AUTHOR COMMENTARIES - 2008

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Professor Roger Powell and Dr. Tim Holland

Featured Scientist Interview

According to Essential Science Indicators℠ *from Thomson Reuters, the paper, "An internally consistent thermodynamic data set for phases of petrological interest," (Holland TJB and Powell R,* J. Metamorph. Geol*. 16[3]: 309-43, May 1998), ranks at #6 among Geosciences Highly Cited Papers, with 911 citations.*

The papers authors are Dr. Tim Holland and Professor Roger Powell. Dr. Holland is a Reader in Petrology in the Department of Earth Sciences at the University of Cambridge. Professor Powell is a Professorial Fellow in the School of Earth Sciences at the University of Melbourne.

In the interview below,* ScienceWatch.com *talks with Professor Powell about this paper.

SW: Would you please sum up your 1998 *Journal of Metamorphic Geology* paper, "An internally consistent thermodynamic data set for phases of petrological interest," for our readers?

First to say that the "I" here is Roger Powell, and I am speaking for both myself and my friend and collaborator, Tim Holland. The work, of which this is the most recent published part, is the result of more than 25 years of ongoing research collaboration, most of which has taken place around the world, with me at the University of Melbourne, Australia, and Tim at the University of Cambridge in the UK.

What this paper provides is a dataset of thermodynamic properties of the constituents (end-members) of the minerals, fluids, and melt that are needed in order to perform calculations on the conditions of formation of rocks. It is an internally consistent dataset because all of the available information has been appraised and combined to establish consistency. This is done statistically (in a least squares sense), giving uncertainties and correlations on the dataset. This then allows calculations with the dataset to be done such that uncertainties on the results can be obtained, an important aim in any science.

Coauthor
Dr. Tim Holland

SW: This data set is an update of a prior data set. How do the sets differ from each other?

The research started in 1982, and the first dataset papers came out in 1985, explaining the philosophy and providing the first actual dataset. The

first published update was in 1990, the second in 1998. With each of these updates, the evolution is firstly in the methodology to process and represent the data, particularly the pressure and temperature dependence of the thermodynamic properties. Secondly it is in the scope and quality of the data themselves. The dataset is calculated from a large body of experimental data (on individual minerals and reactions between them) that encode the thermodynamic properties, and data from new experiments continue to be published. As new data become available the dataset changes and hopefully improves.

SW: Has the data been updated since your 1998 paper, or are there plans to do so?

Although the 1998 paper is the second published upgrade of the dataset, we have continued to release the current version. The dataset that is currently being used is the fifth update of the one in that paper. In the same way our software that uses the dataset, THERMOCALC, was presented in a 1988 paper, and updated in a 1998 paper, but the software has evolved more or less continuously through to the present. The software and the dataset are free downloads on the web.

The third update of the dataset, which is near completion, should be submitted for publication later this year (2008), also in the *Journal of Metamorphic Geology*.

SW: Who uses this data set, and for what tasks?

Petrologists, mainly metamorphic petrologists working on the rocks that form in the bowels of ancient mountain belts, use the dataset primarily to determine the pressure and temperature of formation of rocks now found at the Earth's surface. This information gives critical clues to the processes that form and evolve mountain belts. This is a critical part of geology, as much of the basement of the continents is the stitched-together remains of such ancient mountain belts.

SW: What initially sparked your interest in this particular topic?

Both Tim and I were supervised for our D.Phil. theses at the University of Oxford by a brilliant and far-sighted geologist, Steve Richardson, who saw that the application of equilibrium thermodynamics to rocks could be a supremely powerful tool. He pushed us in that direction. I produced a very rudimentary thermodynamic dataset for use in my thesis work in the early '70s, and when Tim started his work soon after I had left Oxford, he took up a similar approach. The meeting of minds that started our collaboration was the result of Tim, who was keen to take the dataset idea further, wanting to have someone involved who was interested in the maths/stats/computing side of the research, someone who also could see the relevance geologically. The someone was me.

"As new data become available the dataset changes and hopefully improves..."

SW: What should the "take-away lesson" about your work be for laypeople?

The take-away lesson is that it would be very difficult for work of this scope to be done by one person: it requires a collaborative effort, and the effort ideally needs to involve people with different abilities and skills. I have brought to this in some sense the simpler part, the algorithmic and program design, and the writing and upgrading of general software to process the available data to make the dataset (as well as the software THERMOCALC to actually use the dataset). Tim has done the actual appraisal and assembly of all the disparate data and information to run through the software to make the dataset itself.

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Roger Powell and Tim Holland's most-cited paper with 911 cites to date:

Holland TJB and Powell R, "An internally consistent thermodynamic data set for phases of petrological interest," *J. Metamorph. Geol.* 16(3): 309-43, May 1998. Source: *Essential Science Indicators* from Thomson Reuters.

Additional Information:

Roger Powell and Tim Holland are featured in ISIHighlyCited.com.

Keywords: thermodynamic properties, mineral constituents, fluid constituents, melt constituents, rock formation, data set updates, THERMOCALC software, mountain belts, collaboration.

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