Evaluating And Supplementing XRD Results With Elemental Data: Mineral Modelling Examples From The Duvernay Formation

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Introduction

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.

Evaluating the Quality of XRD Results

Understanding the mineralogical composition of shale resource plays is particularly important with regards to the completion of horizontal wells and maximizing well performance. Accurate measurements of clay content are imperative to evaluating the relative brittleness through a shale play, which can greatly improve the effectiveness of fracking strategies. Consequently, confidence in the quality of available mineralogical data is critical. As the relative accuracy of XRD results can vary greatly from vendor to vendor, and reliably differentiating between competing datasets can be critical. The quality of these analyses can be assessed by comparing them to bulk elemental geochemistry analyses performed on the same samples. While the composition of many common mineral phases can vary greatly, this strategy can be extremely useful for generating a first-order evaluation of the quality of the X-ray diffraction results.

Mineral Modeling in Sedimentary Rocks

Traditionally, estimating the mineralogical composition of a rock based on bulk elemental geochemistry is limited predominantly to the field of igneous petrology, where an ideal abundance of mineral species,

or “normative mineralogy”, can be calculated directly using a set of pre-defined rules, such as CIPW. While the results of these models differ to some degree from the actual mineralogical composition of the rock, these normative mineralogical compositions are useful for comparing and classifying rocks where only chemical analyses can be performed.

The problem becomes more difficult when dealing with sedimentary rocks; while a strictly quantitative, CIPW style approach may be taken to identify combinations of minerals that would produce a given chemical concentration, this solution is often non-unique as the suite and even composition of mineral phases in sedimentary rocks can vary greatly for a given bulk chemistry (Braun, 1986; Kolka *et al*, 1994). A more qualitative approach has been taken by some, allowing the algorithm to automatically determine a suite of minerals to model by attempting to classify the rock based on its bulk elemental chemistry (Rosen et al, 2004). Ideally, however, a more accurate solution involves an algorithm that can be “trained” for a geochemical dataset with known mineralogical assemblages, so that the model can be tailored to the system in question.

Conclusions

Evaluating XRD results in conjunction with a highly accurate elemental geochemical dataset allows for greater confidence in the reliability of the XRD data, and more importantly provides the means to calibrate a mineralogical model tailored to the study interval analyzed. The power of this integrated approach is that it is not biased by, or limited to any particular formation, rock type, or geologic setting, and can be applied to any system. In this example, the mineralogical model created for the Duvernay can be applied to equivalent intervals across the study area, allowing accurate estimates of mineralogical composition to be acquired for samples where only elemental data is available. Once calculated, these mineralogical data can be used to better understand the physical characteristics of the field, which is critical for the optimal placement of lateral wells and techniques such as fracking.

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