Improved Calibration of the Absolute Thermal Maturity of Coal-Sourced Oils and Gas Condensates Using PLS Regression

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Abstract

Knowing the absolute maturity of petroleum fluids can help to constrain the depth and timing of expulsion from source rocks and to clarify genetic relationships. For example: do suspected oil shows represent indigenous or migrated oil; are various oils from the same or sequential charge events; and did gas condensates form via phase separation from oils or directly from source rocks at higher maturity?

Absolute maturities are usually established by calibrating the fluids' molecular maturity parameters against equivalent parameters determined for bitumens extracted from source rocks of known maturity. Use of individual parameters can be problematic if the selected parameters reach equilibrium part-way through the oil window or are adversely affected by variation in source organofacies. In this study, we have developed a new method for predicting absolute maturities of coal-sourced oils and gas condensates based on Partial Least Squares (PLS) regression. The use of factor-based regression allows multiple maturity parameters to be used collectively, thus minimising potential errors associated with individual parameters.

Initially, 28 molecular maturity parameters were determined for 129 New Zealand coaly rocks of known Suggate coal rank [Rank(S_r)] and T_{max} values from throughout the oil window. Then, using bivariate correlations, Principal Component Analysis and PLS regression, two PLS regression models were developed for prediction of Rank(S_r) and T_{max}. The first model, optimised for Rank(S_r), uses a training set of 58 source rocks and 5 methylnaphthalene maturity parameters. The second model, optimised for T_{max}, uses 52 source rocks, the same 5 methylnaphthalene parameters and 3 methylphenanthrene parameters. Internal cross-validation shows that the models predict known Rank(S_r) and T_{max} values with standard errors of 0.40 rank units and 2.7°C, respectively, which are comparable to those of measured values.

Application of the PLS models to a set of 132 New Zealand coal-sourced oils and gas condensates predicts maturity values that are largely consistent with Rank(S_r) and T_{max} limits for the oil and gas windows determined independently from source rock pyrolysis studies. The gas condensates are overall more mature than the oils, but with significant overlap in their maturity ranges. The calibrated maturities of petroleum fluids in Taranaki Basin provide useful insight into the migration and charge histories of various fields, prospects and leads.

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Improved calibration of the absolute thermal maturity of coal-sourced oils and gas condensates using PLS regression

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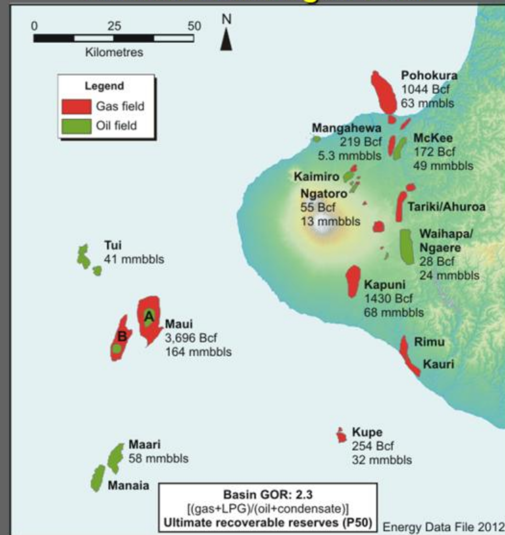
AAPG 2012 International Conference & Exhibition, Singapore, 16–19 September 2012

Talk outline

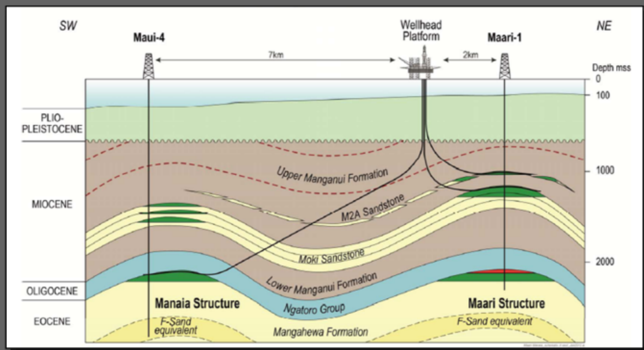
1. Introduction
2. Development of new method
3. Application to Taranaki Basin
4. Conclusions
5. Acknowledgements

Taranaki oil and gas fields



Absolute fluid maturities help clarify genetic relationships

1. Are various oils from the same or sequential charges?
2. When and at what depths were they expelled?
3. Did gas columns form via phase separation from oils or directly from source rocks at higher maturity?



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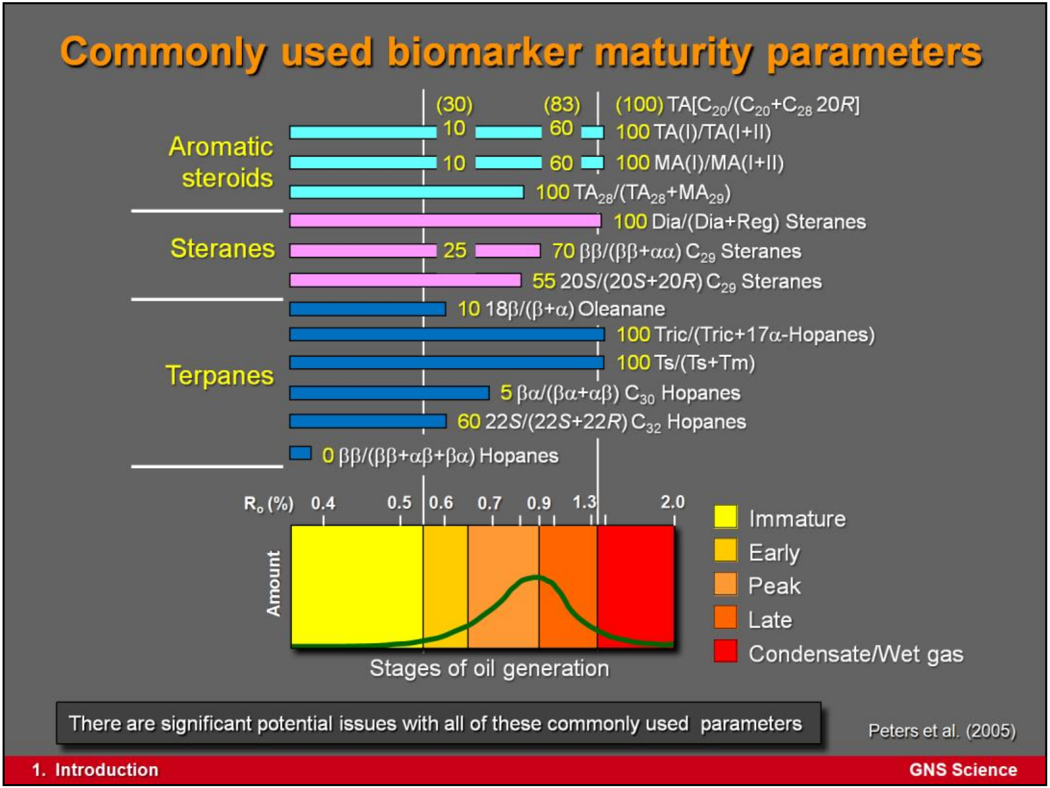


Presenter's notes: Most of them based on the different thermal stability of isomers – the less stable isomer is degraded preferentially; Not rigorously calibrated to R_o. All parameters are more or less influenced by other factors, such as, source organofacies, depositional conditions or biodegradation.

Affected by factors other than maturity *per se*

•Source organofacies and depositional environment

•Solubility differences between oils and gas condensates

•Biodegradation

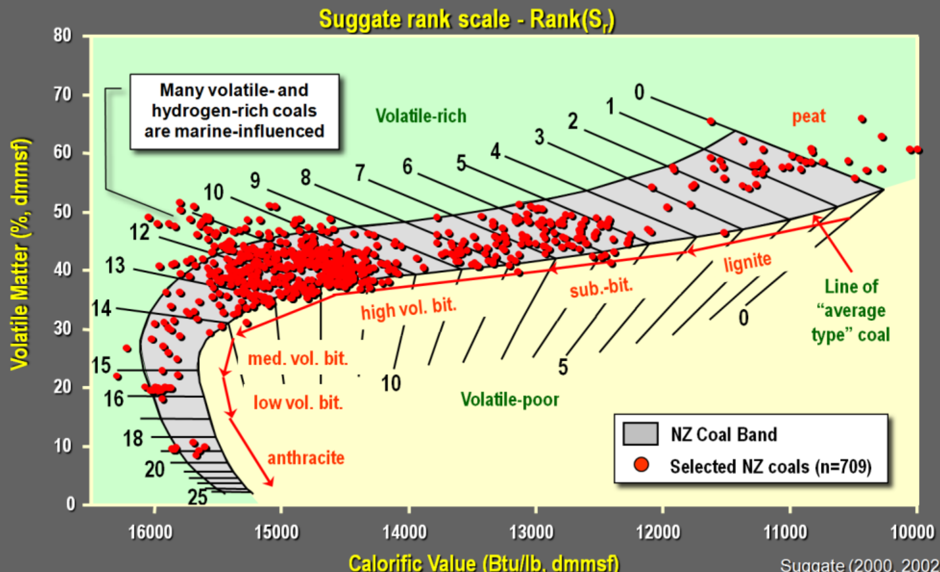
Limited range of applicability

•Reach equilibrium within or even before the oil window

•Do not extend into the gas window

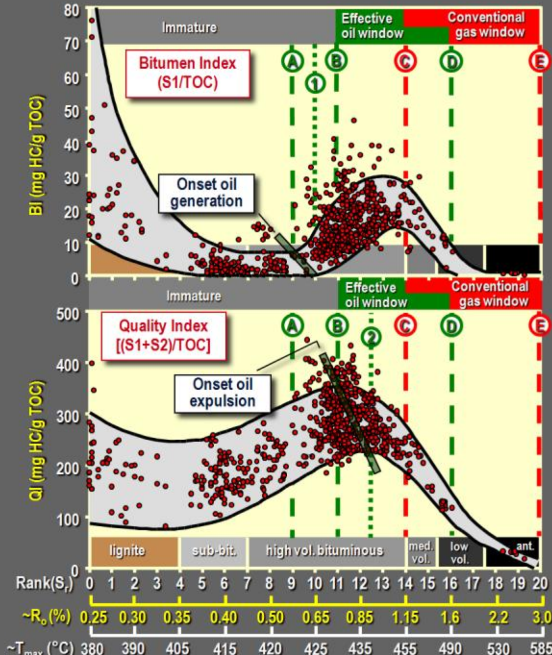
•Non-linear with maturity

Choice of target maturity parameters



- In NZ basins, vitrinite reflectance (R_o) is commonly suppressed due to marine influence
- Rank(S_r) and Rock-Eval T_{max} thus preferred for maturity calibration models [R_o obtained by correlation]

Maturation pathways for NZ coals

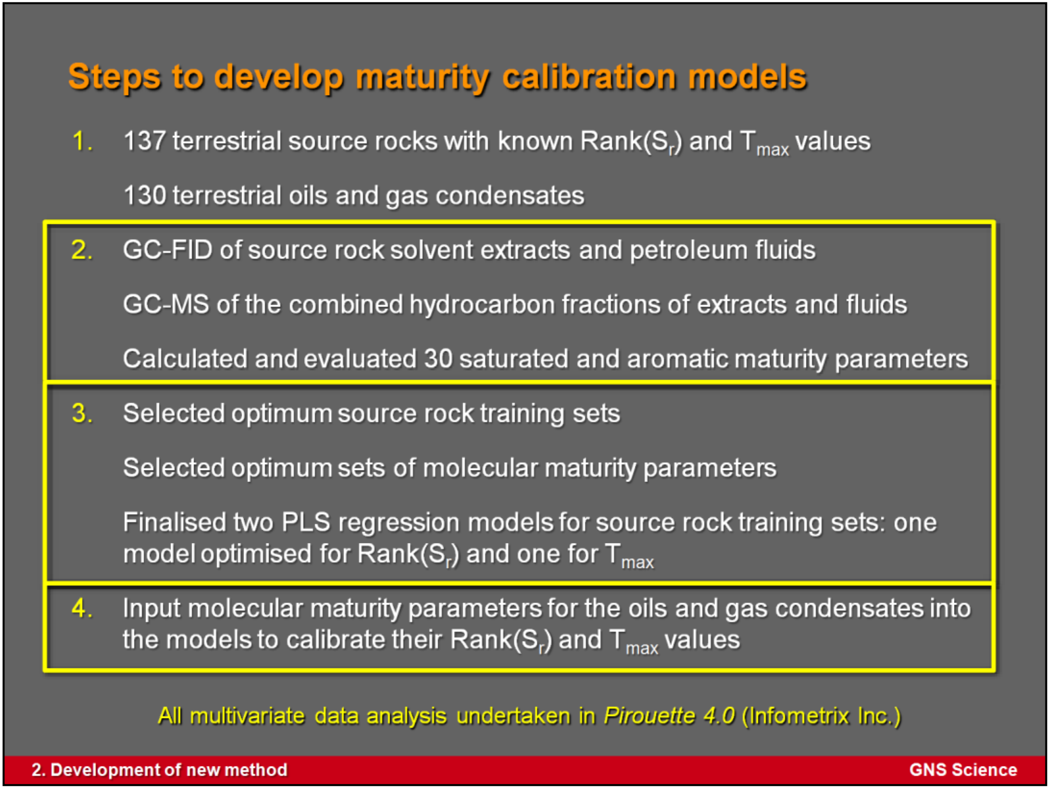


Key maturity thresholds based on Rock-Eval and TEPyGC

- **A** Onset of oil generation for coals near top of Coal Band [Rank(S_r) 9, R_o 0.55%, T_{max} 425°C].
- **1** Onset of oil generation for coals near base of Coal Band [Rank(S_r) 10, R_o 0.65%, T_{max} 425°C].
- **B** Onset of oil expulsion for coals near top of Coal Band [Rank(S_r) 11, R_o 0.70%, T_{max} 430°C].
- **2** Onset of oil expulsion for coals near base of Coal Band [Rank(S_r) 12.5, R_o 0.90%, T_{max} 440°C].
- **C** Onset of primary gas generation [Rank(S_r) 14, R_o 1.15%, T_{max} 455°C].
- **D** End of the oil window [Rank(S_r) 16, R_o 1.6%, T_{max} 490°C].
- **E** Approximate end of the conventional gas window [Rank(S_r) 20, R_o 3.0%, T_{max} 585°C].

- Onset gas generation and end of oil window defined primarily from TEPyGC data
- Correlations of Rank(S_r) with R_o and T_{max} based on coals near middle of Coal Band

Sykes & Snowdon (2002), Sykes & Johansen (2007)

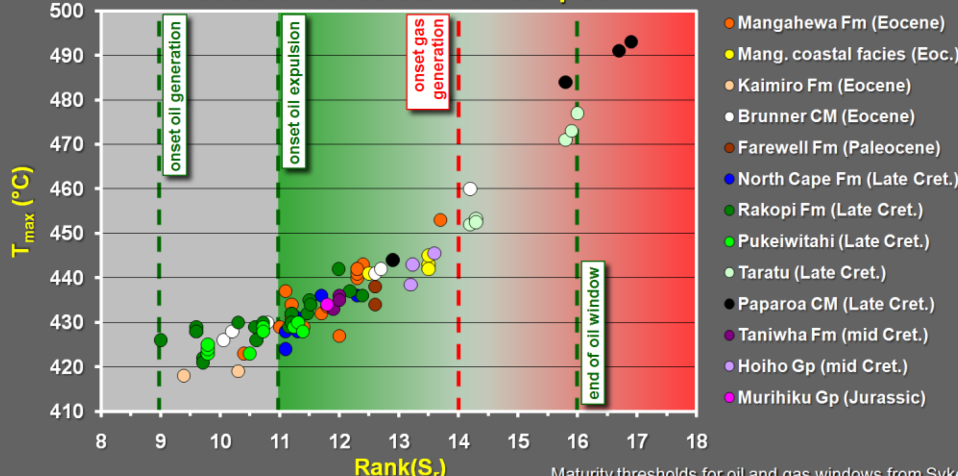


Presenter's notes:

1. All extract and fluid analyses undertaken by one lab (Applied Petroleum Technology, Norway) to maximise comparability.
2. Source rocks and molecular maturity parameters selected using correlations against Rank(Sr) and Tmax, Principal Component Analysis (PCA) and Partial Least Squares (PLS) regression (Pirouette v.4.0.).
3. PLS is a factor-based multivariate regression technique that allows a number of molecular maturity parameters to be used simultaneously, minimising potential errors from individual parameters.
4. Separate models 'predict' known Rank(Sr) and Tmax values of the source rock training sets with minimum error.

Selection of coaly source rock sample training sets

Initial screened set of 87 samples



Maturity thresholds for oil and gas windows from Sykes & Snowdon (2002) and Sykes & Johansen (2007)

Iterative evaluation of extract molecular maturity parameters using cross-plots, PCA and PLS resulted in two final training sets:
1. Rank(S_r), 61 samples [Rank(S_r)>11.0]
2. T_{max}, 57 samples [T_{max}>430°C]

Selection of molecular maturity parameters

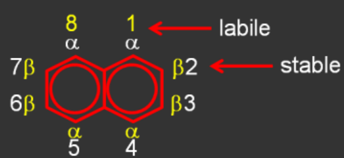
Final sets of molecular maturity parameters

Compound group	Label	Ratio
Trimethylnaphthalenes	TNR	2,3,6TMN/(1,3,5TMN + 1,4,6TMN)
	TNR2	(2,3,6 + 1,3,7)/(1,3,5 + 1,4,6 + 1,3,6)
	TMNr	(1,3,7)/(1,3,7 + 1,2,5)
Tetramethylnaphthalenes	TeMNr	1,3,6,7/(1,3,6,7 + 1,2,5,6 + 1,2,3,5)
	TeMNr2	1,2,6,7/(1,2,6,7 + 1,2,5,6 + 1,2,3,5)
Methylphenanthrenes	MP1a	1.5x(2-MP + 3-MP)/(P + 1-MP + 9-MP)
	MP1b	1.89x(3-MP + 2-MP)/(P + 1.26x(1-MP + 9-MP))
	MP2	2-MP/(1-MP + 2-MP)

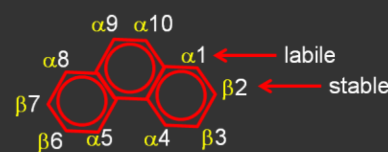
Rank(S_r) model (Trimethylnaphthalenes, Tetramethylnaphthalenes)

T_{max} model (all parameters)

Naphthalene carbon skeleton



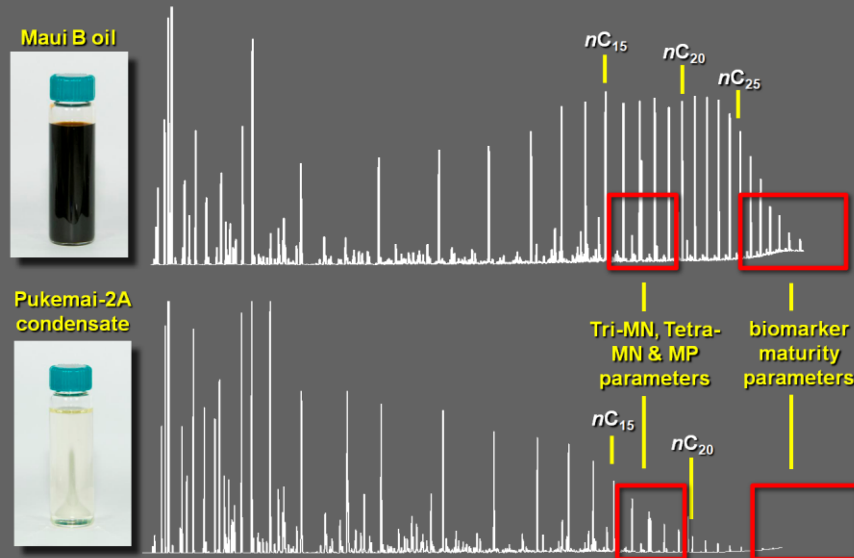
Phenanthrene carbon skeleton



Alexander et al. (1985), Radke et al. (1986), Radke (1988), van Aarssen et al. (1999)

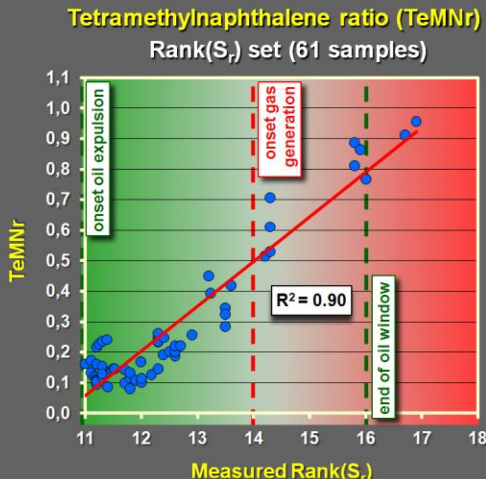
Presenter's notes: These parameters all work on the basis that with increasing maturity there is an increase in the more stable isomers (@beta positions).

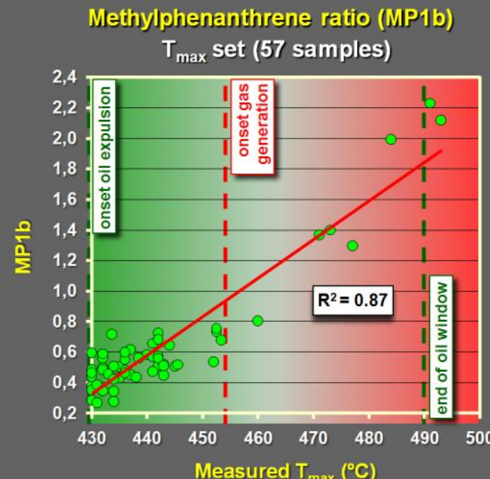
Accommodating gas condensates



Tri- and tetra-methylnaphthalenes (MN) and methylphenathrenes (MP) are present in sufficient concentrations even in the lightest of Taranaki gas condensates, whereas biomarkers are not.

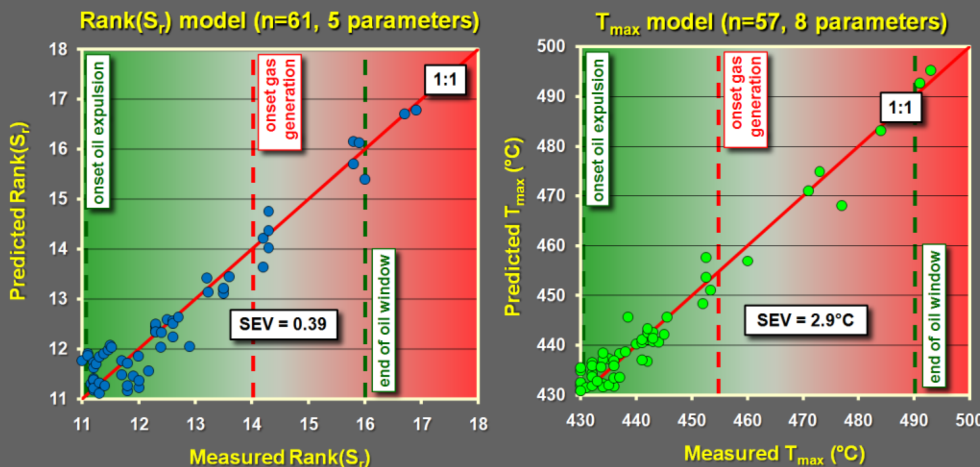
Selected aromatic maturity parameters versus Rank(S_r) and T_{max} for final source rock training sets





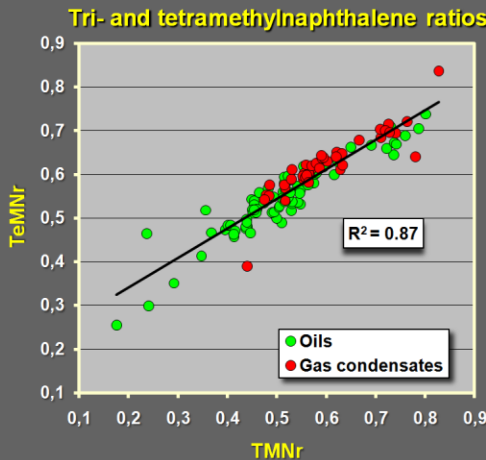
Maturity thresholds for oil and gas windows from Sykes & Snowdon (2002) and Sykes & Johansen (2007)

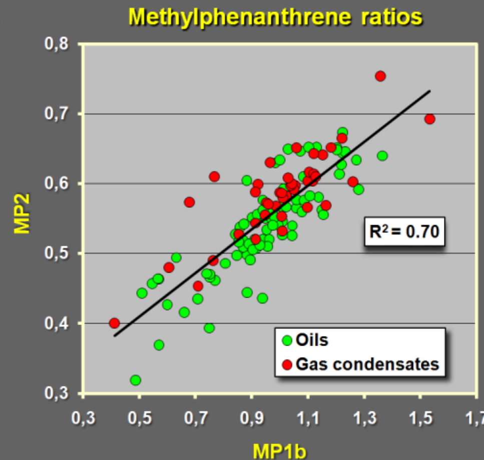
Final PLS regression models



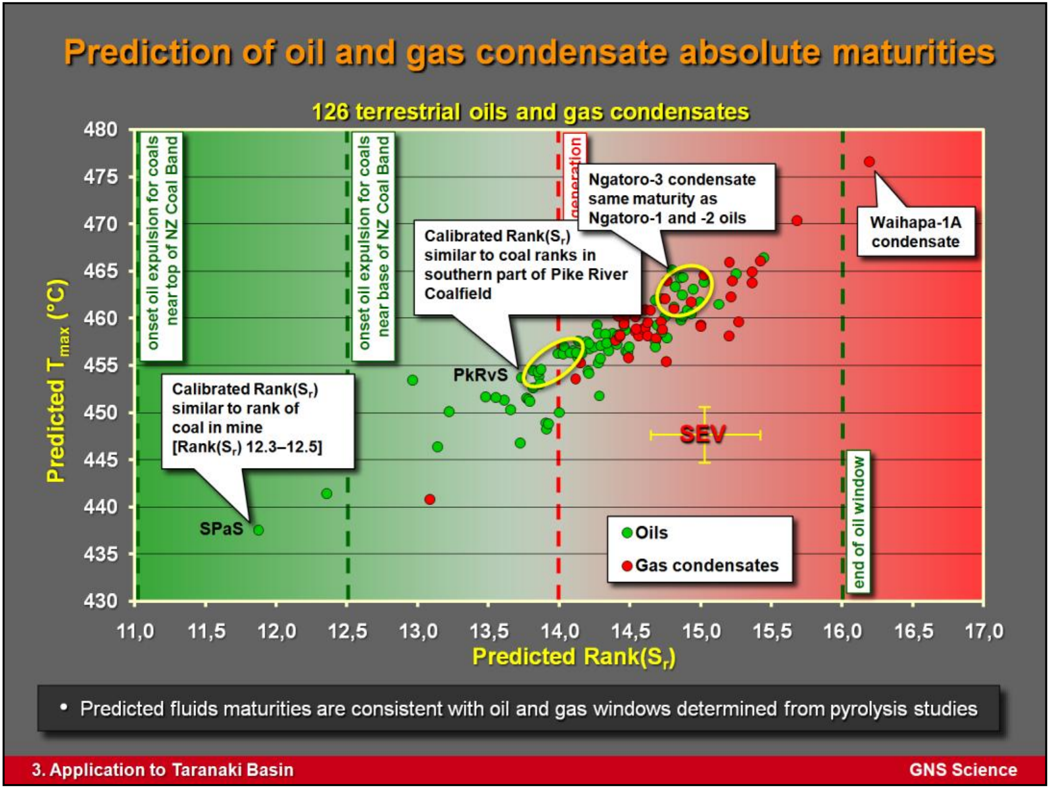
- Internal cross-validation of the final PLS regression models produced Standard Errors of Cross-Validation (SEV) of 0.39 Rank(S$_r$) units and 2.9°C T$_{max}$. These errors are comparable to those of measured values.

Oil and gas condensate input data for prediction



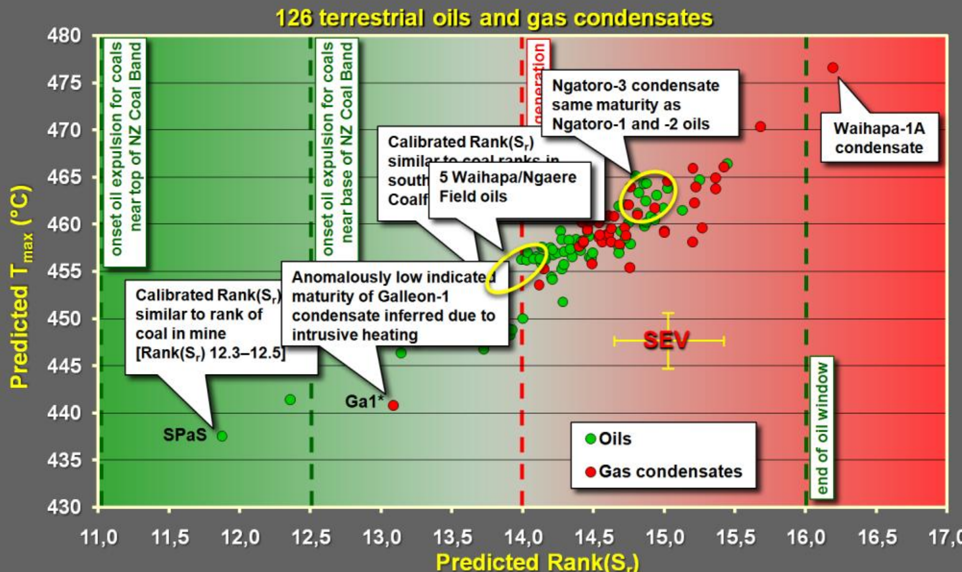


- Valid tri- and tetramethylnaphthalene and methylphenanthrene ratios obtained for all gas condensates.
- Only 4 Kauri Field oils (out of 130 fluids) omitted because of anomalous parameters. Two are biodegraded to Level 3.



Presenter's notes: Rank(S_r) vs T_{max} relation for the fluids closely matches that of the source rocks. Predicted fluid maturities represent cumulative maturities.

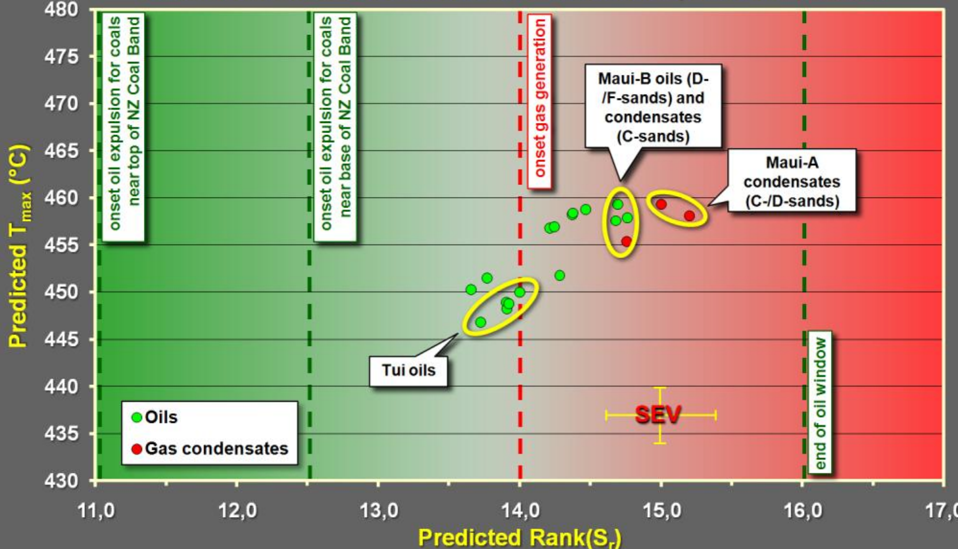
Prediction of oil and gas condensate absolute maturities



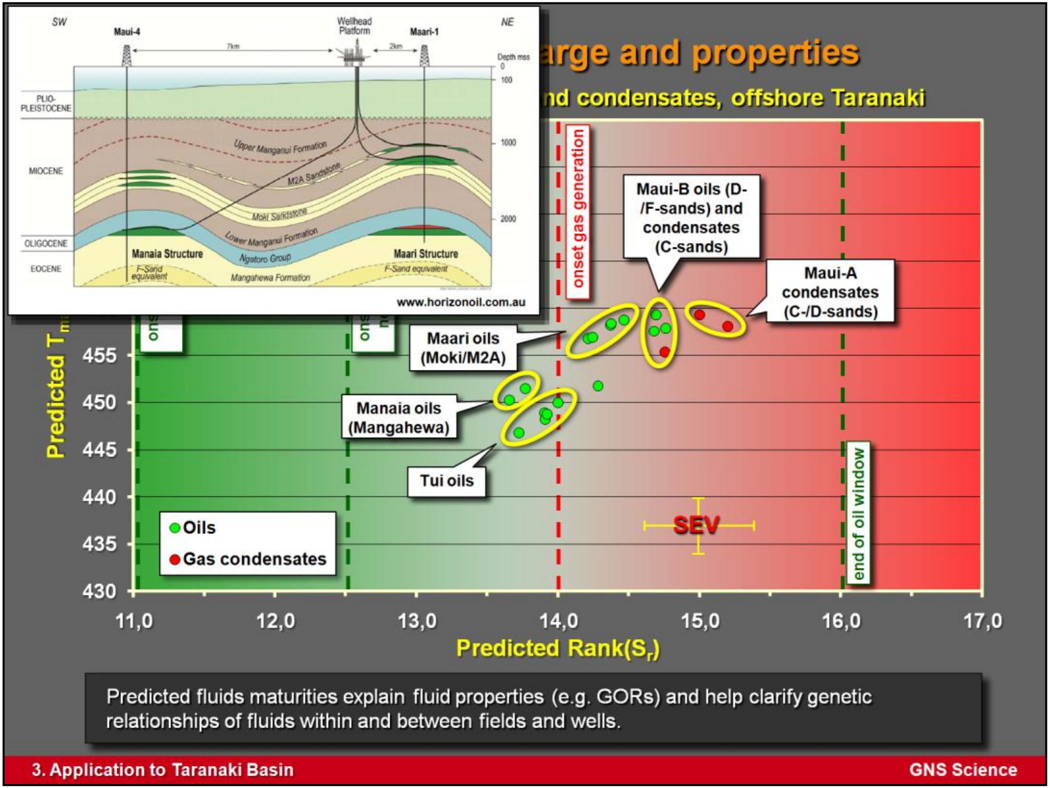
- Predicted fluids maturities are consistent with oil and gas windows determined from pyrolysis studies

Understanding petroleum charge and properties

Late Cretaceous terrestrial oils and condensates, offshore Taranaki



Predicted fluids maturities explain fluid properties (e.g. GORs) and help clarify genetic relationships of fluids within and between fields and wells.



arge and properties
nd condensates, offshore Taranaki
SW
NE
Maui-4
Wellhead Platform
Maari-1
7km
2km
Depth mss
0
100
1000
2000
PLIO-PLEISTOCENE
MIOCENE
OLIGOCENE
EOCENE
Upper Manganui Formation
M2A Sandstone
Moki Sandstone
Lower Manganui Formation
Ngatoro Group
Mangahewa Formation
Manaia Structure
Maari Structure
F-Sand equivalent
F-Sand equivalent
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onset gas generation
Maui-B oils (D-/F-sands) and condensates (C-sands)
Maui-A condensates (C-/D-sands)
Maari oils (Moki/M2A)
Manaia oils (Mangahewa)
Tui oils
SEV
end of oil window
Oils
Gas condensates
Predicted T_{max}
455
450
445
440
435
430
11,0
12,0
13,0
14,0
15,0
16,0
17,0
Predicted Rank(S_r)
Predicted fluids maturities explain fluid properties (e.g. GORs) and help clarify genetic relationships of fluids within and between fields and wells.
3. Application to Taranaki Basin
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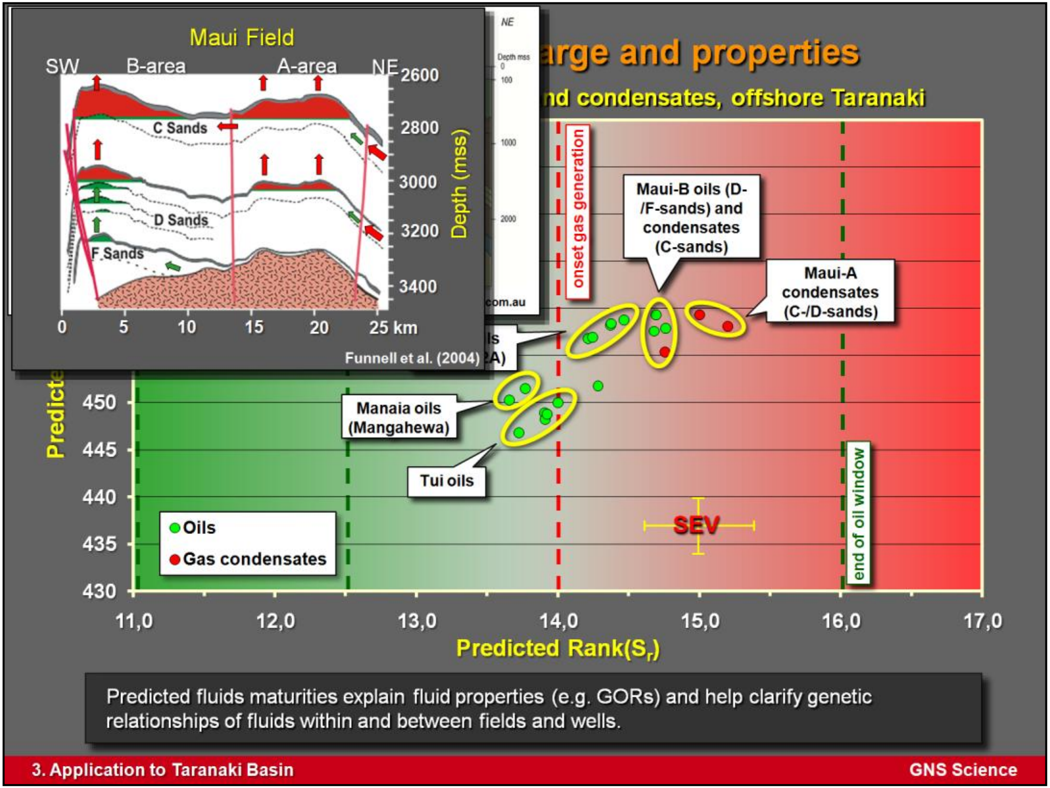

arge and properties
nd condensates, offshore Taranaki
Maui Field
SW
B-area
A-area
NE
C Sands
D Sands
F Sands
2600
2800
3000
3200
3400
Depth (mss)
0
5
10
15
20
25 km
Funnell et al. (2004)
NE
com.au
onset gas generation
Maui-B oils (D-/F-sands) and condensates (C-sands)
Maui-A condensates (C-/D-sands)
Manaia oils (Mangahewa)
Tui oils
Oils
Gas condensates
SEV
end of oil window
450
445
440
435
430
11,0
12,0
13,0
14,0
15,0
16,0
17,0
Predicted Rank(S_r)
Predicted fluids maturities explain fluid properties (e.g. GORs) and help clarify genetic relationships of fluids within and between fields and wells.
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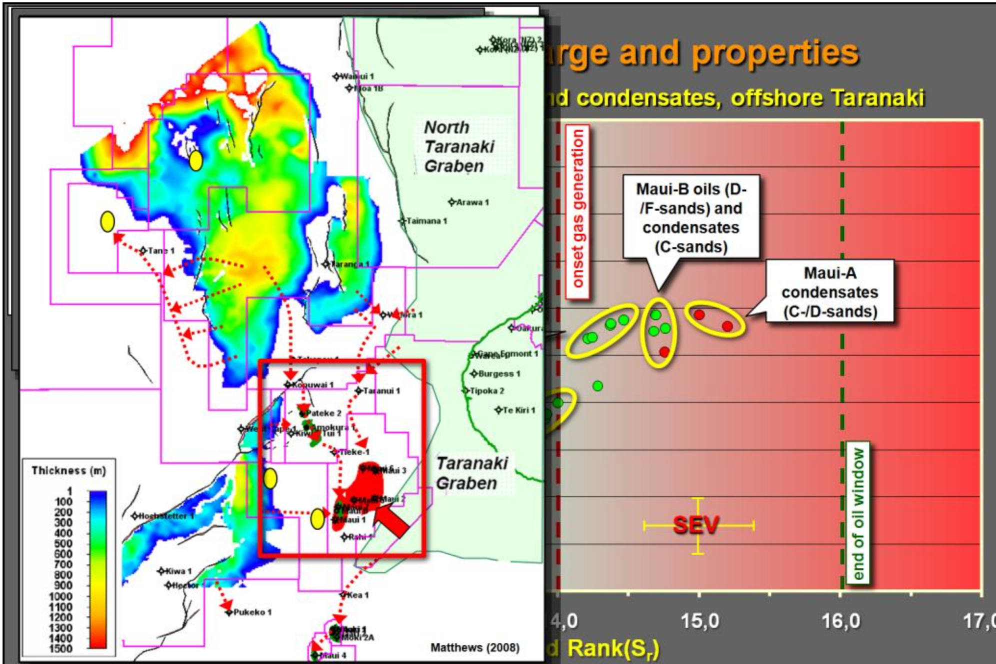

Predicted fluids maturities explain fluid properties (e.g. GORs) and help clarify genetic relationships of fluids within and between fields and wells.

Conclusions

- New PLS regression models have been developed that enable reliable calibration of the absolute maturities of terrestrial-sourced oils and gas condensates in terms of Rank(S_r) and T_{max}.
- Predicted maturities of New Zealand oils and gas condensates are consistent with maturity thresholds for the oil and gas windows determined independently from source rock pyrolysis studies.
- Calibrated absolute maturities of petroleum fluids can provide valuable insights into fluid properties (GORs), genetic relationships, migration pathways, and charge histories.

All results available @ http://data.gns.cri.nz/pbe

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