

Reference	Name in PySulfSat	T-sens?	P-sens?	H ₂ O-sens?	Fe ³⁺ 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"	Fe ³⁺ /Fe _T
O'Neill and Mavrogenes (2022)	"calculate_S6St_CS6_SCSS"	Liquid composition, T, and log(<i>f</i> _{O₂}) or Fe ₃ /Fe _T , SCSS and C _{S6} model

Correcting SCSS²⁻ and SCAS⁶⁺ calculations for S_T

Name in PySulfSat	Input arguments
"calculate_SCSS_Total"	SCSS ²⁻ , S ⁶⁺ /S _T
"Calculate_SCAS_Total"	SCAS ⁶⁺ , S ²⁻ /S _T
"Calculate_S_Total_SCSS_SCAS"	SCSS ²⁻ , SCAS ⁶⁺ , S ⁶⁺ /S _T , or model for S ⁶⁺ /S _T ('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 δ ³⁴ S to ³⁴ S/ ³² S
"Lee_Wieser_sulfide_melting"	Modelling of S and chalcophile element behavoir during mantle melting.

