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# VESIcal: An open-source thermodynamic model engine for mixed volatile ($H_2O$-$CO_2$) solubility in silicate melts

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Modeling the solubility of volatiles in silicate melts is fundamental to the interpretation of volcanic systems and has implications for magma dynamics, eruption style, and material transport between the mantle, crust, and atmosphere. Recent advancements in computational capabilities and access to computing tools has outpaced the functionality and extensibility of previously available modeling platforms. Here we present VESIcal (Volatile Equilibria and Saturation Index calculator), the first comprehensive modeling tool for $H_2O$, $CO_2$, and mixed ($H_2O$-$CO_2$) solubility in silicate melts that: a) allows users access to seven popular models, with easy inter-comparison between models; b) provides universal functionality for all models (e.g., functions for calculating saturation pressures, degassing paths, etc.); c) can process large datasets (1,000's of samples) automatically; d) can output computed data into an Excel spreadsheet or CSV file for post-modeling analysis; e) integrates plotting capabilities directly within the tool; and f) provides all of this within the framework of a python library, making the tool extensible by the user and allowing any of the model functions to be incorporated into any other code capable of calling python.

Here we will provide a demonstration of VESIcal and its capabilities with applications to various volcanic processes affected by volatiles. VESIcal represents the first tool capable of directly comparing multiple solubility models and equations of state. We find that commonly used models predict surprisingly different volatile solubilities, particularly for pure $CO_2$ or mixed $CO_2$-$H_2O$ fluids. Even for melt compositions that are well represented in the calibration datasets of multiple models (e.g., MORBs), calculated solubilities for pure $CO_2$ and pure $H_2O$ can deviate from one another by factors of >2 leading to 2x deviations in calculated saturation pressures (e.g., 5 to 10 kbar). The solubility of $CO_2$ predicted by different rhyolitic models also differs substantially, overwhelming other sources of uncertainty such as analytical errors on measurements of volatile contents or uncertainties in crustal density profiles. This highlights the importance of model choice when drawing geological conclusions based on volatiles in magmas.