How to Make Databases for ESD

Mary Elizabeth Wagner, 05.18.20

To be used with ESD Version 1.2

There are three categories of databases that need to be exported in order to create an ESD. They can be easily generated in FactSage.

Database Type 1: Standard State Free Energy

1. Open FactSage's Equilib module.
2. Ensure your units are set to mol, K, and bar
3. Set your database to FactPS.
4. Enter the element you are interested in generating the standard state data for. Your amount is one mol, and your temperature is T. Click "next".
5. In the next window, select all liquids, solids, and gasses. In the "temperature" window, type *273 2273 1.*
   - This will start your temperature at 273 K, and increase by 1 degree until you reach 2273.
6. Click "calculate".
7. Once your calculation has been completed, you go to "Output" -> "Save or Print" -> "Save Excel Spreadsheet".
   - Click "spreadsheet setup"
   - You will want *one* system property column, Temperature
   - You will want *one* species property column, Activity.
   - Under "species", you should select all phases from the FactPS database.
8. Export your database. Save it as "Symb_ss.xlsx". Symb is your element symbol. For Iron, you would save it as Fe_ss.xlsx.

Database Type 2: $\Delta G_{reaction}$

1. Open FactSage's Reaction module.
2. Ensure your units are set to mol, K, and bar.
3. Set your database to FactPS
4. Enter the *reduction* reaction normalized *per mol of metal.*
5. Set temperature to T.
6. Click next.
7. In the next window, select all liquids, solids, and gasses. In the "temperature" window, type *273 2273 1.*
   - This will start your temperature at 273 K, and increase by 1 degree until you reach 2273.
8. Click "calculate".
9. Go to "Output" -> "Save Tablular Output" -> save "Symb_anion.txt" where "Symb" is your metallic element symbol and anion is the element produce at the anode. For Iron in a sulfide electrolyte, you would save Fe_S.txt.

Database Type 3: Binary Metal Solution Data

1. Open FactSage's Equilib module.
2. Ensure your units are set to mol, K, and bar
3. Set your database to the proper database for whichever binary solution you are interested in.
4. Set your molar amounts as follows:
   - For your more reactive metal, type <A>
   - For your more noble metal, type <1-A>.
     - If you have an additional cathode element, the more noble metal becomes <1-A-B+AB>
     - The cathode element is <B-BA>
5. Your temperature is the temperature of the reaction.
6. Click "next"
7. In the following window, select all phases and solutions that the FactSage documentation tells you for that particular system.
8. Set <B> to whatever proportion of additive you have in relation to the more noble metal. (If the cathode element is fixed to the noble metal. If it is fixed to the more reactive metal, then the more reactive metal is defined as <1-A>, and so on.
   - If you have a cast iron cathode, where C is fixed at the eutectic in the Fe-C diagram, <B> is 0.17.
9. Click "calculate".
10. Once your calculation has been completed, you go to "Output" -> "Save or Print" -> "Save Excel Spreadsheet".
    - Click "spreadsheet setup"
    - You will want *one* system property column, Alpha
    - You will want *one* species property column, Activity.
    - Under "species", you should select all liquid phases from your solution database.
11. Export your database. Save it as TSymbASymb2CathodeB.xlsx.
    - For an Fe-Cu system at 1573K, you would save 1573FeCu.xlsx.
    - For an Fe-Cu-C system where C is fixed at 0.17 C/C+Fe, you would save 1573FeCuC17.
12. If you are setting a special binary to compare with experiments, and have a precise value for the cathode (e.g. 17.65), then you can save the file as whatever you like. Mathematica will ask you to import that file specially.