Evaluating and Supplementing XRD Results with Elemental Data: Mineral Modelling Examples from the Duvernay Formation

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Abstract

X-ray diffraction (XRD) is a powerful tool for evaluating the mineralogical composition of geologic samples, but the degree of accuracy that can be achieved through the analysis can be difficult to establish. Reported errors can vary greatly from operator to operator, and according to some researchers, results within 3 wt.% absolute or 10% relative of the true concentration should be considered “highly accurate” results (Hillier, 2000). Unsurprisingly, routine analyses from similar or even identical samples can return variable results, especially when analyzed by different operators.

This study will use examples from the Upper Devonian (Frasnian) Duvernay Formation of Alberta to demonstrate the use of a paired X-ray diffraction and elemental geochemistry dataset in two ways; first by assessing the relative quality of XRD results by comparing them to highly accurate elemental data from the same samples, and second by using paired XRD and elemental data to train a highly adaptive model for estimating the mineralogical composition of samples where only elemental data is available. The Duvernay Formation is a relatively heterogeneous system, comprising limestones, mudstones and calcareous mudstones (Stoakes and Creaney, 1984). The variety of mineralogical suites present in this study area makes it an excellent example of the ability of this modelling technique to work in relatively complex basins.

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