Header identifies parameter file version number. The following is a description of the version 4 parameter file format.

# Compartments

First blocked section is the number of compartments

--------------------------------------------------------------------------------

Compartment C to M Units label

Water, 0.01, L <----- if "C to M" is -999 then this field is editable, display in interface

BL, 0.0000178, g wt

Soil, 0.003, kg

This is a new section. Why is it needed? One reason it allows us to remove the mass info for BL sites out of the code. Another is that it provides a generic way to have multiple compartments that define immiscible/uncombinable materials, each with their own mass info. The mass of each of these compartments will be used in the conversions between concentration and mass. Other possible compartments would be soil, sediment, organic layers, etc.

# Input variables (non-components)

This could be a useful section and would include parameters that we need information about, that are not components. For example, temperature, and %HA but I suppose Site and Sample could also be in this category. Anything listed here will have a column in the input file.

# Components

The component block looks similar to the existing parameter file format. These are also variables that will be listed in the input file. Maybe we should re-think Type to specify the compartment and little else. In which case, we will need another variable to specify fixed activity.

--------------------------------------------------------------------------------

Component Charge Type Activity Site Den <--- these components are displayed in the interface

H, 1, 1, 2, 1 <--- instead of type, maybe we should specify "Mass compartment" actually, we'll still need type

Cu, 2, 1, 2, 1 to be able to specify fixed activity but we can simplify "Type" if we split out the mass unit info

DOC-FA, -1, 1, 1, 0.0006 <--- WHAM FA component - have to think about the interface and if we still want %HA, also WHAMV vs WHAMVII

Ca, 2, 1, 2, 1 We also need to have a section for other WHAM parameters like proton binding, double layer overlap etc

Mg, 2, 1, 2, 1 this stuff: FA parameters, 4.73E-3, 3.26, 9.64, 3.34, 5.52, -103, 0.4, 8E-10, 1500

Na, 1, 1, 2, 1

K, 1, 1, 2, 1

Al, 3, 1, 2, 1

FeIII, 3, 1, 2, 1

SO4, -2, 1, 2, 1

Cl, -1, 1, 2, 1

CO3, -2, 1, 2, 1

POC, -1, 31, 1, 0.0006 <---- I'm not trying to suggest that HA is interpreted as POC, but that POC is interpreted as HA

# Defined components

These components will not appear in the input file, but will be useful for species reactions. Anything listed here should either be

* A constant such as BL (and in this case we are talking about total BL) – but is that redundant with the BL definition in the compartment?
* A component that is derived from other components or input variables. For example, Humics = DOC \*HA%/100
* WHAM derived components

These all need to be assigned a component number so I think we do need to include numbers in these blocks. No, we should do text matching – less to keep track of and better for humans.

--------------------------------------------------------------------------------

Defined components <--- I'm thinking these components are not displayed in the interface

Component, From, Charge, Compartment, Type, Activity, Site Den

BL1, 1.45E-05, -1, BL, 1, 1, 1

FA1, DOC-FA, 0, Water, 1, 1, .004 <--- we need to think through how to specify WHAM species and WHAMV vs WHAMVII

FA2, DOC-FA, 0, Water, 1, 1, .006 we will also be able to put them into different mass units (e.g. soils vs water)

HA1, POC, 0, Water?, 1, 1, .004 and have master dbs for WHAM distribution as well as an over-ride with

HA2, POC, 0, Water?, 1, 1, .006 a given parameter file (maybe have a parameter file creator)

pCO2, 1E-3.2, 0, Water, 1, 1, 1

# Species

This is the typical species list but defined in a non-tableau format. Type should identify which compartment this species will reside in, the number of components used to form this species, and the component ~~numbers~~ names and stoichiometries for each of those components, followed by log K, ΔH etc. Do we want to keep Monte Carlo info? We’ve never used it in the BLM. Let’s ditch it!

-------------------------------------------------------------------------------- <--- Mass unit should be defined as well

Species Type Act. NC C1 S1 C2 S2 C3 S3 Log K Delta H Temp Conc

BL1-Cu, 21, 1, 2, BL1, 1, Cu, 1, 7.400 0.000 0.000 0.0000E+00 <-- what about searching from a master dbs?

BL1-CuOH,21, 1, 3, BL1, 1, Cu, 1, H, -1, -1.300 0.000 0.000 0.0000E+00

BL1-Ca, 21, 1, 2, BL1, 1, Ca, 1, 3.600 0.000 0.000 0.0000E+00

BL1-H, 21, 1, 2, BL1, 1, H, 1, 5.400 0.000 0.000 0.0000E+00

BL1-Na, 21, 1, 2, BL1, 1, Na, 1, 3.000 0.000 0.000 0.0000E+00

HCO3, 11, 1, 2, CO3, 1, H, 1, 10.329 0.000 0.000 0.0000E+00

H2CO3, 11, 1, 2, CO3, 1, H, 2, 16.681 0.000 0.000 0.0000E+00

MgHCO3, 11, 1, 3, CO3, 1, Mg, 1, H, 1, 11.400 0.000 0.000 0.0000E+00

MgCO3, 11, 1, 2, CO3, 1, Mg, 1, 2.980 0.000 0.000 0.0000E+00

MgSO4, 11, 1, 2, Mg, 1, SO4, 1, 2.370 0.000 0.000 0.0000E+00

CaHCO3, 11, 1, 3, Ca, 1, CO3, 1, H, 1, 11.440 0.000 0.000 0.0000E+00

CaCO3, 11, 1, 2, Ca, 1, CO3, 1, 3.220 0.000 0.000 0.0000E+00

CaSO4, 11, 1, 2, Ca, 1, SO4, 1, 2.300 0.000 0.000 0.0000E+00

CuOH, 11, 1, 2, Cu, 1, H, -1, -7.520 0.000 0.000 0.0000E+00

Cu(OH)2, 11, 1, 2, Cu, 1, H, -2, -16.220 0.000 0.000 0.0000E+00

CuSO4, 11, 1, 2, Cu, 1, SO4, 1, 2.360 0.000 0.000 0.0000E+00

CuCO3, 11, 1, 2, Cu, 1, CO3, 1, 6.750 0.000 0.000 0.0000E+00

Cu(CO3)2,11, 1, 2, Cu, 1, CO3, 2, 9.920 0.000 0.000 0.0000E+00

CuCl, 11, 1, 2, Cu, 1, Cl, 1, 0.400 0.000 0.000 0.0000E+00

CuHCO3, 11, 1, 3, Cu, 1, CO3, 1, H, 1, 14.620 0.000 0.000 0.0000E+00

Cu-FA1, 11, 1, 2, FA1, 1, Cu, 1, 5.000 0.000 0.000 0.0000E+00

Cu-FA2, 11, 1, 2, FA1, 1, Cu, 1, 7.000 0.000 0.000 0.0000E+00

Cu-HA1, 31, 1, 2, HA1, 1, Cu, 1, 5.500 0.000 0.000 0.0000E+00

Cu-HA2, 31, 1, 2, HA1, 1, Cu, 1, 7.500 0.000 0.000 0.0000E+00

# Linked lists

Not sure how useful this is, it was useful for things like cation exchange reactions. Obviously we haven’t done a lot of soils work. Let’s not include this…for now?

# Phase list

Finally we might use this! We can have phase stoichiometry, thermodynamic constants, and finally the amount of moles if there is a finite amount of the phase present (in other words, if there is a possibility it will all dissolve and “poof”, it’s gone).

-------------------------------------------------------------------------------- <-- need to think this one through as well

Phase, NC, C1, S1, C2, S2, C3, S3, Log Ks, Delta H, Temp, Moles

CO2(g), 2 CO3, 1, H, 2, pCO2, 1, -1.5, ??, 0, 0

Most of the file I/O info will disappear. Although it would be fun to be able to do multi-layer soil simulations again. A lot of important info migrated to “user notes” and I think that needs to be formalized better.