Combining concentration-area method with indicator kriging analysis for geochemical anomaly identification of the typical deposit

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Geochemical datasets always include outliers and potentially have skewed distributed data. Althought normal transformation can enhance the robustness of the kriging method, it can smooth the data more seriously. Indicator kriging method does not rely on the stationarity of the datasets, can make more robust and feasible against a series of outliers. The threshold is the most important factor of indicator kriging analysis. The concentration-area method [1] which baesd on the fractal and multifractal theory can provide great help for the threshold calculation.

When we carried out the anomaly identification analysis of Cu concentration in the typical deposit of China, we used the concentration-area method (ACAF) [2] to obtaine the threshold for the indicator kriging. The results of the indicator Kriging interpolation are shown in the figure below.
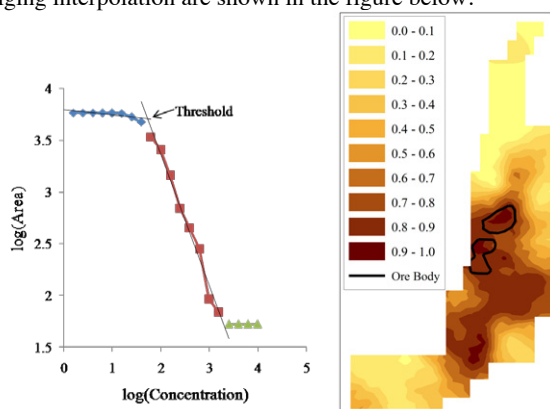

Figure 1: Indicator kriging interpolation results of Cu concentration

Discussion

Combining concentration-area method with indicator kriging analysis can highlight the known ore bodies and delineate mineralization centre more effectively, indicating that it is very suitable for the ore-hunting prognosis which is based on non-stationarity datasets and outliers.

[1] Cheng *et al*. (1994) *Journal of Geochemical Exploration* **43**, 91–109.[2] Xie *et al*. (2004) *Mathematical Geology* **36**, 847–864.

Equilibrium Se isotope fractionation parameters: A first-principles study

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Introduction

Se belongs to one of the most redox-sensitive elements, so Se isotopes might be used to trace some redox and biointerference processes. But there are just a few pioneering studies [1, 2] that provided equilibrium Se isotope fractionation factors.

Based on the Urey model or the Bigeleisen–Mayer equation method, several important equilibrium Se isotope fractionation parameters are investigated by first-principles calculations. All the frequencies are obtained at B3LYP/6-311+G (d, p) level, with a frequency scaling factor of 1.05. Table 1 shows some of the calculated fractionation factors [3].

A-B	$10^3\ln(\alpha_{A-B})=a*10^6/T^2+b*10^3/T+c$
SeO_4^{2-}-SeO_3^{2-}	$10^3\ln(\alpha_{A-B})= 0.524637*10^6/T^2 + 2.94785*10^3/T-2.50587$
SeO_4^{2-}-$HSeO_3^-$	$10^3\ln(\alpha_{A-B})= 0.608479*10^6/T^2 + 2.77841*10^3/T-2.38642$
SeO_4^{2-}-HSe^-	$10^3\ln(\alpha_{A-B})= 1.709258*10^6/T^2 + 5.51101*10^3/T-5.02758$
SeO_3^{2-}-$HSeO_3^-$	$10^3\ln(\alpha_{A-B})= 0.083841*10^6/T^2 -0.16944*10^3/T+0.11944$
SeO_3^{2-}-HSe^-	$10^3\ln(\alpha_{A-B})= 1.184621*10^6/T^2 + 2.56316*10^3/T-2.52171$
SeO_4^{2-}-SeMet	$10^3\ln(\alpha_{A-B})= 1.236799*10^6/T^2 + 5.12772*10^3/T-4.42211$
SeO_4^{2-}-SeCyst	$10^3\ln(\alpha_{A-B})= 1.204255*10^6/T^2 +5.32442*10^3/T-4.59242$
SeO_4^{2-}-DMSe	$10^3\ln(\alpha_{A-B})=1.323029*10^6/T^2 +4.90539*10^3/T-4.22539$
SeO_4^{2-}-DMDSe	$10^3\ln(\alpha_{A-B})=1.306259*10^6/T^2 +5.48531*10^3/T-4.72162$
SeO_2-SeO	$10^3\ln(\alpha_{A-B})=0.438882*10^6/T^2 +2.57817*10^3/T-2.15291$
SeO_2-Se_2	$10^3\ln(\alpha_{A-B})=0.335359*10^6/T^2 +4.14586*10^3/T-3.45764$
SeO_2-H_2Se	$10^3\ln(\alpha_{A-B})=0.725619*10^6/T^2 +2.61754*10^3/T-2.71278$
SeO_2-Se(T)	$10^3\ln(\alpha_{A-B})=0.263308*10^6/T^2 +4.34169*10^3/T-3.63616$
SeO_2-Se(M)	$10^3\ln(\alpha_{A-B})=0.257529*10^6/T^2 +4.34519*10^3/T-3.63933$
SeO-Se(T)	$10^3\ln(\alpha_{A-B})=-0.175574*10^6/T^2 +1.76352*10^3/T-1.48325$
SeO_2-DMSe	$10^3\ln(\alpha_{A-B})=0.198796*10^6/T^2 +3.02243*10^3/T-2.49061$
SeMet-DMSe	$10^3\ln(\alpha_{A-B})=0.086231*10^6/T^2-0.22233*10^3/T+0.19672$

Table 1: The formula for Se isotope fractionations at different temperatures (see [3] for details).

Discussion of Results

Our results suggest that the magnitude of isotope fractionation is depended on Se valence states, and there is a trend of heavy Se isotopes enrichment as SeO_4^{2-} > SeO_3^{2-} > $HSeO_3^-$ > SeO_2 > selenoamino acids > alkylselenides > Se (0) or H_2Se > HSe^-. The equilibrium Se isotope fractionation factors provided here might be useful to explain Se isotope distributions in the biogeochemical cycle and also important to the study of Se global cycling.

[1] Krouse & Thode (1962) *Can. J. Chem*. **40**, 367–375.
[2] Schauble (2004) *Rev. Mineral. Geochem*. **55**, 65–111.
[3] Li & Liu (2011) *EPSL*. **304**, 113–120.