Like Space and Time, Transformation Ratio is Curved*

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Search and Discovery Article #41713 (2015)**
Posted October 26, 2015

*Adapted from oral presentation given at AAPG Annual Convention & Exhibition, Denver, Colorado, May 31-June 3, 2015

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Abstract

Source rock kerogen hydrogen indices and transformation ratios are frequently used as thermal maturation surrogates, and as proxies for calculating the amount of hydrocarbons generated from a thermally mature source rock, assuming an original hydrogen index can be assigned to the source rock. Transformation ratio (TR) and hydrogen index (HI) are commonly assumed to be linearly related via TR = (HIo – HI)/HIo, where HIo is a constant – the immature source rock's average original hydrogen index – and HI is the present day hydrogen index. In reality, however, the TR-HI relationship is shown to be non-linear. That non-linearity manifests itself most markedly in highly oil-prone, high original HI source rocks, which has important petroleum exploration implications. For example, an area where the present day HI is ~550 for an oil-prone source with HIo = 700 would traditionally calculate at a TR = ~20%. However, its true TR is ~40%. Therefore, areas where the source transformation ratio has traditionally been calculated as too low to have generated/expelled commercial amounts of hydrocarbons may in fact have transformation ratios which do imply significant hydrocarbon generation and expulsion. Examples and application are presented.

Reference Cited

Spigolon, L.D., M.D. Lewan, H.L. de Barros Penteado, L.F.C. Coutinho, and J.G.M. Filho, 2015, Evaluation of the petroleum composition and quality with increasing thermal maturity as simulated by hydrous pyrolysis: A case study using a Brazilian source rock with Type I kerogen: Org. Geochem., v. 83-84, p. 27-53.

Like Space and Time, Transformation Ratio is Curved

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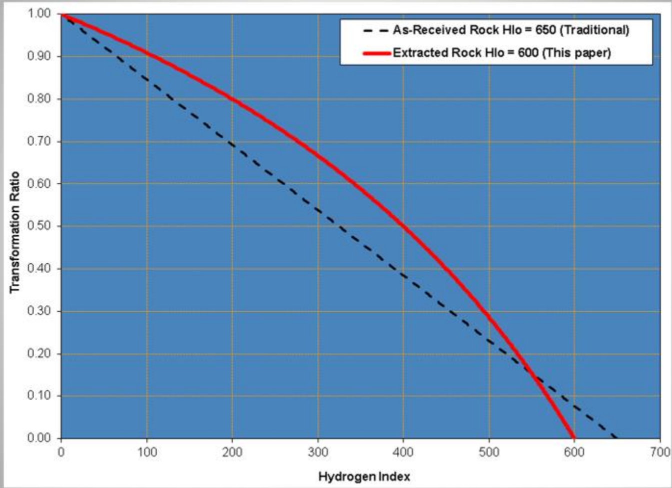
Transformation Ratio – Hydrogen Index Relationship
Traditional method compared to our new one



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Presenter's notes: This talk will show that the TR-HI line is curved rather than straight, and will discuss the significance of this difference for interpretation and decision making.

Transformation Ratio (TR)

A parameter that quantifies the relative progress of hydrocarbon generation

Values from 0.0 to 1.0

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Presenter's notes: We can probably all agree with this philosophical definition of TR. But how can we actually determine TR from laboratory measurements?

Transformation Ratio (TR)

Traditional option 1:

Calculated from Hydrogen Index

$$TR_m = \frac{HI_o - HI_m}{HI_o}$$

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Presenter's notes: Here is one way. The subscript o is the immature value, and the subscript m indicates that it is the measured value

Transformation Ratio (TR)

Traditional option 2:

Calculated from Rock-Eval S2

$$TR_m = \frac{S2_o - S2_m}{S2_o}$$

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Presenter's notes: Here is another way.

Transformation Ratio (TR)

These two formulations

only give the same results if

$TOC_o = TOC_m$,

which only occurs when the source rock

is a closed system.

(No expulsion)

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Presenter’s notes: We must resolve this discrepancy, and that means we must discard what we think we know and start again from the basics.

Definitions of Hydrogen Index (HI)

$$HI = 100 \times \frac{S2}{TOC}$$

Hydrocarbon generative potential per unit of kerogen

Implicit assumptions in this understanding:

- S2 represents only the HCs generated during pyrolysis
- Carbon in TOC is all in the form of kerogen

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Presenter's notes: This is the standard mathematical definition of HI. But what does HI signify, and how should it be used in interpretation?

The reality, for as-received rocks:

$$HI = 100 \times \frac{(S2_{k} + S2_{hb})}{(TOC_{k} + TOC_{b})}$$

k refers to kerogen

hb refers to heavy bitumen

b refers to all bitumen

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Presenter's notes: We can probably all agree with this philosophical definition of TR. But how can we actually determine TR from laboratory measurements?

For immature source rocks:

$$HI = 100 \times \frac{(S2_k + S2_{hb})}{(TOC_k + TOC_b)} \approx 100 \times \frac{S2_k}{TOC_k}$$

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Presenter's notes: For immature rocks the bitumen content may be negligible, and as a result our assumptions are not bad.

For mature source rocks:

$$HI = 100 \times \frac{(S2_k + S2_{hb})}{(TOC_k + TOC_b)} \neq 100 \times \frac{S2_k}{TOC_k}$$

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Presenter's notes: For mature rocks, bitumen content is normally much higher, leading to our original assumption being invalid. A consequence is that HI is no longer telling us what we assume it is telling us. This error creates significant problems.

So how can we measure $S2_k$ and TOC_k?

Answer:

Work with extracted samples

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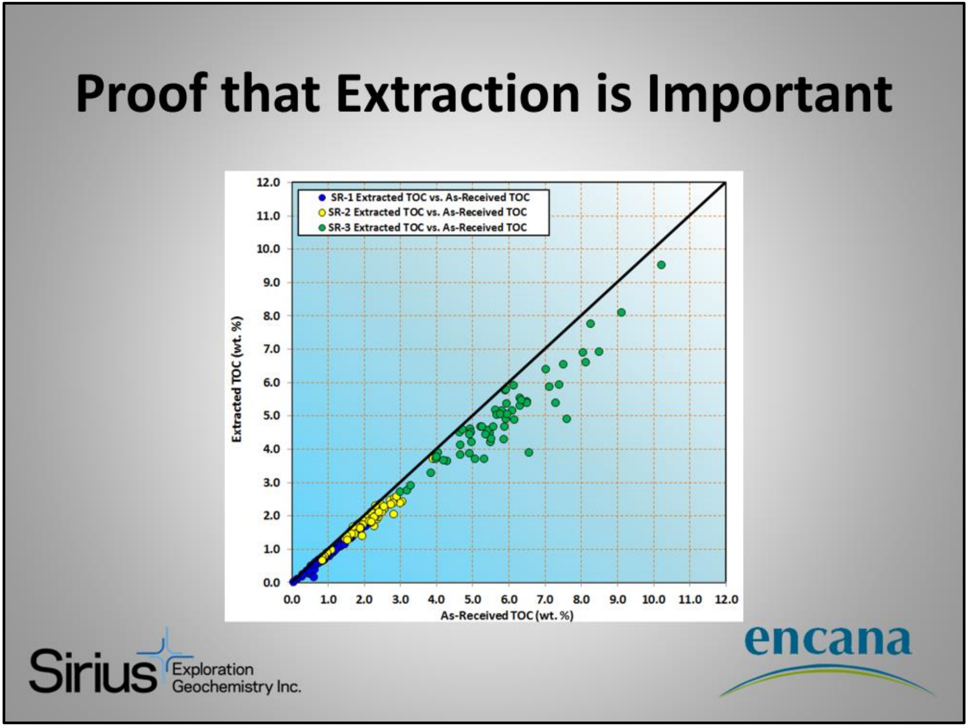
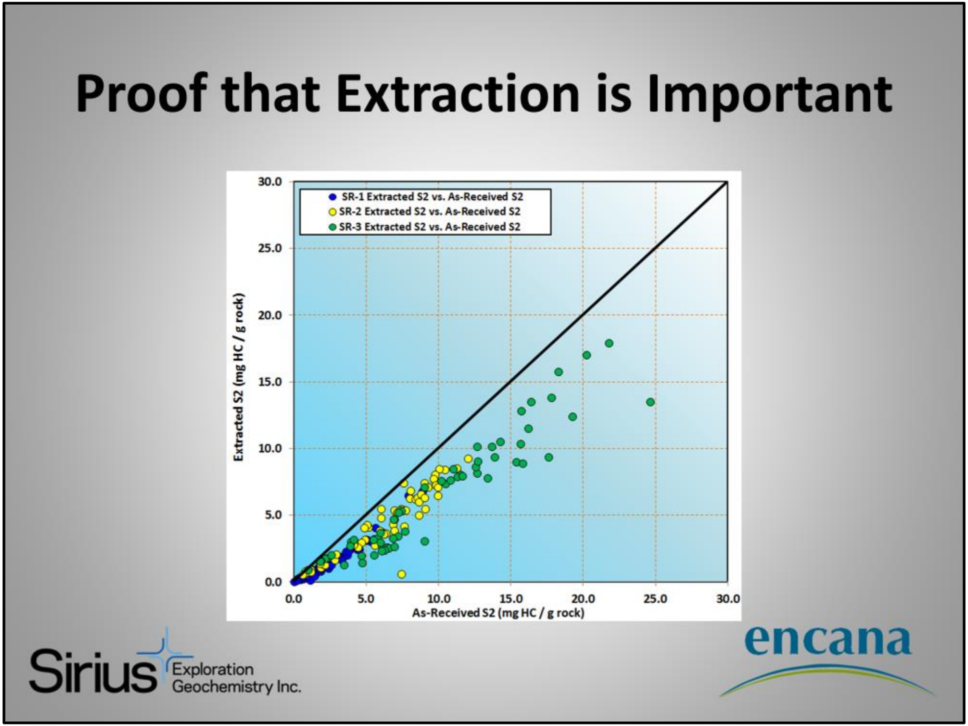
Presenter's notes: So, to make HI live up to its expectations, we need to know S2k and TOCk.

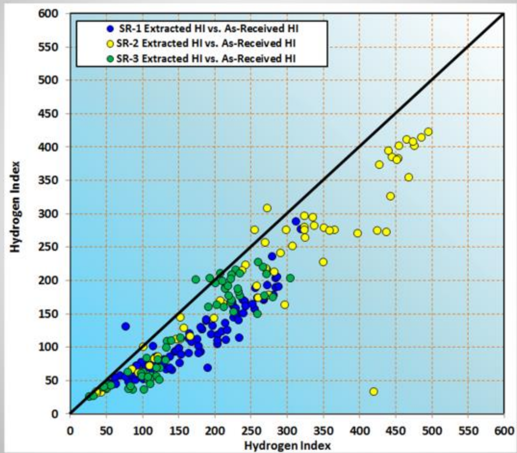


Presenter's notes: TOC values in extracted rocks are consistently less than in unextracted rocks, and by a predictable percentage.



Presenter's notes: S2 values in extracted rocks are consistently less than in unextracted rocks, again by a reasonably predictable percentage.

Proof that Extraction is Important



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Presenter's notes: Because S2 decreases faster during extraction than TOC, HI values in extracted rocks are usually less than in unextracted rocks. However, quantitative prediction is lower. That result makes intuitive sense, since HI is a ratio of the other two parameters.

An important distinction:

HI_{ext} is Hydrogen Index

obtained by analysis of extracted samples

$$HI_{ext} = 100 \times \frac{S2_{ext}}{TOC_{ext}} = 100 \times \frac{S2_k}{TOC_k}$$

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The original purpose in calculating Hydrogen Index is valid

But to achieve our stated goal, we need to work with extracted samples.

The differences in interpretation between HI and HI_{ext} can be very large, and can strongly affect exploration decisions.

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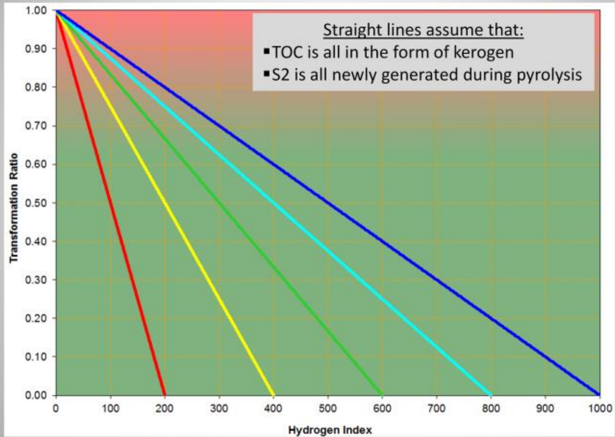
Traditional TR-HI relationship



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This Paper's TR-HI relationship (using extracted rock data)

$$TR = \frac{[HI_o / 100] - [HI_m \times [60 - 5 \times HI_o / 100]] / [6000 - 5 \times HI_m]}{[HI_o / 100]}$$

Assumptions: (1) TOC = [5 x S2] / 60 based on S2 being represented by $C_{10}H_{22}$
(2) TOC_o = 1.0 to simplify derivation

We prefer to calculate TR from HI rather than S2 because it is easier to predict HI_o than $S2_o$.

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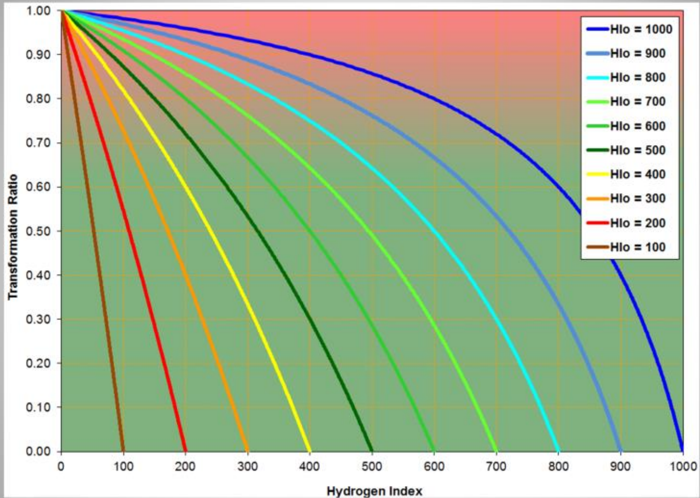
This Paper's TR-HI relationship



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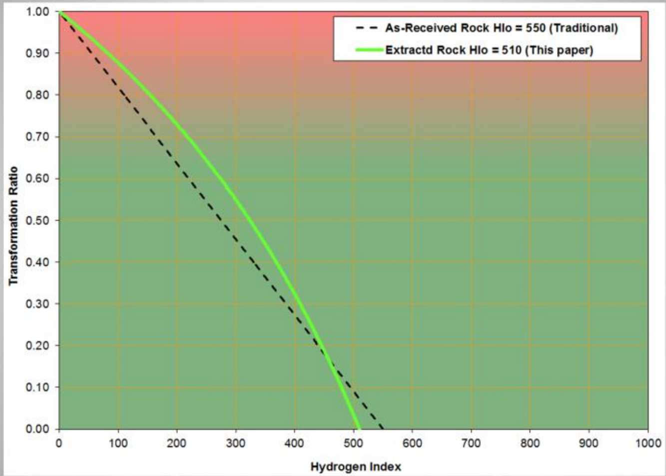
Presenter's notes: We note that the TR-HI relationship for extracted rocks is a family of curved lines, and that curvature increases as HI increases. Therefore, the error resulting from using the traditional method will be greatest for the best source rocks of greatest exploration interest.

Example: Type II Niobrara kerogen A-R vs. Extracted Calculations



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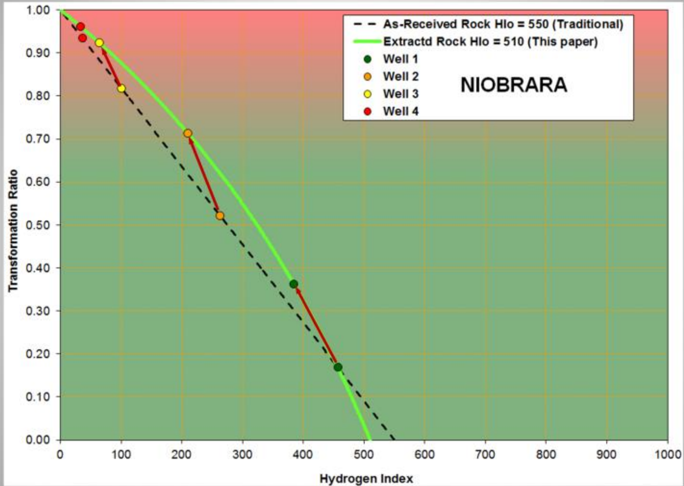
Example: Type II Niobrara kerogen
A-R vs. Extracted Calculations



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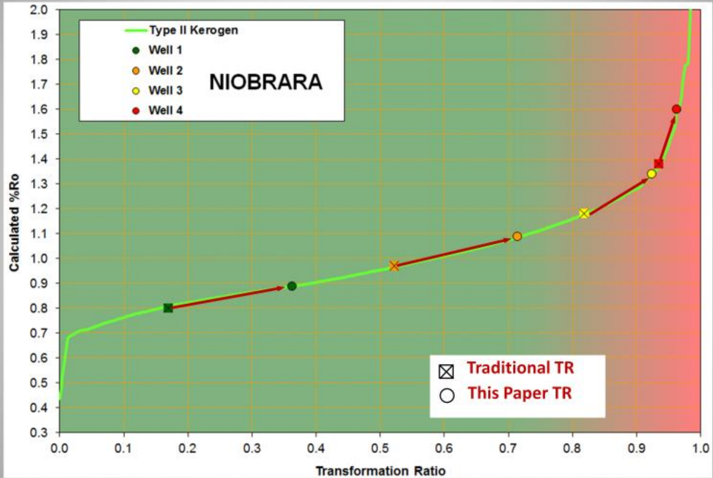
Type II Example:
Niobrara: A-R vs. Extracted Calculations



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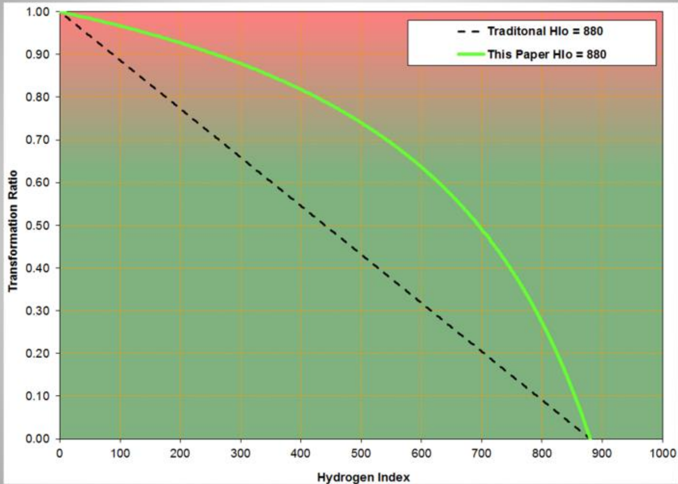
Type I Example:
Barbalha Fm. (Brazil): A-R data only



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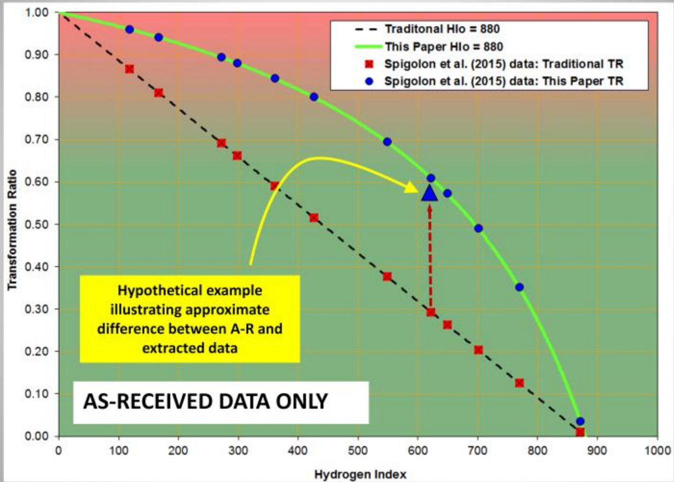
Data from Spigolon *et al.* (2015) Org. Geochem., Vol. 83-84, p. 27-53

Type I Kerogen:
Barbalha Fm., Brazil: A-R data only



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Data from Spigolon *et al.* (2015) Org. Geochem., Vol. 83-84, p. 27-53

Conclusions

- Transformation Ratio is best calculated from the observed transformation of convertible kerogen, as represented by the extracted S2:

$$TR = \frac{S2_{exto} - S2_{extm}}{S2_{exto}}$$

- From a practical standpoint, HI_{ext} is used as a convenient proxy for $S2_{ext:}$

$$TR = \frac{[HI_{exto} / 100] - [HI_{extm} \text{ x } [60 - 5 \text{ x } HI_{exto} / 100]] / [6000 - 5 \text{ x } HI_{extm}]}{[HI_{exto} / 100]}$$

- Transformation Ratio is not linearly related to HI because S2 and TOC vary, and vary independently, during petroleum generation.

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Conclusions (cont.)

- Hydrogen Index obtained from extracted samples (HI_{ext}) is a very powerful direct indicator of hydrocarbon generation.
- HI_{ext} can thus be used to calibrate maturity models, and to calculate Transformation Ratio and volumes of oil and gas generated.
- In contrast, HI obtained from unextracted samples will often significantly underestimate TR and volumes of hydrocarbons generated. Errors will be greatest at moderate levels of maturity, and may lead to overlooking good exploration opportunities.
- Extraction adds very little cost or delay to source-rock evaluation.

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