

May 12th, 2024

New features:

- Added the model of Ding et al. (2018) for sulphide-saturation of silicate melt (New high pressure experiments on sulphide saturation of high-FeO* basalts with variable TiO₂ contents – Implications for the sulphur inventory of the lunar interior. *Geochimica et Cosmochimica Acta*, Volume 222, pages 319–339).
- Added the model of Wallace and Carmichael (1992) for sulphide-saturation of silicate melt (Sulfur in basaltic magmas. *Geochimica et Cosmochimica Acta* 56, 1863-1874).
- Added the model of Boulliang and Wood (2023) for sulphur oxidation state in silicate melt (Sulfur oxidation state and solubility in silicate melts. *Contributions to Mineralogy and Petrology* 178: 56).
- Changed implementation of the Smythe et al. (2017) sulphide saturation model so that it is now not linked to the Kiseeva and Wood (2015) sulphide composition model, but can be used with any model of sulphide composition that involves Ni and Cu contents.
- Added calculations of the saturation pressure by a H₂O-CO₂ fluid when using 'Melt Liquidus Association' calculations option with melt compositions that contain H₂O and/or CO₂. The saturation pressure is calculated for each available fluid saturation model.
- Added an option to model crystallisation ignoring sulphide saturation by choosing 'No S saturation' option among models for sulphide saturation.

Bug fixes:

- Fixed an issue that resulted in parameters 'Apply H₂O and P Corrections To All Models' and "Save Ds file name with parameters' loaded incorrectly when reading a saved file with parameters.
- Fixed an issue that resulted in SO₃ concentration not being reported in the output if S only was present in the data file and the 'Calculate all analyses' option was selected without choosing the 'Sulfide-saturated' option.
- Fixed an issue that resulted in incorrect calculations at elevated pressures when using the oxidation state of Fe model of Kress and Carmichael (1991).
- Fixed an issue that resulted in an error when the model of Ding et al. (2023) for Ds for S and SO₃ between silicate melt and fluid was used with a pure CO₂ system.
- Fixed the behaviour of the 'Open Data File' dialog so that if the user presses the 'Cancel' button the previously loaded file is not removed.