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**Geochemical determination of heavy oil viscosity using multivariate statistical algorithms**

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**Summary**

Accurate prediction of fluid properties such as oil viscosity, for core, cuttings and even contaminated samples, using geochemical proxies correlated to physical measurements of viscosity is viable for heavy oil production and exploration activities. Such predictions rely not only on high precision geochemical measurement to calibrate proxy methods but crucially on accurate, representative viscosity measurements, which often reveal error introduced via sample handling and analysis. Here we present multivariate statistical partial least squares (PLS) and artificial neural network (ANN) oil geochemistry-viscosity prediction methods as well as a storage time viscosity correction (STVC) methodology able to ameliorate core storage effects in large legacy viscosity datasets enabling effective correlations of chemical properties and oil viscosity.

**Introduction**

Modern recovery operations, especially for unconventional resources, rely on accurate physical fluid property estimates for prospecting, resource assessment, risking, and optimal production. In conventional petroleum fields, in-field variations in oil production as a function of oil mobility are primarily controlled by variance in reservoir permeability, which is more heterogeneous than *in situ* oil-phase fluid properties; however, the opposite is true in heavy oil and super heavy oil fields, where oil viscosity varies laterally and horizontally over short distances by orders of magnitude (Adams, 2008; Larter et al., 2008). In these resources, in situ sampling is difficult, horizontal wells common and cuttings and sidewall core are the common sample types.

Lack of core or downhole fluids prohibits collection of representative (unaltered) oil samples and small sample volumes or sample aging or contamination dictate that API gravity and/or viscosity must be estimated using genetic or statistical models and geochemical analysis. Pre-drill fluid property predictions are possible using genetic reactive compositional models (e.g., GNAWD, MPath; Trinity or BioClass) or geostatistical extrapolation of large measured API gravity or viscosity data sets, but typically these data are unavailable for new development and exploration plays. Molecular representation models can predict equation of state parameters, directly (e.g., Crampon et al., 2004) or via critical properties (Marreo and Gani, 2001), but need specialized models and skilled modelers. Chemical correlations with measured properties using multivariate methods, e.g., partial least squares (PLS; Rosipal & Kramer, 2006) and neural networks (Qin & McAvoy, 1992) have been applied to complex oil, coal or other systems to predict key parameters for many applications. These quick, low cost methods need limited

measured or analog data and tiny oil samples for the prediction sample set (Koopmans et al., 1998; Larter et al., 2008).

Fluid property prediction, especially for viscosity is most important in heavy oil reservoirs where up to two orders of magnitude change in viscosity at reservoir conditions occurs within a 30 m interval. In most cases, no single chemical parameter can correlate to measured viscosity of oil across a heavy oil field. We showed earlier (Adams et al., 2008; Larter et al., 2008) that complex relationships between geochemical parameters and dead oil viscosity may be resolved using multivariate methods. This paper addresses best practices for developing correlations and methods for identifying sources of error in large data sets to accurately predict oil viscosity from geochemical data. The same methods can be applied to predict API gravity; however, we caution that using standard correlations to compute viscosity from API gravity are totally unreliable for heavy oils!

## Method

For regression of chemical data, PLS is particularly effective when the number of independent variables (chemical components) is greater than the number of samples (often the case in exploration) and when the independent and predicted variables share a linear correlation. Viscosity commonly varies highly non-linearly with heavy oil composition due to its complex, often non-Newtonian nature and thus non-linear PLS or non-linear neural networks may best predict heavy oil viscosity from oil chemistry. Non-linear PLS, however, is very sensitive to starting values and typically does not produce significantly higher quality predictions than conventional PLS but can account for outliers more effectively (Malthouse et al., 1996). For this reason, we commonly apply a simple log transform to the measured viscosity data and use PLS methods and multi layer perceptron or radial basis network neural networks (ANN model), trained on oil component concentration data and dead oil viscosity (20°C in cP). Although ANN methods require more substantial training sets than PLS, ANN can be run with small data sets.

In this paper, we discuss the advantages and disadvantages of the various methods on large datasets of penecontemporaneously analyzed heavy oil geochemical data and a viscosity data set from Canadian heavy oilfields. For example, in one study, over 300 solvent extracted oils from delineation well core from a heavy oil field were analyzed for SARA, and GC-MS of total hydrocarbons. The viscosity of 120 oil samples mechanically extracted from core using a sealed vessel compaction driven recovery device (Larter et al., 2006) were measured using a Brookfield viscometer. The maturity and source rock facies variations of the oil charge are comparatively uniform in this dataset but the reservoir core was stored frozen under standard storage conditions for a variable time of 2 to ~1800 days prior to mechanical oil extraction and viscosity measurement. Oil API gravities vary from 7.7 to 11 degrees, dead oil viscosities (20°C) as vary from ~3000 to 3,000,000 cP and biodegradation levels from 5 to 6 (Peters and Moldowan scale).

Statistical predictions of viscosity from oil chemistry rely on accurate viscosity measurements to calibrate proxy correlations and an adequate number of precise chemical parameters to span the whole range of compositions in the sample set (e.g., biodegradation can remove key components from some oils) and account for the processes causing variability in oil chemistry and, viscosity (maturity and facies, biodegradation and sample storage effects). Measured oil viscosity is a function of not only intrinsic oil charge chemistry and in reservoir alteration, but also the storage conditions and duration, sample collection, contamination and processing and measurement (Adams, 2008; Adams et al., 2008). Volatilization of light end hydrocarbons (LEH) during core storage, handling, extraction and oil cleaning significantly affects measured

viscosity. Heavy oil core, stored frozen, loses LEH systematically with time, causing order of magnitude increases in bitumen viscosity over 1 year, while relative viscosities in a vertical reservoir profile are maintained. As standard centrifugation of core to extract oil often volatilizes LEH, compaction-based bitumen extraction (Larter et al., 2006) was used to obtain viscosity data.

In addition, experiments investigating contamination of bitumen samples show that even small quantities of dispersed water and reservoir solids can significantly affect measured viscosity. These findings are consistent with the correlation of heavy oil viscosity with solid content defined as asphaltenes and the proportion of solid maltenes at  $< 323$  K (Hasan et al., 2009) that support the rheological model of heavy oil as “a dispersion of non-interacting uniform rigid spherical particles in a Newtonian fluid”. This non-Newtonian behavior at low temperatures may cause viscosity to vary by a factor of 2 to 5 or more with measurement shear rate due to shear thinning. Geochemists need to be aware of these analytical pitfalls in “routine” viscosities.

Proper selection of oil samples representative of produced oil is crucial for viscosity-chemistry calibration data sets but can be challenging due to different sample types and storage and sample preparation procedures prior to viscosity measurement and geochemical analysis. Oil components, tracking oil maturity, source rock facies, in reservoir alteration and LEH recharge, etc., are the dominant parameters in most correlations and thus must be accurately measured. For heavy oils, this means careful LEH retention or assessment of LEH loss during sampling, water removal, then accurate hydrocarbon and thioaromatic separation, with good resolution of key parameters usually by GCMS and quantification with sufficient internal standards to produce accurate, precise concentration data. Our experience is that the thioaromatic compounds are key and thus “total hydrocarbon” analyses have been found to be more effective than analysis of LC separated saturated and aromatic hydrocarbon fractions. Quantitative total hydrocarbon fractions were analyzed by GCMS using internal and recursive standards (Bennett et al., 2009).

Correlations between fluid properties and geochemical data can be developed with similar success using component concentrations or parts of, or whole, chromatograms of key components as time series datasets. Ratios of geochemical components are widely reported in the literature, but PLS regression assumes linear additivity (i.e., variables or concentrations when summed are additive), a condition ratios do not honor. In general peak ratio geochemistry is of limited value in predictive geochemistry and with routine accurate quantitation now available it is no longer as necessary. Here concentrations of aromatic, thioaromatic hydrocarbons and saturated hydrocarbon biomarkers were used as correlation proxies with the lighter aromatics excluded due to volatility and variable loss during storage. To minimize variability related to experimental drift in large datasets data transformation by autoscaling concentrations (Pirouette by Infometrix) or aligning chromatograms is important. To ensure calibration samples span the full compositional range of the prediction set, hierarchical cluster analysis (HCA) and Principal Component Analysis (PCA) were applied to define the most characteristic variables. Here only core oil was used, but different sample types can be used in calibration or prediction datasets if all part of a single population.

Clearly errors in viscosity data will be present in any large dataset collected over a period of time reflecting variable storage and extraction histories. In this case, individual viscosity values varied by up to 30-80% from “true values” equivalent to drill time dead oil viscosity (DTDV) due to long sample storage times and centrifugation. To compare these data, a correlation curve between equivalent compaction and centrifuge extracted oils was used to correct centrifuged oil viscosities. A method to correct measured oil viscosities of stored core to

equivalent dead oil viscosity at drilling time called the storage time viscosity correction (STVC) was developed (Adams et al., 2008). The best algorithm for STVC varies with the natural logarithm of storage time given binary end member mixing of light end and heavy end fraction viscosities consistent with published algorithms of diffusive mass transport through polymers and oil spill evaporation. A similar correction for viscosity using sample storage time as a dependent variable via PLS regression, as described below, is possible using the fraction of the oil not susceptible to evaporation correlated to measured viscosity of fresh oils (short storage time). This PLS method can correct for storage time, mud contamination and sample type (e.g., produced oil, cuttings, core etc) when estimating viscosity from non-ideal calibration data.

## Results

The PLS models using the whole training dataset of oil component concentrations predicted the measured viscosity over the whole viscosity range (5 decades) with RMSE of 139,187 cP. Inclusion of storage time and relative depth from the top of the bitumen pay zone plus removal of the 11 statistical outliers improved prediction accuracy (RMSE = 72,541 cP), but removal of 30 samples with storage time longer than 200 days (old samples) most significantly improved the model (RMSE = 31,503 cP; *best fit model*). The *best fit model* predicts reasonably accurate dead oil viscosity values across this field in the training set (predominantly oils with viscosities  $\gg 100,000$  cP) and with the inclusion of storage time allows for prediction of DTDV at 30 days for all the samples including the additional 200+ chemistry only samples and 30 old samples. Including STVC viscosities of the oil samples in the training set did not significantly improve predictions. Using chromatograms in place of the concentration data also provided good results for the fresher viscosities because of additional chemical information in small peaks not included in the concentration dataset. Chromatograms can be used more reliably in data sets with uniform maturity and oil sources as well as sample handling and storage time, especially if internal standards have not been used. The PLS models poorly predicted the most degraded, high viscosity samples in the data set because of the non-linear variation of chemical composition with viscosity. In the most degraded oils, the key parameters controlling the PLS model like dibenzothiophene had been removed by biodegradation, such that either additional calibration data were needed to refine the linear regression or a separate PLS model was needed to predict viscosity  $> 400,000$  cP.

Generally good linear fits of observed and predicted viscosities are obtained with the ANN model trained on 30-day DTDV data set. The best equivalent ANN model included both relative depth and sample storage time, and better predicted the highest viscosities (RMSE  $\sim 9500$  cP), possibly due to the model's non-linear basis. The ANN model produced similarly accurate results using only a subset of the aromatic hydrocarbon data, which could save on analytical costs. Comparisons of predicted and measured viscosity in a few vertical well profiles showed that STVC estimated 30-day DTDV match the estimated PLS 30-day and ANN 30-day DTDV.

## Conclusions

The accurate prediction of oil mobility is crucial for effective exploration and optimization of production strategies especially in biodegraded heavy oil and bitumen reservoirs which exhibit great fluid property heterogeneity. To build representative geochemical viscosity prediction models to represent subsurface oil variability and which are not susceptible to sample handling and analytical effects, careful, consistent analytical and data processing procedures must be followed. Legacy viscosity data sets typically need correction, thus the STVC model was validated with the

independently determined PLS DTDV 30 days. Multivariate statistical PLS and ANN regression models of heavy oil composition, based on GCMS molecular geochemistry data accurately predicted a wide range of dead oil viscosities (1000 to  $10^6$  cP) stored for times up to 4 years. The best model required storage time and sample relative depth as variables and exclusion of samples stored for > 6 months. Similar studies with smaller datasets and fresh samples typically produce DTDV predictions with accuracies better than 5-10% allowing for assessment of the viability of heavy oil and bitumen field development, especially for cold production operations (DTDV << 100,000 cP) and in areas where representative liquid oil samples are unavailable. In general, long term analytical data quality and reproducibility, the biogeochemical complexity of biodegradation and the magnitude of sample storage effects are the ultimate limits on viscosity prediction using geochemical data.

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