Behavior of organic compounds in black shale heated by igneous intrusion

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Black shale is dark-colored mudrock containing rich organic compounds. Black shales are also important to the natural fuel-resource economy of the world because they constitute the most important accessible reservoir of organic compounds in the Earth's crust [1]. By a long term of thermal effects, they become source rock and eventually generate petroleum or natural gas because of irreversible alteration in them. This leads us to trace thermal history by thermal alteration through their concentration fluctuation. The purpose of this study was to provide mathematical model with thermal alteration of organic compounds in black shales collected rock samples in Koshikijima Island, Kagoshima Prefecture. It could be more easily calculable than known thermal indices (vitrinite reflectance, carbonaceous material graphitization and thermal modeling).

We could recognize from self-organizing map that aliphatic hydrocarbon fraction was overall suitable for model construction compared with aromatic hydrocarbon and resin fraction separated by column chromatography. Organic compounds qualified and quantified with GC-MS were classified into 13 categories by cluster analysis. Among these categories, two clusters showed strong correlation with thermal indices. One mainly included most of *n*-C_{10}-C_{22} saturated hydrocarbon and the other included Pristane and Phytane known as biomarker.

Regression analysis suggested that general linear models to each thermal index with significance level of 5% were derived respectively. As for their compounds, Dodecane fitted closely estimates of vitrinite reflectance and those of thermal modeling. 2-methyl hexadecane fitted carbonaceous material graphitization and estimates of that likewise. These results implied that the thermal alteration could be quantitatively explained by statistical approach.

[1] Tourtelot (1979), *Clays and Clay Minerals* **27**, 313-321.