

PHASE EQUILIBRIUM MODELLING: APPROACHES AND PITFALLS

On-line workshop May 10-14th 2021

Dave Pattison

University of Calgary, Canada

Jacob Forshaw

University of Calgary, Canada

Pierre Lanari

University of Bern, Switzerland

Dave Waters

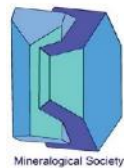
University of Oxford, UK

Mark Caddick

Virginia Tech, USA

Doug Tinkham

Laurentian University, Canada



UNIVERSITY OF CALGARY
FACULTY OF SCIENCE



Welcome to the biggest metamorphic event ever!



Zoom webinar etiquette

- The chat function is disabled.
- You may ask a question by writing it in the Q&A box.
The moderator will pose the question to the speaker(s).
- If the webinar crashes, or if you lose your connection,
log in again as normal (using the same link)

Who are you (we)?

638 registrants

47 countries

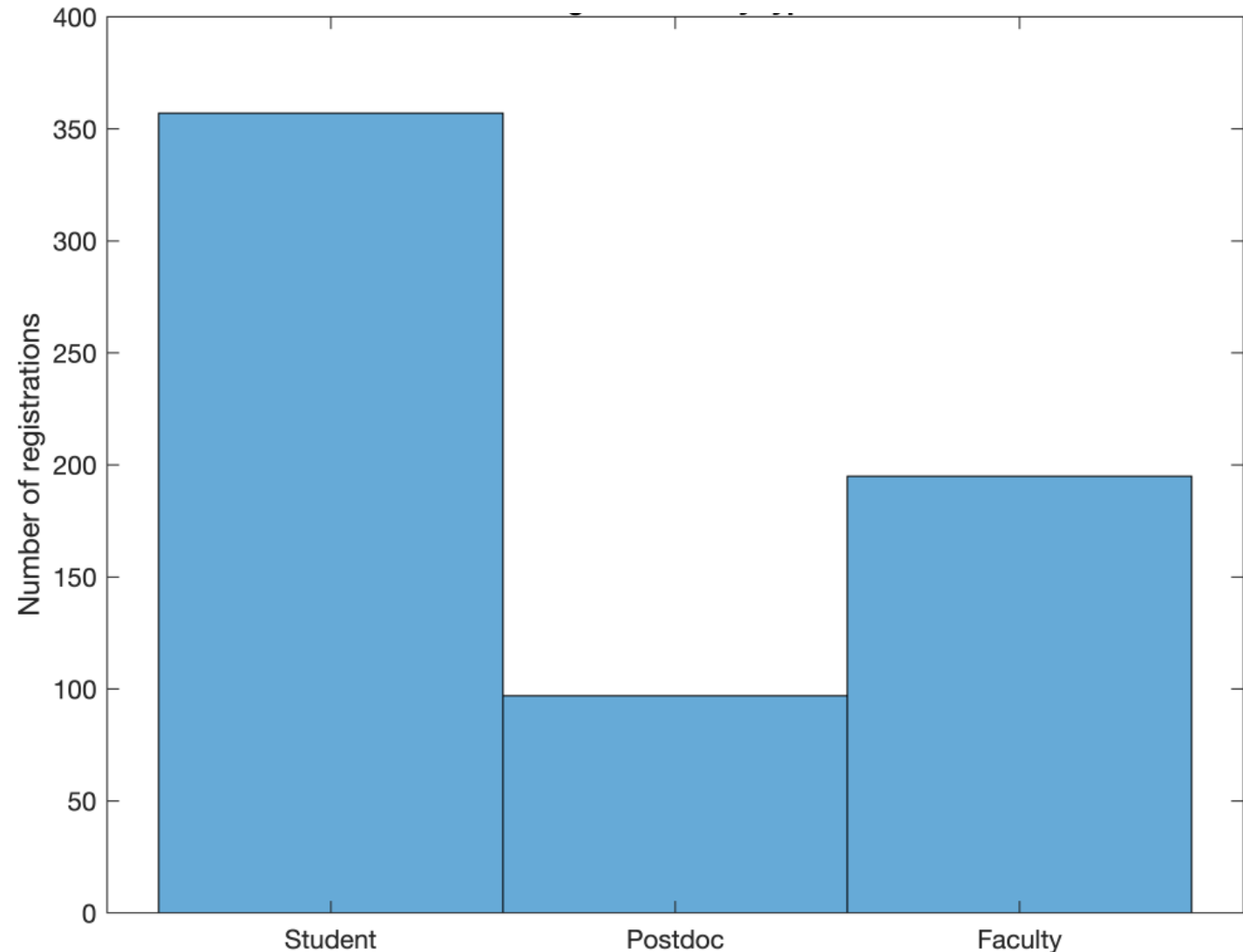
55% students

15% postdocs

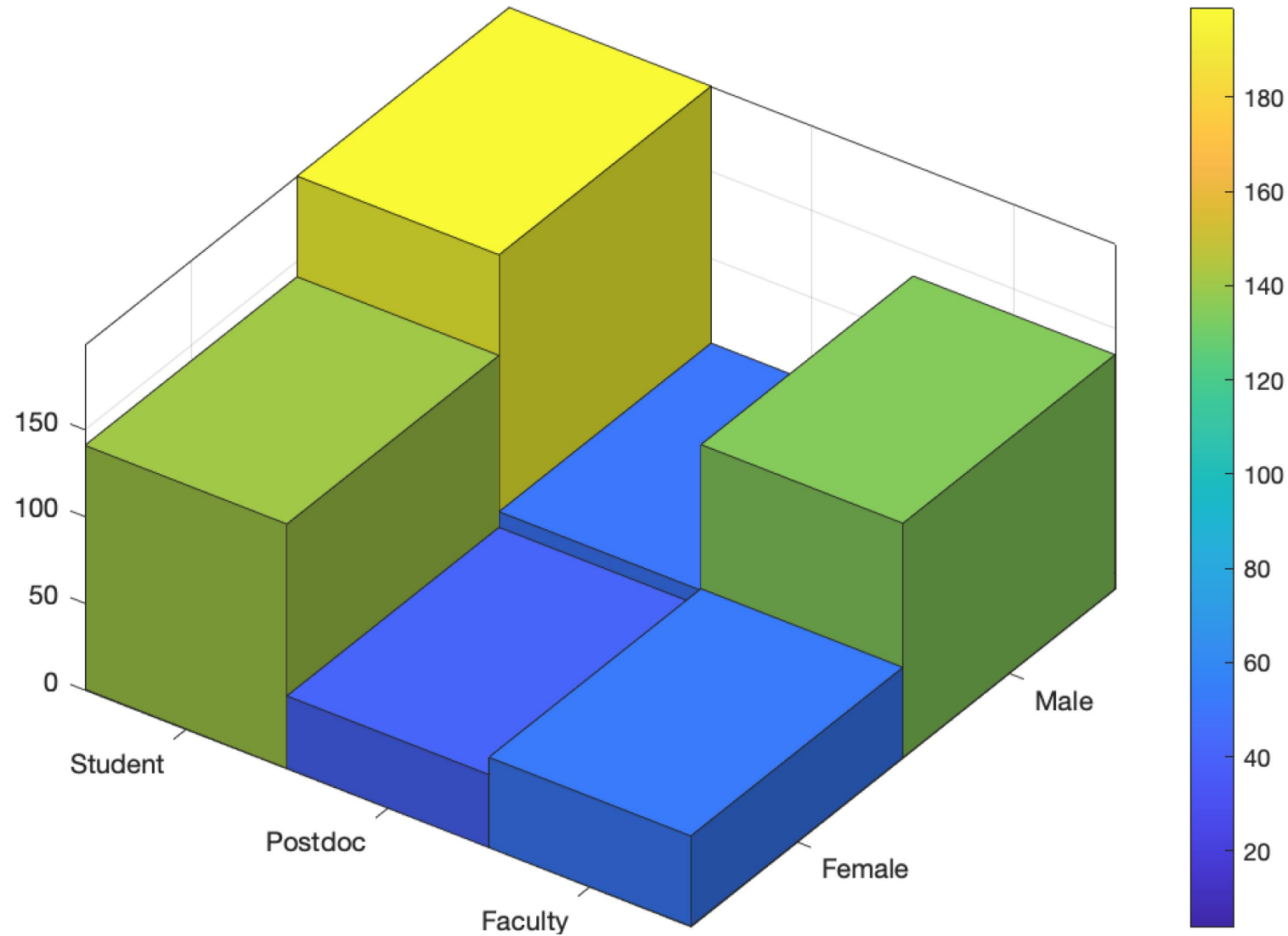
30% faculty

500 registered to attend
the live workshop

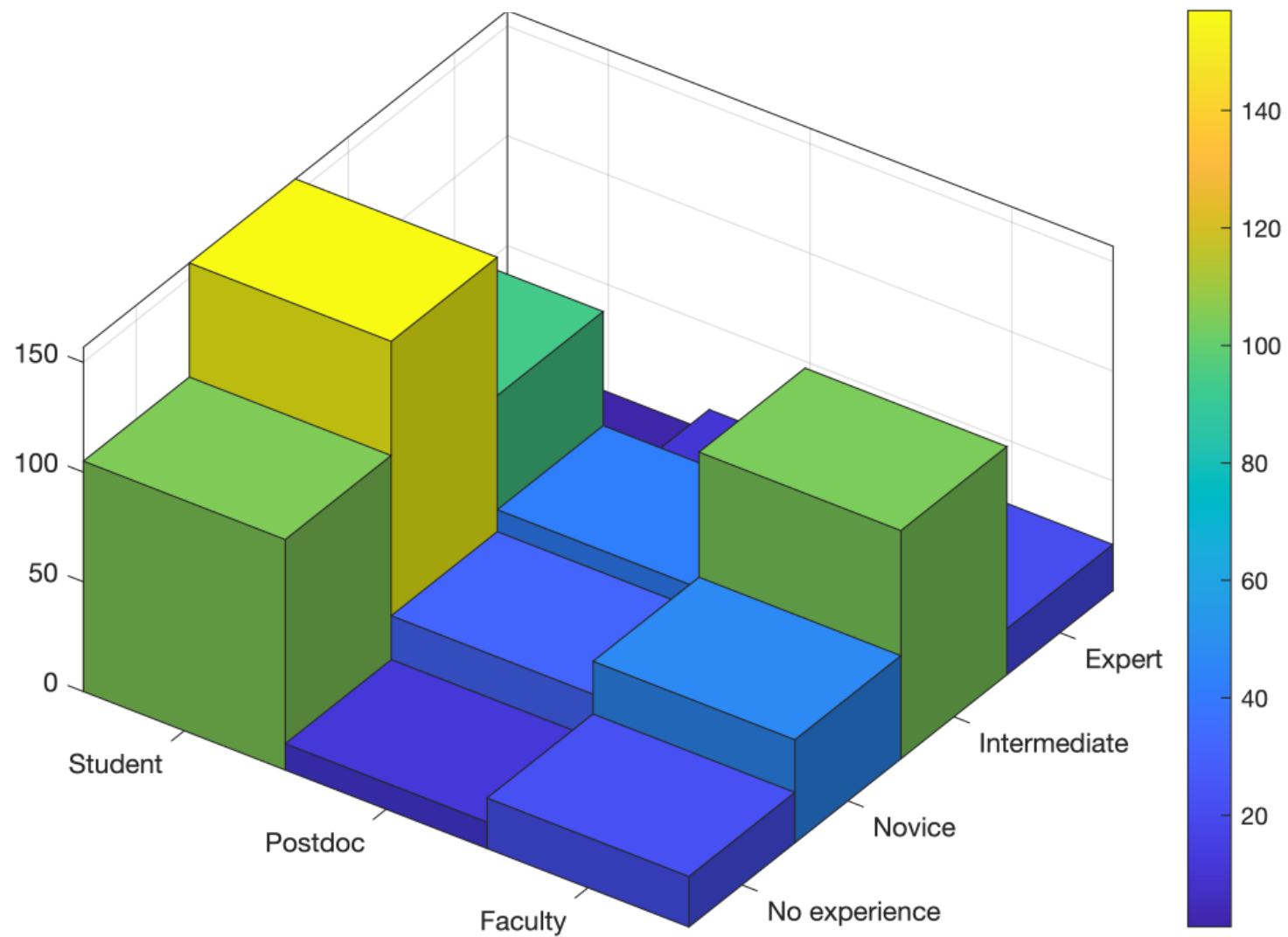
(vs. 35-40 for planned in-person
workshop in Calgary in May 2020)



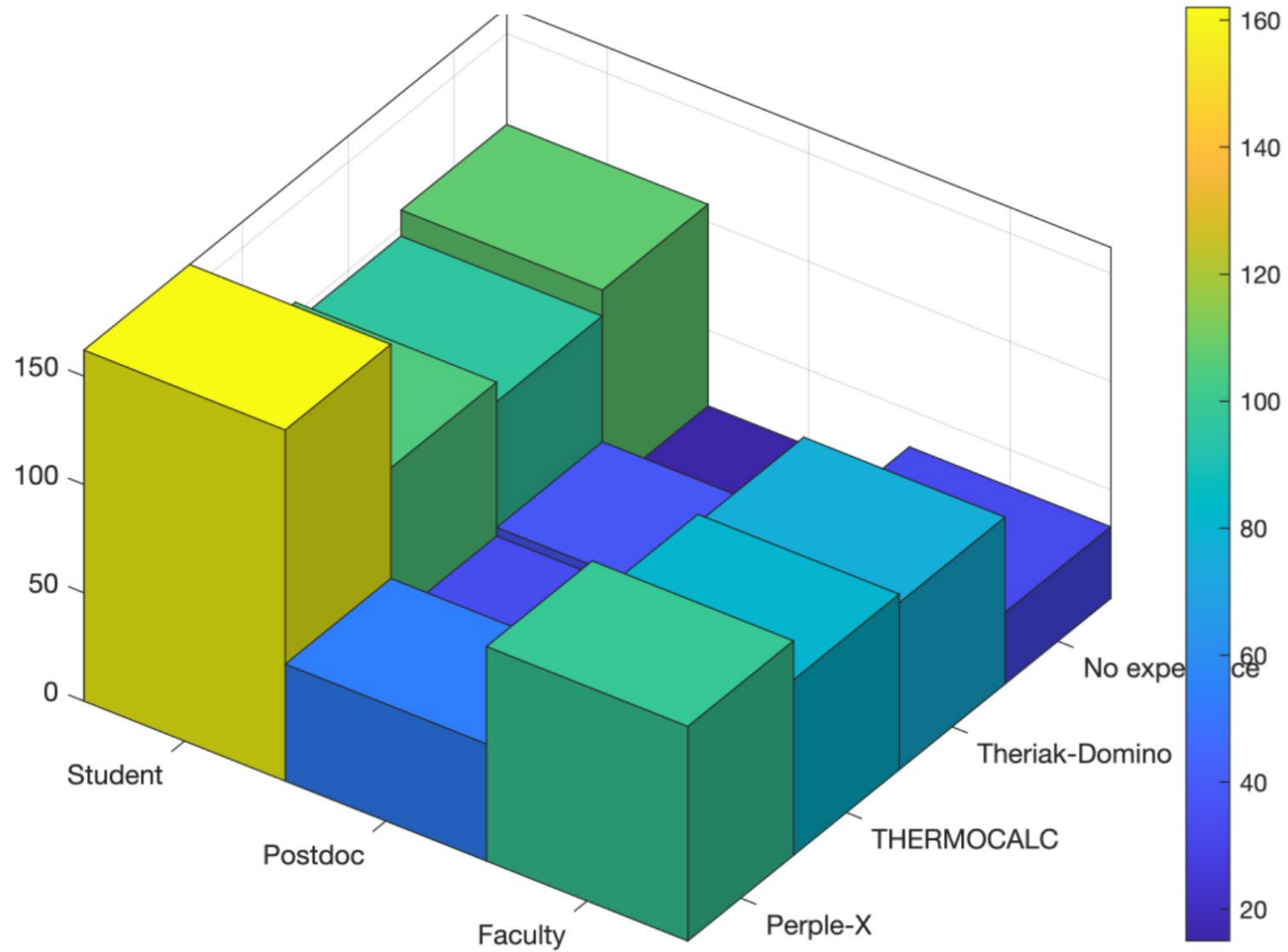
Who are you (we)?



Experience with phase equilibrium modelling



Experience with phase equilibrium modelling software packages



Plan for the week

Days 1 and 2: M May 10 and T May 11, 2021

Thermodynamic databases and phase equilibrium modelling software packages

M May 10, session 1a: Overview of thermodynamic databases (Pierre Lanari)

M May 10, session 1b: THERMOCALC & AvPT (Dave Waters)

Tu May 11, session 2a: Perple_X (Mark Caddick)

Tu May 11, session 2b: Theriak-Domino (Doug Tinkham)

Days 3 and 4: W May 12 and Th May 13, 2021

Factors influencing the interpretation of phase equilibrium modelling

W May 12, session 3a: Uncertainties & best practices in phase equilibrium modelling and thermobarometry (Dave Waters)

W May 12, session 3b: Reactive bulk composition & Bingo-Antidote (Pierre Lanari)

Th May 13, session 4a: Equilibrium & kinetics in metamorphism (Dave Pattison, Jacob Forshaw)

Th May 13, session 4b: Assessment of databases/solution models against the natural record (Jacob Forshaw, Dave Pattison)

Day 5: F May 14, 2021

Topics of interest provided by participants: shorter, more informal presentations and discussions

Participant-requested topics for Friday

1. Overview comparison of THERMOCALC vs Perple_X vs Theriak-Domino

2. Dealing with H₂O when it is the only volatile

a. Subsolidus vs. suprasolidus phase diagrams, and how to handle H₂O (excess vs fixed)

b. Suprasolidus phase diagrams (esp. phase diagrams for granulites and migmatites) – how to handle melt when some of it may be lost

3. Mixed volatile reactions

4. Choosing the best chemical system for modelling

a. Simplicity vs. complexity, using examples from various systems

b. How to handle Fe³⁺

5. XMapTools

Importance of phase equilibrium modelling to metamorphic petrology

1. Provides estimates of pressures (depths) and temperatures of rocks that have been changed by tectonic and magmatic processes - and how these conditions have changed during a rock's history (ie, P-T-t paths). This information is needed by our colleagues in other spheres of Earth Science!
2. After petrography and mineral/rock chemical analysis, phase equilibrium modelling is probably the biggest commonality amongst all metamorphic investigations.

Potential, and responsibility!

Philosophy of workshop

1. We are all here to learn (presenters included)
2. Emphasis is on approach/understanding, rather than recipes
3. The rocks are always right (models are not reality – they are just models)
4. Thermodynamic databases and solution models are not infallible – they are works in progress
5. There is no substitute for careful, critical analysis of the results of phase equilibrium modelling against the natural features of the rocks.

Plan for today (Monday May 10, 2021)

Session	Presenters	Time (MDT)
Introduction	Dave Pattison on behalf of co-organizers	08.00 - 08.10 am
Overview of thermodynamic databases	Pierre Lanari	08.10 - 09.00 am
Q&A	Jacob Forshaw, Moderator	09:00 - 09:30 am
Break		09:30 - 09.45 am
THERMOCALC & AvPT	Dave Waters	09.45 – 10.30 am
Q&A	Jacob Forshaw, Moderator	10.30 - 11.00 am
Open Q&A		11.00 - 11.30 am