**Point Source Calculator**

**User Guidance**

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Purpose: Point Source Calculator for calculating chemical concentrations due to direct chemical inputs to the water body.

**Menu Items**

File manipulations are performed on the menu bar. The first menu item is ***File***, with submenus ***Retrieve All*** and ***Save All***. *Retrieve All* will open a file browser and allow a user to upload a previously created input file into the interface. The input files are text files that can be created either with the PSC interface or with a text editor. The *Save All* command will open a file browser and allow the user to save the inputs from the PSC interface into a text file.

The naming of output files is determined by the name of the file saved or retrieved. The name and directory of the output files are always presented at the bottom of the GUI.

Users must use either Retrieve All or Save All before running a simulation. If not, an error message will appear instructing the user to do so. This is necessary because the use of Save or Retrieve establishes the location where output files will be created.

**Chemical Tab**

The chemical properties tab allows users to enter of chemical properties. The definitions are summarized here:

**Chemical Properties Section**

***Chemical ID*** can be used to name the chemical that is being studied. The content of this box is not used in the program nor is it used for file naming.

***Sorption Coefficient*** either as Koc or Kd both in ml/g. Kd is the linear sorption coefficient, and Koc is the organic-carbon-normalized sorption coefficient (mL/g). Sorption coefficients are the same in all compartments.

***Water Column Half Life*** is the half-life (days) of a chemical in the water column. This parameter acts on all phases of the chemical in the water column (unlike hydrolysis or photolysis inputs). If there is no degradation, leave this parameter blank.

***Temperature Associated with the Water Column Value*** is the temperature (°C) at which the water column degradation study was conducted. During a simulation, the degradation rate is adjusted by temperature, with this temperature input being the reference.

***Photolysis Halflife*** is the near-surface aquatic half-life (days) of the chemical due to photolysis. If there is no degradation, leave this parameter blank.

***Photolysis Reference Latitude*** is the latitude that the photolysis value is intended to simulate.

Hydrolysis Halflife is the half-life (days) of the chemical due to hydrolysis at whatever pH is to be simulated. A half-life of zero is interpreted to mean that the compound does not degrade by this process.

***Benthic Halflife*** is the half-life (days) of the chemical in the benthic compartment. This parameter acts on all phases of the pesticide in the benthic compartment. If there is no degradation, leave this parameter blank.

***Temperature Associated with the Benthic Compartment Value*** is the temperature (°C) at which the benthic metabolism study was conducted.

**Volatilization Section**

***No Volatilization*** – Checking this option will exclude volatilization

***Estimate Henry’s Constant*** – Checking this option will cause the program to calculate Henry’s Constant from molecular weight, vapor pressure, and solubility.

***Use Henry’s Constant*** – Checking this option will cause the program to use the input value for the Henry's Law constant.

***Molecular Weight*** is the molecular weight of the chemical. This parameter only affects the volatilization rate.

***Vapor Pressure*** is the vapor pressure (torr) of the compound at a representative temperature to be simulated. This parameter only affects the volatilization rate and only if "Estimate Henry's Constant" is selected.

***Solubility*** is the solubility (mg/L) of the pesticide at a representative temperature to be simulated. Solubility is used only in the volatilization routine; it does not cap concentrations in this program. This parameter only affects the volatilization rate.

***Heat of Henry*** is the enthalpy of phase change from aqueous solution to air solution (Joules/mole). This enthalpy can be approximated from the enthalpy of vaporization (Schwarzenbach et al., 1993), which can be obtained from EPISuite among other sources. Enthalpy for pesticides obtained in a literature review ranged from 20,000 to 100,000 J/mol (average 59,000 J/mol). Some example enthalpies for pesticides are

Metalochlor 84,000 Feigenbrugel et al. 2004

Diazonon 98,000 Feigenbrugel et al. 2004

Alachlor 76,000 Gautier et al., 2003

Dichlorvos 95,000 Gautier et al., 2003

Mirex 91,000 Yin and Hassett, 1986

Lindane 43,000 Staudinger et al. (2000)

EPTC 37,000 Staudinger et al. (2000)

Molinate 58,000 Staudinger et al. (2000)

Chlorpyrifos 17,000 Staudinger et al. (2000)

Enthalpies can also be estimated by the US EPA EPI Suite software. Open the software, then select the HENRYWIN subprogram on the left of the EPI Suite screen. On the top menu of the HENRYWIN window item, select the ShowOptions, then select Show Temperature Variation with Results. Enter the chemical name of interest and then push the Calculate button. EPI Suite will give the temperature variation results in the form of an equation: HLC (atm-m3/mole) = exp(A-(B/T)) {T in K}. The enthalpy of solvation in Joules/mol is equal to 8.314\*B. Example enthalpies from EPI Suite are:

Pendamethalin 62,000 J/mol

Carbaryl 58,000 J/mol

Carbofuran 54,000 J/mol

Molinate 54,000 J/mol

Endosulfan 37,000 J/mol

***Reference Temperature for Henry’s constant*** is the temperature at which the vapor pressure, solubility, Henry’s Law constant apply or were measured at (°C).

***Henry’s Constant*** (atm m3/mol): Allows Henry’ Law constant to be entered directly when it is available. If Henry’s Constant is not available it can be calculated automatically by checking the appropriate radio button.

**Mass Release Schedule**

There are 3 ways to input mass into the system: by specifying a repeating schedule, by reading an input time series file that specifies the daily mass, or by reading a PRZM5 standard output file.

***Specify Mass***

Choosing this option allows the user to specify a repeating schedule that runs through the entire simulation. Up to three mass input schedules can be superimposed upon each other.

***Offset*** – the number of days after the start of the simulation before the mass input pattern begins

***Days On*** – the number of consecutive days that mass is input into the system for this schedule

***Days Off*** – the number of consecutive days that mass is not input into the system for this schedule

***Mass (kg/day)*** – the mass input into the system during the Days On of this schedule

***Use a Time Series File***

Choosing this option allows the program to read a file that contains daily values for water flow and mass. The structure is one day of data per line with the data separated by whitespace (blanks or tabs with the amount of whitespace being inconsequential). The first three columns are dummies (program does not use them) but a user may wish to reserve these for day, month, year for their own records. The next two columns are water flow (m3) and chemical mass (kg) that occur for that day. A typical file may look like the following:

dummy dummy dummy water (m3) mass (kg)

1 1 2014 123.9 1.7

1 2 2014 144 1.8

A s Q 119.90 1.9e4

OneApril 14 1.23e2 0.01

The length of the file does not have to correspond to the weather file. But the program will assume that the first day of the time series will correspond to the first day of the weather file, and it will assume that the values are in chronological order and that there is no missing days or data.

***Use PRZM5 Output File***

Choosing this option allow the program to read a standard PRZM5 ZTS file which specifies the daily mass as well as water flow into the system. The required file has the same structure as a PRZM5 ZTS file (Young and Fry, 2014). All data are delimited by whitespace and each line represents one day of data. Data must be in chronological order and must include every day of the simulation. In the zts file, the order of the data on a line is as follows:

year, month, day, daily flow (cm), daily sediment (tonnes), mass1 (g/cm2), mass2 (g/cm2), …plus other data

The PSC does not use all data in the zts file. The PSC reads in the zts file as follows:

dummy, dummy, dummy, daily flow (cm), dummy, mass entering (g/cm2), dummy

where *dummy* is a place holder (the number should be in the file, but the PSC does not use it). Only the 4th (daily flow) and the 6th (mass1) are used by the PSC. The remaining data serve only as place holder and can be replaced with a zero, so a typical file with 5 days of data may look like this:

0 0 0 0.12 0 1.34 0

0 0 0 0.17 0 1.34 0

0 0 0 0.13 0 0 0

0 0 0 0.00 0 0 0

0 0 0 0.17 0 100.6 0

***Watershed Area****:*

Because the time series input file is structured as a PRZM5 output file as if the inputs were normalized to an area as represented by a watershed. Thus total flow and total mass delivered into the PSC is the input file values times the watershed area using appropriate unit conversions.

**Toxicity Tab**

This Tab allows the user to enter ***Concentrations of Concern*** that correspond to several time averaging schemes. The program will use these values for analysis if the user chooses to check the ***Do Toxicity Analysis*** box at the top of the page. The program will calculate the number of days that the concentrations are above these values and how many consecutive days that the concentrations remain above these values.

**Scenario Tab**

***Scenario ID*** is text that will be used in the output file naming. It is helpful if it is indicative of the scenario characteristics.

The ***Get Weather*** button allows specification of a weather file. The weather file should be organized without a header and into the following white-space-delimited columns:

date, precipitation (cm), pan evaporation (cm), average temp (°C), wind speed (cm/s)

The date should be presented as a number consisting of the two-digit numerical values for month day year and compiled together for example December 15, 1992 should be written as 121592. January 3, 1991 should be written as 010391 (or 10391). The program will read the entire date value in as a single integer and parse the value. Because the file is recognized as being white-space delimited the date should not contain any internal spaces. For example, February 7, 1992 which is 020792 can be written as 20792 but not as 2 792. Daily metrological files for the United States that will work for PSC are available from the US EPA at: http://www.epa.gov/ceampubl/tools/metdata/index.htm The files at that address contain additional columns of information that have no effect on PSC.

***Width of Mixing Cell [m]*** is the width of receiving water body.

***Depth of Mixing Cell [m]*** is the depth of receiving water body.

***Length of Mixing Cell [m]*** is the width of receiving water body. Note that for a flowing water body such as a stream or river, this length value should correspond roughly to twice the dispersivity (2D/v, where D is the dispersion coefficient and v is the velocity of the stream or river)) characteristic of the flowing water body. A good starting value may be around 30 meters as estimated from the median of data in Fisher et al. (1979).

***Use Constant Flow Rate [m3/sec]*** specifies is the base flow through the receiving water body.

***No Base Flow***—there will be no constant flow through the system

***DFAC [-]*** is a parameter defined as is in the model EXAMS. It represents the ratio of vertical path lengths to depth. Default value is set to 1.19 as suggested by EXAMS documentation.

***Water Column SS [mg/L]*** is the suspended mass in the water column. Default value is set to that used by the USEPA/OPP standard farm pond.

Water Column Biomass [mg/L] is the biomass in water column which impacts photolysios and has a very minor impact on sorption.

***Chlorophyl [mg/L]*** represents the chlorophyll concentration in the water column. Default value is set to that used by the EPA standard farm pond. This parameter only affects the photolysis rate.

***Water Column Foc*** is the fraction of organic carbon associated with suspended sediment. Default values are set to those used by the EPA standard farm pond.

***Water Column DOC [mg/L]*** represents the dissolved organic carbon concentration in the water column. ***Benthic Foc*** is the fraction of organic carbon associated with benthic sediment. Default value is set to that used by the USEPA/OPP standard farm pond. This parameter only affects the photolysis rate.

***Benthic Depth [m]*** is the depth of the benthic compartment. This is another difficult to estimate parameter; however, literature and EPA’s own calibrations suggest about 0.05 m.

***Benthic Porosity*** is the porosity of the benthic compartment: [pore space volume per total volume]. Default value is set to that used by the USEPA/OPP standard farm pond.

***Bulk Density [g/cm3]*** is the rationally defined bulk density: [mass of sediment per total volume of sediment]. Default value is set to that used by the USEPA/OPP standard farm pond.

***Benthic Foc*** is the fraction of organic carbon associated with benthic sediment. Default value is set to that used by the USEPA/OPP standard farm pond.

***Benthic DOC [mg/L]*** represents the dissolved organic carbon concentration in the water column. Default value is set to that used by the USEPA/OPP standard farm pond.

***Benthic Biomass [g/m2]*** biomass per square meter in the benthic zone. This parameter has little influence on results; it is a holdout from early model development. Default value is set to that used by the USEPA/OPP standard farm pond.

***QT [-]*** (not user accessible in PSC) is the Q10 value for metabolism. Fixed in the PSC to a value of 2.

***Mass Transfer Coefficient [m/s]*** represents the mass transfer coefficient between the water column and the benthic zone. It accounts for all means of mass transport and is referenced to the surrogate driving force of aqueous concentration differences. It is a difficult parameter to measure. Literature and EPA’s own calibrations suggests a starting estimate of 10-8 m/s.

**Results Tab**

This page provides a graph of daily aqueous concentrations and some analyses with the *Concentration of Concern* (C0C). The first columns of results (Total Conc. or Pore Water) gives the maximum value of the chemical over the averaging periods specified on the Toxicity page. The Days > CoC column present a fraction which is the ratio of the total number of days exceeding the CoC to the total number of days in the simulation.

Additional analyses and summaries are provided in the main output file, including the maximum number of sequential days above the CoC. The main output file will have a name that starts with the Outfile Family Name (see bottom of the Point Source Calculator GUI) and will be appended with the scenario ID and “\_Parent.txt”. So, for a chemical in which the user save the inputs as ChemA and used a scenario VirginiaMountans, the output file will have the name ChemA\_VirginiaMountains\_Parent.txt. This file will contain all the results from the simulation, some of which does not appear in the interface so a more detailed analysis is available if desired.

**More Info Tab**

This page provides additional useful information characterizing the chemicals behavior. The way the chemical tends to distribute itself is presented as well as a comparison of the different mechanisms of dissipation.

**Output Files**

Two output files are generated. They can both be located in the Working Directory as specified at the bottom of the interface. All files associated with a particular run will have the Outfile Family Name (also specified at the bottom of the interface) in the file name. One output file will contain all the post processed output that is in the Results tab as well as some additional analyses. The other file will contain daily concentraions in both the water column and the benthic region.

**Citations**

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