|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Reference** | **Name in PySulfSat** | **T-sens?** | **P-sens?** | **H2O-sens?** | ***Fe3+ sensitive*?** | **Sulfide/Sulfate comp?** |
| **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” | Fe3+/FeT |
| O’Neill and Mavrogenes (2022) | “calculate\_S6St\_CS6\_SCSS” | Liquid composition, T, and log(*f*o2) or Fe3/FeT, SCSS and CS6 model |

**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 for S6+/ST ( ’Nash’, ‘Jugo’ or ‘Kleinsasser’) |

**Other functions**

|  |  |
| --- | --- |
| “crystallize\_S\_incomp” | Calculates S left in the melt for a given F\_melt, assuming S is entirely incompatible |
| “calculate\_mass\_frac\_sulf” | Calculates mass fraction of sulfide/sulfate removed for a fractional crystallization path where the SCSS or SCAS is modelled |
| “convert\_d34\_to\_3432S” | Converts δ34S to 34S/32S |
| “Lee\_Wieser\_sulfide\_melting” | Modelling of S and chalcophile element behavoir during mantle melting. |