



VESICAL

An open-source thermodynamic model engine for mixed volatile (H₂O-CO₂) solubility in silicate melts... and more!

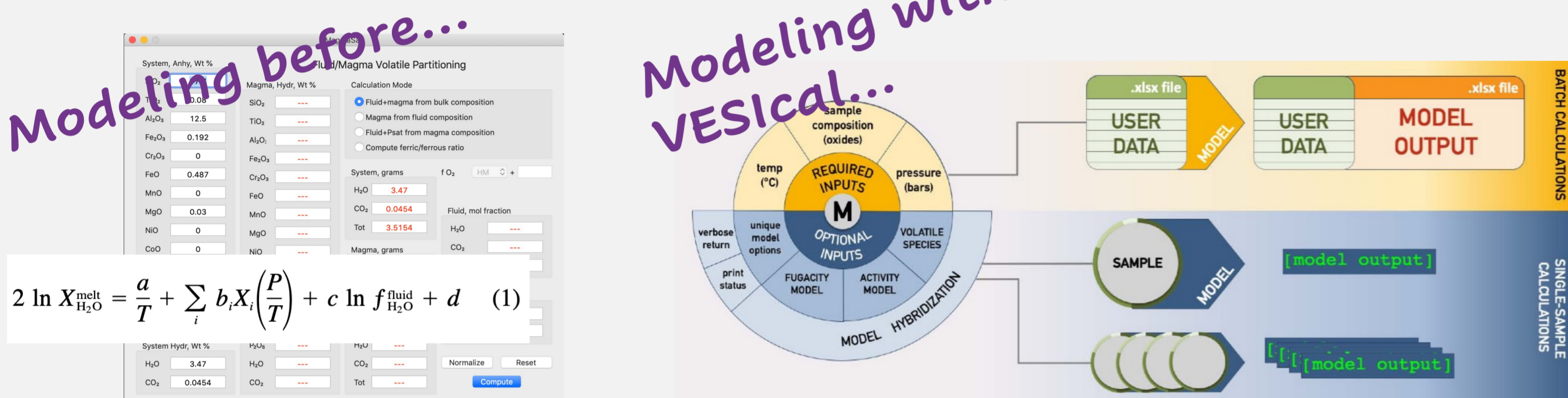


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Solubility Models Today

Despite a communal wealth of H₂O-CO₂ 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 CO₂ and H₂O concentrations to calculate saturation pressures or XH₂O 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.

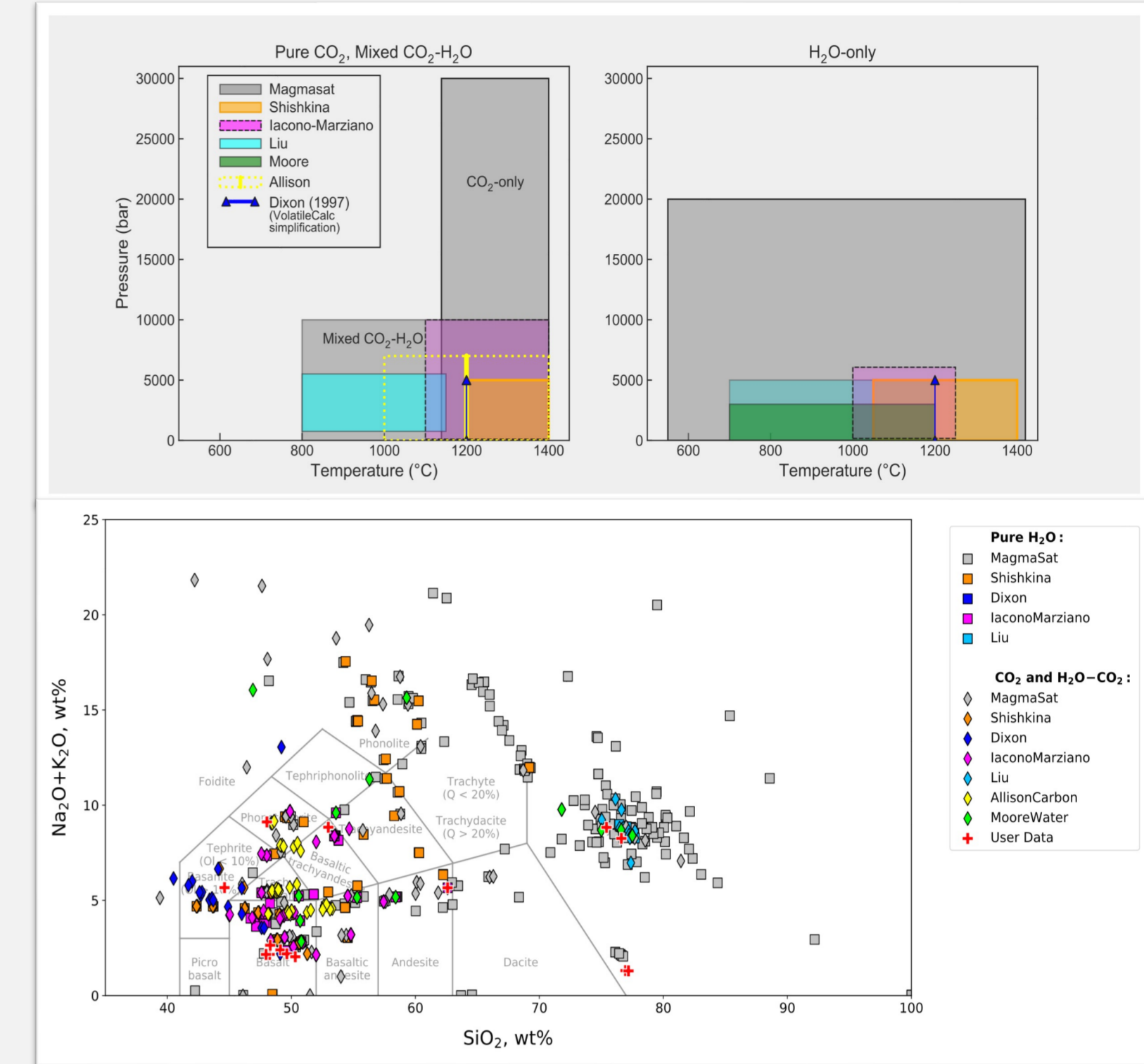


$$2 \ln X_{H_2O} = \frac{a}{T} + \sum b_i X_i \left(\frac{P}{T}\right) + c \ln f_{H_2O} + d \quad (1)$$

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...

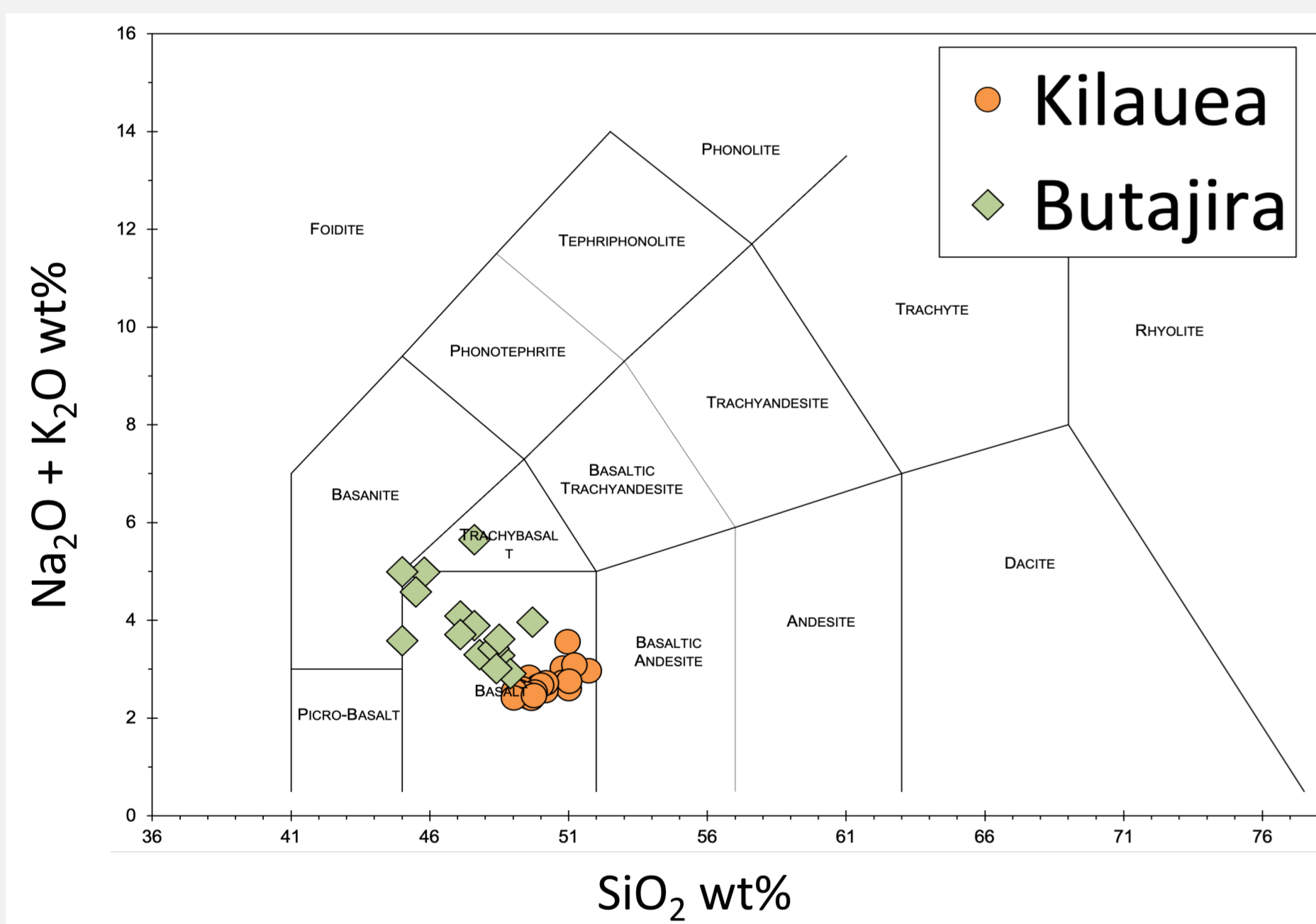
- Utilize any built-in fugacity or activity model
- Write custom calculations right into VESICAL
- Use **model comparison tools to choose the right model for the job**
- New: calculate liquid density and viscosity
- New: **Easy inter-op with python library ThermoBar**

Example use case: Compositional variation matters!

Problem: Plotting polybaric data on isobaric plots

When examining a dataset of related glasses, it is common practice to plot them atop isobars, curves representing the saturation point at constant pressure. Because calculating isobars is computationally intensive to do manually, such isobars are calculated for one composition and may represent the mean, median, or other glass in the set.

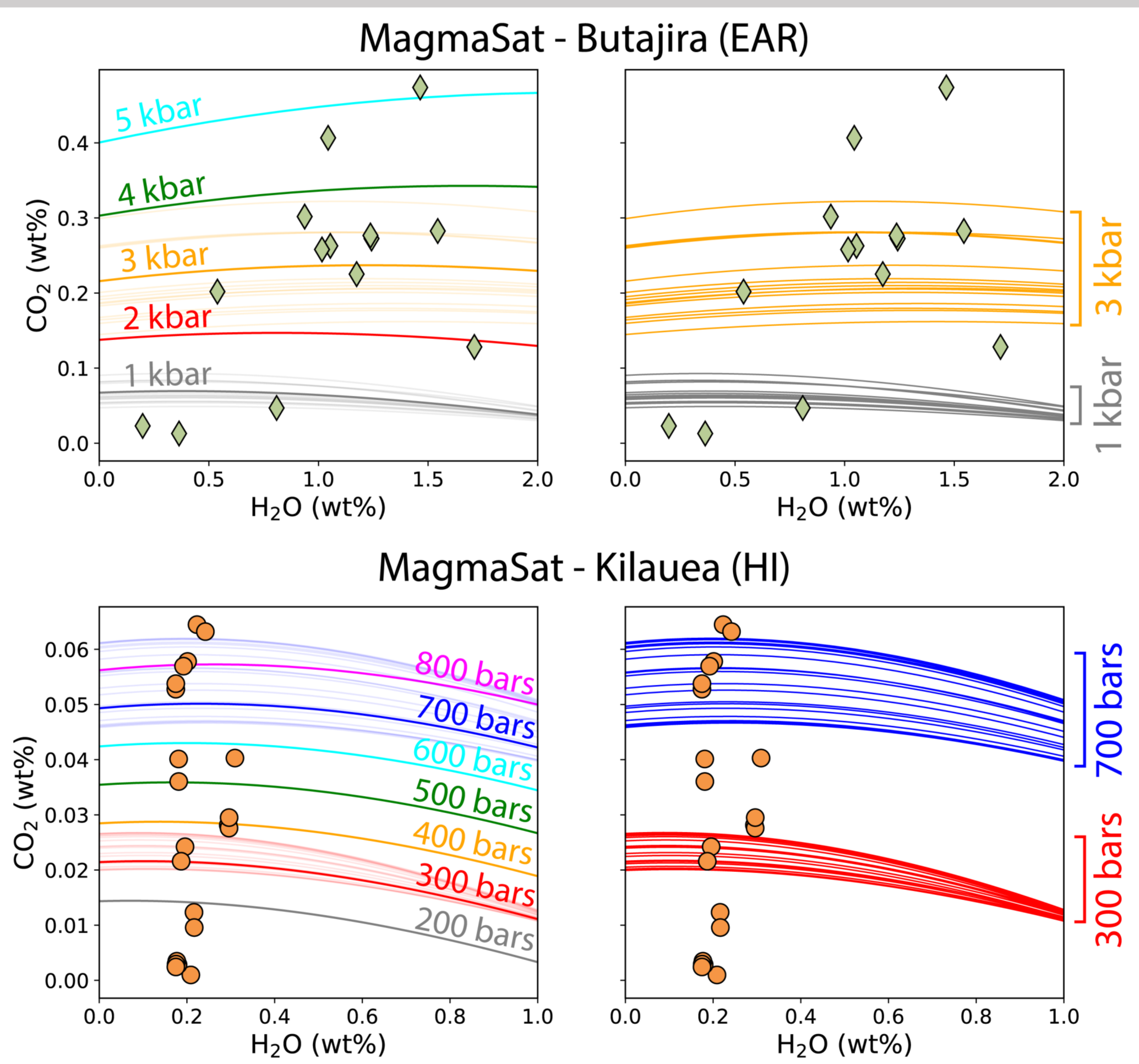
VESICAL now allows us to easily calculate isobars (or, for that matter, saturation pressure, fluid composition, etc) for each glass in our dataset. Here we examine how even minor compositional variation within two sets of melt inclusions (MI) form individual eruptions can lead to significant differences in calculated isobars. This suggests that plotting all MI from a set on top of just one set of isobars can misrepresent the actual saturation pressures of every MI except for the one for which isobars were calculated.



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.

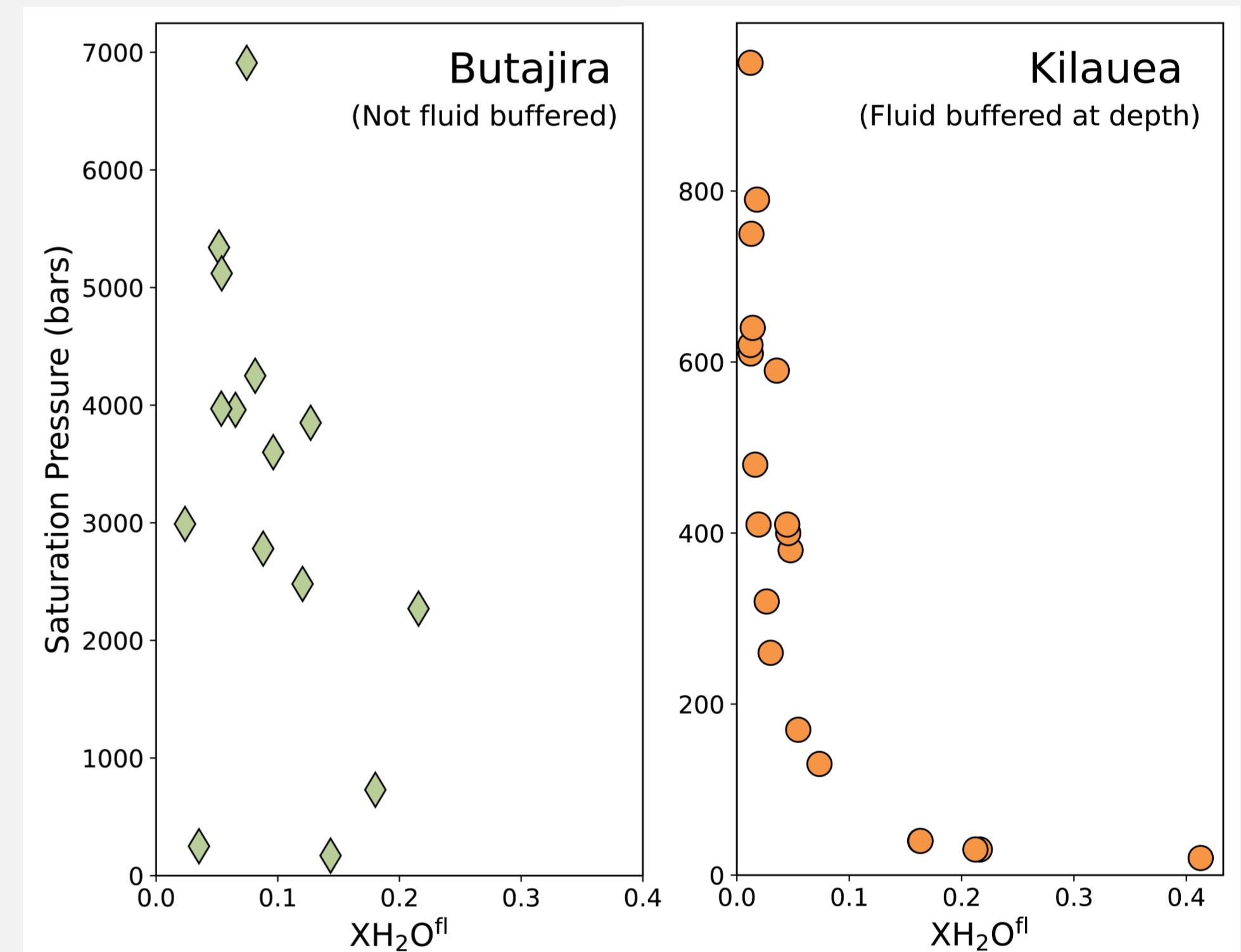
Here we plot isobars calculated with MagmaSat for olivine-hosted melt inclusions from Butajira (Iddon and Edmonds, 2020) and a subset of melt inclusions from Kilauea (Wieser et al., 2021).

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 (Kilauea).



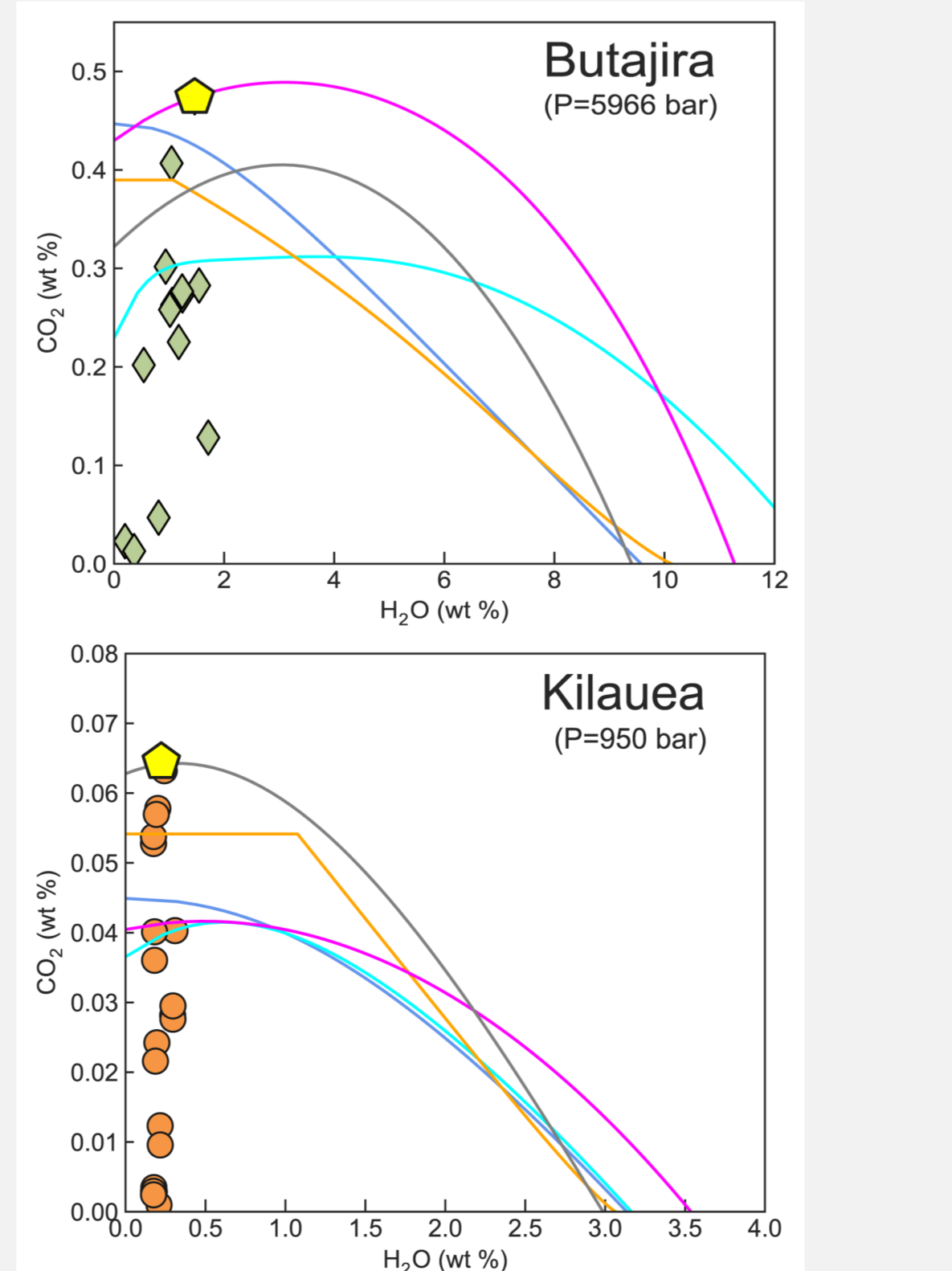
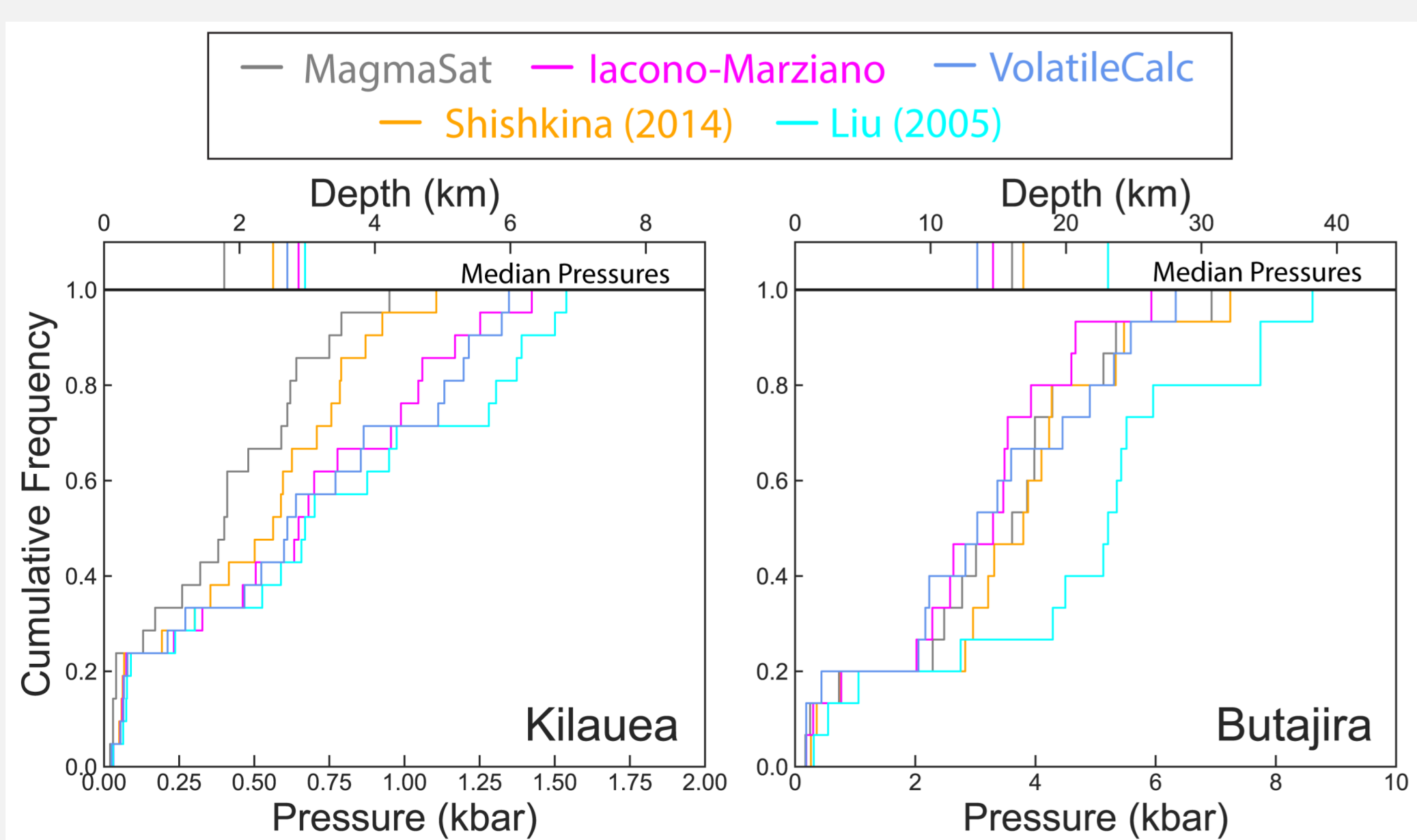
Alternative plotting

Below we show how plotting these datasets differently can represent them more accurately. By calculating the individual saturation pressure and fluid composition (here as mole fraction of H₂O in the fluid, XH₂O^{fl}) for each MI (something made possible for large datasets with VESICAL), true pressure variations can be seen, and new trends may emerge.



Here we see a clear pattern in the Kilauea fluid compositions with pressure, indicating the system may be fluid buffered above ~200 bars such that fluid composition is constant during ascent. At lower pressures, H₂O becomes less soluble and begins to exsolve more strongly, pushing the fluid composition to higher XH₂O^{fl}. Butajira shows no such trend and is likely not fluid buffered.

Model comparison made easy



How to use VESICAL

Start here!



<https://vesical.readthedocs.io/>

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



Installed locally on your computer
(Easy: every model except MagmaSat)
(Hard: every model w/MagmaSat)



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

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

