The OECD P_{OV} and LRTP Screening Tool, Version 2.2[1]

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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

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[1] *The OECD P_{OV} and LRTP Screening Tool 2.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 fixes a bug introduced by changes in Excel 2007.
[2] Industrial usage of the software is explicitly allowed.

and its scientific and technical background can be found in the publication by Wegmann et al. (2009).

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 partition coefficients between air and water and between octanol and water as chemical-specific input parameters. From these inputs The Tool calculates metrics of P_{OV} and LRTP from a 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, instructions for performing different types of calculations and for 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. Before using The Tool, the user should read carefully the license agreement at the end of this document.

1. 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 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 MS Excel 2002 or higher on MS Windows on a PC, or MS Excel 2004 for Macintosh on Mac OS X 10.3 or higher. The Tool does not work with MS Excel 2008 for Macintosh.

Opening the Software and Running The Tool for a Single Chemical
To run The Tool, the Microsoft Excel Workbook The_Tool_2.1.xls needs to be opened. Because The Tool makes use of the Visual Basic for Applications macro language, the user may be asked to enable macros when The_Tool_2.1.xls 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_2.1.xls 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 chemical compounds. 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 contains cells in which chemical properties of a compound can be entered, see Figure 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.

Figure 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 and valid data are provided for a single chemical, clicking the "Calculate" button under the two panels leads to the "**Graphical Results**" page that shows the results for the single chemical in two plots of LRTP vs. P_{OV}. The P_{OV} metric 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 38% of its initial concentration. In the plot on the right, the LRTP metric is the transport efficiency (TE, in %) that estimates the percentage of emitted chemical that is deposited 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.

A more detailed presentation of the results for the single chemical can be obtained by clicking the "Details" button, which leads to a page with a detailed listing of all model results for the chemical selected (see below for a description of the

contents of this page). 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 below, Subsection on "Monte Carlo Uncertainty Analysis" for a description of this option.

Finally, The Tool allows for simultaneous analyis 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 has to 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. There are three databases included in the distribution version of The Tool. Users can create additional custom databases of chemicals of interest. The three databases included in The Tool are named "Reference Chemicals", "Generic PCB Homologues", and "History". The first contains 270 entries representing 10 organic compounds; this database is described in more detail below in the Subsection on Reference Compounds in Section 3 below. The second database contains property data describing 10 generic PCBs with the number of chlorines ranging from one to ten. The third database, "History", is a unique database that stores properties and results for all compounds that are entered as single chemicals on the "**Main Menu**" page.
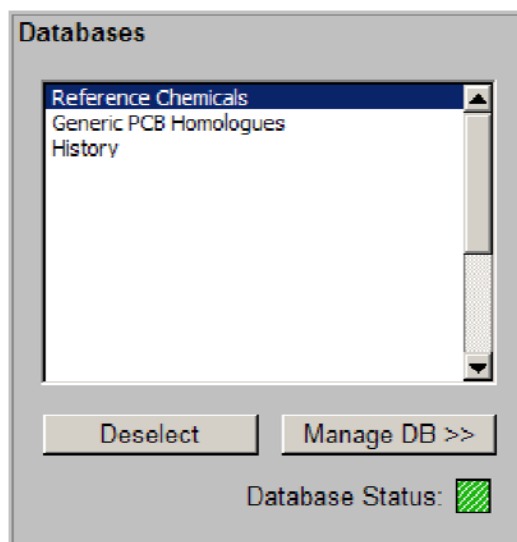
Figure 2: Database list on the "Main Menu" page.

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 "Details" button, which then leads to a page containing detailed results for the chemical selected.

The second option for working with databases from the Main Menu is to click the "Manage DB" button, which leads to a new page that is labeled **Database Management**. 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 3.
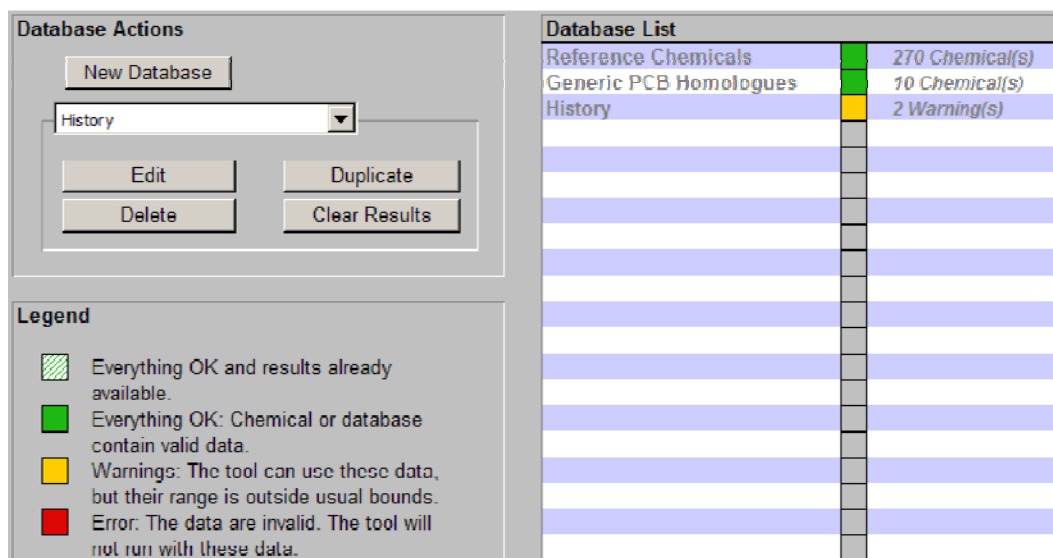
Figure 3: Database actions and database list as shown on the "Database Management" page.

Databases can be created, duplicated, deleted and edited. Click on the "Edit" button to view and edit the database selected with the pull-down menu. Each database is stored on a separate worksheet within the The_Tool_2.1.xls workbook file, with the name, molecular weight and the five chemical properties required by the model as columns of input data (purple column headings). Model results are displayed in columns H to W (light green headings). Columns H to J contain the main results for P_{OV}, CTD, TE, see Section 2 below for the selection of these three values. In columns K to V, all results for P_{OV}, CTD, and TE are given for the three release scenarios (emission to soil, water and air separately). For emission 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. Finally, the chemical's fraction in air that is bound to aerosol particles, Phi, is displayed in column W.

 The name of the database can be changed by selecting the database in the pull-down menu on the "**Database Management**" page, clicking the "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 „Filter" button. The filters allow sub-sets of data to be selected and screened in any data column (see Microsoft Excel help for detailed instructions on using the filters feature).

Changes made within the databases are saved as soon as the The_Tool_2.1.xls file is saved because all databases are stored within that file. As an important consequence, whenever the The_Tool_2.1.xls file is passed on to another user, all databases are passed on as well. It is possible to delete some databases and/or 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 (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 pushed.

Presentation of Detailed Model Results

The results from the multimedia mass balance model employed in The Tool are presented if the "Details" button on the "**Graphical Results**" page is clicked for a selected chemical. This leads to a new page that contains a full list of model output for the selected chemical. In the box right to the chemical's name, the numerical values of P_{OV}, CTD and TE that are displayed on the "**Graphical Results**" page are given. Further to the right, all P_{OV}, CTD and TE values obtained for the three scenarios of emissions to soil, water and air are listed (see below, Section 3). The three pie charts show the chemical's 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 with all mass fluxes calculated by the model (degrading reactions, physical removal, and inter-compartment exchange). With these numbers, the users can identify processes that dominate the observed fate of a particular chemical.

Monte Carlo Uncertainty Analysis

The Tool software allows a simple sensitivity and uncertainty analysis of results for the single chemical if "Include Monte Carlo Analysis for Single Chemical" is checked on the "**Main Menu**" page. Five cells are displayed in which default dispersion factors for the five 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 five 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. If 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 large.

When the Monte Carlo option was selected, the "**Graphical Results**" page contains two unique buttons in the panel "Select a chemical" underneath the plot of TE 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 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 five 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 TE. 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

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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 15 "relationship charts" in which for every metric (P_{OV}, CTD, and TE) the results of the *n* Monte Carlo runs are plotted against every input parameter.

Changing Model Settings

The "**Preferences**" page can be accessed from 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 (no warning at all if value outside limits) or more restrictive (no calculation at all if value 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 TE = 2.248%. These values are model results for reference chemicals that are known as persistent organic chemicals; see Section 3 below for a more detailed description of the use of reference chemicals. Users can replace these numbers by other values at which lines for P_{OV}, CTD and TE shall be drawn.

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 "Clear".

In the fourth panel (right, middle), the "Enable Macros" warning, which might have been switched off, can be activated. This helps other users, to whom the model might be passed on, to properly open the The_Tool_2.1.xls workbook on their computer.

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. 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 Manage Databases 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.

Database Management

Button "<< Main"	Returns to the Main Menu page.
Button "New"	Prepares a new database page, asks for its name and presents an empty database sheet into which substance properties can be entered.
Button "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 "<<"	Returns to the Database Management page.
Button "Check"	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.
Pull-down menu "Sort by:"	Lets you select sorting criteria from all input parameters, results and the problem indicator (see "Check").
Button "Filters"	Displays a subset of the database that fulfills your criteria. See Excel Autofilter help documentation for further details.

Graphical Results

Button "<< Main"	Returns to the Main Menu page.
Button "Details"	Shows detailed 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.

Preferences

Button "<< Main"	Returns to the Main Menu page.
Button "Reset to Default"	Restores the default values in the panels the button is located in.
Button "Clear"	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.

2. 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 with detailed model results for a single chemical ("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 emission of 100 mol/hour to air, water, and soil. In every run, P_{OV} and TE 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 TE and two values for CTD; all of these results are displayed in columns G to J and rows 3 to 5 of the page with detailed model results ("Details" button on the "**Graphical Results**" page). Finally, the P_{OV}, CTD and TE values shown in the plots on the "**Graphical Results**" page are derived by selecting the highest values of P_{OV}, CTD, and TE 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 values in air. However, the lower a chemical's Henry's law constant is, the more important becomes transport in water, and for relatively water soluble compounds, CTDs 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 values is selected. This 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; this effect is not included in the model used in The Tool.

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 transport efficiency, TE) vs. overall persistence, P_{OV}. This type of plot, which has been 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) and others; see Scheringer (2002) for an overview.

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 4. 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.
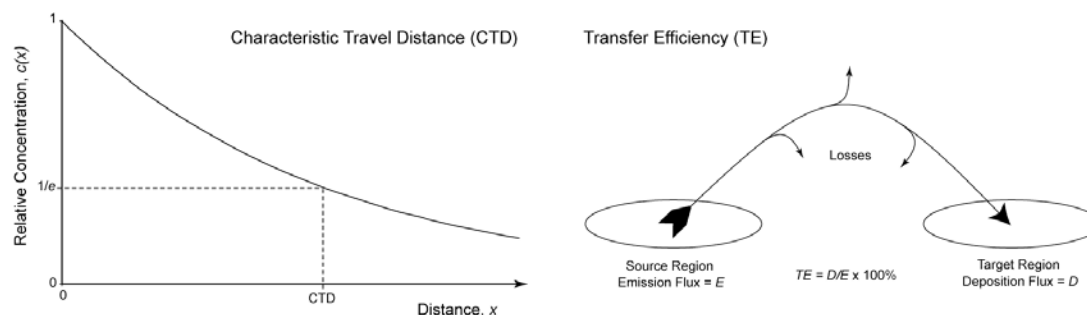

Figure 4: Transport-oriented and target-oriented LRTP metrics in comparison.

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 Transfer Efficiency (TE, %). Transfer Efficiency is calculated from the ratio of the deposition mass flux from air to surface media in a region adjacent to the region to which the chemical is released and the mass flux of the chemical emitted to air in the release region. Both fluxes must be expressed in the same units on a mass basis (eg, kg/year) or on a mole basis (eg. moles/year). TE results are shown in the graph on the right on the "**Graphical Results**" page; the TE is given as the percentage of emission

flux that is deposited 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) rely only on the single-media half-lives as persistence criteria. P_{OV} metrics provide a somewhat different perspective because they take into account 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.[3]

Comparison of Model Results to Result 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 group 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 vs. P_{OV}, see Figure 1 in Klasmeier et al. (2006). The P_{OV} value of the POP-like reference chemical

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[3] 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.

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 2.248 % (TE of PCB-28). To display these boundaries in the plots on the "**Graphical Results**" page, one has to 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.

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

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