

# PHASE EQUILIBRIUM MODELLING: APPROACHES AND PITFALLS REPORT ON THE ON-LINE WORKSHOP

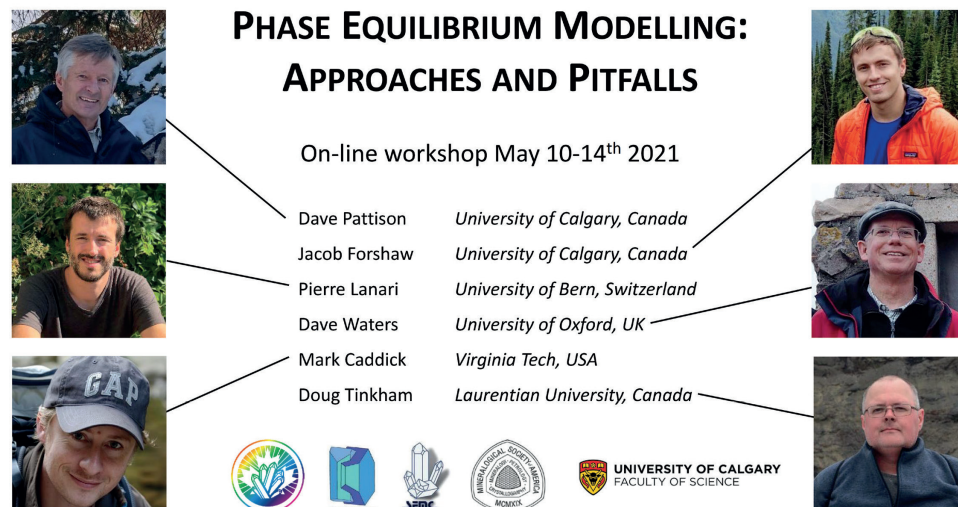
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The no-cost, online phase equilibrium modelling workshop entitled Phase Equilibrium Modelling: Approaches and Pitfalls was held 10–14 May 2021. The workshop was organised and presented by Dave Pattison and Jacob Forshaw (both from the University of Calgary, Canada), Pierre Lanari (University of Bern, Switzerland), Dave Waters (University of Oxford, UK), Mark Caddick (Virginia Tech, USA) and Doug Tinkham (Laurentian University, Canada) (FIG. 1). The meeting was jointly sponsored by the Mineralogical Association of Canada,

question-and-answer (Q&A) session, with a 15 minute break between. A 30 minute open Q&A session concluded each day. Registrants submitted questions to a moderator who posed those questions to the presenters. The presentations and the Q&A sessions on day five were shorter and less structured.

The lectures and associated Q&A sessions were recorded. These, along with pdf documents of the presentations, are available for public access and to download from the workshop's website: <http://e-thermo-workshop-2021.petrochronology.org/>. These materials are, or will be, available on the websites of the Mineralogical Association of Canada, Mineralogical Society of Great Britain and Ireland, the Société Française de Minéralogie et de Cristallographie, and the Mineralogical Society of America.

The large registration was unexpected and encouraging. Of note was the high number of students and post-doctoral fellows (combined, about 70% of the registrants), and the 39:61 ratio of female to male registrants (FIG. 2A). The majority of registrants described themselves as novice or intermediate in terms of their experience with phase equilibrium modelling (FIG. 2B). Of those who had used the different software packages there was a fairly even distribution, with use of Perple\_X being slightly higher than the other two (FIG. 2C).

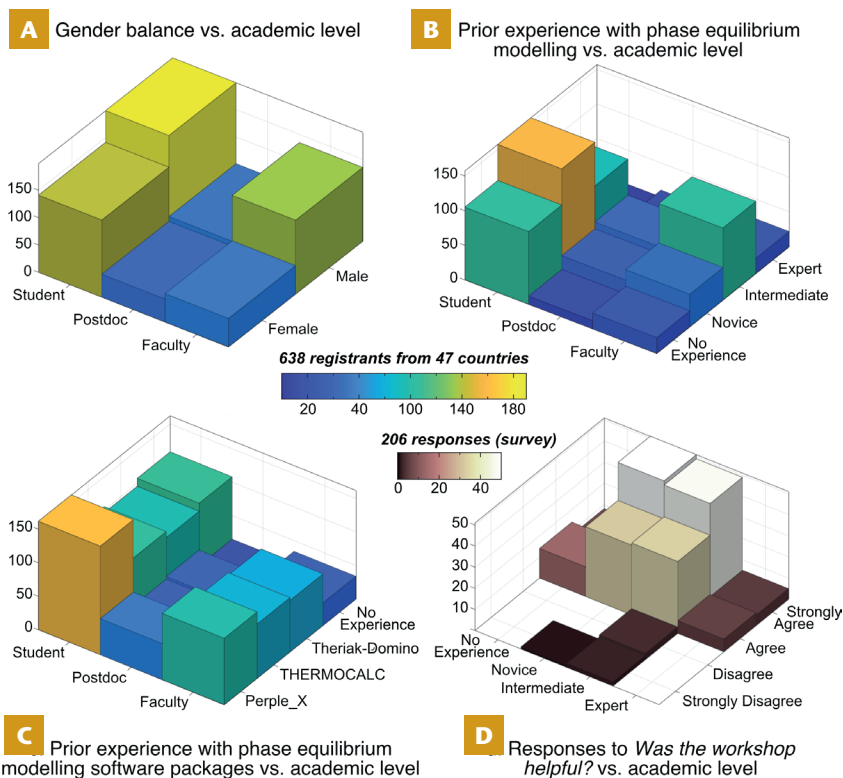


**FIGURE 1** Title slide of the on-line workshop Phase Equilibrium Modelling: Approaches and Pitfalls, which was held 10–14 May 2021.

the Mineralogical Society of Great Britain and Ireland, the Mineralogical Society of America, and the Société Française de Minéralogie et de Cristallographie. A total of 638 scientists from 47 countries registered for the online workshop, compared with 35 registrants for the equivalent COVID-cancelled in-person workshop at the May 2020 Geoconvention meeting in Calgary.

The rationale for the workshop was that all practicing and up-and-coming metamorphic geoscientists should have a nuanced understanding of the potential, but also the pitfalls, of phase equilibrium modelling. The first two days of the workshop focused on thermodynamic databases and three of the most commonly used metamorphic phase equilibrium modelling software packages: THERMOCALC, Perple\_X, and Theriak-Domino. Days three and four focused on factors that influence the interpretation of a phase equilibrium model, including uncertainties in phase equilibrium modelling, reactive bulk composition, the interplay between equilibrium kinetics in petrological interpretation, and an assessment of predicted phase equilibria versus natural constraints. Day five consisted of shorter presentations that addressed topics requested by the registrants.

The workshop was conducted by Zoom webinar and hosted by the Faculty of Science at the University of Calgary. The workshop ran for 3.5 hours each day for the five consecutive days. The first four days featured two 45–60 minute lectures, each followed by a dedicated



**FIGURE 2** Registrant profile and satisfaction of the on-line workshop Phase Equilibrium Modelling: Approaches and Pitfalls.

Reaction to the workshop, based on 206 responses to the post-workshop survey, was positive. Over 97% of attendees said that the workshop was helpful, that they would attend again, and that they would recommend it to others. The most positive reaction to the workshop came from those of intermediate and, especially, novice experience (FIG. 2D), and from the 71% of registrants who attended all five days of the workshop. More than 97% agreed or strongly agreed that the webinar format was effective and that the content was appropriate, and 96% agreed or strongly agreed that the workshop encouraged them to do phase equilibrium modelling. Whilst several respondents remained loyal to the software they had previously used, many expressed interest in trying out other software packages. The three most commonly cited criticisms of the workshop—especially from those with no prior experience of phase equilibrium modelling—were, 1) a desire for more hands-on tutorials and exercises for the different software packages, 2) a desire for more case studies and specific applications, and 3) the fact that there was a lot to digest each day.

Some of the most commonly cited “take-aways” from the workshop included the following: appreciation of the differences between the software packages; the importance of choice of thermodynamic database and solution models for a given phase equilibrium model; the importance of assessing the reactive bulk composition for a successful model; the type and magnitude of uncertainties on calculated phase

equilibria; and the way in which metamorphism is an interplay between equilibrium and kinetics. However, the two biggest ones were that A) the rocks are always right (that is, models are not reality, they are just models); and B) the fact that phase equilibrium modelling is not a “routine” endeavour: it offers great potential while demanding careful thought and analysis.

One aspect of the workshop that was of more than petrological interest was the vast reach of the workshop compared to its in-person precursor (638 vs. 35 registrants). The change to an online format was catalysed by the COVID-19 pandemic, yet the implications of this change go beyond the pandemic. Many registrants had neither the time nor the money to attend the originally planned in-person event yet were able to attend and benefit from the online event. Some noted that an online event can't replicate the depth of interaction of an in-person event—a view we don't dispute—but that this was counterbalanced by the increased reach of the online event. Perhaps a blend of online and in-person events (such as workshops or scientific meetings) will be the way of the future.

Submitted on behalf of the organisers:

**Dave Pattison, Jacob Forshaw, Pierre Lanari, Doug Tinkham, Dave Waters, and Mark Caddick**

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