

## Addendum: Quantitative models linking igneous amphibole composition with magma volatile chemistry

Paul A. Giesting<sup>1\*</sup> and Justin Filiberto<sup>2</sup>

1: Department of Geography-Geology, Illinois State University, Normal, Illinois 61790, USA

2: Department of Geology, Southern Illinois University, Carbondale, Illinois 62901, USA

\* - Corresponding author (giesting@alumni.nd.edu)

In this Addendum, we present three additional resources for those who wish to understand or use the regression model we present for Cl/OH partitioning between an igneous calcic amphibole and coexisting melt.

First, the supporting tables in spreadsheet format had some dangling links to external spreadsheets. We supply corrected spreadsheets with this addendum and apologize for the inconvenience caused to several readers by the mistake. Supporting Table 8 has been exchanged with data from Giesting et al. (2015) for use with the discussion of the third point, below.

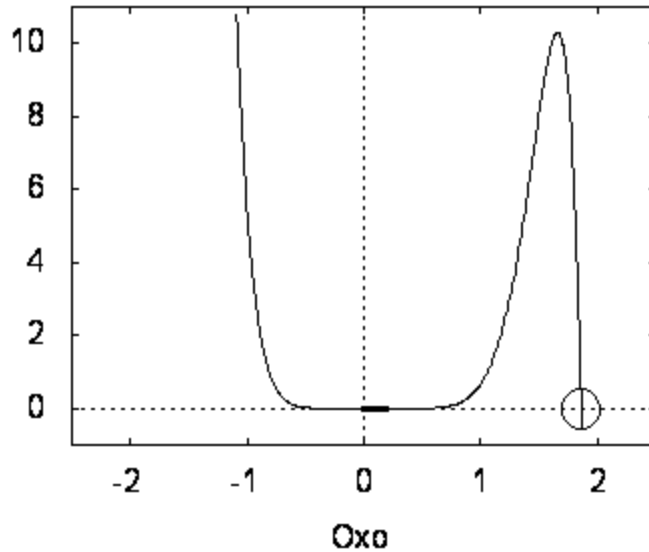
Second, we call attention to the calculated standard error (0.373) for the preferred regression equation, which is needed to calculate prediction intervals for  $\ln K_{Cl}$  (Iman, 1994; De Veaux et al., 2012). The standard error can be found in Supporting Table 4 for each of the regression equations. We remind the reader that this error sweeps up an unquantifiable amount of uncertainty based on the many assumptions and component models used to construct the overall model, especially the Popp et al. (2006) model for OH/O calculation, over and above the ordinary amount of analytical error on the data used to construct the model and any variation due to variables we did not consider in the regression, or whose relationship to  $\ln K_{Cl}$  is not linear.

Third, we wish to discuss the procedure for finding roots of the polynomial equation that results from ordinary usage of the H<sub>2</sub>O-undersaturated version of the model. In Fig. 1 and 2, we show a plot of this polynomial for a specific real amphibole+glass pair (using wxMaxima). This particular polynomial has the simplest behavior we have observed, which is to have two roots in the region of chemical possibility ( $0 < \text{Oxo} < 2$ ), one of them the appropriate root, which in the plotted case is a degenerate real root located at a local minimum for the function, and one is the trivial root that always appears when  $\text{Oxo} + \text{F} + \text{Cl} = 2 \text{ apfu}$ , so  $\text{OH} = 0$  (not a chemically realistic solution). Other possible behaviors appear to include multiple degenerate real roots in the region of interest, and it is not immediately obvious which of these roots should be selected as the real root. However, this choice can be made very simple in a variety of ways; the one we suggest is to recalculate the Popp et al. (2006)  $K_x$  constant in the "forward" direction via Equation 3 using the values of  $f(\text{H}_2\text{O})$ ,  $\text{Oxo}$ ,  $\text{OH}$ ,  $\text{Fe}^{3+}$ , and  $\text{Fe}^{2+}$  that result from the polynomial solution and see if this matches the value previously calculated using the Ti, Al content of the amphibole and the  $T$ ,  $P$  of equilibration. In our experience, only one root will satisfy this condition, and we take this to be the actual value of  $\text{Oxo}$  for the amphibole.

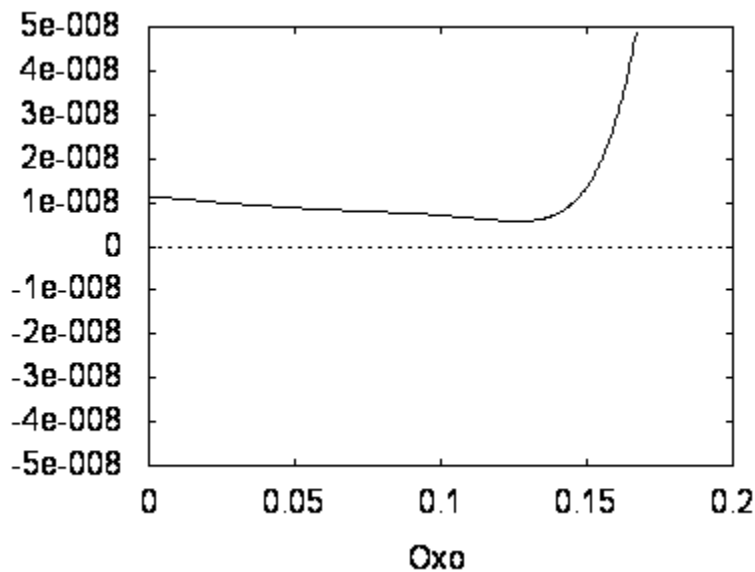
## References

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- Iman, R.L., 1994. *A Data-Based Approach to Statistics*. Duxbury Press, Belmont, California, pp. 561-562.
- Popp, R.K., Hibbert, H.A., and Lamb, W.M. (2006) Oxy-amphibole equilibria in Ti-bearing calcic amphiboles: Experimental investigation and petrologic implications for mantle-derived amphiboles. *American Mineralogist*, 91, 54-66.



**Figure 1.** Plot of the polynomial equation resulting from substitution of Equations 3-7 into one another assuming H<sub>2</sub>O-undersaturated conditions for one of the amphibole analyses in Giesting et al. (2015). The chemically meaningful root, which is a degenerate real root, is in the thickened black segment ( $0 < \text{Oxo} < 0.2$ ; see Fig. 2). The spurious root, which is circled, is located at  $\text{Oxo} + \text{F} + \text{Cl} = 2$ , i.e.,  $\text{OH} = 0$ .



**Figure 2.** The portion of the graph beneath the thickened line segment in Figure 1, zoomed in to show the degenerate real root. Note that due to rounding error, the plot does not quite touch the Oxo axis.