

5 November, 2025

New Models:

- H₂O-CO₂ fluid -silicate melt equilibrium models of Holloway and Blank (1994) and Dixon (1997).

Holloway and Blank (1994) presented two models, one for a pure H₂O fluid for basaltic silicate melt compositions and another for an H₂O-CO₂ fluid for rhyolitic silicate melt compositions. The algorithms involved in the implementation of the models in Petrolog4 (algorithms for finding H₂O and CO₂ concentrations in silicate melt and fluid at equilibrium) differ from those published by Holloway and Blank (1994).

Implementation of the Dixon (1997) involves the compositional dependence of CO₂ solubility in alkaline silicate melts that follows the originally proposed Π parameter. This is different from implementations of this model in other software that use melt SiO₂ content to describe the compositional dependence of CO₂ solubility in alkaline silicate melts.

Improvements to the algorithm:

- Improvements to the algorithm for obtaining equilibrium between H₂O-CO₂ fluids and silicate melts in systems with high H₂O and low CO₂ content (H₂O / CO₂ > 3,000). This improves Petrolog4 ability to model degassing during crystallisation.
- When fluid-saturated and/or sulphide-saturated conditions are selected for crystallisation calculations, these phases now appear on the liquidus without a delay for most starting compositions and selected sets of models.
- During Mineral Liquidus Association calculations with compositions that include H₂O and/or CO₂, the calculated saturation pressures are shown only for fluid saturation models that are applicable to the silicate melt compositions involved (i.e., whether the compositions contain both H₂O and CO₂, only H₂O, or only CO₂. 'N/A' is displayed for the other models.

Changes to the GUI:

- None

Bug fixes:

- Starting from version 4.2.0, the melt S content was incorrectly calculated during modelling of crystallisation, when the starting composition was forced to sulphide saturation. This led to sulphide undersaturation at oxidised conditions (fO₂ > QFM buffer). The saturation was delayed by ~ 3% of crystallisation on average. This is now fixed in version 4.2.3.2.
- When loading data from file that did not contain a pressure column, calculation pressure was reset to 1 bar. This is now fixed in version 4.2.3.1.
- When using components for output during Crystallisation calculations, the magma composition columns in the output files were occasionally incorrectly labelled using components, despite the concentrations in the magma being reported using elemental concentrations.

- Fixed repeat display of component names in cumulate phases for some calculations.
- Under some combinations of chosen parameters, the corrections to the calculated crystallisation temperatures for (1) silicate melt H₂O content and (2) crystallisation pressure were incorrectly displayed as applied for sulphide, H₂O-CO₂ fluids, sulphate, zircon and apatite. This is now fixed.