Canadian Environmental Modeling Centre Water Quality Model and the Simon Fraser University Food Web Model User's Guide

September 11, 2007

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Introduction

The Canadian Environmental Modelling Centre's AGRO modeling system (AGRO) is a MicroSoft Excel® based application that combines a water quality model with a food web model to estimate exposure to aquatic species from pesticides in a user-defined water body. A major feature of this system is its capability to incorporate dynamic functionalities which allow the user to introduce changing environmental and emission conditions so that the fate and bioaccumulation results of numerous chemicals can easily and efficiently be compared.

The AGRO modeling system is written in Visual Basic and has an EXCEL® interface for parameter input and output display. This system can be run in dynamic mode which uses daily input of water, sediment, and pesticide from predicted daily mass loadings generated by US EPA Pesticide Root Zone Model, version 3.12 (PRZM3.12) (Suárez, 2006). [Note: AGRO can also be run in a steady-state mode, but this application is not the focus of this User's Guide]. Daily loading and emission values from PRZM3.12 are then used to generate predicted daily pesticide concentrations in the water column, benthic pore water and benthic sediment of the water body. From these concentrations, the food web model estimates bioaccumulation of pesticide in aquatic organisms.

The water quality model component of the AGRO modeling system is the Quantitative Water, Air, Sediment Interaction (QWASI) Fugacity model developed by Mackay et al. at the Canadian Environmental Modelling Centre (Mackay, Joy and Paterson (1983), Mackay, Paterson and Joy (1983), Webster Lian and Mackay (2005), Mackay and Diamond (1989)). The QWASI model is based on a single receiving water body of user-defined size and depth with an active sediment layer. This model is run in dynamic mode which includes daily input of water from field runoff, dissolved pesticide in field runoff, eroded sediment, pesticide sorbed to eroded sediment, pesticide emissions resulting from application drift and rainfall. These dynamic daily values are generated outside of the AGRO modeling system using the EPA PRZM3.12 model. The AGRO modeling system has built-in capability to import annual mass loading files output from PRZM3.12 and convert these values into the units and configurations needed by the QWASI Fugacity model.

The food web model in AGRO is based on the Bioaccumulation model developed by F.A.P.C. at Simon Fraser University (Gobas, 2007). The Bioaccumulation model is a dynamic or time dependent interpretation of Arnot and Gobas [2004] bioaccumulation equation. This model is based on the assumption that the exchange of hydrophobic organic chemicals between the organism and its ambient environment can be described by a single equation for a large number of aquatic organisms. For each aquatic organism, this equation estimates bioaccumulation as a function of intake of pesticide via respiration and ingestion of prey, and outflow of pesticide via excretion, metabolism to a daughter product and respiratory exhalation.

System Requirements

The AGRO modeling system is designed to run using MicroSoft Excel® 2003 with a minimum hard disk space of 15 MB.

Computation Flow Overview

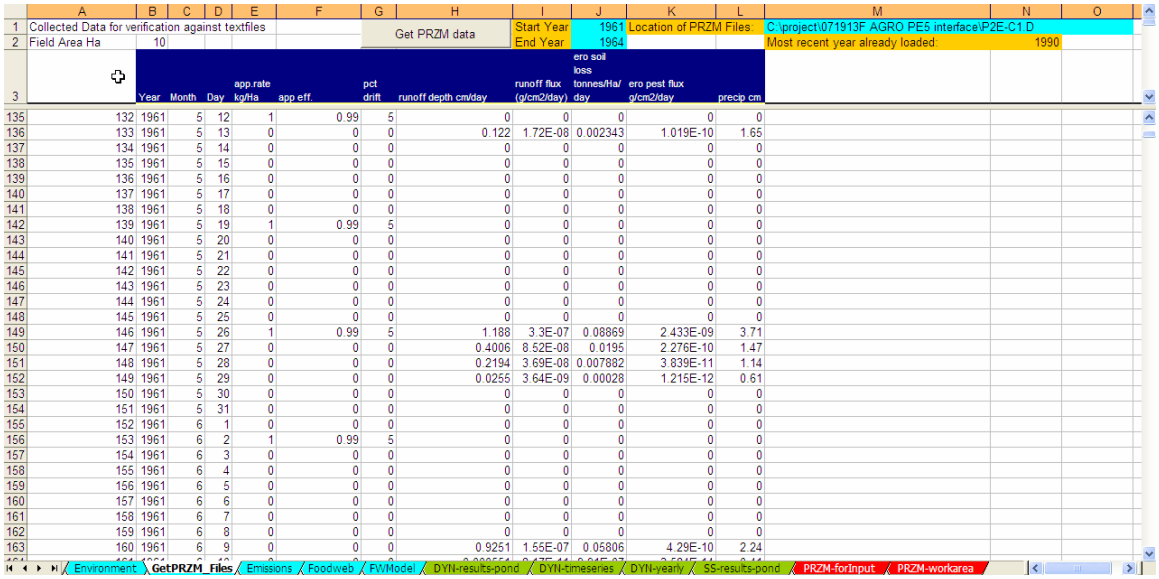
Using Visual Basic for Applications (VBA) as the programming language allows for the AGRO modeling system to function within the framework of EXCEL spreadsheets, thus facilitating the entry and viewing of both the input parameters and the display and analysis of the subsequent output. The following steps detail how to run the AGRO modeling system.

To run the AGRO modeling system in dynamic mode:

Step 1 - Import Daily Mass Loading Data Generated by PRZM3.12 for use in the QWASI model.

Go to the **Get_PRZM_Files** Tab

Here is an example of a Get_PRZM_Files page:



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Collected Data for verification against textfiles							Get PRZM data	Start Year	1961	Location of PRZM Files:		C:\project\071913F AGRO PE5 interface\P2E-C1.D		
2	Field Area Ha	10							End Year	1964			Most recent year already loaded:	1990	
3		Year	Month	Day	app.rate kg/Ha	app eff.	pct drift	runoff depth cm/day	runoff flux (g/cm2/day)	ero soil loss tonnes/Ha/ day	ero pest flux g/cm2/day	precip cm			
135	132	1961	5	12	1	0.99	5	0	0	0	0	0			
136	133	1961	5	13	0	0	0	0.122	1.72E-08	0.002343	1.019E-10	1.65			
137	134	1961	5	14	0	0	0	0	0	0	0	0			
138	135	1961	5	15	0	0	0	0	0	0	0	0			
139	136	1961	5	16	0	0	0	0	0	0	0	0			
140	137	1961	5	17	0	0	0	0	0	0	0	0			
141	138	1961	5	18	0	0	0	0	0	0	0	0			
142	139	1961	5	19	1	0.99	5	0	0	0	0	0			
143	140	1961	5	20	0	0	0	0	0	0	0	0			
144	141	1961	5	21	0	0	0	0	0	0	0	0			
145	142	1961	5	22	0	0	0	0	0	0	0	0			
146	143	1961	5	23	0	0	0	0	0	0	0	0			
147	144	1961	5	24	0	0	0	0	0	0	0	0			
148	145	1961	5	25	0	0	0	0	0	0	0	0			
149	146	1961	5	26	1	0.99	5	1.188	3.3E-07	0.08869	2.433E-09	3.71			
150	147	1961	5	27	0	0	0	0.4006	8.52E-08	0.0195	2.276E-10	1.47			
151	148	1961	5	28	0	0	0	0.2194	3.69E-08	0.007882	3.839E-11	1.14			
152	149	1961	5	29	0	0	0	0.0255	3.64E-09	0.00028	1.215E-12	0.61			
153	150	1961	5	30	0	0	0	0	0	0	0	0			
154	151	1961	5	31	0	0	0	0	0	0	0	0			
155	152	1961	6	1	0	0	0	0	0	0	0	0			
156	153	1961	6	2	1	0.99	5	0	0	0	0	0			
157	154	1961	6	3	0	0	0	0	0	0	0	0			
158	155	1961	6	4	0	0	0	0	0	0	0	0			
159	156	1961	6	5	0	0	0	0	0	0	0	0			
160	157	1961	6	6	0	0	0	0	0	0	0	0			
161	158	1961	6	7	0	0	0	0	0	0	0	0			
162	159	1961	6	8	0	0	0	0	0	0	0	0			
163	160	1961	6	9	0	0	0	0.9251	1.55E-07	0.05806	4.29E-10	2.24			

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

In cell Get_PRZM_Files!J1, enter the beginning year of the simulation.

In cell Get_PRZM_Files!J2, enter the end year of the simulation.

In cell Get_PRZM_Files!M1, enter "C:*xxxxx**yyyyy*\P2E-C1.D" where *xxxxx**yyyyy*\ is the folder structure where the PRZM3.12 generated P2E-C1.D* mass loading files of interest are stored. Remember to type "P2E-C1.D" at the end of the folder structure since this is necessary for the system to identify the P2E-C1 mass loading files.

Click the "**Get PRZM data**" button located on cells Get_PRZM_Files!G(1:2)-Get_PRZM_Files!H(1:2). Clicking this executes a Visual Basic macro which imports the mass loading values from the PRZM3.12 P2E-C1.D* mass loading files and stores them in this tab. This macro also converts the data into the units and variables compatible with the QWASI model. These converted values are stored in the **PRZM-forInput tab**.

Table 1 below summarizes the conversion of massing loading values in the P2E-C1.D* files into the values stored in the **PRZM-forInput tab.**

Table 1: Summary of daily input values for AGRO model derived from PRZM output

Parameter	Description
Simday	assigned to evaluate and loop through the total number of days of data provided by PRZM
Year Month Day	from PRZM
E to Pond kg/y	this is the 5% spray drift from PRZM expressed as kg/y
Inflow-W Conc ng/L	from PRZM expressed in ng/L
Inflow-P Conc ng/L	from PRZM expressed in ng/L
Bulk Inflow Conc ng/L	uses Inflow-W Conc and Inflow-P Conc with the respective volume fractions to calculate a bulk water concentration of chemical
Water Inflow rate m3/h	Standard rate defined on Environment worksheet + PRZM runoff
Particulate Inflow rate m3/h	Standared rate derived from Environment worksheet +PRZM erosion rate
Inflow-P concentration	derived Inflow and Particulate inflow rates
VF-W Inflow	Volume Fraction of water in the inflow
VF-P Inflow	Volume Fraction of particulate in the inflow
rain rate m^3/h	converted from cm/day in PRZM to m3/h

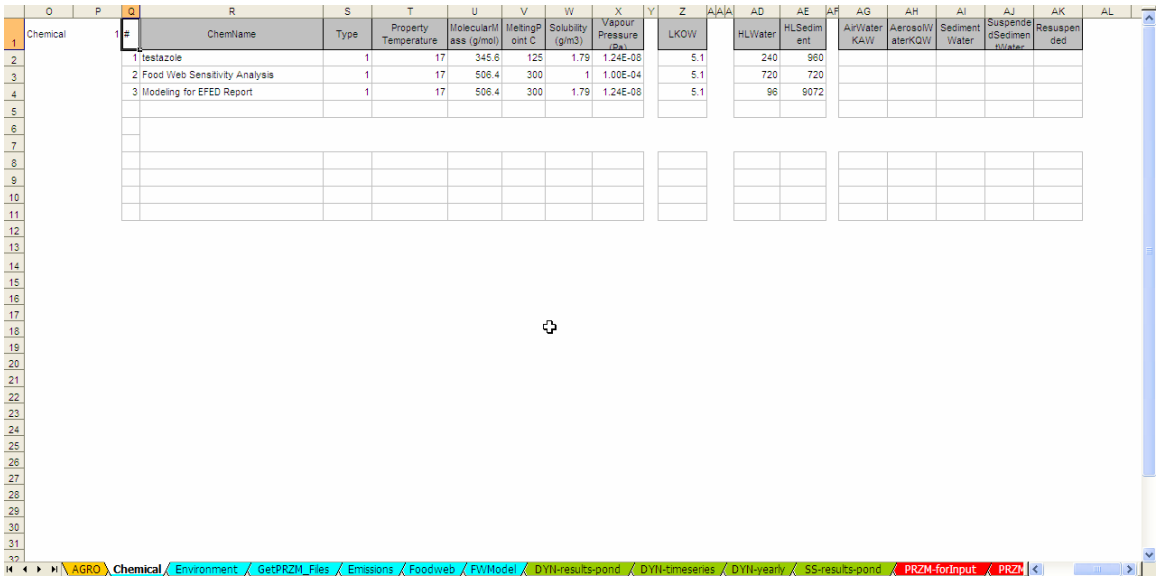
The AGRO modeling system also contains a blank worksheet with tab entitled, **PRZM-workarea**. This worksheet is used by the AGRO Visual Basic module to store internal variable values during processing of the PRZM3.12 input files.

Step 2 – Enter or Select Chemical Input Parameters

Go to the **Chemical** tab

The chemical parameters are defined here. A "database" of chemical parameters is listed in columns Chemical!Q through Chemical!AK.

Here is an example of columns Chemical!Q through Chemical!AK in the **Chemical** Tab:



Chemical	1	#	ChemName	Type	Property Temperature	MolecularMass (g/mol)	MeltingPoint C	Solubility (g/m3)	Vapour Pressure (Pa)	LKOW	HLWater	HLSediment	AirWaterKAW	AerosolWaterKQW	SedimentWater	SuspendedSedimentWater	Resuspended
		1	testazole	1	17	345.6	125	1.79	1.24E-08	5.1	240	960					
		2	Food Web Sensitivity Analysis	1	17	506.4	300	1	1.00E-04	5.1	720	720					
		3	Modeling for EFED Report	1	17	506.4	300	1.79	1.24E-08	5.1	96	9072					

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

More chemicals can be added to this database or existing chemicals can be modified by entering data into the appropriate columns. The names of the newly added chemicals will appear in the list-box entitled "Select a Chemical" in columns Chemical!D-Chemical!F of this tab.

To enter a new chemical with Type I partitioning into the chemical database, enter the following chemical information into the first available empty row:

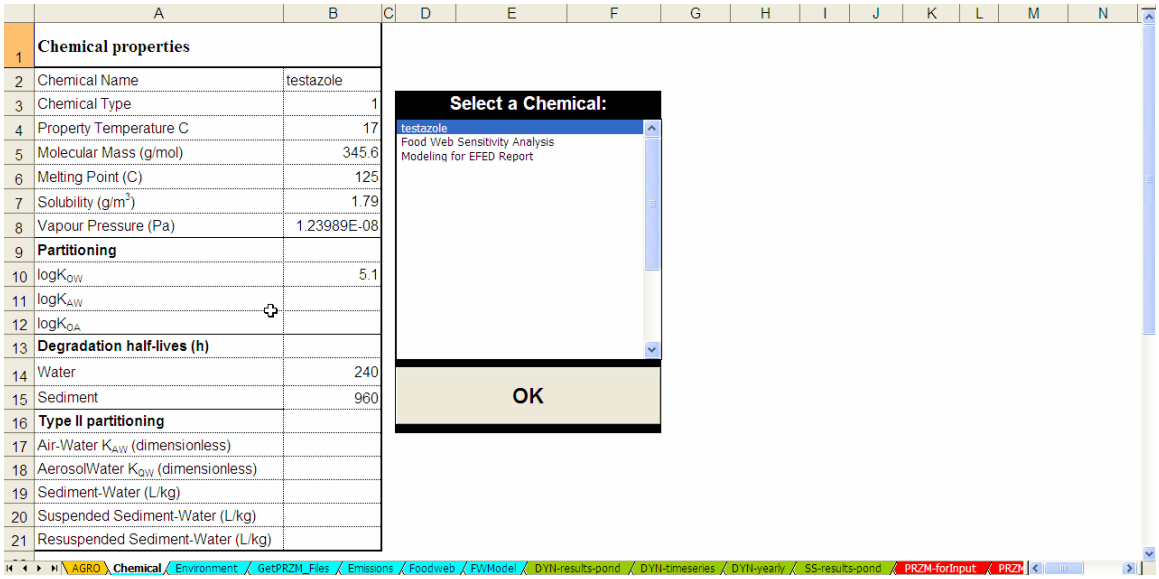
Table 2: Chemical Parameters for Type I Partitioning Simulations

Column	Parameter	Units	Notes
Chemical!Q	Chemical Identifier	---	The row number plus 1. This will be used as the chemical number identifier.
Chemical!R	Chemical Name	---	Name of chemical of interest
Chemical!S	Chemical Type	---	1 for Type I partitioning and 2 for Type II partitioning. For regulatory modeling, Type I partitioning is employed.
Chemical!T	Property Temperature	°C	Default 17°C
Chemical!U	Chemical Molecular Mass	g/mol	Molecular weight of chemical
Chemical!V	Chemical Melting Point °	°C	
Chemical!W	Solubility	g/m^3	Water solubility of chemical. Equivalent units are kg/L.
Chemical!X	Chemical Vapor Pressure	Pa	
Chemical!Z	Log K_{OW}	(mg/L)/(mg/L)	Log 10 of the Octanol-Water Partition Coefficient, K_{OW}
Chemical!AD	Chemical Half-life in Water	hours	Aqueous aerobic half-life
Chemical!AE	Chemical Half-life in Sediment	hours	Aqueous anaerobic half-life

For Type I partitioning, Columns Chemical!AG-Chemical!AK are left blank.

Now, go to the list-box “Select a Chemical” in columns Chemical!D-Chemical!F. Highlight the chemical of interest and click the “OK” button. This will cause the appropriate values of the selected chemical to appear in column Chemical!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Chemical!B without affecting the original values in the database, although these value will be overwritten each time the “OK” button is clicked)

Here is an example of columns Chemical!A through Chemical!N (Rows 1-21) in the **Chemical** tab:



	A	B
1	**Chemical properties**	
2	Chemical Name	testazole
3	Chemical Type	1
4	Property Temperature C	17
5	Molecular Mass (g/mol)	345.6
6	Melting Point (C)	125
7	Solubility (g/m^3)	1.79
8	Vapour Pressure (Pa)	1.23989E-08
9	**Partitioning**	
10	$logK_{OW}$	5.1
11	$logK_{AW}$	
12	$logK_{OA}$	
13	**Degradation half-lives (h)**	
14	Water	240
15	Sediment	960
16	**Type II partitioning**	
17	Air-Water K_{AW} (dimensionless)	
18	AerosolWater K_{OW} (dimensionless)	
19	Sediment-Water (L/kg)	
20	Suspended Sediment-Water (L/kg)	
21	Resuspended Sediment-Water (L/kg)	

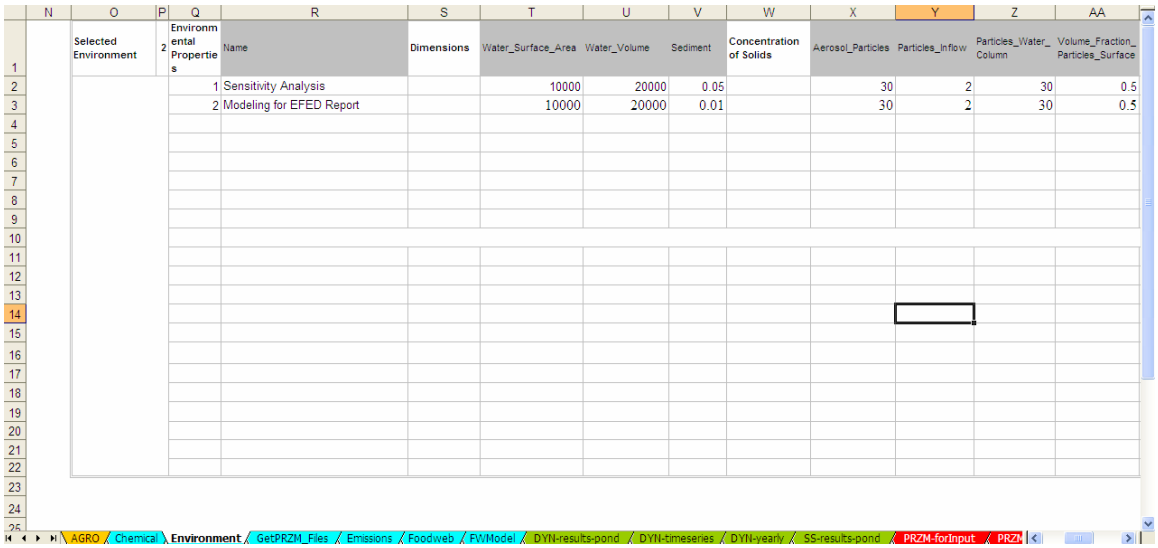
Step 3 – Enter or Select Environment Input Parameters

Go to the **Environment** tab

The environment scenario parameters are defined here. A "database" of environmental scenarios is listed in columns Environment!O through Environment!AW. The environmental parameters listed here are those required to run the QWASI 3.10 model.

The user may add environmental scenarios to this database by entering necessary information into the columns Environment!O through Environment!AW. The names of the newly added environments will appear in the list-box entitled "Select an Environment" in this tab. Each new environment should be entered in the first blank line below the existing environments.

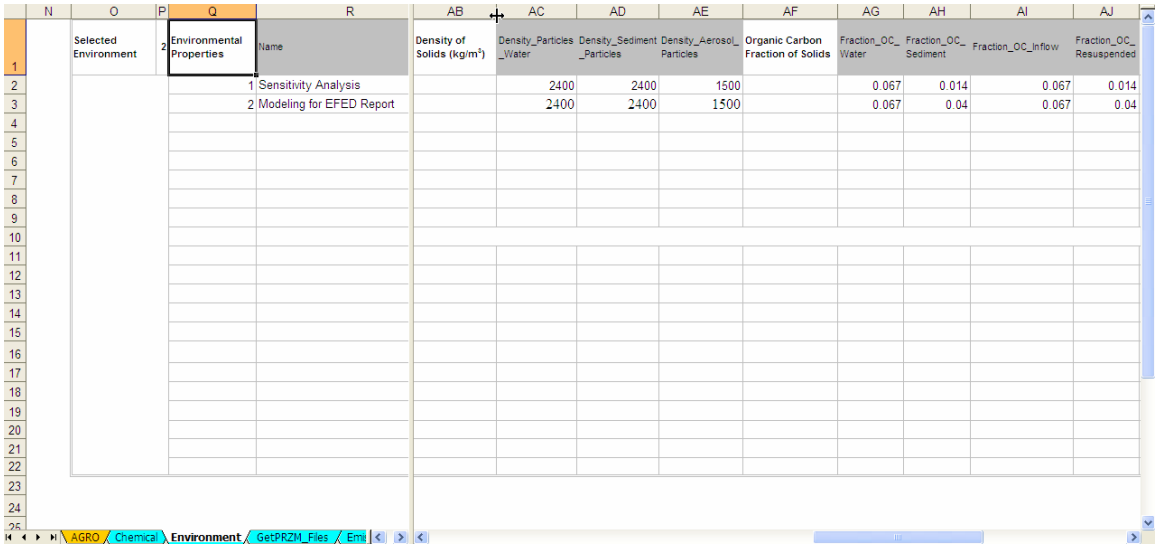
Here is an example of columns Chemical!O through Chemical!AA of the environmental database in the **Environment** tab. Columns Environment!S through Environment!V refer to dimensions of the water body. Columns Environment!W through Environment!AA refer to the concentration of particle solids in the various bulk media..



	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA
1		Selected Environment	2	Environmental Properties	Name	Dimensions	Water_Surface_Area	Water_Volume	Sediment	Concentration of Solids	Aerosol_Particles	Particles_Inflow	Particles_Water_Column	Volume_Fraction_Particles_Surface
2				1	Sensitivity Analysis		10000	20000	0.05		30	2	30	0.5
3				2	Modeling for EFED Report		10000	20000	0.01		30	2	30	0.5

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

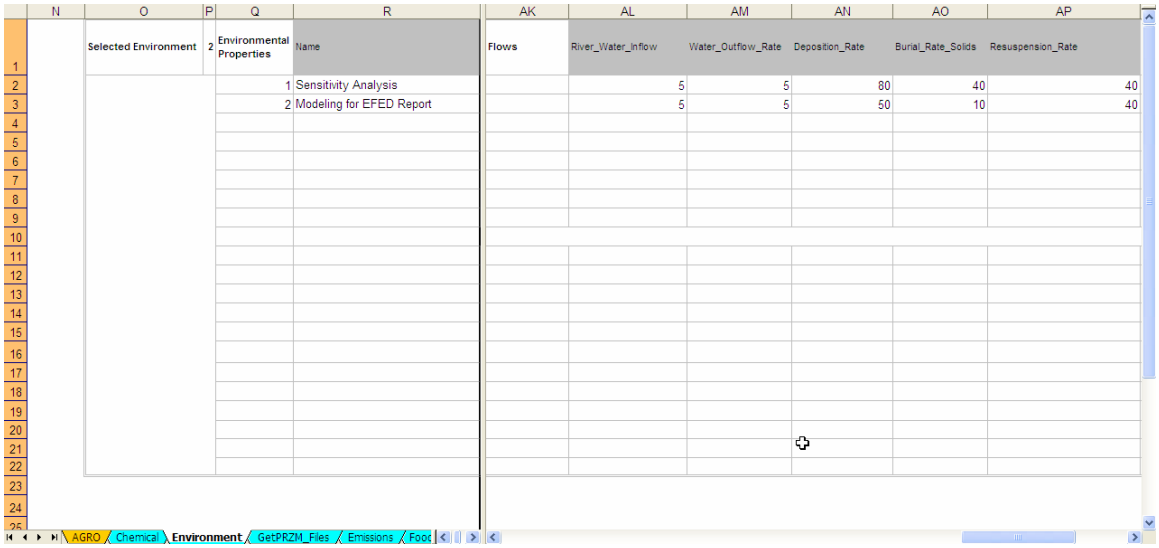
Splitting the screen after column Environment!R and scrolling right, displays columns Environment!AB through Environment!AE which pertain to the density of solids in the various bulk media. Columns Environment!AF through Environment!AJ pertain to the fraction of organic carbon in the various bulk media.



	N	O	P	Q	R	AB	AC	AD	AE	AF	AG	AH	AI	AJ
1		Selected Environment	2	Environmental Properties	Name	Density of Solids (kg/m³)	Density_Particles_Water	Density_Sediment_Particles	Density_Aerosol_Particles	Organic Carbon Fraction of Solids	Fraction_OC_Water	Fraction_OC_Sediment	Fraction_OC_Inflow	Fraction_OC_Resuspended
2				1	Sensitivity Analysis		2400	2400	1500		0.067	0.014	0.067	0.014
3				2	Modeling for EFED Report		2400	2400	1500		0.067	0.04	0.067	0.04

AGRO | Chemical | Environment | GetPRZM_Files | Emi

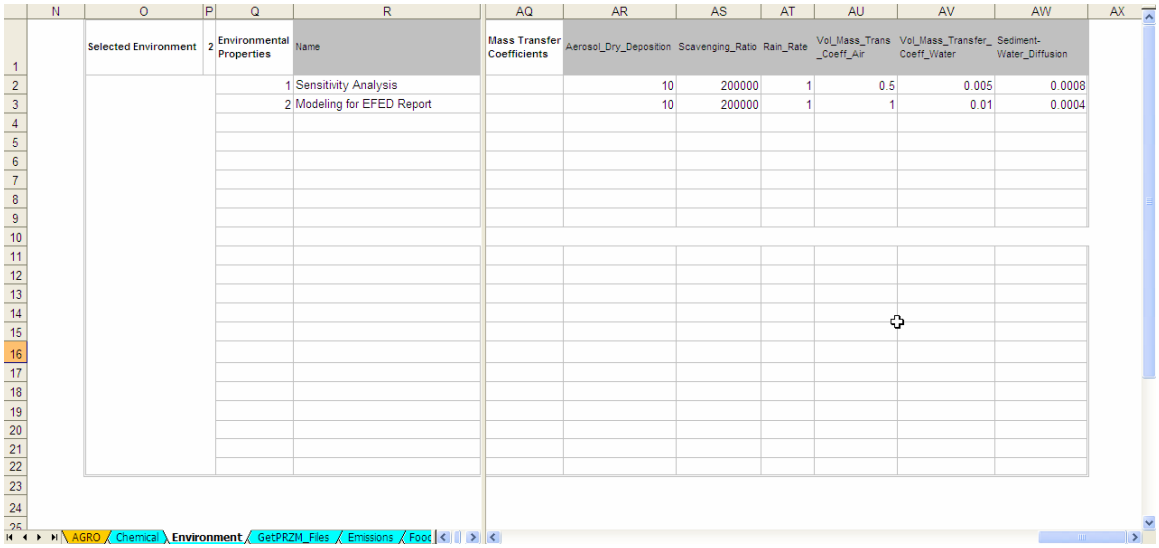
Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AK through Environment!AP which pertain to the flow rates for the water and sediment in various bulk media.



	N	O	P	Q	R	AK	AL	AM	AN	AO	AP
1		Selected Environment	2	Environmental Properties	Name	Flows	River_Water_Inflow	Water_Outflow_Rate	Deposition_Rate	Burial_Rate_Solids	Resuspension_Rate
2				1	Sensitivity Analysis		5	5	80	40	40
3				2	Modeling for EFED Report		5	5	50	10	40

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Food

Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AQ through Environment!AW which pertain to the mass transfer coefficients between various bulk media.



	N	O	P	Q	R	AQ	AR	AS	AT	AU	AV	AW	AX
1		Selected Environment	2	Environmental Properties	Name	Mass Transfer Coefficients	Aerosol_Dry_Deposition	Scavenging_Ratio	Rain_Rate	Vol_Mass_Trans_Coeff_Air	Vol_Mass_Transfer_Coeff_Water	Sediment-Water_Diffusion	
2				1	Sensitivity Analysis		10	200000	1	0.5	0.005	0.0008	
3				2	Modeling for EFED Report		10	200000	1	1	0.01	0.0004	

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Food

Here is a summary of the input Parameters in the **Environment** Tab:

Table 3: Input Parameters in the Environment Tab

Note: Default values for EPA generic pond scenario are listed in notes column.

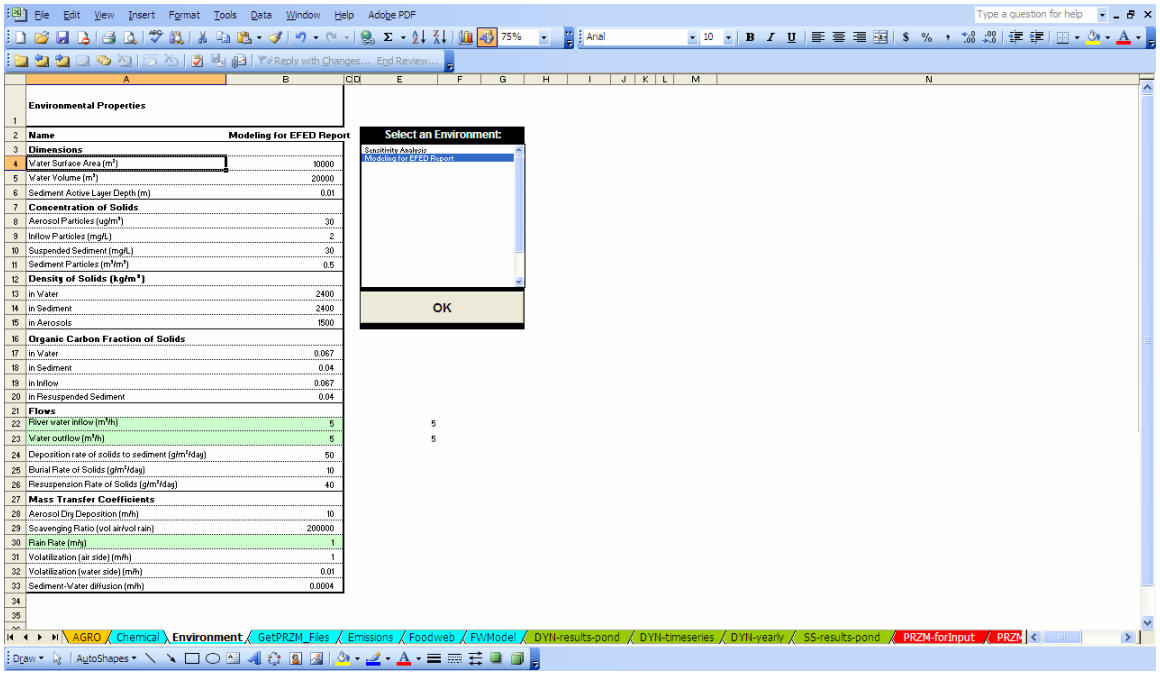
Column	Parameter	Units	Notes
Environment!O	**"Dimensions"**	---	Label for columns associated with dimensions of the water body
Environment!P	Selected Environment Identifier	---	Numeric identifier of environmental scenario highlighted in the "Select an Environment" list-box. Automatically changes with change in highlighted selection.
Environment!Q	Environmental Properties Scenario Identifier	---	User-supplied numeric identifier of environmental scenario of interest
Environment!R	Name of Environmental Scenario	---	Name given to the environmental scenario
Environment!T	Water_Surface_ Area	m^2	Surface area of water body Default value: 10,000
Environment!U	Water_Volume	m^3	Volume of water body Default value: 20,000
Environment!V	Sediment	m	Depth of sediment in benthic layer. Default value: 0.05
Environment!W	**"Concentration of Solids"**	---	Label for columns associated with concentration of solid particles in various bulk media
Environment!X	Aerosol_Particles	ug/m^3	Concentration of solid particles in air bulk media. Default value: 30
Environment!Y	Particles_Inflow	mg/L	Concentration of solid particles in inflow water bulk media. Default Value: 2
Environment!Z	Particles_Water_ Column	mg/L	Concentration of suspended sediment in water column. Default value: 30
Environment!AA	Volume_Fraction _Particles_ Surface	m^3/m^3	Volume fraction of sediment particles in benthic. Default value: 0.5

Column	Parameter	Units	Notes
Environment!AB	**"Density of Solids"**		Label for columns associated with density of solid particles in various bulk media
Environment!AC	Density_Particles _Water	kg/m^3	Density of solid particles in water column bulk media. Default value: 2400
Environment!AD	Density_ Sediment_ Particles	kg/m^3	Density of solid particles in benthic sediment bulk media. Default value: 2400
Environment!AE	Density_Aerosol_ Particles	kg/m^3	Density of solids particles in air bulk media. Default value: 1500
Environment!AF	**"Organic Carbon Fraction of Solids"**		Label for columns associated with organic carbon fraction in various bulk media
Environment!AG	Fraction_OC_ Water	---	Fraction of organic carbon in water column bulk media. Default value: 0.067
Environment!AH	Fraction_OC_ Sediment	---	Fraction of organic carbon in benthic sediment bulk media Default value: 0.014
Environment!AI	Fraction_OC_ Inflow	---	Fraction of organic carbon in inflow water bulk media Default value: 0.067
Environment!AJ	Fraction_OC_ Resuspended	---	Fraction of organic carbon in resuspended sediment. Default value: 0.014

Column	Parameter	Units	Notes
Environment!AK	**"Flows"**		Label for columns associated with flow rates in various bulk media
Environment!AL	River_Water_ Inflow	m^3/h	Flow rate of inflow water into water body. Default value: 5
Environment!AM	Water_Outflow_ Rate	m^3/h	Flow rate of outflow water out of the water body. Default value: 5
Environment!AN	Deposition_Rate	g/m^2	Deposition rate of solid particles to benthic sediment. Default value: 80
Environment!AO	Burial_Rate_ Solids	g/m^2	Burial rate of solid particles in benthic sediment. Default value: 40
Environment!AP	Resuspension_ Rate	g/m^2	Resuspension rate of solid particles out of the benthic and back into the water column. Default value: 40
Environment!AQ	**"Mass Transfer Coefficients"**		Label for columns associated with Mass transfer Coefficients between various bulk media
Environment!AR	Aerosol_Dry_ Deposition	m/h	Deposition rate of dry particles out of air into water body. Default value: 10
Environment!AS	Scavenging_Ratio	Volume of air/Volume of Rain	Scavenging Ratio of air to rain Default value: 20,000
Environment!AT	Rain_Rate	m/year	Rainfall rate in meters per year. Default value: 1
Environment!AU	Vol_Mass_ Trans_Coeff_ Air	m/h	Volatilization rate – air side Default value: 1
Environment!AV	Vol_Mass_ Transfer_Coeff_ Water	m/h	Volatilization rate – water to air Default value: 0.01
Environment!AW	Sediment-Water-Diffusion	m/h	Diffusion rate between benthic sediment and water column. Default value: 0.0004

Now, go to the list-box “Select an Environment” in columns Environment!E through Environment!G. Highlight the environment of interest and click the “OK” button. This will cause the appropriate values of the selected environment to appear in column Environment!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Environment!B without affecting the original values in the database, although these value will be overwritten each time the “OK” button is clicked)

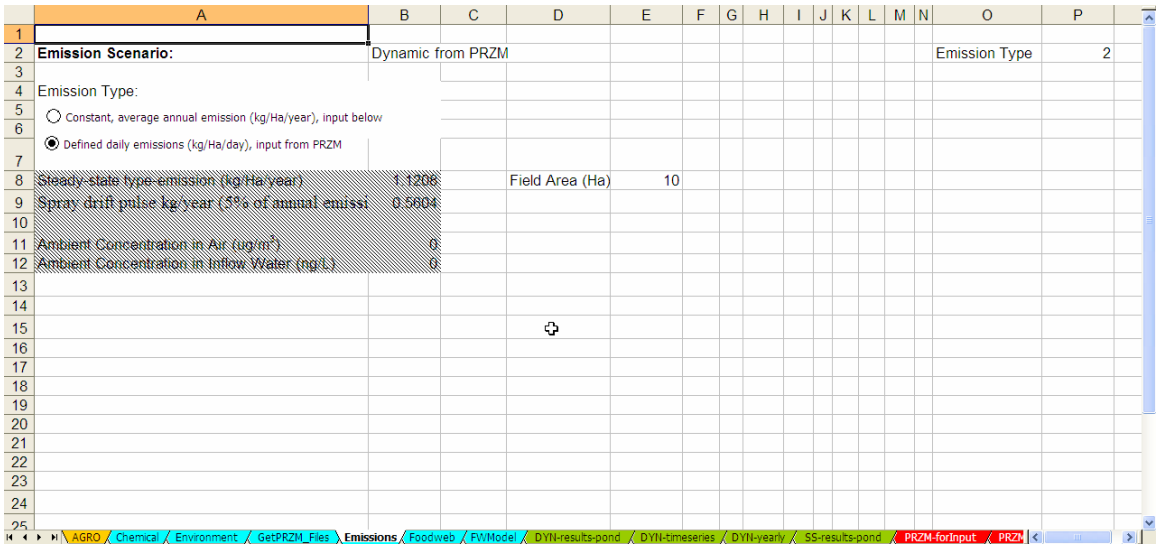
Here is an example of columns Environment!A through Environment!G (Rows 1-33) in the **Environment** tab:



Step 4 – Confirm the Emissions Parameters

Go to the **Emissions** tab

Here is what the Emissions tab page should look like:



Make sure that the "Defined daily emissions (kg/Ha/day), input from PRZM" is selected and that Emission Type is set to 2. Cell Emissions!B2 should say " Dynamic from PRZM". The above set-up with "Defined daily emissions" selected activates the dynamic mode execution of the model where daily values are read from the PRZM-forInput tab.

The internal model code automatically navigates through the PRZM-forInput daily values until it reaches the first non-zero emissions occurrence in PRZM_forInput!E column at which time the model iterations begin.

Step 5 – Review the FWModel tab

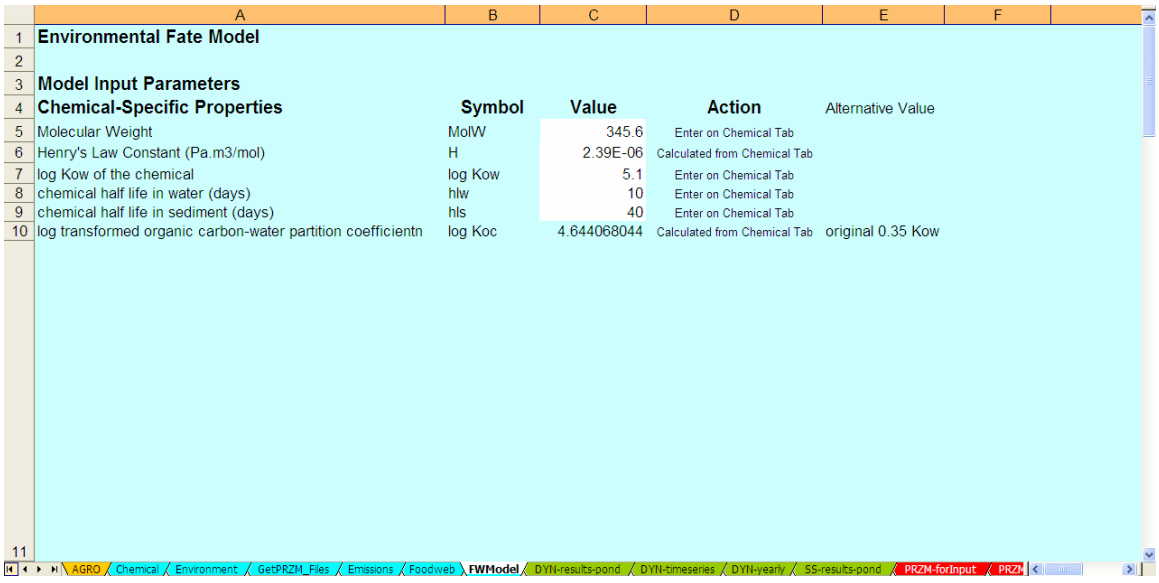
Go to the **FWModel** tab. This tab contains the chemical and ecosystem parameter values used by the Gobas Bioaccumulation model. Review the assigned input values.

Usually, the user will not make any revisions to this tab since the Environmental Fate Parameters are mostly calculated based on values entered in the Chemical tab and the Food Web Bioaccumulation Model values are the recommended values for the embedded organism foodweb. **Note:** There is no database summarizing several possible foodwebs, so any changes made are permanent and it is suggested that an original version of the file be maintained at all times to preserve the original information.

Columns FWModel!A through FWModel!G summarize the Chemical and Environmental Fate input parameters from the QWASI water quality model.

For columns FWModel!A through FWModel!G, rows 4 – 10, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Chemical** tab.

An example of columns FWModel!A through FWModel!G, rows 4 – 10 looks like:



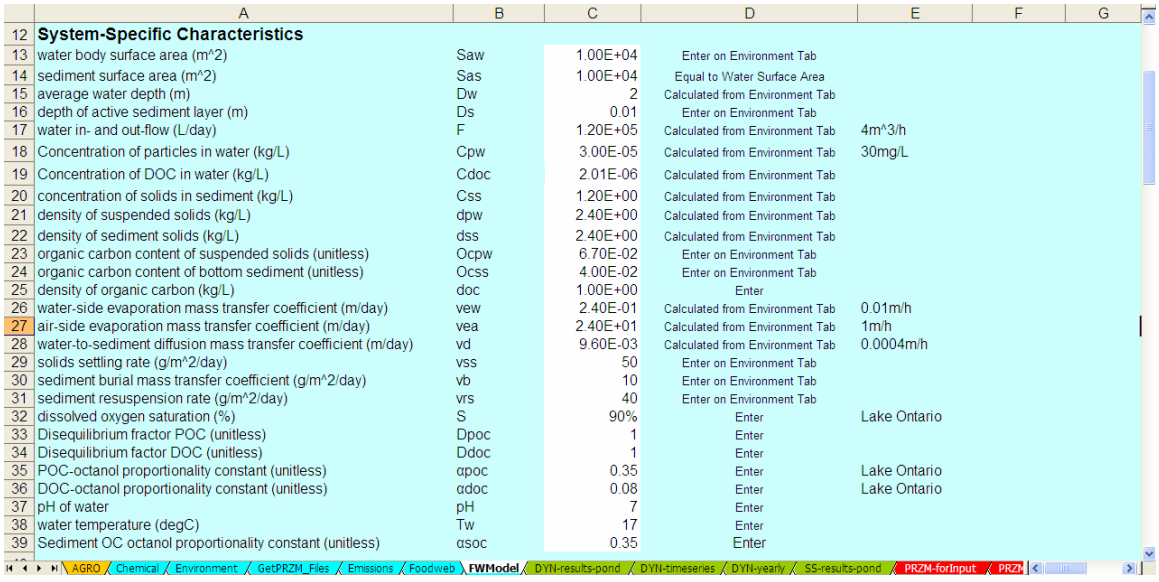
	A	B	C	D	E	F
1	**Environmental Fate Model**					
2						
3	**Model Input Parameters**					
4	**Chemical-Specific Properties**	**Symbol**	**Value**	**Action**	Alternative Value	
5	Molecular Weight	MolW	345.6	Enter on Chemical Tab		
6	Henry's Law Constant (Pa.m3/mol)	H	2.39E-06	Calculated from Chemical Tab		
7	log Kow of the chemical	log Kow	5.1	Enter on Chemical Tab		
8	chemical half life in water (days)	hlw	10	Enter on Chemical Tab		
9	chemical half life in sediment (days)	hls	40	Enter on Chemical Tab		
10	log transformed organic carbon-water partition coefficientn	log Koc	4.644068044	Calculated from Chemical Tab	original 0.35 Kow	
11						

For columns FWModel!A through FWModel!G, rows 12 – 31, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Environment** tab.

The following additional environmental input parameters along with their recommended values are required by the Bioaccumulation model:

Input Parameter	**Recommended Value**
Dissolved oxygen saturation (%)	90%
Disequilibrium fractor POC (unitless)	1
Disequilibrium factor DOC (unitless)	1
POC-octanol proportionality constant (unitless)	0.35
DOC-octanol proportionality constant (unitless)	0.08
pH of water	7
water temperature (degC)	17
Sediment OC octanol proportionality constant (unitless)	0.35
initial chemical mass in water (g)	0
initial chemical mass in sediment (g)	0

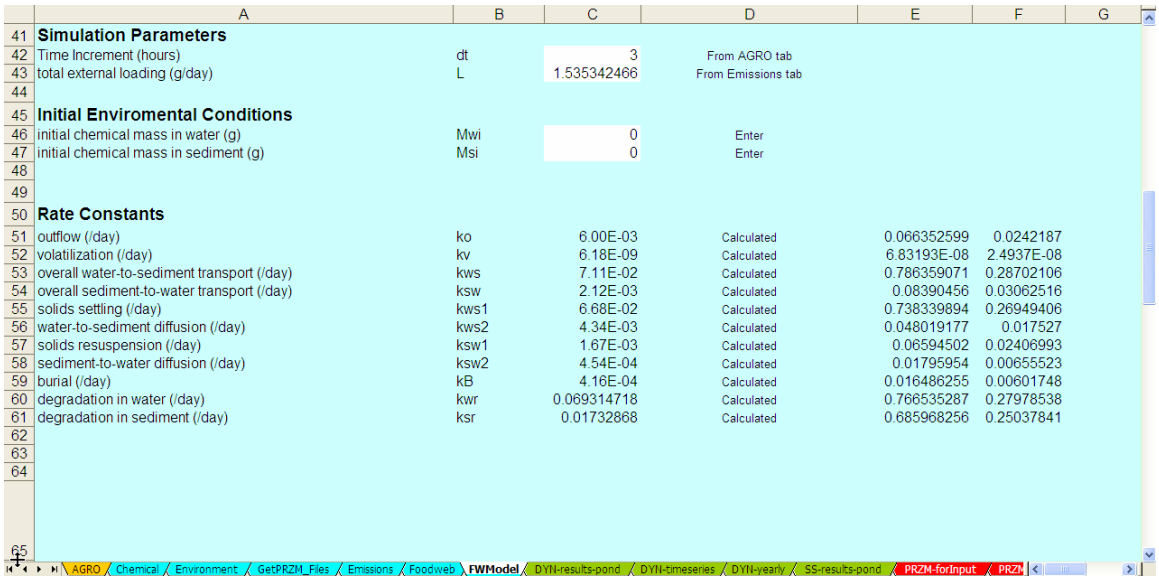
An example of columns FWModel!A through FWModel!G, rows 4 – 10 looks like:



	A	B	C	D	E	F	G
12	**System-Specific Characteristics**						
13	water body surface area (m^2)	Saw	1.00E+04	Enter on Environment Tab			
14	sediment surface area (m^2)	Sas	1.00E+04	Equal to Water Surface Area			
15	average water depth (m)	Dw	2	Calculated from Environment Tab			
16	depth of active sediment layer (m)	Ds	0.01	Enter on Environment Tab			
17	water in- and out-flow (L/day)	F	1.20E+05	Calculated from Environment Tab	4m^3/h		
18	Concentration of particles in water (kg/L)	Cpw	3.00E-05	Calculated from Environment Tab	30mg/L		
19	Concentration of DOC in water (kg/L)	Cdoc	2.01E-06	Calculated from Environment Tab			
20	concentration of solids in sediment (kg/L)	Css	1.20E+00	Calculated from Environment Tab			
21	density of suspended solids (kg/L)	dpw	2.40E+00	Calculated from Environment Tab			
22	density of sediment solids (kg/L)	dss	2.40E+00	Calculated from Environment Tab			
23	organic carbon content of suspended solids (unitless)	Ocpw	6.70E-02	Enter on Environment Tab			
24	organic carbon content of bottom sediment (unitless)	Ocss	4.00E-02	Enter on Environment Tab			
25	density of organic carbon (kg/L)	doc	1.00E+00	Enter			
26	water-side evaporation mass transfer coefficient (m/day)	vew	2.40E-01	Calculated from Environment Tab	0.01m/h		
27	air-side evaporation mass transfer coefficient (m/day)	vea	2.40E+01	Calculated from Environment Tab	1m/h		
28	water-to-sediment diffusion mass transfer coefficient (m/day)	vd	9.60E-03	Calculated from Environment Tab	0.0004m/h		
29	solids settling rate (g/m^2/day)	vss	50	Enter on Environment Tab			
30	sediment burial mass transfer coefficient (g/m^2/day)	vb	10	Enter on Environment Tab			
31	sediment resuspension rate (g/m^2/day)	vrs	40	Enter on Environment Tab			
32	dissolved oxygen saturation (%)	S	90%	Enter	Lake Ontario		
33	Disequilibrium fractor POC (unitless)	Dpoc	1	Enter			
34	Disequilibrium factor DOC (unitless)	Ddoc	1	Enter			
35	POC-octanol proportionality constant (unitless)	αpoc	0.35	Enter	Lake Ontario		
36	DOC-octanol proportionality constant (unitless)	αdoc	0.08	Enter	Lake Ontario		
37	pH of water	pH	7	Enter			
38	water temperature (degC)	Tw	17	Enter			
39	Sediment OC octanol proportionality constant (unitless)	αsoc	0.35	Enter			

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

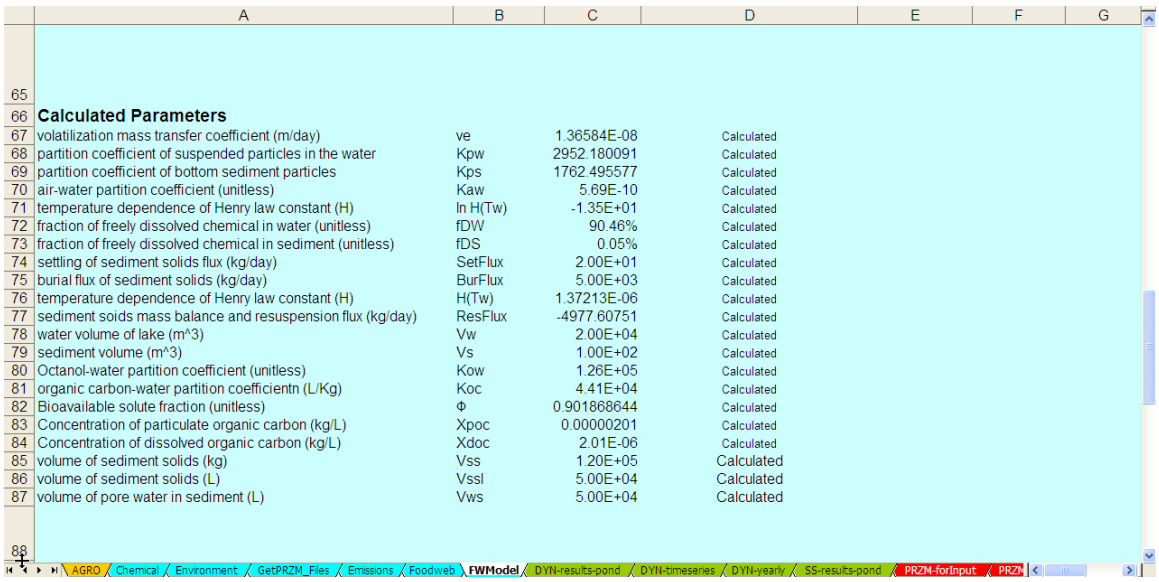
An example of columns FWModel!A through FWModel!G, rows 41 – 65 looks like:



	A	B	C	D	E	F	G
41	**Simulation Parameters**						
42	Time Increment (hours)	dt	3	From AGRO tab			
43	total external loading (g/day)	L	1.535342466	From Emissions tab			
44							
45	**Initial Enviromental Conditions**						
46	initial chemical mass in water (g)	Mwi	0	Enter			
47	initial chemical mass in sediment (g)	Msi	0	Enter			
48							
49							
50	**Rate Constants**						
51	outflow (/day)	ko	6.00E-03	Calculated	0.066352599	0.0242187	
52	volatilization (/day)	kv	6.18E-09	Calculated	6.83193E-08	2.4937E-08	
53	overall water-to-sediment transport (/day)	kws	7.11E-02	Calculated	0.786359071	0.28702106	
54	overall sediment-to-water transport (/day)	ksw	2.12E-03	Calculated	0.08390456	0.03062516	
55	solids settling (/day)	kws1	6.68E-02	Calculated	0.738339894	0.26949406	
56	water-to-sediment diffusion (/day)	kws2	4.34E-03	Calculated	0.048019177	0.017527	
57	solids resuspension (/day)	ksw1	1.67E-03	Calculated	0.06594502	0.02406993	
58	sediment-to-water diffusion (/day)	ksw2	4.54E-04	Calculated	0.01795954	0.00655523	
59	burial (/day)	kB	4.16E-04	Calculated	0.016486255	0.00601748	
60	degradation in water (/day)	kwr	0.069314718	Calculated	0.766535287	0.27978538	
61	degradation in sediment (/day)	ksr	0.01732868	Calculated	0.685968256	0.25037841	
62							
63							
64							
65							

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

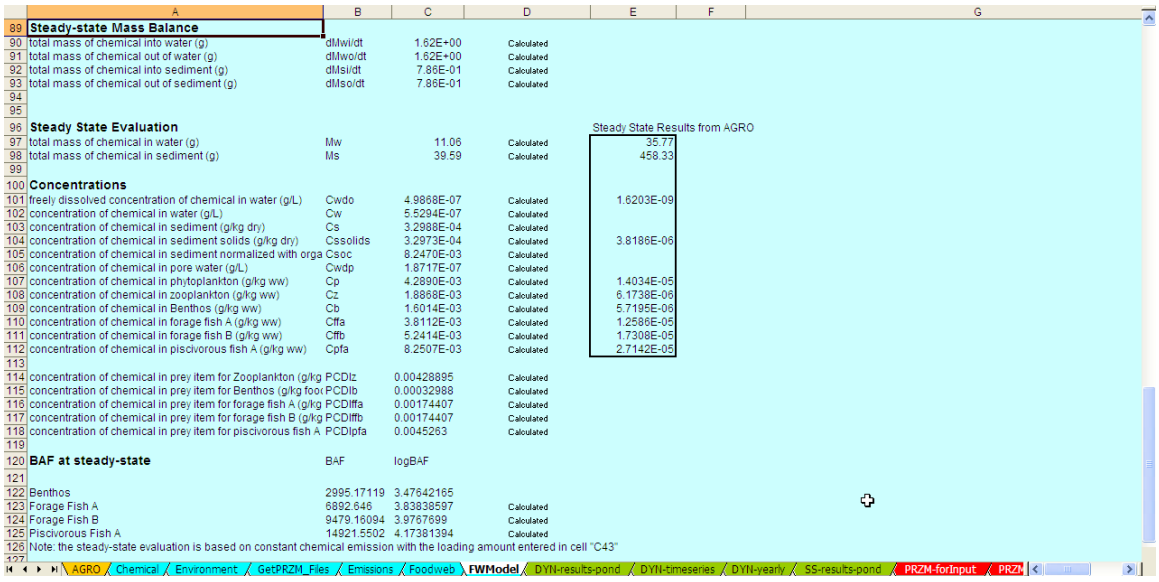
An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:



	A	B	C	D	E	F	G
65							
66	**Calculated Parameters**						
67	volatilization mass transfer coefficient (m/day)	ve	1.36584E-08	Calculated			
68	partition coefficient of suspended particles in the water	Kpw	2952.180091	Calculated			
69	partition coefficient of bottom sediment particles	Kps	1762.495577	Calculated			
70	air-water partition coefficient (unitless)	Kaw	5.69E-10	Calculated			
71	temperature dependence of Henry law constant (H)	ln H(Tw)	-1.35E+01	Calculated			
72	fraction of freely dissolved chemical in water (unitless)	fDW	90.46%	Calculated			
73	fraction of freely dissolved chemical in sediment (unitless)	fDS	0.05%	Calculated			
74	settling of sediment solids flux (kg/day)	SetFlux	2.00E+01	Calculated			
75	burial flux of sediment solids (kg/day)	BurFlux	5.00E+03	Calculated			
76	temperature dependence of Henry law constant (H)	H(Tw)	1.37213E-06	Calculated			
77	sediment soids mass balance and resuspension flux (kg/day)	ResFlux	-4977.60751	Calculated			
78	water volume of lake (m^3)	Vw	2.00E+04	Calculated			
79	sediment volume (m^3)	Vs	1.00E+02	Calculated			
80	Octanol-water partition coefficient (unitless)	Kow	1.26E+05	Calculated			
81	organic carbon-water partition coefficientn (L/Kg)	Koc	4.41E+04	Calculated			
82	Bioavailable solute fraction (unitless)	Φ	0.901868644	Calculated			
83	Concentration of particulate organic carbon (kg/L)	Xpoc	0.00000201	Calculated			
84	Concentration of dissolved organic carbon (kg/L)	Xdoc	2.01E-06	Calculated			
85	volume of sediment solids (kg)	Vss	1.20E+05	Calculated			
86	volume of sediment solids (L)	Vssl	5.00E+04	Calculated			
87	volume of pore water in sediment (L)	Vws	5.00E+04	Calculated			
88							

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:

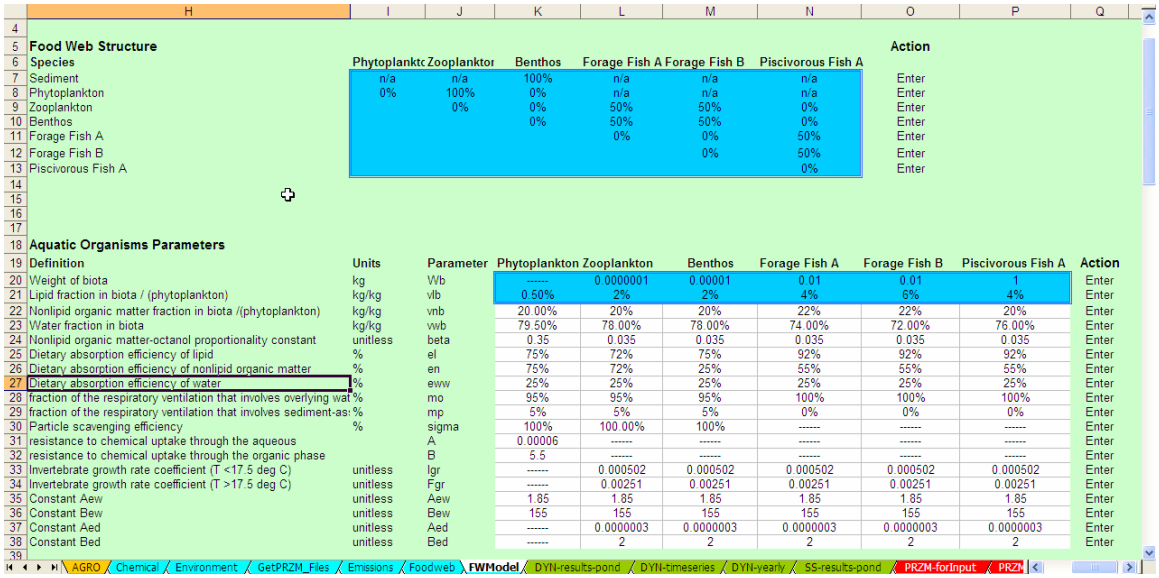


	A	B	C	D	E	F	G
89	**Steady-state Mass Balance**						
90	total mass of chemical into water (g)	dMwi/dt	1.62E+00	Calculated			
91	total mass of chemical out of water (g)	dMwo/dt	1.62E+00	Calculated			
92	total mass of chemical into sediment (g)	dMsi/dt	7.86E-01	Calculated			
93	total mass of chemical out of sediment (g)	dMso/dt	7.86E-01	Calculated			
94							
95							
96	**Steady State Evaluation**				Steady State Results from AGRO		
97	total mass of chemical in water (g)	Mw	11.06	Calculated	35.77		
98	total mass of chemical in sediment (g)	Ms	39.59	Calculated	458.33		
99							
100	**Concentrations**						
101	freely dissolved concentration of chemical in water (g/L)	Cwdo	4.9868E-07	Calculated	1.6203E-09		
102	concentration of chemical in water (g/L)	Cw	5.5294E-07	Calculated			
103	concentration of chemical in sediment (g/kg dry)	Cs	3.2988E-04	Calculated			
104	concentration of chemical in sediment solids (g/kg dry)	Cssolids	3.2973E-04	Calculated	3.8186E-06		
105	concentration of chemical in sediment normalized with orga	Csoc	8.2470E-03	Calculated			
106	concentration of chemical in pore water (g/L)	Cwdp	1.8717E-07	Calculated			
107	concentration of chemical in phytoplankton (g/kg ww)	Cp	4.2890E-03	Calculated	1.4034E-05		
108	concentration of chemical in zooplankton (g/kg ww)	Cz	1.8868E-03	Calculated	6.1738E-06		
109	concentration of chemical in Benthos (g/kg ww)	Cb	1.6014E-03	Calculated	5.7195E-06		
110	concentration of chemical in forage fish A (g/kg ww)	Cffa	3.8112E-03	Calculated	1.2586E-05		
111	concentration of chemical in forage fish B (g/kg ww)	Cffb	5.2414E-03	Calculated	1.7308E-05		
112	concentration of chemical in piscivorous fish A (g/kg ww)	Cpfa	8.2507E-03	Calculated	2.7142E-05		
113							
114	concentration of chemical in prey item for Zooplankton (g/kg	PCDIz	0.00428895	Calculated			
115	concentration of chemical in prey item for Benthos (g/kg foo	PCDIb	0.00032988	Calculated			
116	concentration of chemical in prey item for forage fish A (g/kg	PCDIffa	0.00174407	Calculated			
117	concentration of chemical in prey item for forage fish B (g/kg	PCDIffb	0.00174407	Calculated			
118	concentration of chemical in prey item for piscivorous fish A	PCDIpfa	0.0045263	Calculated			
119							
120	**BAF at steady-state**	BAF	logBAF				
121							
122	Benthos	2995.17119	3.47642165				
123	Forage Fish A	6892.646	3.83838597	Calculated			
124	Forage Fish B	9479.16094	3.9767699	Calculated			
125	Piscivorous Fish A	14921.5502	4.17381394	Calculated			
126	Note: the steady-state evaluation is based on constant chemical emission with the loading amount entered in cell "C43"						

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

Food Web input values for the Bioaccumulation model are included in columns FWModel!G through FWModel!L.

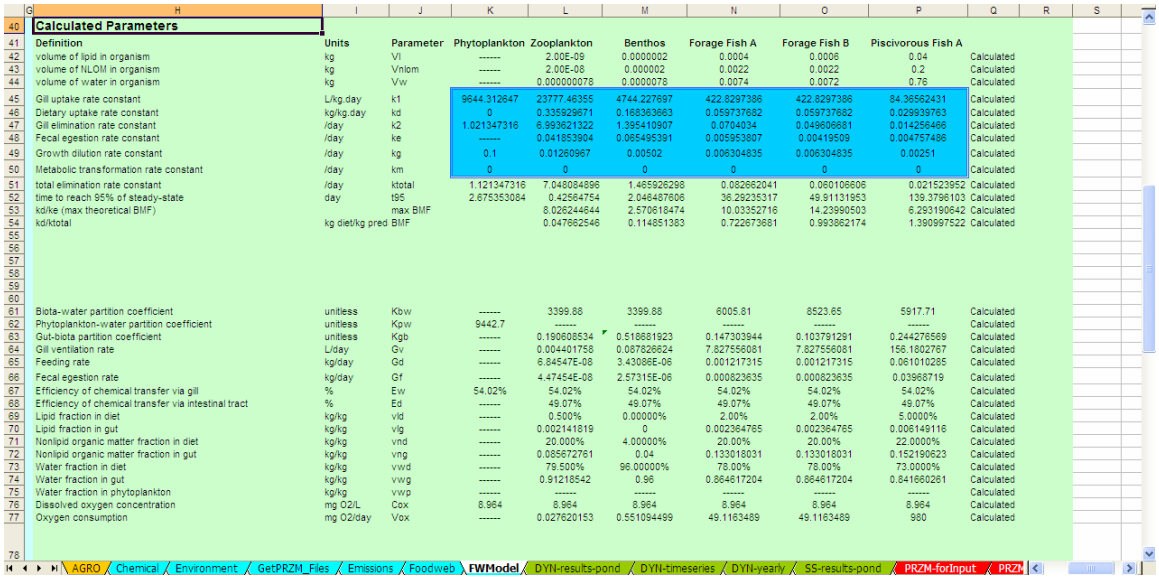
The food web structure is included in rows 5 through 13. . The food web aquatic organism individual parameters are included in rows 18-38. The below page displays the recommended values for these rows:



	H	I	J	K	L	M	N	O	P	Q
4										
5	**Food Web Structure**							**Action**		
6	**Species**	Phytoplanktc	Zooplanktor	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A			
7	Sediment	n/a	n/a	100%	n/a	n/a	n/a	Enter		
8	Phytoplankton	0%	100%	0%	n/a	n/a	n/a	Enter		
9	Zooplankton		0%	0%	50%	50%	0%	Enter		
10	Benthos			0%	50%	50%	0%	Enter		
11	Forage Fish A				0%	0%	50%	Enter		
12	Forage Fish B					0%	50%	Enter		
13	Piscivorous Fish A						0%	Enter		
14										
15										
16										
17										
18	**Aquatic Organisms Parameters**									
19	**Definition**	**Units**	**Parameter**	**Phytoplankton**	**Zooplankton**	**Benthos**	**Forage Fish A**	**Forage Fish B**	**Piscivorous Fish A**	**Action**
20	Weight of biota	kg	Wb	------	0.0000001	0.00001	0.01	0.01	1	Enter
21	Lipid fraction in biota / (phytoplankton)	kg/kg	vlb	0.50%	2%	2%	4%	6%	4%	Enter
22	Nonlipid organic matter fraction in biota /(phytoplankton)	kg/kg	vnb	20.00%	20%	20%	22%	22%	20%	Enter
23	Water fraction in biota	kg/kg	vwb	79.50%	78.00%	78.00%	74.00%	72.00%	76.00%	Enter
24	Nonlipid organic matter-octanol proportionality constant	unitless	beta	0.35	0.035	0.035	0.035	0.035	0.035	Enter
25	Dietary absorption efficiency of lipid	%	el	75%	72%	75%	92%	92%	92%	Enter
26	Dietary absorption efficiency of nonlipid organic matter	%	en	75%	72%	25%	55%	55%	55%	Enter
27	Dietary absorption efficiency of water	%	eww	25%	25%	25%	25%	25%	25%	Enter
28	fraction of the respiratory ventilation that involves overlying wat	%	mo	95%	95%	95%	100%	100%	100%	Enter
29	fraction of the respiratory ventilation that involves sediment-as	%	mp	5%	5%	5%	0%	0%	0%	Enter
30	Particle scavenging efficiency	%	sigma	100%	100.00%	100%	------	------	------	Enter
31	resistance to chemical uptake through the aqueous		A	0.00006	------	------	------	------	------	Enter
32	resistance to chemical uptake through the organic phase		B	5.5	------	------	------	------	------	Enter
33	Invertebrate growth rate coefficient (T <17.5 deg C)	unitless	Igr	------	0.000502	0.000502	0.000502	0.000502	0.000502	Enter
34	Invertebrate growth rate coefficient (T >17.5 deg C)	unitless	Fgr	------	0.00251	0.00251	0.00251	0.00251	0.00251	Enter
35	Constant Aew	unitless	Aew	1.85	1.85	1.85	1.85	1.85	1.85	Enter
36	Constant Bew	unitless	Bew	155	155	155	155	155	155	Enter
37	Constant Aed	unitless	Aed	------	0.0000003	0.0000003	0.0000003	0.0000003	0.0000003	Enter
38	Constant Bed	unitless	Bed	------	2	2	2	2	2	Enter
39										

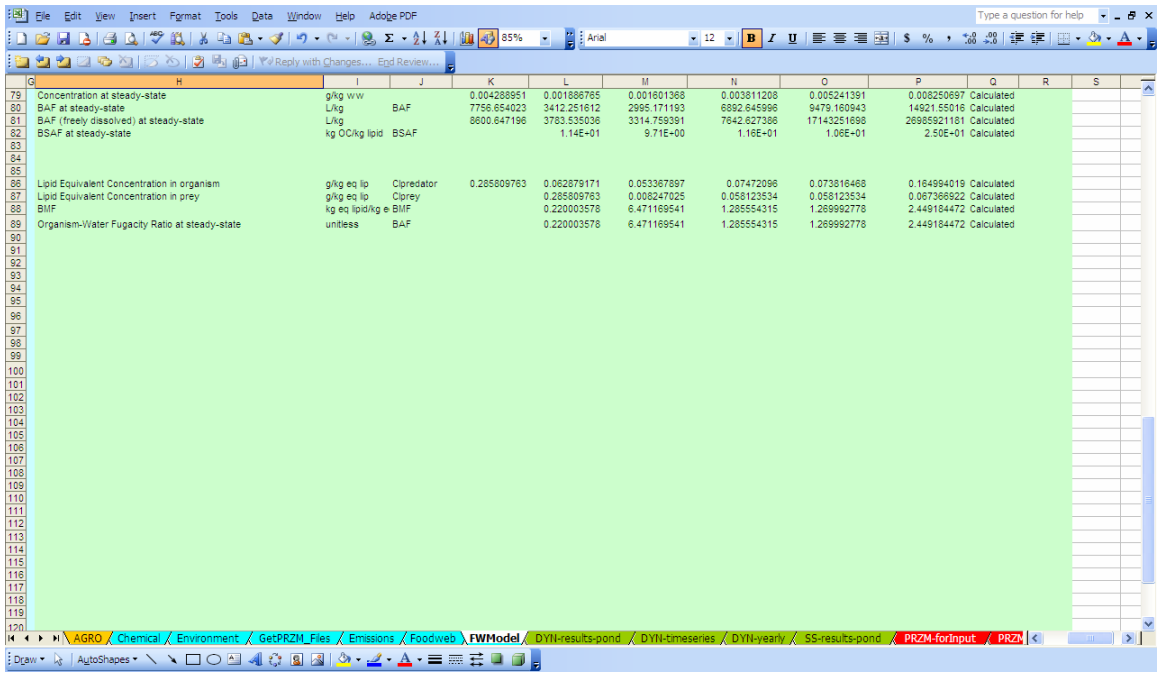
AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

The calculated parameters for each aquatic organism in the food web are included in rows 40 through 77 and 79-89. The below pages display the recommended values for these rows:



	Definition	Units	Parameter	Phytoplankton	Zooplankton	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A	
40	**Calculated Parameters**									
41	Definition	Units	Parameter	Phytoplankton	Zooplankton	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A	
42	volume of lipid in organism	kg	Vl	------	2.00E-09	0.0000002	0.0004	0.0008	0.04	Calculated
43	volume of NLOM in organism	kg	Vnlom	------	2.00E-08	0.000002	0.0022	0.0022	0.2	Calculated
44	volume of water in organism	kg	Vw	------	0.000000078	0.0000078	0.0074	0.0072	0.76	Calculated
45	Gill uptake rate constant	L/kg.day	k1	9644.312647	23777.46355	4744.227697	422.8297386	422.8297386	84.36562431	Calculated
46	Dietary uptake rate constant	kg/kg.day	kd	0	0.335929671	0.168363663	0.059737682	0.059737682	0.029939763	Calculated
47	Gill elimination rate constant	/day	k2	1.021347316	6.993621322	1.395410907	0.0704034	0.049606881	0.014256466	Calculated
48	Fecal egestion rate constant	/day	ke	------	0.041853904	0.085495391	0.005953807	0.00419509	0.004757486	Calculated
49	Growth dilution rate constant	/day	kg	0.1	0.01260967	0.00502	0.006304835	0.006304835	0.00251	Calculated
50	Metabolic transformation rate constant	/day	km	0	0	0	0	0	0	Calculated
51	total elimination rate constant	/day	ktotal	1.121347316	7.048084896	1.465926298	0.082662041	0.060106606	0.021523952	Calculated
52	time to reach 95% of steady-state	day	ts5	2.675353084	0.42564754	2.046487606	36.29235317	49.91131953	139.3796103	Calculated
53	kd/ke (max theoretical BMF)		max BMF		8.026244644	2.570618474	10.03352716	14.23990503	6.293190642	Calculated
54	kd/ktotal	kg diet/kg pred	BMF		0.047662546	0.114851383	0.722673681	0.993862174	1.390997522	Calculated
55										
56										
57										
58										
59										
60										
61	Biota-water partition coefficient	unitless	Kbw	------	3399.88	3399.88	6005.81	8523.65	5917.71	Calculated
62	Phytoplankton-water partition coefficient	unitless	Kpw	9442.7	------	------	------	------	------	Calculated
63	Gut-biota partition coefficient	unitless	Kgb	------	0.190808534	0.518681923	0.147303844	0.103791291	0.244276569	Calculated
64	Gill ventilation rate	L/day	Gv	------	0.004401758	0.087826824	7.827556081	7.827556081	156.1802767	Calculated
65	Feeding rate	kg/day	Gd	------	6.84547E-08	3.43086E-06	0.001217315	0.001217315	0.061010285	Calculated
66	Fecal egestion rate	kg/day	Gf	------	4.47454E-08	2.57315E-06	0.000823635	0.000823635	0.03968719	Calculated
67	Efficiency of chemical transfer via gill	%	Ew	54.02%	54.02%	54.02%	54.02%	54.02%	54.02%	Calculated
68	Efficiency of chemical transfer via intestinal tract	%	Ed	------	49.07%	49.07%	49.07%	49.07%	49.07%	Calculated
69	Lipid fraction in diet	kg/kg	vld	------	0.500%	0.00000%	2.00%	2.00%	5.0000%	Calculated
70	Lipid fraction in gut	kg/kg	vlg	------	0.002141819	0	0.002364765	0.002364765	0.006149116	Calculated
71	Nonlipid organic matter fraction in diet	kg/kg	vnd	------	20.000%	4.00000%	20.00%	20.00%	22.0000%	Calculated
72	Nonlipid organic matter fraction in gut	kg/kg	vng	------	0.085672761	0.04	0.133018031	0.133018031	0.152190623	Calculated
73	Water fraction in diet	kg/kg	vwd	------	79.500%	96.00000%	78.00%	78.00%	73.0000%	Calculated
74	Water fraction in gut	kg/kg	vwg	------	0.91218542	0.96	0.864617204	0.864617204	0.841660261	Calculated
75	Water fraction in phytoplankton	kg/kg	vwp	------	------	------	------	------	------	Calculated
76	Dissolved oxygen concentration	mg O2/L	Cox	8.984	8.984	8.984	8.984	8.984	8.984	Calculated
77	Oxygen consumption	mg O2/day	Vox	------	0.027620153	0.551094499	49.1163489	49.1163489	980	Calculated
78										

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM



79	Concentration at steady-state	g/kg ww		0.004288951	0.001886765	0.001601368	0.003811208	0.005241391	0.008250697	Calculated
80	BAF at steady-state	L/kg	BAF	7756.654023	3412.251612	2995.171193	6892.645996	9479.160943	14921.55016	Calculated
81	BAF (freely dissolved) at steady-state	L/kg		8600.647196	3783.535036	3314.759391	7642.627386	17143251698	26985921181	Calculated
82	BSAF at steady-state	kg OC/kg lipid	BSAF		1.14E+01	9.71E+00	1.16E+01	1.06E+01	2.50E+01	Calculated
83										
84										
85										
86	Lipid Equivalent Concentration in organism	g/kg eq lip	Clpredator	0.285809763	0.062879171	0.053367897	0.07472096	0.073816468	0.164994019	Calculated
87	Lipid Equivalent Concentration in prey	g/kg eq lip	Clprey		0.285809763	0.008247025	0.058123534	0.058123534	0.067366922	Calculated
88	BMF	kg eq lipid/kg e	BMF		0.220003578	6.471169541	1.285554315	1.269992778	2.449184472	Calculated
89	Organism-Water Fugacity Ratio at steady-state	unitless	BAF		0.220003578	6.471169541	1.285554315	1.269992778	2.449184472	Calculated
90										

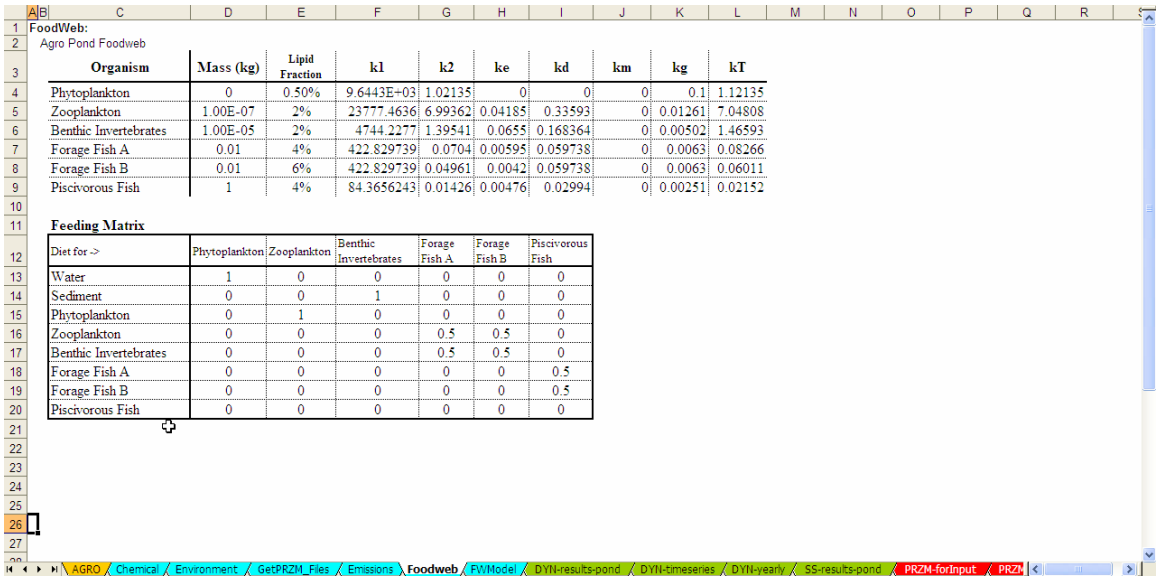
AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

Step 7 – Review the Foodweb tab

Go to the **Foodweb** tab. All values in this tab are automatically calculated from the **FWModel** tab. Thus, the user will never make any revisions to this tab.

The **Foodweb** tab summarizes the calculated k-values and the Feeding Matrix from the **FWModel tab**. The **Foodweb** tab is where the Bioaccumulation model actually reads in its input values to populate the foodweb and generate organism concentrations.

The page below displays a copy of the Foodweb tab with recommended calculated masses, lipid fractions, k-rates, and feeding matrix for the food web.



FoodWeb:

Agro Pond Foodweb

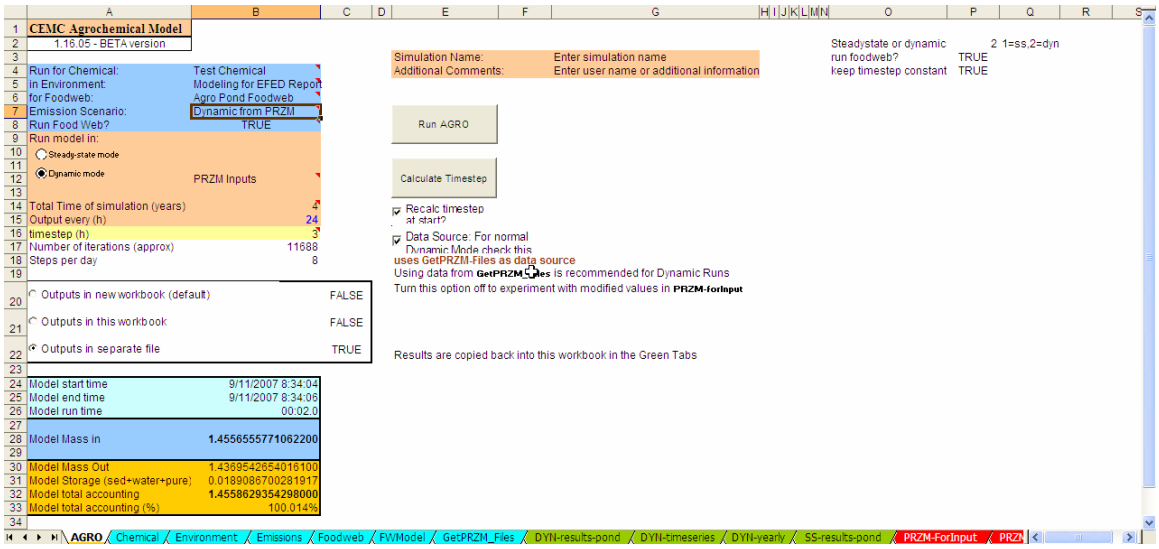
Organism	Mass (kg)	Lipid Fraction	k1	k2	ke	kd	km	kg	kT
Phytoplankton	0	0.50%	9.6443E+03	1.02135	0	0	0	0.1	1.12135
Zooplankton	1.00E-07	2%	23777.4636	6.99362	0.04185	0.33593	0	0.01261	7.04808
Benthic Invertebrates	1.00E-05	2%	4744.2277	1.39541	0.0655	0.168364	0	0.00502	1.46593
Forage Fish A	0.01	4%	422.829739	0.0704	0.00595	0.059738	0	0.0063	0.08266
Forage Fish B	0.01	6%	422.829739	0.04961	0.0042	0.059738	0	0.0063	0.06011
Piscivorous Fish	1	4%	84.3656243	0.01426	0.00476	0.02994	0	0.00251	0.02152

Feeding Matrix

Diet for ->	Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish
Water	1	0	0	0	0	0
Sediment	0	0	1	0	0	0
Phytoplankton	0	1	0	0	0	0
Zooplankton	0	0	0	0.5	0.5	0
Benthic Invertebrates	0	0	0	0.5	0.5	0
Forage Fish A	0	0	0	0	0	0.5
Forage Fish B	0	0	0	0	0	0.5
Piscivorous Fish	0	0	0	0	0	0

Step 8 – Confirm Run Parameters and Run Simulation

Go to the **AGRO** tab



In the above page, cells to be completed by the user are in tan.

The user may enter a name for the simulation in cell AGRO!G3. The user may enter additional comments about the simulation in cell AGRO!G4.

The Dynamic mode button should be selected.

Enter the number of years of the simulation in cell AGRO!B14. Make sure that this number of years is equal to the number of years in the beginning and ending year range entered in the **GetPRZM_Files** tab.

To output daily, enter “24” in cell AGRO!B15. The use of daily output is highly recommended as a default.

Set the minimum timestep to the recommended value of 3 hours by entering “3” in cell AGRO!B16.

Select the “Outputs in separate file” option. This saves the working values into a separate file during a model run which speeds up model execution. At the end of the run the results are read back into this spreadsheet for review.

Cell AGRO!B8 should be set to “TRUE” so that the Bioaccumulation model is run in addition to the QWASI water quality model.

Also, cell AGRO!P4 should also be set to “True” so the timestep set as constant (equal to 3 hours) for the entire simulation.

Examine cells AGRO!B4 – AGRO!B8 to make sure that the correct chemical, environmental scenario, foodweb, and dynamic simulation model options are selected.

Click the "Run AGRO" button to run the simulation.

To monitor the progress of a simulation, each simulation day number is displayed on the lower left-hand corner as it is being processed.

Upon completion of a simulation, Cells AGRO!B24 – AGRO!B33 displays the model run time and simulation mass balance.

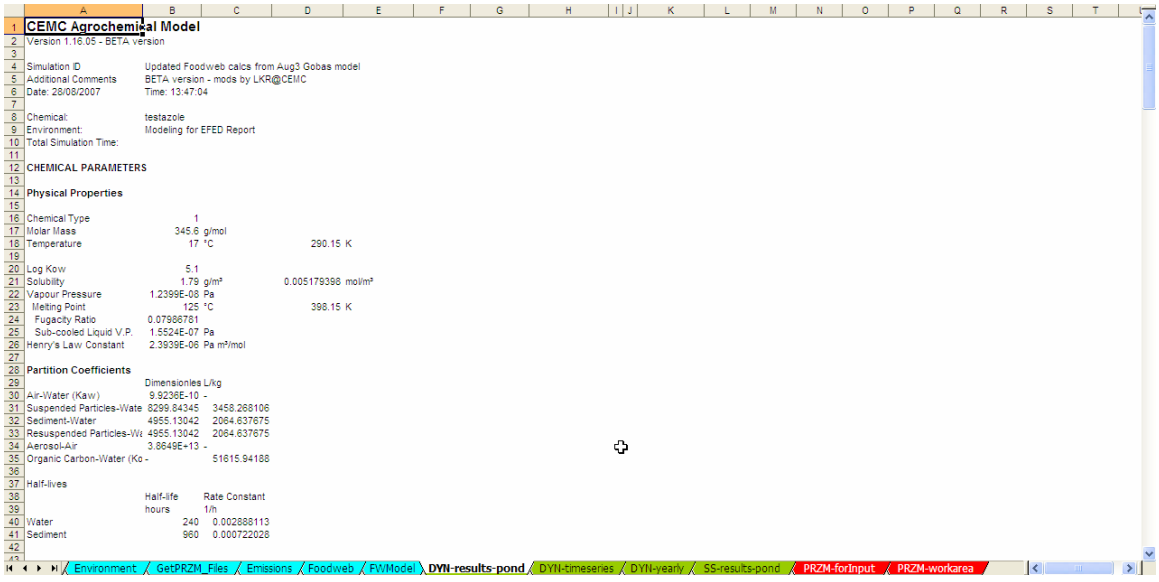
Step 9 – Examine the output from the simulation

The output from the dynamic mode simulation is displayed in tabs **DYN-results-pond**, **DYN-timeseries**, and **DYN-yearly**. (Note: You may see a tab named **SS-results-pond** which is intended to display output for steady-state simulations and is not relevant for dynamic simulations).

The results presented in the **DYN-results-pond** tab are in the same format as the QWASI model with the foodweb results output at the bottom. These results reflect the **conditions at the end of the simulation**.

The following series of pages display an example of output contained in the **DYN-results-pond** tab.

DYN-results-pond tab, Rows 1 - 43 display the model version number, scenario descriptors, and echoes of the chemical input parameters.

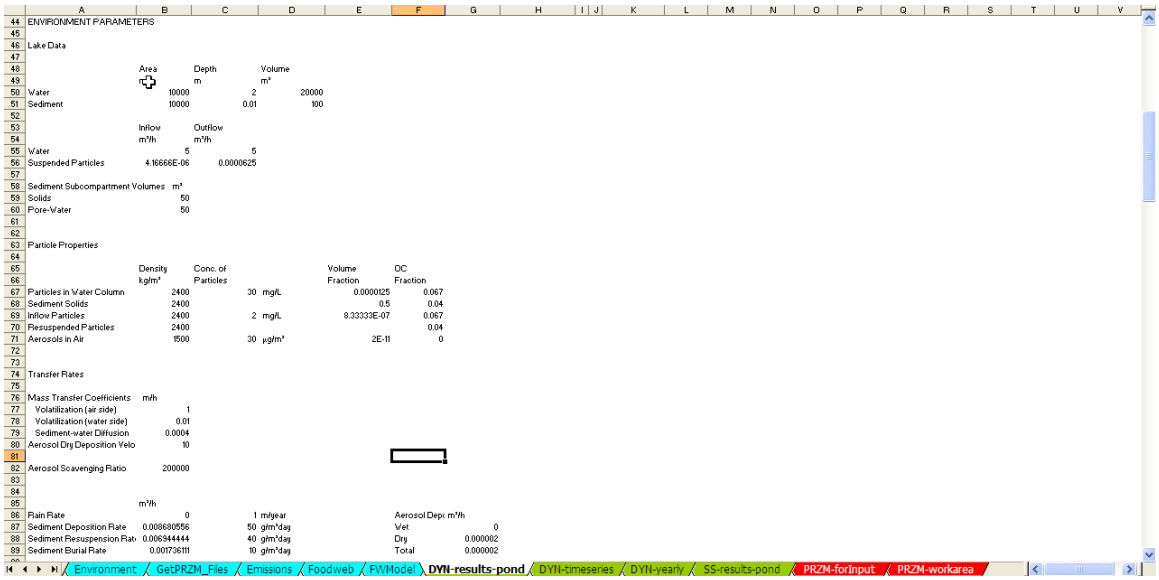


CEMC Agrochemical Model
Version 1.16.05 - BETA version

Simulation ID	Updated Foodweb calcs from Aug3 Gobas model				
Additional Comments	BETA version - mods by LKR@CEMC				
Date: 28/08/2007	Time: 13:47:04				
Chemical:	teatazole				
Environment:	Modeling for EFED Report				
Total Simulation Time:					
CHEMICAL PARAMETERS					
Physical Properties					
Chemical Type	1				
Molar Mass	345.6	g/mol			
Temperature	17	°C	290.15	K	
Log Kow	5.1				
Solubility	1.79	g/m³	0.005179398	mol/m³	
Vapour Pressure	1.2399E-08	Pa			
Melting Point	125	°C	398.15	K	
Fugacity Ratio	0.07986781				
Sub-cooled Liquid V.P.	1.5524E-07	Pa			
Henry's Law Constant	2.3939E-06	Pa m³/mol			
Partition Coefficients					
	Dimensionless	L/kg			
Air-Water (Kaw)	9.9236E-10	-			
Suspended Particles-Wate	8299.84345	3458.268106			
Sediment-Water	4955.13042	2064.637675			
Resuspended Particles-Wa	4955.13042	2064.637675			
Aerosol-Air	3.8649E+13	-			
Organic Carbon-Water (Ko	-	51615.94188			
Half-lives					
	Half-life	Rate Constant			
	hours	1/h			
Water	240	0.002888113			
Sediment	960	0.000722028			

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

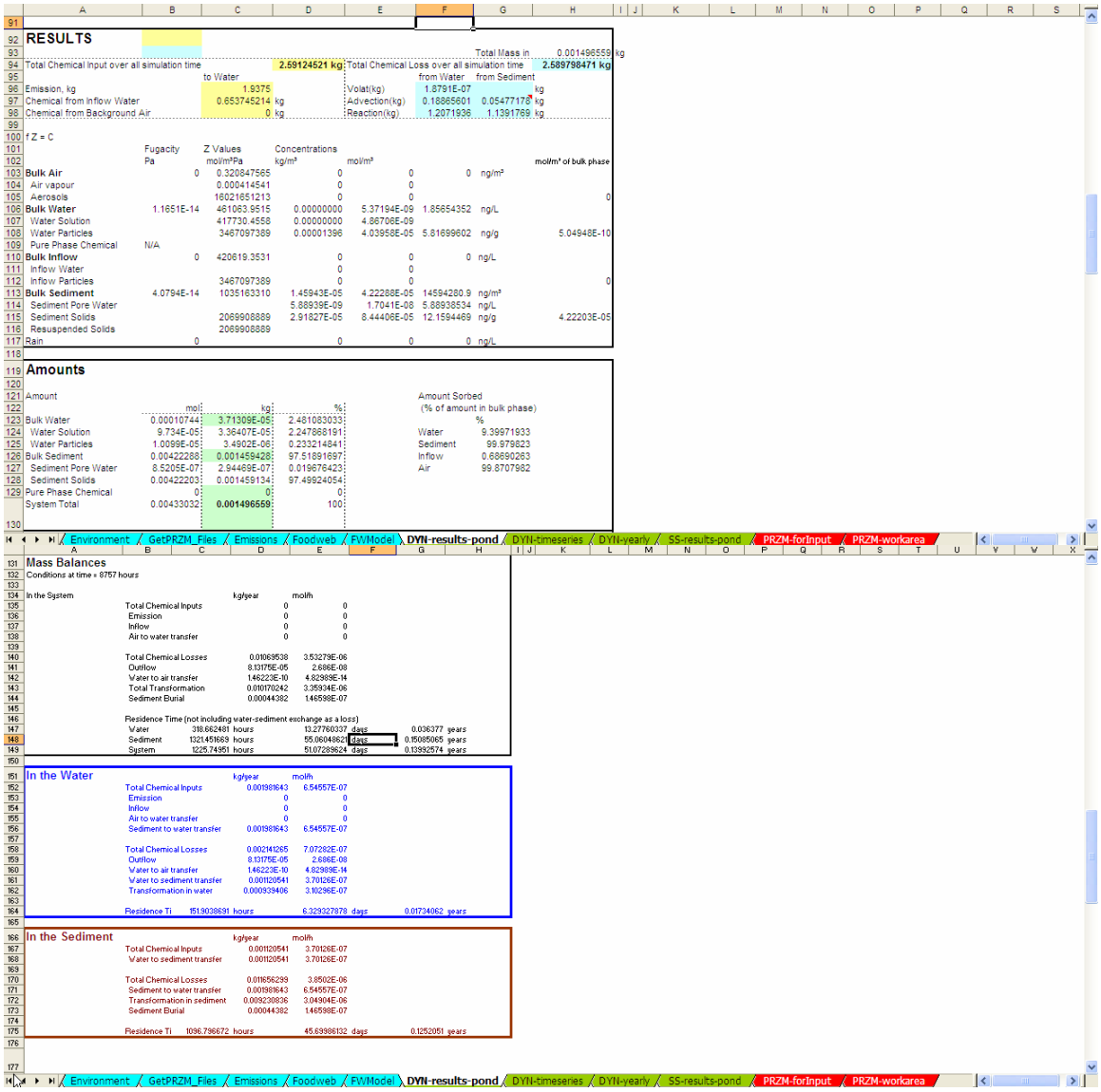
DYN-results-pond tab, Rows 44 - 91 display echoes of the environment input parameters.



	A	B	C	D	E	F	G	H
44	ENVIRONMENT PARAMETERS							
45								
46	Lake Data							
47								
48		Area	Depth	Volume				
49			m	m³				
50	Water	10000	2	20000				
51	Sediment	10000	0.01	100				
52								
53		Inflow	Outflow					
54		m³/h	m³/h					
55	Water	5	5					
56	Suspended Particles	4.16666E-06	0.0000625					
57								
58	Sediment Subcompartment Volumes	m³						
59	Solids	50						
60	Pore-Water	50						
61								
62								
63	Particle Properties							
64								
65		Density	Conc. of			Volume	OC	
66		kg/m³	Particles			Fraction	Fraction	
67	Particles in Water Column	2400	30	mg/L		0.0000125	0.067	
68	Sediment Solids	2400				0.5	0.04	
69	Inflow Particles	2400	2	mg/L		8.33333E-07	0.067	
70	Resuspended Particles	2400					0.04	
71	Aerosols in Air	1500	30	µg/m³		2E-11	0	
72								
73								
74	Transfer Rates							
75								
76	Mass Transfer Coefficients	m/h						
77	Volatilization (air side)	1						
78	Volatilization (water side)	0.01						
79	Sediment-water Diffusion	0.0004						
80	Aerosol Dry Deposition Velo	10						
81								
82	Aerosol Scavenging Ratio	200000						
83								
84								
85		m³/h						
86	Rain Rate	0	1	m/year		Aerosol Depc	m³/h	
87	Sediment Deposition Rate	0.008680556	50	g/m²/day		Wet	0	
88	Sediment Resuspension Rat	0.006944444	40	g/m²/day		Dry	0.000002	
89	Sediment Burial Rate	0.001736111	10	g/m²/day		Total	0.000002	

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

DYN-results-pond tab, Rows 92 - 228 display results from the QWASI water quality model. These include mass balances for the chemical in both water and benthic sediment.



RESULTS

Total Mass in					0.001496559	kg
Total Chemical Input over all simulation time			2.59124521	kg		
Total Chemical Loss over all simulation time					2.589798471	kg
	to Water				from Water	from Sediment
Emission, kg	1.9375					
Chemical from Inflow Water	0.653745214	kg				
Chemical from Background Air	0	kg				
Volat(kg)	1.8791E-07	kg				
Advection(kg)	0.18865601	0.05477175	kg			
Reaction(kg)	1.2071936	1.1391769	kg			

f Z = C

	Fugacity Pa	Z Values mol/m³Pa	Concentrations kg/m³	mol/m³			mol/m³ of bulk phase
Bulk Air	0	0.320847565	0	0	0	ng/m³	
Air vapour		0.000414541	0	0			
Aerosols		16021651213	0	0			0
Bulk Water	1.1651E-14	461063.9515	0.00000000	5.37194E-09	1.85654352	ng/L	
Water Solution		417730.4558	0.00000000	4.86706E-09			
Water Particles		3467097389	0.00001396	4.03958E-05	5.81699602	ng/g	5.04948E-10
Pure Phase Chemical	N/A						
Bulk Inflow	0	420619.3531	0	0	0	ng/L	
Inflow Water			0	0			
Inflow Particles		3467097389	0	0			0
Bulk Sediment	4.0794E-14	1035163310	1.45943E-05	4.22288E-05	14594280.9	ng/m³	
Sediment Pore Water			5.88939E-09	1.7041E-08	5.88938534	ng/L	
Sediment Solids		2069908889	2.91827E-05	8.44406E-05	12.1594469	ng/g	4.22203E-05
Resuspended Solids		2069908889					
Rain	0		0	0	0	ng/L	

Amounts

Amount	mol	kg	%	Amount Sorbed (% of amount in bulk phase)	%
Bulk Water	0.00010744	3.71309E-05	2.481083033		
Water Solution	9.734E-05	3.36407E-05	2.247868191	Water	9.39971933
Water Particles	1.0099E-05	3.4902E-06	0.233214841	Sediment	99.979823
Bulk Sediment	0.00422288	0.001459428	97.51891697	Inflow	0.68690263
Sediment Pore Water	8.5205E-07	2.94469E-07	0.019676423	Air	99.8707982
Sediment Solids	0.00422203	0.001459134	97.49924054		
Pure Phase Chemical	0	0	0		
System Total	0.00433032	**0.001496559**	100		

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | **DYN-results-pond** | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

Mass Balances

Conditions at time = 8757 hours

In the System		kg/year	mol/h
Total Chemical Inputs		0	0
Emission		0	0
Inflow		0	0
Air to water transfer		0	0
Total Chemical Losses		0.01069538	3.53279E-06
Outflow		8.13175E-05	2.68E-08
Water to air transfer		1.46223E-10	4.82989E-14
Total Transformation		0.010702	3.53934E-06
Sediment Burial		0.00044382	1.46598E-07

Residence Time (not including water-sediment exchange as a loss)

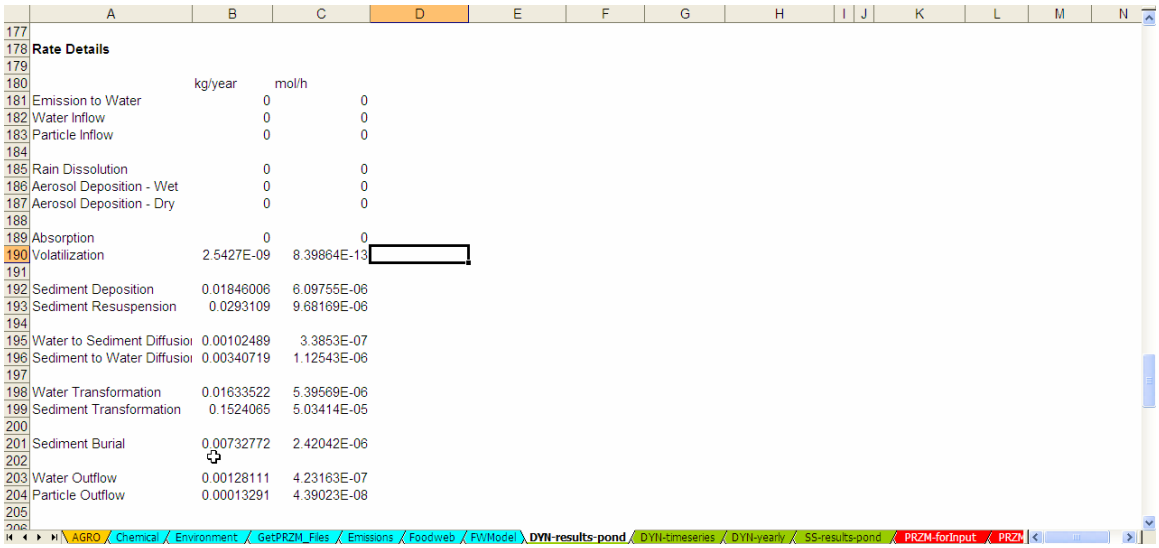
Water	318.662481	hours	13.2760337 days	0.036377 years
Sediment	1321.451669	hours	55.06048621 days	0.15085065 years
System	1225.74951	hours	51.07289624 days	0.13992574 years

In the Water		kg/year	mol/h
Total Chemical Inputs		0.001981643	6.54557E-07
Emission		0	0
Inflow		0	0
Air to water transfer		0	0
Sediment to water transfer		0.001981643	6.54557E-07
Total Chemical Losses		0.002141265	7.07282E-07
Outflow		8.13175E-05	2.68E-08
Water to air transfer		1.46223E-10	4.82989E-14
Water to sediment transfer		0.001120541	3.70126E-07
Transformation in water		0.000939406	3.10286E-07
Residence Ti	1513.938691	hours	63.23327878 days	0.01734062 years

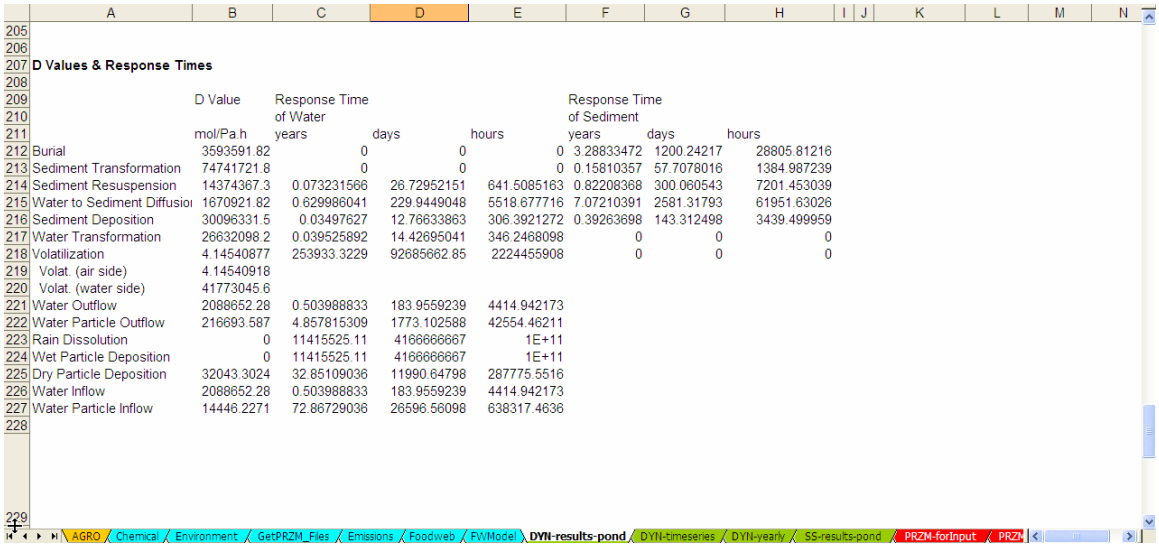
In the Sediment		kg/year	mol/h
Total Chemical Inputs		0.001120541	3.70126E-07
Water to sediment transfer		0.001120541	3.70126E-07
Total Chemical Losses		0.011656299	3.8502E-06
Sediment to water transfer		0.001981643	6.54557E-07
Transformation in sediment		0.009230836	3.04904E-06
Sediment Burial		0.00044382	1.46598E-07
Residence Ti	1096.796672	hours	45.69986132 days	0.1252051 years

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | **DYN-results-pond** | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

DYN-results-pond tab, Rows 92 - 228, continued.

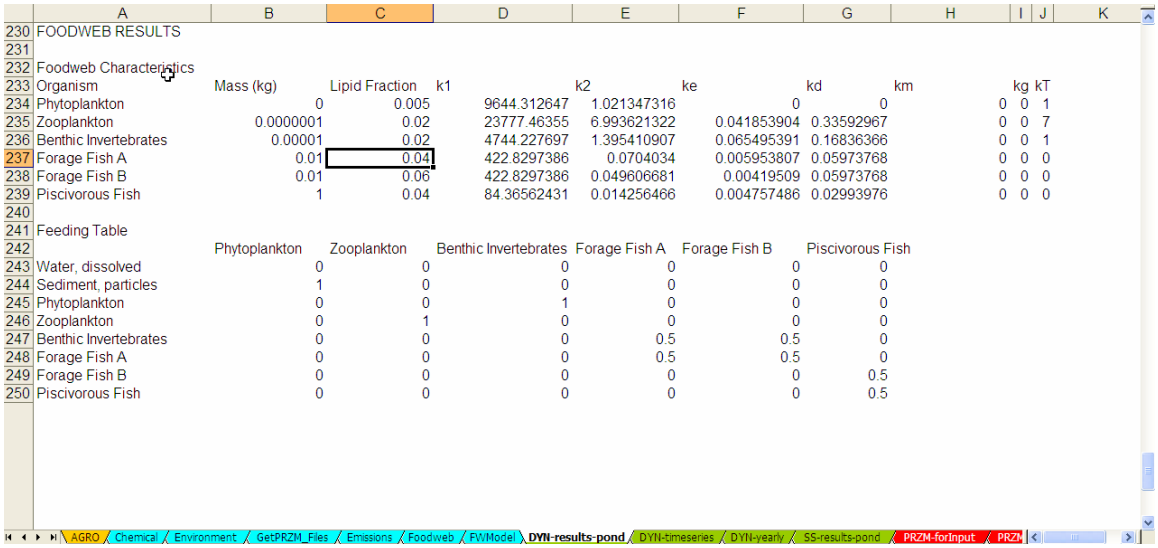


	A	B	C
177			
178	**Rate Details**		
179			
180		kg/year	mol/h
181	Emission to Water	0	0
182	Water Inflow	0	0
183	Particle Inflow	0	0
184			
185	Rain Dissolution	0	0
186	Aerosol Deposition - Wet	0	0
187	Aerosol Deposition - Dry	0	0
188			
189	Absorption	0	0
190	Volatilization	2.5427E-09	8.39864E-13
191			
192	Sediment Deposition	0.01846006	6.09755E-06
193	Sediment Resuspension	0.0293109	9.68169E-06
194			
195	Water to Sediment Diffusio	0.00102489	3.3853E-07
196	Sediment to Water Diffusio	0.00340719	1.12543E-06
197			
198	Water Transformation	0.01633522	5.39569E-06
199	Sediment Transformation	0.1524065	5.03414E-05
200			
201	Sediment Burial	0.00732772	2.42042E-06
202			
203	Water Outflow	0.00128111	4.23163E-07
204	Particle Outflow	0.00013291	4.39023E-08
205			



	A	B	C	D	E	F	G	H
205								
206								
207	**D Values & Response Times**							
208								
209		D Value	Response Time of Water			Response Time of Sediment		
210								
211		mol/Pa.h	years	days	hours	years	days	hours
212	Burial	3593591.82	0	0	0	3.28833472	1200.24217	28805.81216
213	Sediment Transformation	74741721.8	0	0	0	0.15810357	57.7078016	1384.987239
214	Sediment Resuspension	14374367.3	0.073231566	26.72952151	641.5085163	0.82208368	300.060543	7201.453039
215	Water to Sediment Diffusio	1670921.82	0.629986041	229.9449048	5518.677716	7.07210391	2581.31793	61951.63026
216	Sediment Deposition	30096331.5	0.03497627	12.76633863	306.3921272	0.39263698	143.312498	3439.499959
217	Water Transformation	26632098.2	0.039525892	14.42695041	346.2468098	0	0	0
218	Volatilization	4.14540877	253933.3229	92685662.85	2224455908	0	0	0
219	Volat. (air side)	4.14540918						
220	Volat. (water side)	41773045.6						
221	Water Outflow	2088652.28	0.503988833	183.9559239	4414.942173			
222	Water Particle Outflow	216693.587	4.857815309	1773.102588	42554.46211			
223	Rain Dissolution	0	11415525.11	4166666667	1E+11			
224	Wet Particle Deposition	0	11415525.11	4166666667	1E+11			
225	Dry Particle Deposition	32043.3024	32.85109036	11990.64798	287775.5516			
226	Water Inflow	2088652.28	0.503988833	183.9559239	4414.942173			
227	Water Particle Inflow	14446.2271	72.86729036	26596.56098	638317.4636			
228								
229								

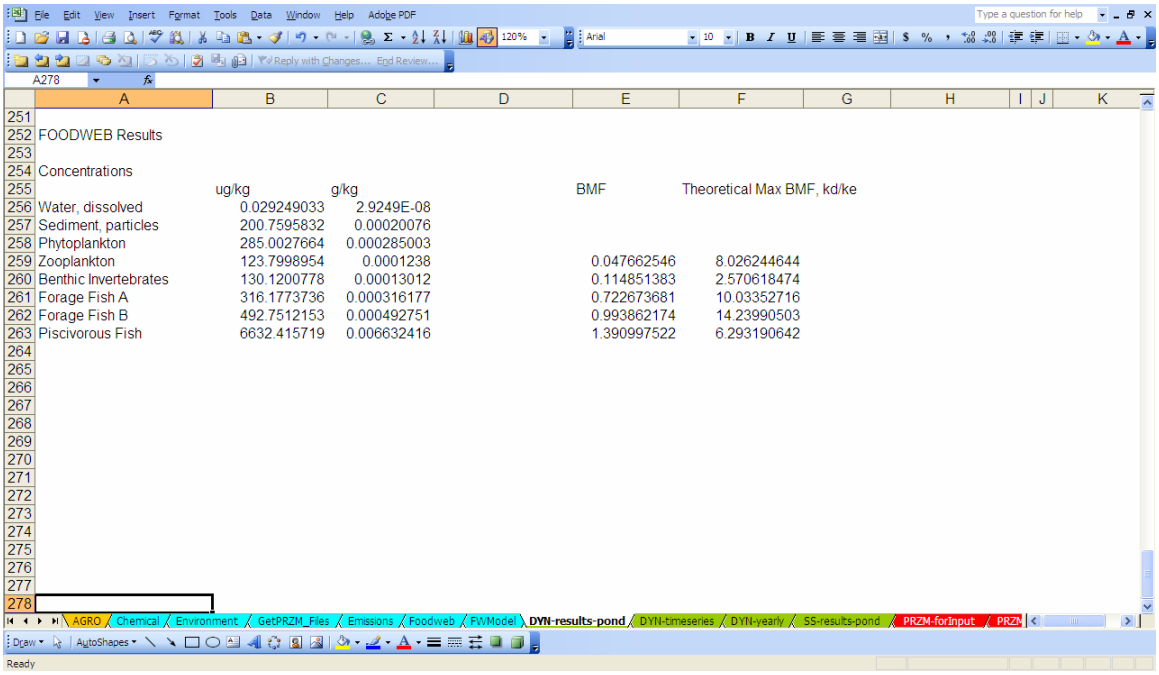
DYN-results-pond tab, Rows 229 - 250 display echoes of the input for the Food Web aquatic organism masses, lipid fraction, k-rates and feeding table matrix used by the Bioaccumulation model.



	A	B	C	D	E	F	G	H	I	J	K
230	FOODWEB RESULTS										
231											
232	Foodweb Characteristics										
233	Organism	Mass (kg)	Lipid Fraction	k1	k2	ke	kd	km	kg	kT	
234	Phytoplankton	0	0.005	9644.312647	1.021347316	0	0	0	0	1	
235	Zooplankton	0.0000001	0.02	23777.46355	6.993621322	0.041853904	0.33592967	0	0	7	
236	Benthic Invertebrates	0.00001	0.02	4744.227697	1.395410907	0.065495391	0.16836366	0	0	1	
237	Forage Fish A	0.01	0.04	422.8297386	0.0704034	0.005953807	0.05973768	0	0	0	
238	Forage Fish B	0.01	0.06	422.8297386	0.049606681	0.00419509	0.05973768	0	0	0	
239	Piscivorous Fish	1	0.04	84.36562431	0.014256466	0.004757486	0.02993976	0	0	0	
240											
241	Feeding Table										
242		Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish				
243	Water, dissolved	0	0	0	0	0	0				
244	Sediment, particles	1	0	0	0	0	0				
245	Phytoplankton	0	0	1	0	0	0				
246	Zooplankton	0	1	0	0	0	0				
247	Benthic Invertebrates	0	0	0	0.5	0.5	0				
248	Forage Fish A	0	0	0	0.5	0.5	0				
249	Forage Fish B	0	0	0	0	0	0.5				
250	Piscivorous Fish	0	0	0	0	0	0.5				

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

DYN-results-pond tab, Rows 251 - 263 display calculated results of pesticide concentrations from the Bioaccumulation model for each aquatic organism in the food web.



	A	B	C	D	E	F	G	H	I	J	K
251											
252	FOODWEB Results										
253											
254	Concentrations										
255		ug/kg	g/kg		BMF	Theoretical Max BMF, kd/ke					
256	Water, dissolved	0.029249033	2.9249E-08								
257	Sediment, particles	200.7595832	0.00020076								
258	Phytoplankton	285.0027664	0.000285003								
259	Zooplankton	123.7998954	0.0001238		0.047662546	8.026244644					
260	Benthic Invertebrates	130.1200778	0.00013012		0.114851383	2.570618474					
261	Forage Fish A	316.1773736	0.000316177		0.722673681	10.03352716					
262	Forage Fish B	492.7512153	0.000492751		0.993862174	14.23990503					
263	Piscivorous Fish	6632.415719	0.006632416		1.390997522	6.293190642					

AGRO | Chemical | Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM

The **DYN-timeseries** tab contains the values of selected output variables for each day of the simulation.

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!P** is displayed below. These columns summarize the daily simulation date, emission, fugacities for each bulk media, and bulk media chemical concentrations in natural units.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1							Fugacity, Pa						Bulk Concentrations (natural units)			
2	Time (h)	Year	Month	Day	Emission kg/year		Water	Sediment	Inflow	Air			Water, ng/L	Sediment, ng/m3	Inflow, ng/L	Air, ug/m3
3	0	1961	5	12	0		0	0	0	0			0	0	0	0
4	24	1961	5	13	0		1.3E-10	4.83385E-13	3.707E-10	0			20306.92813	172932040.5	71616.50282	0
5	48	1961	5	14	0		1.1E-10	1.35508E-12	0	0			17922.30308	484784687.3	0	0
6	72	1961	5	15	0		9.6E-11	2.09168E-12	0	0			15289.41262	748303193.9	0	0
7	96	1961	5	16	0		8.2E-11	2.6999E-12	0	0			13049.06468	965897203.9	0	0
8	120	1961	5	17	0		7E-11	3.1993E-12	0	0			11142.62027	1144556663	0	0
9	144	1961	5	18	0		6E-11	3.60647E-12	0	0			9520.202258	1290224549	0	0
10	168	1961	5	19	182.5		7.1E-11	3.93555E-12	0	0			11264.38615	1407953362	0	0
11	192	1961	5	20	0		1.9E-10	4.81545E-12	0	0			29842.88113	1722739580	0	0
12	216	1961	5	21	0		1.6E-10	5.98684E-12	0	0			25474.53025	2141805650	0	0
13	240	1961	5	22	0		1.4E-10	6.94633E-12	0	0			21757.15283	2485067301	0	0
14	264	1961	5	23	0		1.2E-10	7.72632E-12	0	0			18593.5109	2764108682	0	0
15	288	1961	5	24	0		1E-10	8.34432E-12	0	0			15900.89572	2988777956	0	0
16	312	1961	5	25	0		8.5E-11	8.85374E-12	0	0			13608.95676	3167446801	0	0
17	336	1961	5	26	182.5		1.1E-10	9.24447E-12	5.26211E-10	0			16771.90322	3307231133	254081.866	0
18	360	1961	5	27	0		2.9E-10	1.05366E-11	4.94791E-10	0			46946.14905	3769507763	164049.663	0
19	384	1961	5	28	0		2.7E-10	1.23803E-11	4.16959E-10	0			42979.92547	4429091717	108676.5174	0
20	408	1961	5	29	0		2.4E-10	1.39769E-11	1.6158E-10	0			37866.30352	5000259500	25011.56927	0
21	432	1961	5	30	0		2E-10	1.52963E-11	0	0			32482.18771	5472294134	0	0
22	456	1961	5	31	0		1.7E-10	1.63547E-11	0	0			27789.35146	5850918657	0	0
23	480	1961	6	1	0		1.5E-10	1.71897E-11	0	0			23794.613	6149649959	0	0
24	504	1961	6	2	182.5		1.5E-10	1.7836E-11	0	0			23518.71931	6380880634	0	0
25	528	1961	6	3	0		2.5E-10	1.894E-11	0	0			40376.78899	6775843983	0	0
26	552	1961	6	4	0		2.2E-10	2.02572E-11	0	0			34542.93204	7247060994	0	0

Environment | GetPRZM_Files | Emissions | Foodweb | FWModel | DYN-results-pond | DYN-timeseries | DYN-yearly | SS-results-pond | PRZM-forInput | PRZM-workarea

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!R - DYN-timeseries!Z** is displayed below. These columns summarize the daily chemical concentrations for aquatic organism in the food web.

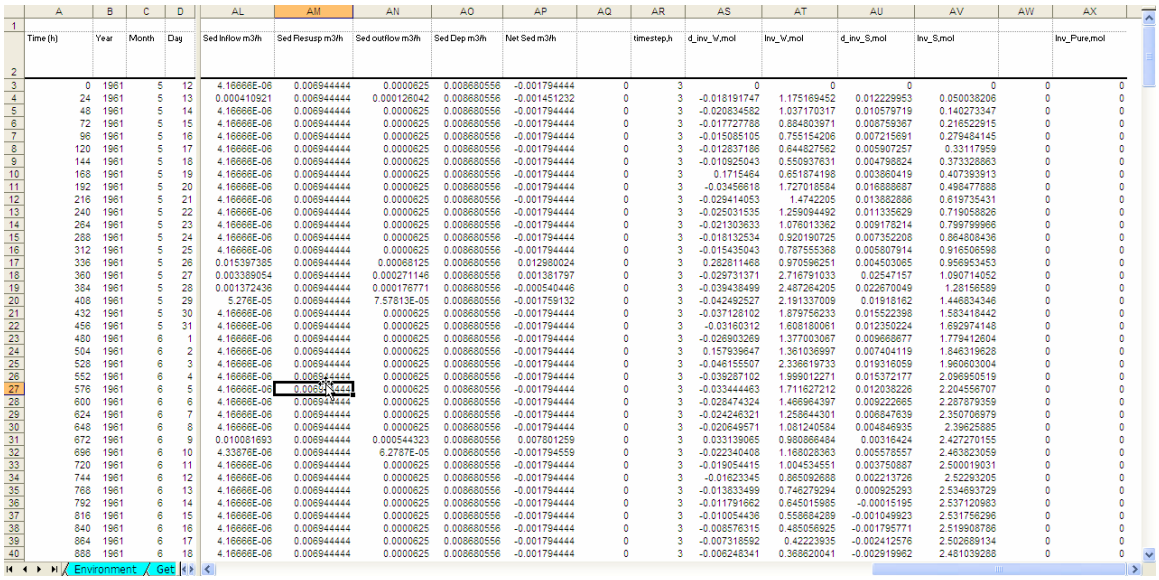
	A	B	C	D	Q	R	S	T	U	V	W	X	Y	Z
1						Foodweb Concentrations, ng/g								
2	Time (h)	Year	Month	Day		Water-dissolved only, ug/L	Sediment-solids only	Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish	
3	0	1961	5	12		0	0	0	0	0	0	0	0	
4	24	1961	5	13		18.3983639	144.0809566	78164.026	62030.63277	35014.77677	6133.13	6173.2782	1045.09162	
5	48	1961	5	14		16.2378599	403.9057268	120730.5011	57853.61079	48710.55016	15653.4	15920.994	2770.38887	
6	72	1961	5	15		13.8524239	623.4601737	120012.5353	50344.87764	45645.77312	23411.4	24086.13	4529.8241	
7	96	1961	5	16		11.822637	804.7519288	107526.3843	43278.37173	39801.94883	29311.7	30521.786	6281.82178	
8	120	1961	5	17		10.0953714	953.6047714	93352.90391	37063.51999	34187.51531	33624.6	35452.438	8003.56073	
9	144	1961	5	18		8.62543778	1074.970183	80230.63547	31714.04962	29281.80141	36629.6	39120.521	9676.38235	
10	168	1961	5	19		10.205693	1173.057733	71987.98925	35137.18164	26675.75931	38721.1	41891.534	11315.8057	
11	192	1961	5	20		27.038072	1435.326652	152532.9679	93506.25142	63046.36948	47362.8	51264.594	14135.0053	
12	216	1961	5	21		23.0802844	1784.477914	185511.8276	83122.19457	72569.92899	58259.2	63083.711	17518.9007	
13	240	1961	5	22		19.7122879	2070.471574	176000.4979	71974.19784	65764.42861	66493.8	72400.716	20831.8332	
14	264	1961	5	23		16.8459836	2302.959139	154528.7067	61832.62265	57018.28398	72273.9	79356.182	24044.9195	
15	288	1961	5	24		14.4064362	2490.145758	133660.5589	53004.93264	48987.85019	76005.2	84300.292	27132.017	
16	312	1961	5	25		12.3299071	2639.00642	114868.1109	45431.66969	42034.92367	78074.6	87576.734	30073.0551	
17	336	1961	5	26		15.1955813	2755.46986	103868.6877	52049.11296	38701.78198	79059.6	89730.105	32902.6031	
18	360	1961	5	27		42.5338745	3140.622656	235288.035	146759.0701	97859.66961	90918.1	102787.3	37580.7892	
19	384	1961	5	28		38.9404199	3690.165048	301279.5108	139552.5357	118842.1362	107564	120901.93	43273.4452	
20	408	1961	5	29		34.3074061	4166.042163	296263.1154	124823.7845	112323.3712	120998	136055.62	48969.7209	
21	432	1961	5	30		29.4293211	4559.32499	267006.4187	107893.5729	99106.75061	130635	147569.74	54516.7726	
22	456	1961	5	31		25.1775451	4874.781763	232734.7769	92627.09826	85579.76433	136799	155678.36	59835.0704	
23	480	1961	6	1		21.5582556	5123.674285	200606.8726	79461.94202	73552.68943	140104	160919.68	64888.0964	
24	504	1961	6	2		21.3082921	5316.327635	175613.9479	76196.64357	64804.72924	141267	163955.8	69681.969	

Environment | GetPRZM_Files | Emi

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AA - DYN-timeseries!AJ** is displayed below. These columns display the daily concentrations in the dissolved water column, benthic sediment and pore water along with the total daily input of chemical mass, total daily output of chemical mass, daily water inflow rate, daily water outflow rate, and net daily water volume flux.

	A	B	C	D	AA	AB	AC	AD	AE	AF	AH	AI	AJ
1													
2	Time (h)	Year	Month	Day	Water-dissolved only-ug/L-2	Sediment solids only ng/g	Conc porewater ug/L		SumInput, kg	SumLoss, kg	Water inflow m3/h	Water outflow m3/h	Net water m3/h
3	0	1961	5	12	0	0	0		0	0	5	5	0
4	24	1961	5	13	18.39836386	0.144080957	0.069785105		0.439666399	0.439666465	10.08333	10.08333	0
5	48	1961	5	14	16.23785987	0.403905727	0.195630319		0.454831194	0.454831721	5	5	0
6	72	1961	5	15	13.8524239	0.623460174	0.301970743		0.454831194	0.454831721	5	5	0
7	96	1961	5	16	11.82263701	0.804751929	0.389778768		0.454831194	0.454831721	5	5	0
8	120	1961	5	17	10.09537143	0.953604771	0.461875119		0.454831194	0.454831721	5	5	0
9	144	1961	5	18	8.625437785	1.074970183	0.520658029		0.454831194	0.454831721	5	5	0
10	168	1961	5	19	10.20569304	1.173057733	0.568166389		0.517331194	0.517331721	5	5	0
11	192	1961	5	20	27.03807204	1.435326652	0.695195418		0.954831194	0.954831721	5	5	0
12	216	1961	5	21	23.08028441	1.784477914	0.864305605		0.954831194	0.954831721	5	5	0
13	240	1961	5	22	19.71228793	2.070471574	1.002825628		0.954831194	0.954831721	5	5	0
14	264	1961	5	23	16.84598363	2.302959139	1.115430163		0.954831194	0.954831721	5	5	0
15	288	1961	5	24	14.40643623	2.490145758	1.206093344		0.954831194	0.954831721	5	5	0
16	312	1961	5	25	12.32990715	2.63900642	1.278193482		0.954831194	0.954831721	5	5	0
17	336	1961	5	26	15.19558134	2.75546986	1.33460214		1.058873579	1.058877616	54.5	54.5	0
18	360	1961	5	27	42.53387448	3.140622656	1.521149543		1.797845806	1.797875133	21.69167	21.69167	0
19	384	1961	5	28	38.94041986	3.690165048	1.787318469		1.87718513	1.877219789	14.14167	14.14167	0
20	408	1961	5	29	34.30740611	4.166042163	2.017807876		1.909914237	1.909950634	6.0625	6.0625	0
21	432	1961	5	30	29.4293211	4.55932499	2.208293031		1.913098522	1.913134945	5	5	0
22	456	1961	5	31	25.17754514	4.874781763	2.36108341		1.913098522	1.913134945	5	5	0
23	480	1961	6	1	21.55825564	5.123674285	2.481633628		1.913098522	1.913134945	5	5	0
24	504	1961	6	2	21.30829206	5.316327635	2.574944601		1.975598522	1.975634945	5	5	0

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AL - DYN-timeseries!AX** is displayed below. These columns display the particle solid fluxes in the water column and benthic sediment along with various water and sediment daily fluxes in mol basis.



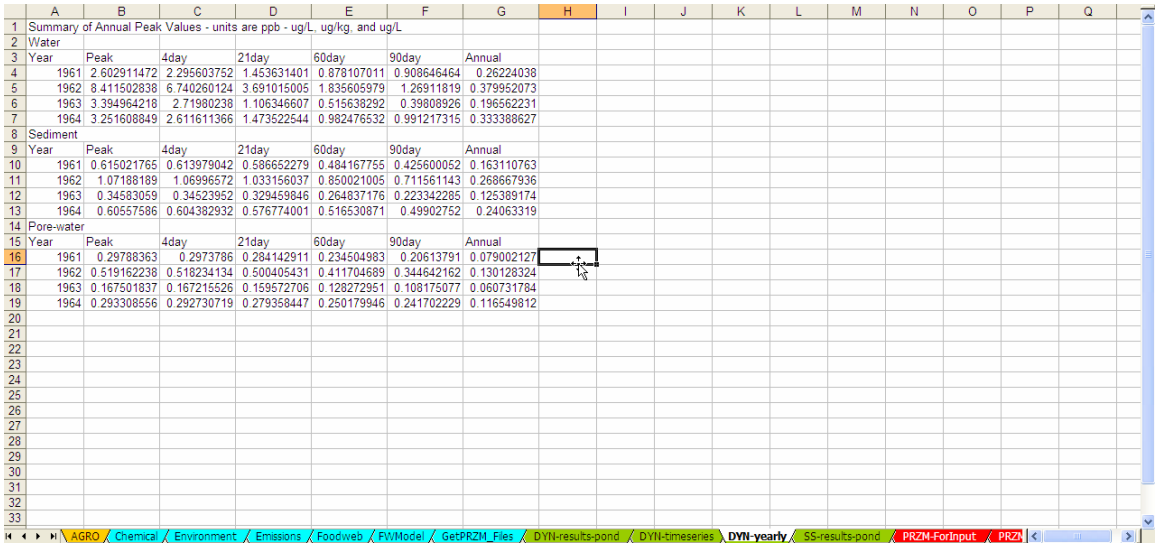
	A	B	C	D	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX
1																	
2	Time (h)	Year	Month	Day	Sed Inflow m3/h	Sed Resusp m3/h	Sed outflow m3/h	Sed Dep m3/h	Net Sed m3/h		timestep,h	d_inv_V,mol	Inv_V,mol	d_inv_S,mol	Inv_S,mol		Inv_Pure,mol
3	0	1961	5	12	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	0	0	0	0	0	0
4	24	1961	5	13	0.000410921	0.006944444	0.000126042	0.008680556	-0.001451232	0	3	-0.018191747	1.175169452	0.012229953	0.050038206	0	0
5	48	1961	5	14	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.020834582	1.037170317	0.010579719	0.140273347	0	0
6	72	1961	5	15	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.017727788	0.884803971	0.008759367	0.216522915	0	0
7	96	1961	5	16	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.015085105	0.755154206	0.007215691	0.279484145	0	0
8	120	1961	5	17	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.012837186	0.644827562	0.005907257	0.33117959	0	0
9	144	1961	5	18	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.010925043	0.550937631	0.004798824	0.373328863	0	0
10	168	1961	5	19	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	0.1715464	0.651874198	0.003860419	0.407393913	0	0
11	192	1961	5	20	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.03456618	1.727018584	0.016888687	0.498477888	0	0
12	216	1961	5	21	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.029414053	1.4742205	0.013882886	0.619735431	0	0
13	240	1961	5	22	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.025031535	1.259094492	0.011335629	0.719058826	0	0
14	264	1961	5	23	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.021303633	1.076013362	0.009178214	0.799799966	0	0
15	288	1961	5	24	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.018132534	0.920190725	0.007352208	0.864808436	0	0
16	312	1961	5	25	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.015435043	0.787555368	0.005807914	0.916506598	0	0
17	336	1961	5	26	0.015397385	0.006944444	0.00068125	0.008680556	0.012980024	0	3	0.282811468	0.970596251	0.004503065	0.956953453	0	0
18	360	1961	5	27	0.003389054	0.006944444	0.000271146	0.008680556	0.001381797	0	3	-0.029731371	2.716791033	0.02547157	1.090714052	0	0
19	384	1961	5	28	0.001372436	0.006944444	0.000176771	0.008680556	-0.000540446	0	3	-0.039438499	2.487264205	0.022670049	1.28156589	0	0
20	408	1961	5	29	5.276E-05	0.006944444	7.57813E-05	0.008680556	-0.001759132	0	3	-0.042492527	2.191337009	0.01918162	1.446834346	0	0
21	432	1961	5	30	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.037128102	1.879756233	0.015522398	1.583418442	0	0
22	456	1961	5	31	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.03160312	1.608180061	0.012350224	1.692974148	0	0
23	480	1961	6	1	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.026903269	1.377003067	0.009668677	1.779412604	0	0
24	504	1961	6	2	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	0.157939647	1.361036997	0.007404119	1.846319628	0	0
25	528	1961	6	3	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.046155507	2.336819733	0.019316059	1.960603004	0	0
26	552	1961	6	4	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.039287102	1.999012271	0.015372177	2.096950519	0	0
27	576	1961	6	5	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.033444463	1.711627212	0.012036226	2.204556707	0	0
28	600	1961	6	6	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.028474324	1.468964397	0.009222665	2.287879359	0	0
29	624	1961	6	7	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.024246321	1.258644301	0.008847639	2.350706979	0	0
30	648	1961	6	8	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.020649571	1.081240584	0.004846935	2.39625885	0	0
31	672	1961	6	9	0.010081693	0.006944444	0.000544323	0.008680556	0.007801259	0	3	0.033139065	0.980866484	0.00316424	2.427270155	0	0
32	696	1961	6	10	4.33876E-06	0.006944444	6.2787E-05	0.008680556	-0.001794559	0	3	-0.022340408	1.168028363	0.005578557	2.463823059	0	0
33	720	1961	6	11	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.019054415	1.004534551	0.003750887	2.500019031	0	0
34	744	1961	6	12	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.01623345	0.865092688	0.002213726	2.52293205	0	0
35	768	1961	6	13	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.013833499	0.746279294	0.000925293	2.534693729	0	0
36	792	1961	6	14	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.011791662	0.645015985	-0.00015195	2.537120983	0	0
37	816	1961	6	15	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.010054436	0.558684289	-0.001049923	2.531756296	0	0
38	840	1961	6	16	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.008576315	0.485056925	-0.001795771	2.519908786	0	0
39	864	1961	6	17	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.007318592	0.42223935	-0.002412576	2.502689134	0	0
40	888	1961	6	18	4.16666E-06	0.006944444	0.0000625	0.008680556	-0.001794444	0	3	-0.006248341	0.368620041	-0.002919962	2.481039288	0	0

The following table summarizes the columns in the columns of the **DYN-timeseries tab:**

Table 4: Summary of timeseries output parameters included with the model

Variable/Parameter	Description (if necessary)
Time (h)	
Year	From PRZM3.12
Month	From PRZM3.12
Day	From PRZM3.12
Emission kg/year	(if it occurs at this output interval)
Fugacity, Pa	
Water	
Sediment	
Inflow	
Air	
Pure Phase Chemical	
Bulk Concentrations (natural units)	
Water, ng/L	
Sediment, ng/m3	
Inflow, ng/L	
Air, ug/m3	
Foodweb Concentrations, ng/g	
Water-dissolved only, ug/L	
Sediment-solids only	
Phytoplankton	
Zooplankton	
Benthic Invertebrates	
Forage Fish A	
Forage Fish B	
Piscivorous Fish	
Other	
SumInput kg	Cumulative system Input of chemical
SumLoss kg	Cumulative system Loss of chemical
Water inflow m3/h	
Water outflow m3/h	
Net water m3/h	Inflow-Outflow
Sed Inflow m3/h	
Sed Resusp m3/h	
Sed outflow m3/h	
Sed Dep m3/h	
Net Sed m3/h	Inflow + Resusp – Outflow – Dep

The **DYN-yearly** tab contains the Estimated Environmental Concentrations (EECs) for the peak, 4-day, 21-day, 60-day, 90-day and Annual running averages for the chemical dissolved water column, benthic sediment sorbed chemical, and chemical dissolved in benthic pore water for each simulation year.



	A	B	C	D	E	F	G
1	Summary of Annual Peak Values - units are ppb - ug/L, ug/kg, and ug/L						
2	Water						
3	Year	Peak	4day	21day	60day	90day	Annual
4	1961	2.602911472	2.295603752	1.453631401	0.878107011	0.908646464	0.26224038
5	1962	8.411502838	6.740260124	3.691015005	1.835605979	1.26911819	0.379952073
6	1963	3.394964218	2.71980238	1.106346607	0.515638292	0.39808926	0.196562231
7	1964	3.251608849	2.611611366	1.473522544	0.982476532	0.991217315	0.333388627
8	Sediment						
9	Year	Peak	4day	21day	60day	90day	Annual
10	1961	0.615021765	0.613979042	0.586652279	0.484167755	0.425600052	0.163110763
11	1962	1.07188189	1.06996572	1.033156037	0.850021005	0.711561143	0.268667936
12	1963	0.34583059	0.34523952	0.329459846	0.264837176	0.223342285	0.125389174
13	1964	0.60557586	0.604382932	0.576774001	0.516530871	0.49902752	0.24063319
14	Pore-water						
15	Year	Peak	4day	21day	60day	90day	Annual
16	1961	0.29788363	0.2973786	0.284142911	0.23450498	0.20613791	0.079002127
17	1962	0.519162238	0.518234134	0.500405431	0.411704689	0.344642162	0.130128324
18	1963	0.167501837	0.167215526	0.159572706	0.128272951	0.108175077	0.060731784
19	1964	0.293308556	0.292730719	0.279358447	0.250179946	0.241702229	0.116549812

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