemicals, *Environmental Science & Technology*, **48**, 3245–3252, https://doi.org/10.1021/es4026003.

Klasmeier, J., Matthies, M., MacLeod, M., Fenner, K., Scheringer, M., Stroebe, M., Le Gall, A.C., McKone, T.E., van de Meent, D., Wania, F. (2006) Application of Multimedia Models for Screening Assessment of Long-Range Transport Potential and Overall Persistence, *Environmental Science & Technology* **40**, 53–60. https://doi.org/10.1021/es0512024.

Mackay, D., Paterson, S. (1981) Calculating Fugacity, *Environmental Science & Technology* **15**, 1006–1014. https://doi.org/10.1021/es00091a001.

Mackay, D., Reid, L. (2008). Local and Distant Residence Times of Contaminants in Multi-Compartment Models. Part I: A Review of the Theoretical Basis. *Environmental Pollution*. **156**. 1196–1203. https://doi.org/10.1016/j.envpol.2008.04.012.

MacLeod, M., Fraser, A.J., Mackay, D. (2002) Evaluating and Expressing the Propagation of Uncertainty in Chemical Fate and Bioaccumulation Models, *Environmental Toxicology & Chemistry* **21**, 700–709. https://doi.org/10.1002/etc.5620210403.

MacLeod, M., Mackay, D. (2004) Modeling Transport and Deposition of Contaminants to Ecosystems of Concern: A Case Study for the Laurentian Great Lakes, *Environmental Pollution* **128**, 241–250. https://doi.org/10.1016/j.envpol.2003.08.029

MacLeod, M., Scheringer, M., Götz, C., Hungerbüler, K., Davidson, C.I., Holsen, T.M. (2010) Chapter 6. Deposition from the atmosphere to water and soils with aerosol particles and precipitation. In Handbook of Chemical Mass Transport in the Environment, Thibodeaux, L.J. and Mackay, D. (eds), CRC Press. Boca Raton, USA. https://doi.org/10.1201/b10262-7.

Morgan, M.G, Henrion, M. (1990) *Uncertainty. A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*. Cambridge University Press, Cambridge, UK.

OECD (2002) *Report of the OECD/UNEP Workshop on the Use of Multimedia Models for Estimating Overall Environmental Persistence and Long-Range Transport in the Context of PBTs/POPs Assessment*, OECD Series on Testing and Assessment No. 36, OECD, Paris, 191 pp. https://doi.org/10.1787/9789264078505-en.

OECD (2004) *Guidance Document on the Use of Multimedia Models for Estimating Overall Environmental Persistence and Long-Range Transport.* OECD Series on Testing and Assessment No. 45, OECD, Paris, 84 pp. https://doi.org/10.1787/9789264079137-en.

OECD (2023) *Review of the OECD $P_{OV}$ and LRTP Screening Tool 15 years after its Release.* OECD Series on Testing and Assessment No. 388, OECD, Paris, 56 pp. https://one.oecd.org/document/ENV/CBC/MONO(2023)36/en/pdf.

Pontolillo, J., Eganhouse, R.P (2001) *The Search for Reliable Aqueous Solubility (Sw) and Octanol-Water Partition Coefficient (Kow) Data for Hydrophobic Organic Compounds: DDT and DDE as a Case Study*. U.S. Geological Survey, Washington, DC, 2001. https://doi.org/10.3133/wri014201

Schenker, U., MacLeod, M., Scheringer, M., Hungerbühler, K. (2005) Improving Data Quality for Environmental Fate Models: A Least-Squares Adjustment Procedure for Harmonizing Physicochemical Properties of Organic Compounds, *Environmental Science & Technology* **39**, 8434–8441. https://doi.org/10.1021/es0502526.

Scheringer, M. (1996) Persistence and Spatial Range as Endpoints of an Exposure-Based Assessment of Organic Chemicals, *Environmental Science & Technology* **30**, 1652–1659. https://doi.org/10.1021/es9506418.

Scheringer, M. (1997) Characterization of the Environmental Distribution Behavior of Organic Chemicals by Means of Persistence and Spatial Range, *Environmental Science & Technology* **31**, 2891–2897. https://doi.org/10.1021/es970090g.

Scheringer, M. (2002) *Persistence and Spatial Range of Environmental Chemicals*. Wiley-VCH, Weinheim, 294 pp.

Scheringer, M., Bennett, D.H., McKone, T.E., Hungerbühler, K. (2001) Relationship Between Persistence and Spatial Range of Environmental Chemicals, in: Lipnick, R., Mackay, D., Jansson, B., Petreas, M. (Eds.) *Persistent Bioaccumulative Toxic Chemicals II: Assessment and New Chemicals.* American Chemical Society, Washington DC, 53–63.

Scheringer, M., Jones, K.C., Matthies, M., Simonich, S. van de Meent, D. (2009) Multimedia Partitioning, Overall Persistence, and Long-Range Transport Potential in the Context of POPs and PBT Chemical Assessments. *Integrated Environmental Assessment and Management*, **5**, 557–576. https://doi.org/10.1897/ieam_2009-007.1.

Stroebe, M., Scheringer, M., Held, H., Hungerbühler, K. (2004a) Intercomparison of Multimedia Fate Models: Modes of Transport, Measures of Long-Range Transport Potential, and the Spatial Remote State, *The Science of the Total Environment* **321**, 1–20. https://doi.org/10.1016/j.scitotenv.2003.09.008.

Stroebe, M., Scheringer, M., Hungerbühler, K. (2004b) Measures of Overall Persistence and the Temporal Remote State, *Environmental Science & Technology* **38**, 5665–5673. https://doi.org/10.1021/es035443s.

USEPA. 2025. CompTox Chemicals Dashboard v2.6.0. comptox.epa.gov/dashboard Developed by: United States Environmental Protection Agency.

Van de Meent, D. (2005) The Mobility Ratio is used with the SimpleBox model as an LRTP metric. Personal communication by D. van de Meent, RIVM, Bilthoven, The Netherlands.

Wania, F. (2003) Assessing the Potential of Persistent Organic Chemicals for Long-Range Transport and Accumulation in Polar Regions, *Environmental Science and Technology* **37**, 1344–1351. https://doi.org/10.1021/es026019e.

Webster, E., Mackay, D., Wania, F. (1998) Evaluating Environmental Persistence, *Environmental Toxicology and Chemistry* **17**, 2148–2158. https://doi.org/10.1002/etc.5620171104.

Wegmann, F., Cavin, L., MacLeod, M., Scheringer, M., Hungerbühler, K. (2009) The OECD software tool for screening chemicals for persistence and long-range transport potential, *Environmental Modeling & Software* **24**, 228–237. https://doi.org/10.1016/j.envsoft.2008.06.014.

# Appendices

## Appendix A. Database Descriptions

### *Reference Chemicals*

This database was described and applied by Klasmeier et al. (2006) as a selection of ten well-studied chemicals that would provide a "yardstick" for assessing the $P_{OV}$ and LRTP of other chemicals. The chemicals included in this database are: PCB-28, PCB-101, PCB-180, alpha-HCH, HCB, aldrin (known POPs), biphenyl, p-cresol, atrazine (not POPs) and $CCl_4$ (not defined as a POP, though volatile and globally distributed in the atmosphere). There are 270 entries in this database, 27 iterations of minimum, maximum and median values for log $K_{AW}$, log $K_{OW}$, log $K_{OA}$, half-life in air, water and soil for each chemical. The median values are labeled as "-14". The results for the median parameterization of the six POPs are assessed to define the model-specific "POP-like" criteria for $P_{OV}$, *CTD* and the dispersed ($\phi 1$), transferred ($\phi 2$) and accumulated ($\phi 3$) emissions fractions. This database was included in v2.x of the Tool. Full details of the parameterization of these chemicals are described in Klasmeier et al. (2006).

### *Generic PCB Homologues*

In the "**Generic PCB Homologues**" database, the generalized physical-chemical properties and results for ten generic PCBs, labeled as mono- to deca-chloro PCBs. This database is automatically sorted by increasing molar mass. It is intended to be representative of PCB homologues, not for specific congeners. This database was included in v2.x of the Tool and was noted, though not described in Wegmann et al. (2009).

### *Neutral POPs 2025*

This new database includes 20 neutral POPs added to the Stockholm Convention since the 2009 version of the Tool. Reported physical-chemical properties as described in Section 1 of this document were collected from published risk profiles developed by the POPs Review Committee (POPRC) under the Stockholm Convention, where available. In some cases, additional properties necessary to run the Tool models were added to the database. To address remaining data gaps, values were selected from the literature and publicly available sources. The values selected in this database generally reflect the median of the acceptable values reported in the POPRC documents. Table A1-1 gives the sources of the data used to derive the physical-chemical properties listed in "**Neutral POPs 2025**".

**Table A1.1. Sources consulted to parameterize chemicals listed in "Neutral POPs 2025" database.**

| ID | Chemical | Sources |
|---|---|---|
| 1 | BDE-47 | EAS-E Suite Database: easesuitedb_v1.0.1 |
| 2 | BDE-99 | UNEP/POPS/POPRC.2/17/Add.1<br>EAS-E Suite Database: easesuitedb_v1.0.1 |
| 3 | BDE-169 | UNEP/POPS/POPRC.3/20/Add.6<br>EAS-E Suite Database: easesuitedb_v1.0.1 |
| 4 | BDE-193 | UNEP/POPS/POPRC.3/20/Add.6<br>EAS-E Suite Database: easesuitedb_v1.0.1 |
| 5 | BDE-209 | UNEP/POPS/POPRC.11/10/Add.1<br>UNEP/POPS/POPRC.10/10/Add.2 |
| 6 | beta-HCH | UNEP/POPS/POPRC.3/20/Add.9 |
| 7 | chlordecone | UNEP/POPS/POPRC.2/17/Add.2<br>Wegmann et al. (2009) |
| 8 | chlorpyrifos | UNEP/POPS/POPRC.19/INF/11 |
| 9 | dechlorane plus | UNEP/POPS/POPRC.15/3<br>Sverko et al. (2011) |
| 10 | dicofol | UNEP/POPS/POPRC.13/7/Add.1 |
| 11 | gamma-HCH | UNEP/POPS/POPRC.2/17/Add.4<br>UNEP/POPS/POPRC.1/10<br>UNEP/POPS/POPRC.1/8<br>UNEP/POPS/POPRC.3/20/Add.4<br>Wegmann et al. (2009)<br>EAS-E Suite Database: easesuitedb_v1.0.1 |
| 12 | HBCD | UNEP/POPS/POPRC.6/13/Add.2<br>Marvin et al. (2011) |
| 13 | HCBD | UNEP/POPS/POPRC.8/16/Add.2 |
| 14 | hexabromobiphenyl | UNEP/POPS/POPRC.3/20Add.3<br>Wegmann et al. (2009) |

| | | |
|---|---|---|
| 15 | MCCPs (C14) | UNEP/POPS/POPRC.17/INF/5<br>UNEP/POPS/POPRC.18/INF/10 |
| 16 | methoxychlor | UNEP/POPS/POPRC.15/4 |
| 17 | pentachlorobenzene | UNEP/POPS/POPRC.3/20/Add.7<br>UNEP/POPS/POPRC.3/INF/21 Annex II |
| 18 | SCCPs (C10) | UNEP/POPS/POPRC.18/INF/10<br>UNEP/POPS/POPRC.6/INF/15 |
| 19 | tech-endosulfan | UNEP/POPS/POPRC.5/10/Add.2 |
| 20 | tri-PCN | UNEP/POPS/POPRC.9/13/Add.1<br>Environment Canada (2011)<br>UNEP (2001)<br>EAS-E Suite Database: easesuitedb_v1.0.1 |

## *References*

EAS-E Suite (Ver.0.981 - BETA, release September, 2025). www.eas-e-suite.com. Phys-chem database version: easesuitedb_v1.01. Accessed Nov 4, 2025. Developed by ARC Arnot Research and Consulting Inc., Toronto, ON, Canada

Environment Canada. (2011) Ecological Screening Assessment. Chlorinated Naphthalenes June 2011. https://www.canada.ca/content/dam/eccc/migration/ese-ees/835522fe-ae6c-405a-a729-7bc4b7c794bf/cns_sar_en.pdf

Klasmeier, J., Matthies, M., MacLeod, M., Fenner, K., Scheringer, M., Stroebe, M., Le Gall, A.C., McKone, T.E., van de Meent, D., Wania, F. (2006) Application of Multimedia Models for Screening Assessment of Long-Range Transport Potential and Overall Persistence, *Environmental Science & Technology* **40**, 53–60. https://doi.org/10.1021/es0512024.

Marvin, C.H., Tomy, G.T., Armitage, J.M., Arnot, J.A., McCarty, L., Covaci, A., Palace, V. (2011) Hexabromocyclododecane: Current Understanding of Chemistry, Environmental Fate and Toxicology and Implications for Global Management. *Environmental Science and Technology*. **45**. 8613–8623. https://doi.org/10.1021/es201548c

Sverko, E., Tomy, G.T., Reiner, E.J., Li, Y.-F., McCarry, B.E., Arnot, J.A., Law, R.J., Hites, R.A. (2011) Dechlorane Plus and Related Compounds in the Environment: A Review. *Environmental Science and Technology*. **45**, 5088–5098. https://doi.org/10.1021/es2003028

UNEP. (2001) Chlorinated Naphthalenes. Concise International Chemical Assessment Document **34**. Geneva. 2001. Accessed Nov 4 2025. https://www.inchem.org/documents/cicads/cicads/cicad34.htm#2.0

Wegmann, F., Cavin, L., MacLeod, M., Scheringer, M., Hungerbühler, K. (2009) The OECD software tool for screening chemicals for persistence and long-range transport potential, *Environmental Modeling & Software* **24**, 228–237. https://doi.org/10.1016/j.envsoft.2008.06.014.

## Appendix B. Credits

### OECD $P_{OV}$ and LRTP Screening Tool v2.x

***Participating Members of the OECD Expert Group (v2.x)***

Mark Bonnell, Jörg Klasmeier, Anne Christine Le Gall, Donald Mackay, Matthew MacLeod, Michael Matthies, Thomas E. McKone, Bernd Scharenberg, Martin Scheringer, Noriyuki Suzuki, Dik van de Meent, Frank Wania

***OECD Project Coordinator***

Take Fukushima

***Model Concept***

Matthew MacLeod, Martin Scheringer

***Model Code***

Matthew MacLeod

***Software Development***

Laurent Cavin, Fabio Wegmann

***Manual Preparation***

Martin Scheringer, Matthew MacLeod, Fabio Wegmann

***Software Beta Testing***

Aurélie Guillossou, Anne-Christine Le Gall, Christian Götz, Urs Schenker, Christian Capello.

Special thanks to Burkhard Wagner for support and inspiration.

### OECD $P_{OV}$ and LRTP Screening Tool v3.0

***Participating Members of the OECD Expert Group on Updating the OECD $P_{OV}$ and LRTP Screening Tool (v3.0)***

Sandrine Andres, Joost Bakker, Michael Beking, Mark Bonnell, Knut Breivik, Andreas Buser, Jed Costanza, John Crosse, Ian Doyle, Yoshitaka Imaizumi, James Lymer, Matthew MacLeod, Qinghong Pu, Emiel Rorije, Eric Verbruggen, Martin Scheringer, Kei Ohno Woodall

***OECD Project Coordinator***

Patience Browne, Asako Hotta, Marie-Ange Baucher

***Additional Model Code and Software Development***

Liisa Toose, Knut Breivik

***Manual Updates***

Liisa Toose, Jon Arnot, Michael Beking, Knut Breivik, Andreas Buser

Project funding by OECD based on grants from the Swiss Federal Office for the Environment (FOEN), the German Federal Environmental Agency (UBA), Environment and Climate Change Canada (ECCC), and the Research Council of Norway (#343110).

## Appendix C. The Tool License Agreement

For details, please refer to the license agreement.