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LEACHABILITY CONCEPT

Leachability as a process-based method to determine the mobility of chemicals in a PMT/vPvM framework

Leachability as a process-based method to determine the mobility of chemicals in a PMT/vPvM framework

Dr. Judith Klein

Dimitrios Skodras

Dr. Michael Klein

Fraunhofer-Institut für Molekularbiologie und Angewandte Oekologie IME
in Schmallenberg

Content

1 Summary

In this study the official version of FOCUS PELMO (version 6.4.4) is used for the prediction of percentage leachability. Numerous simulations are performed for hypothetical substances using different Koc and DT50 values in a broad range. Aim of this concept is to show the potential of leachability as an indication of mobility (M/vM) for PMT and vPvM (persistent, mobile, toxic and very persistent, very mobile) substances.

In this report the following aspects are included:

- Background on current PMT/vPvM assessment
- Description of simulation studies
- Description on the leachability concept as higher tier for mobility within PMT/vPvM hazard assessment
- Results of simulation studies

A tool for result visualization is implemented in Python3 (Van Rossum, G. 2009). The tool is published on the Fraunhofer IME software website (https://software.ime.fraunhofer.de/). Furthermore, the code is made available on https://github.com/IMEDiman/LeachCalc under GNU General Public License v3.0.

2 Introduction

In 2020, the EU Commission published the "Chemicals Strategy for Sustainability – Towards a Toxic-Free Environment". A part of this strategy is to define new hazard classifications for PMT and vPvM (persistent, mobile, toxic and very persistent, very mobile) substances which will be introduced into the CLP Regulation (Classification, Labelling and Packaging; EC No 1272/2008) and REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals; EC No 1907/2006) regulation. The new hazard classification should help to identify chemicals that have the potential to reach and accumulate in drinking water.

Within REACH legislation, there is already guidance available for persistence (P) and toxicity (T) assessment (ECHA 2017). For mobility (M) the log Koc value is listed in the regulation as parameter to classify substances as mobile or very mobile. However, the regulation also takes into account that the log Koc as only parameter is a poor indicator to characterize the potential of substances to reach drinking water sources (ECETOC 2021, Collard et al. 2022, Pawlowski et al. 2023). Therefore, it is mentioned that other methods such as leaching studies, modelling or monitoring should be considered in a Weight of Evidence (WoE) approach.
The reason is that transport of a substance through soil or sediment cannot be described with Koc only but is predominantly controlled by a combination of sorption *and* degradation apart from other substance and environmental parameters. This concept was already used by leaching indices like the GUS index (Gustafson 1989). However, the GUS index (Groundwater Ubiquity Score) is empirically derived. It relates pesticide half-life and Koc from laboratory data of substances that are mostly not registered anymore to US groundwater monitoring data from the 80's and must therefore be considered as outdated.

With regard to *modelling* as Weight-of-Evidence for mobility the FOCUS framework (European Commission, 2014) can be used. The FOCUS models and scenarios are already well established in regulatory context of PPP authorisation for many years to describe the transport of PPP through soil to groundwater. The so-called FOCUS models consider the relevant substance properties as well as the influence of climate, soil and plants. This is done for several representative European scenarios covering a broad range of European pedo-climatic condition with mean annual temperature from 4 to 18 °C and annual precipitation from 500 to 1150 mm. The FOCUS models are continuously tested and part of a version control to ensure the quality and the maintenance of the computer programs.

To determine the leachability as an indication of mobility (M/vM) for PMT, the FOCUS model PELMO is used. PELMO is a one-dimensional simulation model simulating the vertical movement of substances in soil by solving the convection dispersion equation. The first version of PELMO was released in 1991 (Klein, 1991). FOCUS PELMO is an official FOCUS model for PPP registration in the EU. The latest version used for FOCUS groundwater simulations is FOCUS PELMO 6.6.4. The use of PELMO enables a process-based hazard assessment for PMT and vPvM substances. Leachability is only intended to be considered as a higher tier for mobility (M/vM), which implies that the assessment for persistence (P/vP) is not affected.

3 Material and methods

The PMT hazard classification should be based on substance properties and needs to be independent of exposure. In this report, leachability in percentage is proposed as a method to define the mobility of a substance. Leachability is calculated as the fraction (percentage) of mass that can leach through an unsaturated soil barrier of 1 m under realistic European pedo-climatic conditions. Since only linear transport processes are considered, the fraction of leached mass is independent from the level of exposure.

For the simulations, the FOCUS model PELMO 6.6.4 is used. It requires input data on location (soil, climate), considered crop and exposed substance.

- To consider a large range of European pedo-climatic scenarios (4 –18 °C annual average temperature, 500 –1150 mm annual precipitation), simulations for all nine FOCUS groundwater locations (Châteaudun, Hamburg, Jokioinen, Kremsmünster, Okehampton, Piacenza, Porto, Sevilla, Thiva) are performed. To ensure that leachability is independent of exposure, linear sorption (Freundlich exponent = 1.0) is assumed. The reference temperature for the soil DT50 value is set to 12°C in accordance with the ECHA guidance on persistence [1].
- Winter cereals which is the most important agricultural crop is selected as surrogate for all arable crops. The reason is that large areas of winter cereals can be found in almost all agricultural regions of the EU and is therefore available as crop in the parameterization of all nine FOCUS locations.
- The substance is defined by a particular Koc-$DegT50_{soil}$ combination and a set of constant default parameters compiled in **Table A** 2. The substance exposure is assumed on a monthly basis (e.g. application on soil surface) to consider various weather conditions in different seasons. Simulations are performed for a period of 120 years to ensure meaningful results for substances with higher Koc values for which leaching processes are slow and more years are needed to be transported down to 1 m depth. In practice, the 120 years are repetitions of the 20 climate years used in FOCUS.

With this setup a total of 7749 simulations (21 Koc values x 41 $DegT50_{soil}$ values x 9 locations) are performed. Each PELMO simulation creates a KONZCHEM.PLM (see respective file supplied with this report) which contains the annual dissolved mass in the percolate in mg/L for 5 cm thick soil layers. This value is taken for the 21st layer corresponding to 1 m depth for all years neglecting the first six years as so-called warming-up period. To be consistent with the FOCUS principles regarding a realistic worst-case, the 80th percentile annual mass flux transported down to 1 m is used and related to the mass at the soil surface. This results in an overall 90th percentile worst-case due to the conservative assumption related to the selection of the soil profiles (FOCUS, 2000). To take the results of all nine locations into account, the average leachability of the nine locations is calculated. Thus, for each simulated substance defined by a particular Koc-$DegT50_{soil}$ combination one leachability value is assigned.

A whole matrix of multiple Koc-$DegT50_{soil}$ combinations is simulated. The results are compiled in a look-up table which is the basis of a user-friendly software that determines the leachability of a substance within the simulated Koc and DegT50 range. The $DegT50_{soil}$ was varied between 1 and 365 days and the Koc between 0 and 10,000 mL/g (see **Table A** 1).

A substance is defined to be not mobile if the average leachability is less than 1%. If the leachability is greater than 1% the substance is considered to be mobile. Substances with an average leachability greater than 10% are considered to be very mobile (see Table 1).

Table 1: Definition of mobility based on leachability in %

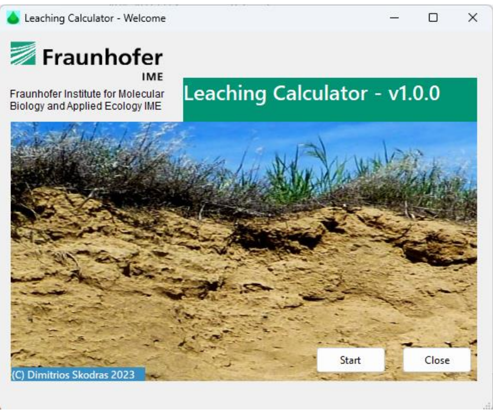
Leachability in %	Mobility
< 1 %	not mobile
1 % - 10 %	mobile
> 10 %	very mobile

4 Development of Leaching Calculator

To facilitate leachability calculations a user-friendly software was developed (Figure 1). The tool is implemented in Python with the graphical user interface (GUI) built in PySide6 (Qt Company 2023). It is published on the Fraunhofer IME software website (https://software.ime.fraunhofer.de/). Furthermore, the code is available on GitHub (https://github.com/IMEDiman/LeachCalc). An additional version as a command-line interface (CLI) is also available.

4.1 Graphical User Interface LeachCalc

Figure 1: Welcome form of the user-friendly tool Leaching Calculator



Source: Screenshot, Fraunhofer IME

The user may enter a Koc and a $DegT50_{soil}$ value at reference temperature of 12 °C. Based on the simulation results of PELMO, the software interpolates the respective average leachability value in % (**Fehler! Verweisquelle konnte nicht gefunden werden.**) as explained below. The name of the substance can be inserted in a text field and the corresponding representative values for KOC and $DegT50_{soil}$ directly into the spin boxes. The respective up- and down arrows can also be used. A condensed result is displayed in the text box below. It is updated if the input parameters are changed. The content can be copied with the "Copy to Clipboard"-button and pasted into an application of choice.

Figure 2: Main form of Leaching Calculator

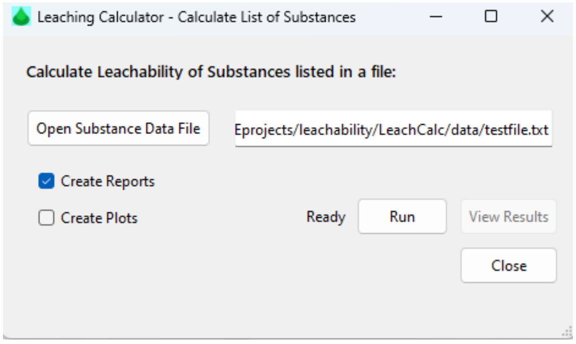
Source: Screenshot, Fraunhofer IME

If a combination of input parameters is not represented in the lookup table an interpolation is performed. This is done with the RectBivariateSpline function from the Python3 module scipy.interpolate (Virtanen et al. 2020). It is based on the concept of spline interpolation, a method of approximating a function from a set of data points. In contrast to the more basic polynomial interpolation, it involves the fitting of multiple polynomial functions to data subsets. These polynomials are to be low-degree for more stability and accuracy and chosen such that the overall deflection curve is continuous and smooth.

Furthermore, based on the lookup-table and the interpolation method a contour plot is created representing the three mobility areas on the KOC-$DT50_{soil}$ plane. The python package matplotlib (Hunter 2007) is used here. Upon changing the input parameters this figure gets updated with a purple cross signifying the mobility of the Koc-$DegT50_{soil}$ input configuration. The figure can be saved as a PNG, JPG or PDF file (300 dpi) with the "Save Figure"-button (**Fehler! Verweisquelle konnte nicht gefunden werden.**).

If the leachability for multiple substances should be computed, clicking "Calculate List" opens a new form (see Figure 3). The list can be loaded by clicking "Open Substance Data File" which opens the common file dialog. An example file can be found in. It can be specified by clicking the respective check boxes whether short reports and plots shall be created. With "View Results" a file dialog with the result files opens.

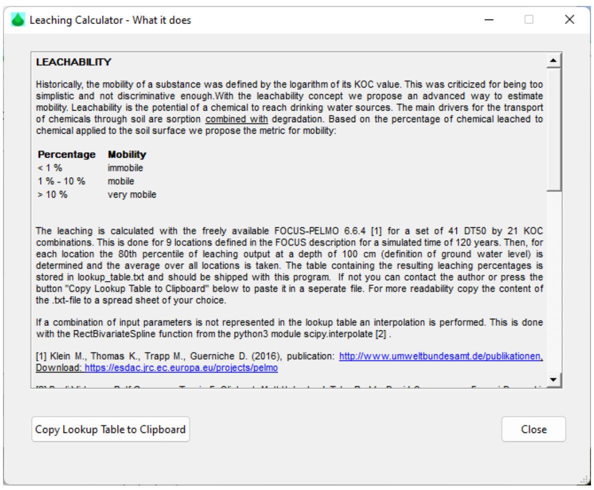
Figure 3: Calculate leachability for a list of substances



Source: Screenshot, Fraunhofer IME

By clicking at "Info", and "What it does", a new form opens (Figure 4) and the Leaching Calculator provides information on the categorization of mobility with regard to leachability and the underlying data (lookup table). The user may click at "Copy Lookup Table to Clipboard" to copy the data. For better readability the content can be pasted into a spread sheet of choice.

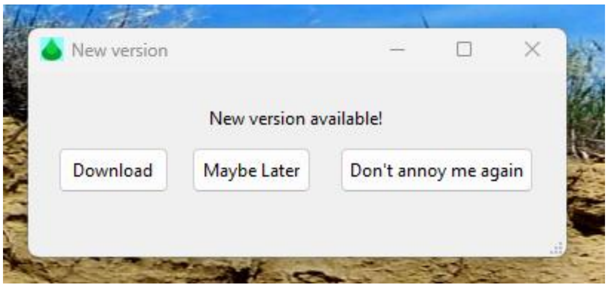
Figure 4: "What it does"- form of the Leaching Calculator



Source: Screenshot, Fraunhofer IME

On start the program looks for updates. If this is the case a new form opens (see Figure 5). Clicking on "Download" will open the user's standard browser directed to the webpage where the new version can be downloaded. Clicking "Don't annoy me again" creates a file named "LC_noUpdate.txt" in the same folder where the program is found. As long as it is present this update form will not be shown again. However, it can be opened either by deleting the file or via the main form -> Info -> Check for Updates.

Figure 5: Form informing the user about new program versions

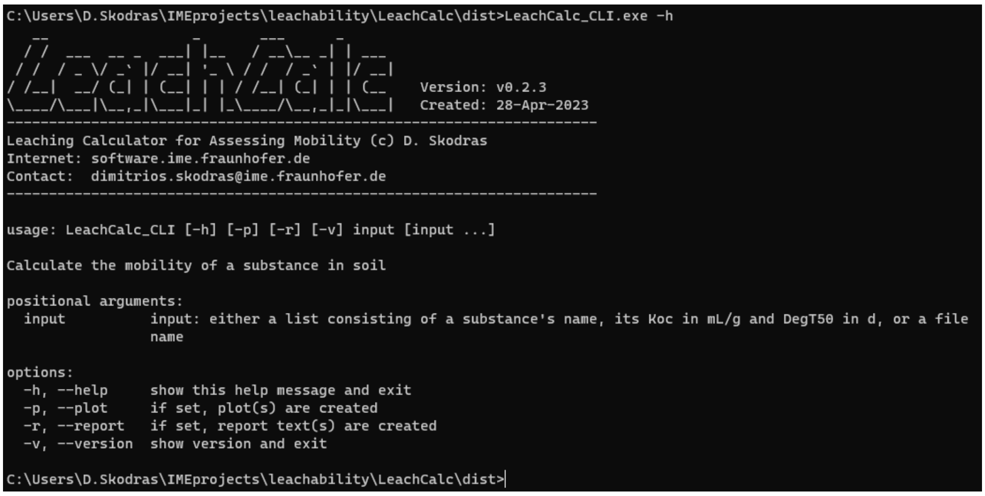


Source: Screenshot, Fraunhofer IME

4.2 Command-Line Interface LeachCalc_CLI

For purposes of interfacing the Leaching Calculator with other programs, a command-line version is also presented. In Figure 6 the program is called from the Windows command line cmd with the "help" flag showing how and with which possible options LeachCalc_CLI.exe can be called.

Figure 6: Command-Line Interface of LeachCalc



Source: Screenshot, Fraunhofer IME

There are two possible ways to specify the input argument, similar to those in the GUI.

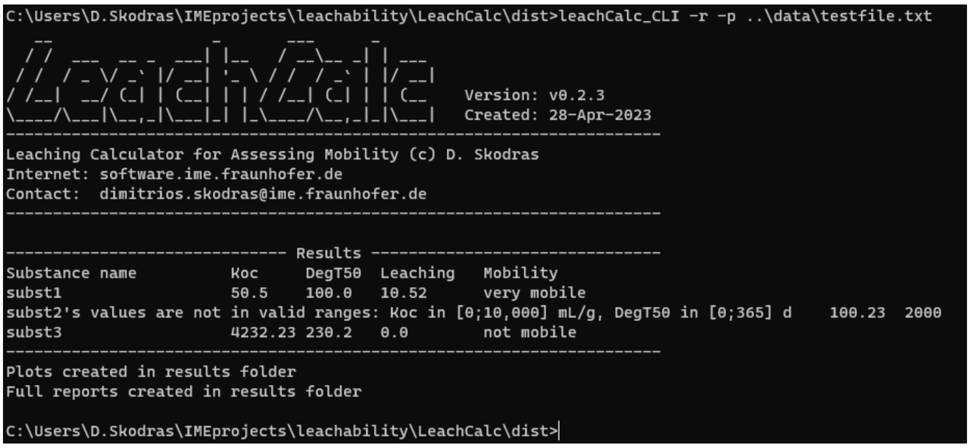
1. Pass three arguments, separated by a space. The first denotes the substance name, the second its Koc value in mL/g and the third its $DegT50_{soil}$ value at 12 °C in d. The latter two have to be floating numbers within the range specified above.
2. Pass a path to a text file containing these three tabulator-separated arguments with one line per substance (see Appendix 0 for an example file)

If the "-r" or the "-p" flags are passed, full reports and plots of the style identical to the GUI version are created. If none are set, the input parameters are repeated with the leaching percentage and the resulting mobility assessment. See Figure 7 and for examples.

Figure 7: LeachCalc_CLI call with a substance name, its Koc and $DegT50_{soil}$

Source: Screenshot, Fraunhofer IME

Figure 8: LeachCalc_CLI with a file containing data for multiple substances



Source: Screenshot, Fraunhofer IME

4.3 Guidance on selecting Koc and $DegT50_{soil}$

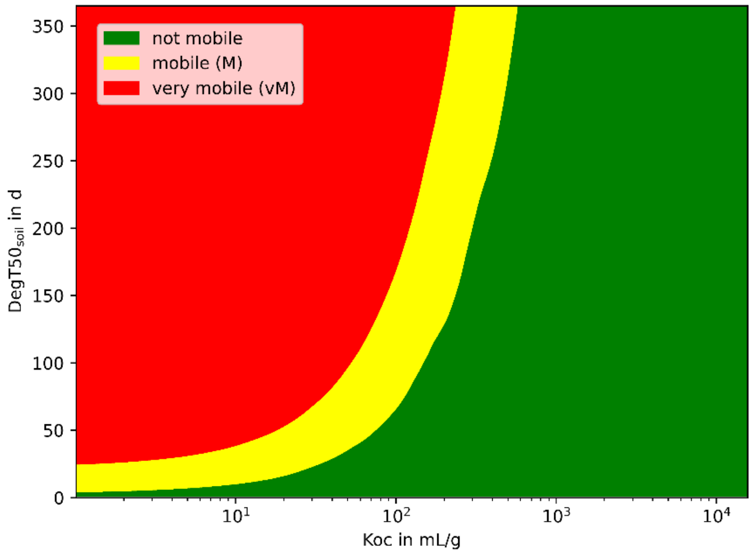
Regarding the input parameters for Koc and $DegT50_{soil}$ it is recommended to be consistent with existing guidance documents that were developed in the context of the FOCUS leaching approach. This includes FOCUS, 2000, EC, 2014 and especially EFSA, 2014. A central point is that due to the conservativeness of the scenarios robust and representative input parameters for sorption and degradation should be used. This means that if a minimum of 4 values are available for a parent compound (3 values for a metabolite) the geometric mean values should be used for both Koc (not for log Koc!) and $DegT50_{soil}$. In case of a lower number of values the worst-case should be used (minimum Koc and maximum $DegT50_{soil}$). EFSA, 2014 also provides guidance for when $DegT50_{soil}$ from field degradation values, if they are available, should be used instead of laboratory degradation values (e.g. from OECD 307). It needs to be stressed that the reference temperature for the DegT590 values is 12 °C which means that DegT50 values that are normalised to 20 °C and need to be multiplied with a factor of 2.58^0.8 according to the EFSA opinion on Q10 values (EFSA, 2007).

5 Result of simulations

Leaching is calculated with the freely available FOCUS-PELMO 6.6.4 (Klein M., 2021) (https://esdac.jrc.ec.europa.eu/projects/pelmo) for a set of 41 $DegT50_{soil}$ by 21 KOC combinations. The $DegT50_{soil}$ is varied between 1 and 365 days and the Koc between 0 and 10,000 mL/g. This is done for nine different locations defined in the FOCUS groundwater scenarios for a simulation time of 120 years. For each location the 80th percentile of leached substance mass at a depth of 100 cm (surrogate for very shallow ground water level) is determined and the average over all locations is taken. The result of the simulations is the average leachability in percentage calculated with FOCUS-PELMO 6.6.4 as function of $DT50_{soil}$ and Koc (Figure 9) covering the EU. The underlying data of the contour plot is presented in the appendix (**Fehler! Verweisquelle konnte nicht gefunden werden.**; Table A 1 continued)

Leachability decreases rapidly with increasing Koc values. For Koc-values greater or equal to 600 ml/g leachability is below 1% (Figure 9, green, not mobile) independently of the value of $DegT50_{soil}$. The lower the Koc values the more depends the leachability on the $DegT50_{soil}$ value.

Figure 9: Average leachability (leached percentage) over all scenarios for each DegT50-Koc combination



Source: Fraunhofer IME, plotted using the Python package Matplotlib (Hunter 2007)

6 Conclusions

In this study it is described how leachability can be used in a Weight-of-Evidence approach to assess the mobility of a substance within PMT/vPvMT hazard assessment.

By using the presented approach it is possible to assess the leaching potential of substances trough soil and sediment to reach drinking water sources. The presented approach is suitable for PMT hazard assessment as leachability is calculated independently of substance emission. The models and scenarios used in this approach take into account all important processes and pedo-climatic boundary conditions that are relevant for the transport of chemicals through the soil. With regard to the substance properties, it is based on two important parameters Koc and $DegT50_{soil}$ which control the degradation and sorption of a chemical in soil or sediment which are the most important processes for the transport of substances down to potential drinking water sources. Substances which degrade rapidly in soil and sediment do not have the tendency to reach drinking water sources regardless of the corresponding Koc value.
The leachability approach therefore represents a much higher degree of realism for the mobility assessment compared to a simplistic log Koc value. The calculations within the leachability approach are based on the concept of FOCUS with the FOCUS model FOCUS PELMO 6.6.4 which is successfully used since more than 20 years in the authorisation of PPP. This ensures that the conservative and protective character of FOCUS is also considered in the leachability approach.

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List of abbreviations

Abbreviation	Description
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
Koc	Soil/sediment adsorption partitioning value normalised to organic carbon content
PELMO	PEsticide Leaching Model
GUS	Groundwater Ubiquity Score, Index method, experimentally calculated value that relates pesticide half-life and Koc (from laboratory data)
SETAC	Society of Environmental Toxicology and Chemistry
PPP	Plant Protection Products

Appendix

A.1 Data Tables

Table A 1: Average Leachability in % for Koc in [0;10,000] and $DegT50_{soil}$ in [1;100]

KOC\ DT50	1	2	3	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	95	100
0	0.5	0.7	1.0	1.6	3.6	6.0	8.6	11.2	13.8	16.5	19.3	21.9	24.2	26.5	28.7	30.8	33.0	35.0	37.0	38.7	42.1	43.6
2	0.2	0.4	0.6	1.1	2.8	4.8	7.1	9.4	11.8	14.3	17.0	19.5	21.9	24.1	26.2	28.3	30.4	32.5	34.5	36.4	39.7	41.3
4	0.1	0.2	0.4	0.7	2.1	3.9	6.0	8.1	10.2	12.6	15.0	17.5	19.7	21.9	24.0	26.0	27.9	29.9	31.9	33.8	37.4	39.0
6	0.1	0.1	0.2	0.5	1.6	3.2	5.0	7.0	9.0	11.1	13.4	15.7	17.9	20.0	22.1	24.0	25.9	27.7	29.6	31.5	35.1	36.8
8	0.0	0.1	0.1	0.3	1.3	2.6	4.2	6.0	7.9	9.8	11.9	14.1	16.2	18.3	20.3	22.2	24.1	25.9	27.7	29.4	32.9	34.6
10	0.0	0.0	0.1	0.3	1.0	2.2	3.6	5.2	7.0	8.7	10.6	12.6	14.6	16.7	18.6	20.5	22.4	24.2	25.9	27.6	30.9	32.5
20	0.0	0.0	0.0	0.1	0.4	0.9	1.6	2.5	3.6	4.9	6.3	7.7	9.2	10.7	12.2	13.7	15.3	16.8	18.4	19.9	22.9	24.3
40	0.0	0.0	0.0	0.0	0.1	0.2	0.4	0.7	1.1	1.6	2.2	3.0	3.8	4.6	5.6	6.5	7.5	8.6	9.6	10.7	12.8	13.9
60	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.4	0.6	0.9	1.3	1.7	2.2	2.7	3.3	3.9	4.6	5.2	6.0	7.5	8.3
80	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.3	0.4	0.6	0.8	1.1	1.4	1.7	2.1	2.5	3.0	3.5	4.5	5.0
100	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.2	0.3	0.4	0.6	0.8	1.0	1.2	1.5	1.8	2.1	2.8	3.2
200	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.4	0.4
400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
600	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
800	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

10000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Source: Fraunhofer IME

Table A 1 continued: Average Leachability in % for KOC in [0;10,000] and DegT50$_{soil}$ in [105;365]

KOC\DT50	105	115	120	125	135	145	155	165	175	185	205	225	245	265	285	305	325	345	365
0	45.3	48.2	49.5	50.8	53.3	55.6	57.8	59.8	61.8	63.7	67.6	71.1	74.2	77.2	80.1	82.8	85.4	87.8	90.0
2	42.8	45.9	47.3	48.7	51.3	53.7	55.9	58.0	60.0	61.8	65.3	68.7	71.9	74.7	77.4	80.0	82.5	84.9	87.3
4	40.6	43.5	45.0	46.4	49.1	51.5	53.8	56.0	58.1	60.1	63.6	66.8	69.8	72.7	75.5	78.0	80.5	82.8	85.0
6	38.4	41.4	42.8	44.3	46.9	49.4	51.7	53.9	56.0	58.0	61.7	65.0	68.2	71.0	73.7	76.2	78.5	80.9	83.1
8	36.3	39.4	40.8	42.2	44.9	47.4	49.8	52.1	54.2	56.1	59.9	63.3	66.4	69.3	72.0	74.5	76.8	79.0	81.1
10	34.1	37.3	38.8	40.2	42.8	45.4	47.9	50.2	52.3	54.3	58.1	61.5	64.6	67.6	70.3	72.8	75.2	77.4	79.5
20	25.7	28.4	29.8	31.1	33.6	36.1	38.5	40.7	42.8	44.8	48.6	52.1	55.4	58.5	61.4	64.0	66.6	69.0	71.3
40	15.0	17.2	18.3	19.4	21.6	23.6	25.6	27.5	29.3	31.0	34.5	37.7	40.6	43.3	45.9	48.4	50.8	53.1	55.2
60	9.1	10.7	11.6	12.4	14.1	15.8	17.6	19.2	20.9	22.5	25.7	28.7	31.4	34.0	36.5	39.0	41.3	43.5	45.6
80	5.6	6.8	7.4	8.1	9.4	10.7	12.1	13.5	14.9	16.2	19.0	21.8	24.4	27.0	29.5	31.8	34.1	36.3	38.4
100	3.6	4.4	4.9	5.4	6.4	7.4	8.5	9.6	10.8	11.9	14.3	16.6	18.9	21.2	23.5	25.8	28.0	30.1	32.2
200	0.5	0.7	0.8	0.9	1.2	1.5	1.8	2.1	2.5	2.9	3.8	4.8	5.9	7.1	8.3	9.6	10.9	12.2	13.5
400	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.5	0.7	0.9	1.2	1.5	1.8	2.2	2.6	3.0
600	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.3	0.3	0.5	0.6	0.7	0.9
800	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.3
1000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1
2000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Source: Fraunhofer IME

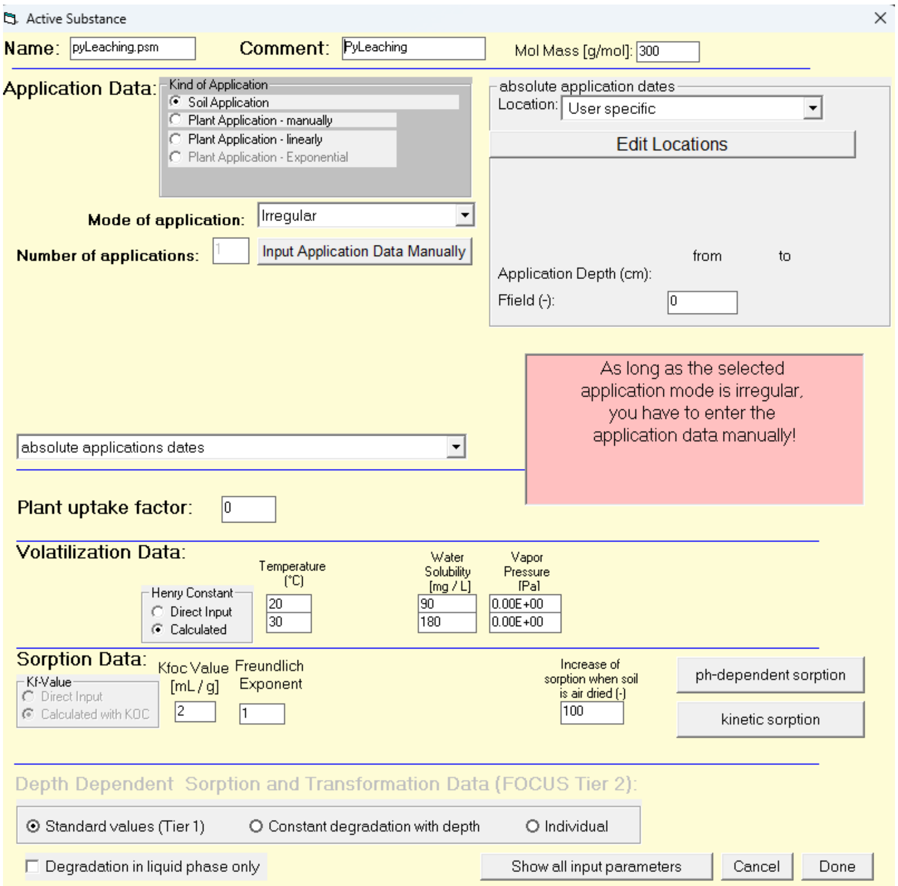
Table A 2: Constant and default parameters used for PELMO simulations

Application Rate	0.1 kg*	Molar Mass	300 g/mol
Application Date	1st of each month	Water solubility (at 20 °C)	90 mg/L
Kind of Application	Soil Application	Vapor Pressure (at 20 °C)	0.0 Pa
Application Depth	0 cm	Diffusion coefficient Air (at 20 °C)	4.98E-02 cm^2/s
Plant Uptake Factor	0.0	Q10-Value	2.58
Freundlich Exponent	1.0	Moisture Exponent	0.7
Stoichiometric Factor	1	Temperature during Study	12 °C
Reference Irradiance	100 W/m^2	Increase of sorption when soil is dried	1
Relative Moisture during Study	100 %	pKa (pH-dependent Sorption)	20

*The choice for the application rate is arbitrary. With linear sorption (Freundlich exponent = 1.0) the leached mass does not depend on the applied rate that we checked explicitly.

A.2 Generic Substance in PELMO GUI

Figure 10: Representation of substance information in PELMO's GUI



Source: Screenshot, Fraunhofer IME

A.3 Leaching Calculator – Substance list example

In the substance list file three tab-separated entries are required for each substance. The first is its name, the second is the koc value in mL/g and the third is the $DegT50_{soil}$ value in d.

################
Testfile.txt
subst1 50.5 100
subst2 100.23 2000
subst3 4232.23 230.2