|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Reference** | **Name in PySulfSat** | **Melt composition?** | **T-sens?** | **P-sens?** | **H2O-sens?** | ***Fe3+ sensitive*?** | **Sulfide/Sulfate comp?** | **Cali dataset available?** |
| **SCAS models** | | | | | | | | |
| Chowdhury & Dasgupta (2019) | “calculate\_CD2019\_SCAS” | **🗸** | **🗸** | **✗** | **🗸** | **✗** | **✗** | **🗸** |
| Zajacz & Tsay (2019) | “calculate\_ZT2022\_SCAS” | **🗸** | **🗸** | **✗** | **🗸** | **✗** | **✗** | **🗸** |
| Masotta & Keppler (2015) | “calculate\_MK2015\_SCAS” | **🗸** | **🗸** | **✗** | **🗸** | **✗** | **✗** | **🗸** |
| **SCSS models** | | | | | | | | |
| Li and Zhang (2022) | “calculate\_LiZhang2022\_SCSS” | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** |
| Blanchard et al. (2021) | “calculate\_B2021\_SCSS” | **🗸** | **🗸** | **🗸** | **🗸** | **✗** | **🗸** | **🗸** |
| O’Neill (2021) | “calculate\_O2021\_SCSS” | **🗸** | **🗸** | **🗸** | **✗** | **🗸** | **🗸** |  |
| O’Neill and Mavrogenes (2022)\*1 | “calculate\_OM2022\_SCSS” | **🗸** | **🗸** | **🗸** | **✗** | **🗸** | **🗸** | **🗸** |
| Liu et al. (2021) | “calculate\_Liu2021\_SCSS” | **✗** | **🗸** | **🗸** | **🗸** | **✗** | **🗸** | **🗸** |
| Smythe et al. (2017) | “calculate\_S2017\_SCSS” | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** |
| Fortin et al. (2015) | “calculate\_F2015\_SCSS” | **🗸** | **🗸** | **🗸** | **🗸** | **✗** | **✗** | **🗸** |
| **Sulfide composition models** | | | | | | | | |
| O’Neill (2021) | “Calc\_ONeill” | **🗸** | **✗** | **✗** | **✗** | **🗸** |  |  |
| Smythe et al. (2017) using Kiseeva et al. (2015) | “Calc\_Smythe” | **🗸** | **🗸** | **✗** | **✗** | **🗸** |  |  |

**Calculating Proportion of S6+ using empirical approaches**

|  |  |  |
| --- | --- | --- |
| **Reference** | **Name in PySulfSat** | **Input parameters** |
| Jugo et al. (2010) | “calculate\_S6St\_Jugo2010\_eq10” | ΔQFM |
| Nash et al. (2019) | “calculate\_S6St\_Nash2019” | T, Fe3+/FeT |
| O’Neill and Mavrogenes (2022) | “calculate\_OM2022\_S6St” | Melt comp, T, log(*f*o2) **or** Fe3/FeT |

**Correcting SCSS2- and SCAS6+ calculations for ST**

|  |  |
| --- | --- |
| **Name in PySulfSat** | **Input arguments** |
| “calculate\_SCSS\_Total” | SCSS2-, S6+/ST |
| “Calculate\_SCAS\_Total” | SCAS6+, S2-/ST |
| “Calculate\_S\_Total\_SCSS\_SCAS” | SCSS2-, SCAS6+, S6+/ST, or model ( ’Nash’, ‘Jugo’, ‘OM2022’, ‘Kleinsasser’) |

**Other functions**

|  |  |
| --- | --- |
| “crystallize\_S\_incomp” | Calculates S left in the melt for a given Fmelt  (assuming S is entirely incompatible |
| “calculate\_mass\_frac\_sulf” | Calculates mass fraction of sulfide removed for a model of changes in SCSS with fractional crystallization |
| “convert\_d34\_to\_3432S”, “convert\_3432S\_to\_d34” | Converts δ34S to 34S/32S and vice versa |
| “Lee\_Wieser\_sulfide\_melting” | Modelling of S and chalcophile element behaviour during mantle melting. |
| **For Monte Carlo simulations** | |
| ‘add\_noise\_2\_dataframes’ | Generate duplicated rows in df1 based on errors present in df2 |
| ‘add\_noise\_series’, ‘duplicate\_dataframe’ | Used to simulate uncertainty in specific variables |
| ‘av\_noise\_samples\_series’ | Average outputs from Monte Carlo simulations per sample |