Workshop report:
Modelling volatile behaviour in magmas

Sunday 29th January 2023 - IAVCEI pre-conference workshop - Rotorua, Aotearoa

Ery Hughes[1]*, Shuo Ding[2], Kayla Iacovino[3], Penny Wieser[4], Geoff Kilgour[1]

1 Te Pū Ao | GNS Science, Aotearoa (@eryhughes, @NZvolcanologist)
2 Lamont-Doherty Earth Observatory, Columbia University, USA (@ShuoDing4)
3 Jacobs/NASA Johnson Space Centre, USA (@kaylai)
4 University of California – Berkley, USA (@Penny_Wieser)
*e.hughes@gns.cri.nz

Disclaimer: This is a workshop report that has not been peer reviewed.

Co-signers (alphabetically by first name):
Alex Nichols (University of Canterbury, New Zealand)
Ana Casas Ramos (Australian National University, Australia)
Christina Cauley (University of Oregon, USA)
Clara Waelkens (University of Hannover, Germany)
Diego F. Narváez (Departamento de geología, Escuela Politécnica Nacional, Quito, Ecuador)
Elaine R. Smid (Waipapa Taumata Rau | The University of Auckland, Aotearoa New Zealand)
Emma Nicholson (University College London, UK)
Francesca Haywood (University of Bristol, UK)
Gui Aksit (University of Oregon, USA)
Kara Brugman (Arizona State University, USA)
Kelly McCartney (University of Hawaii at Manoa, USA)
Lissie Connors (University of Oregon, USA)
Margaret Hartley (University of Manchester, UK)
Matthew Varnam (Lunar and Planetary Laboratories, The University of Arizona, USA)
Paul Wallace (Department of Earth Sciences, University of Oregon, USA)
Roberto Moretti (Università della Campania "L. Vanvitelli", Dipartimento di Ingegneria, Italy)
Rose Gallo (University of Hawai'i at Manoa, USA)
Terry Plank (Lamont Doherty Earth Observatory, Columbia University, USA)
Will Hutchison (University of St Andrews, UK)

Table of Contents

Workshop description

Volatiles are a critical component of magmas, driving volcanic eruptions, creating and modifying planetary atmospheres, and generating ore deposits. There has been an immense amount of work quantifying the solubility of individual volatile species in a wide variety of magma compositions and the creation of various modelling capabilities to look at magmatic degassing.

This workshop aimed to bring together experimentalists, numerical modellers, and observational researchers with an interest in volatile solubility in magmas. Through group discussions, model demonstrations, and keynote talks, we explored the current landscape and looked for future directions. We started with a demonstration session of existing models and codes. There is currently no benchmarking for such codes, so we discussed options for a benchmarking exercise and test datasets. This was followed by discussions on future directions, covering:

1. What are the experimental gaps (e.g., melt compositions, volatile species, pressure-temperature (PT) ranges, fugacity coefficients, non-ideal mixing, etc.)?
2. What do observational researchers need these codes to be able to do?
3. Can we link monitoring needs to solubility outputs?

Format

The workshop was hybrid, with the opportunity for pre-submitted written work, to ensure as many people as possible could participate – accessibility was high on our priority list. As required for IAVCEI 2023, masks were required for in-person attendees and testing prior to attending if this was a participant's first IAVCEI event. The cost was NZ$50 to attend, which was set by IAVCEI 2023. Prior to the workshop, we sent out a form where people who would not attend the workshop could give answers to the questions we would be discussing – only one person gave feedback this way.

Most of the workshop was recorded and has been uploaded to a YouTube playlist in multiple parts: https://www.youtube.com/playlist?list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL.

1 Introduction	https://www.youtube.com/watch?v=dli2IeL3Zxw&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=1
2.1 Introduction to VESIcal	https://www.youtube.com/watch?v=yVEvR-jNPZ8&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=2
2.2 Introduction to Sulfur_X	https://www.youtube.com/watch?v=1wHvDy4Q9rU&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=3
2.3 Introduction to CHOSETTO	https://www.youtube.com/watch?v=zlyEOkaR3Yg&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=4
2.4 Introduction to SCHOFe	https://www.youtube.com/watch?v=8U27ph5D45g&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=5

2.5 Model benchmarking and intercomparison	https://www.youtube.com/watch?v=Wx785sir0vU&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=6
3.1 Keynote: What are the gaps?	https://www.youtube.com/watch?v=SYxRCRR-nlo&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=7
3.2 Keynote: What do observational researchers need codes to do?	https://www.youtube.com/watch?v=wanPnJTchdM&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=8
4 Breakout report and wrap-up	https://www.youtube.com/watch?v=aHDUx_sbPe4&list=PLDSC0wbXSKIziryb7vgWOFdYhMlvkd4KL&index=9

Participants

We had 33 virtual and 48 in-person registered participants (including convenors and speakers). Due to the flooding in Auckland and the travel problems this caused, we ended up with ~30 in-person and ~20 online, which made for great discussions on each and across both platforms. We sent out a form prior to the workshop to those attending and others interested in the topic – 74 people filled out the form. Most registered participants were part of organisations from the United States, United Kingdom, and Aotearoa New Zealand (Fig. 1). There were a variety of career positions for respondents (Fig. 2).

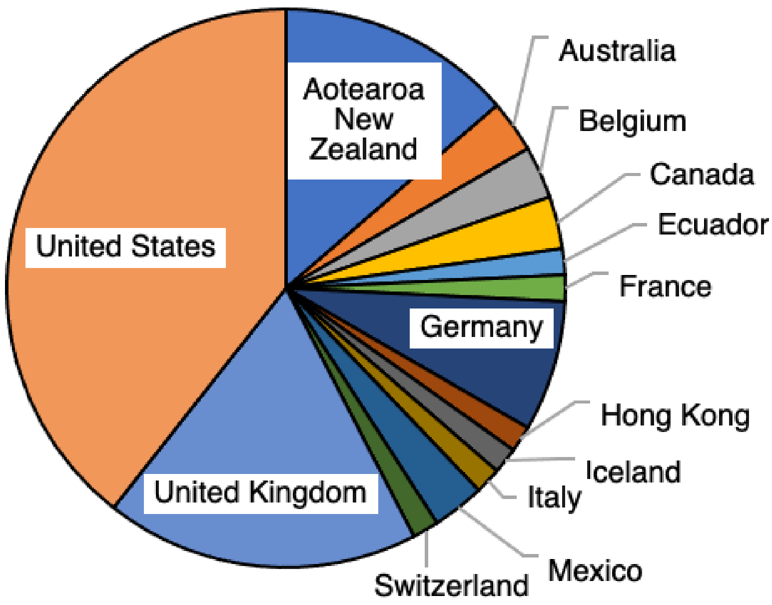

Figure 1 Country of organisation where provided for registered participants (*n* = 66).

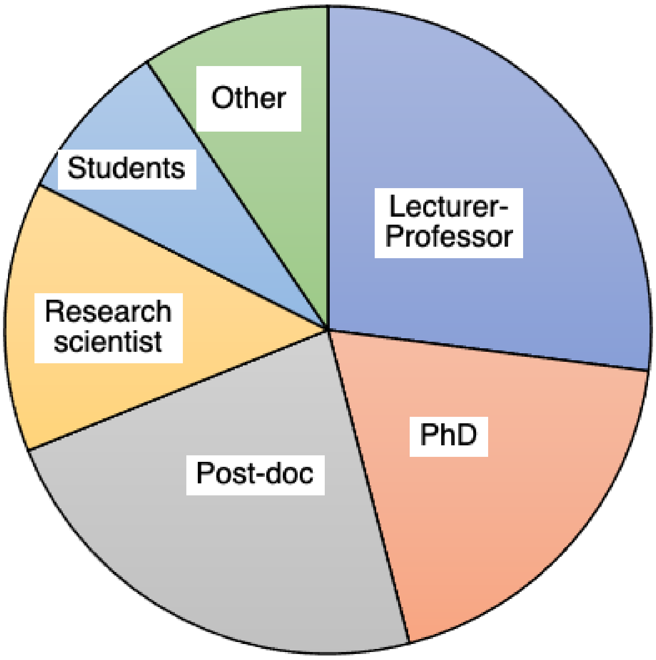

Figure 2 Career position where provided for survey respondents (*n* = 74).

Most respondents were specialists in modelling, then microanalysis, followed by experiments then field measurements (respondents could identify as many specialties as they wanted; Fig. 3). This confirmed we had engagement from a range of disciplines, which was key to a successful workshop. We also asked what solubility codes respondents had used. The vast majority had used VolatileCalc or MagmaSat, with all other codes having been used by <18 % of respondents (Fig. 4).

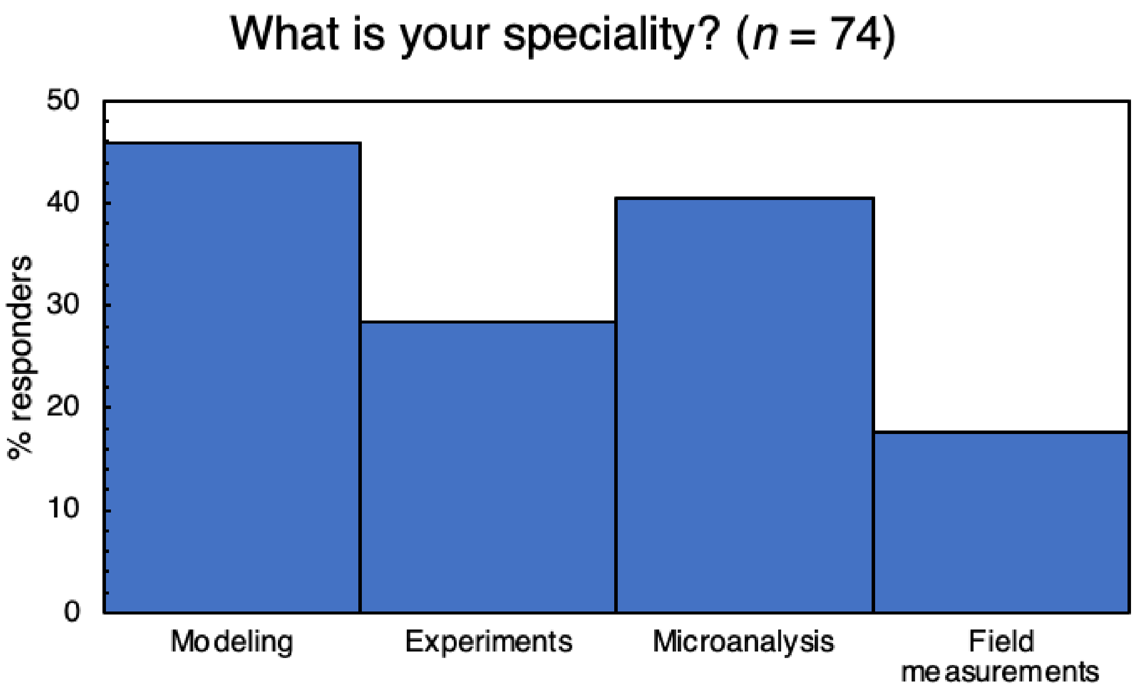

Figure 3 What is your speciality? Respondents selected as many specialities as they wanted using a free-text box.

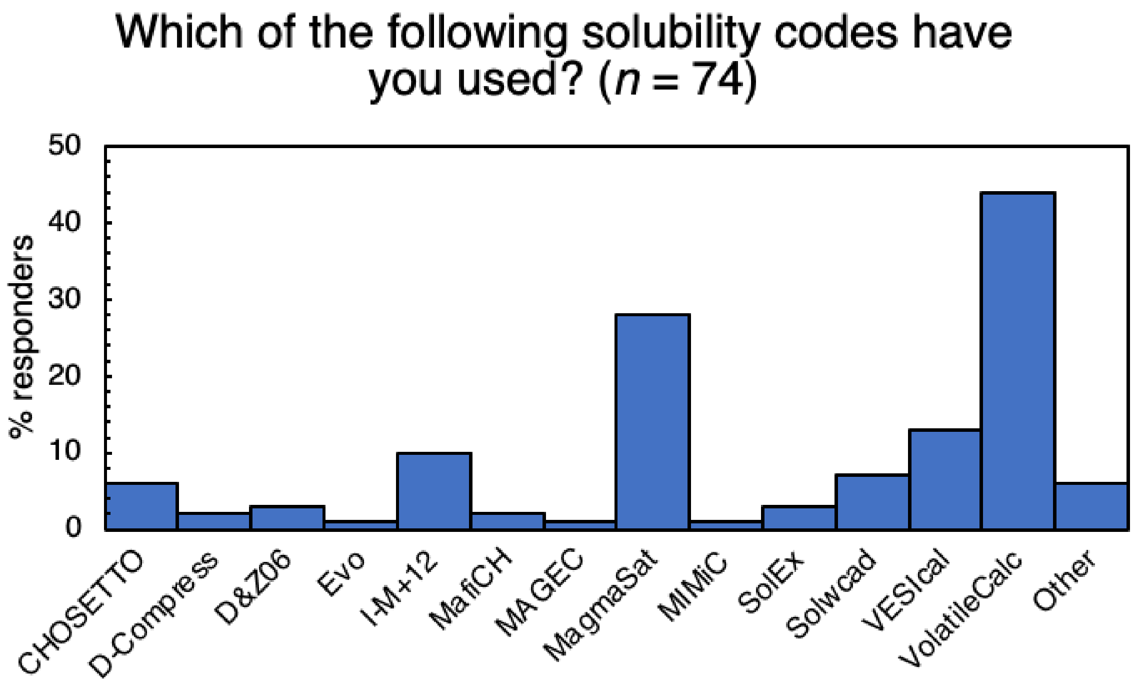

Figure 4 Which of the following solubility codes have you used? Respondents could select as many as they wanted and include models not listed in the survey. CHOSETTO (Moretti *et al.*, 2003; Moretti & Papale, 2004), D-Compress (Burgisser *et al.*, 2015), D&Z06 (Duan & Zhang, 2006), EVo (Liggins *et al.*, 2020; 2022), I-M+12 (Iacono-Marziano *et al.*, 2012), MafiCH (Allison *et al.*, 2022), MAGEC (Sun & Lee, 2022), MagmaSat (Ghiorso & Gualda, 2015), MIMiC (Rasmussen *et al.*, 2020), SolEx (Witham *et al.*, 2012), Solwcad (Papale *et al.*, 2006), VESIcal (Iacovino *et al.*, 2021), and VolatileCalc (Newman & Lowenstern, 2002).

Models and benchmarking

To directly compare disparate volatile models, we selected four compositions: MORB (SiO_2 = 47.4 wt%), arc magmas from Fuego (SiO_2 = 49.67 wt%) and Soufrière Hills (SiO_2 = 60.3 wt%), and a rhyolite from Mono Craters (SiO_2 = 77.2 wt%). The full compositions are given below (including their volatile contents; Table 1). We asked authors of different models for two types of calculations to be performed:

1) Pressure of vapour-saturation
2) Isothermal closed-system degassing path

Table 1 Melt compositions (including volatile contents) used for comparison calculations.

Name	**MORB2**[1]	**Fuego**[2]	**Mono craters**[3]	**Soufrière Hills**[4]
SiO_2 (wt%)	47.4	49.67	77.19	60.3
TiO_2 (wt%)	1.01	1.17	0.06	0.81
Al_2O_3 (wt%)	17.64	16.5	12.8	15.8
Fe_2O_3 (wt%)	0.89	1.65	0.26	1.22
FeO (wt%)	7.18	8.43	0.71	4.392
FeO_T (wt%)	7.98	9.91	0.94	5.49
MnO (wt%)	0	0.19	0	0
MgO (wt%)	7.63	4.38	0.03	2.8
CaO (wt%)	12.44	7.9	0.53	6.56
Na_2O (wt%)	2.65	3.37	3.98	1.94
K_2O (wt%)	0.03	0.79	4.65	0.32
P_2O_5 (wt%)	0.08	0.22	0	0
H_2O-eq (wt%)	0.2	4	5	5
CO_2-eq (ppm)	1100	3500	500	300
S-eq (ppm)	1400	2700	0	300
fO_2 (ΔFMQ)	0	1	1	2
Fe^{3+}/Fe_T	0.10	0.15	0.25	0.2
T (°C)	1100	1100	800	1000

References: 1 Allan *et al.* (1989), Ghiorso & Gualda (2015), Cottrell *et al.* (2021), Wieser *et al.* (2022); 2 Lloyd *et al.* (2013), Rasmussen *et al.* (2020), Wieser *et al.* (2022); 3 Liu *et al.* (2005), Wieser et al. (2022); 4 Cassidy *et al.* (2015).

We prepared model results from VESIcal by K. Iacovino (Shishkina, Dixon, Iacono-Marziano, MagmaSat; Iacovino *et al.*, 2021), SCHOFe by E. Hughes (Hughes on these diagrams; Hughes *et al.* in prep), MAGEC by C. Sun (CSun on these diagrams; Sun & Lee, 2022), and Sulfur_X by S. Ding (SulfurX in these diagrams; Ding *et al.*, 2023). It was clear from trying to compile the different outputs that it would be very helpful for there to be consensus and descriptions of column naming and associated units, which can seriously hinder model intercomparison.

The saturation pressures from different models are shown in Fig. 5 (note, Sulfur_X employs the Iacono-Marziano or Dixon model to calculate the initial saturation pressure). As highlighted in Wieser *et al.* (2022), there is a concerning difference between the different models, requiring detailed interrogation of the calibration dataset of each model.

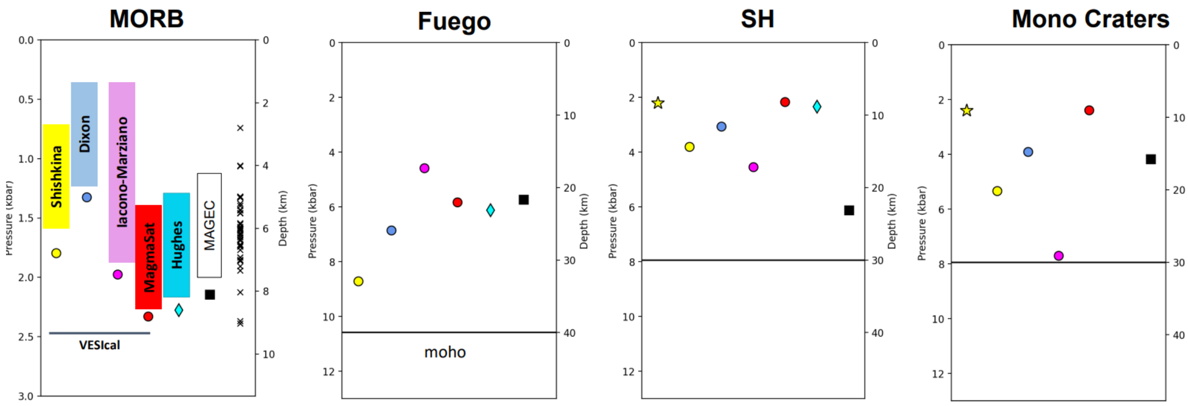

Figure 5 Saturation pressures calculated with different models. Approximate moho positions are shown as black lines, except for MORB (where different estimates are shown as black crosses).

For degassing calculations, we examined trends of S, CO_2, and H_2O in the melt against pressure, as well as the trajectory in CO_2-H_2O space (e.g., Fig. 6 for MORB). As previously noted (Wieser *et al.* 2022), different solubility models show reasonably similar behaviour for H_2O vs. pressure, while there is significantly more divergence in CO_2 vs. pressure. For example, at ~100 MPa, Dixon predicts almost twice as much CO_2 as MagmaSat. Differences in S between models are mostly dominated by the difference in the initial S content prior to the onset of S degassing. This is because MAGEC accounts for sulfide saturation (so the S content cannot exceed the sulfide content at sulfide saturation [SCSS]), which is not the case for Hughes or Sulfur_X. This makes it hard to tell apart different degassing behaviours. For arc magmas (e.g., Fuego in Fig. 7), Hughes and Sulfur_X show very similar degassing behaviour for S. MAGEC predicts very low S contents (likely because the SCSS is not being corrected for the presence of S^{6+}, which would greatly increase total S solubility prior to the onset of degassing). There are also substantial differences in CO_2 behaviour.

We also calculated the CO_2/SO_2 molar ratio of the degassing fluid (note that S is not included in the models in VESIcal, so we only show comparisons for Hughes, Sulfur_X, and MAGEC; Fig. 8). This is a particularly interesting comparison because it has been suggested that CO_2/SO_2 is a barometer. However, it is clear from drawing a horizontal line on any of these plots that the pressure obtained from the gas composition is highly model dependent.

Overall, these model comparisons showed that the result is highly dependent on the model. Part of this is because models are only calibrated on a restricted compositional spectrum (e.g., the andesitic Soufrière Hills and rhyolitic Mono Craters magma is outside the calibration range of many models). However, all the models discussed should behave well on MORB, and yet there are still substantial differences. It became clear from the associated discussion that modelling remains 'piecemeal', with different models focussed on specific calculations, but not all models can do all calculations. In particular, the inclusion (or absence) of sulfide saturation produces a wide discrepancy in the modelled behaviour for S. This makes it difficult to attribute differences in degassing behaviour. It is clear that a model including S in all its species (e.g., S partitioning into the fluid, sulfide and anhydrite saturation, calculation of S^{6+} proportions to get total S) is required to progress.

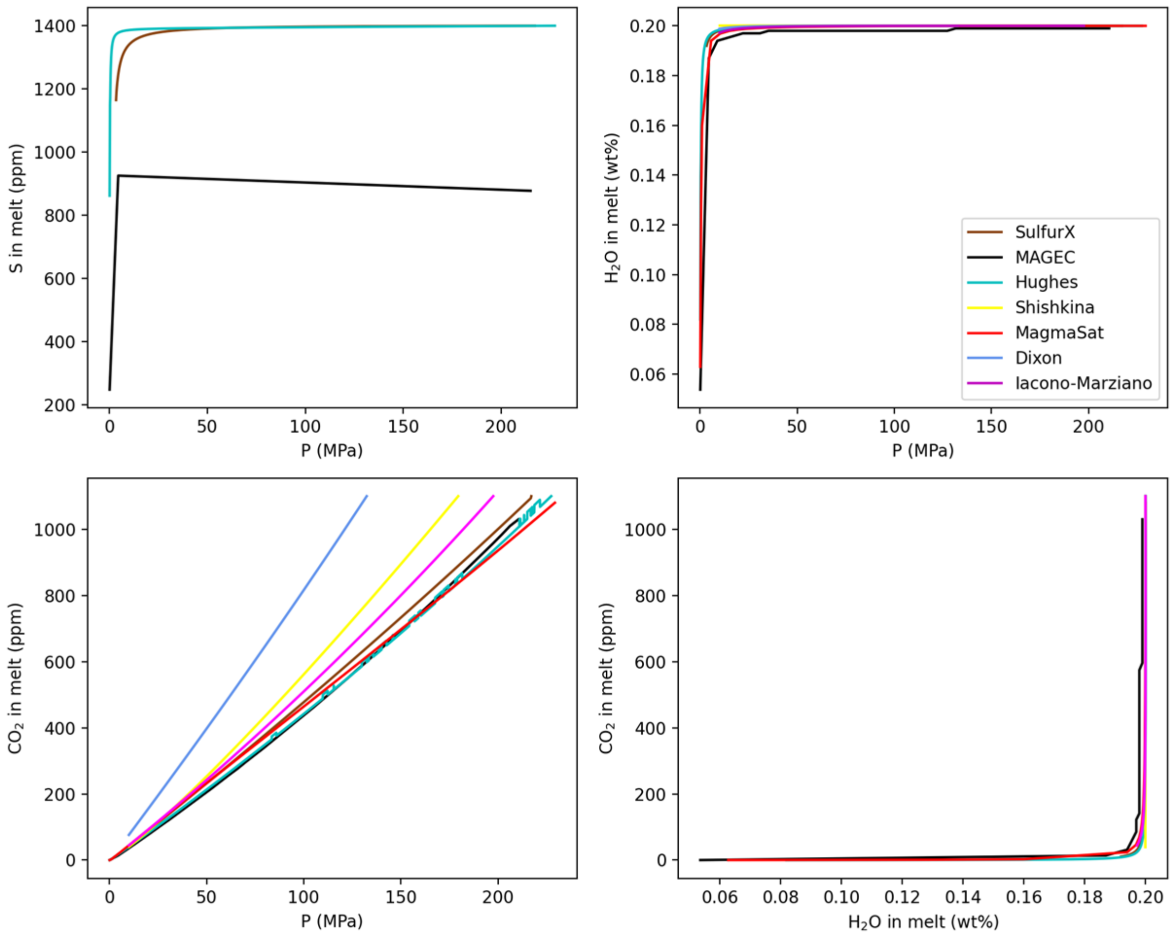

Figure 6 Degassing paths for MORB.

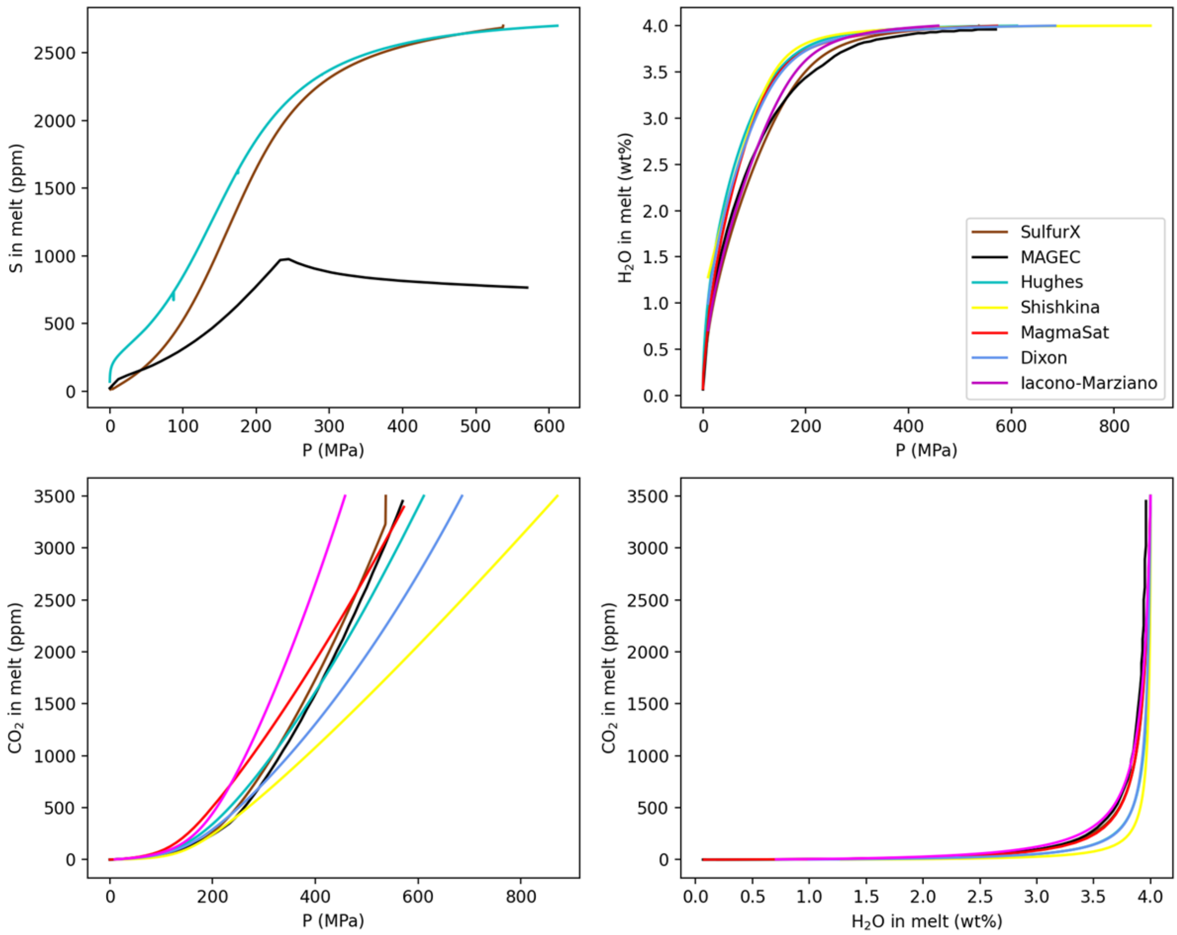

Figure 7 Degassing paths for Fuego.

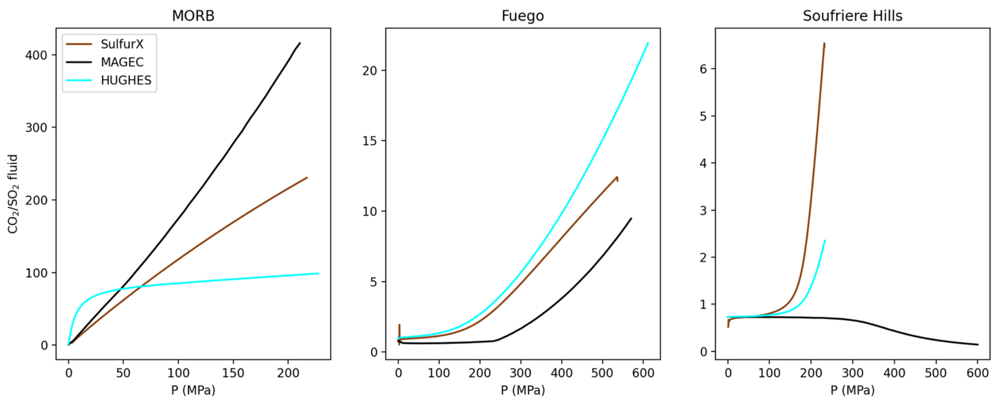

Figure 8 CO_2/SO_2 molar ratios in the fluid.

Summary of discussions of high-level topics

We covered three high-level topics, underlain by three sub-questions, for discussion at the workshop:

Q1: What are the experimental and modelling gaps e.g., melt compositions, volatile species, PT ranges, fugacity coefficients, non-ideal mixing, etc.?	Q2: What do observational researchers need these codes to be able to do?	Q3: Can we link monitoring needs to solubility outputs?
• What are the key open questions or needs related to this topic? • What are some existing challenges to answering these questions and potential solutions to these challenges? • What is a potential target area (in physical or P/T/X space) where a multidisciplinary (observational + experimental + analytical + modelling) study could take place to answer some of these big questions?		

For each high-level topic, we invited a keynote speaker to give a 20 min talk, which was followed by 5 min of questions. A 30 min discussion was achieved via small groups either in-person or online, where the group would take notes on a shared google-doc and choose one key point to relay back to the main group at the end. We had five groups in person and at least one group online: breakout groups were either online or in-person for ease of discussion. All feedback was presented to the whole group, as well as the final breakout report and wrap-up. The notes from these discussions are summarised below and included in full in the appendix.

Q1: Where are the gaps in our experimental and modelling knowledge, and how do we fill them?

In this section, we discussed the gaps in both our ability to perform experiments and our ability to model magmatic systems. Shuo Ding and Penny Wieser presented a keynote talk on this topic. The recorded talk is available on YouTube at: https://youtu.be/SYxRCRR-nlo

As discussed above, breakout sessions focused on the following questions: What are the key open questions? What are the existing challenges in addressing these questions? What are potential target areas? Answers to all of these points are discussed together below.

During breakout sessions, both modelling and experimental needs were discussed. Within the field of magmatic volatile modelling, the models have become complex yet disparate enough to the point that model intercomparison and benchmarking are crucial in making further discoveries. While the creation of new niche models is not seen as a negative thing, the community discussed how comparing our existing models is an area ripe for progress. Consistency between models was noted as an area needing improvement. Namely, are models broadly deployable, and are parameters and outputs comparable? This first step in model intercomparison began in this workshop, and the community is keen to continue this effort on a larger and more in-depth scale. Not only will this lead to furthering progress in modelling capability, but it will also allow observational researchers to efficiently pick the right model for their use case without necessarily needing to know the low-level details of each model implementation (e.g., calibration range shortfalls, equation of state used, etc.).

This led into a discussion of how we communicate models. How can modellers clearly communicate the limitations of their model? From a hazards perspective, what constitutes a useful result (e.g., how do we interpret differences in model outputs given the same inputs)? Benchmarking is seen as a critical step in addressing these issues.

The need for open and accessible data and models was highlighted as something that should be strongly considered for model communication. Using open-source best practices will help address current issues surrounding uncertainty in model choice by a user and in interpreting results. For example, codes should be well documented with guides that explain how to choose parameters, what model shortfalls exist, etc. Additional tools (e.g., jupyter notebooks, scripting languages, web-apps and applications with a GUI) will allow more access to these models particularly for users with little to no coding experience. Hopefully, we can leverage practices in other fields to encourage open data, e.g., NASA's Open-source Science Initiative and Transform to Open Science (TOPS).

An important step in addressing model communication is in clearly communicating model and experimental uncertainty. Currently, uncertainties are extremely difficult to compare between experimental studies, meaning that propagating those errors into a model becomes essentially impossible. Thoughtful discussion on how to quantify, report, and propagate errors is a major need in improving model utilisation.

Making models extensible through open-source practices is critical to pushing models further. For example, we can integrate existing databases into our codes (e.g., a user could automatically pull data from a repository such as EarthChem and model them). There is a great benefit in writing models in such a way that allows them to be integrated into both geodynamic and conduit flow models. This requires a non-GUI way to call the functions, compatibility between the coding languages, and thought into the choice of variables (e.g., enthalpy vs. PT). Model standardisation, increased usability and extensibility, and collaboration among larger groups to bring models together and perform intercomparisons and benchmarking are all seen as critical needs to move the field into the next decade.

Bridging both the modelling and experimental aspects was the ever present question of disequilibrium. Many volcanic processes in nature are not equilibrium processes, but thermodynamic models are by design created for systems in equilibrium. Models that incorporate known kinetics for bubble nucleation and crystal growth would be highly useful to the community. Studies aimed at determining these parameters including the kinetics of sulfide resorption in particular were identified as good next steps.

Gaps in our experimental knowledge are many, but which gaps are the most important to fill? The community identified both a better understanding of volatile solubility in arc magmas and the solubility of halogens in all magmas as two critical needs. There is currently a lack of experimental data for intermediate compositions, even in the otherwise well documented

H_2O-CO_2 space. Experimental data accounting for more alkalic and silicic compositions are also important. Halogens (F, Cl, Br, I) have been the focus of more and more observational studies, but our experimental knowledge of their solubilities is distinctly lacking. The interactions between halogens and other major volatile components (particularly H_2O) mean that the experiments are complex and can be difficult to perform, but even individual studies on small magma compositional ranges will be immediately useful to the community.

It was noted that funding targeted experimental efforts can be difficult. Workshops like this one and derivative reports will help in establishing the need for such studies, aiding in motivating grant proposals. Networking with large community efforts such as SZ4D who have identified a need for more experimental studies is another important avenue for funding. Fostering the inclusion of early career scientists into the field of volatile modelling will also aid in the effort by growing the community and setting the groundwork for the future of the field.

In summary, the community highlighted several gaps in our ability to accurately and effectively model volatiles in magmas. Existing models and those moving forward must be more accessible, with extensive documentation and open-source code. Experiments are difficult in many ways (choice of capsule material, method of buffering oxygen fugacity, high failure rates resulting in long duration projects) and can be equally difficult to fund. Community reports, engaging with ongoing large-scale studies such as SZ4D, and including early career researchers in the field are all seen as important ways to help convince funding agencies of the need for experimental studies. Experiments and modelling should be coordinated to fill literature gaps. Future critical experimental studies would focus on halogens in all systems, volatiles in intermediate magmas, and disequilibrium processes and kinetics. Efforts to undertake re-analysis of existing experimental products may provide a significant advance in our knowledge with relatively little investment compared to conducting multiple new experimental studies.

Q2: What do observational researchers need these codes to be able to do?

This breakout session focuses on the question: “Which models does the community need to interpret observational data from inclusions, volcanic gases, and geochemistry and to infer magmatic processes?” The keynote talk was given by Margaret Hartley (University of Manchester, UK) and is available on YouTube here: https://youtu.be/wanPnJTchdM.

The use of models to interpret CO_2/S ratio in volcanic gases, which ultimately leads to understanding volcanic unrest, and connecting degassing modelling to magma ascent/fluid dynamics were of the most interest to participants. Discussions on these overarching topics led to the discussion of several specific needs for models including: the inclusion of halogens, sulfur, and other trace gases that can be measured as gas fluxes and in accessory minerals like apatite; incorporation of processes like redox evolution of the system; disequilibrium degassing; magma recharge; fluid immiscibility; post entrapment modification correction (PEM); vapour bubble growth; C and S isotope fractionation during magma ascent and degassing; and switching between open- and closed-system degassing.

Moreover, intermediate and more alkaline (e.g., nephelinites) compositions are scarcely included in existing models.

Some of the processes, like sulfur and halogen degassing and redox change, are included in some existing models, while others are either not integrated in a degassing model (e.g., correction of PEM and vapour bubble growth, magma recharge), or simply do not exist. However, as shown in our benchmarking exercises, even among existing degassing models, discrepancies in predicting saturation pressures, sulfur behaviour, and co-existing vapour compositions exist. Moreover, each model is calibrated in different P-T-compositional space and with its own advantages and disadvantages. A question continuing to plague observational researchers is in understanding which model to use. This depends on the specific modelling purpose and targeted system. From a modelling perspective, providing calibration information, being clear with data issues and quantifying errors and uncertainties are essential. For example, the option to plot a user's samples along with the calibration data in P-T-compositional-fO_2 space could be very helpful for users to visualise which model's parameters fit the observational data the best. To address the discrepancies among existing models, a paper comparing models with benchmarking calculations on different and well-constrained volcanoes (from melt inclusions, volcanic gas, geophysical observations, targeted experiments, etc.) appears to be much needed. Such a paper would be extremely helpful for data interpretation; for example, to interpret volcanic gas data. To include other processes (kinetic degassing, isotope fractionation) and elements (halogens and other measurable trace gases), more targeted experiments are needed. Moreover, revisiting old data/experimental-products with more recently developed analytical methods (e.g., XANES [X-ray Absorption Near-Edge Structure] spectroscopy, SIMS [Secondary Ion Mass Spectrometry]) would be useful.

In terms of model usage, potential solutions and future directions were discussed. Well-annotated and adaptable scripts are important for both individual users and for constructing some kind of forum/platform where easy comparisons among different models are possible, and users with less coding skills can get centralised help. Common input and output files/structure and standardised vocabulary would make the comparison practice easier. To keep a broader community involved, regular workshops for model updates, hands-on demos, better code documentation, tutorials (YouTube videos, jupyter notebooks) would be necessary. If the community requires more integrated, well-maintained, and user-friendly models that incorporate different processes, a core development team with stable funding and clearly assigned credits for contributions are needed.

Q3: Can we link monitoring needs to solubility outputs?

Building upon the previous session, which gave the observational researchers' perspective on what they need from models, in this session we discussed how to put into practice a better link between these two fields. A keynote was given by Tricia Nadeau (from USGS, not recorded).

The top highlighted points chosen by the community in this session largely focused on the challenges and possible paths forward in combining disparate datasets. Currently, linking observations at active volcanoes with solubility models is non-trivial due to fundamental differences in how data are expressed, differences in monitoring techniques, and complexities in choosing and using a solubility model. In particular, workshop attendees stressed the need to relate petrology, geophysics, and numerical modelling to surface gas observations. For example, leveraging geophysical estimates of total gas content (e.g., compressibility combined with inflation/deflation measurements) was seen as an area that would require inputs from the petrologic modelling and observational data.

The key point raised in the talk and discussion was the problem of disequilibrium. All of our solubility models currently assume degassing occurs in equilibrium, and yet S, H and C all have different diffusion rates. Disequilibrium degassing makes it very difficult to link measured gas ratios to solubility models. It was suggested that what requires improvement is a coupling of diffusivity and gas emission models. Another issue that was raised is the role of the hydrothermal system altering gas ratios from the point of emission to the point of measurement, and the clear need for better thermodynamic models of these processes.

A proposed path forward involves the selection of a few volcanoes where we can perform high quality experiments to build a volcano-specific model that would allow direct comparison to monitoring data. This would be possible in many mafic volcanoes (e.g., Kīlauea). However, for the more silicic volcanoes where the solubility models differ the most, there is no guarantee we would have an eruption in our lifetime to check the models against real data.

It was also raised that at many volcanoes around the world, we have no gas record, so the first time we get gas is when unrest is already established or an eruption has begun. In many instances, there is also very little petrological work. This means that as a community, we need to improve at doing petrology quickly, to be able to conduct meaningful work during an eruption to help gas geochemists understand what they are seeing. Conversely, utilising modelling techniques that require fewer petrologic constraints, even if results had large error bars, would be a new and innovative way to make solubility modelling more useful to observatories.

The issue of funding was brought up many times. We do not have enough funding to conduct basic petrology on all volcanoes that present a hazard. We also simply do not have enough experiments, nor enough money to pay people to develop the codes we need as a community. Similarly, there are not enough gas geochemists at most volcano observatories and these gas geochemists do not have enough sensors or deployment systems (i.e., drones) to obtain pristine gas chemistry data. In many cases, even with all the funding in the world, access is still restricted (e.g., in national parks and wilderness in the US).

The elephant in the room during the entire workshop was the influence of other volatiles. No model yet can do H-C-S-Cl-F. Experiments on other volatiles are challenging: for instance, Cl can simply strip all the cations out of the melt during Cl-saturation experiments.

Summary and next steps

Five key findings from this workshop are outlined below:

1. **Review paper on existing models:** There is a clear need for a review paper that discusses the state of the field of modelling volatile behaviour in magmas. As discussed during the workshop, there are currently a number of different models available, but it can be difficult to know which one to use in a given situation. Participants suggested that a review paper would help to provide guidance on the strengths and weaknesses of different models, and make recommendations for which ones to use in different scenarios. It would be particularly helpful in the hazard and monitoring space in understanding how to interpret model results. This review paper would also be useful in establishing benchmarking tests that could be employed as new models are developed.
2. **Making models user-friendly and transparent:** Pressure-temperature-composition calculations for volatile solubility should be simpler, integrated, and transparent. Participants discussed the challenges of working with such calculations, and suggested that making them more user-friendly could help to broaden the use of volatile solubility models beyond the small volatile community. Participants emphasised the importance of making volatile solubility models accessible and open (e.g., by following open-source best practices), well documented, easy to use and install, and easy to link with other observations.
3. **Integrating different data types:** Participants suggested that better integration of different types of data (e.g., petrology, geophysics, numerical models, and surface gas observations) could help to improve our understanding of volatile behaviour in magmas.
4. **The importance of understanding disequilibrium processes:** The workshop participants emphasised the need for better understanding of disequilibrium processes and kinetics. Disequilibrium likely plays a large role in degassing processes, which is particularly relevant to monitoring, making it difficult to fully utilise solubility models for monitoring. By improving our understanding of disequilibrium, we can better predict and monitor volcanic activity. This will require a combination of experimental studies and modelling efforts.
5. **New solubility data to expand volatile and major element composition space:** Two key areas for further experimental study were highlighted by the workshop participants. In terms of magma compositions, it was highlighted that there is a major lack of solubility data for intermediate melts, even though such melts are often associated with the highest risk volcanoes. Even in H_2O-CO_2 space, which is the volatile space most well constrained in general, andesitic experiments are lacking. Participants pointed out in all three sessions the need for expanding our understanding of halogen solubility (F, Cl, Br, I) in all magmas. All are critical in understanding nuanced degassing trends measured at active volcanoes. Bromine in particular was highlighted as a key need since it can be measured by UV spectroscopy, a technique that already dominates the volcano monitoring field.

References

Allan, J. F., Batiza, R., Perfit, M. R., Fornari, D. J., & Sack, R. O. (1989). Petrology of lavas from the Lamont seamount chain and adjacent East Pacific Rise, 10 N. Journal of Petrology, 30(5):1245–1298. https://doi.org/10.1093/petrology/30.5.1245

Allison, C.M., Roggensack, K. and Clarke, A.B. (2022). MafiCH: a general model for H_2O–CO_2 solubility in mafic magmas. Contributions to Mineralogy and Petrology, 177(3):40. https://doi.org/10.1007/s00410-022-01903-y

Burgisser, A., Alletti, M. and Scaillet, B. (2015). *Simulating the behavior of volatiles belonging to the C–O–H–S system in silicate melts under magmatic conditions with the software D-Compress*. Computers & Geosciences, 79:1–14. https://doi.org/10.1016/j.cageo.2015.03.002

Cassidy, M., Edmonds, M., Watt, S. F., Palmer, M. R., & Gernon, T. M. (2015). *Origin of basalts by hybridization in andesite-dominated arcs.* Journal of Petrology, 56(2):325–346. https://doi.org/10.1093/petrology/egv002

Cottrell, E., Birner, S.K., Brounce, M., Davis, F.A., Waters, L.E. and Kelley, K.A. (2021). *Oxygen fugacity across tectonic settings*. Magma redox geochemistry, 33–61. https://doi.org/10.1002/9781119473206.ch3

Ding, S., Plank, T., Wallace, P. and Rasmussen, D. (2023). *Sulfur_X: A model of sulfur degassing during magma ascent.* Geochemistry, Geophysics, Geosystems, 24(4): e2022GC010552. https://doi.org/10.1029/2022GC010552

Duan, Z., & Zhang, Z. (2006). *Equation of state of the H_2O, CO_2, and H_2O-CO_2 systems up to 10 GPa and 2573.15 K: Molecular dynamics simulations with ab initio potential surface*. Geochimica et Cosmochimica Acta, 70:2311–2324. https://doi.org/10.1016/j.gca.2006.02.009

Ghiorso, M. S., & Gualda, G. A. (2015). *An H_2O–CO_2 mixed fluid saturation model compatible with rhyolite-melts*. Contributions to Mineralogy and Petrology, 169(6):1–30. https://doi.org/10.1007/s00410-015-1141-8

Iacovino, K., Matthews, S., Wieser, P.E., Moore, G.M. and Bégué, F. (2021). *VESIcal Part I: An open-source thermodynamic model engine for mixed volatile (H_2O-CO_2) solubility in silicate melts.* Earth and Space Science, 8(11):e2020EA001584. https://doi.org/10.1029/2020EA001584

Iacono-Marziano, G., Morizet, Y., Le Trong, E. and Gaillard, F. (2012). *New experimental data and semi-empirical parameterization of H_2O–CO_2 solubility in mafic melts*. Geochimica et Cosmochimica Acta, 97:1–23. https://doi.org/10.1016/j.gca.2012.08.035

Liggins, P., Shorttle, O. and Rimmer, P.B. (2020). *Can volcanism build hydrogen-rich early atmospheres?*. Earth and Planetary Science Letters, 550:116546. https://doi.org/10.1016/j.epsl.2020.116546

Liggins, P., Jordan, S., Rimmer, P.B. and Shorttle, O. (2022). *Growth and evolution of secondary volcanic atmospheres: I. Identifying the geological character of hot rocky planets*. Journal of Geophysical Research: Planets, 127(7):e2021JE007123. https://doi.org/10.1029/2021JE007123

Liu, Y., Zhang, Y., & Behrens, H. (2005). *Solubility of H_2O in rhyolitic melts at low pressures and a new empirical model for mixed H_2O–CO_2 solubility in rhyolitic melts*. Journal of Volcanology and Geothermal Research, 143(1–3):219–235. https://doi.org/10.1016/j.jvolgeores.2004.09.019

Lloyd, A. S., Plank, T., Ruprecht, P., Hauri, E., & Rose, W. (2013). *Volatile loss from melt inclusions in pyroclasts of differing sizes*. Contributions to Mineralogy and Petrology, 165(1):129–153. https://doi.org/10.1007/s00410-012-0800-2

Moretti, R., Papale, P., & Ottonello, G. (2003). *A model for the saturation of C-H-O-S fluids in silicate melts.* In C. Oppenheimer, D. M. Pyle, & J. Barclay (Eds.). Geological Society of London Special Publication: Volcanic Degassing, 213:81–101 https://doi.org/10.1144/gsl.sp.2003.213.01.06

Moretti, R., & Papale, P. (2004). *On the oxidation state and volatile behavior in multicomponent gas melt equilibria.* Chemical Geology, 213:265–280. https://doi.org/10.1016/j.chemgeo.2004.08.048

Newman, S. and Lowenstern, J.B. (2002). *VolatileCalc: a silicate melt–H_2O–CO_2 solution model written in Visual Basic for excel*. Computers & Geosciences, 28(5):597–604. https://doi.org/10.1016/S0098-3004(01)00081-4

Papale, P., Moretti, R. and Barbato, D. (2006). *The compositional dependence of the saturation surface of H_2O+CO_2 fluids in silicate melts*. Chemical Geology, 229(1-3):78–95. https://doi.org/10.1016/j.chemgeo.2006.01.013

Rasmussen, D. J., Plank, T. A., Wallace, P. J., Newcombe, M. E., & Lowenstern, J. B. (2020). *Vapor-bubble growth in olivine-hosted melt inclusions*. American Mineralogist, 105(12)1898–1919. https://doi.org/10.2138/am-2020-7377

Sun, C. and Lee, C.T.A. (2022). *Redox evolution of crystallizing magmas with CHOS volatiles and its implications for atmospheric oxygenation.* Geochimica et Cosmochimica Acta, 338:302–321. https://doi.org/10.1016/j.gca.2022.09.044

Wieser, P.E., Iacovino, K., Matthews, S., Moore, G. and Allison, C.M. (2022). *VESIcal: 2. A Critical Approach to Volatile Solubility Modeling Using an Open-Source Python3 Engine.* Earth and Space Science, 9(2):e2021EA001932. https://doi.org/10.1029/2021EA001932

Witham, F., Blundy, J., Kohn, S.C., Lesne, P., Dixon, J., Churakov, S.V. and Botcharnikov, R. (2012). *SolEx: A model for mixed COHSCl-volatile solubilities and exsolved gas compositions in basalt*. Computers & Geosciences, 45:87–97. https://doi.org/10.1016/j.cageo.2011.09.021

Appendices

Schedule

Time (NZDT)	Session	
08:00-08:15	Opening remarks	E. Hughes
08:15-10:00	Introduction to models *VESIcal* *Sulfur_X* *CHOSETTO* *SCHOFe* *MAGEC*	Chair: G. Kilgour K. Iacovino, P. Wieser S. Ding R. Moretti E. Hughes C. Sun
10:00-10:20	*Break*	
10:20-10:35	Model benchmarking	P. Wieser
10:35-11:00	What are the gaps? *Keynote* *Discussion*	Chair: K. Iacovino K. Iacovino, P. Wieser, S. Ding
11:40-12:00	*Break*	
12:00-13:05	What do observational researchers need codes to do? *Keynote* *Discussion*	Chair: S. Ding M. Hartley
13:05-14:05	*Lunch*	
14:05-15:10	Can we link monitoring needs to outputs? *Keynote* *Discussion*	Chair: P. Wieser P. Nadeau
15:10-15:40	Feedback from breakouts *What are the gaps* *Observational needs* *Links to monitoring*	Chair: E. Hughes K. Iacovino S. Ding P. Wieser
15:40-15:55	Next steps discussion	Chair: E. Hughes
15:55-16:00	Closing remarks	Chair: E. Hughes

Raw notes from breakout discussions

Q1: What are the experimental and modelling gaps e.g., melt compositions, volatile species, PT ranges, fugacity coefficients, non-ideal mixing, etc.?

Top points

- How can we make models more accessible?
- Disequilibrium conditions never included in models? (But already complicated enough as it is to model equilibrium) (+ facilitate how to pick 'best' and most applicable model for samples)
- Coordinated experiments to fit the literature and model gaps, but push these towards accessible/user friendly platforms for multidisciplinary use (something like vesical which meets these goals but would need extensions to make it callable from 3D parallel thermo-mechanical codes).
- Can we undertake re-analysis of older experimental products? Could be a significant advance in knowledge with relatively little investment.
- Spin w/arc volcanism → immediate need!
- Connect to economic mining

What are the key open questions or needs related to this topic?

- Consistency–are models broadly deployable, and are parameters comparable?
- Sulfur benchmarking
- How can we clearly communicate model limitations?
- From a hazards perspective, what is a useful result? If a magma could be stored at 100 MPa according to one model, and 200 according with another, how do we interpret this?
- Can we leverage practices in other fields (e.g. astronomy) to encourage open data, and codes that we can build off of? (hopefully yes) If so, can we put this information all in one place?
- Need: Guide for how to choose parameters to input for models (e.g. what is a reasonable fH_2O? How should I estimate temperature) Further documentation would be helpful.
- How can we integrate databases in our codes (e.g. would it be possible to automatically pull earthchem data and model it in VESIcal?
- How can we encourage collaboration among larger groups?
- How can models be accessible (e.g. for people without programming experience)
- Solid comparison of different models (as started in this workshop, but expanded to include even more models) to allow observational researchers to efficiently pick the right model without knowing the details of each model. Also to allow one to understand how two models that might both be within the calibration range of own samples differ and which one is more applicable
- Possibility to include the added complication of melt inclusion with vapour bubbles? How include this in modelling when melt inclusion and vapour bubble are measured separately (assuming vapour bubble is pure CO_2 not always applicable?)

- Disequilibrium processes and kinetics: there is no solid solubility model that includes delayed bubble nucleation and disequilibrium
- Need more solubility data and models for intermediate arc compositions
- Experimental data for more alkalic and silicic compositions; calibration of models that more fully account for compositional dependence.
- Halogens - solubility involving multi-component vapour phase; determination of vapour-melt partitioning Do halogens contribute significantly to total pressure in vapour saturated system
- Lack of experimental data for intermediate compositions.
- More experimental data on halogens.
- Dependency of water and carbon solubility behaviours.
- Model standardisation (both formatting and benchmarking).
- Model usability and extensibility
- Uncertainties – very difficult to compare models with no uncertainties, being able to begin to constrain these, experimental error, and fitting data
- Balance open access vs. utility and accuracy - Making sure it is not just black box
- Choice of model - How did you know which ones to choose, why this specific one, how far can you push them – what is reasonable, then what does this mean for uncertainties
- But actually, if you want uncertainty – may require much more processing capability
- What about disequilibrium effects re: degassing and differences in diffusivities? This can cause diffusive fractionation re: C/S ratios
- What are kinetics of sulfide resorption, how does that play into degassing? How quickly can sulfides be resorbed when degassing begins?
- Accounting for non-ideality, EOS
- Experiments: innovations and more expts in general
    - More specific data for speciation T/P
    - Capture a wide range of compositions
        - dacitic expts in progress, andesite is next
    - Systematic increase of elements
    - New/improved capsule materials
    - Better/easier fO_2 control
- Effect of Cl
- Multicomponent vapour species' interactions
- Models that require less well-constrained parameterization of the magma – usefulness for volcano monitoring
- What proportion of volatiles dissolved in a magma prior to eruption exsolve during vesiculation, and what proportion remain dissolved in the magma?
- How does the changing balance between exsolved versus dissolved affect the rheology of the erupting magma and then eruption style, including the explosivity?

What are some existing challenges to answering these questions and potential solutions to these challenges?

- Challenge: experiments are hard. Funding research with lower publication rates.
- Not always easy to obtain funding for very specific experimental studies that target filling in very specific gaps in models (new and very specific studies sometimes preferred by funding agencies)

- (Similar issue with intermediate compositions: sometimes more challenging to 'sell' to funding agencies)
- Disequilibrium experiments complicated as no efficient way to extract gas phase from capsule
- Practical challenge with oxygen fugacity: not possible in all experimental set-ups to measure the oxygen fugacity?
- Predicting volcanic gas compositions - experiments between 1 atm and a few 100 bars
- More uniformity in data output and formats. Usability incredibly important - e.g., success of VolatileCalc. Also, legacy issues, eg. web models
- Graphical user interface for running models - will allow a much wider range of users to do model calculations (but can also lead to misuse, e.g. if model isn't calibrated for a certain composition of interest).
- Difficult experimental apparatus set-up and funding challenges.
- Experiments are very challenging! Variability in set-up between different labs translates to variability in results.
- No one knows errors -
- Untouched regions in P,T space
- Experimental challenges – S is a nightmare, are we speaking to materials scientists (who might know about avoiding
- Grant structure suited for this challenge? Time consuming, costly, dedicated labs, techs, a few labs where you can get gas compositions in small quantities, access to labs is it possible
    - Emphasis outcomes and impacts, S solubility,
    - Being very clear and specific about how this ties to mineral resources
    - Showing community demand for this – formal group, website
- Computational challenges – distributed to cluster, needs
- Funding may be difficult to get, community is rather small. Are enough early career folks being added to community/supported?
- Can we improve info on past experiments by reanalyzing run products? Prev. efforts in other types of expts have not been fruitful; no large repository where all old expts live. Would have to be community effort, but could be (relatively) low-hanging fruit
- Two levels of of gap - 1) better covering the ranges of composition/conditions, which is building on current knowledge, and 2) gaps that have not yet been addressed much (e.g., non-equilibrium degassing) such that we simply don't have much knowledge at all
- Capsule materials
    - Finding an alloy that doesn't react with sulfur at T > 1100 (Au works at T's < 1050)
    - Longer experiments in basalt-andesite composition space not possible due to capsule reaction when looking at COHS at higher temp
- Measuring the exsolved fluid (limited by analytical precision/accuracy)
- Amph mucking up the works
- What are the funding opportunities for experimental studies?
    - Expet proposals hard to get funded
        - Expts are hard and take a while, so the resulting papers are limited in number if you want them to be quality studies

    - wants to get funding to gather up all of the experimental charges for like 3 decades and re-analyze them
        - In progress
            - Cites Penny's cpx-barometer paper
    - Bigger project/grant to unify the effort?
        - SZ4D recently put out a report relating to this https://purl.stanford.edu/hy589fc7561
- Underreporting of redox conditions in experimental studies

What is a potential target area (in physical or P/T/X space) where a multidisciplinary (observational + experimental + analytical + modelling) study could take place to answer some of these big questions?

- Need: experiments on silica-undersaturated systems, or other extreme compositions
- Intermediate compositions: potential for combination of experimental + monitoring (observational) studies (lots of very actively degassing intermediate volcanoes): maybe multidisciplinary works including all four types of study should be more of a focus
- Having a few supersites, case study volcanoes – Mt St Helens in this compositional gap
- Showing a community need for this and an organised group, structure dependent on this
- Effect of Cl
- Intermediate compositions

Q2: What do observational researchers need these codes to be able to do?

Top points

- Not knowing best model to use and a review paper that covers. Perhaps after inputting chemical compositional range of e.g., MI then an automated recommendation could be provided that reduces errors where possible.
- Making PEC easy and integrated and transparent
- User friendly, easy to use and install, easy link with other observations
- **Usability**, to extend beyond small volatile community, but avoid it becoming black box, maintaining code, and legacy access
    - Challenge: making it a black box, balancing availability of source code and graphical user interface, invisible labour needs to be incentivised
    - Solution: have options available, app and python interface, code documentation, tutorials (youtube videos, but still challenges using the models exist), workshops on models available
- If we want to move towards more integrated and user friendly models that incorporate more different data, and away from a system where people make many different narrow case models, might need a core development team/stable funding, and also figure out how to assign credit for contributions to the more integrated system
- How do the halogens fit in? We need them incorporated in experiments and solubility models. How do brines affect everything as a second fluid phase? Easier said than done. Can we leverage info from fluid inclusions, etc. in economic geology/ore deposits?
- How to interpret emitted C/S ratios and link to what is going on in the subsurface if the volatile saturation models do not agree

What are the key open questions or needs related to this topic?

- Relating gas composition changes to magmatic processes, which ultimately leads to understanding volcanic unrest
- Not a strong coder so having the right software and where you can get centralised help - access to forums that people help others, e.g., MELTS. Python communities help wrt open access
- Comments in the code would also help
- Skill is making the measurement but then a gulf between the analysis and the interpretation of the data for processes
- Existing models are applied to conventional systems that don't include brines, Vulcanian systems where switches in closed vs open system degassing
- Choosing the best fitting model depending on the parameter that fits best e.g., TAS plots seem ok but unusual CaO for example, puts the sample along way out of calibration
- Option or model recipe for best modelling approach
- Risk in using a model that others are using instead of best one
- Sulfur behaviour through the magmatic system, including in fluids (e.g. sulfur-fluid partitioning)

- Models that account for presence of bubbles in melt inclusions
- Pre-processing - post-entrapment processes built-in
- Models for Cl and F
- Trying to establish volatile saturation (or not)
- Dealing with new magma inputs/recharge - how can volatile exchange/addition be accounted for?
- How to treat supercritical fluids vs. just gas? Do we need to treat them differently? How do we deal with transitioning from one to the other?
- Apatite - improving use of apatite as a tool to back out volatile behaviour with well-calibrated models
- Discrepancies between models - how does one deal with this?
- Efficiency of running the code
- Modelling disequilibrium behaviour; more experiments are needed.
- Easy to use for both input and output
- Linking geochemical modelling to geophysical observations
- Usability, to extend beyond small volatile community, but avoid it becoming black box (youtube videos and tutorials that exist are great, but still challenges exist)
- Maintaining code and legacy access
- Halogens
- Intermediate and alkalic compositions
- Disequilibrium
- Degassing relationship with bubble number densities important step in understanding disequilibrium
- Really important to start including sulfur, maybe other traces gases (since these are the things we can measure gas fluxes of)
- Clarity in issues with data (both used to make models and in application of interest)
- Better documentation, try to move towards integrating into one system (vesical)
- How can we connect solubility models to magma ascent/fluid dynamics? What about kinetic effects that could affect gas compositions? How can we bridge these gaps?
- What are rates of exsolution? What are the kinetics on the timescale of seconds, which is the rate at which eruptions may be happening? How do fluids evolve at different timescales in different settings?
- What can experimentalists do re: bubble growth, etc. to inform magma rise models? Is bubble growth diffusion-limited or viscosity/rheology-limited?
- How do the halogens fit in? We need them incorporated in experiments and solubility models. How do brines affect everything as a second fluid phase?
- Unsure how to quantify error and uncertainty in solubility models
- Ways to model C and S isotope fractionation during degassing
- Be able to easily run different models for comparison
- Nested equation of state - gas speciation enabled
- Need to be able to batch process lots of melt inclusions in a single calculation
- Non-specialists need to be able to critically evaluate which models are best to apply for their case study
- To track changes in oxidation state during magma ascent
- Solubility models that are well calibrated for particular redox conditions
- Would be helpful to have common input file requirements so that inputs can be transferred between different codes. And common output file formats so that outputs can be easily compared.

What are some existing challenges to answering these questions and potential solutions to these challenges?

- Kinetics of disequilibrium
- Not knowing best model to use and a review paper that covers. Perhaps after inputting chemical compositional range of e.g., MI then an automated recommendation could be provided that reduces errors where possible.
- Better compositional coverage - nephelinites as well as intermediates
- Well-annotated and adaptable scripts/codes that can be tailored to specific needs
- Lack of open-source/easy access databases
- Working across platforms - need a universal language!
- Lack of a standardised vocabulary
- Need more experiments for multi-component systems involving Cl and F
- Having a standard format of output
- Better usability, challenge: making it a black box, balancing availability of source code and graphical user interface, invisible labour needs to be incentivised, solution: have options available, app and python interface, code documentation, tutorials
- S and halogens: difficulty in analysing fluid compositions in experiments, solution: getting experimental work funded and people to do the experiments
- Solution: regular workshops to keep people aware and up to date on latest models, also hands-on demos at conferences, less secretive about experimental practices
- Solution: revisiting old data/experimental run products
- Understanding errors
- How to give credit for contributions (e.g., new experiments) if we move towards more integrated models rather than people continuing to publish their own models that work in limited conditions
- Can we develop a “best practices” guide by compositional type, volcano type, region, etc. that recommends the codes to use/start with? Might make it easier for researchers new to the field. Are we even at that point, or are we still all trying to figure out exactly that issue via workshops like this?
- Need new experiments for constraining diffusion/disequilibrium effects
- Which model to choose when we are no experts
    - Open vs closed system ?
    - Can measure emitted gas ratios, but some species get oxidised by atmosphere. Also if have open system degassing, very challenging.
- What are the dissolved species e.g. carbon in very reduced lunar magmas?
- Analytical challenges between labs e.g. US SIMS labs hold Dixon standards, UK SIMS holds Shiskhina standards, different set-ups, unsure how high H2O contents affect CO2 solubility
- How to conduct benchmarking - are we comparing like with like, i.e. compositions that lie within the calibration range of the models being compared

What is a potential target area (in physical or P/T/X space) where a multidisciplinary (observational + experimental + analytical + modelling) study could take place to answer some of these big questions?

- Somewhere where there is a lot of historical, constrained data. Philosophically close to vulnerable communities.
- Intermediate, alkalic compositions

- S and halogen-bearing phases
- Disequilibrium
- Look at a few otherwise well constrained volcanoes (e.g., MSH for andesite gap)
- Designated “developer” team with stable funding
- Stromboli - Nice deep degassing with changes in C/S for benchmarking emissions with melt inclusion studies
- An arc volcano with persistent variable C/S outgassing?

Q3: Can we link monitoring needs to solubility outputs?

Top points

- Better understanding the relationship between redox state and surficial gas composition
- Relate petrology, geophysics, numerical models to surface gas observations.
- Think more about mobility of helium and radon isotopes
- We need to develop community efforts to collect and integrate different types of volatile data.
- Address the need to better understand disequilibrium - for degassing this is a really big feature which is particularly relevant to monitoring so it makes it difficult to include solubility models with monitoring
- Can we look at bromine in melts? Can be identified by UV spectroscopy. Possible stand in for the halogens.

What are the key open questions or needs related to this topic?

- Relating sampled gas to source magma (through measurement of Fe oxidation state?)
- Compare detectable S at lava lakes vs. fissure fountaining
- Correlating geophysical data with surface measurements of emissions
- How to better constrain the presence of an exsolved gas phase?
- More halogen solubility data (e.g., Cl)
- What would new models incorporating disequilibrium degassing look like?
- Role of disequilibrium processes
- How to connect fumarole gas measurements (150C) to the magma? Lots of stuff happened to them already.
- At what depth does the magma sit?
- Understand CO_2 sulfur ratios, limited direct data
- Leveraging geophysical estimates of total gas content (e.g., compressibility)
- Think more about helium and radon
- What do the gases that are detected actually represent?
- How can disequilibrium conditions be accounted for?
- How do hydrothermal systems influence what gases will be measured
- Measurements + interpretation of isotopes and wider variety of gases (ex: halogens)
- What kind of petrologic monitoring is possible and feasible during an active eruption?
- Address the need to better understand disequilibrium - for degassing this is a really big feature
- How easy is it to couple models to models of diffusion kinetics and exsolution kinetics
- Monitoring capabilities; ability to measure different species (e.g. we don't even know how the plume evolves, it could be fractionating inside the plume but drones are currently limited in measuring this)
- Measurements of dissolved volatiles in surface emissions, difficulty measuring
- How much does diffuser degassing effect measurements, cannot always measure the full budget
- Accessibility: are there limitations in using these models easily and quickly to match the real-time monitoring efforts

- What are the uncertainties of volatile solubility models, how do these affect the messages to the public
- Can we improve field measurements of fountains/features etc to constrain syn-eruptive disequilibrium/diffusion processes
- Differences between lava flows and vents in degassing
- How much does technique and group affect measurements obscuring the solubility output link? E.g. FTIR vs multi-gas
- Uncertainty in SO2 flux measurements
- Understanding C/S ratios and link to barometry
- How generally applicable are volatile solubility models to different volcanoes? Vs volcano-specific models
- When are gas emissions predictive of future activity, and on what timescales
- How to improve sampling capability of drones?
- How do signals at the surface reflect processes underground?
- To what extent are gases predictive of future eruptions?
- Are there conditions where Kilauea changes from an open system to a closed system and back?
  - Same gases as since 2008 in spite of eruption
  - The interesting time would likely have been before the 80s
  - Sampling at site can be incredibly difficult to arrange with park officials. Monitoring is easier to arrange than scientific sampling - “sometimes the decision isn’t up to us.”

What are some existing challenges to answering these questions and potential solutions to these challenges?

- Challenging surface measurements (how is background minimised?)
- Challenging measurements: XANES → beam damage
- Challenging experiments (discussed earlier)
- Getting volcano-specific models
- Forecast eruptions based on some criteria
- Go to andesitic and rhyolitic compositions
- Harder to get trace gas data, especially in more polluted atmospheres
- More direct sampling (via drones, vacuum chambers), but then need to be able to compare to other types of data
- Look at time series for different gases together, try to deconvolve for different processes
- Thermodynamic models + long-term experiments to consider effects of hydrothermal systems
- Can methods for petrologic monitoring be made faster to make their involvement more feasible? Community efforts could be organised to streamline petrologic monitoring and connect it to other monitoring efforts
- Money: limit in money therefore limit in experiments, there are too many gaps in known models but no one has the money to fix this
- Limitation in who has the money and motivation to adapt a pre-existing model to be more useable for monitoring efforts, with possible limited credit
- Solution - could you make volcano specific models, so you have more targeted solutions which has a clear model for a specific volcano

- Limitation - difficulty in measuring degassing of submarine volcanoes
- Understanding Br behaviour better because it can be measured easily by UV spectroscopy
-
- Person power (not enough people working on this)
- Not enough attention paid to the behaviour of bromine
    - Can be detected by UV
    - Possibly a proxy for other halogens
    - Experimental work would be beneficial
    - What is the concentration in un-degassed samples in the crust (10s of ppm?)
        - SIMS detection limit ~3 ppm for basalts, lower concentrations hindered by mass interferences (Fe, Ti, Mn). Rhyolites easier to measure because higher Br contents and fewer mass-interfering species; det lim maybe ~5 ppm?
        - Might be possible with electron probe - need standards for this
- Drone capabilities
- Lack of historical datasets
- Loss of equipment due to eruptions (such as the loss of multi-gas at Kilauea).

What is a potential target area (in physical or P/T/X space) where a multidisciplinary (observational + experimental + analytical + modelling) study could take place to answer some of these big questions?

- Stromboli, Etna, Hawaii
- Drone sampling
- Stromboli exciting with a shallow and a deep plumbing systems; monitoring is being done.
- Good andesitic system, ideally without strong hydrothermal systems.
- Sakurajima
- Focus more on experiments relating to isotopes and sulfur
- Focus more on halogens/trace gases, including in lakes/spring output
- Data for non-basaltic systems continues to be slim due to rarity of activity
- Community benchmarking activity for all different types of degassing data on a few highly active systems
- Pick a specific volcano to base a reliable solubility model on - e.g. Mt St Helens as there is already a good framework of data there, and this would fill the gap of intermediate experiments. Limit - not large populations there so the importance is limited.