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Estimating Total Organic Carbon Content in Green River Formation Oil Shales Using Elemental Data and Multivariate Analysis

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Abstract

Relationships between total organic carbon (TOC) content and concentrations of major and trace elements, particularly redox-sensitive metals, are well documented in the source rock literature. Over the last ten years, a range of studies using multivariate, neural networking, and machine learning approaches have been applied to source rock TOC prediction based on inorganic elemental concentration data. Another use of these models is identification of key elements that relate to organic enrichment due to their sensitivity to enhanced productivity or preservation conditions, or that reduce organic richness due to dilution. In this study, major and trace element concentration data from inductively coupled plasma (ICP) optical emission spectroscopy-mass spectrometry were related to TOC measured on the same thermally immature oil shale and mudstone samples from two cores collected in distal areas of the Eocene Green River Formation in the Piceance Basin (approx. 100 samples from each core). Several modeling approaches were tested, including multi-linear regression, random forest, and gradient boosting algorithms. Performance of the models was compared and evaluated in terms of mean square error, mean absolute error, and correlation coefficients between measured and predicted TOC values (R^2). Multi-linear regression showed a significant overfitting issue with low bias and high variance. The remaining three models also indicated some overfitting, but generated relatively high R2 values (≥0.66) in the test dataset. This indicates that ensemble tree methods perform better in general for predicting TOC from inorganic elemental data. Among the elements examined, Mo, P, Ti, Ni, and Cr were found to be the top predictors for TOC. This is consistent with results from hierarchical cluster analysis (HCA) applied to these datasets, which also showed many of these elemental associations with organic-rich samples. Results from additional modeling tests comparing different sample groupings, based on stratigraphic sorting or chemofacies clusters identified using HCA, will be presented. In general, the better performance of ensemble tree methods indicates that relationships between TOC and elemental proxies for redox, productivity, and dilution are non-linear.

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