6.0 Specifications for the Chemical Properties Processor

The CPP gathers appropriate chemical properties data from the chemical properties database to supply necessary information to the SDP and modules within the MMSP. The CPP receives input from the chemical properties database. Output from the CPP provides the chemical portion of the SSFs and provides direct data to some modules within the MMSP.

6.1 Read and Write Expectations for the Chemical Properties Processor

Like all processors and modules, any errors that occur in the CPP are expected to be written to the GRF directory. The variable definitions for the header SSF can be found in Appendix A, Table A.1.1. The CPP is required to read and write in the following manner:

Call Arguments	**Description**
SSF_Dir	Call for Site Simulation Files Directory
GRF_Dir	Call for Global Results Files Directory
Header File Name	Header file contains all information needed to run entire simulation

Read expectations	Chemical Properties Database (format described in Section 6.2)
Write expectations	Chemical portion of the Site Simulation Files (format described in Section 7.2)

6.2 Chemical Properties Database Format

The chemical properties database consists of thirteen data tables, which are described in the sections following. Each file format is defined by the column definitions of the data. The data tables will be represented by a flat ASCII comma-separated values file that has the following general format:

1) First line will have number of rows in the data table, excluding the four header lines and the parameter Number of Columns in the data table
2) Second line will contain column names
3) Third line will contain column units
4) Fourth line will contain column data types
5) Fifth to End of File (EOF) will contain the rows of information.

An example would be:

```
5,3
“CHName"      ,”Volume"      ,”VolumeB"
              ,”mL”          ,”mL”
“String(32)”  ,”Real”        ,”Real”
“Ammonia”     ,              ,
“Acrylic Acid” ,4.96e+1      ,6.65e-2
“Acetamide”   ,4.19e+1       ,6.16e-2
“Acenapthene” ,1.22e+2       ,6.75e-2
“Acetic Acid” ,3.91e+1       ,6.16e-2
```

In Sections 6.2.1 through 6.2.13, Column, Units, and Types are defined for all the data tables read by the CPP. The Category and Description were added to clarify the intent of that column.

6.2.1 Format for the Organic Chemical Properties Data Table

This table provides data so that pH- and temperature-dependent organic chemical characteristics may be computed. Many of the organic chemical properties are defined by a two-parameter fit of the property based on temperature or pH. The data are expected to be defined in a comma-separated file that is formatted according the format specified in Section 6.2. Table 6.1 provides the composition of the Organic Chemical Properties Data Table.

Table 6.1 Composition of the Organic Chemical Properties Data Table

Column	Category	Name	Description	Units	Type
A	--	CHName	Standard name of Chemical	--	String(32)
B	--	CASNum	CAS number of chemical (including dashes)	--	String(32)
C	--	SMILES	SMILES String	--	String(32)
D	Air Diffusion	AirDifA	First parameter fit	cm^2/sec	Real
E	Air Diffusion	AirDifB	Second parameter fit	--	Real
F	Volume	VolumeA	First parameter fit	mL	Real
G	Volume	VolumeB	Second parameter fit	--	Real
H	Vapor Pressure	VPA	First parameter fit	torr	Real
I	Vapor Pressure	VPB	Second parameter fit	--	Real
J	Ka1	Ka1A	First parameter fit	mg/L	Real
K	Ka1	Ka1B	Second parameter fit	--	Real
L	Ka2	Ka2A	First parameter fit	mg/L	Real

Column	Category	Name	Description	Units	Type
M	Ka2	Ka2B	Second parameter fit	--	Real
N	Solubility	SolA	First parameter fit	mg/L	Real
O	Solubility	SolB	Second parameter fit	--	Real
P	Henry's Law Constant	HLCA	First parameter fit	atm m^3/mol	Real
Q	Henry's Law Constant	HLCB	Second parameter fit	--	Real
R	Kow	KowA	First parameter fit	--	Real
S	Kow	KowB	Second parameter fit	--	Real

6.2.2 Format for the Metals/Inorganic Chemical Properties Data Table

This table provides distributions for metal and inorganic chemical characteristics that will be sampled from. The solubility and partition coefficient (Kd) have distributions defined for the four environments of soil, sediment, surface water, and solid waste. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2. Table 6.2 provides the composition of the Metals/Inorganic Chemical Properties Data Table. The valid distribution types for tables 6.2, 6.5, and 6.6 are Constant, Normal, LogNormal, Exponential, Uniform, JohnsonSB, JohnsonSU, and Triangular. Tables 6.7 and 6.8 also allow an eighth distribution type (DEmp), which is a Discrete Empirical distribution that allows the user to enter a number of value that will have equal probabilty.

Table 6.2 Composition of the Metals/Inorganic Chemical Properties Data Table

Column	Category	Name	Description	Units	Type
A	--	CHName	Standard name of Chemical	--	String(32)
B	--	CASNum	CAS number of chemical (including dashes)	--	String(32)
C	--	MW	Molecular Weight	g/mole	Real
D	Soil	sol	solubility (most likely estimate)	mg/L	Real
E	Soil	sol_min	solubility (minimum estimate)	mg/L	Real
F	Soil	sol_max	solubility (maximum estimate)	mg/L	Real
G	Soil	sol_sd	solubility (standard deviation)	mg/L	Real
H	Soil	sol_dist	solubility (distribution type)	--	String(10)
I	Soil	Kd	partition coefficient (most likely estimate)	L/kg	Real

Column	Category	Name	Description	Units	Type
J	Soil	Kd_min	partition coefficient (minimum estimate)	L/kg	Real
K	Soil	Kd_max	partition coefficient (maximum estimate)	L/kg	Real
L	Soil	Kd_sd	partition coefficient (standard deviation)	L/kg	Real
M	Soil	Kd_dist	partition coefficient (distribution type)	--	String(10)
N	Sediment	sol	solubility (most likely estimate)	mg/L	Real
O	Sediment	sol_min	solubility (minimum estimate)	mg/L	Real
P	Sediment	sol_max	solubility (maximum estimate)	mg/L	Real
Q	Sediment	sol_sd	solubility (standard deviation)	mg/L	Real
R	Sediment	sol_dist	solubility (distribution type)	--	String(10)
S	Sediment	Kd	partition coefficient (most likely estimate)	L/kg	Real
T	Sediment	Kd_min	partition coefficient (minimum estimate)	L/kg	Real
U	Sediment	Kd_max	partition coefficient (maximum estimate)	L/kg	Real
V	Sediment	Kd_sd	partition coefficient (standard deviation)	L/kg	Real
W	Sediment	Kd_dist	partition coefficient (distribution type)	--	String(10)
X	Surface Water	sol	solubility (most likely estimate)	mg/L	Real
Y	Surface Water	sol_min	solubility (minimum estimate)	mg/L	Real
Z	Surface Water	sol_max	solubility (maximum estimate)	mg/L	Real
AA	Surface Water	sol_sd	solubility (standard deviation)	mg/L	Real
AB	Surface Water	sol_dist	solubility (distribution type)	--	String(10)
AC	Surface Water	Kd	partition coefficient (most likely estimate)	L/kg	Real
AD	Surface Water	Kd_min	partition coefficient (minimum estimate)	L/kg	Real
AE	Surface Water	Kd_max	partition coefficient (maximum estimate)	L/kg	Real

Column	Category	Name	Description	Units	Type
AF	Surface Water	Kd_sd	partition coefficient (standard deviation)	L/kg	Real
AG	Surface Water	Kd_dist	partition coefficient (distribution type)	--	String(10)

6.2.3 Format for the Catalyzation Data Table

The Catalyzation Data Table provides distributions and estimates for organic, metal, and inorganic chemical biodegradation and reduction that will be sampled from or used directly. This table also provides mass ratios and product identification for each chemical reduction and biodegradation. Many of the rates in this table are defined for certain ranges of pH and temperature. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2. Table 6.3 provides the composition of the Catalyzation Data Table.

Table 6.3. Composition of the Catalyzation Data Table

Column	Category	Name	Description	Units	Type
A	--	CHNAME	standard name of chemical	--	string (32)
B	--	CASNUM	CAS number of chemical (including dashes)	--	string (32)
C	Medium Independent	k_HA	acid-catalyzed hydrolysis rate constant	L/mole-day	real
D	Medium Independent	RXPNA(1)	name of reaction product 1	--	string (32)
E	Medium Independent	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
F	Medium Independent	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
G	Medium Independent	RXPNA(2)	name of reaction product 2	--	string (32)
H	Medium Independent	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
I	Medium Independent	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
J	Medium Independent	RXPNA(3)	name of reaction product 3	--	string (32)

Column	Category	Name	Description	Units	Type
K	Medium Independent	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
L	Medium Independent	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
M	Medium Independent	k_HN	neutral hydrolysis rate constant	day^{-1}	real
N	Medium Independent	RXPNA(1)	name of reaction product 1	--	string (32)
O	Medium Independent	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
P	Medium Independent	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
Q	Medium Independent	RXPNA(2)	name of reaction product 2	--	string (32)
R	Medium Independent	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
S	Medium Independent	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
T	Medium Independent	RXPNA(3)	name of reaction product 3	--	string (32)
U	Medium Independent	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
V	Medium Independent	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
W	Medium Independent	k_HB	base-catalyzed hydrolysis rate constant	L/mole-day	real
X	Medium Independent	RXPNA(1)	name of reaction product 1	--	string (32)
Y	Medium Independent	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
Z	Medium Independent	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
AA	Medium Independent	RXPNA(2)	name of reaction product 2	--	string (32)

Column	Category	Name	Description	Units	Type
AB	Medium Independent	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
AC	Medium Independent	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
AD	Medium Independent	RXPNA(3)	name of reaction product 3	--	string (32)
AE	Medium Independent	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
AF	Medium Independent	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real

6.2.4 Format for the Aerobic Biodegradation Data Table

Table 6.4 provides the properties required for distributions and estimates of the aerobic biodegradation rates of organic chemicals being addressed by the HWIR Assessment. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2.

Table 6.4 Composition of the Aerobic Biodegradation Data Table

Column	Category	Name	Description	Units	Type
A	Aerobic	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
B	Aerobic	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
C	Aerobic	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
D	Aerobic	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
E	Aerobic	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
F	Aerobic	RXPNA(1)	name of reaction product 1	--	string (32)
G	Aerobic	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
H	Aerobic	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
I	Aerobic	RXPNA(2)	name of reaction product 2	--	string (32)
J	Aerobic	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
K	Aerobic	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
L	Aerobic	RXPNA(3)	name of reaction product 3	--	string (32)
M	Aerobic	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
N	Aerobic	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real

6.2.5 Format for the Activated Biodegradation Data Table

Table 6.5 provides the properties required for distributions and estimates of the activated biodegradation rates of organic chemicals being addressed by the HWIR Assessment. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2.

Table 6.5 Composition of the Activated Biodegradation Data Table

Column	Category	Name	Description	Units	Type
A	Activated	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
B	Activated	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
C	Activated	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
D	Activated	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
E	Activated	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
F	Activated	RXPNA(1)	name of reaction product 1	--	string (32)
G	Activated	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
H	Activated	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
I	Activated	RXPNA(2)	name of reaction product 2	--	string (32)
J	Activated	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
K	Activated	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
L	Activated	RXPNA(3)	name of reaction product 3	--	string (32)
M	Activated	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
N	Activated	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real

6.2.6 Format for the Anaerobic Biodegradation Data Table

Table 6.6 provides distributions and estimates for organic, metal, and inorganic chemical biodegradation and reduction that will be sampled from or used directly. This table also provides mass ratios and product identification for each chemical reduction and biodegradation. Many of the rates in this table are defined for certain ranges of pH and temperature. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2.

Table 6.6 Composition of the Anaerobic Biodegradation Data Table

Column	Category	Name	Description	Units	Type
A	Anaerobic	k_red	reduction rate constant (most likely estimate)	day^{-1}	real
B	Anaerobic	k_red_min	reduction rate constant (minimum estimate)	day^{-1}	real
C	Anaerobic	k_red_max	reduction rate constant (maximum estimate)	day^{-1}	real
D	Anaerobic	k_red_sd	reduction rate constant (standard deviation)	day^{-1}	real
E	Anaerobic	k_red_dist	reduction rate constant (distribution type)	--	string (32)
F	Anaerobic	RXPNA(1)	name of reaction product 1	--	string (32)
G	Anaerobic	RXPNUM(1)	CAS number of reaction product 1	--	string (3P)
H	Anaerobic	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
I	Anaerobic	RXPNA(2)	name of reaction product 2	--	string (32)
J	Anaerobic	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
K	Anaerobic	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
L	Anaerobic	RXPNA(3)	name of reaction product 3	--	string (32)
M	Anaerobic	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
N	Anaerobic	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real

Column	Category	Name	Description	Units	Type
O	Anaerobic T<15 pH<6	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
P	Anaerobic T<15 pH<6	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
Q	Anaerobic T<15 pH<6	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
R	Anaerobic T<15 pH<6	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
S	Anaerobic T<15 pH<6	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
T	Anaerobic T<15 pH<6	RXPNA(1)	name of reaction product 1	--	string (32)
U	Anaerobic T<15 pH<6	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
V	Anaerobic T<15 pH<6	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
W	Anaerobic T<15 pH<6	RXPNA(2)	name of reaction product 2	--	string (32)
X	Anaerobic T<15 pH<6	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
Y	Anaerobic T<15 pH<6	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
Z	Anaerobic T<15 pH<6	RXPNA(3)	name of reaction product 3	--	string (32)

Column	Category	Name	Description	Units	Type
AA	Anaerobic T<15 pH<6	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
AB	Anaerobic T<15 pH<6	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
AC	Anaerobic T<15 6<pH<8	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
AD	Anaerobic T<15 6<pH<8	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
AE	Anaerobic T<15 6<pH<8	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
AF	Anaerobic T<15 6<pH<8	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
AG	Anaerobic T<15 6<pH<8	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
AH	Anaerobic T<15 6<pH<8	RXPNA(1)	name of reaction product 1	--	string (32)
AI	Anaerobic T<15 6<pH<8	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
AJ	Anaerobic T<15 6<pH<8	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
AK	Anaerobic T<15 6<pH<8	RXPNA(2)	name of reaction product 2	--	string (32)
AL	Anaerobic T<15 6<pH<8	RXPNUM(2)	CAS number of reaction product 2	--	string (32)

Column	Category	Name	Description	Units	Type
AM	Anaerobic T<15 6<pH<8	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
AN	Anaerobic T<15 6<pH<8	RXPNA(3)	name of reaction product 3	--	string (32)
AO	Anaerobic T<15 6<pH<8	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
AP	Anaerobic T<15 6<pH<8	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
AQ	Anaerobic T<15 pH>8	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
AR	Anaerobic T<15 pH>8	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
AS	Anaerobic T<15 pH>8	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
AT	Anaerobic T<15 pH>8	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
AU	Anaerobic T<15 pH>8	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
AV	Anaerobic T<15 pH>8	RXPNA(1)	name of reaction product 1	--	string (32)
AW	Anaerobic T<15 pH>8	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
AX	Anaerobic T<15 pH>8	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real

Column	Category	Name	Description	Units	Type
AY	Anaerobic T<15 pH>8	RXPNA(2)	name of reaction product 2	--	string (32)
AZ	Anaerobic T<15 pH>8	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
BA	Anaerobic T<15 pH>8	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
BB	Anaerobic T<15 pH>8	RXPNA(3)	name of reaction product 3	--	string (32)
BC	Anaerobic T<15 pH>8	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
BD	Anaerobic T<15 pH>8	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
BE	Anaerobic T>15 pH<6	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
BF	Anaerobic T>15 pH<6	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
BG	Anaerobic T>15 pH<6	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
BH	Anaerobic T>15 pH<6	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
BI	Anaerobic T>15 pH<6	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
BJ	Anaerobic T>15 pH<6	RXPNA(1)	name of reaction product 1	--	string (32)

Column	Category	Name	Description	Units	Type
BK	Anaerobic T>15 pH<6	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
BL	Anaerobic T>15 pH<6	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
BM	Anaerobic T>15 pH<6	RXPNA(2)	name of reaction product 2	--	string (32)
BN	Anaerobic T>15 pH<6	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
BO	Anaerobic T>15 pH<6	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
BP	Anaerobic T>15 pH<6	RXPNA(3)	name of reaction product 3	--	string (32)
BQ	Anaerobic T>15 pH<6	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
BR	Anaerobic T>15 pH<6	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
BS	Anaerobic T>15 6<pH<8	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
BT	Anaerobic T>15 6<pH<8	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real
BU	Anaerobic T>15 6<pH<8	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
BW	Anaerobic T>15 6<pH<8	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real

Column	Category	Name	Description	Units	Type
BX	Anaerobic T>15 6<pH<8	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
BY	Anaerobic T>15 6<pH<8	RXPNA(1)	name of reaction product 1	--	string (32)
BZ	Anaerobic T>15 6<pH<8	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
CA	Anaerobic T>15 6<pH<8	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
CB	Anaerobic T>15 6<pH<8	RXPNA(2)	name of reaction product 2	--	string (32)
CC	Anaerobic T>15 6<pH<8	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
CD	Anaerobic T>15 6<pH<8	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
CE	Anaerobic T>15 6<pH<8	RXPNA(3)	name of reaction product 3	--	string (32)
CF	Anaerobic T>15 6<pH<8	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
CG	Anaerobic T>15 6<pH<8	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real
CH	Anaerobic T>15 pH>8	k_bio	biodegradation rate constant (most likely estimate)	day^{-1}	real
CI	Anaerobic T>15 pH>8	k_bio_min	biodegradation rate constant (minimum estimate)	day^{-1}	real

Column	Category	Name	Description	Units	Type
CJ	Anaerobic T>15 pH>8	k_bio_max	biodegradation rate constant (maximum estimate)	day^{-1}	real
CK	Anaerobic T>15 pH>8	k_bio_sd	biodegradation rate constant (standard deviation)	day^{-1}	real
CL	Anaerobic T>15 pH>8	k_bio_dist	biodegradation rate constant (distribution type)	--	string (32)
CM	Anaerobic T>15 pH>8	RXPNA(1)	name of reaction product 1	--	string (32)
CN	Anaerobic T>15 pH>8	RXPNUM(1)	CAS number of reaction product 1	--	string (32)
CO	Anaerobic T>15 pH>8	YCOEF(1)	molar yield coefficient for reaction 1	moles/ mole	real
CP	Anaerobic T>15 pH>8	RXPNA(2)	name of reaction product 2	--	string (32)
CQ	Anaerobic T>15 pH>8	RXPNUM(2)	CAS number of reaction product 2	--	string (32)
CR	Anaerobic T>15 pH>8	YCOEF(2)	molar yield coefficient for reaction 2	moles/ mole	real
CS	Anaerobic T>15 pH>8	RXPNA(3)	name of reaction product 3	--	string (32)
CT	Anaerobic T>15 pH>8	RXPNUM(3)	CAS number of reaction product 3	--	string (32)
CU	Anaerobic T>15 pH>8	YCOEF(3)	molar yield coefficient for reaction 3	moles/ mole	real

6.2.7 Format for the SO_4 and the Methanogenic Reduction Biodegradation Data Table

Table 6.7 provides distributions and estimates for organic, metal, and inorganic chemical SO_4 biodegradation and reduction and methanogenic biodegradation and reduction that will be sampled from or used directly. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2. The MethBio and SO4Bio tables are of identical format, but are stored in two separate files. The MethBio.csv file contains the methanogenic biodegradation rates, and the SO4Bio.csv file contains the sulfate-reducing biodegradation rates.

Table 6.7. Composition of the SO_4 and the Methanogenic Reduction Biodegradation Data Table

Column	Name	Description	Units	Type
A	Name	Chemical Name	-	String(32)
B	CASID	Chemical Abstract ID	-	String(32)
C	k_bio T<15 pH<6	biodegradation rate constant (most likely estimate)	day^-1	Real
D	k_bio T<15 pH<6_min	biodegradation rate constant (minimum estimate)	day^-1	Real
E	k_bio T<15 pH<6_max	biodegradation rate constant (maximum estimate)	day^-1	Real
F	k_bio T<15 pH<6_sd	biodegradation rate constant (standard deviation)	day^-1	Real
G	k_bio T<15 pH<6_p5	literature biodegradation rate constant 5	day^-1	Real
H	k_bio T<15 pH<6_p6		day^-1	Real
I	k_bio T<15 pH<6_p7		day^-1	Real
J	k_bio T<15 pH<6_p8		day^-1	Real
K	k_bio T<15 pH<6_p9		day^-1	Real
L	k_bio T<15 pH<6_p10		day^-1	Real
M	k_bio T<15 pH<6_p11		day^-1	Real
N	k_bio T<15 pH<6_p12		day^-1	Real
O	k_bio T<15 pH<6_p13		day^-1	Real
P	k_bio T<15 pH<6_p14		day^-1	Real
Q	k_bio T<15 pH<6_p15		day^-1	Real
R	k_bio T<15 pH<6_dist	biodegradation rate constant (distribution type)	-	String(10)
S	T<15 pH<6RXPNA(1)	name of reaction product 1	-	String(32)
T	T<15 pH<6RXPNUM(1)	CAS number of reaction product 1	-	String(32)
U	T<15 pH<6YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
V	T<15 pH<6RXPNA(2)	name of reaction product 2	-	String(32)
W	T<15 pH<6RXPNUM(2)	CAS number of reaction product 2	-	String(32)
X	T<15 pH<6YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
Y	T<15 pH<6RXPNA(3)	name of reaction product 3	-	String(32)
Z	T<15 pH<6RXPNUM(3)	CAS number of reaction product 3	-	String(32)

Column	Name	Description	Units	Type
AA	T<15 pH<6YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real
AB	k_bio T<15 6<=pH<=8	biodegradation rate constant (most likely estimate)	day^-1	Real
AC	k_bio T<15 6<=pH<=8_min	biodegradation rate constant (minimum estimate)	day^-1	Real
AD	k_bio T<15 6<=pH<=8_max	biodegradation rate constant (maximum estimate)	day^-1	Real
AE	k_bio T<15 6<=pH<=8_sd	biodegradation rate constant (standard deviation)	day^-1	Real
AF	k_bio T<15 6<=pH<=8_p5	literature biodegradation rate constant 5	day^-1	Real
AG	k_bio T<15 6<=pH<=8_p6		day^-1	Real
AH	k_bio T<15 6<=pH<=8_p7		day^-1	Real
AI	k_bio T<15 6<=pH<=8_p8		day^-1	Real
AJ	k_bio T<15 6<=pH<=8_p9		day^-1	Real
AK	k_bio T<15 6<=pH<=8_p10		day^-1	Real
AL	k_bio T<15 6<=pH<=8_p11		day^-1	Real
AM	k_bio T<15 6<=pH<=8_p12		day^-1	Real
AN	k_bio T<15 6<=pH<=8_p13		day^-1	Real
AO	k_bio T<15 6<=pH<=8_p14		day^-1	Real
AP	k_bio T<15 6<=pH<=8_p15		day^-1	Real
AQ	k_bio T<15 6<=pH<=8_dist	biodegradation rate constant (distribution type)	-	String(10)
AR	T<15 6<=pH<=8RXPNA(1)	name of reaction product 1	-	String(32)
AS	T<15 6<=pH<=8RXPNUM(1)	CAS number of reaction product 1	-	String(32)
AT	T<15 6<=pH<=8YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
AU	T<15 6<=pH<=8RXPNA(2)	name of reaction product 2	-	String(32)
AV	T<15 6<=pH<=8RXPNUM(2)	CAS number of reaction product 2	-	String(32)
AW	T<15 6<=pH<=8YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
AX	T<15 6<=pH<=8RXPNA(3)	name of reaction product 3	-	String(32)
AY	T<15 6<=pH<=8RXPNUM(3)	CAS number of reaction product 3	-	String(32)
AZ	T<15 6<=pH<=8YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real
BA	k_bio T<15 pH>8	biodegradation rate constant (most likely estimate)	day^-1	Real
BB	k_bio T<15 pH>8_min	biodegradation rate constant (minimum estimate)	day^-1	Real
BC	k_bio T<15 pH>8_max	biodegradation rate constant (maximum estimate)	day^-1	Real
BD	k_bio T<15 pH>8_sd	biodegradation rate constant (standard deviation)	day^-1	Real
BE	k_bio T<15 pH>8_p5	literature biodegradation rate constant 5	day^-1	Real
BF	k_bio T<15 pH>8_p6		day^-1	Real
BG	k_bio T<15 pH>8_p7		day^-1	Real
BH	k_bio T<15 pH>8_p8		day^-1	Real
BI	k_bio T<15 pH>8_p9		day^-1	Real
BJ	k_bio T<15 pH>8_p10		day^-1	Real

Column	Name	Description	Units	Type
BK	k_bio T<15 pH>8_p11		day^-1	Real
BL	k_bio T<15 pH>8_p12		day^-1	Real
BM	k_bio T<15 pH>8_p13		day^-1	Real
BN	k_bio T<15 pH>8_p14		day^-1	Real
BO	k_bio T<15 pH>8_p15		day^-1	Real
BP	k_bio T<15 pH>8_dist	biodegradation rate constant (distribution type)	-	String(10)
BQ	T<15 pH>8RXPNA(1)	name of reaction product 1	-	String(32)
BR	T<15 pH>8RXPNUM(1)	CAS number of reaction product 1	-	String(32)
BS	T<15 pH>8YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
BT	T<15 pH>8RXPNA(2)	name of reaction product 2	-	String(32)
BU	T<15 pH>8RXPNUM(2)	CAS number of reaction product 2	-	String(32)
BV	T<15 pH>8YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
BW	T<15 pH>8RXPNA(3)	name of reaction product 3	-	String(32)
BX	T<15 pH>8RXPNUM(3)	CAS number of reaction product 3	-	String(32)
BY	T<15 pH>8YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real
BZ	k_bio T>=15 pH<6	biodegradation rate constant (most likely estimate)	day^-1	Real
CA	k_bio T>=15 pH<6_min	biodegradation rate constant (minimum estimate)	day^-1	Real
CB	k_bio T>=15 pH<6_max	biodegradation rate constant (maximum estimate)	day^-1	Real
CC	k_bio T>=15 pH<6_sd	biodegradation rate constant (standard deviation)	day^-1	Real
CD	k_bio T>=15 pH<6_p5	literature biodegradation rate constant 5	day^-1	Real
CE	k_bio T>=15 pH<6_p6		day^-1	Real
CF	k_bio T>=15 pH<6_p7		day^-1	Real
CG	k_bio T>=15 pH<6_p8		day^-1	Real
CH	k_bio T>=15 pH<6_p9		day^-1	Real
CI	k_bio T>=15 pH<6_p10		day^-1	Real
CJ	k_bio T>=15 pH<6_p11		day^-1	Real
CK	k_bio T>=15 pH<6_p12		day^-1	Real
CL	k_bio T>=15 pH<6_p13		day^-1	Real
CM	k_bio T>=15 pH<6_p14		day^-1	Real
CN	k_bio T>=15 pH<6_p15		day^-1	Real
CO	k_bio T>=15 pH<6_dist	biodegradation rate constant (distribution type)	-	String(10)
CP	T>=15 pH<6RXPNA(1)	name of reaction product 1	-	String(32)
CQ	T>=15 pH<6RXPNUM(1)	CAS number of reaction product 1	-	String(32)
CR	T>=15 pH<6YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
CS	T>=15 pH<6RXPNA(2)	name of reaction product 2	-	String(32)
CT	T>=15 pH<6RXPNUM(2)	CAS number of reaction product 2	-	String(32)

Column	Name	Description	Units	Type
CU	T>=15 pH<6YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
CV	T>=15 pH<6RXPNA(3)	name of reaction product 3	-	String(32)
CW	T>=15 pH<6RXPNUM(3)	CAS number of reaction product 3	-	String(32)
CX	T>=15 pH<6YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real
CY	k_bio T>=15 6<=pH<=8	biodegradation rate constant (most likely estimate)	day^-1	Real
CZ	k_bio T>=15 6<=pH<=8_min	biodegradation rate constant (minimum estimate)	day^-1	Real
DA	k_bio T>=15 6<=pH<=8_max	biodegradation rate constant (maximum estimate)	day^-1	Real
DB	k_bio T>=15 6<=pH<=8_sd	biodegradation rate constant (standard deviation)	day^-1	Real
DC	k_bio T>=15 6<=pH<=8_p5	literature biodegradation rate constant 5	day^-1	Real
DD	k_bio T>=15 6<=pH<=8_p6		day^-1	Real
DE	k_bio T>=15 6<=pH<=8_p7		day^-1	Real
DF	k_bio T>=15 6<=pH<=8_p8		day^-1	Real
DG	k_bio T>=15 6<=pH<=8_p9		day^-1	Real
DH	k_bio T>=15 6<=pH<=8_p10		day^-1	Real
DI	k_bio T>=15 6<=pH<=8_p11		day^-1	Real
DJ	k_bio T>=15 6<=pH<=8_p12		day^-1	Real
DK	k_bio T>=15 6<=pH<=8_p13		day^-1	Real
DL	k_bio T>=15 6<=pH<=8_p14		day^-1	Real
DM	k_bio T>=15 6<=pH<=8_p15		day^-1	Real
DN	k_bio T>=15 6<=pH<=8_dist	biodegradation rate constant (distribution type)	-	String(10)
DO	T>=15 6<=pH<=8RXPNA(1)	name of reaction product 1	-	String(32)
DP	T>=15 6<=pH<=8RXPNUM(1)	CAS number of reaction product 1	-	String(32)
DQ	T>=15 6<=pH<=8YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
DR	T>=15 6<=pH<=8RXPNA(2)	name of reaction product 2	-	String(32)
DS	T>=15 6<=pH<=8RXPNUM(2)	CAS number of reaction product 2	-	String(32)
DT	T>=15 6<=pH<=8YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
DU	T>=15 6<=pH<=8RXPNA(3)	name of reaction product 3	-	String(32)
DV	T>=15 6<=pH<=8RXPNUM(3)	CAS number of reaction product 3	-	String(32)
DW	T>=15 6<=pH<=8YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real
DX	k_bio T>=15 pH>8	biodegradation rate constant (most likely estimate)	day^-1	Real
DY	k_bio T>=15 pH>8_min	biodegradation rate constant (minimum estimate)	day^-1	Real
DZ	k_bio T>=15 pH>8_max	biodegradation rate constant (maximum estimate)	day^-1	Real
EA	k_bio T>=15 pH>8_sd	biodegradation rate constant (standard deviation)	day^-1	Real
EB	k_bio T>=15 pH>8_p5	literature biodegradation rate constant 5	day^-1	Real
EC	k_bio T>=15 pH>8_p6		day^-1	Real

Column	Name	Description	Units	Type
ED	k_bio T>=15 pH>8_p7		day^-1	Real
EE	k_bio T>=15 pH>8_p8		day^-1	Real
EF	k_bio T>=15 pH>8_p9		day^-1	Real
EG	k_bio T>=15 pH>8_p10		day^-1	Real
EH	k_bio T>=15 pH>8_p11		day^-1	Real
EI	k_bio T>=15 pH>8_p12		day^-1	Real
EJ	k_bio T>=15 pH>8_p13		day^-1	Real
EK	k_bio T>=15 pH>8_p14		day^-1	Real
EL	k_bio T>=15 pH>8_p15		day^-1	Real
EM	k_bio T>=15 pH>8_dist	biodegradation rate constant (distribution type)	-	String(10)
EN	T>=15 pH>8RXPNA(1)	name of reaction product 1	-	String(32)
EO	T>=15 pH>8RXPNUM(1)	CAS number of reaction product 1	-	String(32)
EP	T>=15 pH>8YCOEF(1)	molar yield coefficient for reaction 1	moles/moles	Real
EQ	T>=15 pH>8RXPNA(2)	name of reaction product 2	-	String(32)
ER	T>=15 pH>8RXPNUM(2)	CAS number of reaction product 2	-	String(32)
ES	T>=15 pH>8YCOEF(2)	molar yield coefficient for reaction 2	moles/moles	Real
ET	T>=15 pH>8RXPNA(3)	name of reaction product 3	-	String(32)
EU	T>=15 pH>8RXPNUM(3)	CAS number of reaction product 3	-	String(32)
EV	T>=15 pH>8YCOEF(3)	molar yield coefficient for reaction 3	moles/moles	Real

6.2.8 Format for the Human Health Benchmarks Data Table

Table 6.8 provides human health factors for all constituents to be used directly. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2.

6.2.9 Format for the Ecological Benchmarks Data Table

Table 6.9 provides the complete list of ecological species evaluated in the HWIR Assessment. This table shows the ecological benchmarks for mammals, birds, reptiles, amphibians and ecological communities for all constituents; data are to be used directly. The benchmarks are grouped by species type.

Table 6.8 Composition of the Human Health Benchmarks Data Table

Column	Name	Description	Units	Type
A	ChemName	Chemical Name	-	String(32)
B	ChemCASID	Chemical Abstracts ID	-	String(32)
C	ChemHuman	Flag that represents whether human health assessment is to be performed for this chemical. 0 implies no assessment, 1 implies an assessment	-	logical
D	ChemC_Add	Flag that represents whether Carcinogen results can be added together for ingestion and inhalation pathways. 1 implies they are additive.	unitless	integer
E	ChemCSFfood	Food ingestion Cancer Slope Factor	(mg/kg-d)-1	float
F	ChemCSFinhal	Inhalation Cancer Slope Factor	(mg/kg-d)-1	float
G	ChemCSFwater	Water ingestion Cance Slope Factor	(mg/kg-d)-1	float
H	ChemHealthEffect	Value which idetifies the type of health effect.	unitless	integer
I	ChemNC_Add	Flag that represents whether Hazard Quotients for ingestion and inhalation pathways can be added together. 1 implies they are additive.	unitless	integer
J	ChemRfC	Inhalation Reference Concentration	mg/m3	Float
K	ChemRfDfish	Fish ingestion Reference Dose	mg/kg-d	Float
L	ChemRfDfood	Food ingestion Reference Dose	mg/kg-d	float
M	ChemRfDwater	Water ingestion Reference Dose	mg/kg-d	float
N	ChemBreastMilkExp	Flag that represents whether Breast Milk Ingestion pathway is to be considered. 1 implies it is to be considered.	unitless	integer
O	ChemBM	Breast Milk Reference Dose.	mg/kg-d	float
P	Chemfai	fraction of contaminant ingested by the infant that is absorbed	fraction	float
Q	ChemFam	fraction of contaminant ingested by mother that is absorbed	fraction	float
R	ChemFbl	fraction of contaminant in whole blood compartment	fraction	float
S	ChemFf	fraction of contaminant stored in maternal fat	fraction	float
T	Chemkpm	concentration proportionality constant between plasma and breast milk aqueous phase	unitless	float
U	ChemKrbc	concentration proportionality constant between red blood cells and plasma	unitless	float
V	Chemt_halfb	Half time of chemical in breast milk	d	float

Table 6.9 Complete List of Ecological Species Evaluated in the HWIR Assessment

Mammals	**Birds**	**Reptiles**
mule deer	belted kingfisher	snapping turtle
black bear	osprey	alligator snapping turtle
red fox	burrowing owl	eastern box turtle
black-tailed jack rabbit	loggerhead shrike	painted turtle
mink	western meadowlark	southern hognose snake
coyote	green heron	racer snake
long-tailed weasel	american kestrel	pine snake
raccoon	Cooper's hawk	**Amphibians**
river otter	least tern	bullfrog
kit fox	bald eagle	gopher frog
eastern cottontail	red-tailed hawk	green frog
muskrat	marsh wren	eastern newt
beaver	lesser scaup	flatwood salamander
short-tailed shrew	mallard	**Communities**
prairie vole	cerulean warbler	Aquatic Biota(dslvd)
pine vole	american robin	Aquatic Biota(total)
least weasel	herring gull	Sediment Biota
little brown bat	spotted sandpiper	Soil Biota
meadow vole	northern bobwhite	Plants
deer mouse	american woodcock	
great basin pocket mouse	great blue heron	
short-tailed weasel	canada goose	
	tree swallow	

The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2. Table 6.10 provides the composition of the Ecological Benchmarks Data Table.

Table 6.10 Composition of the Ecological Benchmarks Data Table

Column	Name	Description	Units	Type
A	CHNAME	standard name of chemical	--	string (32)
B	CASNUM	CAS number of chemical (including dashes)	--	string (32)
C	SpecType	Species Type	--	string(32) selected from the following list "mammals" "birds" "reptiles" "amphibians" "community"

Column	Name	Description	Units	Type
D	Species	Species Name	--	string(32)
E	Benchmark	Ecologicial Benchmark	"mg/kg-day" for mammals, birds and reptiles. "mg/L" for amphibians and aquatic biota community. "mg/kg soil" for soil biota community and plant community. "mg/kg sediment OC" for sediment biota community.	Real
F	Weight	Weight of evidence indicator	--	Integer -1 implies low -2 implies medium -3 implies high

6.2.10 Format for the Ecological Bioaccumulation Factors Data Table

Table 6.11 provides the composition of the Ecological Bioaccumulation Factors Data Table. This table provides ecological biologicial transfer, accumulation, and concentration factors for all constituents for terrestrial species; data are to be used directly. The data are expected to be defined in a comma-seperated file that is formatted according the format specified in Section 6.2.

Table 6.11 Composition of the Ecological Bioaccumulation Factors Data Table

Column	Name	Description	Units	Type
A	CHNAME	standard name of chemical	-	string (32)
B	CASNUM	CAS number of chemical (including dashes)	-	string (32)
C	Type	Chemical Type HG implies Mercury M implies Metal O implies Organic D implies Dioxin like	-	string(2) selected from the list of
D	Br_exveg	soil-to-plant BCF (exveg)	(µg/g dry weight plant)/(µg/g soil)	Real
E	Bv_exveg	air-to-plant BTF (exveg)	(µg/g dry weight plant)/(µg/g air)	Real
F	Br_proveg	soil-to-plant BCF (proveg)	(µg/g dry weight plant)/(µg/g soil)	Real

Column	Name	Description	Units	Type
G	Br_exfruit	soil-to-plant BCF (exfruit)	(µg/g dry weight plant)/(µg/g soil)	Real
H	Bv_exfruit	air-to-plant BTF (exfruit)	(µg/g dry weight plant)/(µg/g air)	Real
I	Br_profruit	soil-to-plant BCF (profruit)	(µg/g dry weight plant)/(µg/g soil)	Real
J	Br_root	soil-to-plant BCF (root)	(µg/g dry weight plant)/(µg/g soil)	Real
K	RCF_root	root concentration factor (RCF)	(µg/g wet weight plant)/(µg/mL soil)	Real
L	Br_grain	soil-to-plant BCF (grain)	(µg/g dry weight plant)/(µg/g soil)	Real
M	Br_silage	soil-to-plant BCF (silage)	(µg/g dry weight plant)/(µg/g soil)	Real
N	Bv_silage	air-to-plant BTF (silage)	(µg/g dry weight plant)/(µg/g air)	Real
O	Br_forage	soil-to-plant BCF (forage)	(µg/g dry weight plant)/(µg/g soil)	Real
P	Bv_forage	air-to-plant BTF (forage)	(µg/g dry weight plant)/(µg/g air)	Real
Q	Ba_milk	Milk transfer factor	d/g	Real
R	Ba_beef	Beef biotransfer factor	d/g	Real
S	Ba_water	Biotransfer factor for surface water	d/g	Real
T	Bs	bioavailablility fraction for contaminantion in soil	unitless	Real
U	BCF_worm	earthworm BCF	(µg/g dry weight worm)/(µg/g soil)	Real
V	BCF_invert	inverterbrate BCF	(µg/g dry weight invert)/(µg/g soil)	Real
W	BAF_smamm	small mammal BAF	(µg/g dry weight sm mam)/(µg/g soil)	Real

Column	Name	Description	Units	Type
X	BAF_vert	other verterbrate BAF	(µg/g dry weight vert)/(µg/g soil)	Real

6.2.11 Format for the Aquatic Bioaccumulation Factors Data Table

Table 6.12 provides the composition of the Aquatic Bioaccumulation Factors Data Table. This table provides aquatic biologcial accumulation and concentration factors for all constituents for aquatic species; data are to be used directly. The data are expected to be defined in a comma-separated file that is formatted according to the format specified in Section 6.2.

Table 6.12. Composition of the Aquatic Bioaccumulation Factors Data Table

Column	Name	Description	Units	Type
A	CHNAME	standard name of chemical	-	string (32)
B	CASNUM	CAS number of chemical (including dashes)	-	string (32)
C	km	Metabolic transformation rate	day^{-1}	Real
D	aqpBCFm	Aquatic plant BCF	L/kg plant	Real
E	finBCFm	Wholebody finfish BCF	L/kg finfish	Real
F	shellBCFm	Wholebody shellfish BCF	L/kg shellfish	Real
G	ppBCFm	Phytoplankton BCF	L/kg phtyoplankton	Real
H	zpBCFm	Zooplankton BAF	L/kg zooplankton	Real
I	b1BAFm	Benthos category 1 BAF	L/kg benthos	Real
J	b2BAFm	Benthos category 2 BAF	L/kg benthos	Real
K	T2BAFm	T2 aquatic invertebrates BAF	L/kg aq invert	Real
L	T3BAFm	T3 fish BAF	L/kg finfish	Real
M	T4BAFm	T4 fish BAF	L/kg finfish	Real

6.2.12 Format for the Concentration in the Waste Stream Data Table

This file contains the concentration in both the liquid and solid waste streams. The data can be input to simulate from 1 to 5 different concentration levels in the HWIR sofware system. The format of the concentration in the waste stream data table is define in Table 6.13.

Table 6.13. Composition of the Concentration in the Waste Stream Data Table

Column	Name	Description	Units	Type
A	ChemName	Chemical Name	-	string(32)
B	ChemCASID	Chemical Abstract ID	-	string(32)
C	ChemNumSol	Number of Solid Wast Concentrations	-	Integer
D	ChemSolCw1	First Solid Waste Concentration	μg/g	Real
E	ChemSolCw2		μg/g	Real
F	ChemSolCw3		μg/g	Real
G	ChemSolCw4		μg/g	Real
H	ChemSolCw5		μg/g	Real
I	ChemNumLiq	Number of Liquid Waste Concentrations	-	Integer
J	ChemLiqCw1	First Liquid Waste Concentration	mg/L	Real
K	ChemLiqCw2		mg/L	Real
L	ChemLiqCw3		mg/L	Real
M	ChemLiqCw4		mg/L	Real
N	ChemLiqCw5		mg/L	Real