Reference	Name in PySulfSat	Melt composition?	T-sens?	P-sens?	H_2O-sens?	*Fe^{3+} 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 S^{6+} 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, Fe^{3+}/Fe_T
O'Neill and Mavrogenes (2022)	"calculate_OM2022_S6St"	Melt comp, T, log(fo_2) **or** $Fe3/Fe_T$

Correcting $SCSS^{2-}$ and $SCAS^{6+}$ 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 ('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 removed for a fractional crystallization path where the SCSS is modelled
"convert_d34_to_3432S"	Converts $\delta^{34}S$ to $^{34}S/^{32}S$
"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