VESIcal

An open-source thermodynamic model engine for mixed volatile (H_2O-CO_2) solubility in silicate melts… and more!

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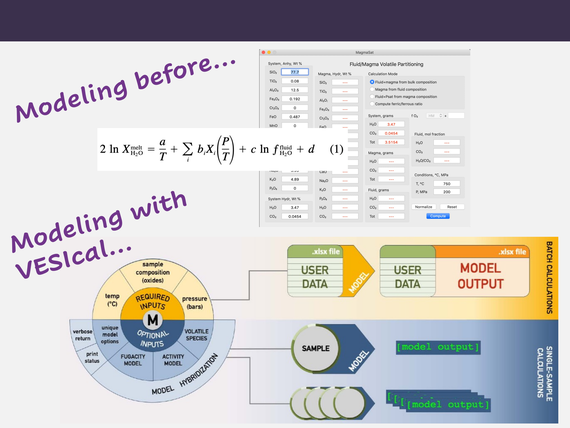
Solubility Models Today

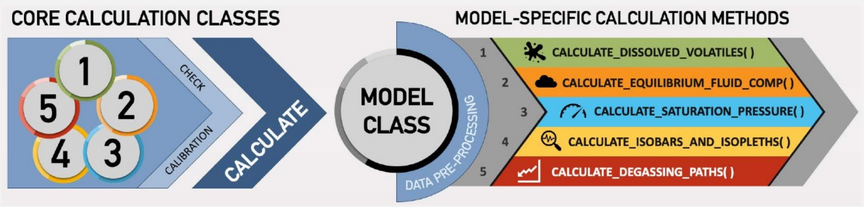
Despite a communal wealth of H_2O-CO_2 solubility models, **quantitative calculations of volatile solubility, and by extension saturation pressures, equilibrium fluid compositions, and degassing paths, remains a time-consuming endeavor**. Modeling tools, when published alongside models, are typically unable to process more than one sample at a time, requiring manual entry of the concentrations of 8-10 major oxides, temperature, as well as CO_2 and H_2O concentrations to calculate saturation pressures or XH_2O to calculate dissolved volatile contents.

Enter VESIcal (Volatile Equilibria and Saturation Identification calculator): a python-based thermodynamic volatile solubility model engine that incorporates seven popular solubility models under one proverbial roof.



$$2 \ln X_{H_2O}^{melt} = \frac{a}{T} + \sum_i b_i X_i \left(\frac{P}{T}\right) + c \ln f_{H_2O}^{fluid} + d \quad (1)$$

What is VESIcal, and what models?

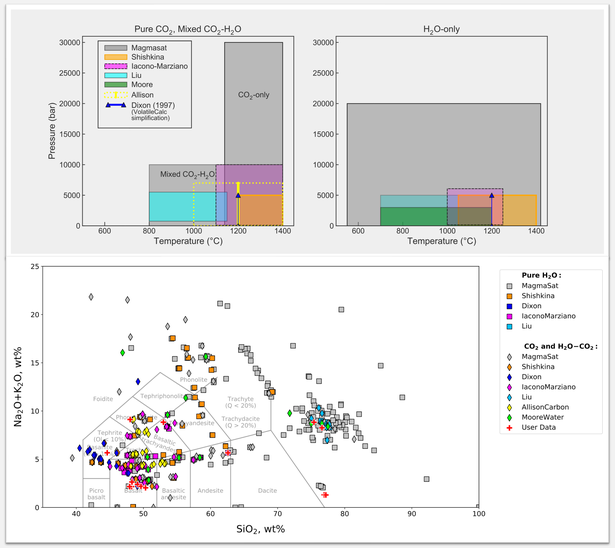


We built a model *engine* that…

- Can perform an array of useful calculations automatically and on large datasets
- Allows selection of a multitude of different models
  - And informs the user if their calculation is outside of the calibrated range of the model chosen
- Has automatic plotting capability built-in
- Allows for solubility, fugacity, and activity models to be combined and interchanged (model hybridization)
- Is open-source and extensible
- Is highly usable to people of all skill levels
  - Run VESIcal locally, on the ENKI server, or in easy mode on the Anvil web app

Plus! You get access under the hood…

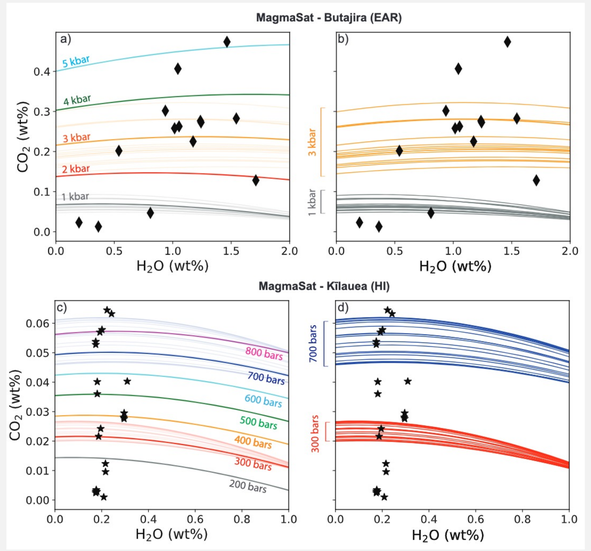
- Utilize any built-in fugacity or activity model
- Write custom calculations right into VESIcal
- Use model comparison tools to choose the right model for the job
- New: calculate liquid density and viscosity
- New: Easy inter-op with python library ThermoBar

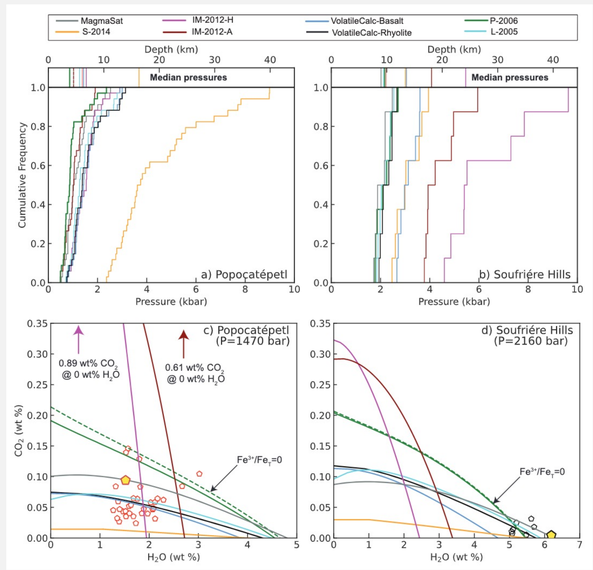


Example use cases

Inter-model comparison

VESIcal allows for easy comparison of how different models treat different melt compositions. Here we plot cumulative distribution functions of saturation pressures for melt inclusions from Popocatépetl (Atlas et al., 2006) and Soufriére Hills (Cassidy et al., 2015) modeled with MagmaSat (gray), Shishkina (yellow), Iacono-Marziano hydrous (pink) and anhydrous (dark red), VolatileCalc basalt (sky blue) and rhyolite (black), Papale et al. 2006 (not yet in VESIcal, green), and Liu (cyan). Bottom panels are isobars calculated at the saturation pressure from MagmaSat (1470 bar) for the melt inclusion shown by the yellow pentagon at 1050 °C for Popocatépetl and 1000 °C for Soufriére Hills. Isobars computed with Papale use Fe^{3+}/Fe^{T} = 0 (dotted line) and 0.15 (solid line).





Compositional variation matters!

Here we demonstrate how compositional variation within a single dataset can affect interpretations. Using one set of isobars for a suite of melt inclusions may often misrepresent actual saturation pressure variation within a dataset.

Here we plot isobars calculated with MagmaSat for olivine-hosted melt inclusions from Iddon and Edmonds (2020) (a and b) and a subset of melt inclusions from Kīlauea (Wieser et al., 2021) (c and d).

Left: MagmaSat isobars for a single melt inclusion within each dataset. **Right**: MagmaSat isobars calculated for every inclusion shown at 1 and 3 kbars (Butajira) or 300 and 700 bars (Kīlauea).

How to use VESIcal

Installed locally on your computer
(works best on mac, can be tricky)

On the ENKI server
http://enki-portal.org/
No install required
Easy to get running

On the Anvil web app
https://vesical.anvil.app/
No install required
No coding required
Limited functionality

Start here!
Read the Docs
https://vesical.readthedocs.io/

- Code documentation
- YouTube tutorials
- Workshop materials
- Jupyter notebook tutorials and examples
- Installation and use instructions

VESIcal Part 1 manuscript

VESIcal Part 2 manuscript

VESIcal github repo

http://vesical.rocks

Links to documentation, servers for running VESIcal, manuscript PDFs, manuscript Jupyter notebooks, and more

References:

K. Iacovino, S. Matthews, P. E. Wieser, G. M. Moore, F. Bégué (2021) VESIcal Part I: An open-source thermodynamic model engine for mixed volatile (H2O-CO2) solubility in silicate melts. Earth and Space Science 8:11.

P. E. Wieser, K. Iacovino, S. Matthews, G. M. Moore, C. M. Allison (2022) VESIcal 2: A critical approach to volatile solubility modeling using an open-source Python3 engine. Earth and Space Science 9:2