A new era of H-O-C-S magma solubility modeling: Better, faster, stronger

DR. KAYLA IACOVINO[1], ALAIN BURGISSER[2], SHUO DING[3], ERY C HUGHES[4], GEOFF KILGOUR[5], PHILIPPA LIGGINS[6], CHENGUANG SUN[7] AND PENNY WIESER[8]

[1]Jacobs, NASA Johnson Space Center
[2]ISTerre
[3]Lamont-Doherty Earth Observatory
[4]Te Pū Ao GNS Science
[5]GNS Science
[6]University of Oxford
[7]The University of Texas at Austin
[8]University of California, Berkeley
Presenting Author: kayla.iacovino@nasa.gov

H_2O, CO_2, and S are the most abundant volatiles in magmatic systems and are critical to understanding magma storage, phase equilibria, and volcanic eruptions. Models that consider all three of these components, however, may not allow for critical examination and adjustment of assumptions underlying the model, or provide benchmark testing or extensible interfaces. Thus, understanding why models produce different results can be challenging. We have gathered authors of established (D-Compress [1]) and recent (VolFe, EVo, Sulfur_X, MAGEC [2–5]) H-O-C-S volatile solubility models to work together to understand how and why our models diverge. We present a series of benchmark basalt degassing scenarios revealing that often understated model assumptions such as fO_2 buffer equations, fO_2-Fe^{3+}/SFe relationships, and even major element normalization routines have outsized effects on model results. All models consider S^{2-} and S^{6+} melt species but with different approaches to sulfate/sulfide capacities, partition coefficients, and species fugacities, leading to divergence in the evolution of modeled gas compositions, melt S and Fe speciation, and fO_2, with the extent of divergence depending on melt composition. Such scenarios enable meaningful intercomparison of existing models and lay the groundwork for a user-friendly yet powerful solubility modeling framework. Given our wealth of existing solubility literature, we suggest that the field of magmatic volatiles should focus now on the creation of modern tools and the modular implementation of existing model equations or methods, and that the evaluation of code usability, transparency, and benchmarking should be codified pillars of the peer-review process. As an example of such an endeavor, we present early work coupling these sulfur solubility models with VESIcal [6], an extensible and rigorously tested python library containing seven existing H_2O-CO_2 solubility models. VESIcal includes the ability to extract, edit, and even interchange assumptions underlying any model. For example, users may combine or swap separately published H_2O, CO_2, and S models, as well as underlying model choices, such as Equations of State and redox models.

[1] Burgisser+ (2015) *Comp. Geosci.*

[2] Hughes+ (2023) *Journ. Geolog. Soc.*
[3] Liggins+ (2020) *EPSL*
[4] Ding+ (2023) *G3*
[5] Sun and Lee (2022) *GCA*
[6] Iacovino+ (2021) *Earth Space Sci.*