Recent Advances in Petroleum System Modeling of Geochemical Processes: TSR, SARA, and Biodegradation*

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Abstract

Basin and petroleum system modeling (BPSM) simulates the generation, expulsion, migration, accumulation, and loss of hydrocarbons in conventional and unconventional petroleum systems. This paper describes three new advances in modeling of geochemical processes: thermochemical sulfate reduction (TSR) modeling for H_2S prediction, as well as saturates-aromatics-resins-asphaltene (SARA) modeling and biodegradation modeling for prediction of oil quality.

TSR is a complex redox reaction controlled by reservoir chemistry and thermal history that converts petroleum and pore water sulfate to solid bitumen, carbon dioxide, and hydrogen sulfide. Accurate TSR modeling is important because it predicts H_2S, which is toxic, corrosive, and increases production costs. A new approach to model TSR enables concentrations of Mg^{2+}, Ca^{2+}, and SO_4^{2-} in pore water and sulfur in oil to be estimated based on reservoir lithology and oil quality. Model output as H_2S-risk distribution identifies areas where TSR can occur.

Predictions of aromatic and asphaltene content in oil cannot be made using standard published kinetics. A new SARA kinetic modeling approach includes 11 components (four bitumen, two oil, three hydrocarbon gas, CO_2, and H_2S) and can be used to improve predictions of oil quality. Additional features include complex secondary cracking through a multi-stage reaction network for bitumen-oil, oil-gas, and bitumen-gas, as well as a special adsorption model for the bitumen components. Components are lumped according to physical and chemical properties in order to minimize processing time. The approach allows prediction of asphaltene flocculation and tar mats as well as CO_2 and H_2S formation.

Biodegradation modeling was previously performed using BPSM simulation results, such as reservoir charge and temperature history. Decoupled post-processing was then applied to determine biodegradation risk. However, accurate predictions of petroleum properties are not possible using this approach. The new approach features full coupling of biodegradation into the BPSM simulation. Phase kinetics (14-

component model) is used with component-specific biodegradability, relative biodegradation ratios, temperature-dependent biodegradation rates, and paleopasteurization for more accurate predictions of API, GOR, viscosity, and CO_2 yields.

Selected References

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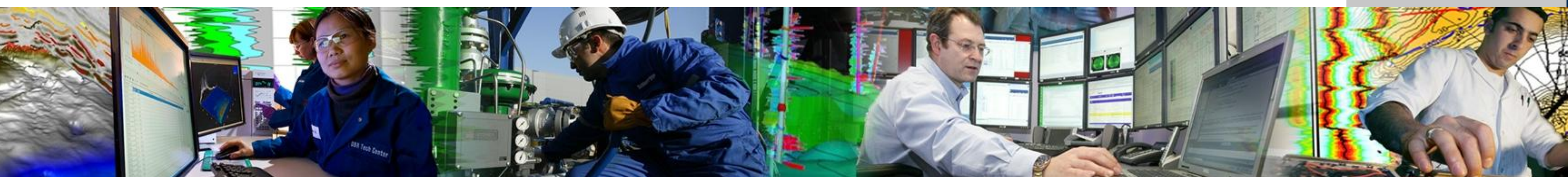

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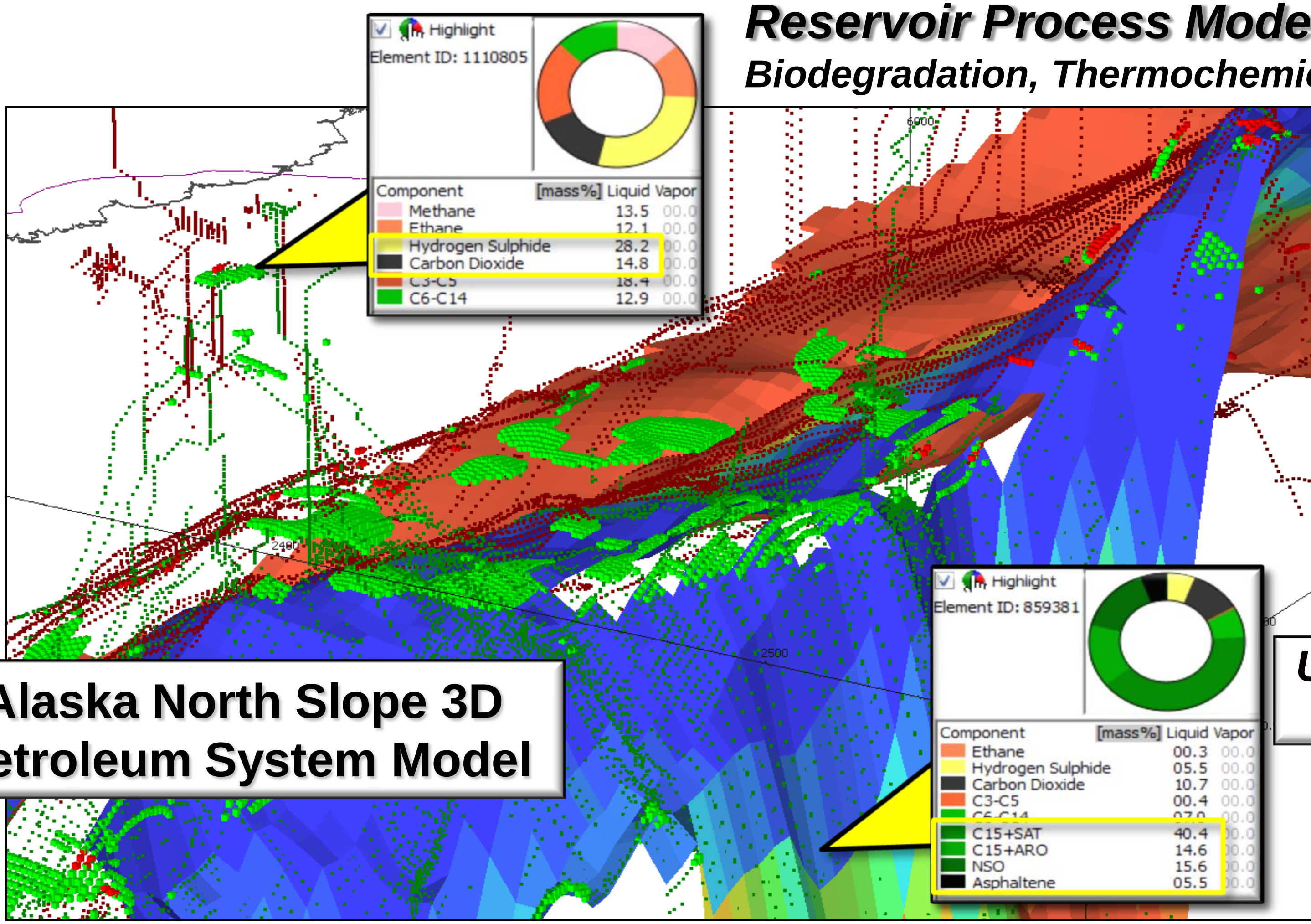
R&D Focus: Reservoir and Source Rock Process Models

Reservoir Process Models

Biodegradation, Thermochemical Sulfate Reduction

Conventional Target



Alaska North Slope 3D Petroleum System Model

Unconventional Target

Source Rock Process Models

SARA (Saturates, Aromatics, Resins, Asphaltenes)

Outline: Modeling of Three Key Subsurface Processes

- **Thermochemical Sulfate Reduction (TSR)**
  - ✓ Goal: Improve regional H_2S predictions
  - ✓ Example: Reservoirs in Offshore Tunisia
- **Biodegradation**
  - ✓ Goal: Improve predictions of oil quality
  - ✓ Example: Reservoirs in Campos Basin, Offshore Brazil
- **Saturates, Aromatics, Resins, Asphaltenes (SARA)**
  - ✓ Goal: Improve oil predictions of oil quality
  - ✓ Example: Shale oil quality prediction on Alaska North Slope
- Conclusions

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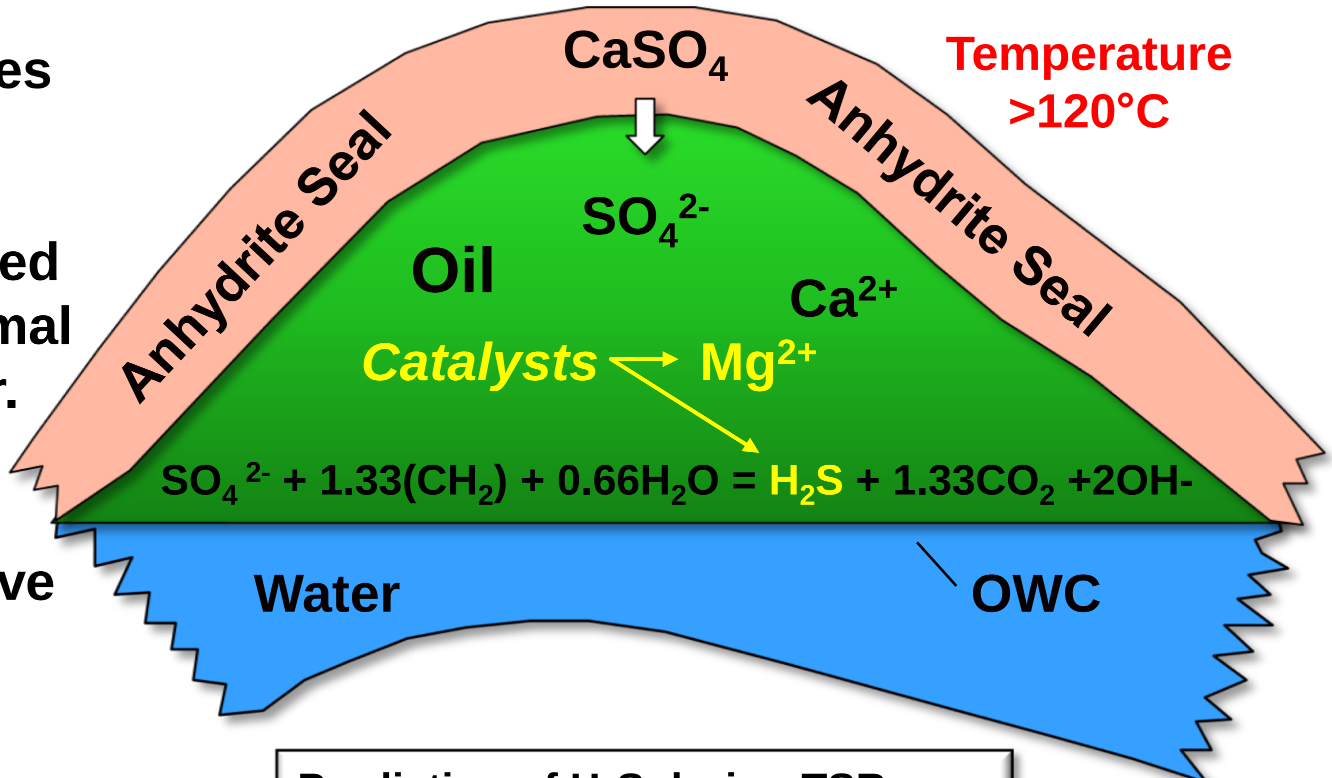
Thermochemical Sulfate Reduction (TSR) is Complex

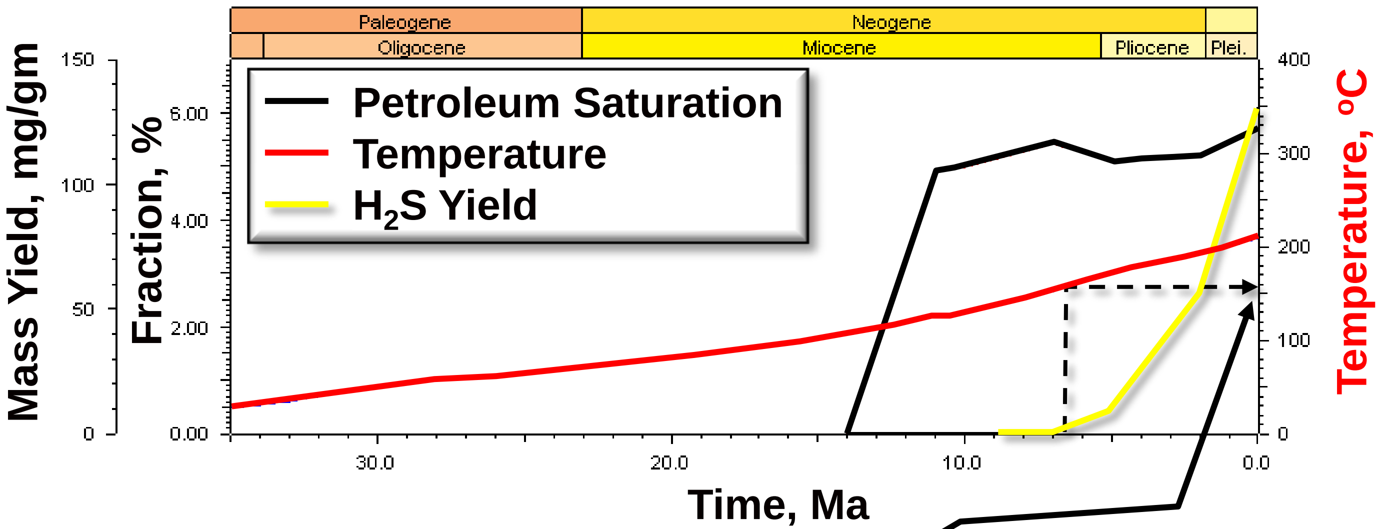
- H_2S is toxic, highly corrosive, and increases production costs.
- H_2S content is controlled by chemistry and thermal history of the reservoir.
- Accurate prediction of H_2S trends = competitive advantage.



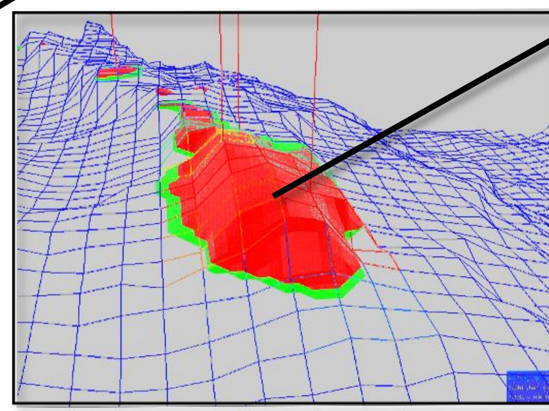
Prediction of H_2S during TSR

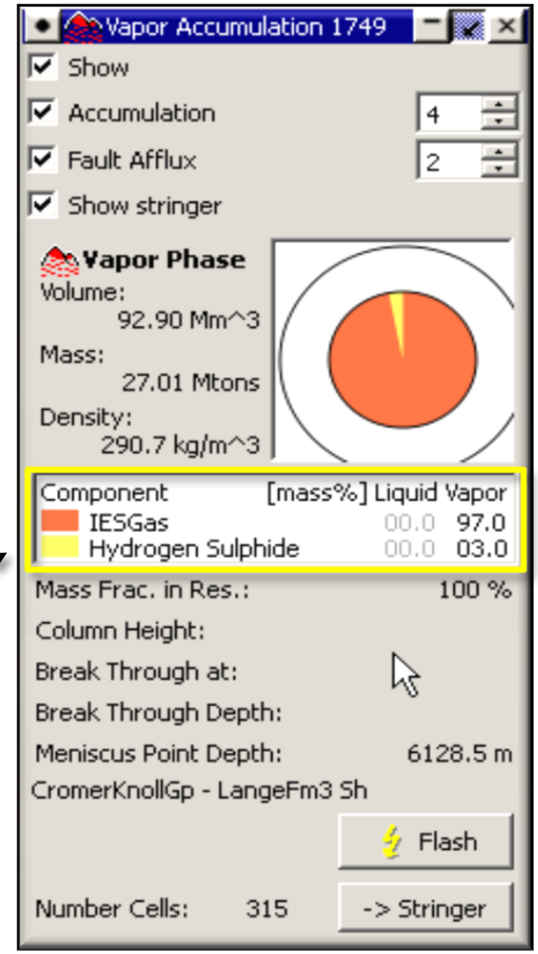
- Catalysts: Mg^{2+} and H_2S
- H_2S tracking during migration

H_2S is Handled as a Separate Component in Modeling

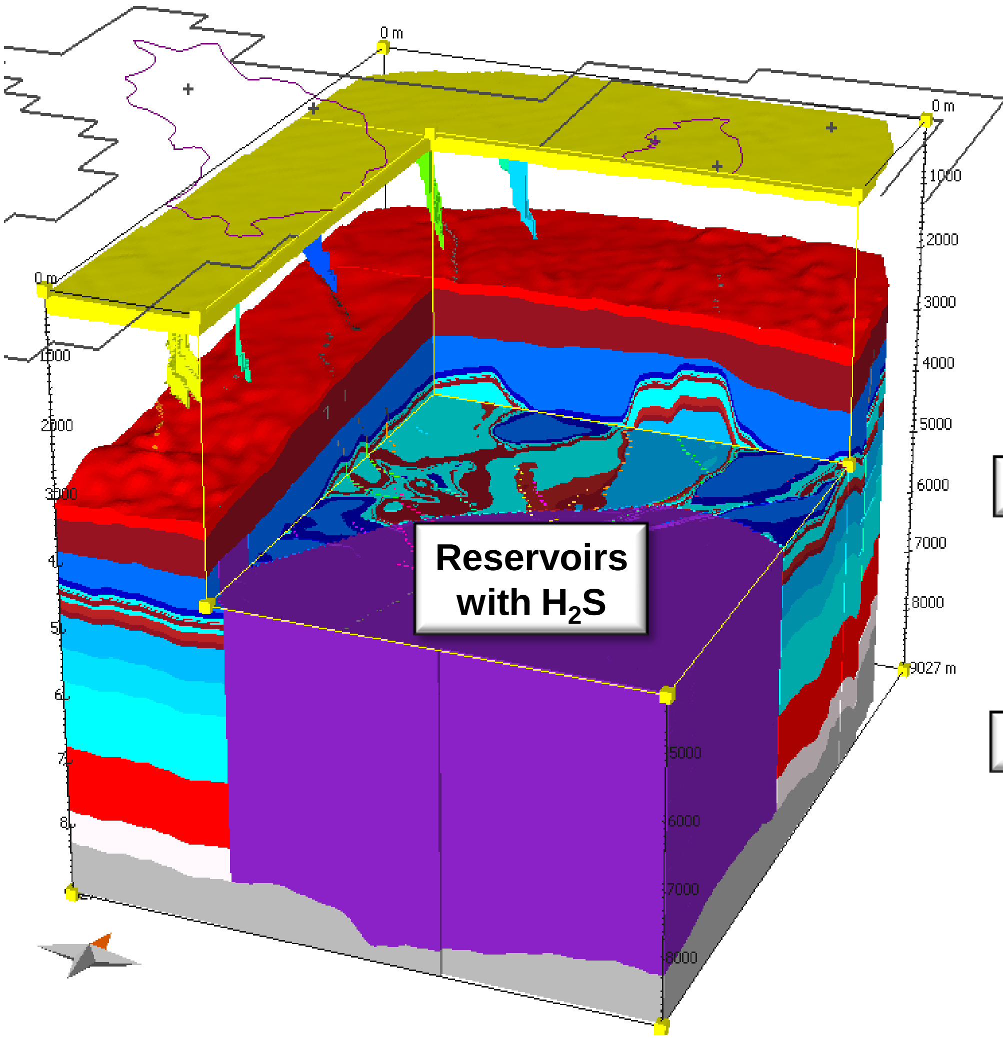


Note critical temperature threshold at ~160ºC

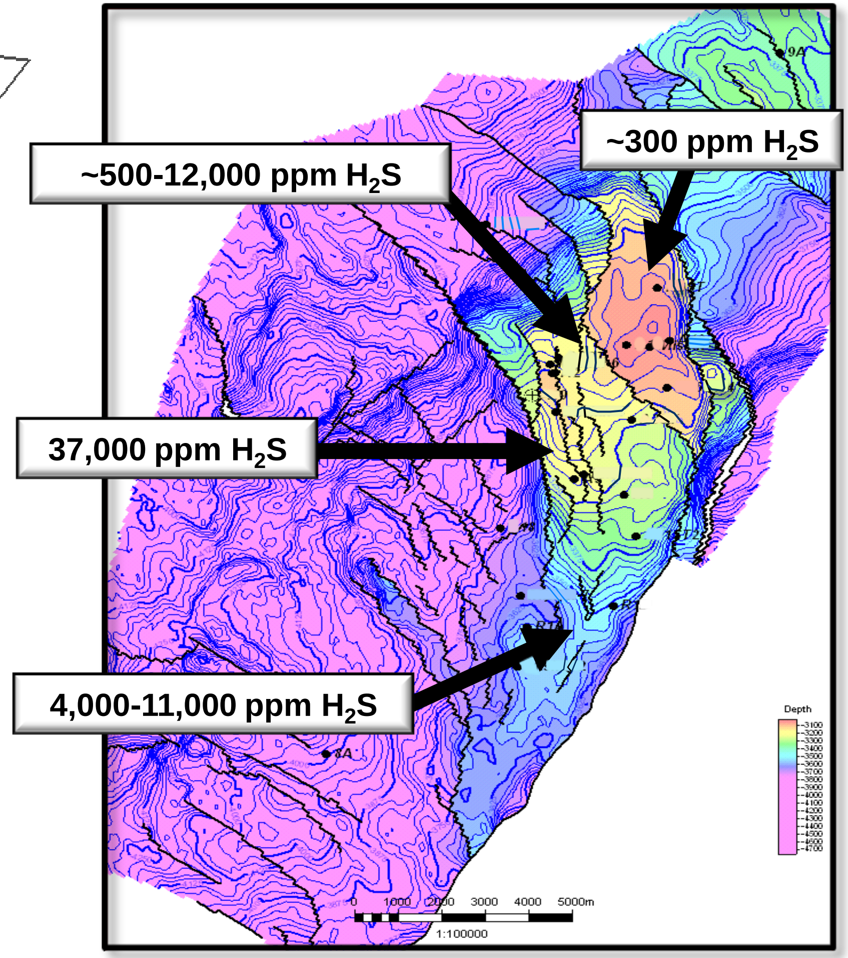




3D Model Predicts H_2S in Reservoirs, Offshore Tunisia

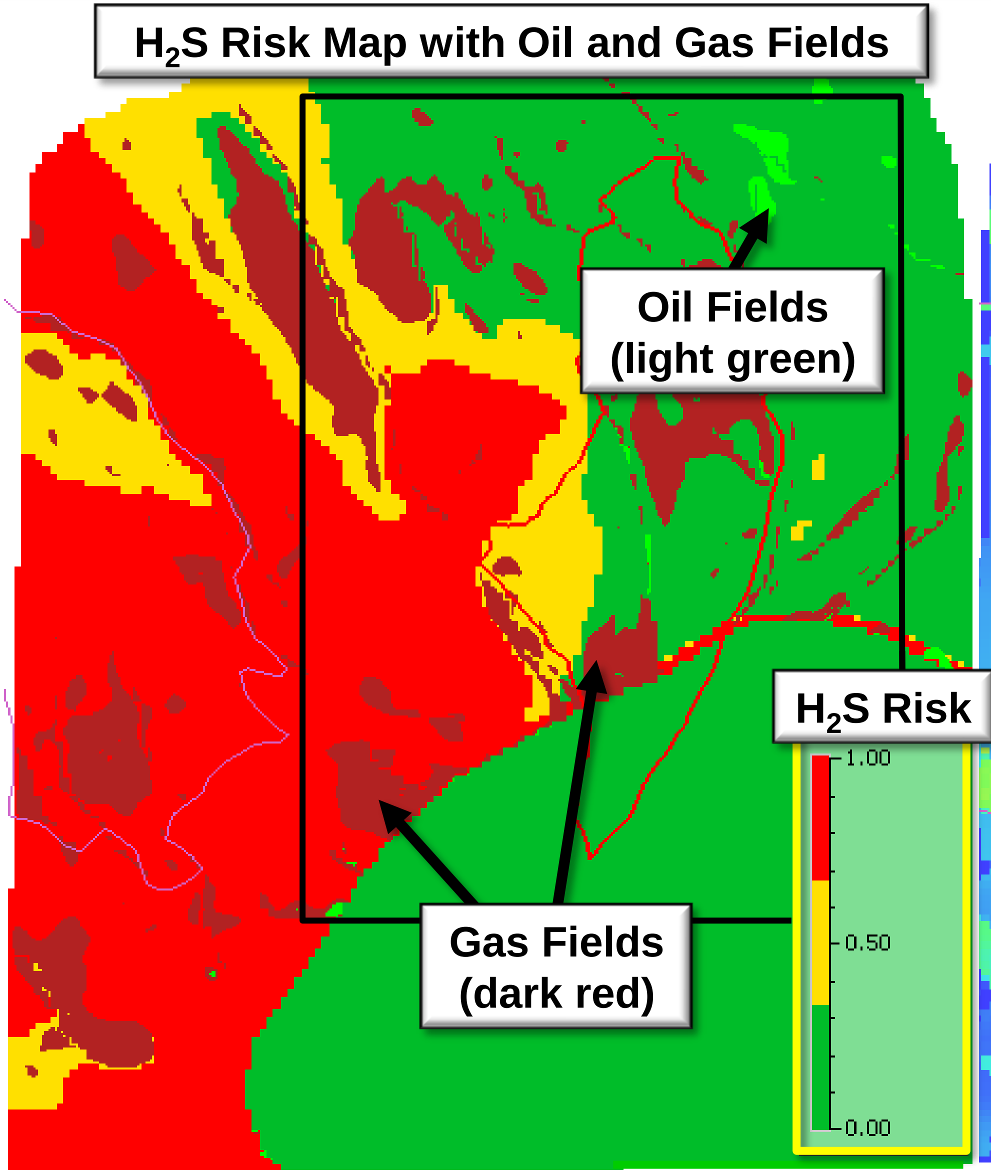


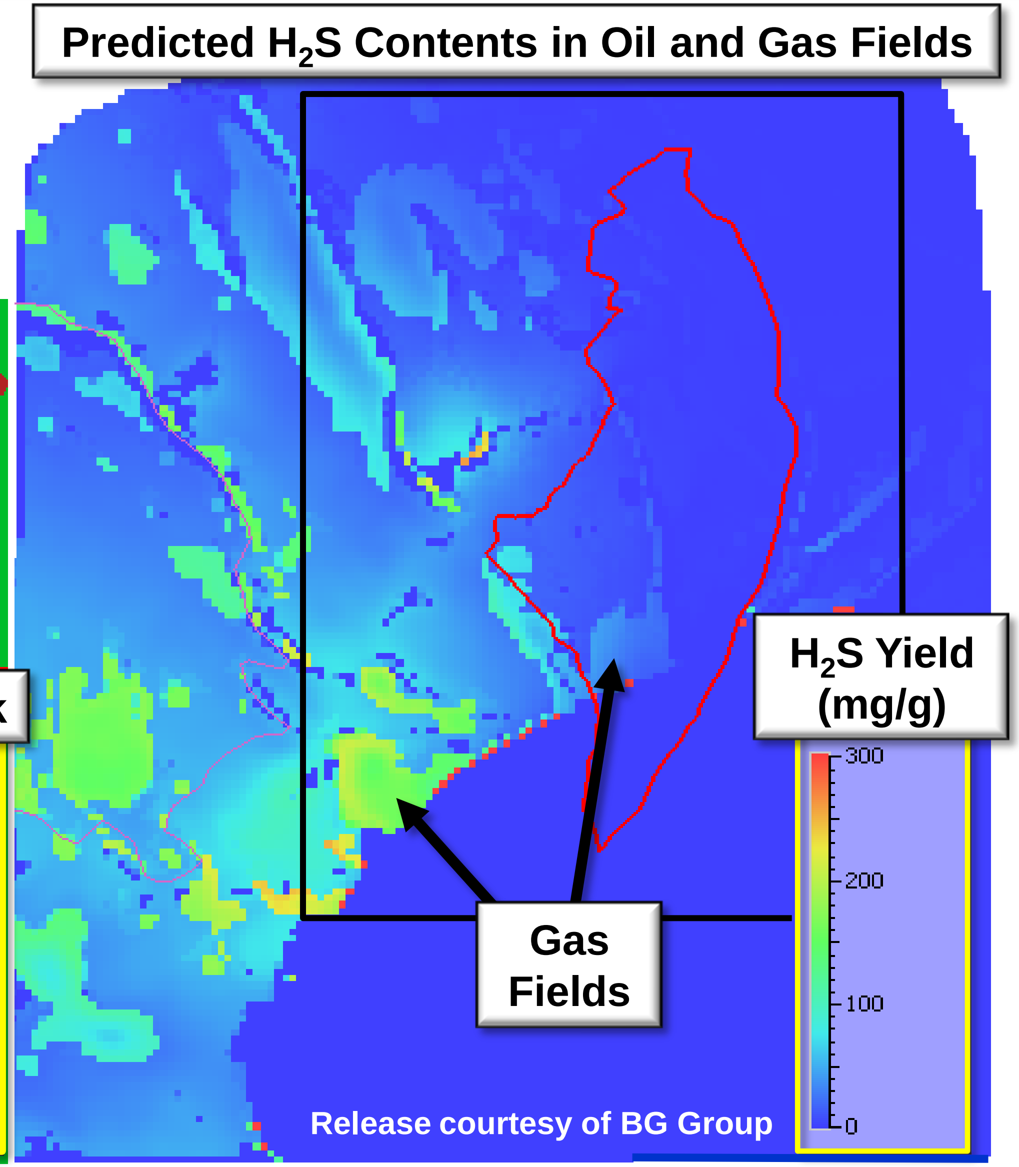
Grimmer et al. (2011)



Release courtesy of BG Group

TSR Modeling Provides Maps of H_2S Risk and Concentration





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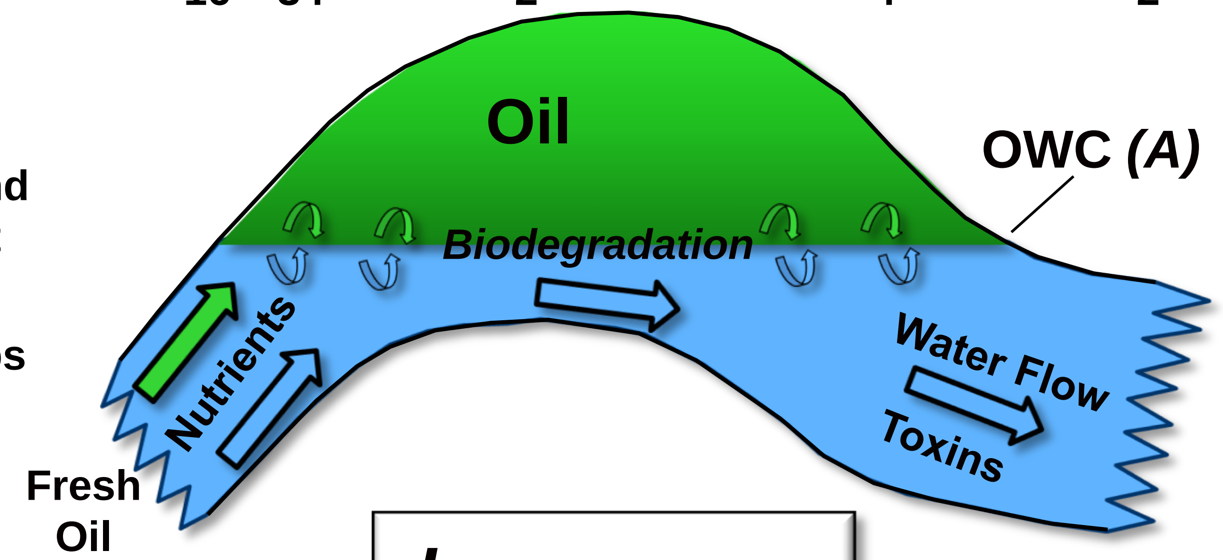
Biodegradation Modeling: Temperature, Degradability

$$4C_{16}H_{34} + 30H_2O \longrightarrow 49CH_4 + 15CO_2$$

- In-reservoir biodegradation can reduce crude oil quality.
- Biodegradation is controlled by reservoir temperature, charge and residence time, oil-water-contact surface area, and other factors.
- Paleopasteurization (>80°C) stops biodegradation.
- Accurate prediction of gas-oil ratio (GOR), API, CO_2 trends = competitive advantage.



Mass m_i

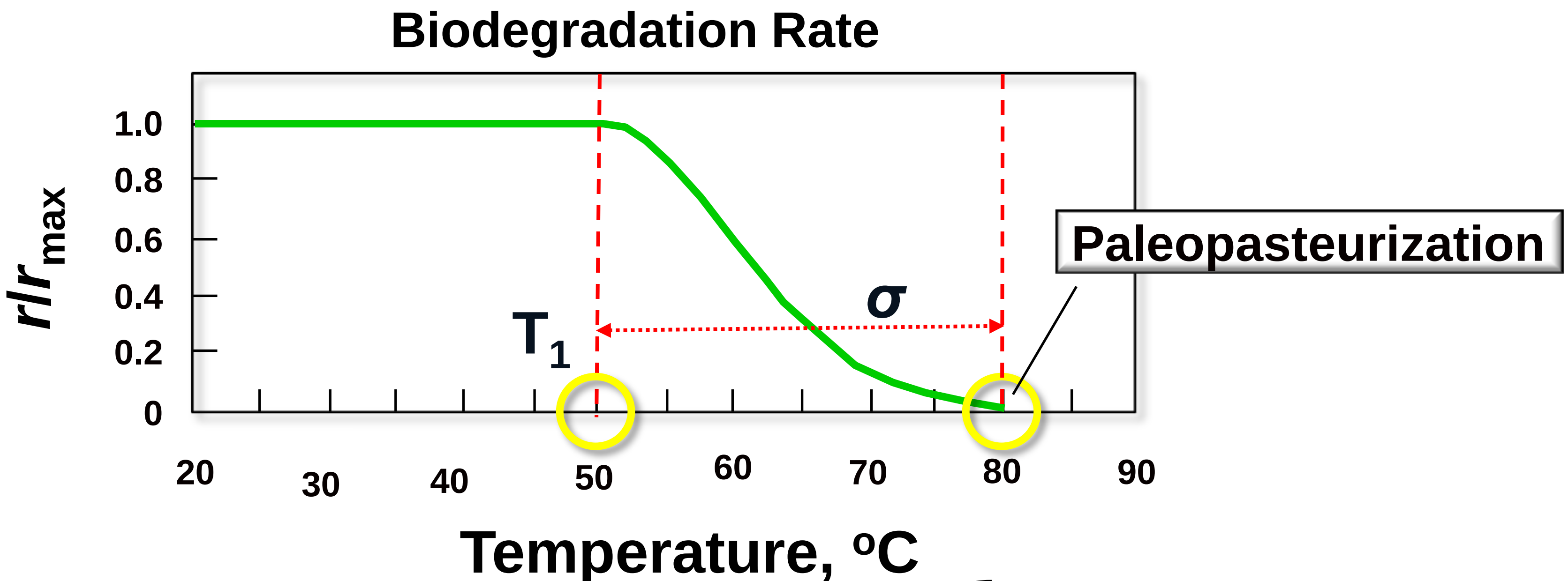
$$\frac{dm_i}{dt} = -r_i r\, A$$

Degradation Rate $r_i r$

Biodegradation Model Features
- Component-specific biodegradability model
- Includes paleopasteurization
- Output of corrected GORI, API, and CO_2 content

Hantschel and Kauerauf (2009)

Degradation Declines Near Paleopasteurization Temperature



$$r = \begin{cases} r_{max}, & T \leq T_1 \\ r_{max} \exp\left(-\frac{(T-T_1)^2}{2\sigma^2}\right), & T > T_1 \end{cases}$$

- r = total degradation rate
- T_1 = temperature above which biodegradation decreases
- σ = temperature range where biodegradation decreases
- r_{max} = max. rate of degradation depends on oil composition, environmental conditions

Blumenstein et al. (2008),
Hantschel and Kauerauf (2009)

‘Degradability’ Limits Degradation within Compound Classes

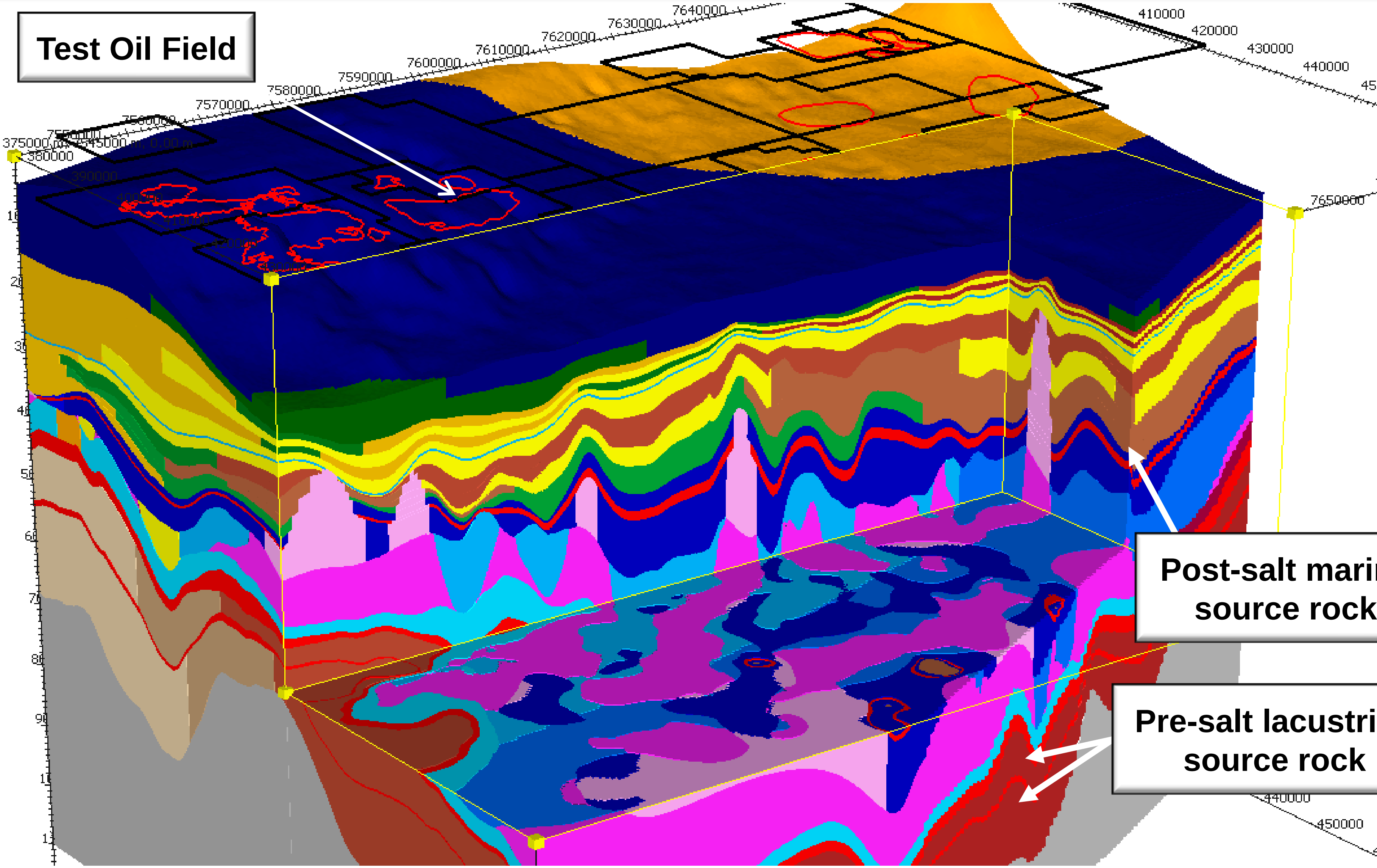
$$4C_{16}H_{34} + 30H_2O \rightarrow 49CH_4 + 15CO_2$$

Compound Class	Degradation Rate, r_i	Degradability
Methane	0.00	0.00
Ethane	0.40	1.00
Propane	1.00	1.00
i-Butane	0.80	1.00
n-Butane	1.00	1.00
i-Pentane	0.70	1.00
n-Pentane	0.80	1.00
n-Hexane	0.80	1.00
C_7-C_{15}	1.00	0.80
C_{16}-C_{25}	1.00	0.60
C_{26}-C_{35}	0.80	0.40
C_{36}-C_{45}	0.30	0.20
C_{46}-C_{55}	0.20	0.10
C_{56+}	0.10	0.02

Lighter alkanes are more easily biodegraded.

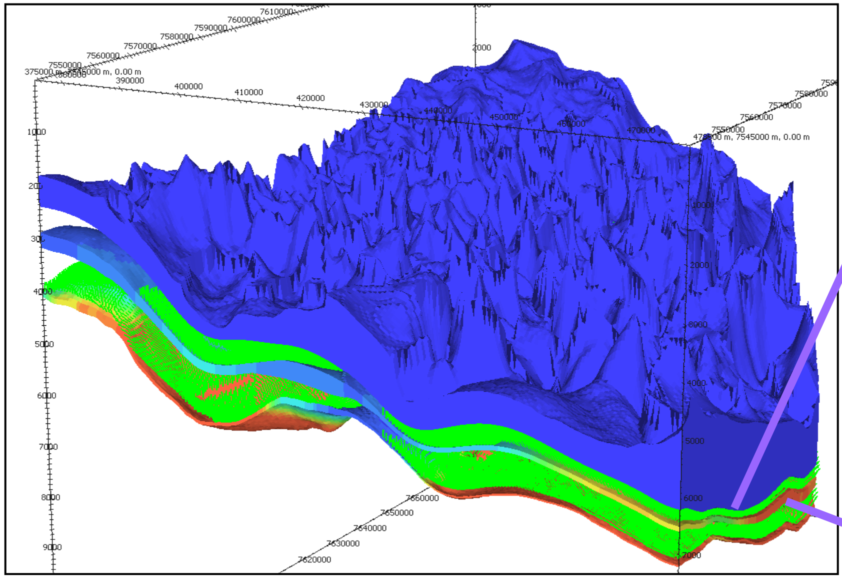
Blumenstein et al. (2008), Hantschel and Kauerauf (2009)

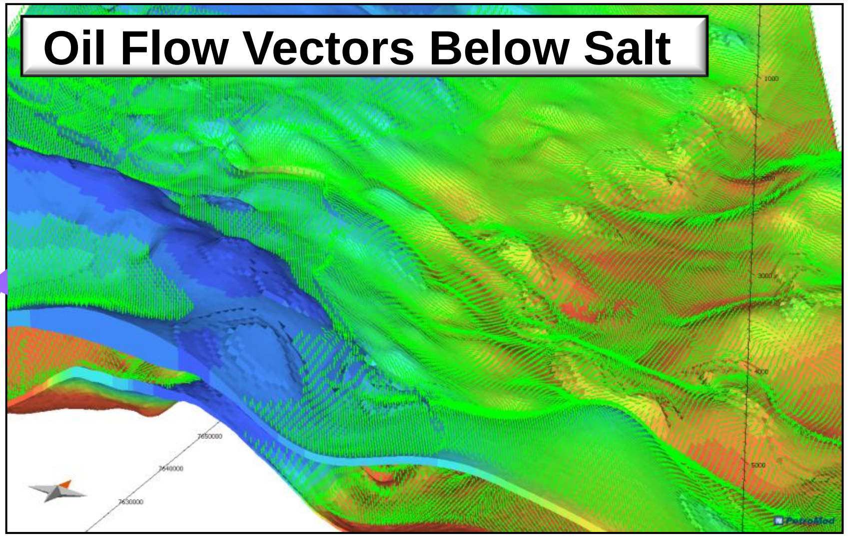
A Test Field was Selected for Study, Offshore Brazil

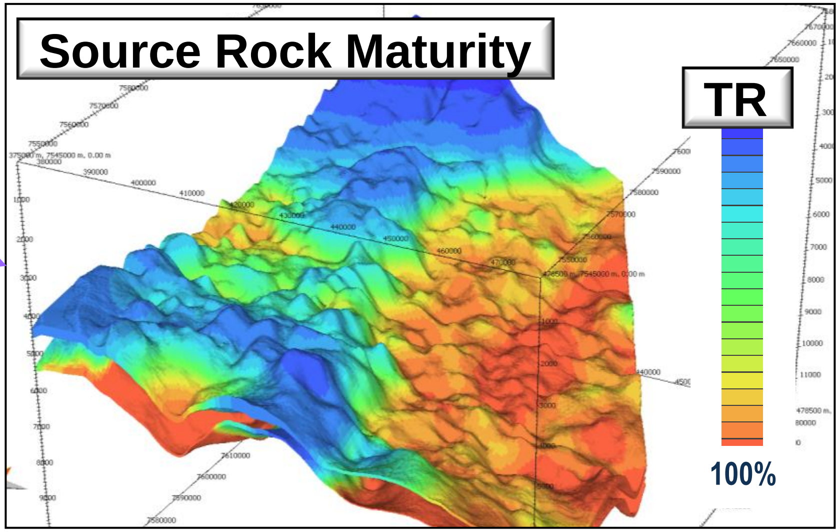


Flowpaths, Source Maturity Before Opening Salt Windows

56 Ma: *Before* Opening of Salt Windows

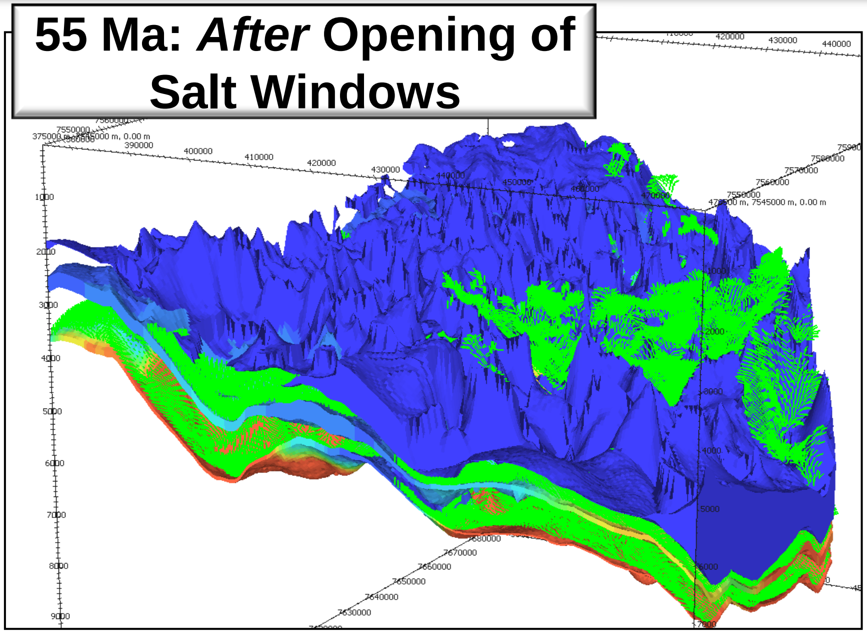


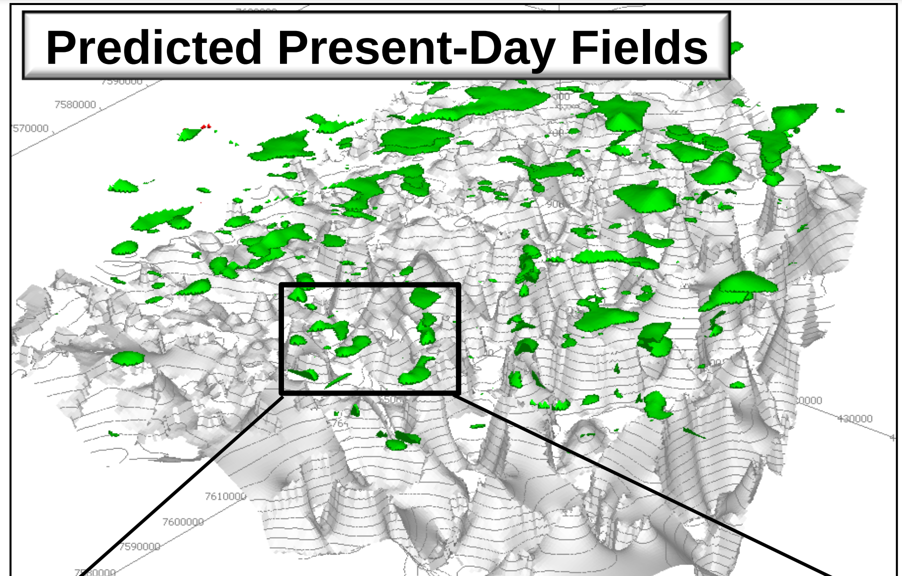


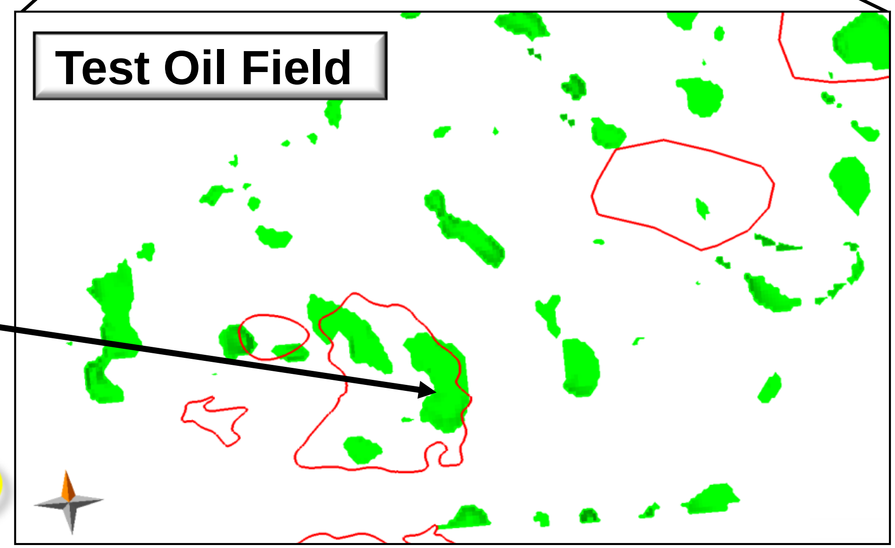


Release courtesy of Petrobras

Fields and Compositions After Opening of Salt Windows







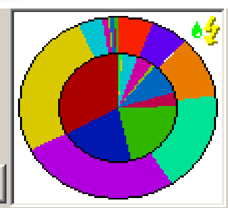
Field Report: OOIP 2200 Mbarrels, API 28-31°,GOR: 110 m^3/m^3

Component	(mass%) Liquid	Vapor
PK_P60+	05.7	00.0
Methane_C	00.0	01.1
PK_P50	06.3	00.0
PK_P40	10.9	00.0
PK_P30	17.9	00.0
PK_P20	26.5	00.0
PK_P10	26.2	00.2
n-Hexane	03.9	04.4
n-Pentane	01.1	04.2
i-Pentane	00.2	01.1
n-Butane	00.7	09.6
i-Butane	00.2	04.0
Propane	00.4	21.8
Ethane	00.1	20.5
Methane	00.0	33.1

Flashed to surface conditions (PR):

- [x] from Liquid
- [ ] from Vapor

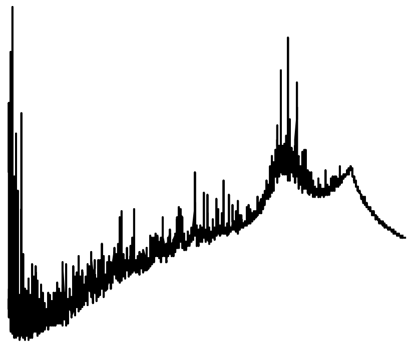
PetroFlash...



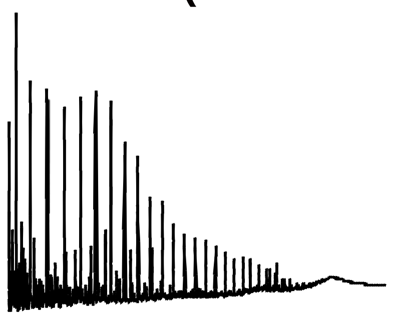
Liquid:	(Mbarrels)	604.47
Vapor:	(mcm)	13306.04
API:		25.84
GOR:	(m^3/m^3)	138.46
CGR:	(m^3/m^3)	0.01

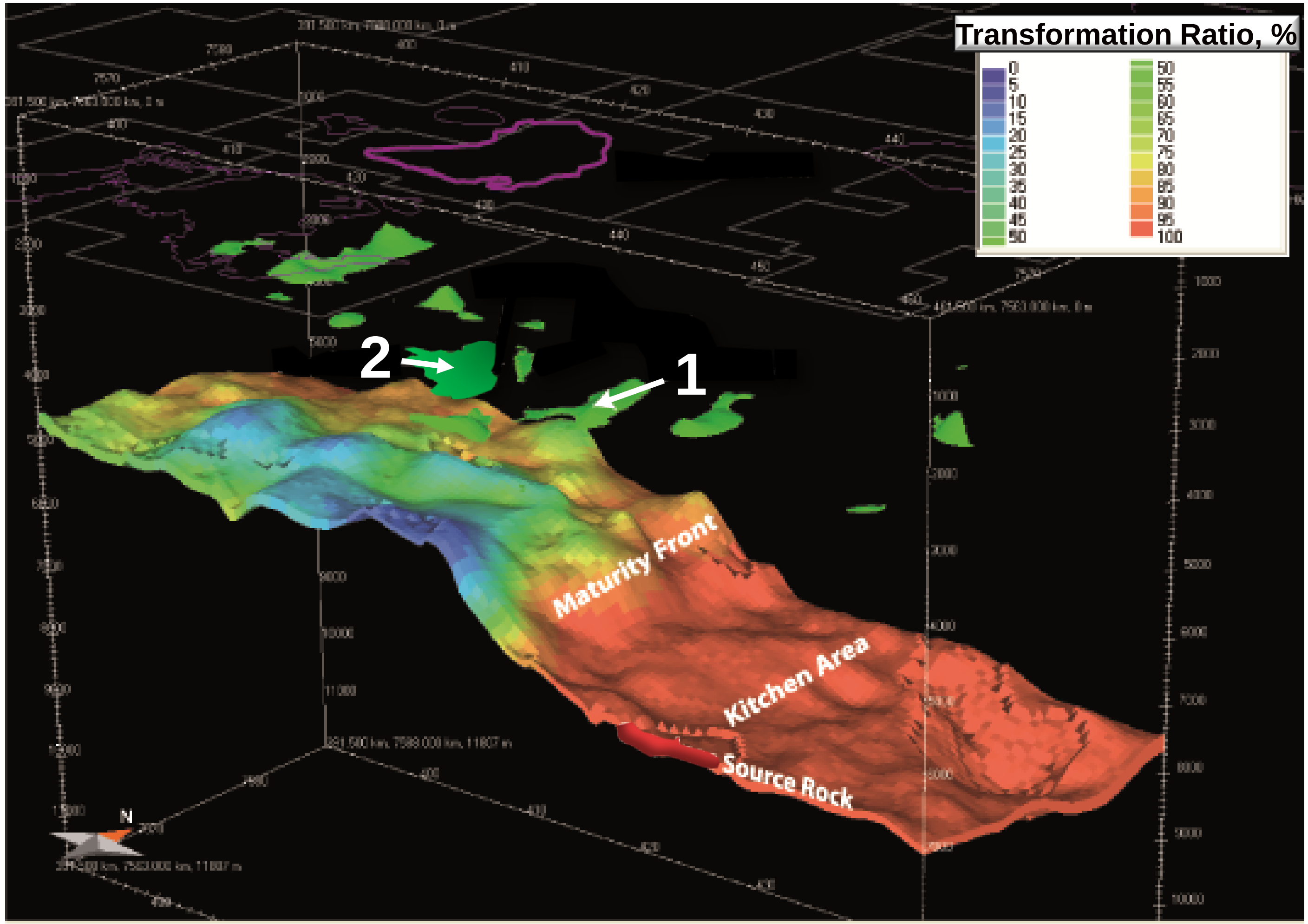
Compartments in Test Field Show Variable API Gravity

Compartment 2
18^{o}API (measured)



Compartment 1
28^{o}API (measured)





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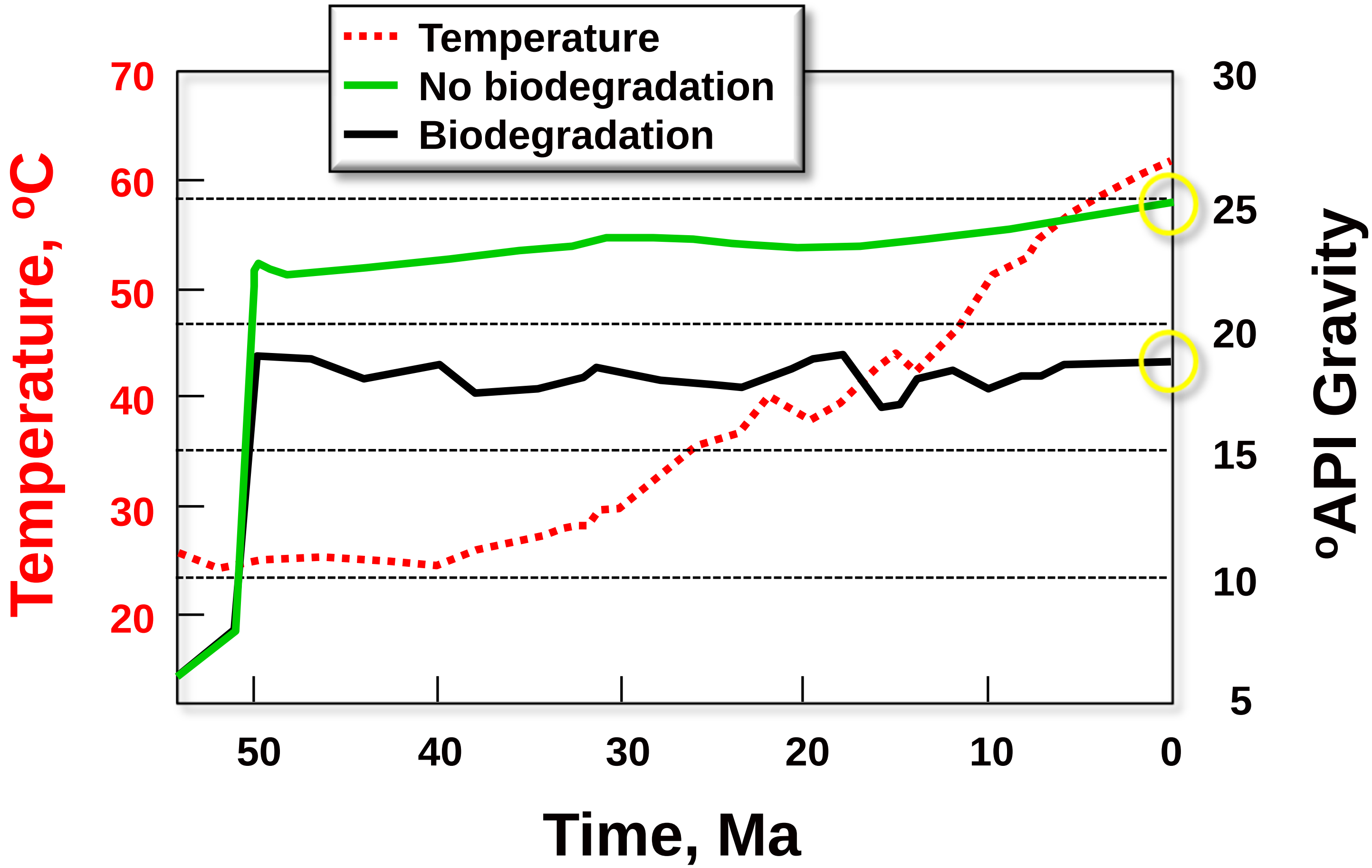
Model Improves API Prediction in Compartment 2



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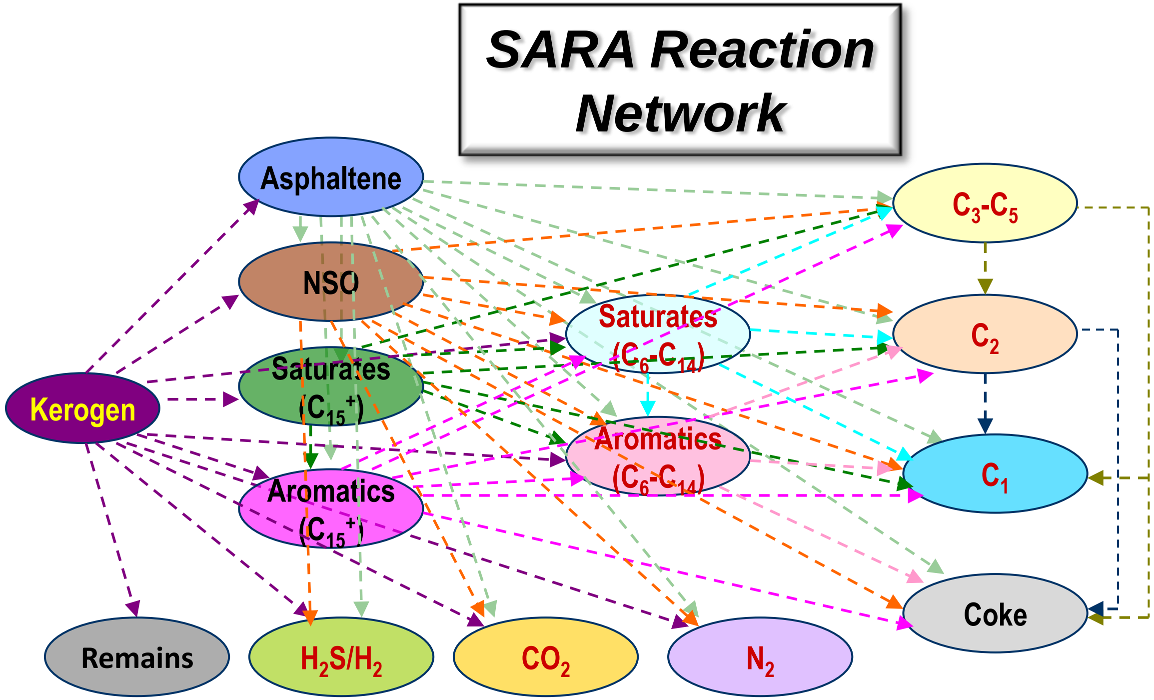
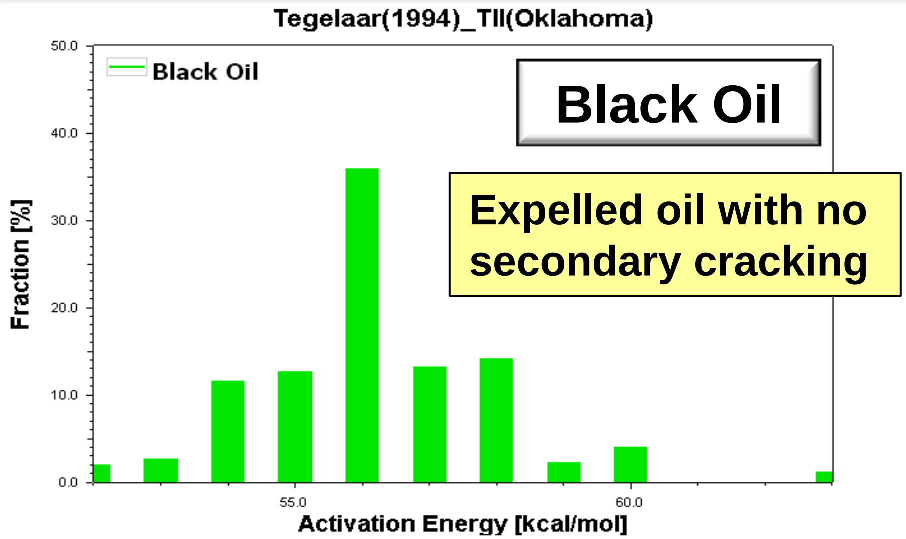
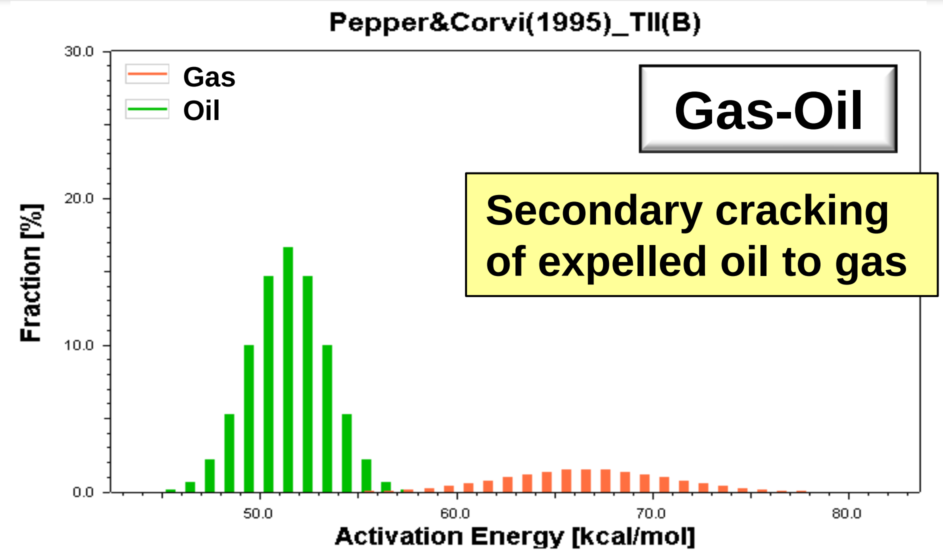
Modeling Saturates, Aromatics, Resins, Asphaltenes (SARA)

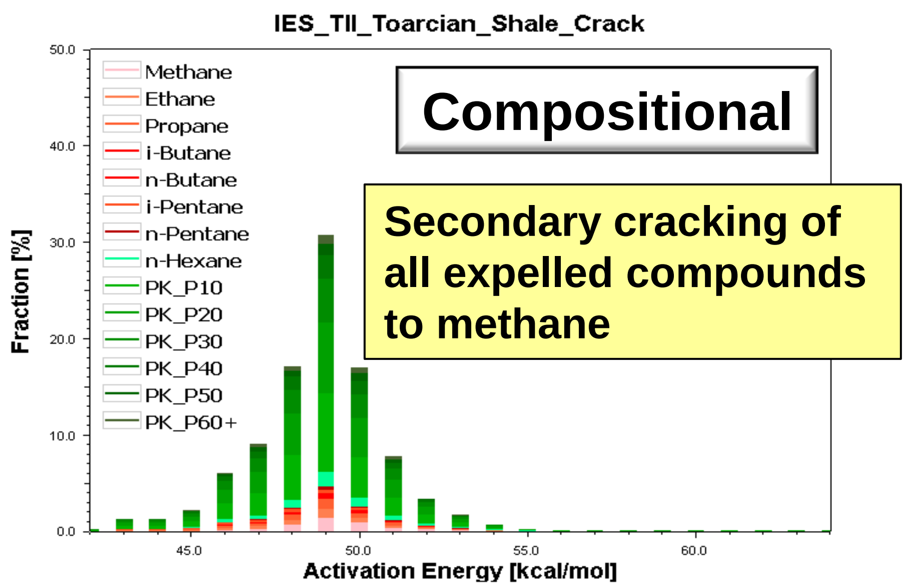
- SARA kinetics can be used to predict oil quality.
- Component cracking is controlled by a multi-stage reaction network.
- Components are lumped by physicochemical properties to optimize compute time.
- SARA model accounts for asphaltene flocculation, H_2S, and CO_2.



Early Kinetic Methods: Predict Quality of *Expelled* Petroleum

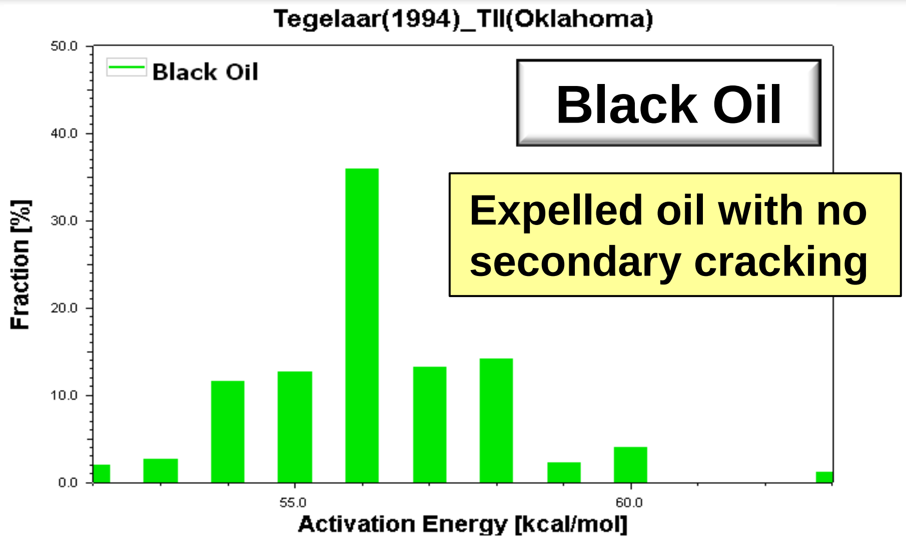


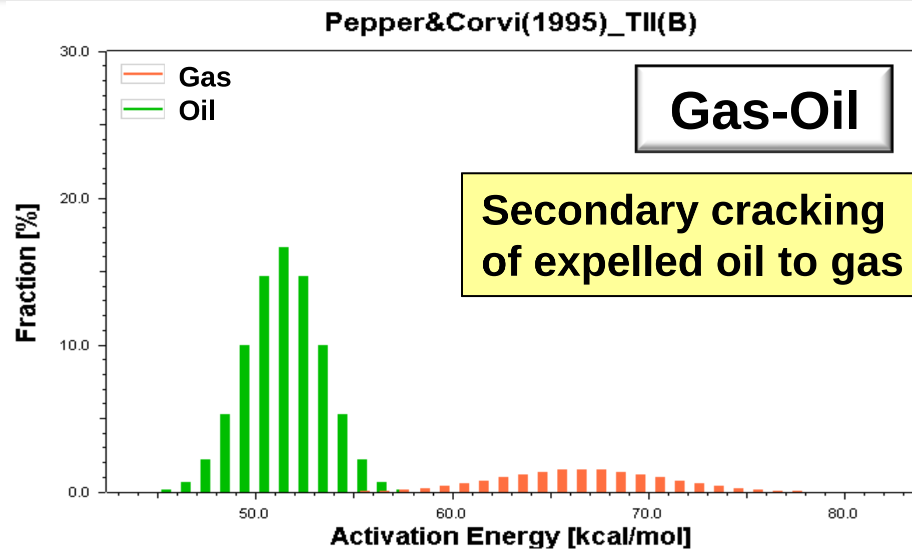


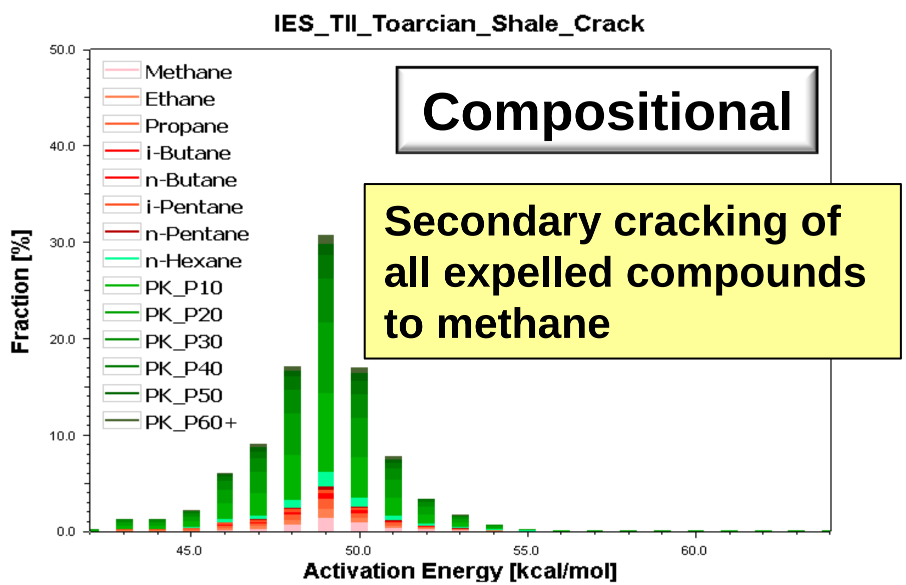


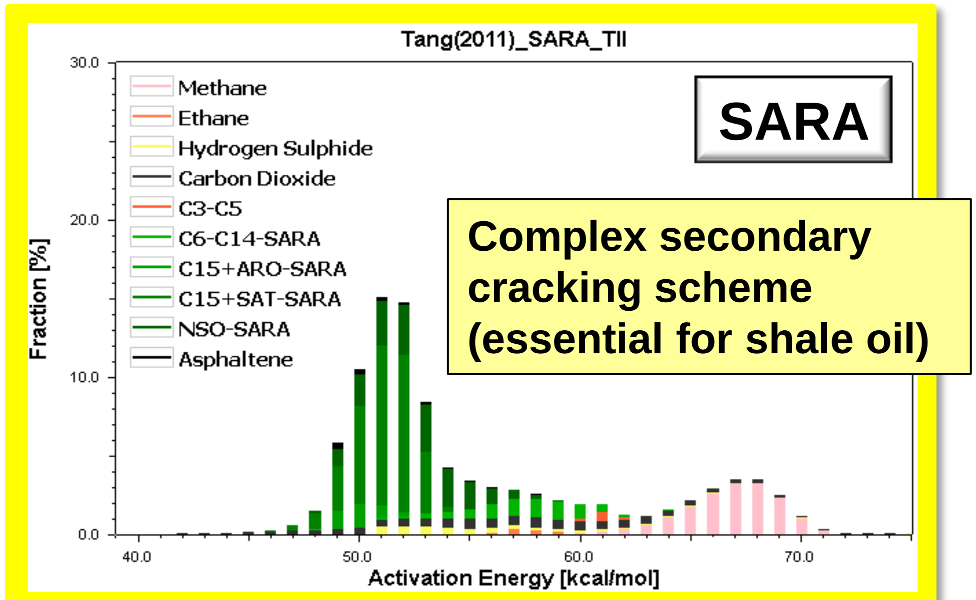
The goal of these methods is to predict the quality of *expelled* (conventional) oil. They do not predict properties of *retained* (unconventional) oil.

New Kinetic Methods: Properties of *Retained* Petroleum



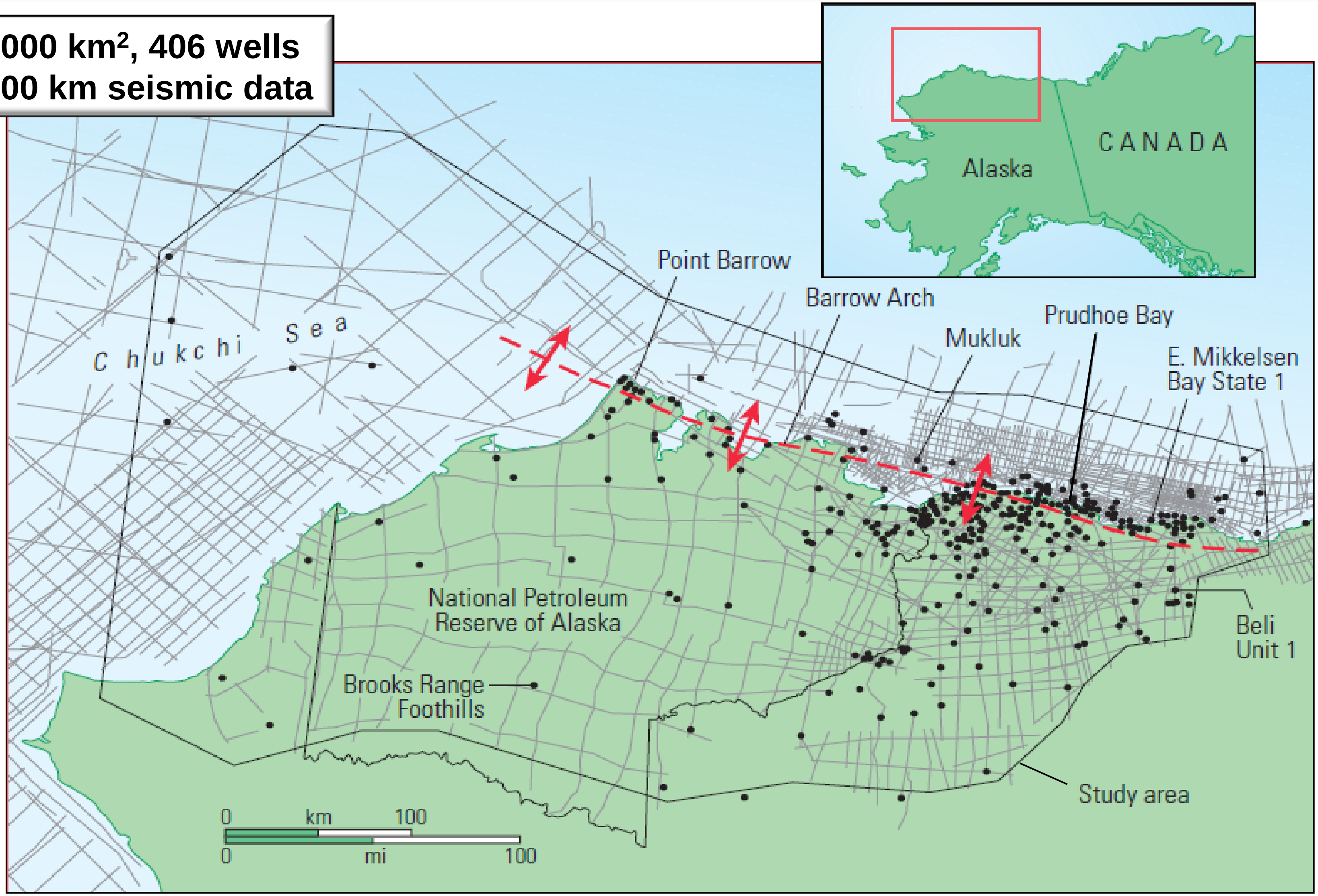






Alaska North Slope Study Illustrates SARA Modeling

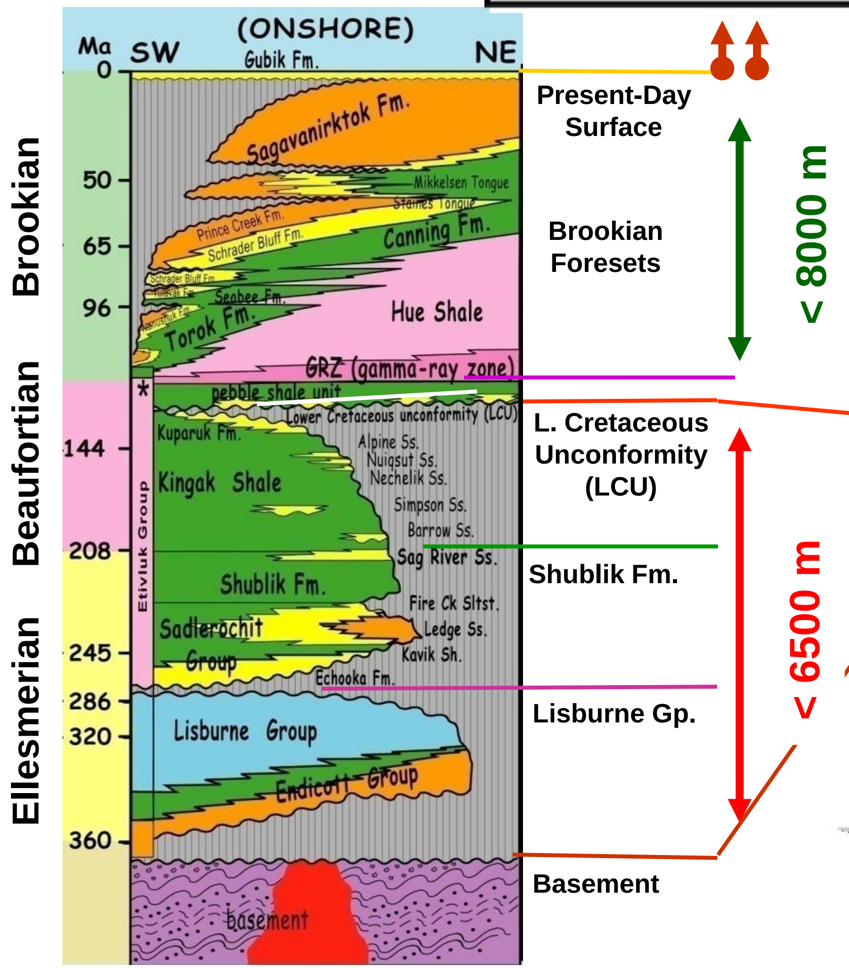
275,000 km^2, 406 wells
48,000 km seismic data



Schenk et al. (2012)

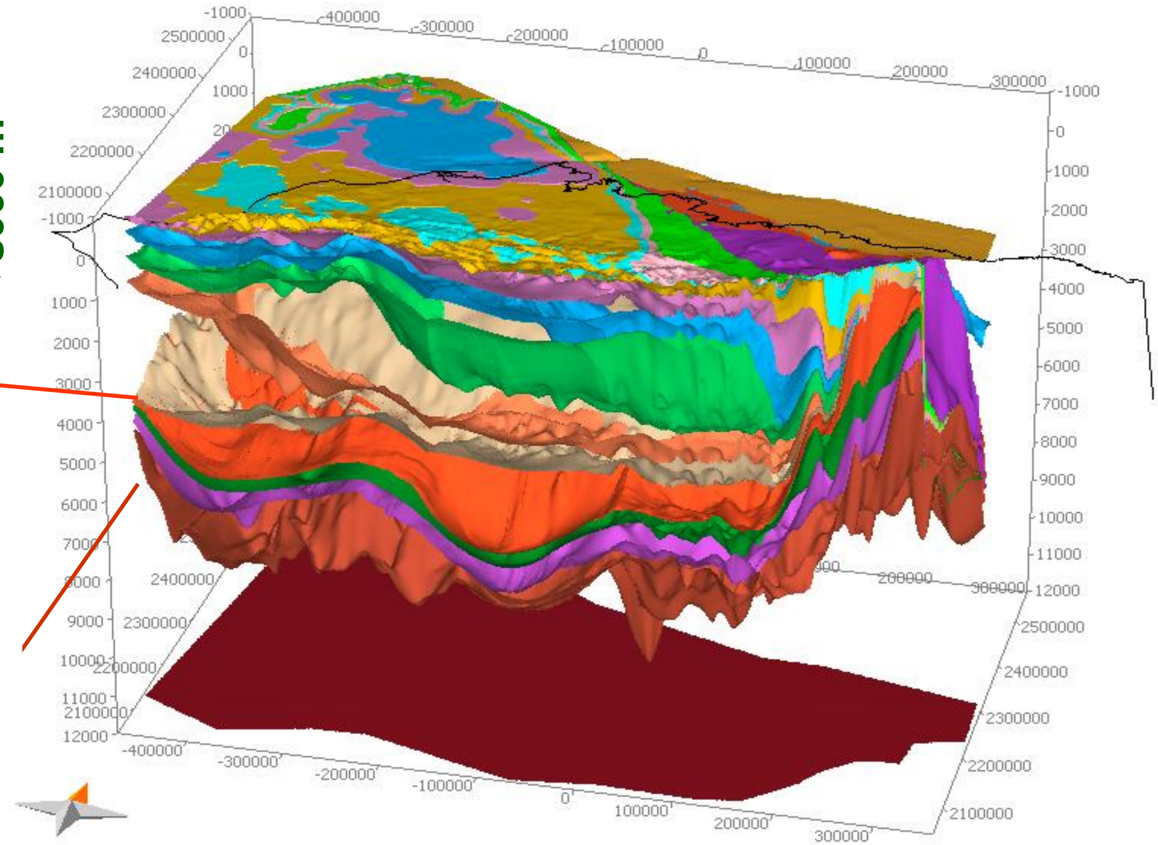
Model Includes Detailed Stratigraphy and Subsurface Maps

Erosion: < 5000 m



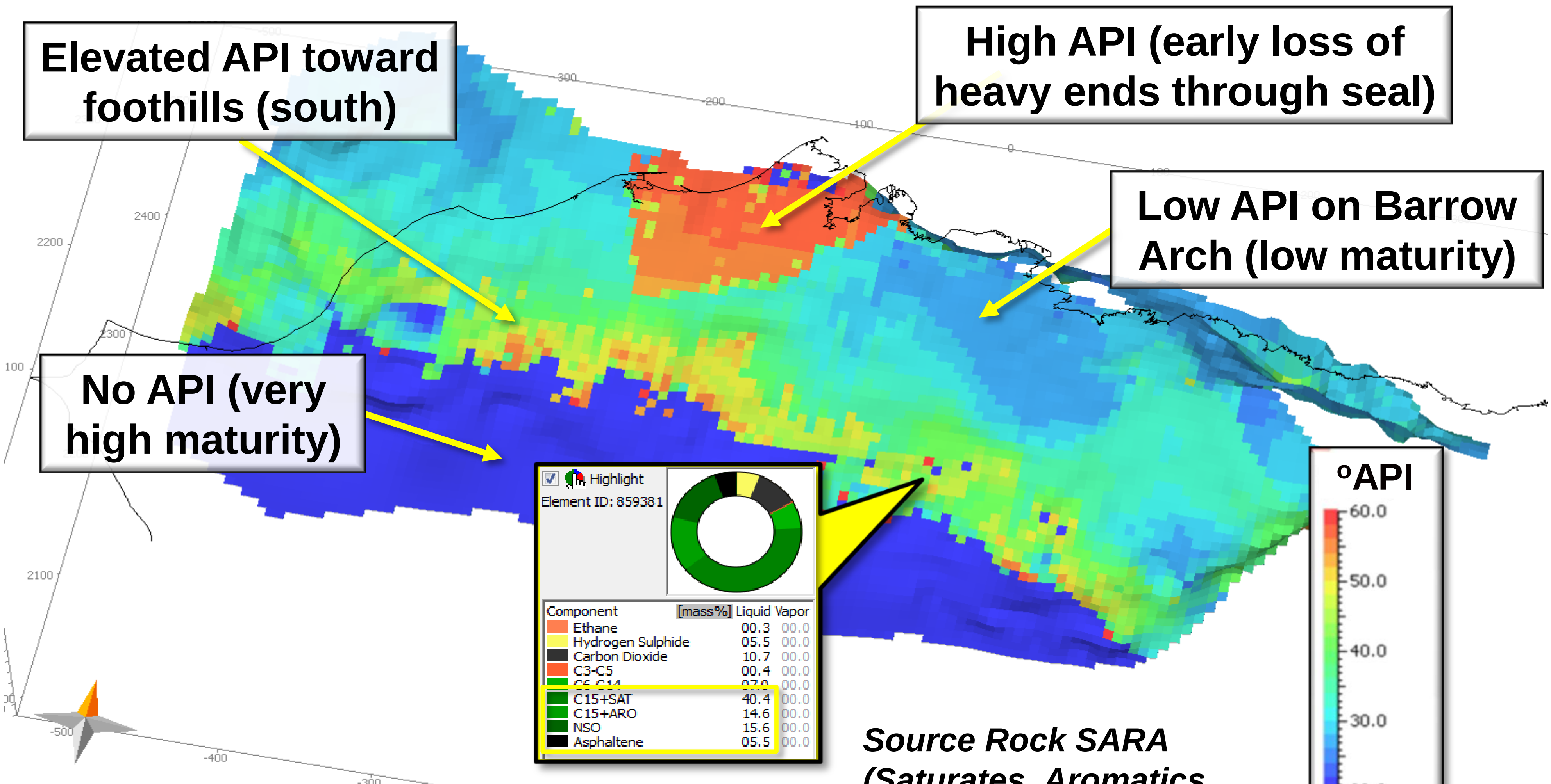
Houseknecht and Bird (2005)

Present-day Geometry



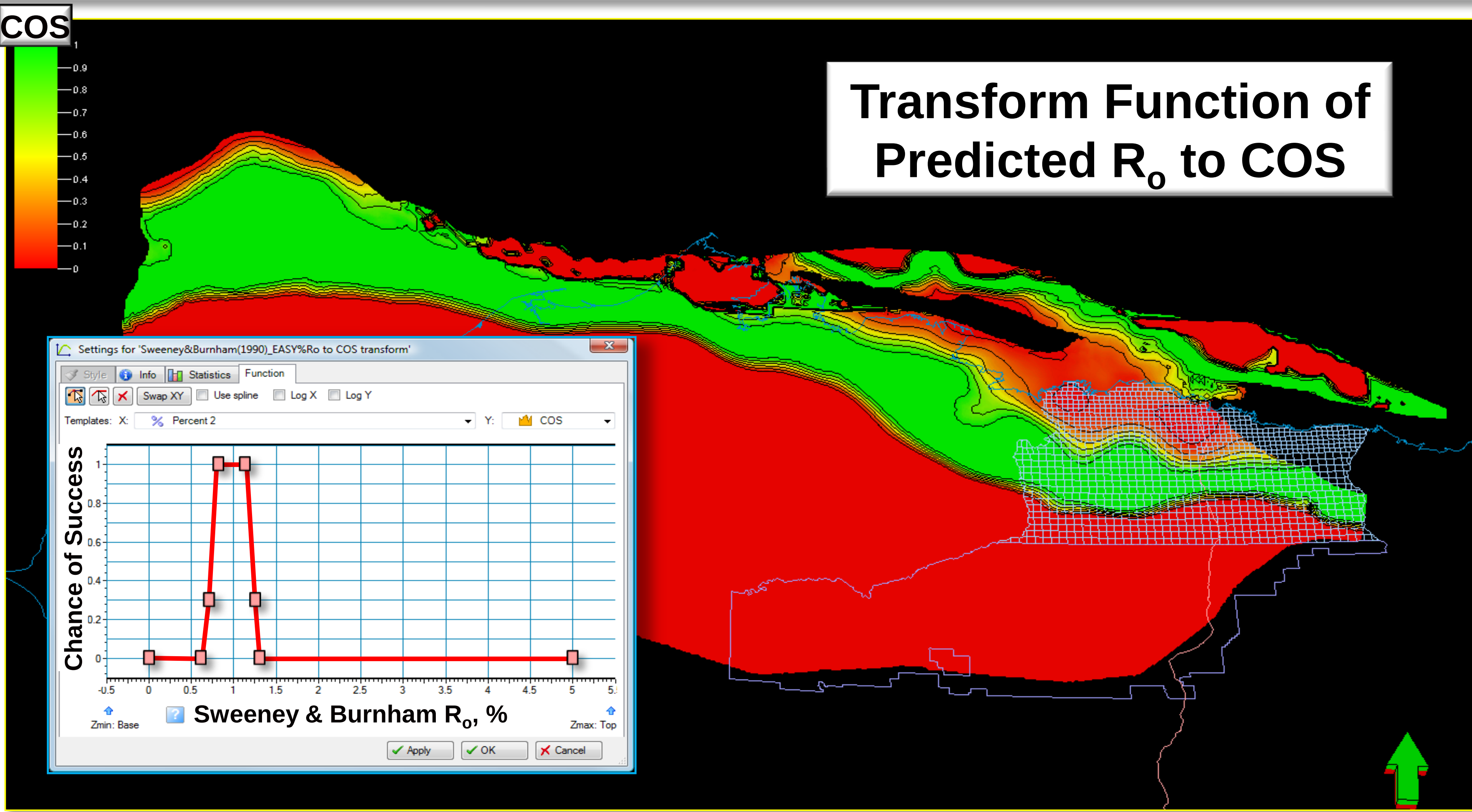
Schenk et al. (2012)

SARA Simulation: Properties of Oil *Retained* in Source Rock



Source Rock SARA (Saturates, Aromatics, Resins, Asphaltenes)

Play Chance Map: Maturation of Shublik Fm. from 3D Model

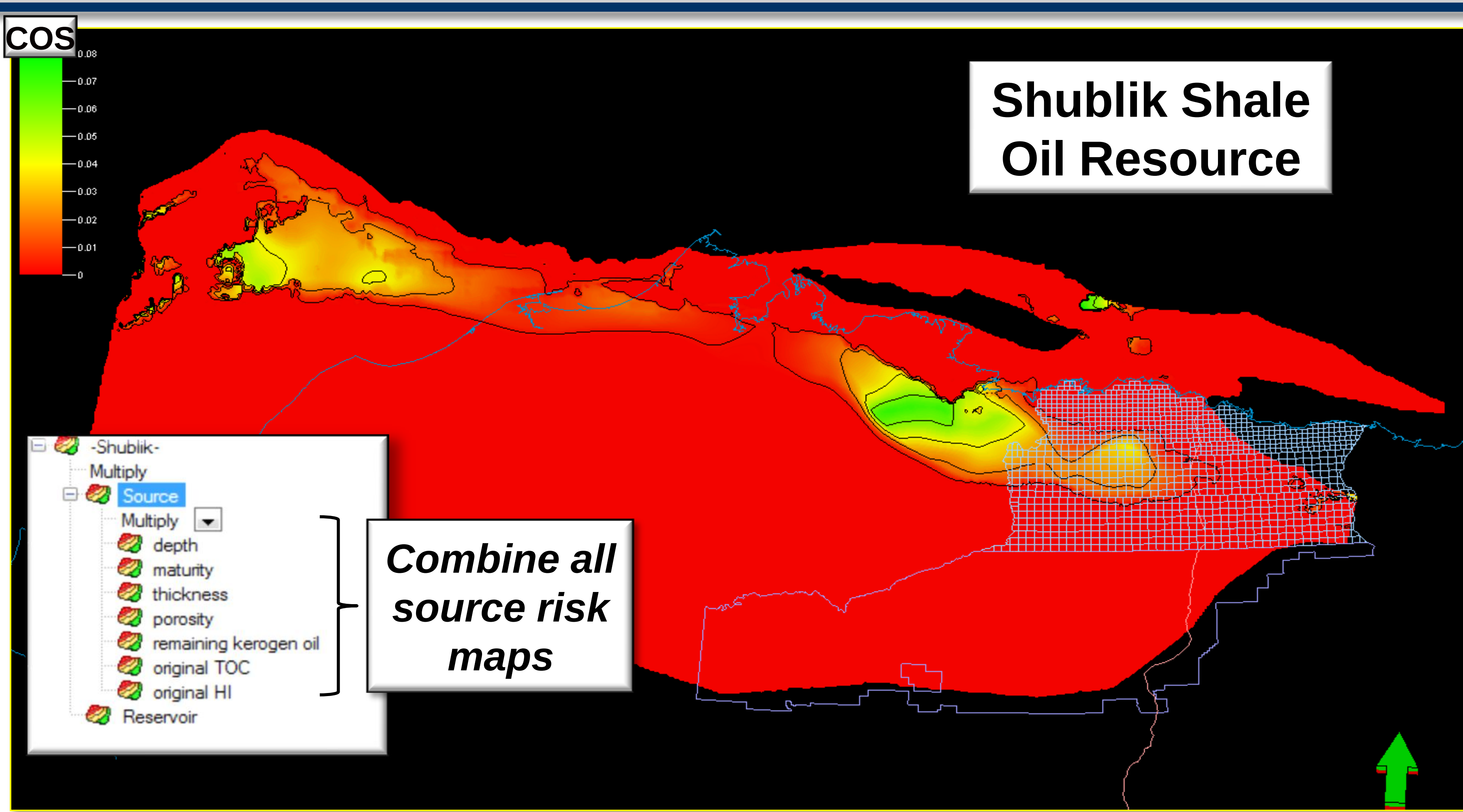


** COS = Chance of Success*

1 = good

0 = bad

Total Play Chance Map Combines Many Source Risk Maps



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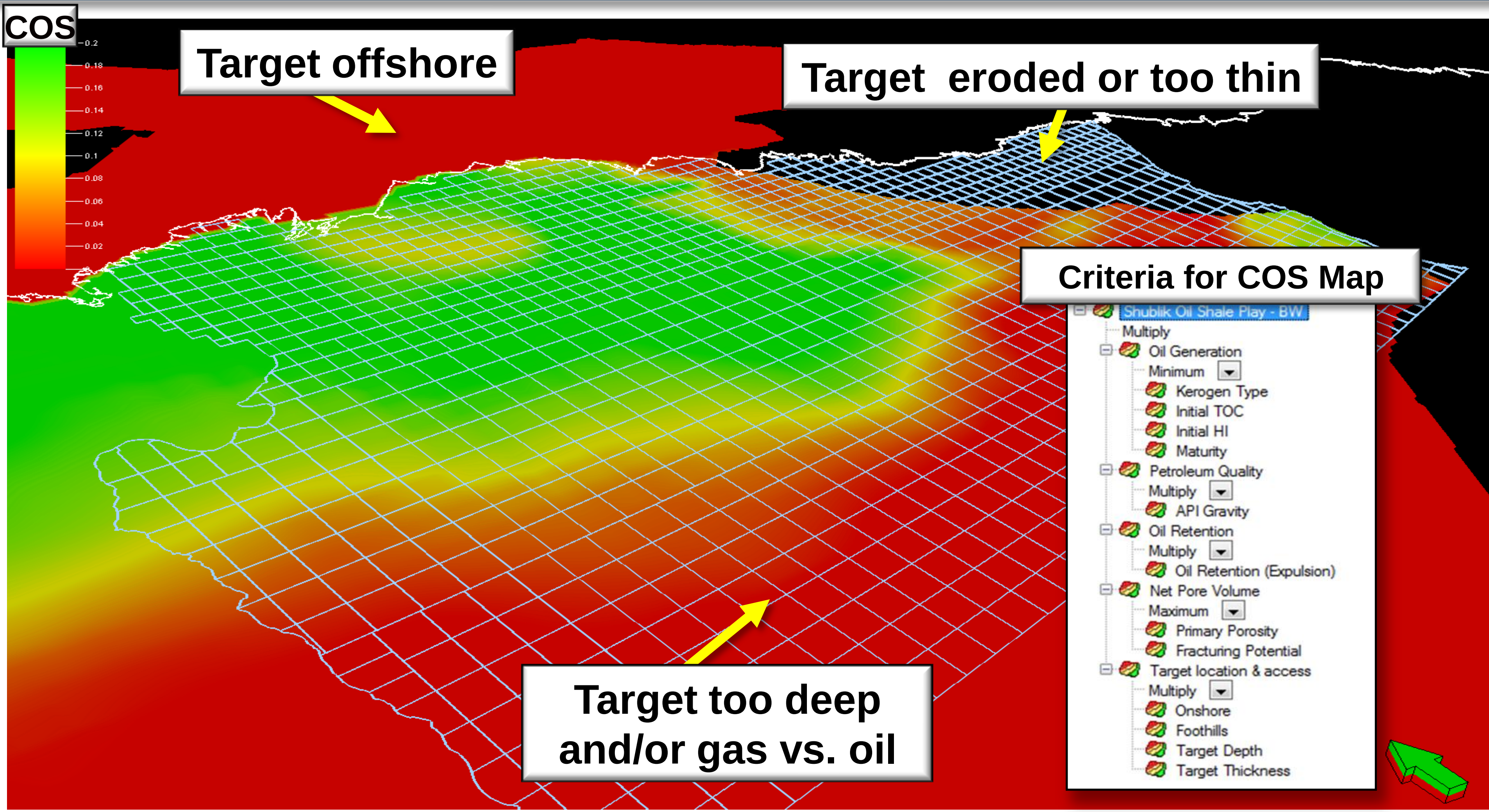
Focused Total Play Chance Map for Shublik Shale Oil



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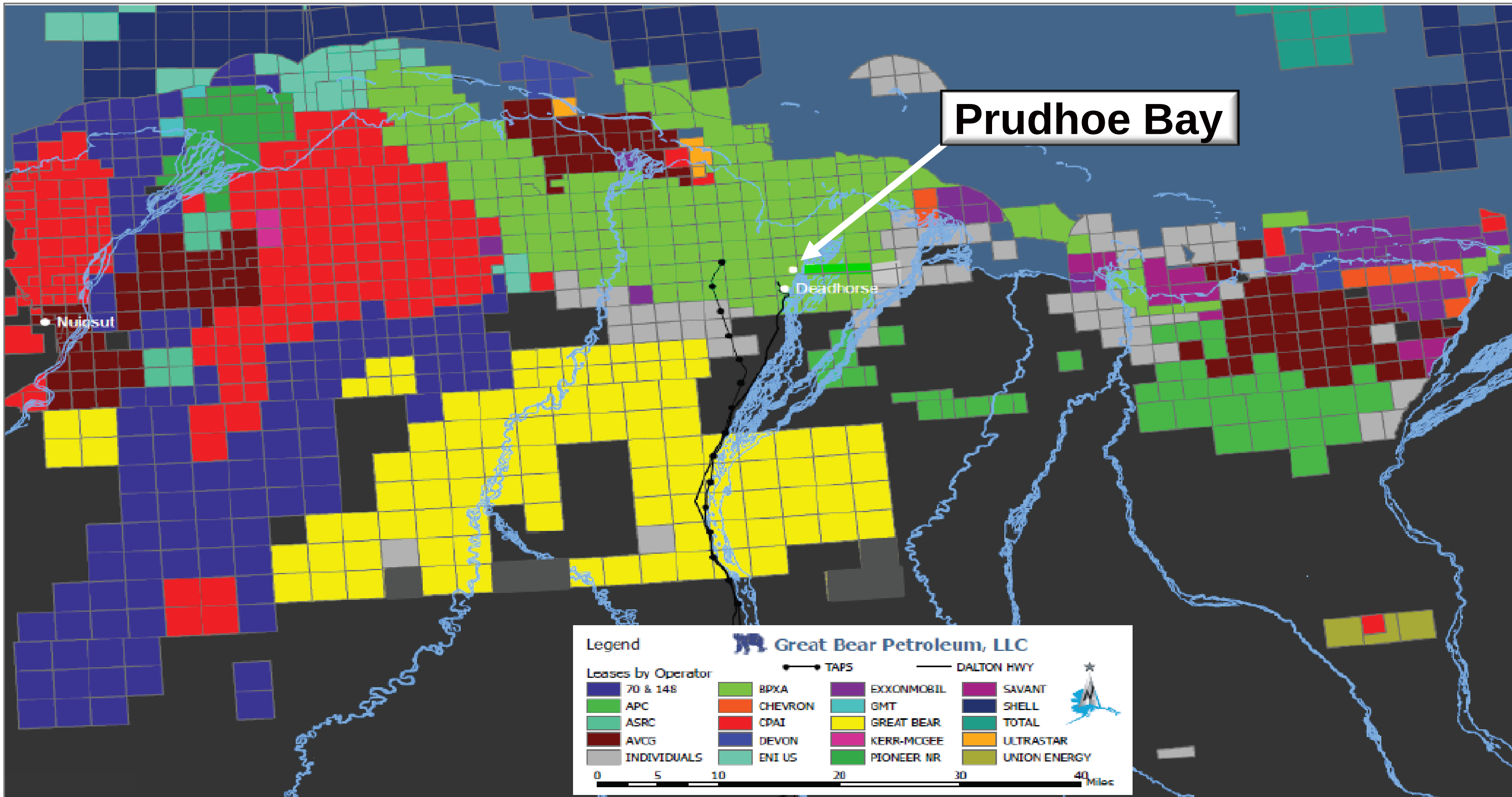
3D Model Identified Shublik Sweet Spots *Early*



Conclusions

- **Recent R&D has focused on new tools to more accurately model reservoir (e.g., TSR, biodegradation) and source rock (e.g., SARA) processes.**
- **Correlations between measured and predicted variables, e.g., API gravity or GOR, are generally good, but exact predictions are not expected due to input uncertainties.**
- **The principal goal of current TSR, biodegradation, and SARA models is to predict regional trends.**
- **More R&D and careful parameter calibration will lead to more accurate results.**

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