

Attachment 2. How to obtain sediment EECs from pe5 and Validation of Equation 1 and Alternatives to Estimating the Chemical Concentration in Sediment on a Dry Weight Basis.¹

1. How do we obtain sediment EECs from pe5?

PRZM/EXAMs can be used to estimate NOC concentration in pore water, NOC concentration in bulk sediment concentrations on a wet weight basis, and NOC concentrations in bulk sediment concentrations on a dry weight basis. Concentrations of pesticide dissolved in pore water (*e.g.*, that are compared to pore water concentrations of sediment tests or used to compare to results water column toxicity tests) are estimated using the pe5 shell and PRZM/EXAMs by selecting “Write Benthic pore water concentrations” in the pe5 shell and then running pe5 as specified by EFED guidance (USEPA, 2006, 2009). Chemical concentrations in pore water are then reported in an EXAMs summary output file (filename_ben.out). **Figure 1** provides an example output file providing pore water concentrations from the EXAMs summary output file. The units in the file where results are reported in parts per billion (ppb) or µg pesticide/L water and the units reported in the file are correct. Use the 1 in 10 year peak concentration to evaluate the potential for acute risk to aquatic invertebrates and the 1 in 10 year 21 day concentration to evaluate the potential for chronic risk to aquatic invertebrates.

Currently, a Tier I model does not exist for estimating sediment EECs. However, the MScotton scenario can be used as a high end screening scenario, similar to the way that GENECC is used.

Chemical concentrations in bulk sediment are also calculated by EXAMs; however, 1 in 10 year peak and 21-day values are not generated in the standard pe5 output files. The pesticide concentration in pore water can be converted to pesticide concentration in bulk sediment on a dry weight basis using equation 1. **Table 1** summarizes the symbols and nomenclature used in the equation.

$$C_{\text{sed-dw}} = \frac{C_{\text{pw-fd}} 1000 (m_{\text{sed}} f_{\text{OC}} K_{\text{OC}} + m_{\text{biota}} K_{\text{biota}} + m_{\text{DOC}} K_{\text{DOC}} + V_{\text{pw}})}{m_{\text{sed}}} \quad (\text{Equation 1})$$

Table 1. Explanation of Symbols and Nomenclature for Equations 1

Symbol	Description	Value or Source of Value ¹	Units	Citation
$C_{\text{sed-dw}}$	Concentration of pesticide in bulk sediment on a dry weight basis	Calculated	mg-pesticide/kg-sediment dry weight	NA
$C_{\text{pw-fd}}$	Concentration of pesticide dissolved in pore water	Output from PRZM/EXAMs and pe5	µg pesticide/L-water	NA
V_{pw}	Volume pore water or volume water in benthic compartment	249.8	m ³	Page 16 of USEPA (2004)
$m_{\text{sed-dw}}$	Mass sediment	675,200	kg	Page 16 of USEPA (2004)
K_{OC}	Organic-carbon normalized solid water distribution coefficient	Value used in modeling in different units	m ³ /kg-organic carbon	NA
m_{biota2}	Mass biota (<i>i.e.</i> , plankton) in benthic compartment	0.06	kg	Page 16 of USEPA (2004)

¹ Attachment 2 to the 2014 USEPA/OPP/EFED Guidance memo on sediment toxicity testing and risk assessment.

Symbol	Description	Value or Source of Value ¹	Units	Citation
K_{biota}	Biota-water partition coefficient	$0.436 \times \left(\frac{K_{OC}}{0.35}\right)^{0.907}$ See footnote 2	m ³ /kg	Page 20 (2004)
m_{DOC2}	Mass of dissolved organic carbon in benthic compartment	1.249	kg	Page 16 of USEPA (2004)
K_{DOC}	Dissolved organic carbon-water partition coefficient for benthic compartment	Assumed to be the K_{OC} used in modeling using different units	m ³ /kg-organic carbon	NA
f_{OC}	Fraction of organic carbon in sediment	0.04	None	Page 16 of USEPA (2004)

1 The values that are not specific to the chemical are default values or equations for the EPA standard pond and were obtained from USEPA (2004).

2 The K_{OC} used in the equation must be in units of m³/kg.

stored as benben.out							
Chemical: ChemX							
PRZM environment: PAturfSTD.txt				modified Thuday, 23 February 2006 at 17:55:08			
EXAMS environment: pond298.exv				modified Tuesday, 26 August 2008 at 05:14:08			
Metfile: w14751.dvf				modified Tuesday, 26 August 2008 at 05:15:00			
Benthic segment concentrations (ppb)							
Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly	
1961	0.1353	0.1352	0.134	0.1302	0.1253	0.04443	
1962	0.1588	0.1588	0.1587	0.1584	0.1578	0.1462	
1963	0.1589	0.1589	0.1589	0.1589	0.1588	0.1558	
1964	0.1737	0.1737	0.1737	0.1737	0.1735	0.162	
1965	0.1736	0.1736	0.1735	0.1733	0.1732	0.1707	
1966	0.4724	0.4715	0.4629	0.4343	0.3991	0.2254	

Sorted results							
Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly	
0.032258065	2.159	2.159	2.158	2.158	2.157	2.115	
0.064516129	2.15	2.15	2.146	2.129	2.107	2.007	
0.096774194	2.063	2.062	2.06	2.056	2.052	1.939	

Pore water concentrations used							
1935	0.1353	0.1352	0.134	0.1302	0.1253	0.04443	
0.1	2.0525	2.0516	2.0495	2.0456	2.0418	1.9336	
						Average o 1.173884	

Figure 1. Excerpt from an example summary EXAMS output file (filename_ben.out) from PRZM/EXAMS providing pesticide concentration in pore water. The units in pore-water are µg pesticide/L water.

See Section 2 for a validation of this method. For equation 1, K_{OC} , K_{biota} , and K_{DOC} are in m³/kg. These must be

converted from the L/kg units in which they are typically reported. The 1000 in the equation is a conversion factor to convert from m³ to L. There are 1000 L in 1 m³.

Finally, in most risk assessments $C_{\text{sed-dw}}$ will need to be converted to an organic carbon normalized sediment concentration ($C_{\text{sed-TOC}}$) using equation 2.

$$C_{\text{sed-TOC}} = \frac{C_{\text{sed-dw}}}{f_{\text{OC}}} \quad (\text{Equation 2})$$

Pe5 also produces a time series file (filename_TS.out). The time series file provides concentrations of pesticide dissolved in the water column in the column titled, "conc.ppm" in units of mg pesticide/L water and the concentration of pesticide in bulk sediment on a fresh or wet weight basis in the column titled, "benthic_conc.ppm" in units of mg pesticide/kg-sediment wet weight.

2. Validation of Equation 1 and Alternatives to Estimating the Chemical Concentration in Sediment on a Dry Weight Basis

PRZM/EXAMs calculates concentrations of pesticide dissolved in the water column, concentrations of pesticide dissolved in sediment pore water, concentration of pesticide in plankton on a dry weight basis, concentration of pesticide in benthos on a dry weight basis, and concentration of pesticide in the total water, and concentration of pesticide in sediment on a dry weight basis. These results are normally reported in the Table 20.XX of the report.xml file for each year of the simulation. A program is available (TAB20AB.exe) that reads each Table 20 and reports the 24-hour, 96-hour, 21-day, 60-day, 90-day, and annual average concentrations for each year. It also sorts the values and reports the 1 in 10 year corresponding value similar to the pe5 output files for pesticide concentrations in the water column and pesticide concentration in pore water. To use pe5 in conjunction with the TAB20AB.exe program or to view the report.xml file, pe5 must be modified so that it does not delete the report.xml file. To do this open pe5.pl in a text editor file. Search for report.xml. The search will identify report.xml is in the following line of code:

```
my @todelete = ("*.ZPM","p2e.exe","restart.prz","fget*.xml","report.xml","VVWM.txt","KECHO.PRN","P2E-C*");  
# "*.ZTS"
```

Delete "report.xml" from the line of code as follows.

```
my @todelete = ("*.ZPM","p2e.exe","restart.prz","fget*.xml","VVWM.txt","KECHO.PRN","P2E-C*"); # "*.ZTS"
```

Save the file with a new filename and use the new file to run pe5. When the new pe5 is used it will produce a report.xml file and it will place it in the folder where other results are saved for that model simulation.

To get the PRZM/EXAMs output files that provide 1 in 10 year summarized results place the TAB20AB.exe file in the same folder as the report.xml file. Double click on the file to open the program. Answer the questions of the program and label the files as appropriate. The first year of EFED PRZM simulations is 1961 and the final year is

1990. This was completed for a couple of simulations using a high and low K_{oc} . The results from the runs are presented in **Table 2** along with calculated values using the conversions described in Equation 1 in Section 1. Calculated values are very similar to EXAMs estimated values and values developed using the TAB20AB.exe program. Supporting files for the runs are provided in Attachment 3 so that the results may easily be reproduced. It is acceptable to determine the total sediment dry weight concentrations 1) by converting pe5 pore water concentrations using equation 6 in Attachment 2, 2) using the report.xml file results, or 3) using the TAB20AB.exe program.

Table 2. Comparison of model estimated values pesticide in sediment concentrations on a dry weight basis with values calculated from pesticide concentration in pore water using equation 1 in Section 1

3. Simulation Name	4. Pore Water Concentration 5. (μg pesticide/L water)		6. Bulk Sediment 7. (μg pesticide/kg-sediment dw)	
	Peak	21-day	Peak	21-day
Test $K_{oc} = 227$ L/kg-organic carbon				
1989 Value from pe5 output and sediment results from report.xml	11.74	11.74	111.00	111.00
1989 Value Calculated using Equation 6	--	--	110.99	110.99
1989 Value Table 20 program	11.74	11.74	111.00	111.00
1 in 10 year value from pe5	11.734	11.734	--	--
1 in 10 year value Table 20 program	11.734	11.734	110.90	110.90
Test 2 $K_{oc} = 10,000$ L/kg-organic carbon				
1980 Value from pe5 output and sediment results from report.xml	2.913	2.91	1170	1170
1980 value Calculated using Equation 6	--	--	1167	1166
1980 value Table 20 program	2.913	2.913	1170	1170
1 in 10 year value from pe5	2.8814	2.8781	--	--
1 in 10 year value from Table 20 program	2.881	2.881	1158	1158

Literature Cited

- USEPA. 2004. *A Discussion with the FIFRA Scientific Advisory Panel Regarding the Terrestrial and Aquatic Level II Refined Risk Assessment Models (Version 2.0). Support Document for Scientific Advisory Panel Meeting Scheduled from March 30 - April 2, 2004.* March 4, 2004. Environmental Fate and Effects Division. Office of Pesticide Programs. United States Environmental Protection Agency. Available at http://www.epa.gov/scipoly/sap/meetings/2004/033004_mtg.htm (Accessed December 15, 2011).
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