Mass Fraction Maturity — Next Generation Geochemical Constraint of Basin Models*

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Abstract

Thermal maturity measurement on oil accumulations are crucial for resource assessment. However, the current concept of an oil maturity is flawed and simplistic, as all oils are mixtures with different components charged from source rocks at different temperatures. With typical geological heating rates of 1-10 °C/Ma at any location within a petroleum system, this means that source rocks are charging traps for timescales on the order of a few million years, to a few tens of millions of years. During this period of time, the expelled and trapped petroleum shows a progressive evolution of both bulk and molecular compositions. The concentrations of various components in oil vary greatly for a single facies source rock of differing maturities nonetheless for the different facies. However, petroleum geochemists have continued to use relative abundances of, in particular, saturated hydrocarbon and other biomarkers to a large degree in oil-source rock and oil-oil correlations and maturity and facies assessment of reservoired oils, leading to many confusing and inconsistent approaches to characterizing maturity. We have suggested an alternative approach is needed which tracks the maturity/petroleum mass fraction relationships for a reservoired oil, in a more complex but realistic manner and allows the more effective bracketing of source kitchen maturity. The maturity distribution of oil would then represent the mass fraction versus source temperature at expulsion profile, for all the components in that reservoired fluid. This concept, called Mass Fraction Maturity (MFM), aims to develop the tools, protocols, and calibration data sets to enable the assessment of the reservoired oil mass fraction and source charge temperature interval relationship. Having this relationship, and knowing what a typical complete charge mass fraction maturity profile would look like for a given source rock type, would enable estimation of any missing charge in the basin (validating additional exploration activity), detection of complex multi-history charge scenarios, and also a much more robust and complete data set for calibration of basin model charge history assessments. We will demonstrate the importance of MFM for understanding the properties of reservoir fluids, post-burial uplift and petroleum mass loss, instantaneous versus cumulative charge events and exploration potential by using case studies from Western Canada and elsewhere.

References Cited

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Department of Geoscience
University of Calgary
The oil window

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Diagenesis</th>
<th>Catagenesis (OIL WINDOW)</th>
<th>Metagenesis</th>
</tr>
</thead>
<tbody>
<tr>
<td>80 °C</td>
<td>Biogenic gas: CH₄, CO₂, H₂S, etc.</td>
<td>Heavy oil and gas</td>
<td>Dry gas (methane)</td>
</tr>
<tr>
<td>120 °C</td>
<td></td>
<td>Medium and light oil and gas</td>
<td>Residuum (graphite)</td>
</tr>
<tr>
<td>150 °C</td>
<td></td>
<td>Condensate and wet gas</td>
<td></td>
</tr>
</tbody>
</table>
Change in Color and Vitrinite Reflectivity

%Ro = 0.55

%Ro = 0.70

%Ro = 0.90

%Ro = 1.10

%Ro = 1.40
# Correlation Chart

<table>
<thead>
<tr>
<th>ASTM Standards</th>
<th>Organic Petrology</th>
<th>Organic Geochemistry</th>
<th>Inorganic Petrology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon Content</td>
<td>Vitrinite Reflectance</td>
<td>TAI</td>
<td>CAI</td>
</tr>
<tr>
<td>Peat</td>
<td>0.2</td>
<td>Light Yellow</td>
<td></td>
</tr>
<tr>
<td>Brown Coal</td>
<td>0.3</td>
<td>Yellow</td>
<td></td>
</tr>
<tr>
<td>Lignite</td>
<td>0.4</td>
<td>Yellow Orange</td>
<td>1</td>
</tr>
<tr>
<td>Sub-bituminous</td>
<td>0.5</td>
<td>Orange</td>
<td></td>
</tr>
<tr>
<td>High</td>
<td>0.6</td>
<td>Golden</td>
<td></td>
</tr>
<tr>
<td>Volatile</td>
<td>0.7</td>
<td>Amber</td>
<td>1.5</td>
</tr>
<tr>
<td>Bituminous</td>
<td>0.8</td>
<td>Red Brown</td>
<td>2</td>
</tr>
<tr>
<td>A</td>
<td>1.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medium</td>
<td>1.5</td>
<td>Dark Red Brown</td>
<td></td>
</tr>
<tr>
<td>Volatile</td>
<td></td>
<td>Brown</td>
<td>3</td>
</tr>
<tr>
<td>Bituminous</td>
<td></td>
<td>Dark Brown</td>
<td>4</td>
</tr>
<tr>
<td>Low</td>
<td></td>
<td>Black</td>
<td>5</td>
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<tr>
<td>Volatile</td>
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</tr>
<tr>
<td>Bituminous</td>
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</tr>
<tr>
<td>Semi-Anthracite</td>
<td>2.1</td>
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</tr>
<tr>
<td>Anthracite</td>
<td>2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meta-Anthracite</td>
<td>6.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
How to assess oil maturity?

I adamantane

II diamantane
Ranges of individual biomarker molecular measurements for thermal maturation

Use several different parameters to define the stage of maturation with respect to oil generation

(Modified from Mackenzie et al., 1982)
Oil maturity derived from biomarkers

Estimated Ro ~0.6–0.7%
Oil maturity derived from PAHs

Estimated Ro $\sim 0.7$–$1.0\%$
Oil maturity derived from diamondoids

Estimated $Ro > 1.2\%$
$n-C_{17}/Pr$ vs. $n-C_{18}/Ph$
TMNr vs. TeMNr
Almost no correlation!
Concentration effects on molecular ratios!

The high concentrations ratio is consistent facies indicator.

At low concentrations coelution and concentration errors result in erroneous facies indicators.
Concentrations of major compound classes in oils

(Wilhelms and Larter, 2004)
The distribution of fraction specific maturity for the oils and condensates (Wilhelms and Larter, 2004).
Summary of oil maturity

- Most commonly used maturity parameters have very different correlations to measured vitrinite reflectance;
- Biomarker parameters are sensitive at low to moderate maturity range;
- PAH parameters are sensitive at moderate to high maturity range;
- Light HCs and diamondoids are sensitive at high maturity range;
- Current oil maturity is a misconception as oil is mixture of charges;
- An alternative approach to track petroleum mass fraction relationships for a reservoired oil (mass fraction maturity) is needed.
Case History of MFM

- Samples collected from the Second White Specks Formation (SWS) in WCSB ranging from immature to high mature form a natural evolution case history
Tmax increase with burial depth

- Immature
- Mature
- Post mature
Ro is controlled by burial depth

\[ y = 10029x^3 - 30366x^2 + 31765x - 8829 \]

\[ R^2 = 0.9921 \]

Depth (m)

Ro (%)
Representative total ion current show systematic variation with increasing maturity.
Representative sterane distributions in different maturity samples

m/z 217

520.96 m
$R_c=0.49$

1900.65 m
$R_c=0.69$

2626.75 m
$R_c=0.94$
Representative TIC of aromatic fraction in different maturity samples

520.96 m
Ro=0.49%

1900.65 m
Ro=0.69%

2626.75 m
Ro=0.94%
$n$-Alkane concentration profile

C10-15 $n$-alkanes ($\mu$g/g EOM)

Ro (%)
Isoprenoids concentration profiles
Biomarkers concentration profiles

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PT (µg/g EOM)

Ro (%) vs. PT (µg/g EOM)
- Core
- Outcrop

ST (µg/g EOM)

Ro (%) vs. ST (µg/g EOM)
- Core
- Outcrop
Diamondoids concentration profiles

**Total Adamantanes (μg/g EOM)**

- Core
- Outcrop

**Total Diamontanes (μg/g EOM)**

- Core
- Outcrop
Concentration profiles of alkylnaphthalenes

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C0-1N (µg/g EOM)

C2N (µg/g EOM)

C3N (µg/g EOM)

C4N (µg/g EOM)

Ro (%) vs C0-1N, C2N, C3N, and C4N concentrations.
Concentration profiles of alkylphenanthenes

P (μg/g EOM)

Ro (%)

Core
Outcrop

MP (μg/g EOM)

Ro (%)

Core
Outcrop

C2P (μg/g EOM)

Ro (%)

Core
Outcrop

C3P (μg/g EOM)

Ro (%)

Core
Outcrop
Conceptual concentration profile of various components

- **1,2 – Biomarkers**
- **3,5 – Aromatic Hydrocarbons**
- **6,7 – Light Hydrocarbons**
- **8-10 – Diamondoids**
Concept of mass fraction maturity
Both concentrations and molecular ratios are applied for maturity constraints.
Mass fraction maturity in a trap

If this could be assessed, it would be a game changing tool!

Age of charge and mass fraction maturity assessment currently lacking viable proxies.
Summary

- Tracking petroleum mass fraction relationships for reservoired oils.
- Elucidation of complex charge histories.
- Defining a quantitative approach to assess kitchen maturity in oil and gas accumulations basins.
- If this could be assessed, it would be a game changing tool!
Thank You
Acknowledgement