Convert name

Length of min3p species name is 12 maximum while TOUGHREACT species name is 20,

At present, the name is truncated by the first 12 characters, not well readable. Create a table for full name and alias?

2.

Convert Debye-Huckel constants

In TOUGHREACT, Ion effective or hydrated radius is used to compute the Debye-Huckel a0 parameter (see Appendix H of Toughreact\_V2\_User\_Guide.pdf for details).

!DHA = 2(r + 1.91|Z|)/(|Z| + 1) for

!DHA = 2(r + 1.81|Z|)/(|Z| + 1) for cations

r is the effective ionic radius, z is the charge.

When z == 0, what is the formulation?

3.

Second species in TOUGHREACT include elements of Complexation Reactions and Redox Reactions in min3p, judged by o2(aq)? For some complex.dbs in MIN3P, it also includes o2(aq) ?

At present, all the reactant or product that contain o2(aq) are treated as redox reactions and the others are treated as the complexation reaction.

The second temperature in TOUGHREACT is 25C. The equilibrium constants (log(K) in base 10) Should modify if 25C does not exist or in the different position.

Convert all the aqueous species to complex.dbs at present.

4.

How to convert surface complex in TOUGHREACT database to MIN3P? In the given database, there is no surface complex. But the database supports adding surface complexes data.

**Not needed.**

5.

How to know from TOUGHREACT if the mineral is reversible or reversible and the parallel reaction pathways, which are needed in MIN3P?

At present, exported to as ‘surface’ and 'reversible'

* 'uo3(c)'
* 'surface'
* 286.0272 **8.0435**
* 3 'h+1' -2.000 'uo2+2' 1.000 'h2o' 1.000
* 'reversible' -7.7190 **19.3150**

6. Warning message

Some of the aqueous/minerals in TOUGHREACT have more than 5 reactant or product, but min3p can only support 5, at present, the program only export 5.