

## Appendix 5

# BROWSE\_ PEARL-OPS Parameterisation for the BROWSE Exposure Scenarios for Residents and Bystanders

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## Summary

OPS (**O**perational Atmospheric Transport Model for **P**riority **S**ubstances) OPS is an atmospheric dispersion model that simulates atmospheric concentration and dry deposition of pollutants in a given area of interest. It simulates the atmospheric process sequence of dispersion, transport, chemical conversion and finally deposition (Van Jaarsveld, 1995, 2004). The special high-resolution model version of OPS used for the BROWSE Scenarios, OPS-St (St for Short term) allows hour-to-hour variations in emissions to be included (Smits et al., 2005; Van Pul et al., 2008).

The model is based on a Gaussian plume dispersion formulation extended with a formulation of vertical wind speed and dispersion profiles that allows the most important meteorological influences on atmospheric dispersion at the local scale to be taken into account: The model also takes into account the effect of deposition on the concentration in the plume (Van Jaarsveld, 1995, 2004). OPS has been set up as a universal framework supporting the modelling of a wide variety of pollutants and specific applications.

For the BROWSE vapour exposure scenarios, OPS computes the concentration in air at multiple receptors around the field at the target distance as well as at the receptor in the centre of the field. The hourly data on the source strength of the emission is calculated by the PEARL model. PEARL (Pesticide Emission Assessment at Regional and Local scales) is a consensus model developed by three Dutch institutes (Alterra, PBL and RIVM) in close co-operation (Leistra et al., 2001; Tiktak et al., 2000; Van den Berg and Leistra, 2004).

The PEARL model is based on (i) the convection/dispersion equation including diffusion in the gas phase with a temperature dependent Henry coefficient, (ii) a two-site Freundlich sorption model (one equilibrium site and one kinetic site), (iii) a transformation rate that depends on water content, temperature and depth in soil, (iv) a passive plant uptake rate. The model includes formation and behaviour of transformation products and describes also lateral pesticide discharge to drains. PEARL can simulate preferential flow. Volatilisation from the soil surface or crop surface is calculated assuming a laminar air layer at the soil surface or plant surface. The model also includes a description of the processes occurring on the crop canopy, phototransformation, wash-off, volatilisation and penetration into plant tissue.

For the BROWSE exposure scenarios for volatilisation from plants, the PEARL option to consider only the plant system has been used. For the exposure scenarios for volatilisation from soils the soil-plant

system is considered, which requires a simulation of the hydrology of the soil system. PEARL does not simulate water flow and soil temperatures itself but uses the Soil Water Atmosphere Plant (SWAP) model for that purpose. In SWAP, flow of water is described with Richard's equation and the flow of heat with Fourier's Law using finite implicit difference schemes (Kroes et al., 2008). SWAP can handle a wide variety of hydrological boundary conditions. Soil evaporation and plant transpiration can be calculated via multiplying a reference evapotranspiration rate with soil and crop factors. SWAP can simulate groundwater levels that fluctuate in response to the rainfall input.

The BROWSE interface includes the option to assess the vapour exposure of bystanders and residents after application of plant protection products to bare soils or crops. Key properties of the substance need to be introduced by the user. Using the BROWSE interface, the user can select the type of assessment needed, e.g. acute or chronic exposure. For each assessment type a post-processing procedure has been developed to obtain the required target output, i.e. various percentiles of exposure concentrations at the target distance.

## Parameterisation of BROWSE PEARL-OPS

For the vapour exposure scenarios for volatilisation from plants or soils the combination of the PEARL and OPS are used. The atmospheric dispersion model OPS simulates atmospheric dispersion and dry deposition of pollutants at the local scale. The scenarios developed have been parameterised for PEARL-OPS. Input data needed are meteorological data, data on physicochemical properties, application data, field size and receptor configuration data. The source strength is computed with the PEARL model. After starting the OPS model, OPS prepares the input files to run PEARL, starts the PEARL model and after completion of the PEARL run uses the PEARL output file with emission data to calculate the dispersion in air around the treated field. From the output of OPS the target outputs are obtained using a post-processing procedure implemented in the interface software of BROWSE.

### General description of PEARL-OPS input

#### *Source configuration*

Source configurations have been defined by BROWSE. Three field sizes have been defined: 200 by 200 m, 500 by 500 m and 2000 by 2000 m. In the scenarios for volatilisation from plants the source height was set at 0.1 m, whereas for the scenarios for volatilisation from soil it was set at 0.0 m.

#### *Emission source*

For each BROWSE application scenario, the emission is computed with the PEARL model and it will depend on the combination of application characteristics, substance properties and meteorological conditions. OPS prepares the input files for PEARL using the substance and application data in the .cmp file, the meteorological data in the .met file and the scenario data in the template file. The .prl input file is prepared by combining the data in the .cmp file to the data in the .tmp file. Template files are created for each crop/ meteorology combination. The emission output file generated by PEARL is input to OPS.

### *Receptor configuration*

Receptor configurations have been defined by BROWSE. In each field a receptor was defined in the centre. Around each field receptors were defined at 10 m from the edge in all directions. Two series of receptors were defined: one for a height of 0.7 m and another for a height of 1.4 m.

### *Weather*

The hourly weather data were collected for locations with an average annual air temperature during the growing season corresponding to the 90th percentile of average annual air temperature during the growing season for the entire Zone (Northern, Central or Southern). The growing season was taken to be from 1 April to 1 October. One site was selected for the Northern Zone (Denmark), two sites in the Central Zone (Germany and Hungary) and two sites in the Southern Zone (Spain and Italy).

### *Soils*

The soil profiles for the vapour exposure scenarios for volatilisation from bare soil were taken from the EFSA persistence scenarios for concentrations in the liquid phase. These soils are low in organic matter content, therefore comparatively high concentrations in the liquid phase can be expected. Because of the equilibrium between the amount of substance in the gas and liquid phase, the selection of use of these soils would also result in comparatively concentrations in the gas phase and hence in volatilisation flux densities from soil. For the Northern, Central and Southern Zone, the corresponding soil profile of the EFSA persistence scenario for the liquid phase was selected (EFSA, 2012). The hourly weather data for these scenarios were taken from the Danish, Hungarian and Spanish scenario for volatilisation from plants (see above).

## **Description – BROWSE\_OPS\_PEARL INPUT**

In this section a description is given of the files needed to assess the vapour exposure using the PEARL-OPS models. These files are created by the BROWSE interface:

1. X.OPS file containing all main input parameters with X as the run identification
2. Y.MET file containing meteorological input in which Y is the name of the meteorological station
3. X.CMP file containing substance data and application data; substance data entered by user using interface
4. X.TMP template file containing scenario data to prepare PEARL input for the scenarios for volatilisation from plants.

Below we specify the input in these four input files. The scenario and parameter definitions are based on:

- 1) **BROWSE DEFINITION** = Definitions made by the BROWSE project group
- 2) **BROWSE SCENARIO SPECIFIC** = Definitions made by the BROWSE group for a specific vapour exposure scenario

3) **DEVELOPMENT DEFINITION** = Definitions made during the BROWSE vapour exposure scenario development

4) **USER INPUT** = Input to be specified by the user in the BROWSE interface.

**X.OPS file**

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>
<p><b>RECORD 1</b>      <b>General Settings</b></p> <p>Quit_After_Run      Option for multiple run sessions with bat file</p> <p>Detailed_Information_To_Screen      Option for output to screen</p> <p>Run_Name      Name of simulation run</p> <p>Caseld      Simulation Case</p>	<p>Set to 'y' (Yes). <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 'n' (No). <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 'RunId'. Input from BROWSE interface <b>DEVELOPMENT DEFINITION</b></p> <p>Set to '5', option for coupling with PEARL. <b>DEVELOPMENT DEFINITION</b></p>
<p><b>RECORD 2</b>      <b>Select component</b></p> <p>Component      Selection of component; component 5 is 'pesticides'</p> <p>Particle_Size_Distribution:      option for particle size Distribution; option 0 is 'None'</p> <p>Name_Particle_Size_Distribution_File      Name of particle size distribution file</p>	<p>Set to '5'. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to '0'. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 'User_Defined'. Dummy value if Particle_Size_Distribution set to '0'. <b>DEVELOPMENT DEFINITION</b></p>
<p><b>RECORD 3</b>      <b>Area characteristics</b></p> <p>Position data      Latitude and longitude of meteorological station</p> <p>Name .met file      Name of meteorological file</p> <p>Surface_Resistance      Option for calculation of surface resistance at receptor point. Options are '0' (constant) and '1' (variable)</p> <p>Overall, large-scale <i>average</i> surface resistance (<math>s\ m^{-1}</math>); also surface resistance at receptor point if Surface_Resistance is '0'</p>	<p><b>BROWSE SCENARIO SPECIFIC.</b></p> <p><b>BROWSE SCENARIO SPECIFIC</b></p> <p>Set to '1'. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to 79 s/m. <b>BROWSE DEFINITION.</b></p>

<p>Roughness_Length_Data Options for data are '0' (single value) or '1' (Roughness length map)</p>	<p>Set to '0'. <b>DEVELOPMENT DEFINITION.</b></p>
<p>Overall_Roughness_Length If Roughness_Length_Data option set to '0'.</p>	<p>Set to 0.10 m. <b>BROWSE DEFINITION..</b></p>
<p>Name_Roughness_Length_Map Name file_roughness-length_map(.rgh) If Roughness_Length_Data option set to '1'.</p>	<p>Set to RoughnessFileName. Dummy name, because only single value specified. <b>DEVELOPMENT DEFINITION</b></p>
<p><b>RECORD 4 Time period and averaging</b></p>	
<p>Start_Run Starting time of simulation Format: yyyy mm dd hh</p>	<p>Set to '2005 04 15 09'. <b>BROWSE DEFINITION</b></p>
<p>End_Run End time of simulation Format: yyyy mm dd hh</p>	<p>Set to '2009 12 31 23'. <b>BROWSE DEFINITION</b></p>
<p>Type_of_averaging Options are: '0' (Total period), '1' (Year), '2' (Month), '3' (Day), '4' (Hour)</p>	<p>Set to '4' (hourly) Specified (yyyy mm dd hh) for the scenarios. <b>DEVELOPMENT DEFINITION</b></p>
<p><b>RECORD 5 Source configuration</b></p>	
<p>Source_Type Options are '0' (constant) or '1' (variable=hourly)</p>	<p>Set to '1'. <b>BROWSE DEFINITION.</b></p>
<p>Name_Source_File If Source_Type set to '0'. Source configuration file (.src)</p>	<p>Set to 'nh3_3_01'. Dummy file name. <b>DEVELOPMENT DEFINITION.</b></p>
<p>Source_Category If Source_Type set to '0' Category number (nnnn)</p>	<p>Set to '0000'. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p>
<p>Country_Area If Source_Type set to '0' Area number (nnnn)</p>	<p>Set to '0000'. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION</b></p>
<p>Emission_Configuration If Source_Type set to '1' Options are '0' (single source) or '1' (emission file)</p>	<p>Set to '1'. <b>BROWSE DEFINITION.</b></p>
<p>Source_coordinates If emission configuration set to '0'. Source coordinates (x,y).</p>	<p>Set to '0.0 0.0'. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p>
<p>Stack height If emission configuration set to '0' Height in m.</p>	<p>Set to '100'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p>
<p>Emission_File_Name If emission configuration set to '1' Emission file (.ems)</p>	<p>The name consists of the OPS file name (RunID) with extension 'ems' <b>DEVELOPMENT DEFINITION.</b></p>

Field definitions	If special case set to '5'. Options are '1' (file) or '2' (rectangular field)	Set to 2. <b>BROWSE DEFINITION.</b>
x-coordinate field	x-coordinate (m) centre	Set to 2500.0 m. <b>BROWSE DEFINITION</b>
y-coordinate field	y-coordinate (m) centre	Set to 2500.0 m. <b>BROWSE DEFINITION</b>
x-dimension field	field length (m)	Set to 200, 500 or 2000 m. <b>BROWSE SCENARIO SPECIFIC</b>
y-dimension field	field width (m)	Set to 200, 500 or 2000 m. <b>BROWSE SCENARIO SPECIFIC</b>
size source segment	grid cell size (m)	Set to 6.25, 25.0 and 125.0 m
source height	source height	Set to 0.1 m for scenarios for volatilisation from plants and to 0.0 m for scenarios for volatilisation from soils. <b>BROWSE DEFINITION</b>
RECORD 6	Receptor configuration	
Configuration_Type	Options are '0' (Model grid), '1' (Specific receptors) or '2' (predefined)	Set to '2'. 50 points around rectangular field (at centre and 1 distance at 2 heights). <b>BROWSE DEFINITION.</b>
Receptor_Grid_Height	If Configuration_Type set to '0' Receptor height in m.	Set to '0'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Grid_Centre_Coordinates	If Configuration_Type set to '0' Coordinates centre (x,y)	Set to '0.0 0.0'. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Number_Grid_Elements	If Configuration_Type set to '0' Number of elements in x and y direction	Set to '10 10 '. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Grid_Resolution	If Configuration_Type set to '0' Resolution in m.	Set to '100'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Receptor_File_Name	If Configuration_Type set to '1' Name of file (.rcp)	Set to SQ100. Dummy file name with extension .rcp. <b>DEVELOPMENT DEFINITION.</b>
Distance from edge of field	Target distance	Set to 10 m. <b>BROWSE DEFINITION</b>
Receptor heights	Target heights	Set to 0.7 m (children) and 1.4 m (adults ). <b>BROWSE DEFINITION</b>
Local roughness length	Local roughness length (m)	Set to 0.05 m. <b>BROWSE DEFINITION.</b>
RECORD 7	Output options	

Percentile_Output	Options are 'n' (No) or 'y' (Yes)	Set to 'n'. <b>DEVELOPMENT DEFINITION.</b>
Target_percentile	If Percentile_Output set to 'y'. Percentile value (001-100)	Set to '98'. Dummy value. <b>DEVELOPMENT DEFINITION</b>
Background concentration	Option to include background concentrations; options are 'n' (No) or 'y' (Yes)	Set to 'n'. <b>BROWSE DEFINITION</b>
RECORD 8	Deposition options	
Dry_deposition	Option to include dry deposition; options are 'n' (No) or 'y' (Yes).	Set to 'n'. <b>BROWSE DEFINITION.</b>
RECORD 9	Input and output paths	
annual source-emission	Path to emission source (.src) file	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
hourly emission	Path to emission file (.ems)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
meteorological data	Path to meteorological file (.met)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
partical size-distribution	Path to partical size-distribution file (.psd)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
receptor	Path to receptor file (.rcp)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
map roughness length	Path to roughness length map file (.rgh)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
PEARL input	Path to PEARL input file (.prl)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
Pesticide input	Path to compound data input file (.cmp)	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>
Output_Path	Path to output files	<b>Set to '\'. DEVELOPMENT DEFINITION.</b>

### X.CMP file

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>	
RECORD 1	General Settings	
Quit_After_Run	Option for multiple run sessions with bat file	Set to 'y' (Yes). <b>DEVELOPMENT DEFINITION</b>
Detailed_Information_To_Screen	Option for output to screen	Set to 'n' (No). <b>DEVELOPMENT DEFINITION</b>

Run_Name	Name of simulation run	Set to 'RunId'. Input from BROWSE interface <b>DEVELOPMENT DEFINITION</b>
Caseld	Simulation Case	Set to '5', option for coupling with PEARL. <b>DEVELOPMENT DEFINITION</b>
RECORD 2	Select component	
Component	Selection of component; component 5 is 'pesticides'	Set to '5'. <b>DEVELOPMENT DEFINITION</b>
Particle_Size_Distribution:	option for particle size Distribution; option 0 is 'None'	Set to '0'. <b>DEVELOPMENT DEFINITION</b>
Name_Particle_Size_Distribution_File	Name of particle size distribution file	Set to 'User_Defined'. Dummy value if Particle_Size_Distribution set to '0'. <b>DEVELOPMENT DEFINITION</b>
RECORD 3	Area characteristics	
Position data	Latitude and longitude of meteorological station	<b>BROWSE SCENARIO SPECIFIC.</b>
Name .met file	Name of meteorological file	<b>BROWSE SCENARIO SPECIFIC</b>
Surface_Resistance	Option for calculation of surface resistance at receptor point. Options are '0' (constant) and '1' (variable)	Set to '1'. <b>DEVELOPMENT DEFINITION.</b>
Overall, large-scale average surface resistance	Overall, large-scale <i>average</i> surface resistance ( $s\ m^{-1}$ ); also surface resistance at receptor point if Surface_Resistance is '0'	Set to 79 s/m. <b>BROWSE DEFINITION.</b>
Roughness_Length_Data	Options for data are '0' (single value) or '1' (Roughness length map)	Set to '0'. <b>DEVELOPMENT DEFINITION.</b>
Overall_Roughness_Length	If Roughness_Length_Data option set to '0'.	Set to 0.10 m. <b>BROWSE DEFINITION..</b>
Name_Roughness_Length_Map	Name file_roughness-length_map(.rgh) If Roughness_Length_Data option set to '1'.	Set to RoughnessFileName. Dummy name, because only single value specified. <b>DEVELOPMENT DEFINITION</b>
RECORD 4	Time period and averaging	
Start_Run	Starting time of simulation Format: yyyy mm dd hh	Set to '2005 04 15 09'. <b>BROWSE DEFINITION</b>
End_Run	End time of simulation Format: yyyy mm dd hh	Set to '2009 12 31 23'. <b>BROWSE DEFINITION</b>



Type_of_averaging	Options are: '0' (Total period), '1' (Year), '2' (Month), '3' (Day), '4' (Hour)	Set to '4' (hourly) Specified (yyyy mm dd hh) for the scenarios. <b>DEVELOPMENT DEFINITION</b>
RECORD 5	Source configuration	
Source_Type	Options are '0' (constant) or '1' (variable=hourly)	Set to '1'. <b>BROWSE DEFINITION.</b>
Name_Source_File	If Source_Type set to '0'. Source configuration file (.src)	Set to 'nh3_3_01'. Dummy file name. <b>DEVELOPMENT DEFINITION.</b>
Source_Category	If Source_Type set to '0' Category number (nnnn)	Set to '0000'. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Country_Area	If Source_Type set to '0' Area number (nnnn)	Set to '0000'. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION</b>
Emission_Configuration	If Source_Type set to '1' Options are '0' (single source) or '1' (emission file)	Set to '1'. <b>BROWSE DEFINITION.</b>
Source_coordinates	If emission configuration set to '0'. Source coordinates (x,y).	Set to '0.0 0.0'. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Stack height	If emission configuration set to '0' Height in m.	Set to '100'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b>
Emission_File_Name	If emission configuration set to '1' Emission file (.ems)	The name consists of the OPS file name (RunID) with extension 'ems' <b>DEVELOPMENT DEFINITION.</b>
Field definitions	If special case set to '5'. Options are '1' (file) or '2' (rectangular field)	Set to 2. <b>BROWSE DEFINITION.</b>
x-coordinate field center	x-coordinate (m)	Set to 2500.0 m. <b>BROWSE DEFINITION</b>
y-coordinate field center	y-coordinate (m)	Set to 2500.0 m. <b>BROWSE DEFINITION</b>
x-dimension field	field length (m)	Set to 200, 500 or 2000 m. <b>BROWSE SCENARIO SPECIFIC</b>
y-dimension field	field width (m)	Set to 200, 500 or 2000 m. <b>BROWSE SCENARIO SPECIFIC</b>
size source segment	grid cell size (m)	
source height	source height	Set to 6.25, 25.0 and 125.0 m
		Set to 0.1 m for scenarios for volatilisation from plants and to 0.0 m for scenarios for volatilisation

<p>RECORD 6 Receptor configuration</p> <p>Configuration_Type Options are '0' (Model grid), '1' (Specific receptors) or '2' (predefined)</p> <p>Receptor_Grid_Height If Configuration_Type set to '0' Receptor height in m.</p> <p>Grid_Centre_Coordinates If Configuration_Type set to '0' Coordinates centre (x,y)</p> <p>Number_Grid_Elements If Configuration_Type set to '0' Number of elements in x and y direction</p> <p>Grid_Resolution If Configuration_Type set to '0' Resolution in m.</p> <p>Receptor_File_Name If Configuration_Type set to '1' Name of file (.rcp)</p> <p>Distance from edge of field Target distance</p> <p>Receptor heights Target heights</p> <p>Local roughness length Local roughness length (m)</p>	<p>from soils. <b>BROWSE DEFINITION</b></p> <p>Set to '2'. 50 points around rectangular field (at centre and 1 distance at 2 heights). <b>BROWSE DEFINITION.</b></p> <p>Set to '0'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to '0.0 0.0'. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to '10 10 '. Dummy values. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to '100'. Dummy value. Not relevant for BROWSE. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to SQ100. Dummy file name with extension .rcp. <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to 10 m. <b>BROWSE DEFINITION</b></p> <p>Set to 0.7 m (children) and 1.4 m (adults ). <b>BROWSE DEFINITION</b></p> <p>Set to 0.05 m. <b>BROWSE DEFINITION.</b></p>
<p>RECORD 7 Output options</p> <p>Percentile_Output Options are 'n' (No) or 'y' (Yes)</p> <p>Target_percentile If Percentile_Output set to 'y'. Percentile value (001-100)</p> <p>Background concentration Option to include background concentrations; options are 'n' (No) or 'y' (Yes)</p>	<p>Set to 'n.' <b>DEVELOPMENT DEFINITION.</b></p> <p>Set to '98'. Dummy value. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 'n'. <b>BROWSE DEFINITION</b></p>
<p>RECORD 8 Deposition options</p> <p>Dry_deposition Option to include dry deposition; options are 'n' (No) or 'y' (Yes).</p>	<p>Set to 'n.' <b>BROWSE DEFINITION.</b></p>
<p>RECORD 9 Input and output paths</p> <p>annual source-emission Path to emission source (.src) file</p>	

hourly emission	Path to emission file (.ems)	<b>Set to ‘\’. DEVELOPMENT DEFINITION.</b>
meteorological data	Path to meteorological file (.met)	
partical size-distribution	Path to partical size-distribution file (.psd)	<b>Set to ‘\’. DEVELOPMENT DEFINITION. Set to ‘\’. DEVELOPMENT DEFINITION.</b>
receptor	Path to receptor file (.rcp)	
map roughness length	Path to roughness length map file (.rgh)	<b>Set to ‘\’. DEVELOPMENT DEFINITION.</b>
PEARL input	Path to PEARL input file (.prl)	<b>Set to ‘\’. DEVELOPMENT DEFINITION.</b>
Pesticide input	Path to compound data input file (.cmp)	<b>Set to ‘\’. DEVELOPMENT DEFINITION. Set to ‘\’. DEVELOPMENT DEFINITION.</b>
Output_Path	Path to output files	
		<b>Set to ‘\’. DEVELOPMENT DEFINITION.</b>

#### X.CMP file

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>
<i>General</i>	
MolMas_subst1 Substance Molar Mass	In g/mol. <b>USER INPUT</b>
<i>Gas/liquid partitioning</i>	
PreVapRef_subst1 Saturated vapour pressure of substance	In Pa. Measured at temperature TemRefVap. <b>USER INPUT</b>
TemRefVap_subst1 Temperature of reference at which the saturated vapour pressure was measured	In degrees Celsius. <b>USER INPUT</b>
SlbWatRef_subst1 Water solubility of substance	Mass concentration in water at saturation (in mg/L) measured at reference temperature TemRefSlb. <b>USER INPUT</b>
TemRefSlb_subst1 Temperature of reference at which the water solubility was measured	In degrees Celsius. <b>USER INPUT</b>
LogKom_sub1 Log of coefficient of equilibrium sorption of substance on organic matter	Kom in L/kg. <b>USER INPUT</b>
<i>Management events</i>	
Nappscen Number of application scenarios	Dimensionless. <b>BROWSE SCENARIO SPECIFIC</b>

<p>Applications ((from 1 to Nappscen) 01-May-2003-0000 AppCrpLAI 1.00 . . 08-May-2003-0000 AppCrpLAI 1.00</p>	<p>The columns of each line with data for a single application contain: 1) application date (dd-mmm-yyy-hhhh), 2) application option, i.e. application to the crop, and 3) dosage (kg/ha). Dosage: <b>USER INPUT</b>. Other items: <b>BROWSE SCENARIO SPECIFIC</b></p>
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### Y.MET file

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>
<p><b>Meteo file</b>                      <b>File with meteorological data</b></p>	<p>The meteo data for the scenarios have been converted into the format needed for OPS. The file contains 9 columns: 1) <b>Date</b> (format is yyyyymmddhh), 2) <b>global radiation</b> (J/cm<sup>2</sup>), 3) <b>temperature</b> (°C), 3) <b>rainfall</b> (mm), 4) <b>rainfall duration</b> (h), 5) <b>rainfall duration</b>, 6) <b>wind direction</b> at 10 m (degrees), 7) <b>wind speed</b> at 10 m, 8) <b>air humidity</b> (%) at 1.5 m and 9) <b>snow indicator</b> (set at 0: no snow).  <b>BROWSE SCENARIO SPECIFIC</b></p>

### Y.TMP file for scenarios for volatilisation from plants

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>
<p><b>Section 1: Control Section</b> CallingProgram    Release type  CallingProgramVersion    Version of calling program  TimStart            Starting time of simulation TimEnd              End time of simulation  InitYears            Duration of warming-up period.  AmaSysEnd           Stopcondition (kg.ha<sup>-1</sup>)</p>	<p>Set to BROWSEPEARL. <b>DEVELOPMENT DEFINITION</b>  Set to 1. <b>DEVELOPMENT DEFINITION</b>  Specified (dd-mm-yy) for BROWSE scenarios. TimStart set at 15-Apr-2005 and TimEnd set at 01-Oct-2009. <b>BROWSE DEFINITION</b>  Set to 0. <b>DEVELOPMENT DEFINITION</b>  Set to 0. <b>DEVELOPMENT DEFINITION</b></p>

OptSys	System simulation option	OptSys set to PlantOnly for scenarios for volatilisation from plants. Only the plant system is considered. <b>BROWSE DEFINITION</b>
OptHyd	Hydrology simulation option	OptHyd set to Automatic. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
RepeatHydrology	Repeat the same hydrology each year	Set to No. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
OptDelTimPrn	Option to set output interval	Set to 'Hour'. <b>BROWSE DEFINITION</b>
OptScreen	Option to write output to screen	Set to Yes. <b>DEVELOPMENT DEFINITION</b>
OptDelOutput	Option to delete detailed output	Set to No. <b>DEVELOPMENT DEFINITION</b>
PrintCumulatives	Option to output cumulative data	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptMacropore	Option to consider preferential flow	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptPersistency	Option to assess persistency in soil	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptPaddy	Option to assess paddy rice	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptAux	Option to produce output for specific models	Set to OPS. Data on source strength of volatilisation from crop output to file in OPS format. <b>DEVELOPMENT DEFINITION.</b>
<b>Section 2: Soil Section</b>		
SoilTypeID	Identification of soil type	Set to dummy name. Not relevant for OptSys is 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
Location		Set to dummy name. Not relevant for OptSys is 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
<b>Section 3: Meteo Section</b>		
MeteoStation	Name of MeteoStation	Set to 'RunId'. Input from BROWSE interface <b>DEVELOPMENT DEFINITION</b>
OptMetInp	Option for daily or hourly meteorology	Set to 'Hourly'. <b>BROWSE DEFINITION.</b>
OptTraRes	Option to select the method to calculate the resistance to volatilisation	Set to 'Laminar'. <b>BROWSE DEFINITION</b>
OptResBou	Option to select the method to calculate the boundary layer resistance	Set to 'Hicks'. Not used in BROWSE. <b>BROWSE DEFINITION.</b>
OptEvp	Option to select the type of data used by the model.	OptEvp set to PenmanMonteith. Not relevant for OptSys 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>

Lat	Latitude of the meteo station	Maximum is 60°. <b>BROWSE SCENARIO SPECIFIC.</b>
Alt	Altitude of the meteo station (m)	<b>BROWSE SCENARIO SPECIFIC.</b>
TemLboSta [-	Initial lower boundary soil temperature 20 40]	Set to 10.0 Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION.</b>
ZMeaWnd	Height of wind speed measurement (m)	Set to 10.0. <b>DEVELOPMENT DEFINITION.</b>
ZMeaTem	Height of temperature measurement (m)	Set to 2.0. <b>DEVELOPMENT DEFINITION.</b>
FacPrc	Correction factor for precipitation	Set to 1.0. <b>DEVELOPMENT DEFINITION.</b>
DifTem	Correction for temperature	Set to 0.0. <b>DEVELOPMENT DEFINITION.</b>
FacEvp	Correction factor for evapotranspiration	Set to 1.0. <b>DEVELOPMENT DEFINITION.</b>
OptIrr with	Option to choose between a scenario and a scenario without irrigation	OptIrr set to 'No'. Not relevant if OptSys 'PlantOnly'. <b>DEVELOPMENT DEFINITION.</b>
IrrigationScheme	Identification of the irrigation scheme	Set to 'No'. Not relevant if OptSys 'PlantOnly'. <b>DEVELOPMENT DEFINITION.</b>
Section 4: Drainage/infiltration section		
OptDra	Option to consider drainage	Set to 'No'. Drainage not considered in BROWSE. <b>BROWSE DEFINITION</b>
Section 5: Substance section		
Table compounds Sub1 End_table	List of substances.	First substance is parent, the others are metabolites. <b>USER INPUT.</b>
Table FraPrtDau (mol.mol-1) end_table		Transformation table (parent-daughter relationships). Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION..</b>
OptCntLiqTraRef_sub1	Option to use the moisture content during the incubation study (CntLiqTraRef)	Set to 'OptimumConditions'. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
DT50Ref_sub1	Half-Life of transformation in soil	Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
TemRefTra_sub1	Temperature of reference at which the half-life of transformation was measured	In Celsius. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
ExpLiqTra_sub1	Coefficient describing the relation between the transformation rate of the substance and the volume fraction of liquid	Dimensionless. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>

<p>CntLiqTraRef_sub1 Reference content of liquid in transformation study from which DT50 was derived</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>MolEntTra_sub1 Molar activation enthalpy of transformation</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>Table horizon FacZTra Hor_sub1 Factor for the influence of depth on transformation rate of the substance in soil as a function of soil layer [0 1]</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>OptCofFre Option to choose between pH-dependent or pH-independent sorption</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>ConLiqRef_sub1 Reference liquid content for the sorption coefficient</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>ExpFre_sub1 Freundlich exponent</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>KomEqL_sub1 Coefficient of equilibrium sorption of substance on organic matter</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>KomEqLMax_sub1 Coefficient of maximum equilibrium sorption of substance on organic matter</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>MolEntSor_sub1 Molar enthalpy of sorption on organic matter in soil</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>TemRefSor_sub1 Temperature of reference at which the sorption coefficient was measured</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p><i>Gas/liquid partitioning</i></p>	
<p>MolEntSlb_sub1 Molar enthalpy of the dissolution</p>	<p>Set to 27 kJ/mol. Describing the relation between the water solubility of the substance and temperature. <b>BROWSE DEFINITION</b></p>
<p>MolEntVap_sub1 Molar enthalpy of the vaporization process</p>	<p>Set to 95 kJ/mol. Describing the relation between the saturated vapour pressure of the substance and temperature. <b>BROWSE DEFINITION.</b></p>
<p><i>Non-equilibrium sorption</i></p>	
<p>CofDesRat_sub1 Rate of desorption</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p>FacSorNeqEqL_sub1 Factor relating coefficient for equilibrium and non-equilibrium sorption</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
<p><i>Uptake</i></p>	
<p>FacUpt_sub1 Coefficient for uptake by plant roots</p>	<p>Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>

<p><b>Volatilization</b></p> <p>ThiAirBouLay      Thickness of the stagnant air layer at the soil surface</p> <p><i>Canopy processes</i></p> <p>OptDspCrp_sub1    Option for the description of the loss routes of substance from the crop surface</p> <p>DT50DspCrp_sub1    Half-life for the disappearance of the substance on the crop</p> <p>DT50TraCrp_sub1    Half-life for the photo-transformation of the substance on the crop</p> <p>DT50PenCrp_sub1    Half-life for the penetration of the substance in the plant tissue</p> <p>FacWasCrp_sub1    Factor for the wash-off of substance from the crop by rainfall or irrigation.</p> <p>RadGloRef          Reference global radiation for the factor for the effect of radiation on the pesticide on the plant</p> <p>FacTraDepRex      Factor for the effect of restricted exposure of deposit on transformation (-)</p> <p>FacVolDepRex      Factor for the effect of restricted exposure of deposit on volatilisation (-)</p> <p>FacPenDepRex      Factor for the effect of restricted Exposure of deposit on penetration (-)</p> <p>FacWasDepRex      Factor for the effect of restricted exposure of deposit on wash-off (-)</p> <p>FraDepRex          Fraction of applied mass to be put in deposit with reduced exposure (-)</p> <p>OptAmaCrpReset    Option to reset mass remaining on Plant surface to zero at next application</p> <p><i>Diffusion of solute in liquid and gas phases</i></p> <p>TemRefDif_sub1    Temperature of reference at which diffusion coefficients were measured</p> <p>CofDifWatRef_sub1    Coefficient of diffusion of the substance in water</p>	<p>Set to 0.006 m. <b>BROWSE DEFINITION..</b></p> <p>Option set to 'Calculated'. <b>BROWSE DEFINITION.</b></p> <p>Not relevant (dummy) if OptDspCrp set to 'Calculated'. <b>DEVELOPMENT DEFINITION.</b></p> <p>In days. <b>USER INPUT.</b></p> <p>In days. <b>USER INPUT.</b></p> <p>Set to 50.0 m<sup>-1</sup>. <b>BROWSE DEFINITION.</b></p> <p>Set to 500 W/m<sup>2</sup>. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. If set to 0.0 then no deposit with reduced exposure. <b>BROWSE DEFINITION.</b></p> <p>Set to 'Yes' for acute exposure assessment and to 'No' for chronic exposure assessment <b>BROWSE SCENARIO SPECIFIC</b></p> <p>Set to 20° C. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 4.3E-5 m<sup>2</sup>/d. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p>
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CofDifAirRef_sub1	Coefficient of diffusion of the substance in air	Set to 0.43 m <sup>2</sup> /d. <b>BROWSE DEFINITION.</b>
<b>Section 6: Management section</b>		
Application-Scheme	Name of application scheme.	Dummy name. <b>DEVELOPMENT DEFINITION</b>
ZTgt	Evaluation target depth (m)	Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
DelTimEvt	Time difference in years between two subsequent events	Not relevant (dummy) for BROWSE. <b>DEVELOPMENT DEFINITION</b>
<i>Management events</i>		The first two columns of the Applications table contain: 1) The application dates and 2) The application option. In the BROWSE scenarios the application option is set to AppCrpLAI. The third column contains the dosage (kg/ha).
table Applications dd-mmm-yyyy-hhhh end_table	AppCrpLAI 0.69	
table TillageDates end_table	Date and depth of tillage for each tillage event.	No ploughing is considered, so no dates are entered. <b>BROWSE DEFINITION.</b>
<i>Initial conditions</i>		Set to 0 mg.kg <sup>-1</sup> . Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
Table interpolate CntSysEq z B 0.00 0.00 50.0 0.00 end_table	Concentration in equilibrium domain	
Table interpolate CntSysNeq B 0.00 0.00 50.0 0.00 end_table	Concentration in non-equilibrium domain	Set to 0 mg.kg <sup>-1</sup> . Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
<i>Upper boundary flux</i>		No dates are entered, so the flux is zero throughout the simulation period. <b>BROWSE DEFINITION.</b>
table FlmDep end_table	Date and flux of deposition (kg.ha <sup>-1</sup> .da <sup>-1</sup> )	
<b>Section 7: Crop section</b>		
RepeatCrops	Option to repeat the growth of the same crop each year	Set to 'Yes'. <b>BROWSE DEFINITION.</b>
Table Crops 20-May 30-Oct	Crop calendar table CropName	Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>

end_table		.
OptLenCrp	Option to select the type of plant growth model	Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
Table CrpPar_cropname end_table	Table with crop parameters	Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
FraCovCrpInp	Fraction of soil covered with crop.	Set to 1.0. Dimensionless. Used if OptSys is set to 'PlantOnly'. <b>BROWSE DEFINITION.</b>
HgtCrpInp	Height of crop	Set at 0.1 m. Specifies height of crop. Used if OptSys is set to 'PlantOnly'. <b>BROWSE DEFINITION.</b>
<b>Section 8: Output Control</b>		
OutputDepths	Option to specify the depths for which output is requested	Set to None. <b>DEVELOPMENT DEFINITION.</b>
OptDelOutFiles		Set to No. <b>DEVELOPMENT DEFINITION.</b>
SoilReport		Set to No. Not relevant if OptSys is set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b>
LeachingReport		Set to No. Not relevant if OptSys is set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION.</b>
AirReport		Set to Yes. <b>DEVELOPMENT DEFINITION.</b>
DrainageReport		Set to No. Not relevant if OptSys is set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION.</b>
table OutputDepths (m) end_table		Not relevant if OptSys is set to 'PlantOnly'.
DateFormat		Set to DaysFromSta. <b>DEVELOPMENT DEFINITION.</b>
RealFormat		Set to G12.4. <b>DEVELOPMENT DEFINITION.</b>

**Y.TMP file for scenarios for volatilisation from soils**

<u>Parameter and description</u>	<u>Value, source &amp; comments</u>
<b>Section 1: Control Section</b>	
CallingProgram    Release type	Set to BROWSEPEARL. <b>DEVELOPMENT DEFINITION</b>
CallingProgramVersion    Version of calling program	Set to 1. <b>DEVELOPMENT DEFINITION</b>
TimStart            Starting time of simulation	Specified (dd-mm-yy) for BROWSE scenarios. TimStart set at 1-Jan-2005 and TimEnd set at 31-Dec-2009. <b>BROWSE DEFINITION</b>
TimEnd              End time of simulation	
InitYears            Duration of warming-up period.	Set to 0. <b>DEVELOPMENT DEFINITION</b>
AmaSysEnd          Stopcondition (kg.ha <sup>-1</sup> )	Set to 0. <b>DEVELOPMENT DEFINITION</b>
OptSys              System simulation option	OptSys set to 'All' for scenarios for volatilisation from soil. <b>BROWSE DEFINITION</b>
OptHyd              Hydrology simulation option	OptHyd set to 'Standard'. <b>DEVELOPMENT DEFINITION</b>
RepeatHydrology    Repeat the same hydrology each year	Set to No. Not relevant (dummy) for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
OptDelTimPrn      Option to set output interval	Set to 'Hour'. <b>BROWSE DEFINITION</b>
OptScreen          Option to write output to screen	Set to 'Yes'. <b>DEVELOPMENT DEFINITION</b>
OptDelOutput      Option to delete detailed output	Set to No. <b>DEVELOPMENT DEFINITION</b>
PrintCumulatives    Option to output cumulative data	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptAux              Option to produce output for specific models	Set to OPS. Data on source strength of volatilisation from crop output to file in OPS format. <b>DEVELOPMENT DEFINITION.</b>
OptMacropore      Option to consider preferential flow	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptPersistency    Option to assess persistency in soil	Set to No. <b>DEVELOPMENT DEFINITION</b>
OptPaddy            Option to assess paddy rice	Set to No. <b>DEVELOPMENT DEFINITION</b>
ThetaTol            Maximum difference in water content between iterations	Set at the default value of 0.001 (m <sup>3</sup> .m <sup>-3</sup> ). <b>DEVELOPMENT DEFINITION</b>
DelTimSwaMin      Minimum time step	The values for the minimum and maximum time steps for the discretization of the Richards' equation are

DelTimSwaMax	Maximum time step	taken to be 1.0 E-7 d and 0.2 d, respectively. <b>DEVELOPMENT DEFINITION</b>
		Set to 1 m. <b>DEVELOPMENT DEFINITION</b>
GWLTol	Tolerance for groundwater level	Set to 30. <b>DEVELOPMENT DEFINITION</b>
MaxItSwa	Maximum number of iterations in SWAP	Set to 'No'. <b>DEVELOPMENT DEFINITION</b>
OptHysteresis	Option to include hysteresis	Set to 0.2. Treated as a dummy. <b>DEVELOPMENT DEFINITION</b>
PreHeaWetDryMin	Minimum pressure head to switch drying/wetting	Set to 'Constant'. <b>DEVELOPMENT DEFINITION</b>
	Option for ponding water	Set to 'No'. <b>DEVELOPMENT DEFINITION.</b>
OptSnow	Option for snow	Set to 'No'. Switch on or switch off vertical resistance. <b>DEVELOPMENT DEFINITION.</b>
OptNoResVert	Switch on or switch off vertical resistance	Set to 'No'. Switch on or switch off option for discharge layer. <b>DEVELOPMENT DEFINITION.</b>
OptDisLay	Option selected for discharge layer	Set to ScenarioID. <b>BROWSE SCENARIO SPECIFIC.</b>
SWAP_ID	ID for SWAP *.pfo output file	
Section 2: Soil Section		
SoilTypeID	Identification of soil type	Name of the soil type. <b>BROWSE SCENARIO SPECIFIC.</b>
Location		The name of the BROWSE location <b>BROWSE SCENARIO SPECIFIC.</b>
Table horizon SoilProperties	Table specifying the soil composition for each horizon	Specify for each horizon: 1) The horizon number [1 10] <b>BROWSE SCENARIO SPECIFIC</b> , 2) Depth of the lower boundary (m) <b>BROWSE SCENARIO SPECIFIC</b> , 3) The number of soil compartments [1 500] <b>DEVELOPMENT DEFINITION.</b> The nodes are distributed evenly over each horizon.
Table horizon VanGenuchtenPar	Table specifying the VanGenuchten parameters for each horizon	Specify for each soil horizon: 1) the mass content of sand, expressed as a fraction of the mineral soil ( $\text{kg.kg}^{-1}$ ) [0 1], 2) the mass content of silt, expressed as a fraction of the mineral soil ( $\text{kg.kg}^{-1}$ ) [0 1], 3) the mass content of clay, expressed as a fraction of the mineral soil ( $\text{kg.kg}^{-1}$ ) [0 1], 4) the organic matter mass content ( $\text{kg.kg}^{-1}$ ) [0 1], and 5) the pH-KCl [1,13]. The format [x,y] is used to specify the acceptable range (i.e. from x to y) of an input parameter. <b>BROWSE SCENARIO SPECIFIC.</b>
OptRho	Option for input of bulk density data	OptRho set to 'Calculate'. Rho ( $\text{kg.m}^{-3}$ ) specified for each horizon. <b>DEVELOPMENT DEFINITION.</b>
ZPndMax	Maximum thickness of ponding water	The default value for the maximum thickness of ponding water layer is used, i.e. 2 mm. When the

	layer Ponding depth	computed thickness of the ponding water layer exceeds 2 mm, the excess of water will be removed as run-off. <b>DEVELOPMENT DEFINITION.</b>
OptSolEvp	Option to select evaporation reduction method	Set to 'Boesten'. <b>BROWSE DEFINITION.</b>
FacEvpSol	Coefficient for evaporation from bare soil	Set to 1.0. <b>BROWSE DEFINITION.</b>
CofRedEvp	Soil evaporation coefficient	The coefficient is set at 0.79 cm <sup>1/2</sup> . <b>DEVELOPMENT DEFINITION.</b>
PrcMinEvp	Minimum rainfall to reset reduction	Set to 0.01 m d <sup>-1</sup> . <b>DEVELOPMENT DEFINITION.</b>
Table horizon LenDisLiq	Dispersion length of solute in liquid phase [at least 0.5 times the compartment thickness]	Set to 2.5 cm for all layers. <b>DEVELOPMENT DEFINITION</b>
OptCofDifRel	Option for Tortuosity	The option of the relation of Millington & Quirk (1960) is selected. OptCofDifRel set to MillingtonQuirk. <b>DEVELOPMENT DEFINITION</b>
ExpDifLiqMilNom	Exponent in nominator of relation of Millington & Quirk for diffusion in the liquid phase.	Set to 2 (-). <b>DEVELOPMENT DEFINITION</b>
ExpDifLiqMilDen	Exponent in denominator of relation of Millington & Quirk for diffusion in the liquid phase.	Set to 0.6667 (-). <b>DEVELOPMENT DEFINITION</b>
ExpDifGasMilNom	Exponent in nominator of relation of Millington & Quirk for diffusion in the gas phase.	Set to 2 (-). <b>DEVELOPMENT DEFINITION</b>
ExpDifGasMilDen	Exponent in denominator of relation of Millington & Quirk for diffusion in the gas phase.	Set to 0.6667 (-). <b>DEVELOPMENT DEFINITION</b>
	Option for ponding water	Set to constant. <b>DEVELOPMENT DEFINITION</b>
<b>Section 3: Meteo Section</b>		
MeteoStation	Name of MeteoStation	Set to 'Runld'. Input from BROWSE interface <b>BROWSE SCENARIO SPECIFIC.</b>
OptMetInp	Option for daily or hourly meteorology	Set to 'Hourly'. <b>BROWSE DEFINITION.</b>
OptTraRes	Option to select the method to calculate the resistance to volatilisation	Set to 'Laminar'. <b>BROWSE DEFINITION</b>
OptResBou	Option to select the method to calculate the boundary layer resistance	Set to 'Hicks'. Not used in BROWSE. <b>BROWSE DEFINITION.</b>

OptEvp	Option to select the type of data used by the model.	OptEvp set to PenmanMonteith. <b>DEVELOPMENT DEFINITION</b>
Lat	Latitude of the meteo station	Maximum is 60°. <b>BROWSE SCENARIO SPECIFIC.</b>
Alt	Altitude of the meteo station (m)	<b>BROWSE SCENARIO SPECIFIC.</b>
TemLboSta [-	Initial lower boundary soil temperature 20 40]	<b>BROWSE SCENARIO SPECIFIC.</b>
FacPrc	Correction factor for precipitation	Set to 1.0. <b>DEVELOPMENT DEFINITION.</b>
DifTem	Correction for temperature	Set to 0.0. <b>DEVELOPMENT DEFINITION.</b>
FacEvp	Correction factor for evapotranspiration	Set to 1.0. <b>DEVELOPMENT DEFINITION.</b>
OptIrr	Option to choose between a scenario with and a scenario without irrigation	OptIrr set to 'No'. <b>DEVELOPMENT DEFINITION.</b>
IrrigationScheme	Identification of the irrigation scheme	Set to 'No'. <b>DEVELOPMENT DEFINITION.</b>
Section 4: Drainage/infiltration section		Set to 'No'. Drainage not considered in BROWSE. <b>BROWSE DEFINITION</b>
OptDra	Option to consider drainage	
Section 5: Substance section		
Table compounds Sub1 End_table	List of substances.	First substance is parent, the others are metabolites. <b>USER INPUT.</b>
Table FraPrtDau (mol.mol-1) end_table		Transformation table (parent-daughter relationships). No metabolites considered. <b>DEVELOPMENT DEFINITION..</b>
OptCntLiqTraRef_sub1	Option to use the moisture content during the incubation study (CntLiqTraRef)	Set to 'OptimumConditions'. <b>DEVELOPMENT DEFINITION</b>
DT50Ref_sub1	Half-life of transformation in soil	In days. <b>USER INPUT.</b>
TemRefTra_sub1	Temperature of reference at which the half-life of transformation was measured	In Celsius. <b>USER INPUT.</b>
ExpLiqTra_sub1	Coefficient describing the relation between the transformation rate of the substance and the volume fraction of liquid	Set to 0.7 (-). <b>DEVELOPMENT DEFINITION</b>
CntLiqTraRef_sub1	Reference content of liquid in transformation study from which DT50 was derived	Set to 1. <b>DEVELOPMENT DEFINITION</b>

MolEntTra_sub1	Molar activation enthalpy of transformation	Set to 65.4 kJ mol <sup>-1</sup> . <b>DEVELOPMENT DEFINITION</b>
Table horizon FacZTra Hor sub1	Factor for the influence of depth on transformation rate of the substance in soil as a function of soil layer [0 1]	Set to 1. <b>DEVELOPMENT DEFINITION</b>
OptCofFre	Option to choose between pH-dependent or pH-independent sorption	Set to 'pH-independent'. <b>DEVELOPMENT DEFINITION</b>
ConLiqRef_sub1	Reference liquid content for the sorption coefficient	Set to 1 mg L <sup>-1</sup> . <b>DEVELOPMENT DEFINITION</b>
ExpFre_sub1	Freundlich exponent	Set to 0.9. <b>DEVELOPMENT DEFINITION</b>
KomEqL_sub1	Coefficient of equilibrium sorption of substance on organic matter	<b>USER INPUT.</b>
KomEqLMax_sub1	Coefficient of maximum equilibrium sorption of substance on organic matter	Set to value of KomEqL. <b>DEVELOPMENT DEFINITION</b>
MolEntSor_sub1	Molar enthalpy of sorption on organic matter in soil	Set to 0. <b>DEVELOPMENT DEFINITION</b>
TemRefSor_sub1	Temperature of reference at which the sorption coefficient was measured	Set to 20 °C. <b>DEVELOPMENT DEFINITION</b>
<i>Gas/liquid partitioning</i>		Set to 27 kJ/mol. Describing the relation between the water solubility of the substance and temperature. <b>BROWSE DEFINITION</b>
MolEntSlb_sub1	Molar enthalpy of the dissolution	Set to 95 kJ/mol. Describing the relation between the saturated vapour pressure of the substance and temperature. <b>BROWSE DEFINITION.</b>
MolEntVap_sub1	Molar enthalpy of the vaporization process	Set to 0. Not considered (dummy value). <b>DEVELOPMENT DEFINITION</b>
<i>Non-equilibrium sorption</i>		Set to 0. Not considered (dummy value). <b>DEVELOPMENT DEFINITION</b>
CofDesRat_sub1	Rate of desorption	Set to 0. Not considered (dummy value). <b>DEVELOPMENT DEFINITION</b>
FacSorNeqEqL_sub1	Factor relating coefficient for equilibrium and non-equilibrium sorption	Set to 0.5. <b>DEVELOPMENT DEFINITION</b>
<i>Uptake</i>		Set to 0.006 m. <b>BROWSE DEFINITION..</b>
FacUpt_sub1	Coefficient for uptake by plant roots	
<b>Volatilization</b>		

<p>ThiAirBouLay            Thickness of the stagnant air layer at the soil surface</p> <p><i>Canopy processes</i> OptDspCrp_sub1 Option for the description of the loss routes of substance from the crop surface</p> <p>DT50DspCrp_sub1    Half-life for the disappearance of the substance on the crop</p> <p>DT50TraCrp_sub1    Half-life for the photo-transformation of the substance on the crop</p> <p>DT50PenCrp_sub1    Half-life for the penetration of the substance in the plant tissue</p> <p>FacWasCrp_sub1    Factor for the wash-off of substance from the crop by rainfall or irrigation.</p> <p>RadGloRef            Reference global radiation for the factor for the effect of radiation on the pesticide on the plant</p> <p>FacTraDepRex        Factor for the effect of restricted exposure of deposit on transformation (-)</p> <p>FacVolDepRex        Factor for the effect of restricted exposure of deposit on volatilisation (-)</p> <p>FacPenDepRex        Factor for the effect of restricted Exposure of deposit on penetration (-)</p> <p>FacWasDepRex        Factor for the effect of restricted exposure of deposit on wash-off (-)</p> <p>FraDepRex            Fraction of applied mass to be put in deposit with reduced exposure (-)</p> <p>OptAmaCrpReset    Option to reset mass remaining on Plant surface to zero at next application</p> <p><i>Diffusion of solute in liquid and gas phases</i> TemRefDif_sub1    Temperature of reference at which diffusion coefficients were measured</p> <p>CofDifWatRef_sub1    Coefficient of diffusion of the substance in water</p> <p>CofDifAirRef_sub1    Coefficient of diffusion of the substance in air</p>	<p>Option set to 'Calculated'. <b>BROWSE DEFINITION.</b></p> <p>Not relevant (dummy) if OptDspCrp set to 'Calculated'. <b>DEVELOPMENT DEFINITION.</b></p> <p>In days. <b>USER INPUT.</b></p> <p>In days. <b>USER INPUT.</b></p> <p>Set to 50.0 m<sup>-1</sup>. <b>BROWSE DEFINITION.</b></p> <p>Set to 500 W/m<sup>2</sup>. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. Not relevant if FraDepRex set to 0.0. <b>BROWSE DEFINITION.</b></p> <p>Set to 0.0. If set to 0.0 then no deposit with reduced exposure. <b>BROWSE DEFINITION.</b></p> <p>Set to 'Yes' for acute exposure assessment and to 'No' for chronic exposure assessment <b>BROWSE SCENARIO SPECIFIC</b></p> <p>Set to 20° C. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 4.3E-5 m<sup>2</sup>/d. Not relevant (dummy) if OptSys set to 'PlantOnly'. <b>DEVELOPMENT DEFINITION</b></p> <p>Set to 0.43 m<sup>2</sup>/d. <b>BROWSE DEFINITION.</b></p>
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Section 6: Management section		
Application-Scheme	Name of application scheme.	Dummy name. <b>DEVELOPMENT DEFINITION</b>
ZTgt	Evaluation target depth (m)	Not relevant (dummy value) for BROWSE vapour exposure scenarios. Set to 1.0 m. <b>DEVELOPMENT DEFINITION</b>
DelTimEvt	Time difference in years between two subsequent events	Set to 'No repeat'. <b>DEVELOPMENT DEFINITION</b>
<i>Management events</i>		
table Applications dd-mmm-yyyy-hhhh end_table	AppSolSur 0.500	The first two columns of the Applications table contain: 1) The application dates and 2) The application option. In the BROWSE scenarios the application option is set to AppSolSur, i.e. application to the soil surface. The third column contains the dosage (kg/ha).
table TillageDates end_table	Date and depth of tillage for each tillage event.	No ploughing is considered, so no dates are entered. <b>BROWSE DEFINITION.</b>
<i>Initial conditions</i>		
Table interpolate z B 0.00 0.00 50.0 0.00 end_table	Concentration in equilibrium domain	Set to 0 mg.kg <sup>-1</sup> . Not relevant (dummy) for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
Table interpolate B 0.00 0.00 50.0 0.00 end_table	Concentration in non-equilibrium domain	Set to 0 mg.kg <sup>-1</sup> . Not relevant (dummy) for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
<i>Upper boundary flux</i>		
table FlmDep end_table	Date and flux of deposition (kg.ha <sup>-1</sup> .da <sup>-1</sup> )	No dates are entered, so the flux is zero throughout the simulation period. <b>BROWSE DEFINITION.</b>
Section 7: Crop section		
CropCalendar	Id of Cropcalendar	Set to 'No'. <b>BROWSE DEFINITION.</b>
RepeatCrops	Option to repeat the growth of the same crop each year	Set to 'Yes'. Not relevant (dummy) for vapour exposure scenarios for volatilisation from bare soil. <b>DEVELOPMENT DEFINITION</b>
Table Crops	Crop calendar table	

end_table		No crops listed in table. Not relevant for vapour exposure scenarios for volatilisation from bare soil. <b>DEVELOPMENT DEFINITION</b>
OptLenCrp	Option to select the type of plant growth model	Set to 'Fixed'. Not relevant (dummy) for vapour exposure scenarios for volatilisation from bare soil. <b>DEVELOPMENT DEFINITION</b>
Section 8: Output Control		
OptDelOutFiles		Set to 'Yes'. <b>DEVELOPMENT DEFINITION.</b>
SoilReport		Set to 'No'. Not relevant for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
LeachingReport		Set to 'No'. Not relevant for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
AirReport		Set to 'No'. Not relevant for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
DrainageReport		Set to 'No'. Not relevant for BROWSE vapour exposure scenarios. <b>DEVELOPMENT DEFINITION</b>
table OutputDepths (m)		Empty table. Not relevant for BROWSE vapour exposure scenarios for volatilisation from bare soil
end_table		
DateFormat		Set to DaysFromSta. <b>DEVELOPMENT DEFINITION.</b>
RealFormat		Set to G12.4. <b>DEVELOPMENT DEFINITION.</b>