**Inorganic/BL components**

Definitions

= residual of component

= calculated total moles of component

= known total moles of component

= known total concentration of component

= stoichiometric coefficient of component in species

= concentration of species

= concentration-to-moles conversion volume for species

Residual

I’m not sure if the term is necessary. In terms of how much of a difference it makes mathematically…from what I can see, it’s usually quite small compared to , but will on occasion be at least as significant as . That just leaves the question of whether it is correct to include it…is the constant value or is ? Or are they both because the bulk solution volume remains the same while the and portions of the volume only matter on a species basis, not when talking about totals?

I think it makes more sense than be calculated from at the beginning of the run, based on the bulk solution MassAmt volume….and from there it should be constant.

Solving for :

Solving for :

When , and are considered constant:

When and are considered constant, but is variable with :

Solving for :

When is a WHAM species:

When is an inorganic species, or a Donnan species, is constant, and when is a component,

Solving for :

Solving for :

**Diffuse/Donnan layer components**

Definitions:

= Boolean value indicating whether species is part of humic substance (0=not part of HS h, 1 = part of HS h)

= charge of species

= concentration of species

= concentration of component , which is consistently going to be the component we’re taking derivatives wrt in these equations

= total concentration of humic substance (g HS / L)

= total charge in the Donnan layer per liter of solution

= residual of Donnan layer component

= stoichiometric coefficient of the Donnan layer component in species …this should be the absolute value of the charge of the species

= stoichiometric coefficient of component in species

NS = number of species

= net humic charge (charge / g HS)

= Donnan layer volume for humic substance h

= max Donnan layer volume for humic substance h, before it’s constrained by the Donnan layer overlap factor

= max Donnan layer volume for humic substance h per gram of humic substance h

= humic charge adjusting factor to force diffuse layer volume to diminish as charge decreases

= molecular weight of humic substance h

= molecular radius of humic substance h

= Avogadro’s number

= ionic strength

= temporary identifiers for applying rules for derivatives…what they represent is context-specific

Residuals:

Solving for :

…depending on the equation, either of these may be useful.

Solving for :

…where , we would expect to follow the rules for a non-constant ….

Solving for :

When is an inorganic species that specifically binds DOC

When is an inorganic species that does not specifically bind DOC

When is an organic (DOC) species

When is a Donnan species…

Solving for :

Solving for :

…we can assume is relatively constant since the only thing that varies is ionic strength (I), but ionic strength is pretty easy to get right off the bat. Th and KZ are also constant, so the only thing that should vary significantly with Cj is Zh.

**WHAM components**

Definitions:

= known total concentration of DOC component (site abundance (mol/g HS) times Th (g HS / L))

= stoichiometric coefficient of DOC component in species

= residual of DOC component

, where I is ionic strength and P is a WHAM parameter…

Residuals:

**Metal in Tox Mode**

Definitions:

= residual of the toxic metal

= calculated total concentration of toxic metal bound to the biotic ligand

= critical accumulation (critical concentration of toxic metal bound to the biotic ligand that caused a toxic effect)

= number of toxicity-associated species, consisting of a metal or metal species bound to the biotic ligand (e.g., BL-Me or BL-MeOH)

Residuals:

Let’s try calculating :