FactSage Custom database (14 November 2024)

The FactSage custom database uses the unified interaction parameter formalism (UIPF) [13, 14], specifying only the $\ln\gamma_i^0$ terms (i = Al, Ti, Si, Ca, and Mg) [15]. The procedure to create the custom database is briefly as follows:

Specify pure-substance references by dragging pure substance data of Fe, Ca. Al, Mg, Si, and Ti, and gas phase O_2 from FactPS database and drop these into the "Function" module :

- Fe: L1 (pure liquid)
- Al: L1 (pure liquid)
- Ti: L1 (pure liquid)
- Si: L1 (pure liquid)
- Ca: G1(pure gas)
- Mg: G1 (pure gas)
- O: 0.5*O2 (pure gas)

Second, right click on "A" under the tab "Sublattice" and click "Add species", enter the name, the formula, and the species of element i of interest (Fe, Al, Ti, Si, Ca, Mg, O). Fe is main solvent, with other "normal" species. The Gibbs Energy function use 1 mol of pure liquid/gas (in the form of number of moles*species#phase, e.g., 1*Fe#Liquid for pure Fe end member, and 0.5*O2#Gas).

Third, right click species in the sublattice "A" under the tab "Sublattice", click "Add" -> "GE"->and add $\varepsilon_1 = \ln\gamma_i^0$ (activity coefficient of I in dilute solution) and $\varepsilon_2 = \ln\gamma_i^i$ (self-interaction term of element i) using the generic data for liquid Fe alloy from Table I of Jung [15] and Table II of Sigworth and Elliott work [16].

The activity coefficients were adjusted as follows:

- Oxygen: the activity coefficient was adjusted until an Fe-0.0005 wt%O binary system gave $p_{O2} = 10^{-16}$ atm (based on Sigworth & Elliott)
- Magnesium: adjusted to give dissolved concentration of 20 ppm
- Calcium: $\varepsilon_{Ca} = 0$ to give near-zero dissolution of Ca into liquid steel
- Aluminum: adjusted $\ln\gamma_{Al}^0$ to give a dissolved oxygen concentration 5E-04 wt% in the mixture (100 g Fe-0.03g Al-10 g Al_2O_3) (based on Sigworth & Elliott)
- Silicon: Adjusted the activity coefficient to match the experimental and industrial data for Al-SiO_2-Al_2O_3-Si reactions for double-saturated ladle slag (at 1600 °C)
- Titanium: Adjusted the activity coefficient to match the experimental and industrial data for Al-TiO_x-Al_2O_3-Ti reactions for double-saturated ladle slag (at 1600 °C)

The final set of values was as follows:

- O: $\ln\gamma_O^0 = 0.18$
- Al: $\ln\gamma_{Al}^0 = 0.71$
- Si: $\ln\gamma_{Si}^0 = 0.43$
- Ti: $\ln\gamma_{Ti}^0 = -1.93$
- Ca: $\ln\gamma_{Ca}^0 = 0$
- Mg: $\ln\gamma_{Mg}^0 = -0.6$

When using the custom database with FToxid and FactPS, select FToxid A-monoxide (activate CaO and MgO only), O_2 in gas (choose "ideal"), 14 PactPS pure liquids and 94 pure solid species (turning off metallic compounds and perovskite-based Ca-Ti and Ca-Ti-Al oxides out of originally 124 pure solids).

With these settings, the predicted $C_1 = [\%Al]^{4/3} \times (\%SiO_2)_{slag}/[\%Si]_{steel} \sim 0.1$ and $C_2 = [\%Al]^{4/3} \times (\%TiO_2)_{slag}/[\%Ti]_{steel} = 0.30$ when using initial compositions as for ET2 initial slag; the calculated activities for MgO, CaO, and Al_2O_3 are respectively 0.99, 0.96, and 5.6×10^{-3} (pure solid references), agreeing with Tang [11] and Kumar [9].

Matching the final compositions of laboratory tests required the addition of a certain amount of extra oxygen to the initial slag and steel, to reflect oxygen in electrolytic iron and oxygen ingress during high-temperature experiments. The amount of extra oxygen was adjusted to match the experimentally determined final compositions.

Table VI. Initial slag and steel with extra oxygen for FeL3+FToxid+FactPS calculations for experiments-vs-chemically analyzed equilibrium slag and steel composition obtained from induction furnace experiments.

Initial system for calculations	Al (FeL3/Experiment)	Ti (FeL3/Experiment)	Si (FeL3/Experiment)	$\%SiO_2$ (FeL3/Experiment)	"$\%TiO_2$" (FeL3/Experiment)
ET1+0.26%O	0.023/0.019	0.030/0.019	0.33/0.35	4.84/5.05	1.09/0.87
ET2+0%O	0.046/0.046	0.058/0.04	0.48/0.4	2.44/3.08	1.02/0.98
ET1 repeat +0.1%O	0.031/0.031	0.039/0.028	0.39/0.33	3.78/3.53	1.07/1.01
ET2 repeat +0.3%O	0.026/0.026	0.034/0.028	0.34/0.43	4.16/3.10	1.10/1.07