

APPLICATIONS OF PETROLEUM SYSTEMS MODELING IN CCUS

2017 CO₂ for EOR as CCUS Conference: Houston, TX

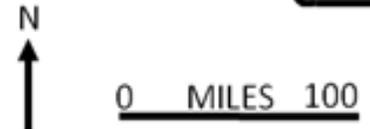
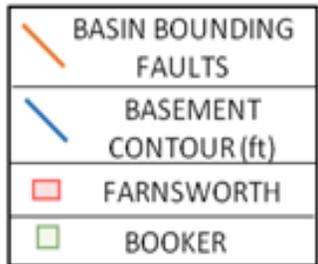
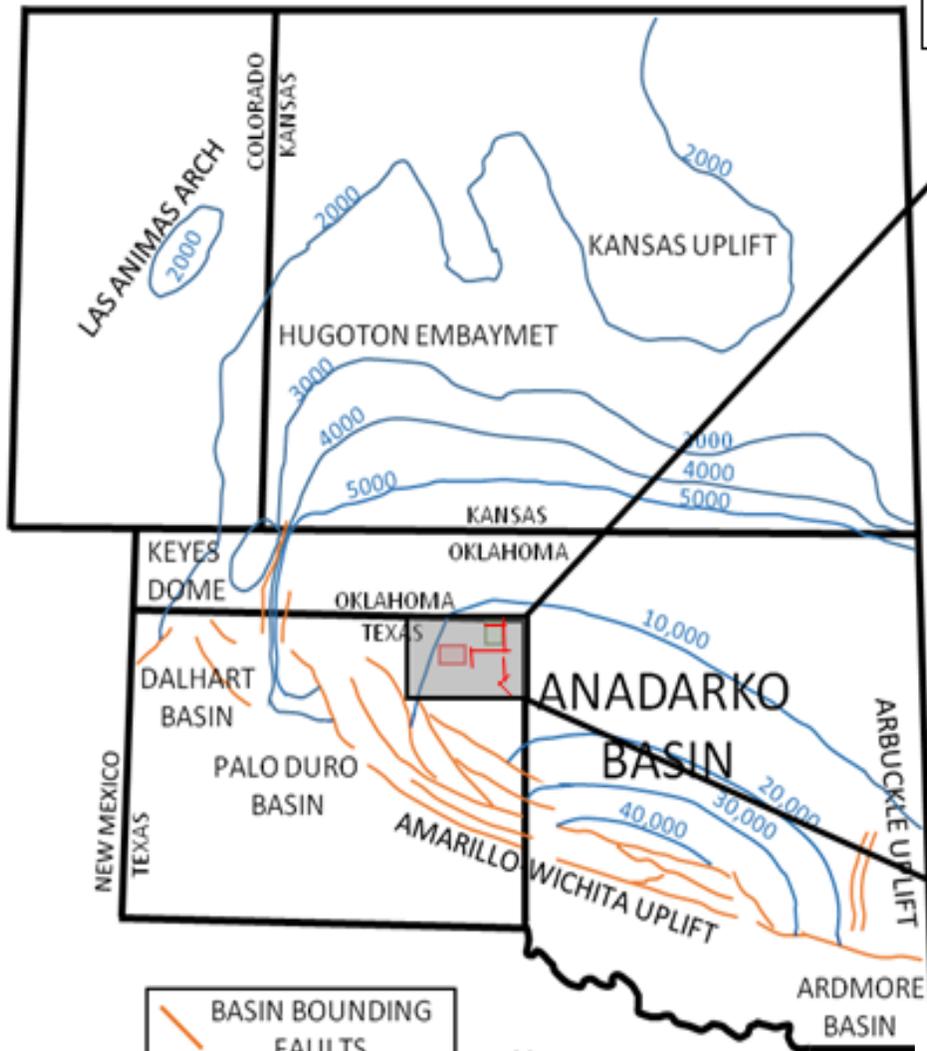
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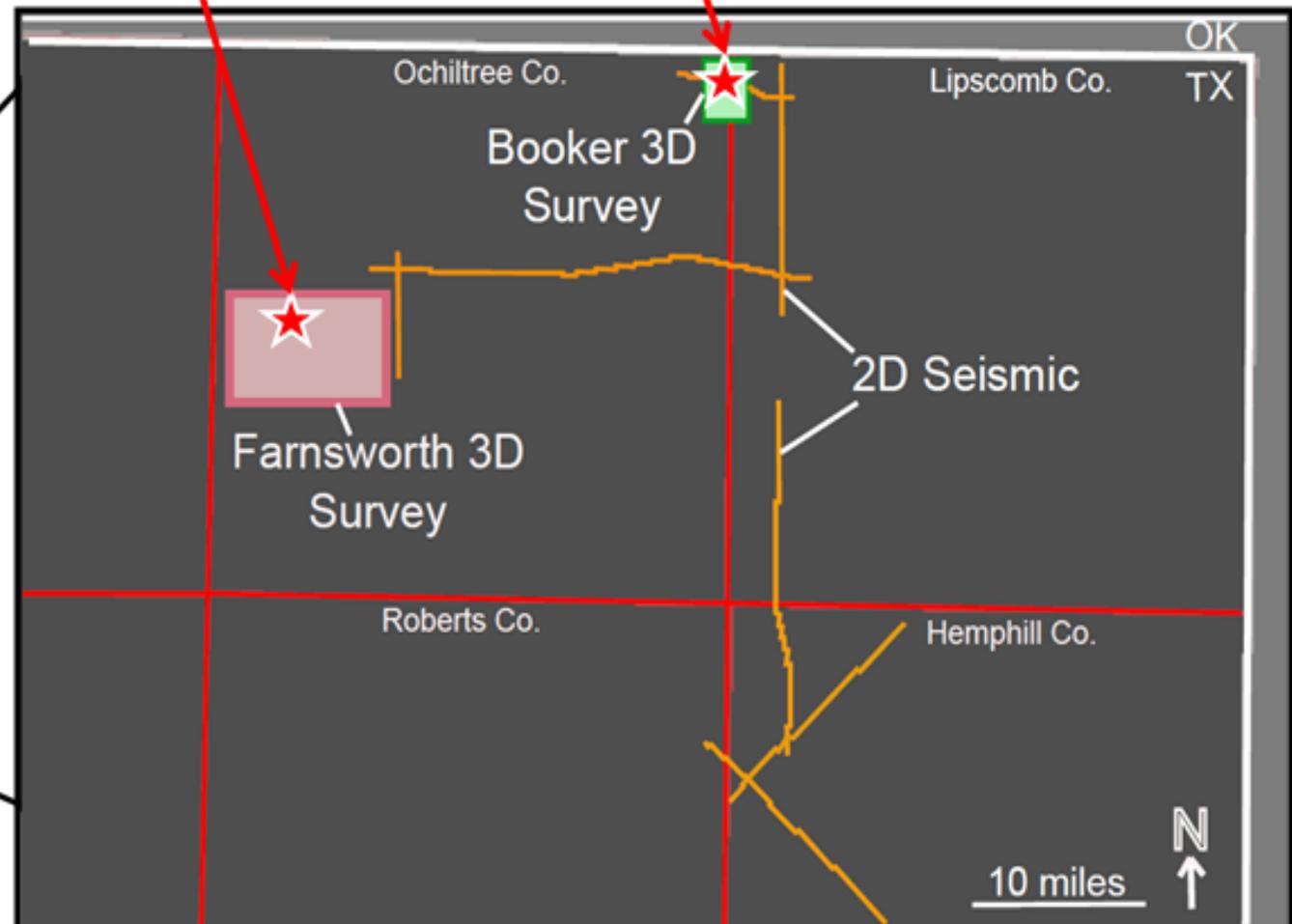
RESEARCH QUESTIONS

- Can we use petroleum system characterization models to help assess current and future carbon storage sites?
- What are the regional scale geologic risks to CO₂ migration?
- What does the NE Texas Morrowan Petroleum system look like and what are the implications for carbon storage: portability of results?



13-10A, 1D Model

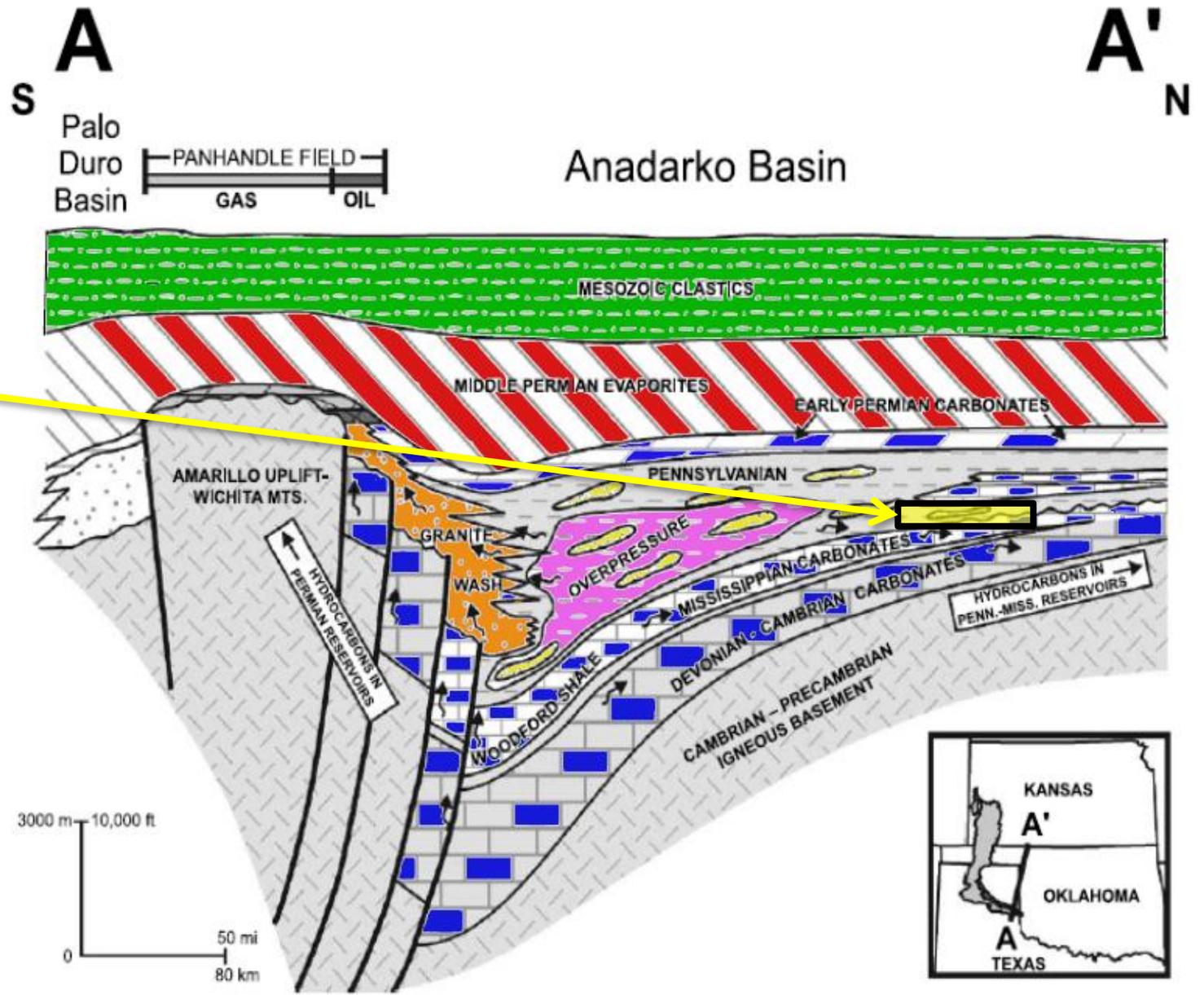
Killingsworth, 1D Model



2D seismic lines

REGIONAL STRATIGRAPHY

Approximate location of study interval (Morrow Sandstone)



modified from Sorenson (2005)

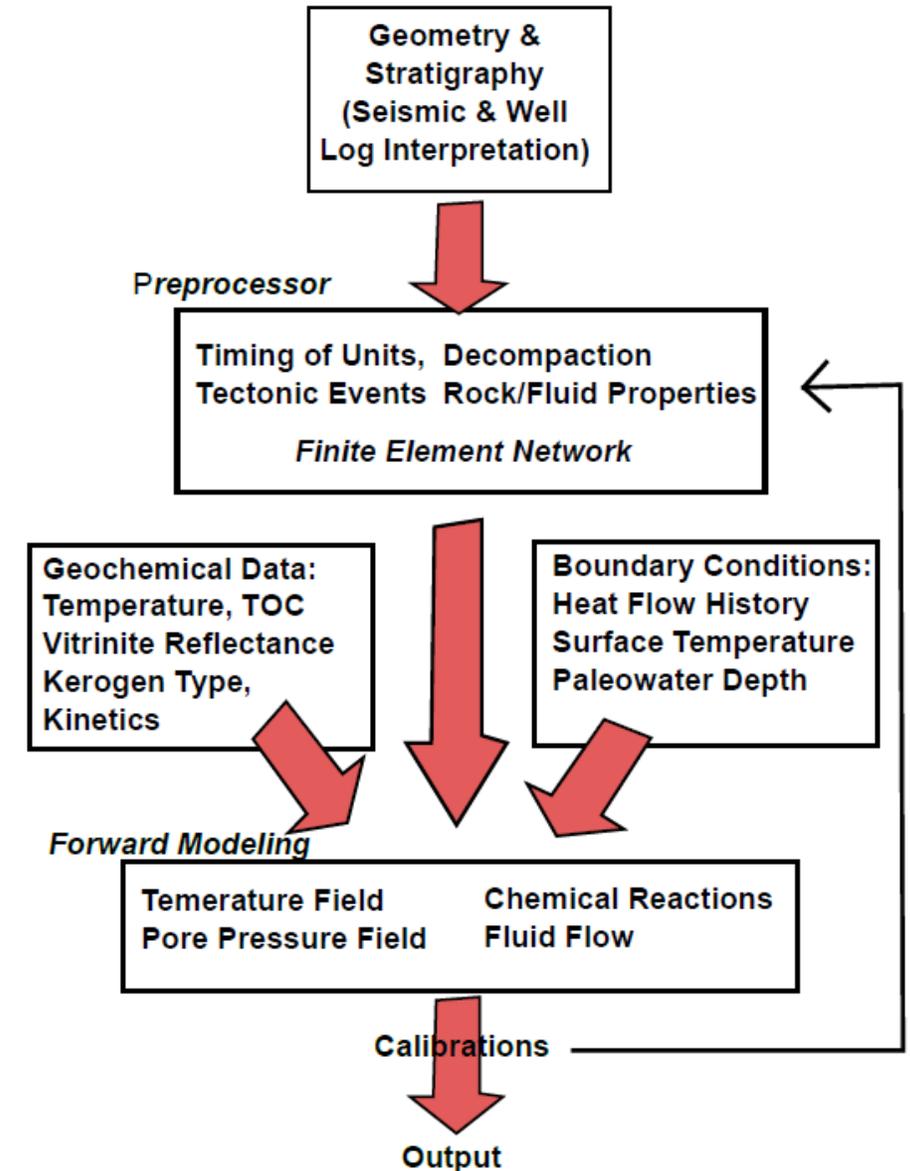
BASICS OF PETROLEUM SYSTEM MODELING (PSM)

- Burial history: **Compaction Modeling**
- Thermal history: **Heat Flow Modeling**
- Maturation history: **Geochemical Kinetic Modeling**
- Hydrocarbon migration: **Flow Modeling**

Purpose of PSM:

Reconstruct the physical/chemical processes that occur in sedimentary basins over geologic time

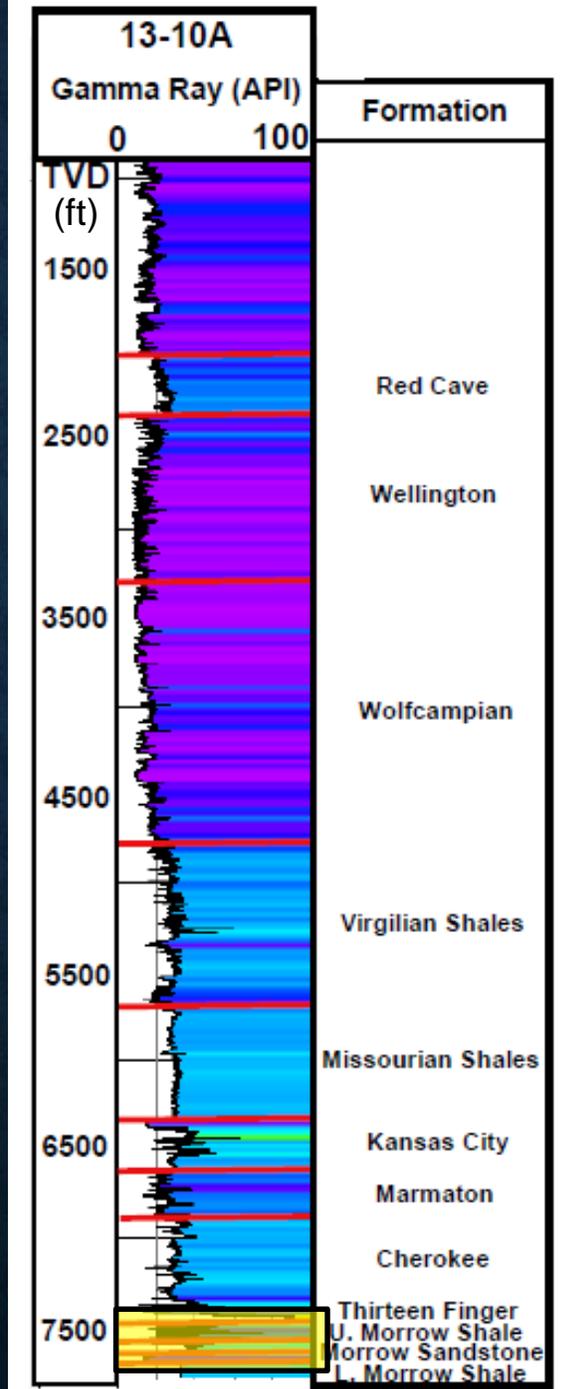
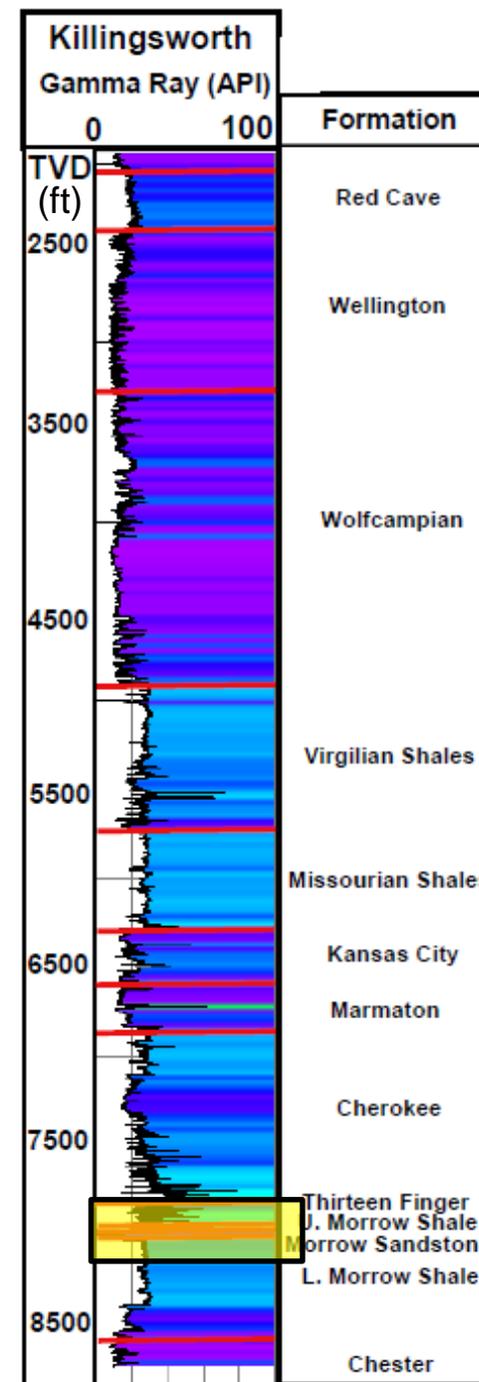
PSM WORKFLOW



Modified from (Peters, K.E., 2009)

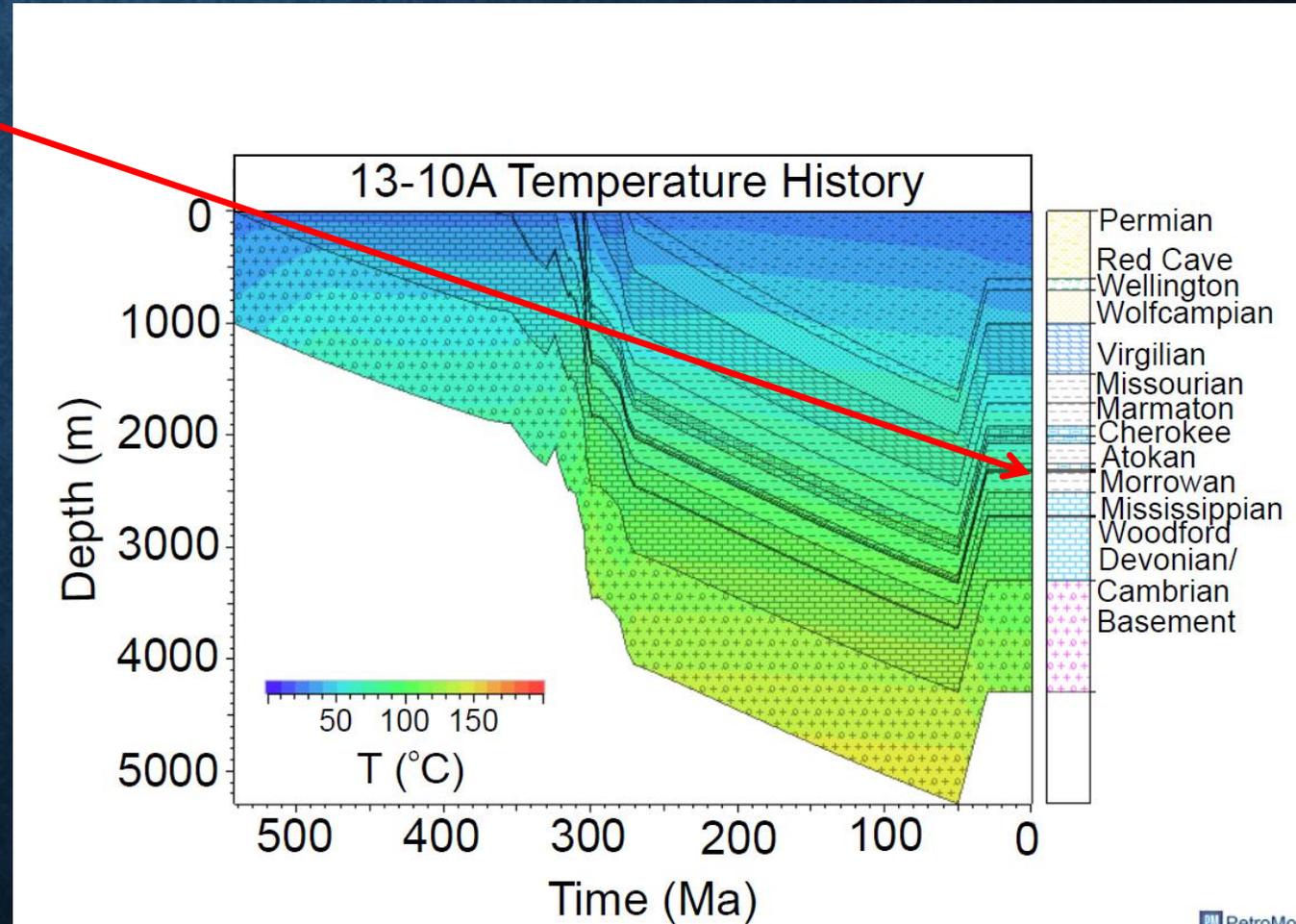
MODEL CONSTRAINTS

- Formation picks produce geometries, core and well data provide lithology
- Seismic data used to pick layers below well data, and construct 2D models
- Core data provide vitrinite reflectance (Rock-Eval), sealing properties, kerogen types, TOC



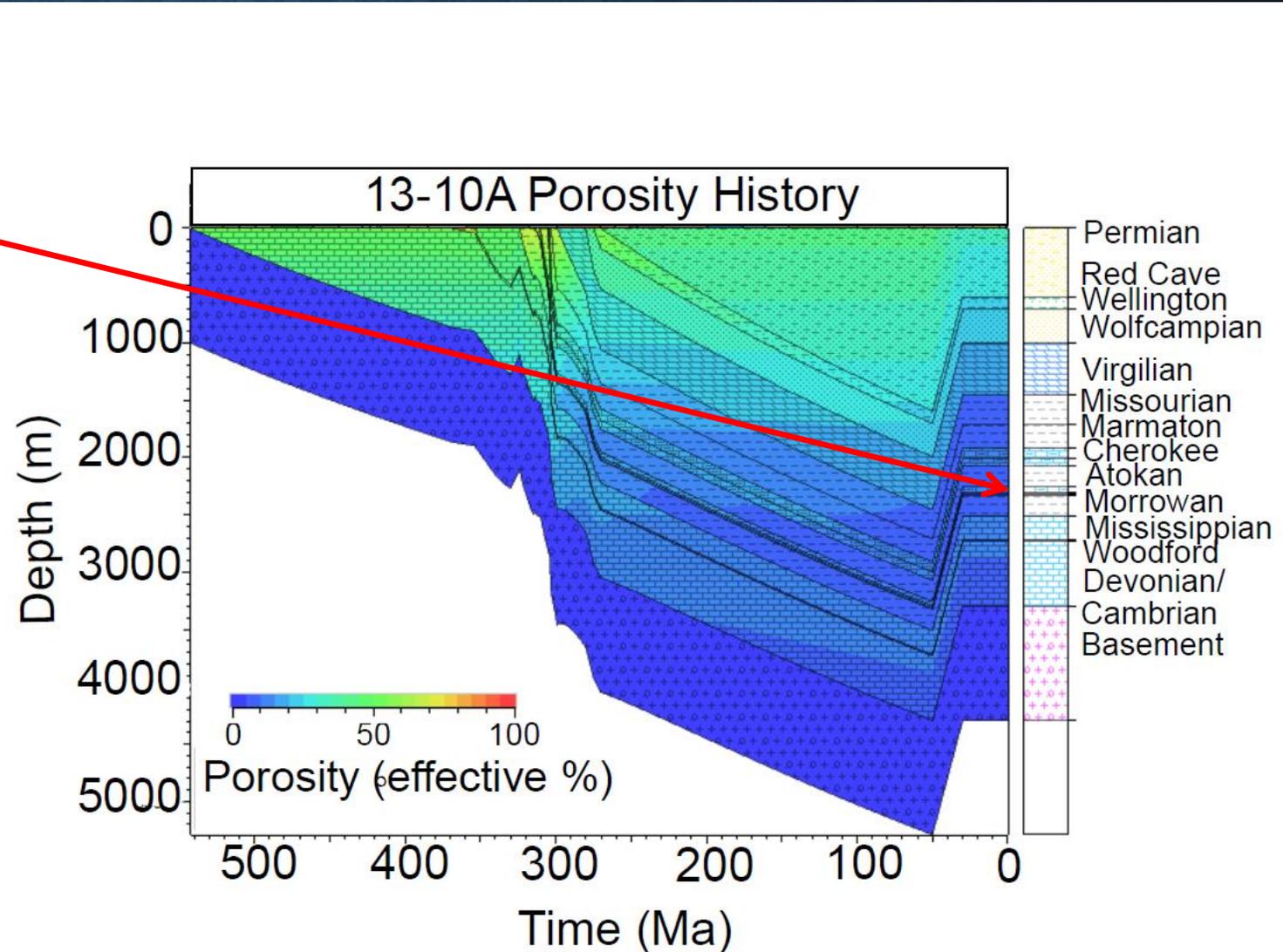
WELL 13-10A RESULTS: BURIAL / TEMPERATURE HISTORY

- Predicted Morrowan reservoir temperature of 165 °F
- Original measured temperature 168 °F (Hinds, 1956)
- Current measured temperature ~160 °F (2015)



WELL 13-10A RESULTS: POROSITY DEVELOPMENT

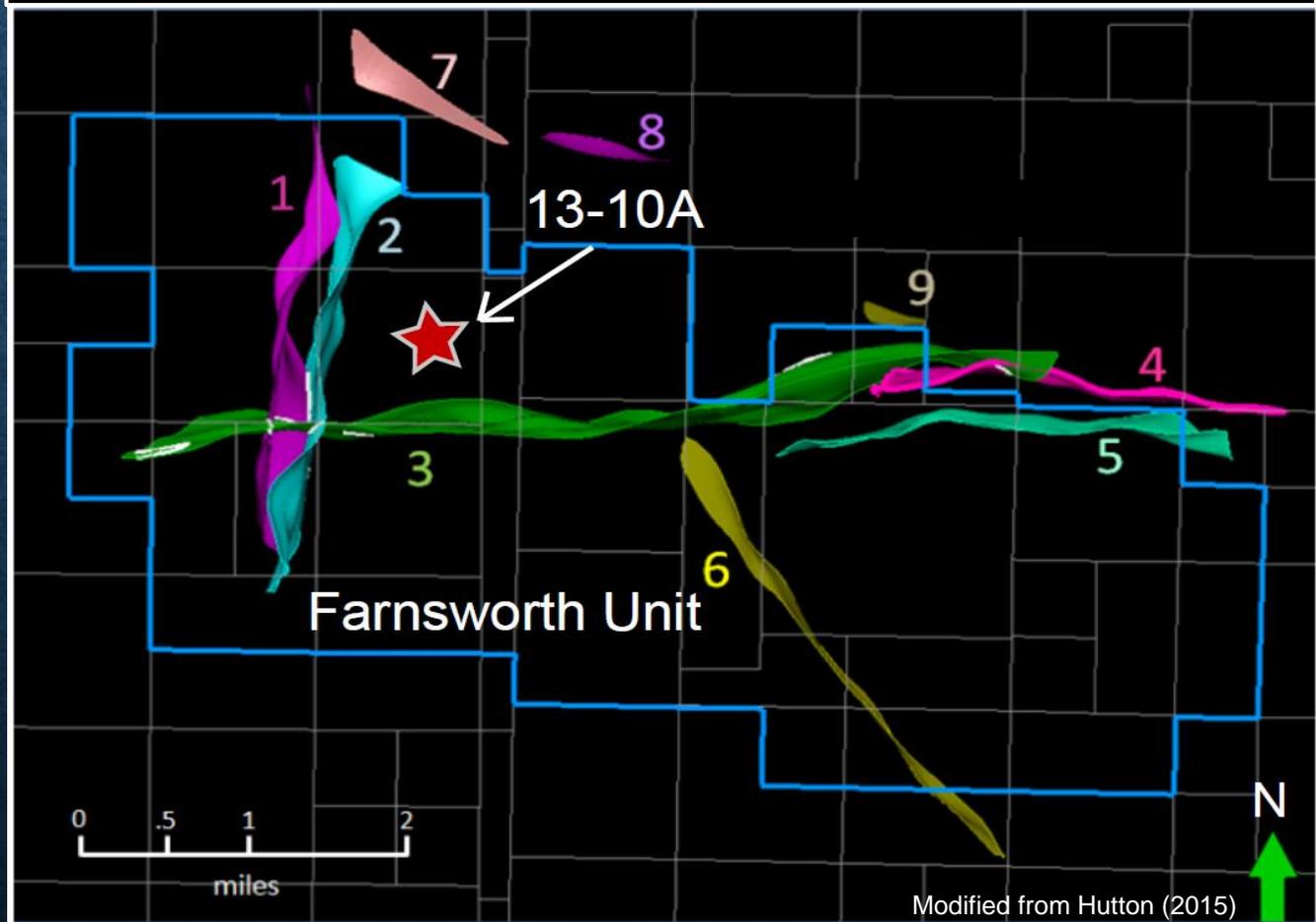
- Present predicted Morrowan sandstone (effective) porosity of 15.5%
- Actual mean measured 14.53% (Munson, 1988)
- Porosity development of Morrowan: rapid decrease during early burial



FIELD SCALE APPLICATION

- Burial history allows tracking of reservoir depth and faults through time
- May help to quantify fault transmissibility

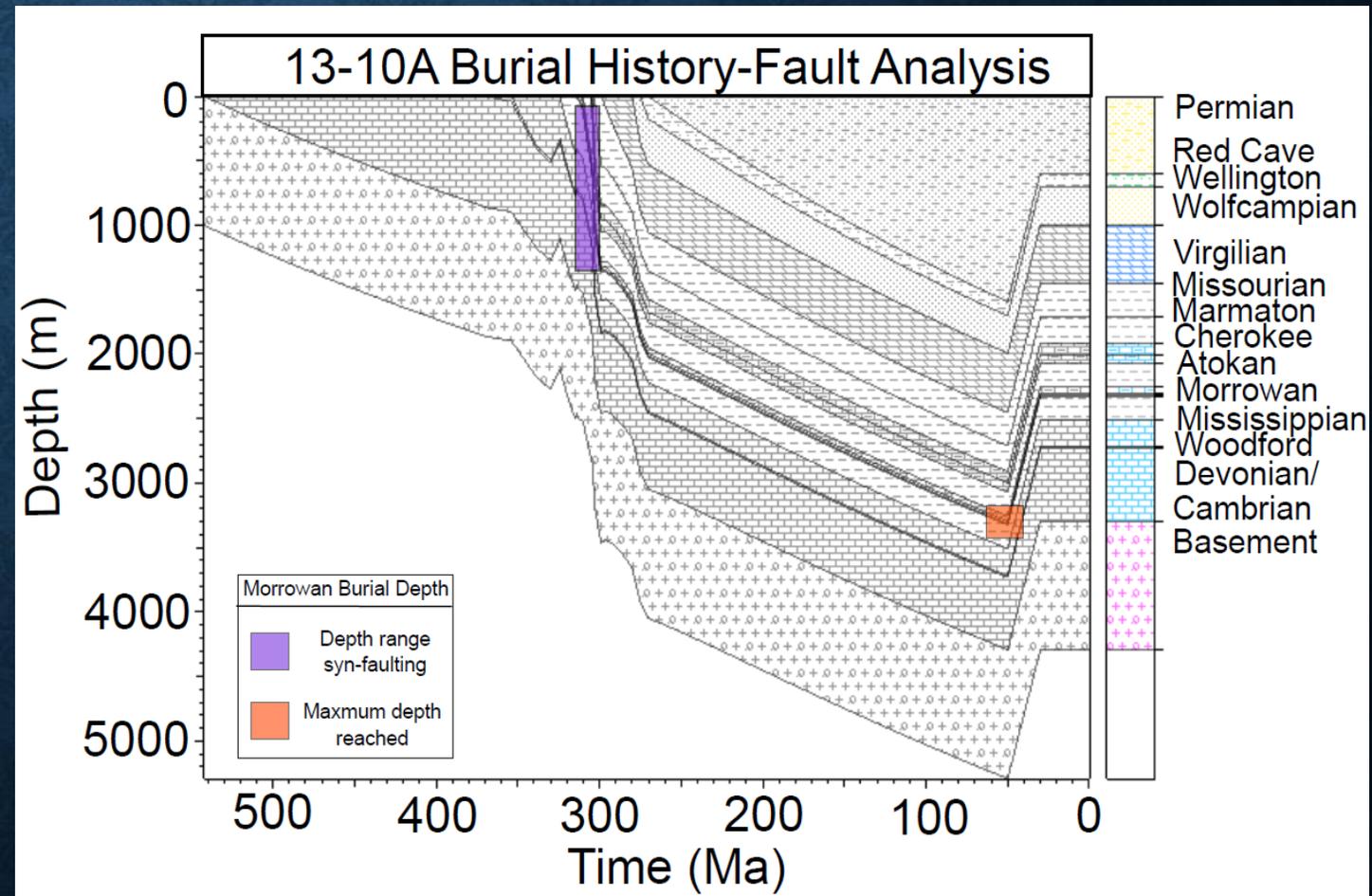
Field area, polygons are potential faults



Modified from Hutton (2015)

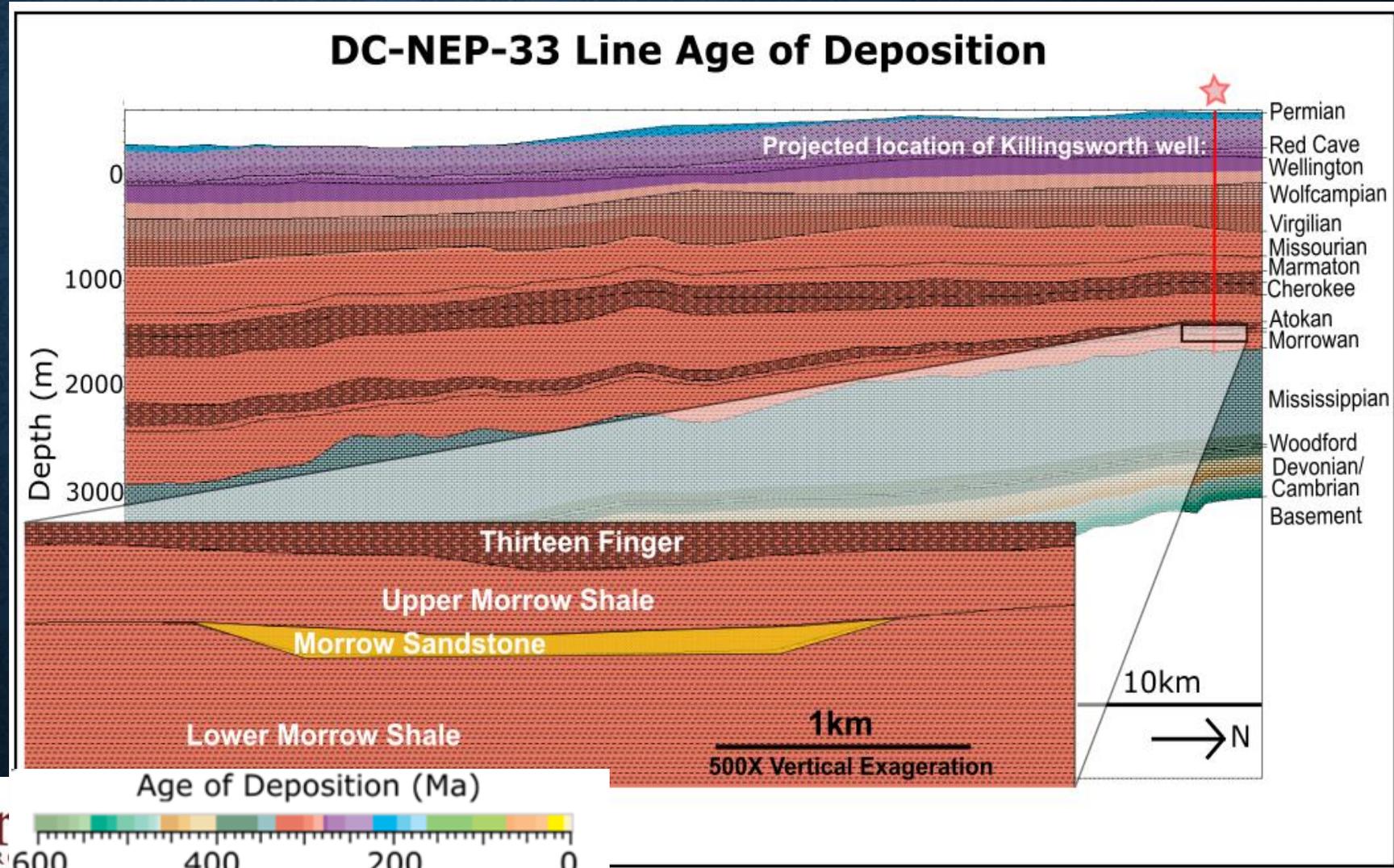
BURIAL HISTORY: AN AID TO FAULT ANALYSIS

- Sperrevik et al. (2002) fault transmissibility model
- Empirical relationships of transmissibility can be derived from burial history parameters plus shale-gouge ratio, throw and fault zone thickness
- These values are used as a proxy for compaction level, clay content, and deformation style



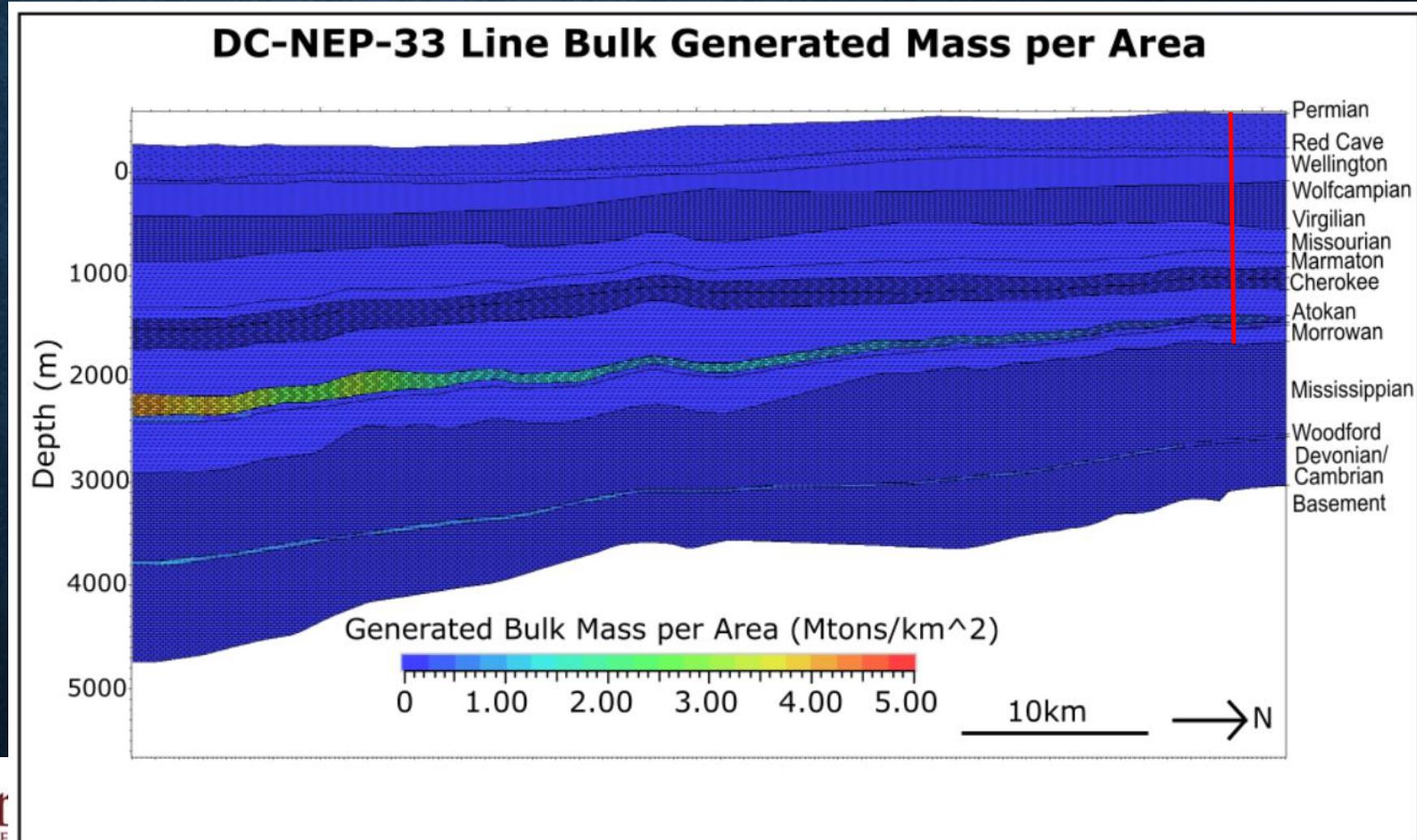
2D MODEL BURIAL HISTORY

- Period of maximum subsidence (~330Ma-280Ma)
- Represents section through Booker Field Morrowan reservoir



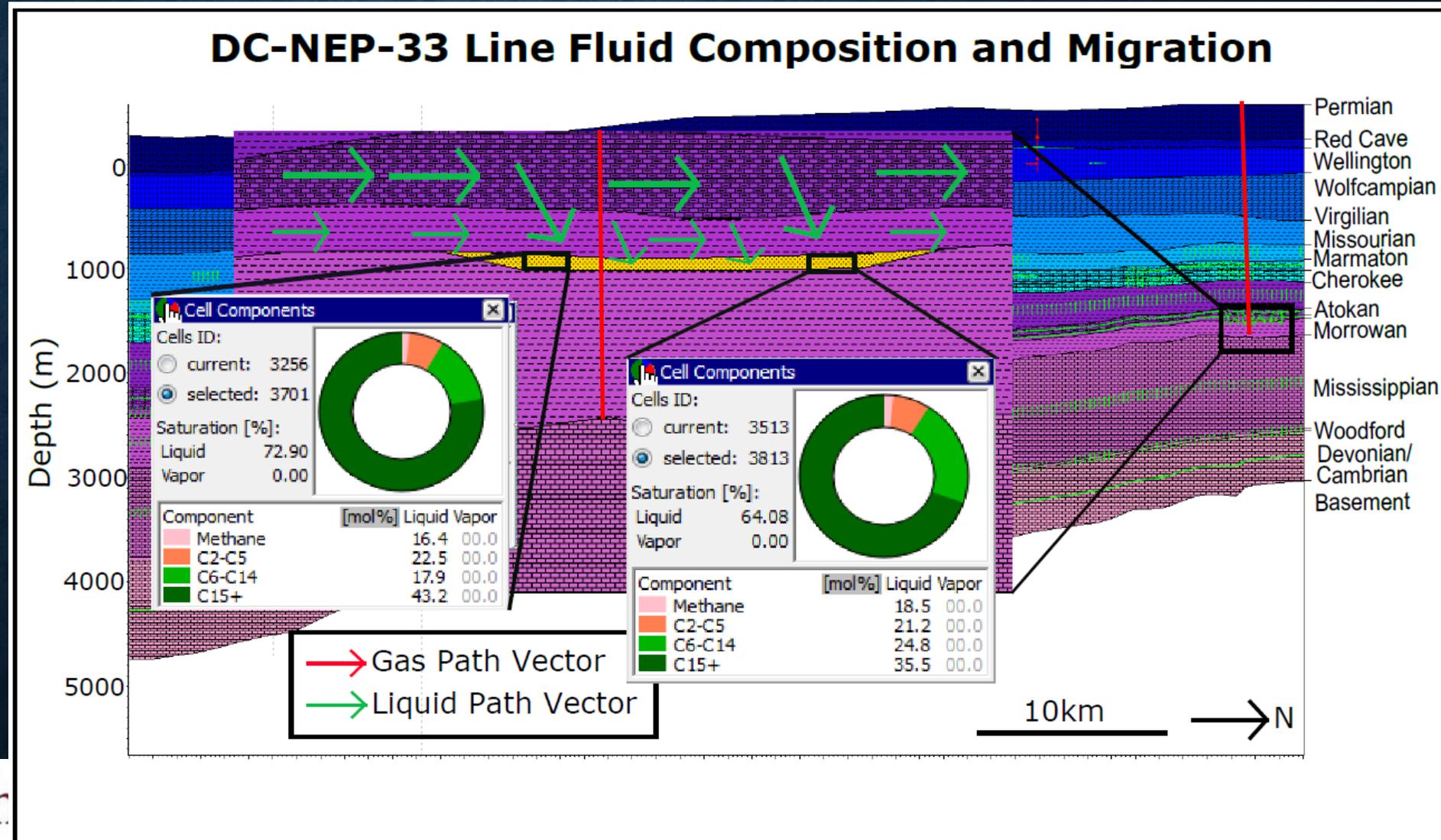
GENERATED MASS PER AREA (MTON/KM²)

- Deduce probable source locations, units & volumetrics
- Most hydrocarbons migrate from the deeper basin



Compositional Results

- Hydrocarbons migrate from the deep basin and charge reservoir
- Some inter-reservoir compositional variability
- Fluid properties are important to storage and field performance predictions



CONCLUSIONS

- 1st order capacity estimation tool for future carbon storage sites, especially when data limited (porosity, temperature, oil composition etc.)
- Informs subsurface fault transmissibility models
- Regional geologic CO₂ plume migration risk is NW-N and appears low
- NE Texas panhandle Morrowan hydrocarbons: Sourced from deeper basin, dominantly Thirteen Finger and upper Morrowan black shales
- Compositional predictions help inform decision makers about potential field response to CO₂-EOR

THANK YOU!

Comments and questions are welcome...



ACKNOWLEDGMENTS

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- Dylan Rose-Coss
- William Ampomah
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- Franciszka Stopa
- Lindsey Rasmussen
- Family & Friends
- REACT/SWP TEAM

Disclaimer:

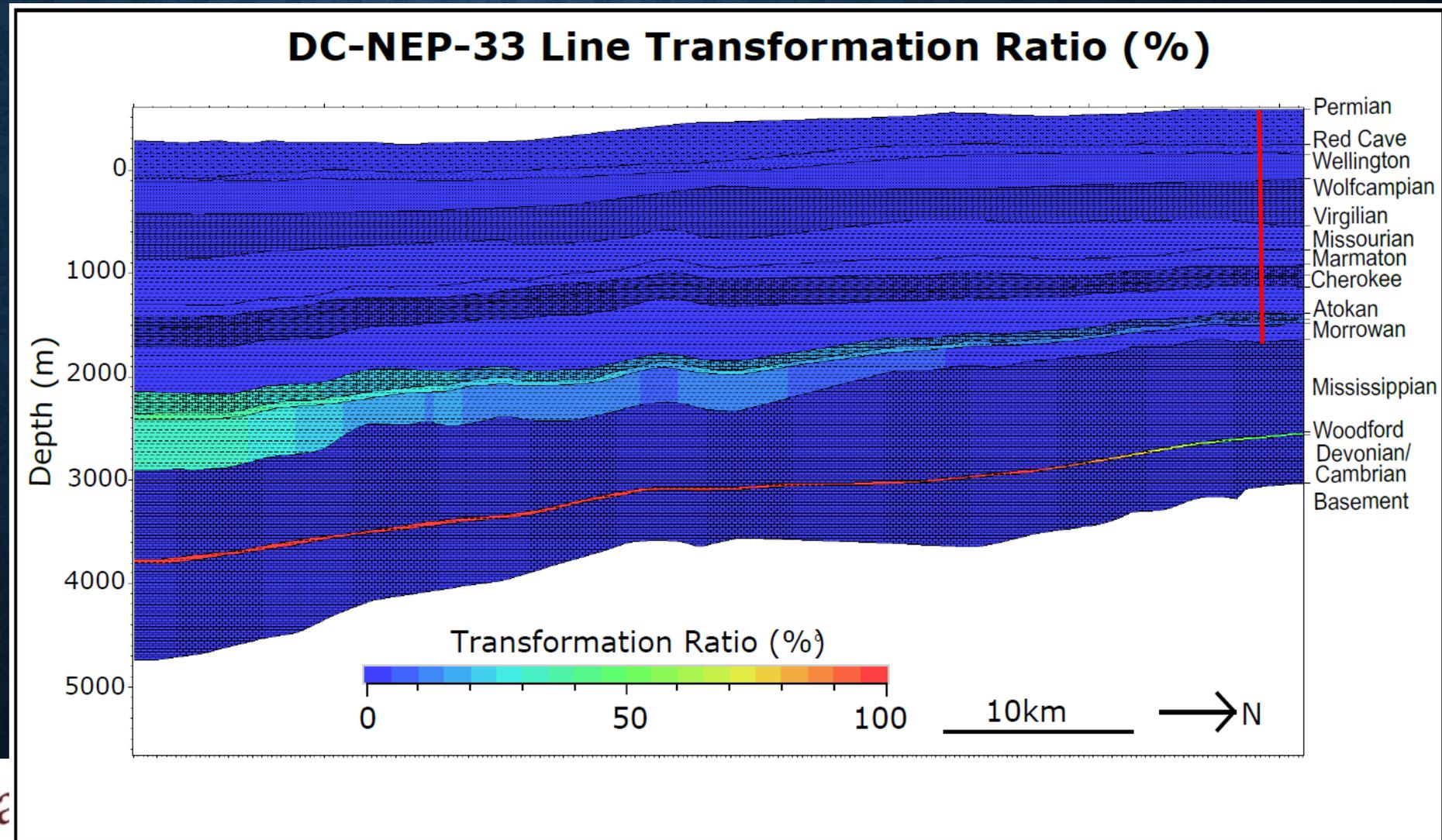
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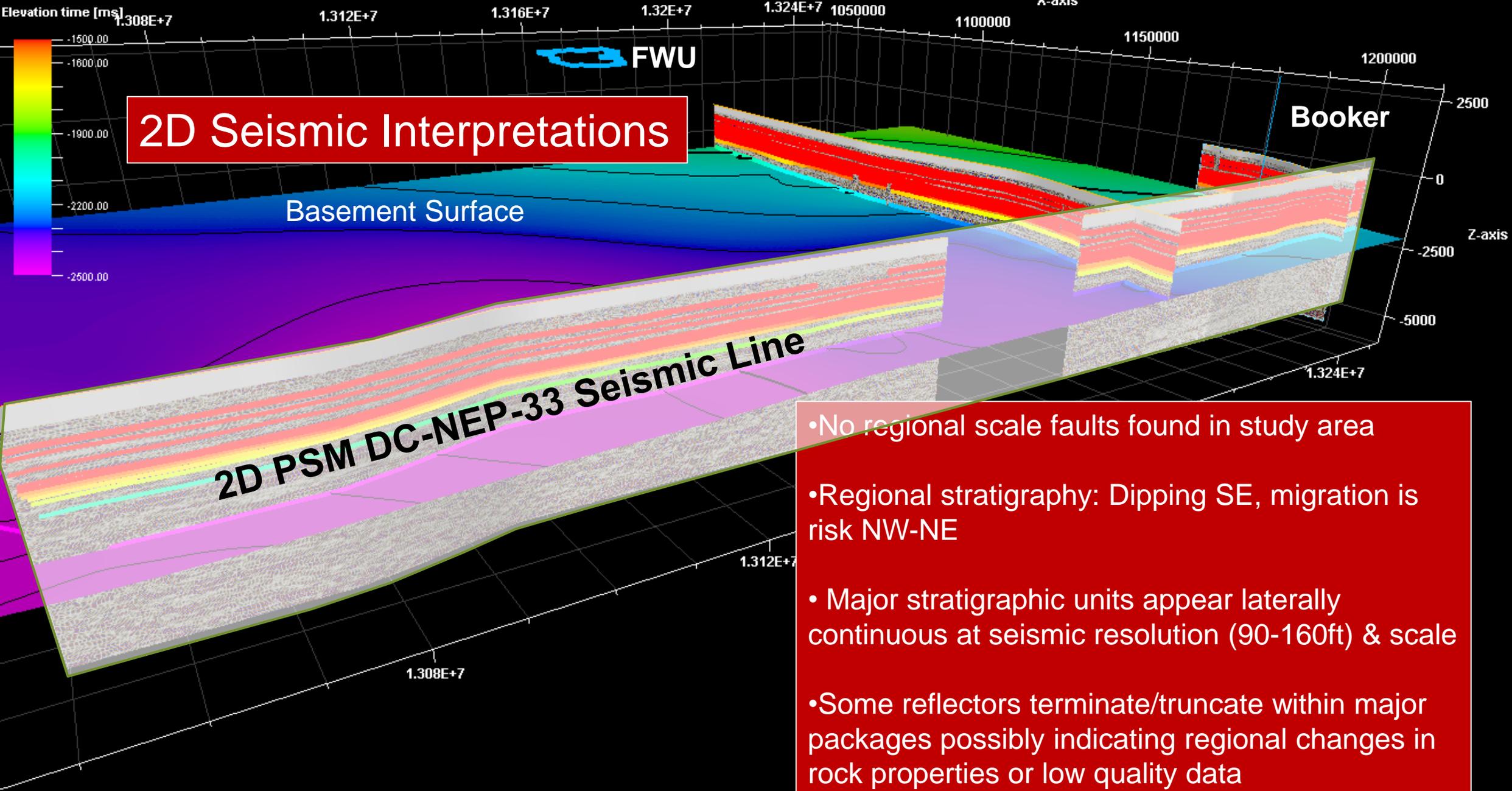
FUTURE WORK

- Mechanism(s) and timing of depressurization?
- Paleo to present stress evolution in the region?
- Use seismic techniques (geomorphic), log and core data to examine hydraulic properties, distribution, geometry of fractures?
- Does the Booker Survey have similar seismic features?
- Construction of a (DFN) hydro-structural models?

TRANSFORMATION RATIO (%)

- Thirteen Finger:
30.5% - 6%
- Upper Morrow Shale:
40% - 7%
- Lower Morrow Shale:
33% - 1.32%
- Woodford: 100%-42%

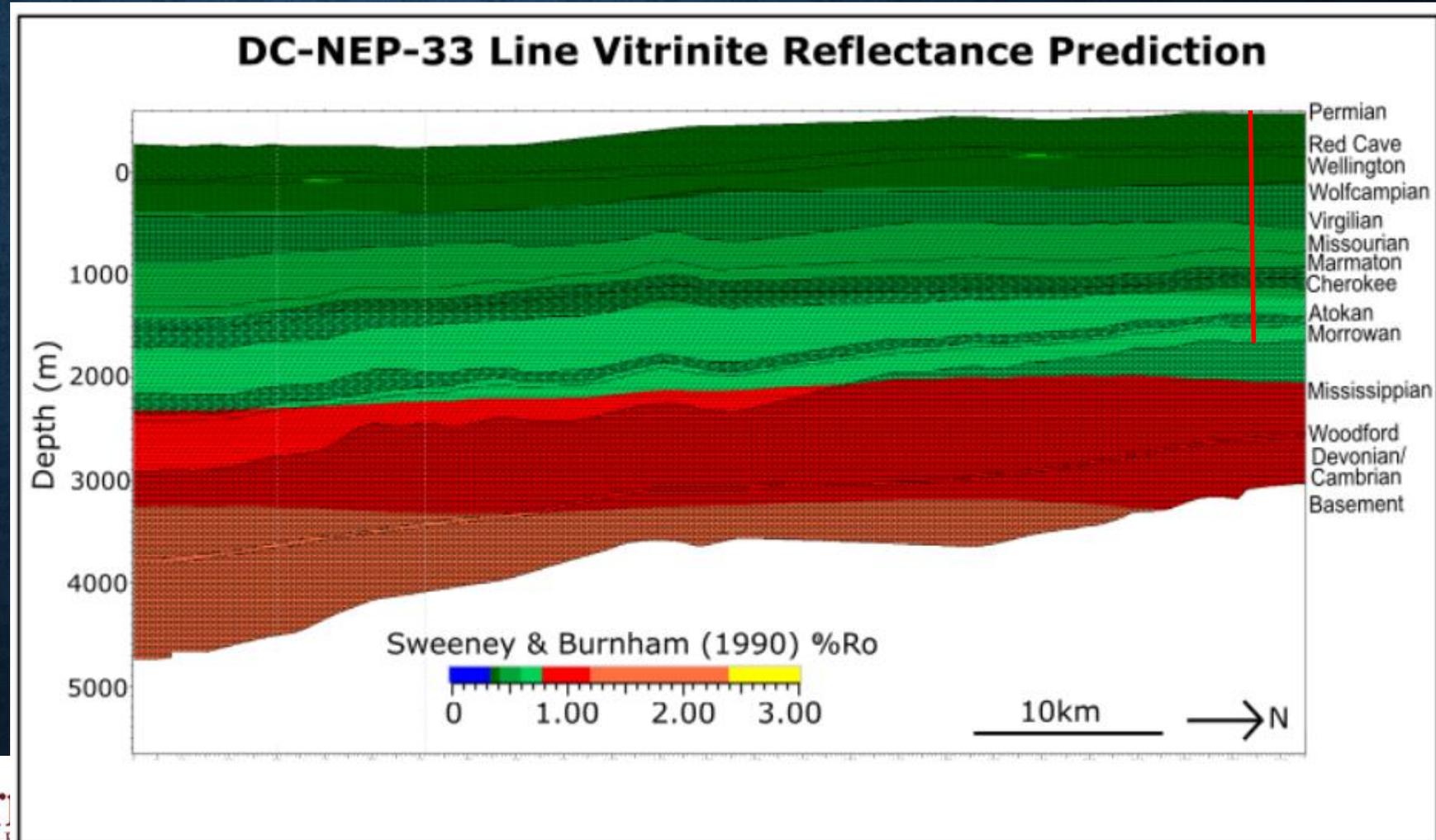




- No regional scale faults found in study area
- Regional stratigraphy: Dipping SE, migration is risk NW-NE
- Major stratigraphic units appear laterally continuous at seismic resolution (90-160ft) & scale
- Some reflectors terminate/truncate within major packages possibly indicating regional changes in rock properties or low quality data
- Regional CO₂ plume migration risk: Low

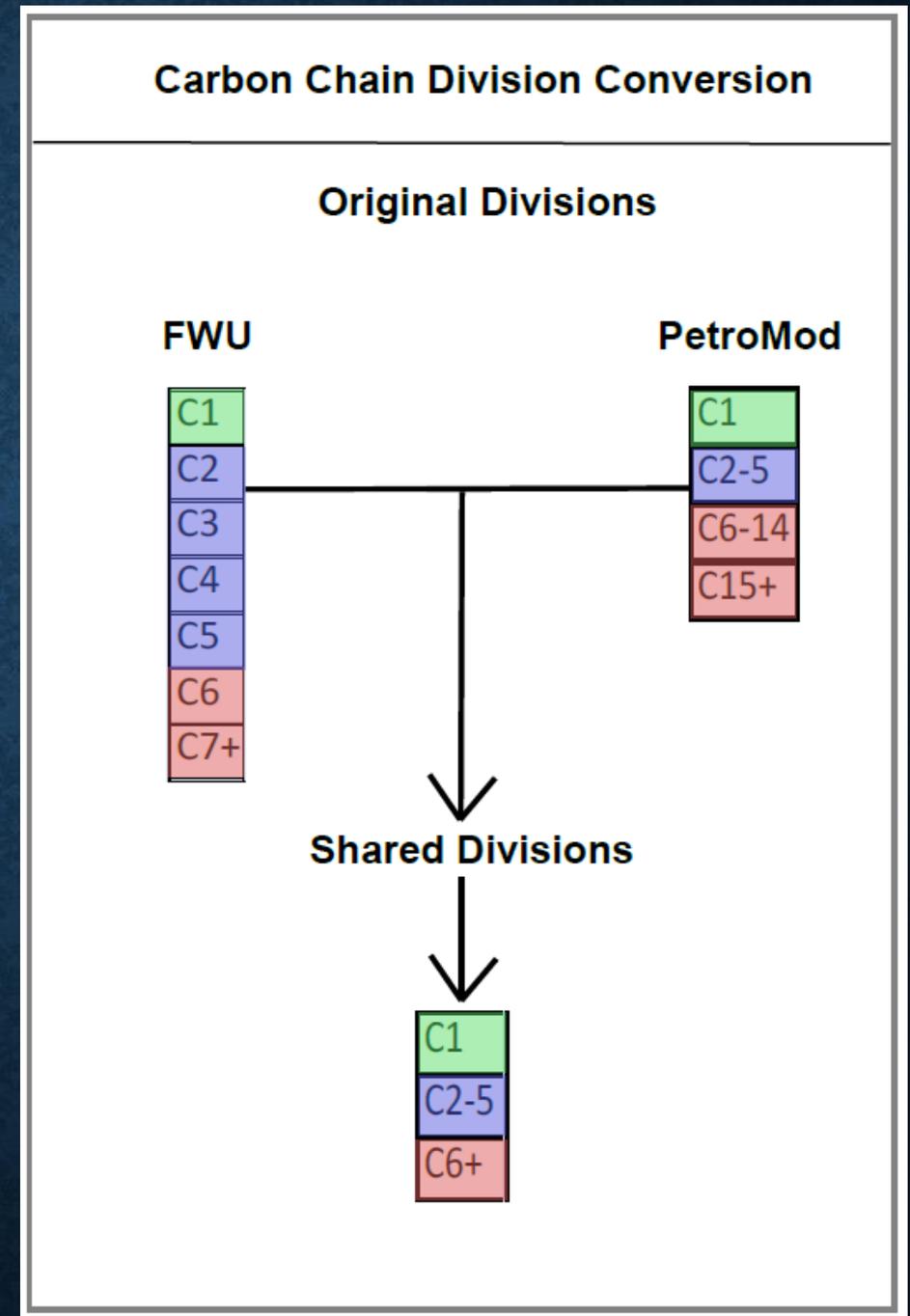
MATURATION PROFILE

- Maturation increases basinward
- Woodford: 1-1.4 %R_o
- Thirteen Finger: 0.65-0.8 %R_o
- Shales encasing Booker Field are marginally mature



Compositional Results

- Compositional data divisions for FWU and PetroMod are different
- Converted both into “common divisions”



Compositional Results Cont.

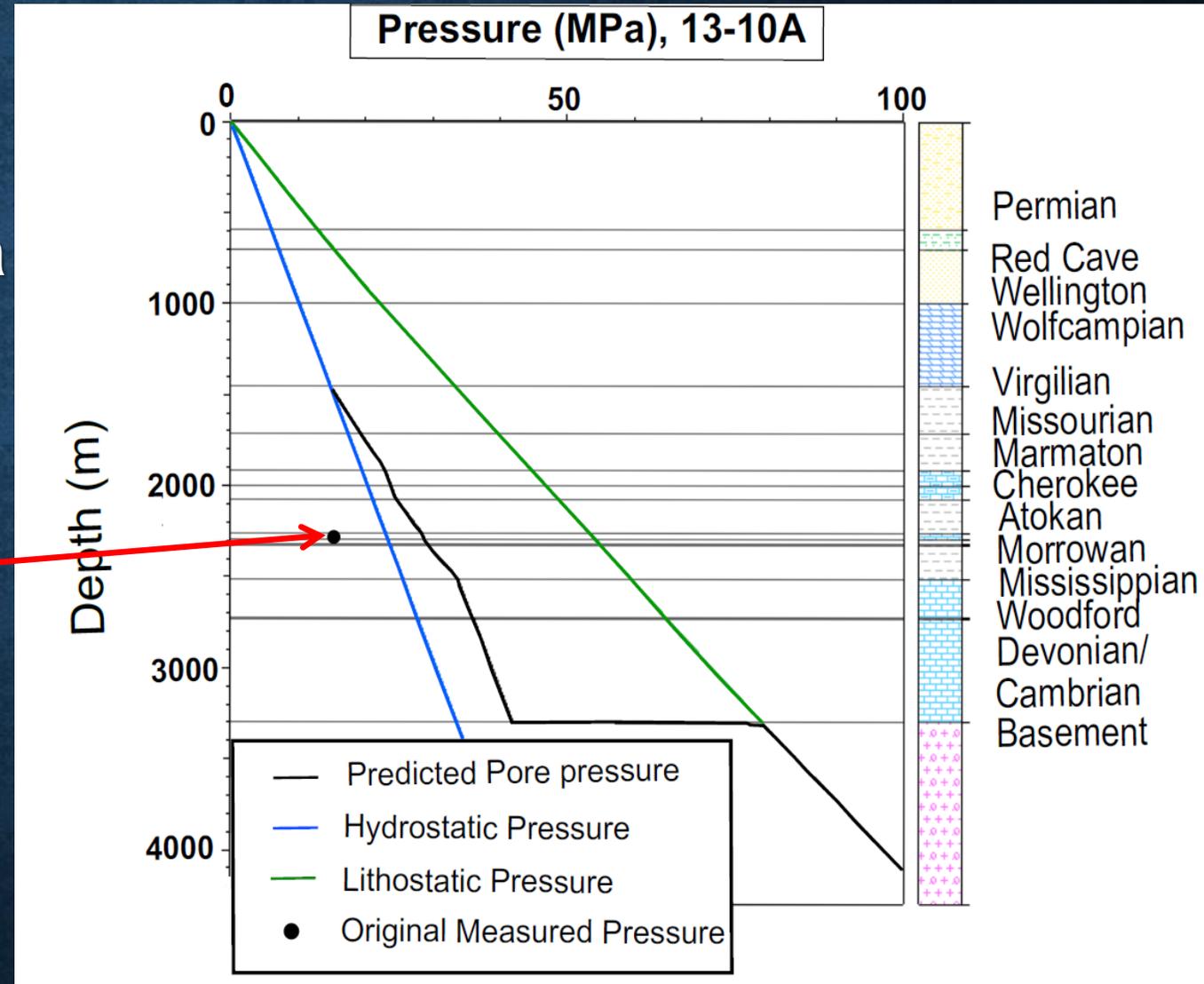
Compositional Data				
Component	FWU measured mol%	Booker predicted mol%	FWU measured mass %	Booker predicted mass %
C1	38.44	18.50	3.98	1.90
C2-5	10.05	21.20	3.02	7.10
C6+	51.51	60.30	93.00	91.00

FWU data from (Hinds, 1956)

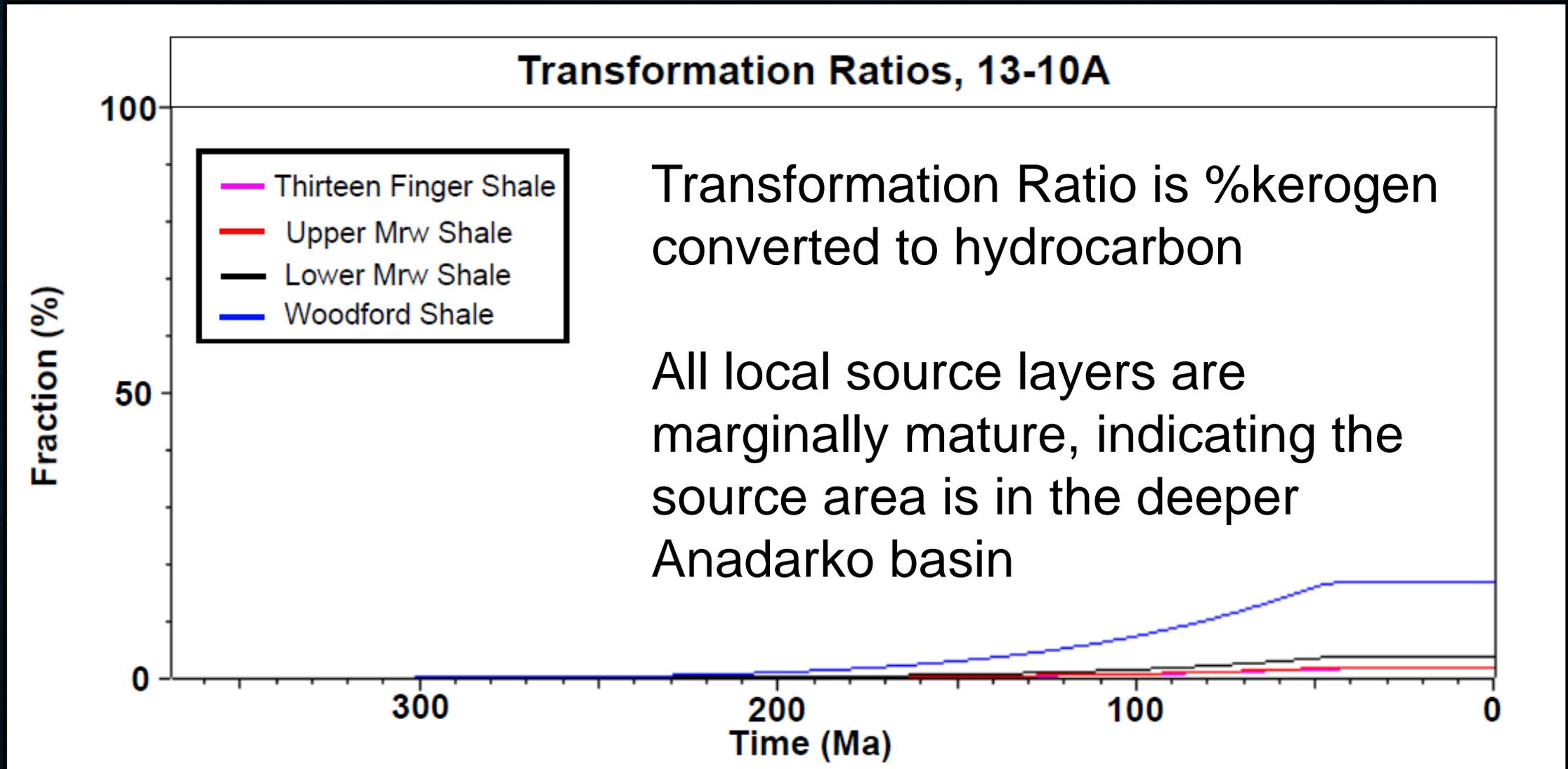
- Insights into the fluid composition and properties of the NE Texas panhandle Morrowan play for potential carbon storage sites

WELL 13-10A RESULTS: PRESSURE

- Current predicted pressure for Morrowan sandstone is ~29 MPa
- Actual measured (1956) in-situ pressure ~15 MPa

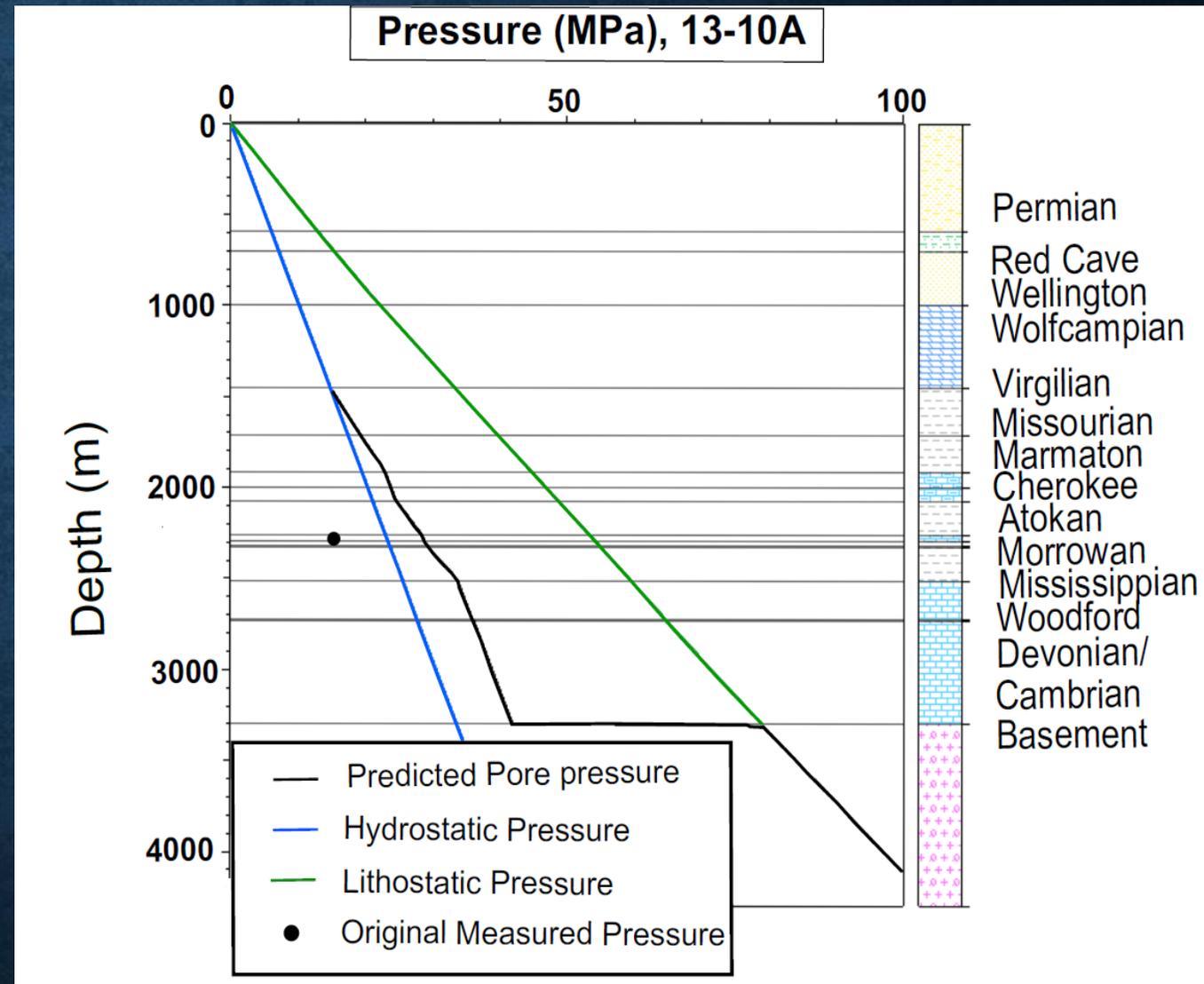


WELL 13-10A RESULTS: TRANSFORMATION RATIO



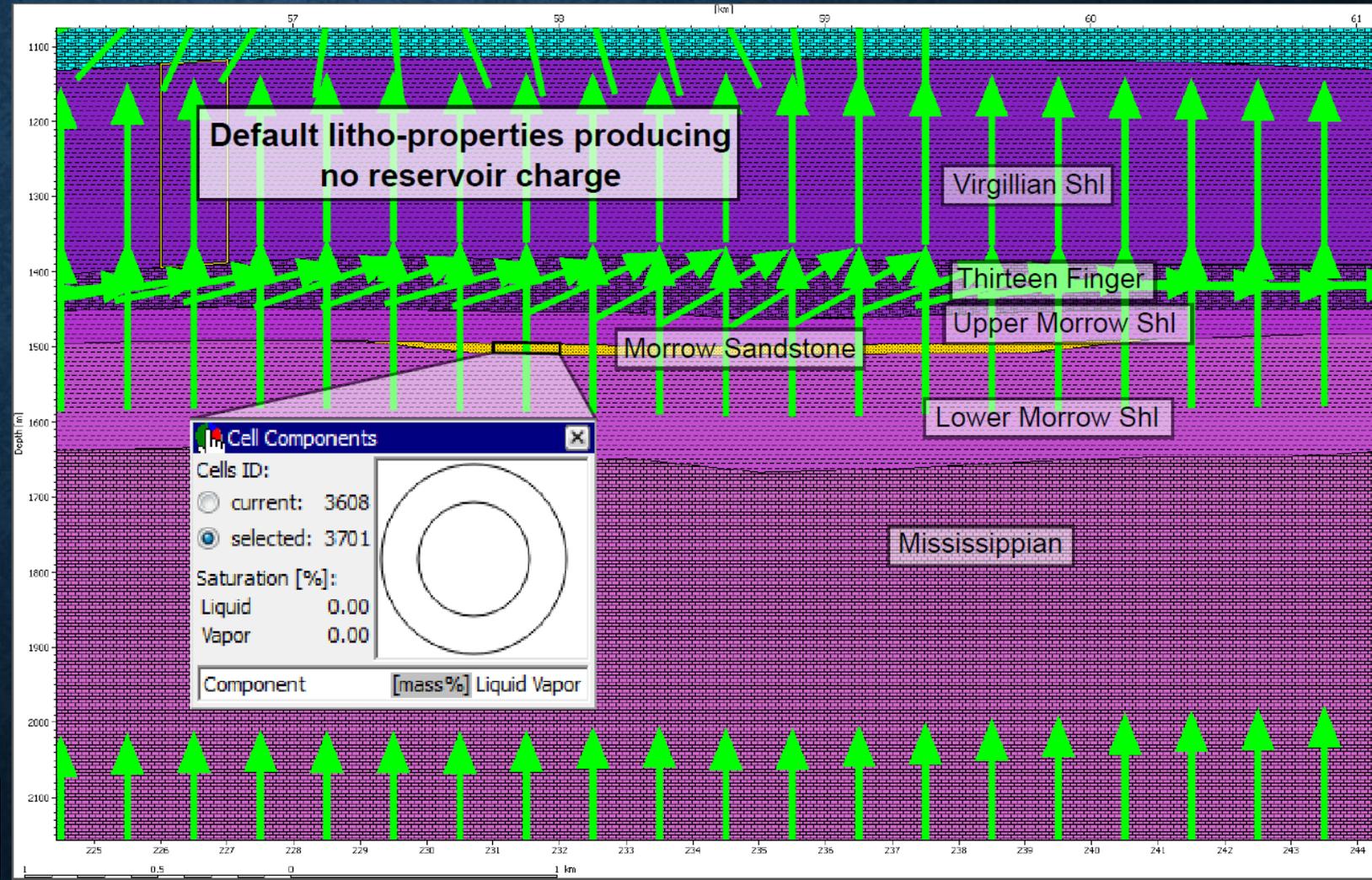
WELL 13-10A RESULTS: PRESSURE

- Area is underpressured
 - Reservoir appears to have depressurized
 - Attributed to Laramide erosion, regional groundwater discharge & restricted recharge (Sorenson, 2005)
 - Plausible paleo-hydraulic connectivity along faults
- Mechanism needs more research, important consideration for CO₂ storage



2D MODEL: NO ACCUMULATION

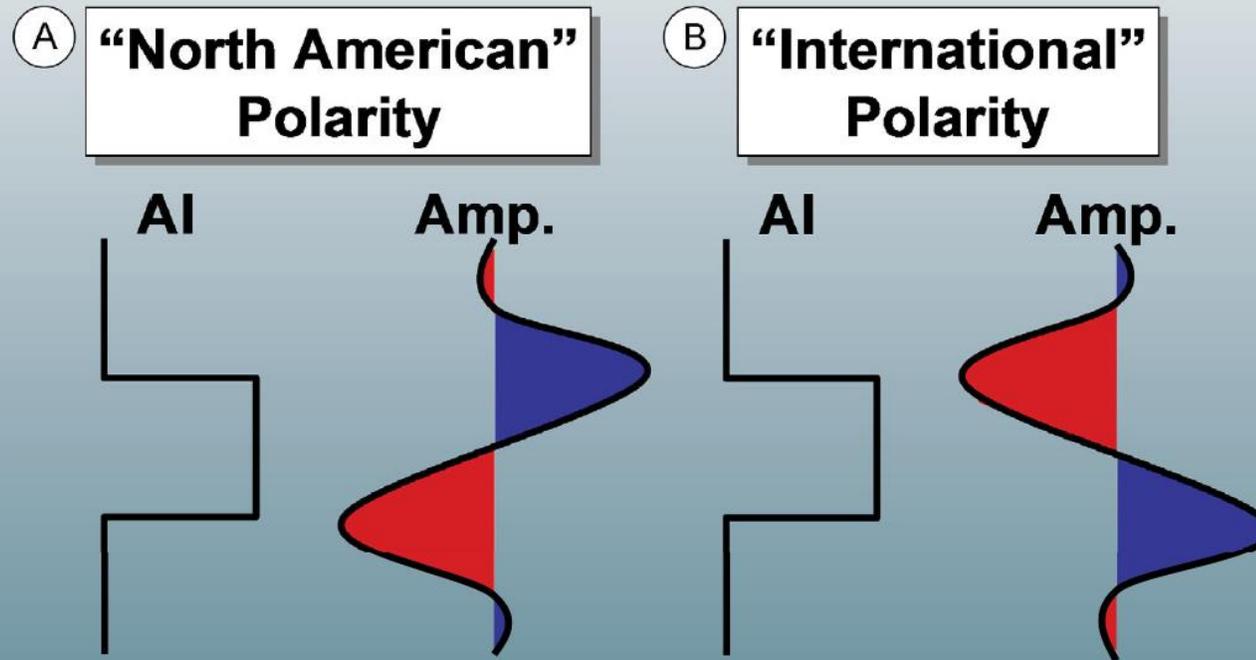
- Results prior to integrating in entry pressure and permeability data for Upper Morrow and Thirteen Finger Shales



SEISMIC POLARITY

◀ Back to Chapter

Figure 4.7: Polarity standards for seismic data display



A) Most interpreters in North America prefer to view seismic data such that an increase in acoustic impedance (positive reflection coefficient) corresponds to a peak (here colored blue) in seismic data. This is the SEG-Y standard.

B) Elsewhere in the world, interpreters prefer to view data such that an increase in acoustic impedance (positive reflection coefficient) corresponds to a trough (here colored red) in seismic data.

BASIN MODELING SEDIMENT FILL

- Fundamental concept: **Backstripping**

$$TS = S^* \frac{\rho_m - \bar{\rho}_s}{\rho_m - \rho_w} + W_d - \Delta_{sl} \frac{\rho_m}{\rho_m - \rho_w}$$

- TS is tectonic subsidence, S^* is layer thickness, W_d is average water depth at time of deposition, Δ_{sl} is change in sea level between the present and deposition time, $\rho_m - \rho_w - \rho_s$ represent mantle, water and sediment density, respectively
- Decompacts stratigraphic layers to their original thicknesses, and bulk densities
- Calculates the amount of isostatic subsidence caused by each layer

BACKSTRIPPING

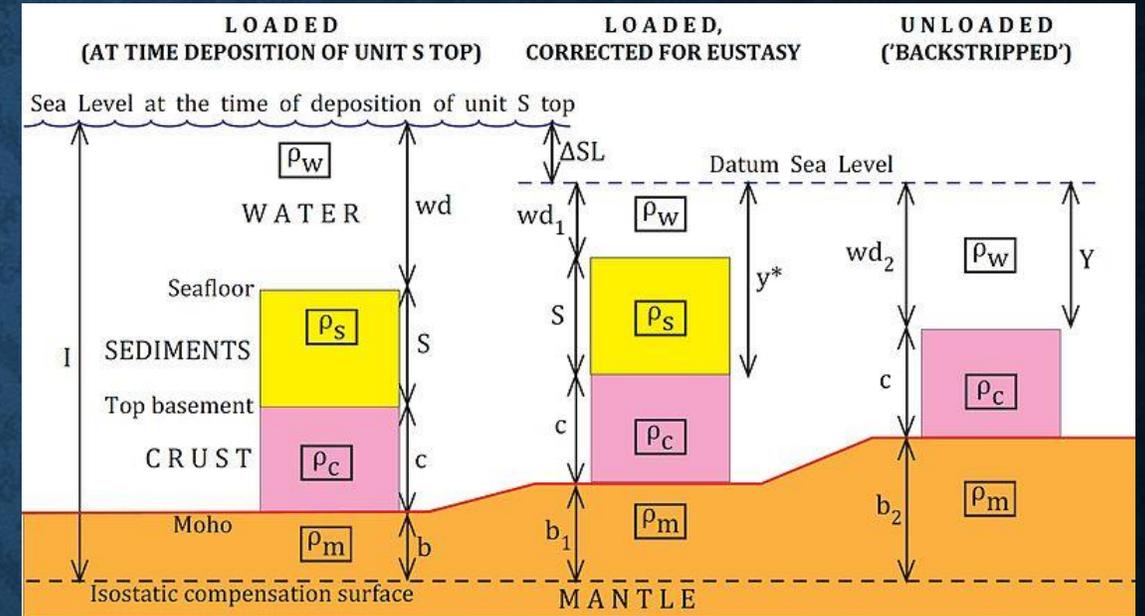
Airy vs flexural isostasy

$$TS = S^* \frac{\rho_m - \bar{\rho}_s}{\rho_m - \rho_w} + W_d - \Delta_{sl} \frac{\rho_m}{\rho_m - \rho_w}$$

Pure AIRY ISOSTASY (no strength)

$$D \frac{d^4 w(x)}{dx^4} = -(\rho_m - \rho_{fill}) g w(x) + q(x)$$

Flexural EQN (elastic strength)



I = thickness between the sea level at the time of deposition of unit S top and the isostatic compensation surface
 wd = water depth at the time of deposition of unit S top
 S = decompacted or partly decompacted thickness of the sedimentary unit whose base we want to "backstrip"
 c = thickness of the crustal basement lying below the horizon we want to backstrip
 b = thickness of the mantle between the Moho and the isostatic compensation surface at the time of deposition of unit S top
 ΔSL = eustatic difference between sea level at the time of deposition of unit S top and a datum sea level (usually, the present day sea level stand)

$wd1$ = water depth we would have had at the time of deposition of unit S top if the sea level had been the same as the datum
 $wd2$ = water depth we would have had at the time of deposition of unit S top if the sea level had been the same as the datum and if there had been no loading due to sedimentary unit S
 $b1$ = thickness of the mantle between the Moho and the isostatic compensation surface we would have had at the time of deposition of unit S top if the sea level had been the same as the datum
 $b2$ = thickness of the mantle between the Moho and the isostatic compensation surface we would have had at the time of deposition of unit S top if the sea level had been the same as the datum and if there had been no loading due to sedimentary unit S

By Stefano Patruno (2012)

y^* = depth of base sedimentary unit S corrected for eustasy and water depth =
 = total subsidence in a water-filled basin below sea level datum, accumulated during deposition of unit S and previously =
 $= S + wd - \Delta SL(\rho_m / (\rho_m - \rho_w)) \approx S + wd - (1.45 \cdot \Delta SL)$

Y = tectonic subsidence in a water-filled basin below sea level datum, accumulated during deposition of unit S and previously =
 $= S((\rho_m - \rho_s) / (\rho_m - \rho_w)) + wd - \Delta SL(\rho_m / (\rho_m - \rho_w)) \approx (1.45 \cdot S) - [S(\rho_s / 2,270)] + wd - (1.45 \cdot \Delta SL)$

PYROLYSIS TERMS

•**Tmax** = the temperature at which the maximum release of hydrocarbons from cracking of kerogen occurs during pyrolysis (top of S2 peak). Tmax is an indication of the stage of maturation of the organic matter.

•**HI** = hydrogen index ($HI = [100 \times S2]/TOC$). HI is a parameter used to characterize the origin of organic matter. Marine organisms and algae, in general, are composed of lipid- and protein-rich organic matter, where the ratio of H to C is higher than in the carbohydrate-rich constituents of land plants. HI typically ranges from ~100 to 600 in geological samples.

•**OI** = oxygen index ($OI = [100 \times S3]/TOC$). OI is a parameter that correlates with the ratio of O to C, which is high for polysaccharide-rich remains of land plants and inert organic material (residual organic matter) encountered as background in marine sediments. OI values range from near 0 to ~150.

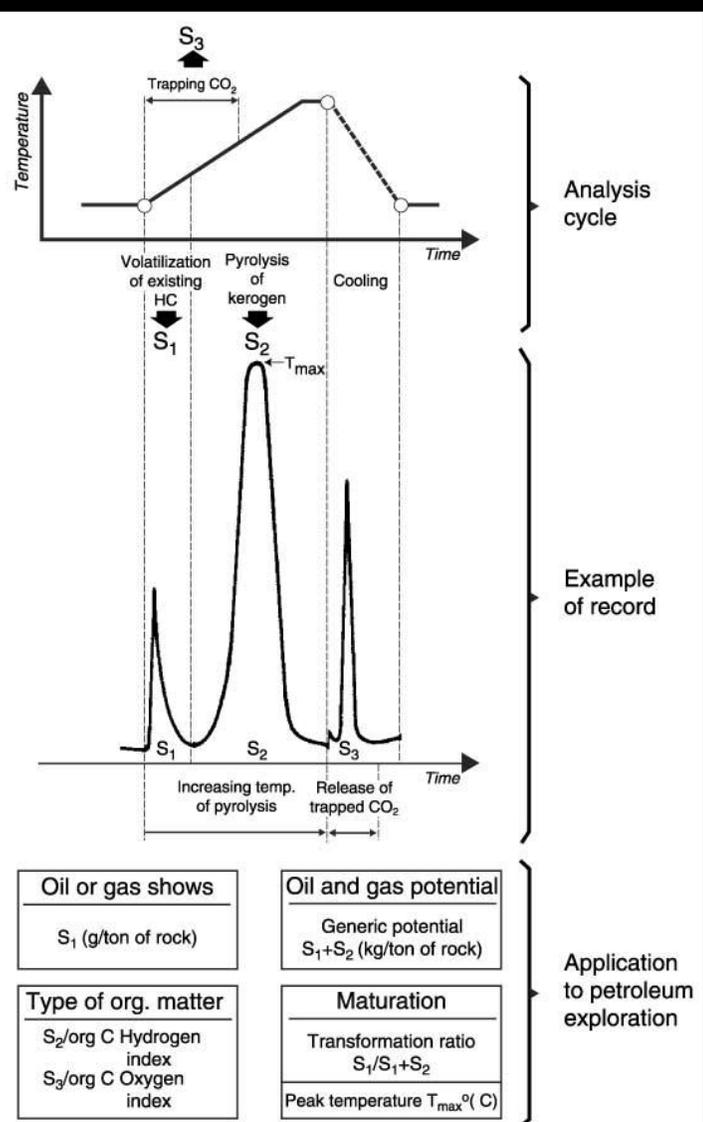
•**PI** = production index ($PI = S1/[S1 + S2]$). PI is used to characterize the evolution level of the organic matter.

•**S1** = the amount of free hydrocarbons (gas and oil) in the sample (in milligrams of hydrocarbon per gram of rock). If $S1 > 1$ mg/g, it may be indicative of an oil show. S1 normally increases with depth. Contamination of samples by drilling fluids and mud can give an abnormally high value for S1

•**S2** = the amount of hydrocarbons generated through thermal cracking of nonvolatile organic matter. S2 is an indication of the quantity of hydrocarbons that the rock has the potential of producing should burial and maturation continue. This parameter normally decreases with burial depths > 1 km.

•**S3** = the amount of CO₂ (in milligrams CO₂ per gram of rock) produced during pyrolysis of kerogen. S3 is an indication of the amount of oxygen in the kerogen and is used to calculate the oxygen index (see below). Contamination of the samples should be suspected if abnormally high S3 values are obtained. High concentrations of carbonates that break down at lower temperatures than 390°C will also cause higher S3 values than expected.

PYROLYSIS



LECO Carbon Analyzer



Sediment is combusted in oxygen & converted to CO₂. gas flows into a non-dispersive infrared detection cell to measures mass of CO₂, converted to percent carbon. The TOC content is subtracted from the total carbon content to get total inorganic carbon



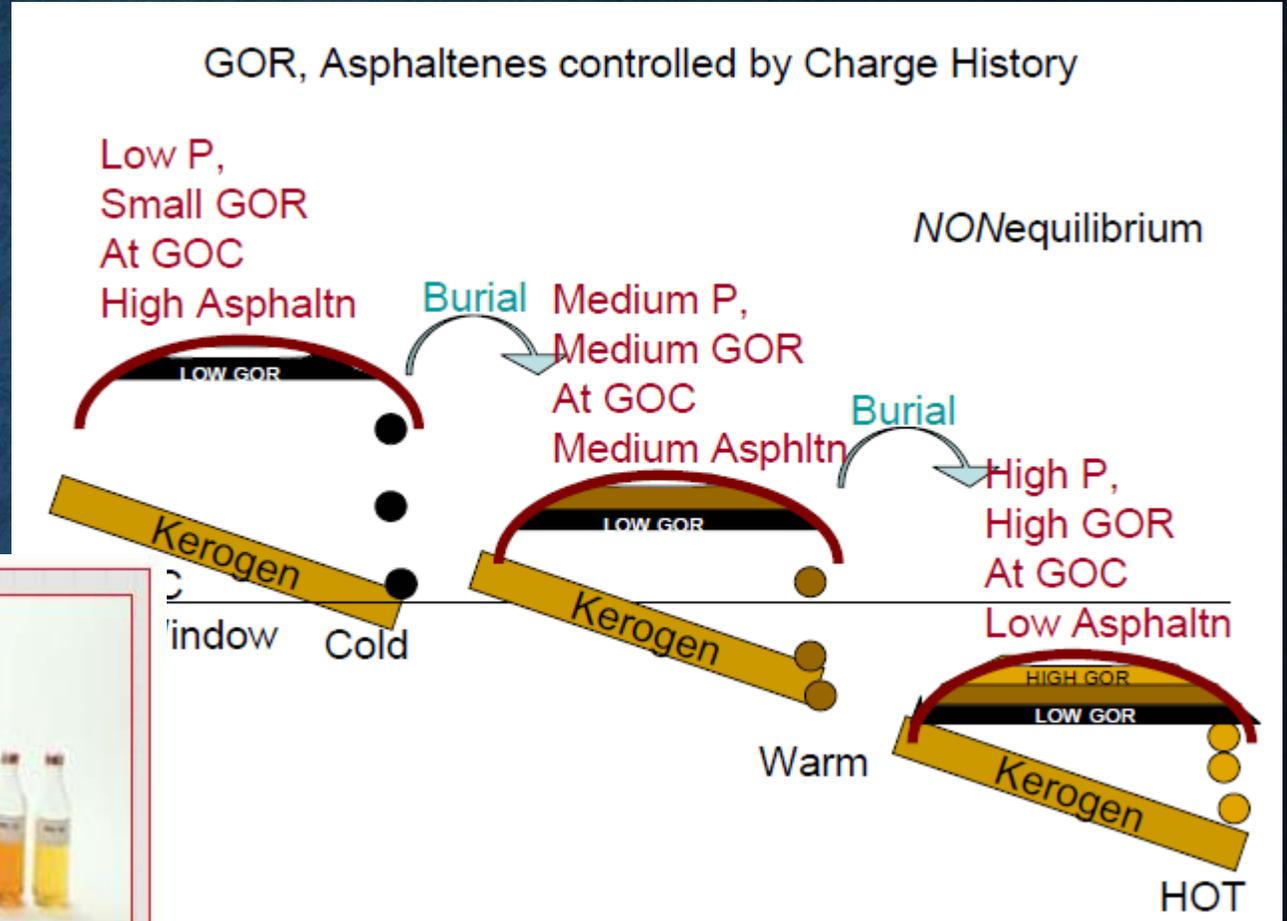
PRIMARY INPUT FILE 13-10A

Primary Inputs for 13-10A

Layer	Top (m)	Base (m)	Thick (m)	Eroded (m)	Depo From (Ma)	Depo to (Ma)	Eroded From (Ma)	Eroded to (Ma)	Lithology	TOC	Kinetic	HI
Permian/Ceno	0	600	600	1000	270	50	50	30	Sandstone (subarkose, clay rich)			
Red Cave	600	712	112		275	270			Siltstone (organic lean)			
Wellington	712	1006	294		280	275			Sandstone (typical)			
Wolfcampian	1006	1472	466		299	280			Dolomite (typical)			
Virgilian	1472	1731	259		303	299			Shale (typical)			
Missourian	1731	1932	201		304	303			Shale (typical)			
Kansas City	1932	2021	89		305	304			Limestone (shaly)			
Marmaton	2021	2094	73		305.3	305			Limestone (shaly)			
Cherokee	2094	2279	185		310	305.3			Shale (typical)			
Thirteen Finger	2279	2320	41		311	310			Limestone (shaly)	9.18	Lewan(2002)_TII(WoodSh)	355
Upper Morrow Shale	2320	2339	19		313.7	311			Shale (organic rich, typical)	3.62	Lewan(2002)_TII(WoodSh)	57
Morrow B	2339	2350	11		314	313.7			Sandstone (subarkose, typical)			
Lower Morrow Shale	2350	2533	183	15	324	314.5	314.5	314	Shale (organic rich, typical)	1.1	Lewan(2002)_TII(WoodSh)	10
Mississippian	2533	2745	212	150	354	330	330	324	Limestone (organic rich - typical)			
Woodford	2745	2758	13		369	354			Shale (organic rich, typical)	1.8	Lewan(2002)_TII(WoodSh)	300
Cambrian-Devonian	2758	3320	562		542	369			Limestone (organic rich - typical)			
Basement	3320	4320	1000		1500	542			Granite (> 1000 Ma old)			

Fluid Properties

- Important for simulations, injection, production, CO₂ migration and carbon storage potential and performance

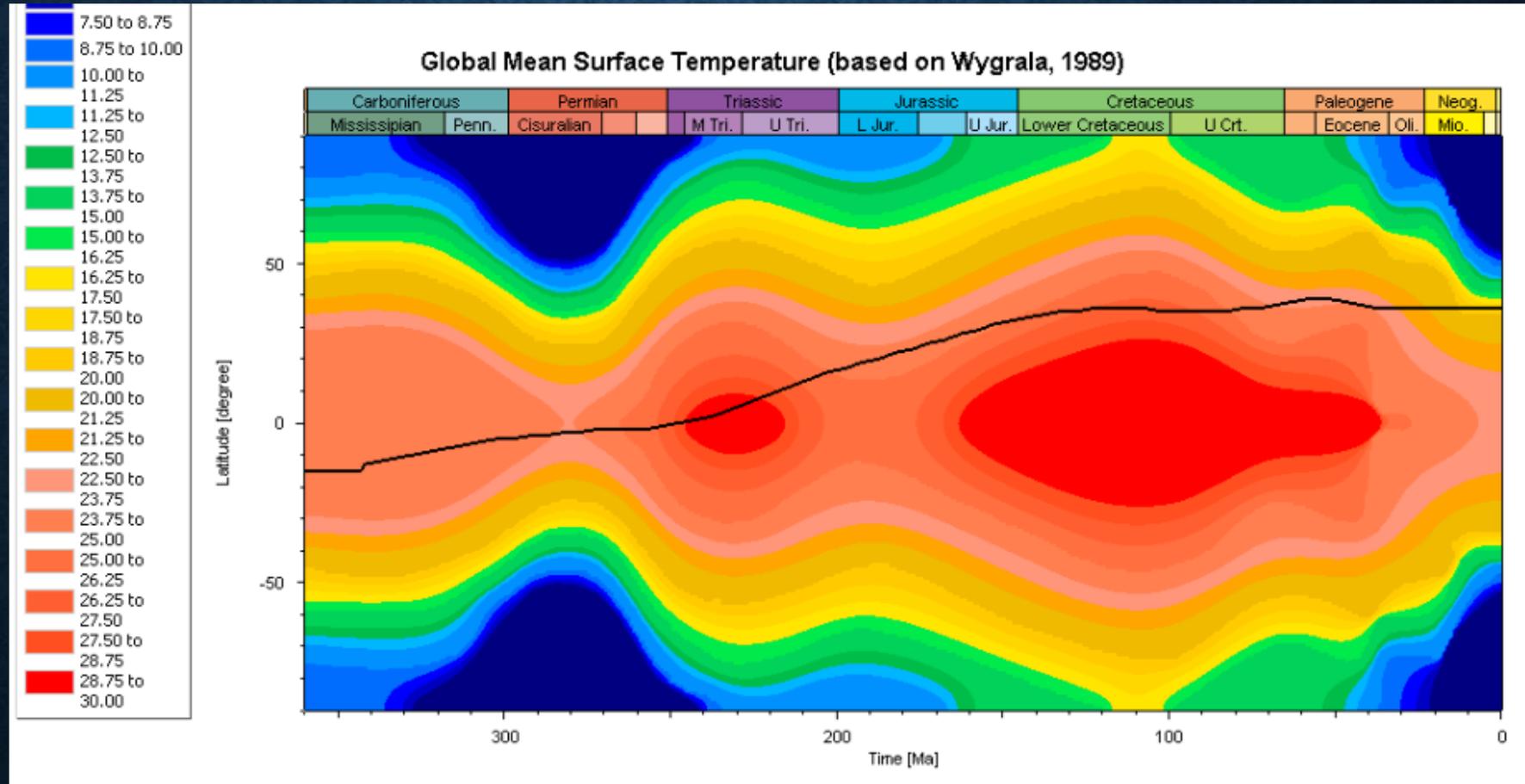


Conceptual model of multi-component expulsion



Example variability of oil samples from a single reservoir

PALEOCLIMATE MODELS



SOURCE ROCK DATA

LECO TOC and Rock Eval
Chaparral Energy L.L.C.
Farnsworth 13-10 A
Project No: 811108



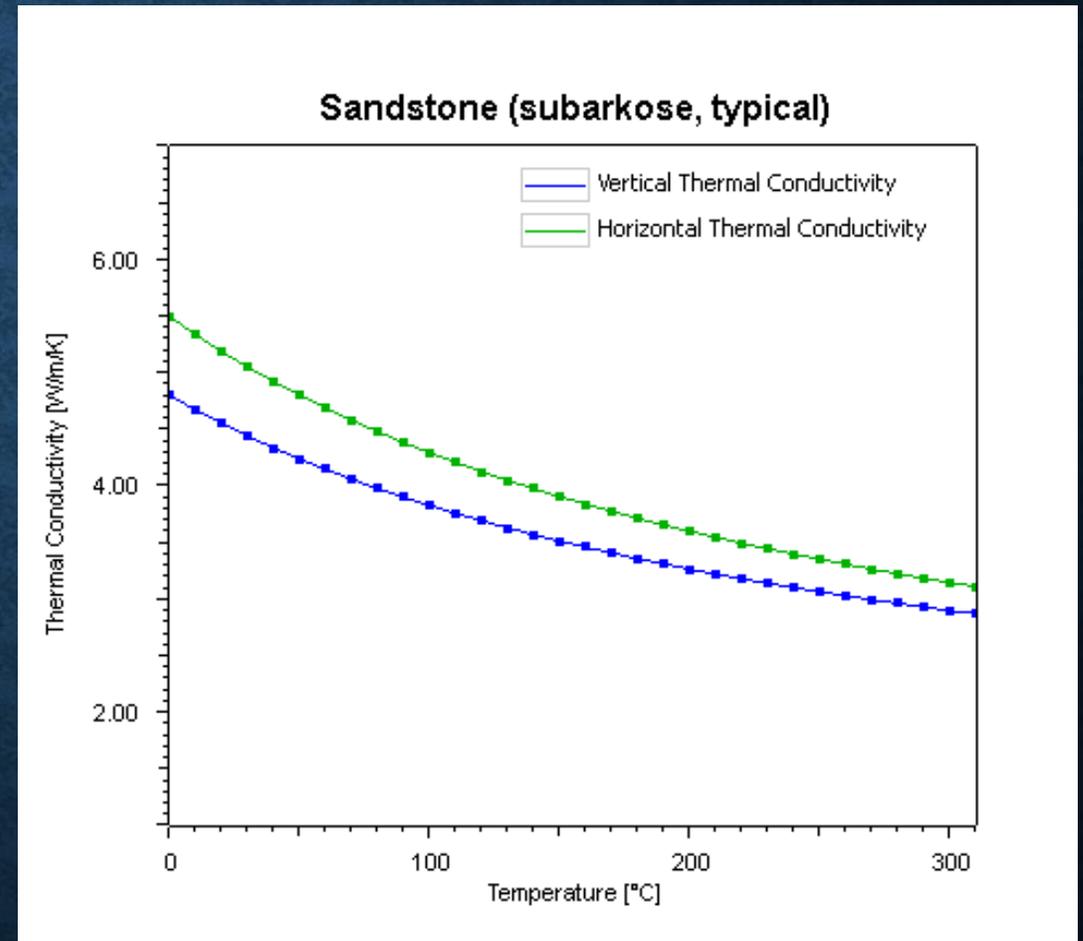
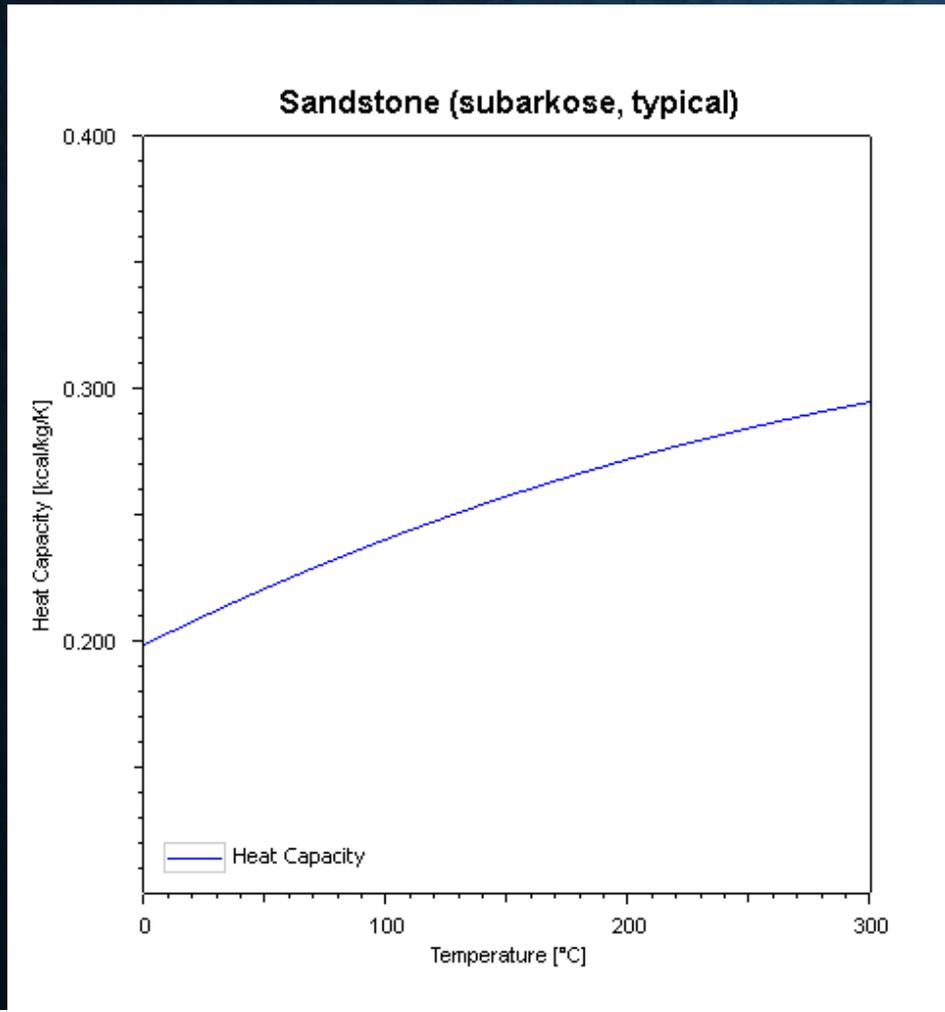
Sample ID	Core Depth ft.	As-Received Bulk Density g/cc	TOC Wt. %	S1 mg/g	S2 mg/g	S3 mg/g	Tmax	HI	OI	S1/TOC	PI	Calc Ro
78	7543.97	2.428	8.49	3.08	30.10	0.41	438	355	5	36	0.09	0.72
79	7612.16	1.403	59.80	27.95	158.35	1.07	430	265	2	47	0.15	0.58
80	7633.76	2.451	2.76	0.30	1.57	0.37	443	57	13	11	0.16	0.81
81	7654.50	2.538	0.34	0.05	0.07	0.21	0	21	62	15	0.42	n/a
82	7658.25	2.564	0.33	0.05	0.01	0.37	0	3	112	15	0.83	n/a
83	7716.26	2.590	0.53	0.07	0.05	0.27	0	10	51	13	0.58	n/a

•Used Rock Eval data to predict initial TOC content, calculation involves 10 variables (8 from above), 2 are educated assumptions from visual maceral data, according to SLB no industry lab in the world does this.



Sample	Type	Top Depth (m)	Bottom Depth (m)	Rock unit	S3	Tmax	OI	PI	TOC	S1	S2	HI	HIO	PIO	Initial TOC %
13 Finger Black Shale	Core	2337	2337	Shale	0.27	442.3	3.33	0.11	8.86	2.6	27.5	295.3	350	0.02	9.18
Upper Morrow Black Shale	Core	2370	2370	Shale	0.22	440	7.5	0.12	2.88	0.4	3.41	116	350	0.02	3.62
Lower Morrow Black Shale	Core	2352	2352	Shale	0.27	451	51	0.58	0.8	0.1	0.31	31	350	0.02	1.1

HEAT CAPACITY & THERMAL CONDUCTIVITY MODELS



RADIOGENIC HEAT MODEL

Uranium: [ppm]
 Thorium: [ppm]
 Potassium: [%]
 Porosity: [%]
 [API]
 [microW/m³]
 [m]

	Porosity [%]	Bulk value [microW/m ³]
1	0.00	0.60
2	10.00	0.54
3	20.00	0.48
4	30.00	0.42
5	40.00	0.36

Rybach (1973)

PetroMod's Lithology Editor

File Edit Windows Help

Lithology Browser

- Sedimentary rocks
 - Clastic sediments
 - Sandstone (typical)
 - Sandstone (clay rich)
 - Sandstone (clay poor)
 - Sandstone (quartzite, typical)
 - Sandstone (quartzite, very quartz rich)
 - Sandstone (subarkose, typical)
 - Sandstone (subarkose, quartz rich)
 - Sandstone (subarkose, clay rich)
 - Sandstone (subarkose, clay poor)
 - Sandstone (subarkose, dolomite rich)
 - Sandstone (arkose, typical)
 - Sandstone (arkose, quartz rich)
 - Sandstone (arkose, quartz poor)
 - Sandstone (arkose, clay rich)
 - Sandstone (arkose, clay poor)
 - Sandstone (arkose, dolomite rich)
 - Sandstone (wacke)
 - Shale (typical)
 - Shale (organic lean, typical)
 - Shale (organic lean, sandy)
 - Shale (organic lean, silty)
 - Shale (organic lean, siliceous, typical)
 - Shale (organic lean, siliceous, 95% opal-...)
 - Shale (black)
 - Shale (organic rich, typical)
 - Shale (organic rich, 3% TOC)
 - Shale (organic rich, 8% TOC)
 - Shale (organic rich, 20% TOC)
 - Siltstone (organic lean)
 - Siltstone (organic rich, typical)
 - Siltstone (organic rich > 10% TOC)
 - Siltstone (organic rich, 2-3% TOC)
 - Conglomerate (typical)
 - Conglomerate (quartzitic)
 - Tuff (felsic)
 - Tuff (basaltic)
 - Carbonate rocks
 - Chemical sediments
 - Biogenic sediments
 - Metamorphic and igneous rocks
 - Crustal rocks
 - Minerals

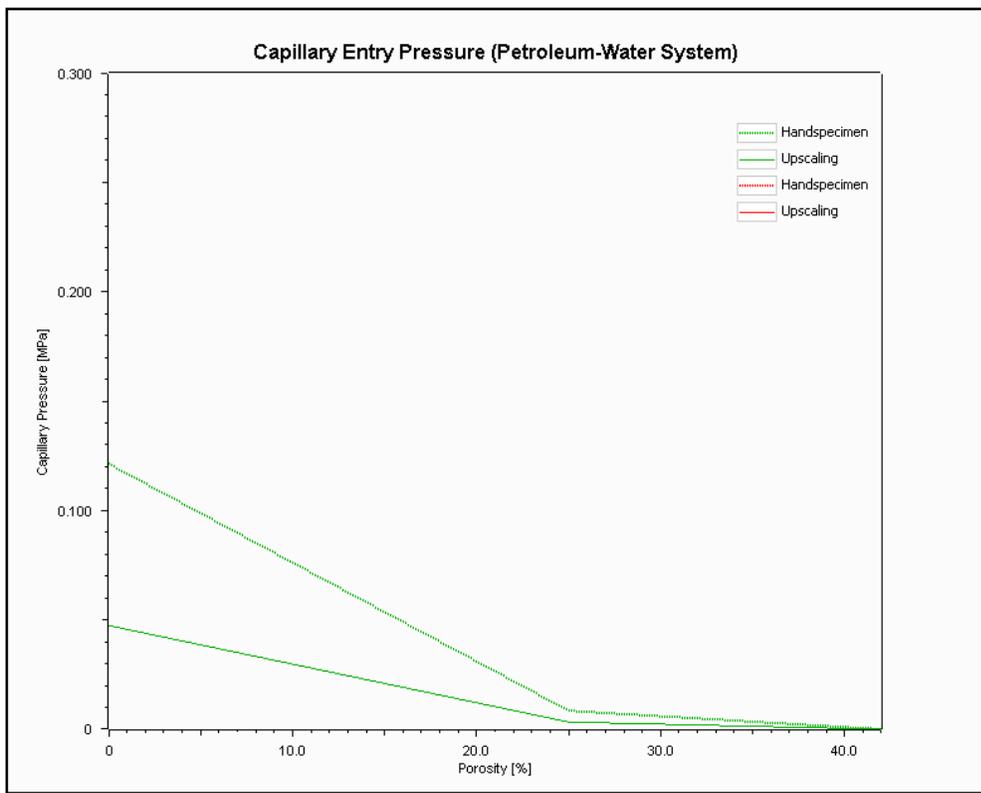
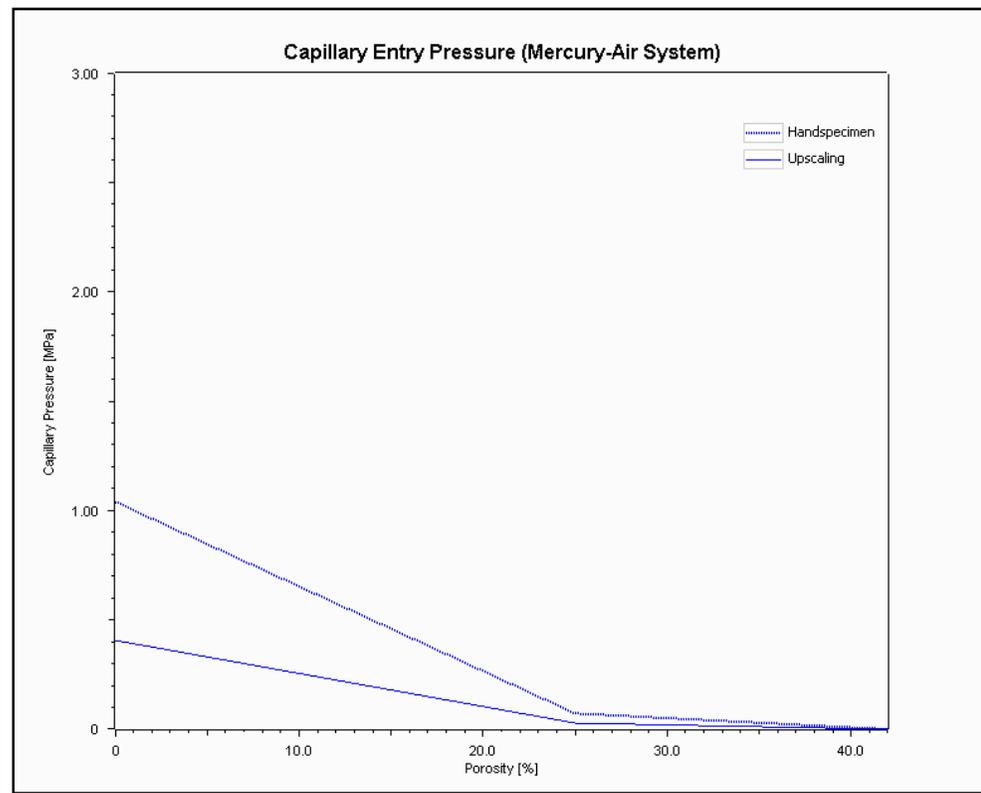
Thermal conductivity Radiogenic heat Heat capacity Mechanical compaction Chemical compaction Permeability Seal properties Fracturing Geomechanics Miscellaneous Mixing Pattern editor

a*por+b a = b =

IFT **liquid**: [mN/m]

IFT **vapor**: [mN/m]

NOTE: Values shown are only for test purposes. Set/change IFT in Phase Editor to use in simulation.



Saturation endpoints:

s**wc [%] Upscaling Factor

s**oc [%]

s**gc [%]

PetroMod's Lithology Editor Cont.

- Lithology Browser
- Sedimentary rocks
 - Clastic sediments
 - Sandstone (typical)
 - Sandstone (clay rich)
 - Sandstone (clay poor)
 - Sandstone (quartzite, typical)
 - Sandstone (quartzite, very quartz rich)
 - Sandstone (subarkose, typical)
 - Sandstone (subarkose, quartz rich)
 - Sandstone (subarkose, clay rich)
 - Sandstone (subarkose, clay poor)**
 - Sandstone (subarkose, dolomite rich)
 - Sandstone (arkose, typical)
 - Sandstone (arkose, quartz rich)
 - Sandstone (arkose, quartz poor)
 - Sandstone (arkose, clay rich)
 - Sandstone (arkose, clay poor)
 - Sandstone (arkose, dolomite rich)
 - Sandstone (wacke)
 - Shale (typical)
 - Shale (organic lean, typical)
 - Shale (organic lean, sandy)
 - Shale (organic lean, silty)
 - Shale (organic lean, siliceous, typical)
 - Shale (organic lean, siliceous, 95% opal-...)
 - Shale (black)
 - Shale (organic rich, typical)
 - Shale (organic rich, 3% TOC)
 - Shale (organic rich, 8% TOC)
 - Shale (organic rich, 20% TOC)
 - Siltstone (organic lean)
 - Siltstone (organic rich, typical)
 - Siltstone (organic rich > 10% TOC)
 - Siltstone (organic rich, 2-3% TOC)
 - Conglomerate (typical)
 - Conglomerate (quartzitic)
 - Tuff (felsic)
 - Tuff (basaltic)
 - Carbonate rocks
 - Chemical sediments
 - Biogenic sediments
 - Metamorphic and igneous rocks
 - Crustal rocks
 - Minerals

Thermal conductivity | Radiogenic heat | Heat capacity | Mechanical compaction | Chemical compaction | Permeability | Seal properties | Fracturing | Geomechanics | Miscellaneous | Mixing | Pattern editor

Elastic properties

Poisson's ratio:

Modulus of elasticity: For initial porosity: [MPa]

For minimum porosity: [MPa]

Plastic properties

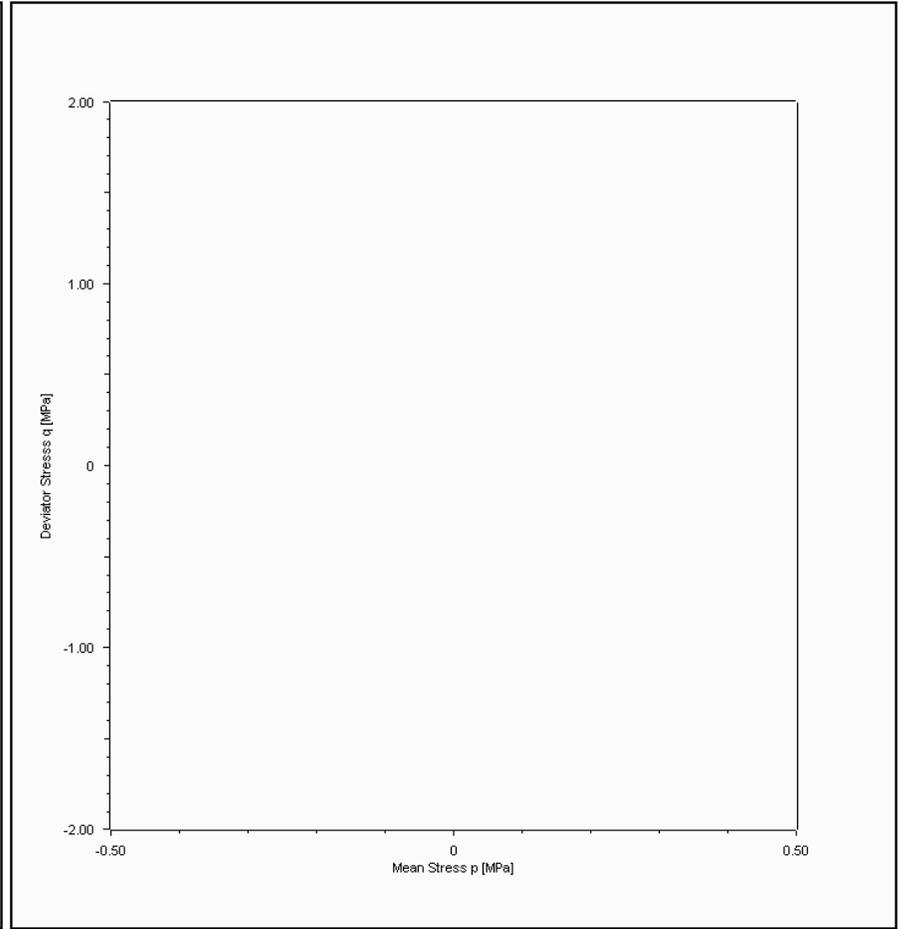
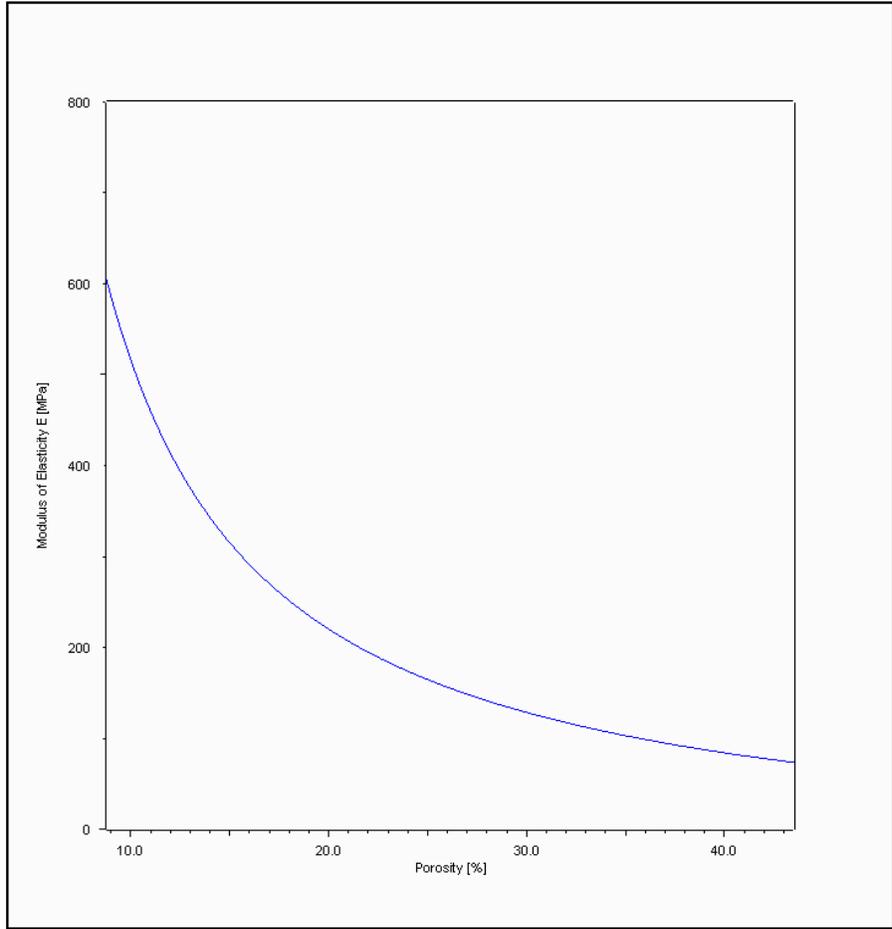
Plastic model: Tensile strength p0: [MPa]

Critical state pressure pc: [MPa]

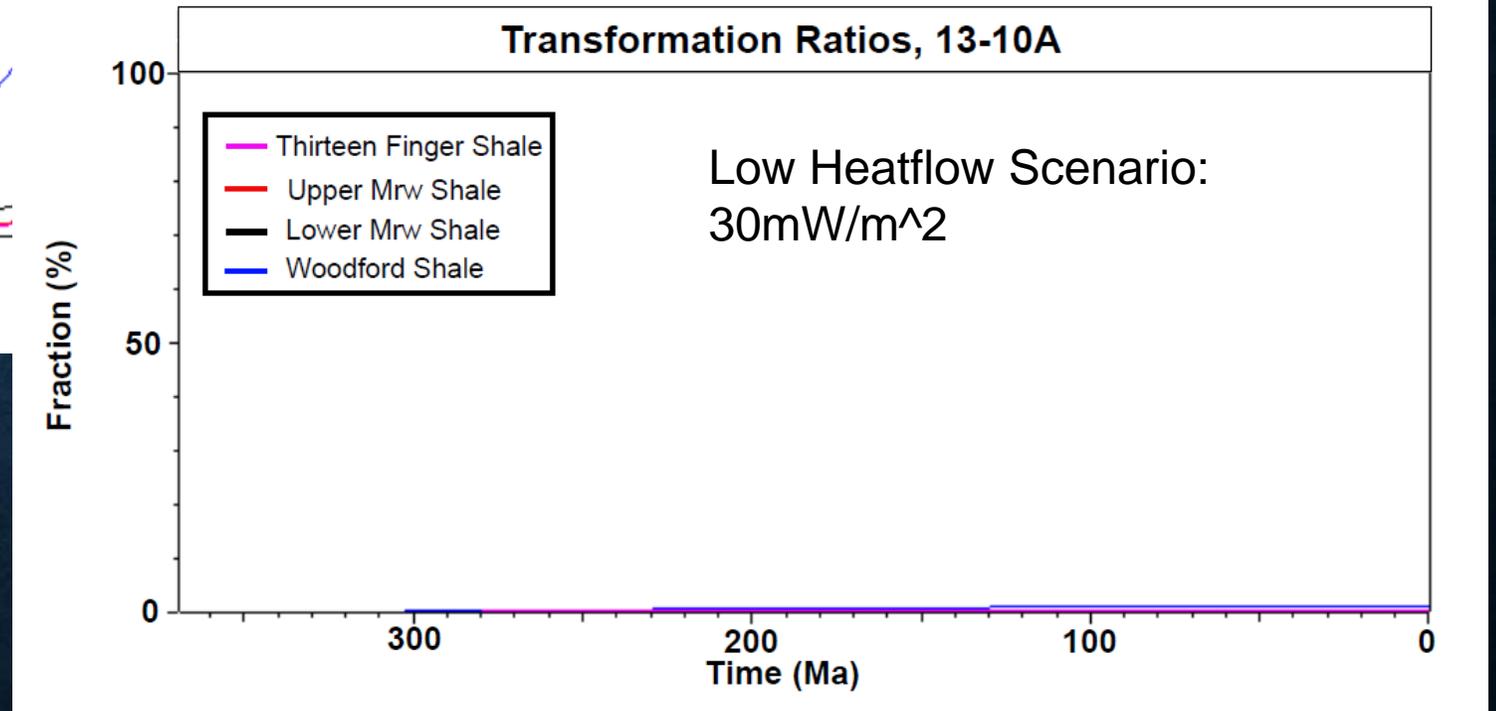
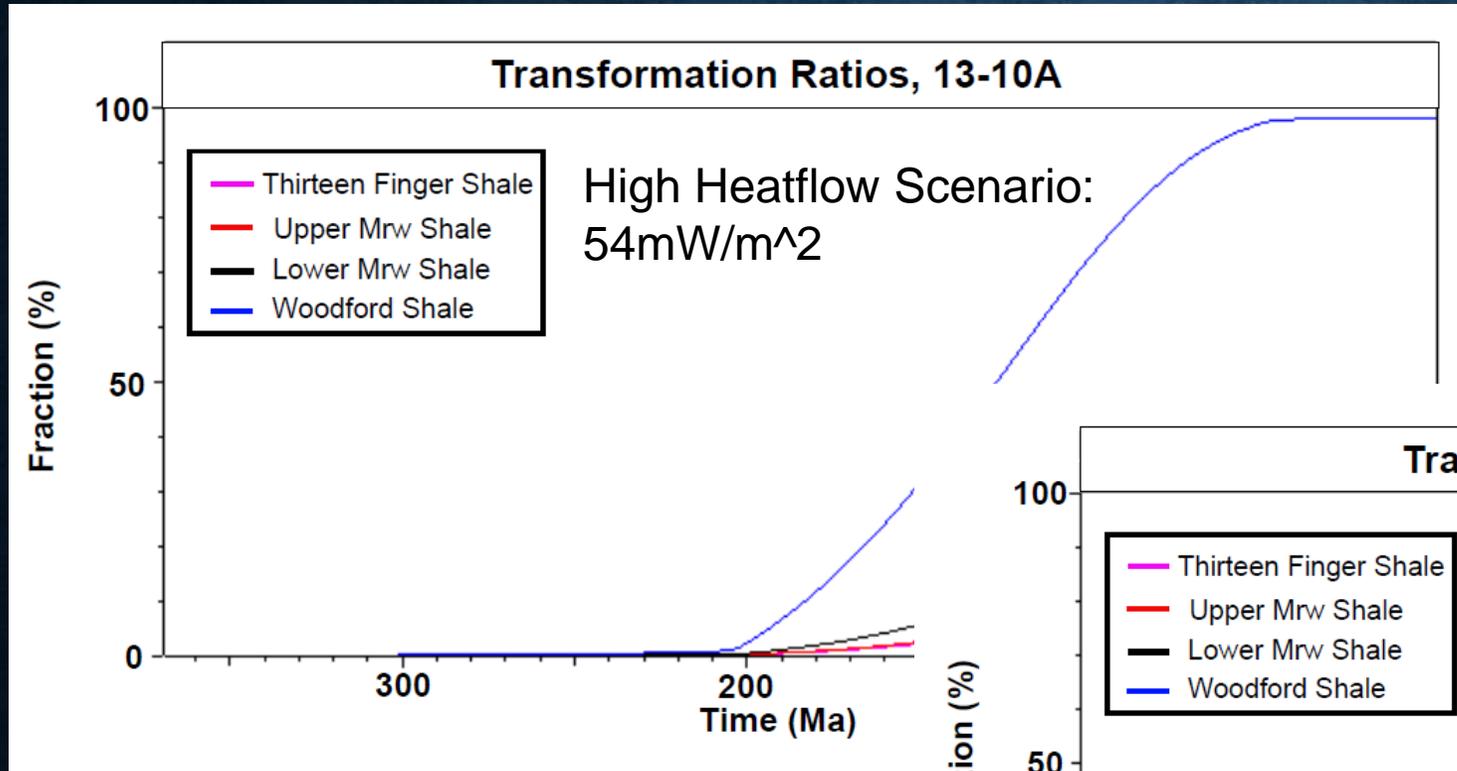
Critical state pressure qc: [MPa]

Maximum mean pressure pm: [MPa]

Calculate

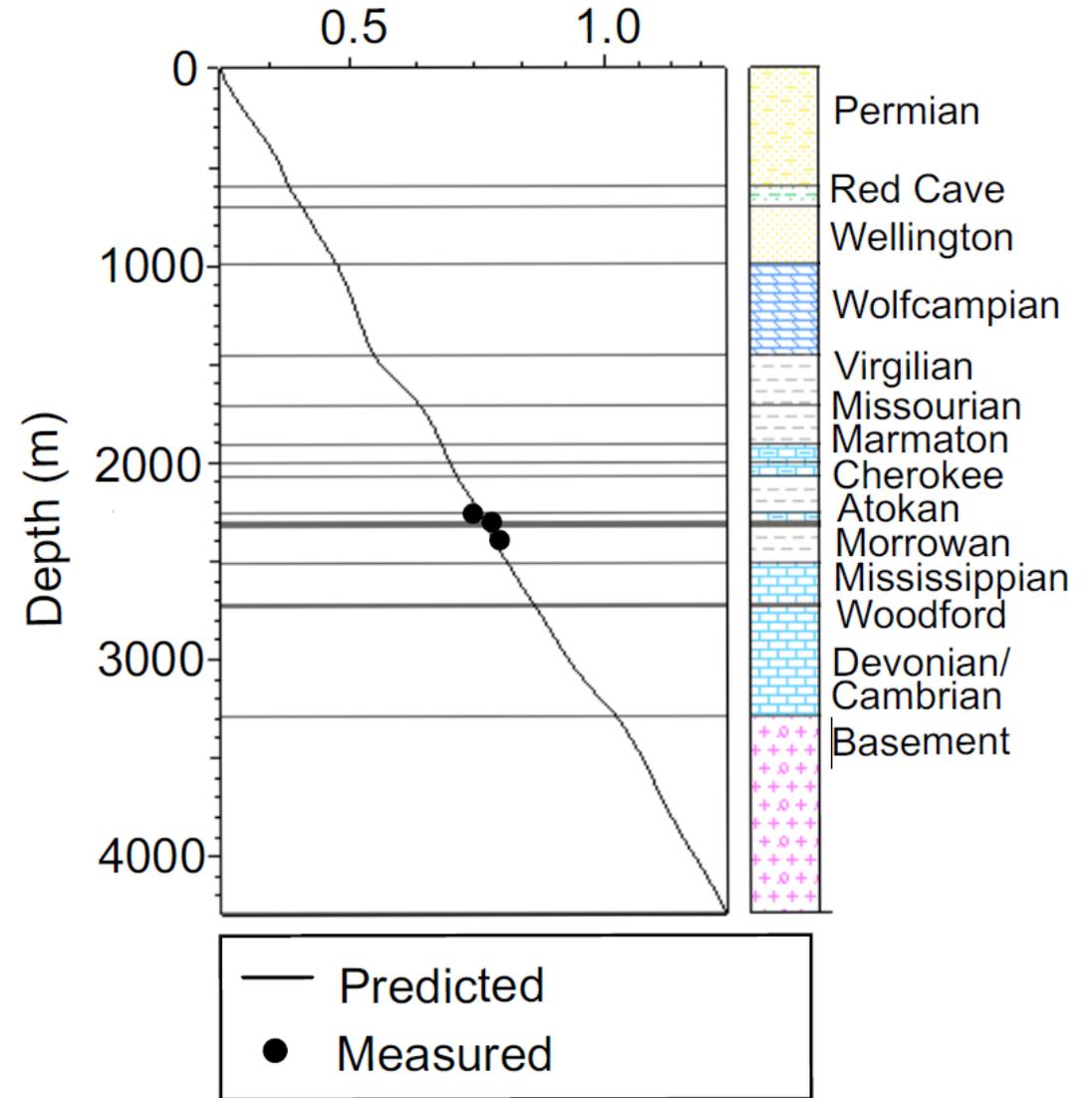


TRANSFORMATION RATIOS & HEATFLOW



VITRINITE CALIBRATION AT FWU

Sweeney & Burnham (1990) %Ro

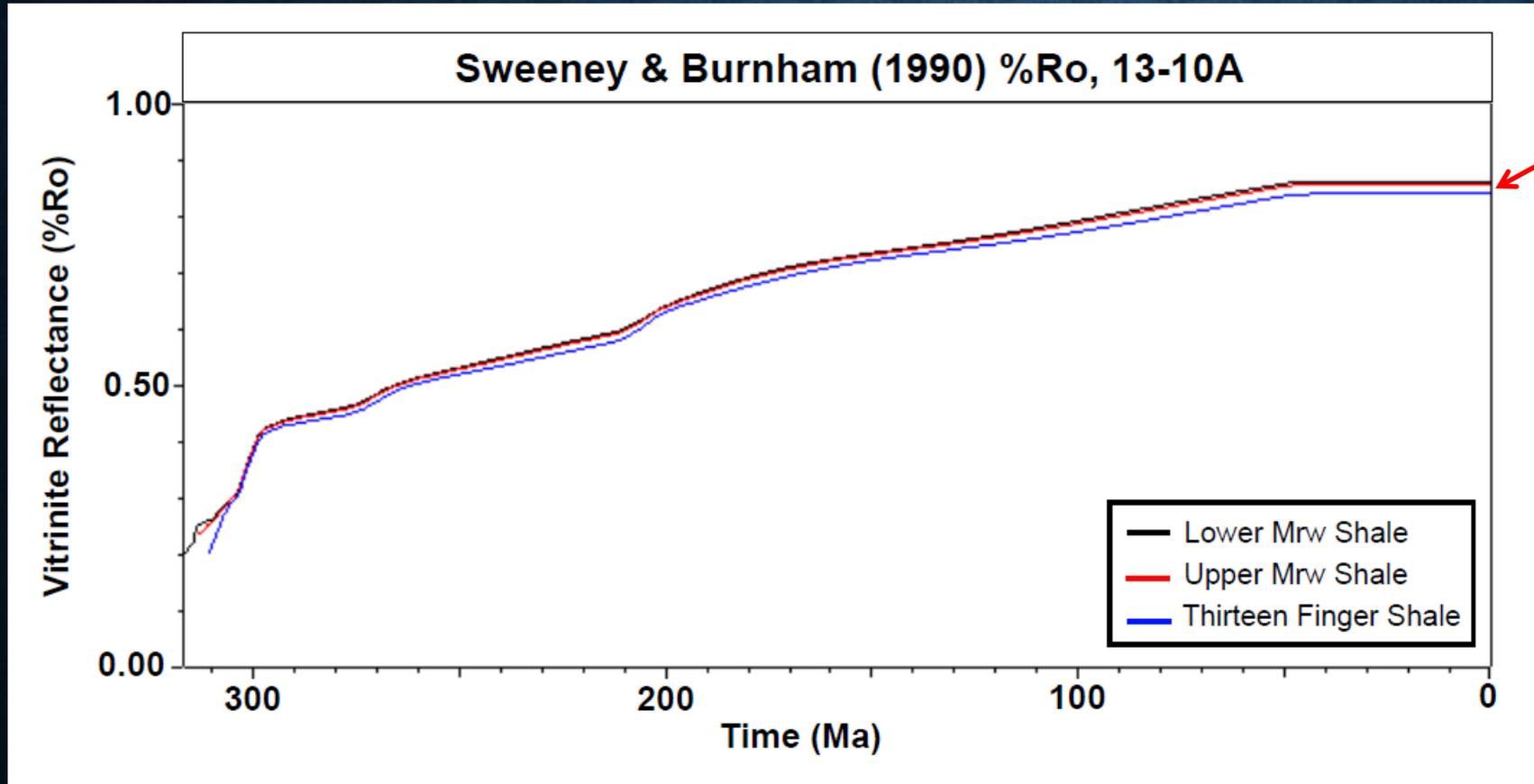


HEATFLOW SENSITIVITY

- Three different basal heatflow scenarios tested against vitrinite data
 - Carter et al., 1998: 54mW/m² (high)
 - Lee and Deming, 1999: 30 mW/m² (Low)
 - 42mW/m² (mid)

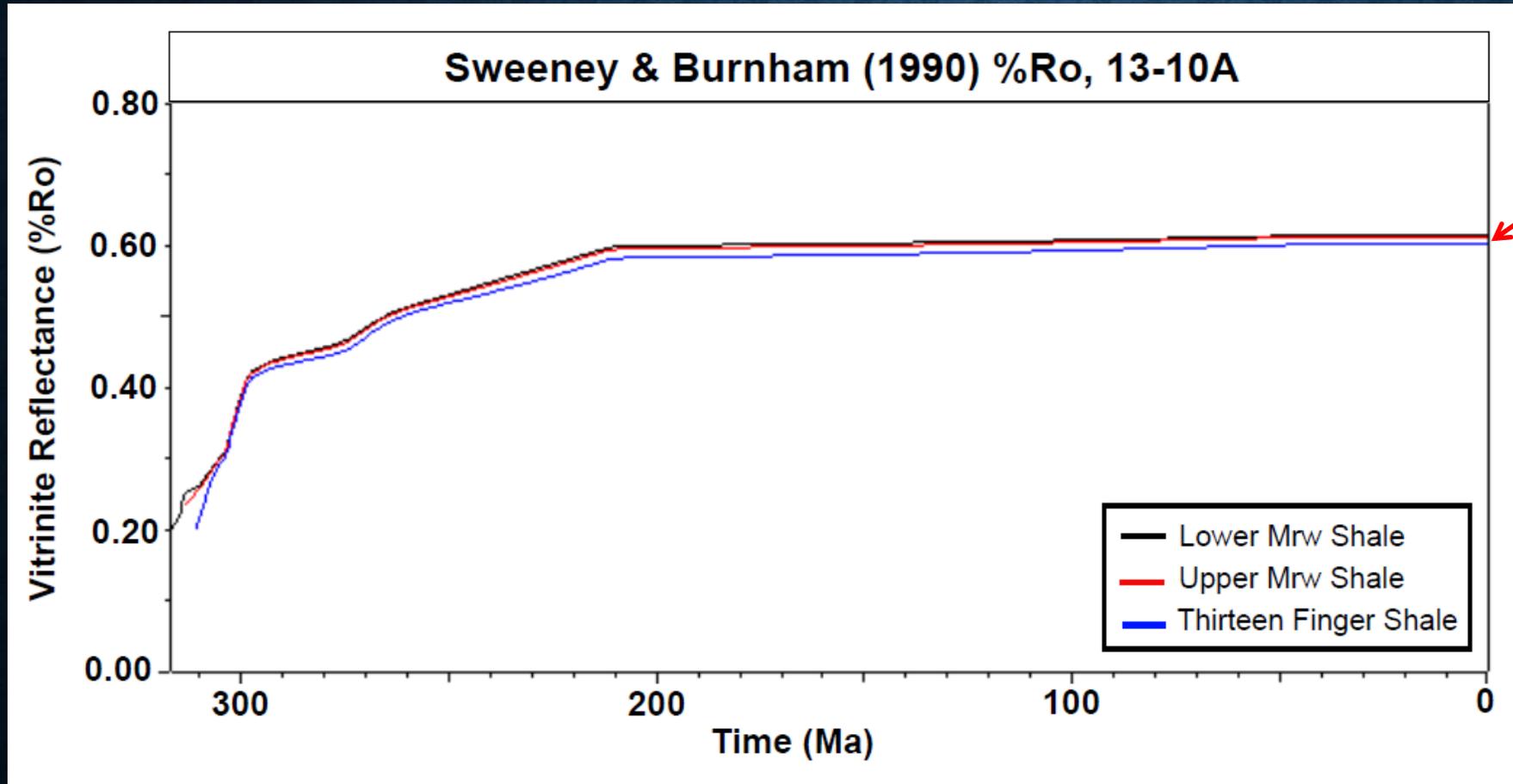
- 13-10A vitrinite reflectance values range from 0.60-0.83 %Ro, mean: 0.72 %Ro

HIGH HEATFLOW VITRINITE PREDICTION



54mW/m² scenario:
Predicted values ~0.8 %Ro

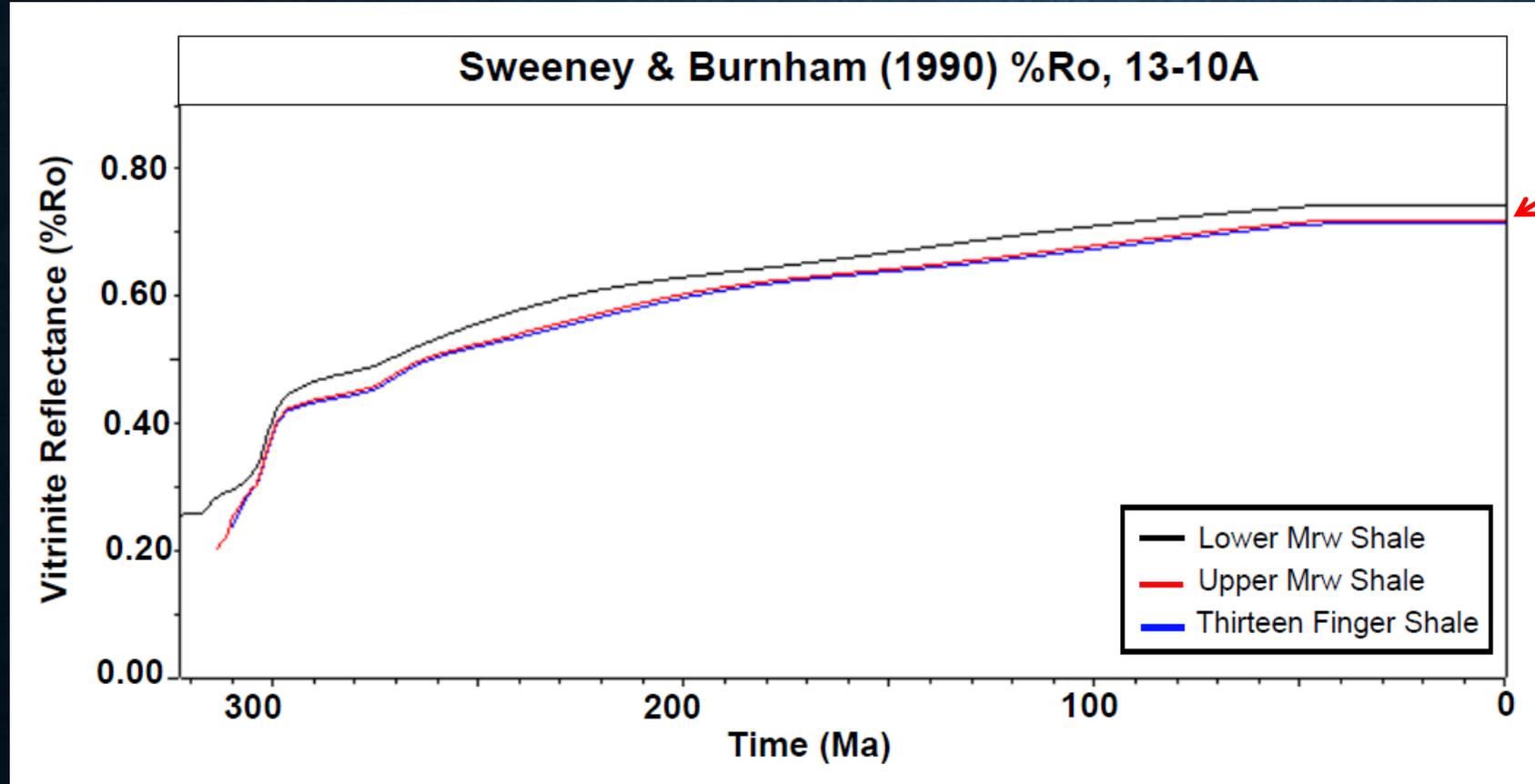
LOW HEATFLOW VITRINITE PREDICTION



30mW/m² scenario:

Predicted values ~0.6 %Ro

MID HEATFLOW VITRINITE PREDICTION

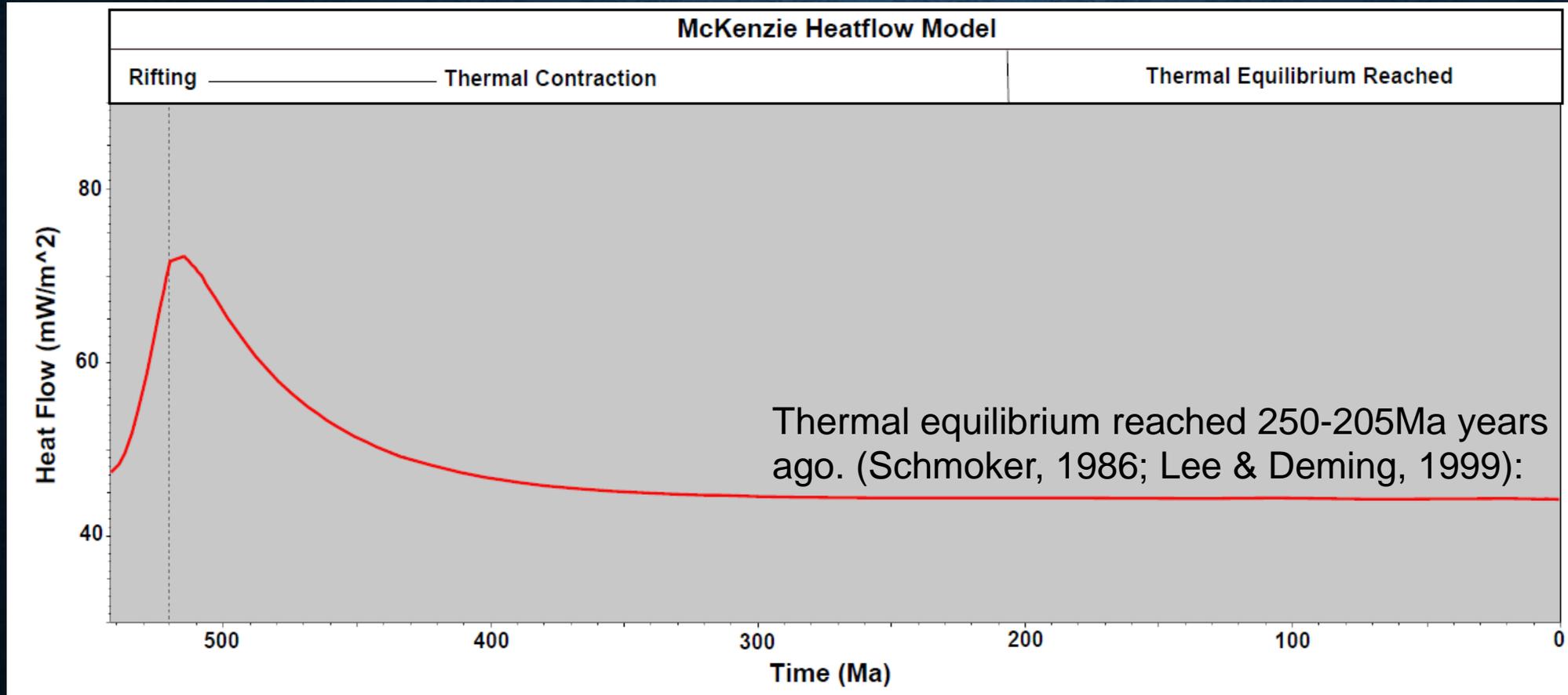


42mW/m² scenario:

Predicted values ~0.7 %Ro

*Closest match to 13-10A
lab measured mean 0.72%Ro

BOUNDARY CONDITIONS 1D: BASAL HEAT FLOW MID SCENARIO



Others Boundary Conditions: Surface Temperature
(Paleo-Climates Models: Wygrala, 1989)

*Model also does radiogenic heat

Models for Capillary Entry Pressure Curves

The following models describe the capillary entry pressure values for hand specimens, in a mercury(Hg)-air system.

1. **"a*perm^b" model:** A general relationship between permeability and capillary entry pressures of the following type is proposed by several authors (Ibrahim, 1970; Hildebrand, 2004; Hirasaki 2006):

$$P_c[MPa] = a \cdot k[mD]^b$$

Default parameters are (a=0.37, b=-0.24) according to Hildebrand.

(A.Hildebrand, S.Schlömer, B.M.Krooss and R.Littke: Gas breakthrough experiments on pelitic rocks: comparative study with N₂, CO₂ and CH₄. Geofluids, 4:61-80, 2004)

2. **"a*(10^(b*por))" model:** This model combines the above P_c(k) relationship with the linear relationship of log k(φ). This gives the following equation for capillary entry pressure: $P_c[MPa] = a \cdot 10^{b\phi}$
The default parameters use the lower part of the bilinear (multipoint model) log k(φ) curves and the above "a*perm^b" law with the Hildebrand parameters. The curve is then identical to model 1 for porosities < 25%, but with lithotype dependent parameters. This allows pressure and seal capacity calibration to be handled separately.

3. **"a*por+b" model (Default):** This model comes in 3 types – constant, linear and bilinear. In the first, P_c has no porosity dependence. In the linear type, P_c is calculated from porosity using the linear parameters a and b. In the bilinear type, these are used only for porosities up to 25%; at greater porosities, P_c drops linearly towards a value of 0 at the initial porosity. By default a and b are fitted to P_c values obtained from model 1, using the Hildebrand parameters (0.37, -0.24) for P_c at 1% porosity and Ibrahim's parameters (0.548, -0.33) for P_c at 25% porosity.

4. **Formula:** A user-defined formula giving capillary entry pressure as a function of several possible variables. Syntax is similar to that used by the Overlay Calculator. Available variables are listed below the entry box. During formula input, the syntax will be checked and any errors in the current formula will be shown in red.

Mixing: All capillary entry pressures are mixed arithmetically. This is a strong simplification.

Upscaling: Basin scale values are calculated from the hand specimen values divided by the upscaling factor. Upscaling decreases the P_c values. An upscaling factor of 2.56 is proposed for clastic rocks and carbonates, no upscaling (factor=1) otherwise.

Conversion to Oil-Water and Gas-Water Systems: is controlled by the interfacial tension values of oil and gas (IFT_{o,g}). The IFT values are temperature and pressure dependent. They are calculated during simulation.

$$P_{c_{o,g}} = P_{c_{Hg}} \cdot \frac{IFT_{o,g}}{360.8 \text{ mNm}^{-1}}$$

Column Heights: are controlled by the differences between water and petroleum densities (ρ_w, ρ_{o,g}).

$$h_{o,g} = \frac{P_{c_{o,g}}}{9.81 \frac{m}{s^2} \cdot (\rho_w - \rho_{o,g})}$$

Models for Chemical Compaction

Chemical effects can cause local re-arrangement of rock matrix material, leading to compaction, porosity loss and associated pressure generation. Chemical compaction models give the rate of porosity loss with time as a function of temperature, possibly effective stress, and model-specific parameters.

Mudstone Chemical Compaction Model: This model can only be used when the mudstone *mechanical* compaction model is also used. In that model, the material parameters e_{100} and β are constant; this model causes them to decay with time via a thermally activated reaction, causing additional porosity reduction. The parameters are the frequency factor and activation energy of the decay reaction, and the maximal e_{100} and β reductions; the latter are the percentages of the initial e_{100} and β values, respectively, that are subject to decay.

Schneider Chemical Compaction Model: This model applies a temperature and effective-stress dependent *viscoplastic* compaction. That is, a porosity loss rate related to the current effective stress is introduced, described by a viscosity which drops with increasing temperature. The physical mechanism is not specified; therefore, the model could be applied to chalk, quartz, etc. The porosity loss rate is:

$$\frac{\partial \phi_{CC}}{\partial t} = (1 - \phi) \frac{\sigma}{\mu} \quad \text{where} \quad \mu = \mu^0 e^{\frac{E_\mu}{R} \left(\frac{1}{T} - \frac{1}{T^0} \right)}$$

where μ is the viscosity, μ^0 is its reference value at temperature T^0 , and E_μ is the associated activation energy.

F. Schneider et al.: *Mechanical and chemical compaction model for sedimentary basin simulators*, Tectonophysics 263 (1996) 307-317

Walderhaug Quartz Cementation Model: Quartz cementation is modelled as a precipitation rate-limited reaction, controlled by the temperature and the quartz surface area available for precipitation. The porosity loss rate is:

$$\frac{\partial \phi_{CC}}{\partial t} = \frac{M}{\rho} \frac{(1 - C) f \phi}{D \phi_b} A e^{-E_a/RT}$$

where C is the quartz grain coating factor, the fraction (0 to 1) of the quartz grain surfaces that are coated and unsuitable for precipitation (therefore, a value of 1 will completely prevent cementation); f is the quartz grain volume fraction, the fraction (0 to 1) of the detrital grains that are quartz; D is the quartz grain size, the average size of the quartz grains; and A and E_a are the frequency factor and activation energy, respectively, of quartz precipitation. The fixed parameters M and ρ are quartz mol mass and density, respectively.

O. Walderhaug: *Modeling Quartz Cementation and Porosity in Middle Jurassic Brent Group Sandstones of the Kvitebjøen Field, Northern North Sea*, AAPG Bulletin, V.84, No.9 (September 2000), P. 1325-1339

Calibration Kinetic Model: Porosity loss due to chemical compaction is described by a selected reaction kinetic; the start value should be zero, the end value gives the maximum porosity loss (in percent), which is achieved when the reaction is complete.

Mixing: By default, no chemical compaction model is assigned to mixed lithologies.

Models for Geomechanical Properties

In the elastic model Hooke's law is used to relate stress and strain tensor by the 4th order stiffness tensor C: $\sigma = C : \varepsilon$. For an isotropic material the stiffness tensor is characterized by two parameters ν and E.

Poisson's Ratio: Poisson's ratio ν is defined as the negative ratio of transverse strain to longitudinal strain under conditions of uniaxial stress: $\nu = - \varepsilon_{\text{trans}} / \varepsilon_{\text{long}}$.

Modulus of elasticity: For an uniaxial stress state, the modulus of elasticity E is defined as the ratio of this stress to the strain in the respective direction: $E = \sigma_1 / \varepsilon_1$.

The following models determine the bulk modulus of elasticity for a lithology:

1.Constant: In this model the modulus of elasticity is fixed at the value E_{const} .

2. Linear from Porosity: In the range between initial and minimal porosity (ϕ_{initial} and ϕ_{min}) the modulus of elasticity is determined by a linear function of porosity:

$$E(\phi) = \frac{E_{\text{max}} - E_{\text{initial}}}{\phi_{\text{min}} - \phi_{\text{initial}}} \phi + E_{\text{max}} - \frac{E_{\text{max}} - E_{\text{initial}}}{\phi_{\text{min}} - \phi_{\text{initial}}} \phi_{\text{min}}$$

where E_{initial} and E_{max} are the moduli of elasticity at initial and minimal porosity, respectively.

3. From Compaction Curve: In this model the modulus of elasticity is based on the compressibility K used in mechanical compaction:

$$E = 3(1 - 2\nu) / C_v, \quad C_v = C_r \frac{3(1 - \nu)}{1 + \nu} = \frac{1}{K}$$

The plastic model comprises a yield surface $f(q,p,h)=0$, where q is the stress deviator, p the mean effective stress, and h the hardening parameter. The function $f(q,p,h)$ may depend on additional constant parameters: the tensile strength p_0 , the critical state pressures p_c and q_c , and the maximum mean pressure p_m .

Drucker Prager with Cap:

$$f(q,p,h) = \begin{cases} q - \chi p - k, & \chi = \frac{q_c}{p_c + p_0}, \quad k = q_0 + \chi p_0, \quad p \leq p_c' \\ \frac{q^2}{q_c^2} + \frac{(p - p_c')^2}{(p_c' - p_0)^2} - 1, & p \geq p_c' \end{cases}, \quad p_c' = p_c + h, \quad q_c' = q_c + h$$

D.C. Drucker and W. Prager, *Soil mechanics and plastic analysis or limit design*, Quart. Appl. Maths, **10**, 157 (1952).

Models for Permeabilities

The following models describe vertical and horizontal hand specimen permeabilities.

- 1. Multipoint Model (Default):** Any (multipoint) curves can be used for vertical hand specimen permeabilities k_{vh} dependent on porosity. The corresponding horizontal hand specimen permeabilities k_{hh} are calculated from the vertical values multiplied with the anisotropy factor a : $k_{hh} = a \cdot k_{vh}$

The permeability values are shown on logarithmic scale in log(mD), that means:
10 mD = 1 log(mD); 1 mD = 0 log(mD); 0.1 mD = -1 log(mD); 0.01 mD = -2 log(mD) ...

The default curves for most of the lithotypes are bilinear in terms of logarithmic values for permeabilities.

- 2. Kozeny-Carman Model:** This very popular relationship is based on tube-like models of rock pore space and has been modified by several authors. The following equation describes vertical hand specimen permeabilities.

$$k[m^2] = F \cdot \frac{20\phi^5}{S^2(1-\phi)^2} \quad \text{if } \phi < 10\% \qquad k[m^2] = F \cdot \frac{0.2\phi^3}{S^2(1-\phi)^2} \quad \text{if } \phi > 10\%$$

with $\phi' = \phi - 3.1 \cdot 10^{-10} S$ and the specific surface area S in m^2/m^3 and scaling Factor F .

The corresponding horizontal hand specimen permeabilities k_{hh} are calculated from the vertical values multiplied with the anisotropy factor a .

(P.C.Carman: Flow of gases through porous media: Academic Press Inc., 1956)

- 3. Formula:** A user-defined formula giving permeability as a function of several possible variables. Syntax is similar to that used by the Overlay Calculator. Available variables are listed below the entry box. During formula input, the syntax will be checked and any errors in the current formula will be shown in red.

Mixing: Permeabilities are mixed geometrically for homogeneous mixtures of lithotypes. In layered mixtures the horizontal values are mixed arithmetically and the vertical values are mixed harmonically.

Upscaling: Basin scale values for horizontal and vertical permeabilities are calculated from the hand specimen values multiplied with the horizontal and vertical upscaling factor respectively. Upscaling factors are measured for sandstones: 500 (horizontal) and 10 (vertical). IES suggests upscaling factors of 50 (horizontal) and 1 (no upscaling vertical) for all clastic rocks and carbonates and no upscaling (factor =1) otherwise.

Models for Radiogenic Heat Production

The Radiogenic heat values are given as rock matrix values (Q_r) and converted to bulk values during the simulation via multiplication with $(1-\phi)$. The following models can be used to define the rock matrix value for radioactive heat production.

- 1. Estimation from Lithology (Default):** Estimated or measured Uranium (U in ppm), Thorium (Th in ppm) and Potassium (K in %) concentrations within the rock material are used to calculate the rock matrix heat production rate after Rybach as follows.

$$Q_r [\mu W / m^3] = 0.00001 \cdot \rho [kg / m^3] \cdot (9.52U + 2.56Th + 3.48K)$$

(L. Rybach: Wärmeproduktionsbestimmungen an Gesteinen der Schweizer Alpen, Beiträge zur Geologie der Schweiz. Geotechnische Serie(51)43, 1973, Kümmerly & Frei.)

- 2. Spectral Gamma Ray:** Concentrations of U, Th and P can also be obtained from spectral gamma ray measurements. These values are bulk values measured with a core sample porosity ϕ_c . The corresponding rock matrix values are calculated using the above equation from Rybach and multiplying the (core sample bulk) radioactive heat production value with $1/(1-\phi_c)$.

- 3. Gamma Ray API:** Gamma ray API values can be used to calculate rock matrix values for heat production after Bückner and Rybach as follows.

$$Q_r [\mu W / m^3] = 0.0158 \cdot (API - 0.8)$$

(C.Bücker and L. Rybach: A simple method to determine heat production from gamma logs. Marine and Petroleum Geology, (13):373-377, 1996)

- 4. Matrix Heat Production Values:** Enter values directly into the field. Choose this option to influence the radiogenic heat in the **Create Heatflow Maps from McKenzie Crustal Model** process in **PetroBuilder 2D** and **PetroBuilder 3D**. Changing the Uranium, Thorium or Potassium values will not affect the McKenzie

Geological Age Correction: Concentrations of radioactive elements are present-day values (U, Th, K). Paleo-values (U_p , Th_p , K_p) are higher corresponding to their half-lives as follows (with t in My). The correction can only be applied to models 1 and 2.

$$U_p = U \cdot (1 + 2.77 \cdot 10^{-4}t - 7.82 \cdot 10^{-3}t^2 + 4.53 \cdot 10^{-12}t^3) \quad Th_p = Th \cdot \exp(0.00005t); \quad K_p = K \cdot \exp(0.000555t)$$

Mixing: Rock matrix values of heat production are always averaged arithmetically for mixtures of lithotypes. Bulk values are obtained from rock matrix values multiplied with $(1-\phi)$.

Models for Specific Heat Capacity

The following models describe temperature dependent specific heat capacity values for rocks (c_r , in kcal/kg/K):

- 1. Waples Model for Rocks (Default):** This equation can be applied to any mineral, lithology or rock value except for kerogen and coal.

$$c_r = c_{20}(0.953 + 2.29 \cdot 10^{-3}T - 2.835 \cdot 10^{-6}T^2 + 1.191 \cdot 10^{-9}T^3) \quad (\text{T in } ^\circ\text{C})$$

(D.W. Waples and J.S. Waples: A review and evaluation of specific heat capacities of rocks, minerals and subsurface fluids. Part1: Minerals and nonporous rocks, natural resources research. 13: 97-122, 2004a)

- 2. Multipoint Model:** A multipoint curve is given for specific heat capacity values vs. temperatures in an interval between the minimum and maximum temperature. Outside the interval the curve is continued with a constant value.

- 3. Kerogen/Coal:** The following function can be used for kerogen and coal (reference same as for model 1).

$$c_r = 2.39 \cdot 10^{-4} (1214.3 + 6.2657 \cdot 10T - 0.12345T^2 + 1.7165 \cdot 10^{-3}T^3 - 1.1491 \cdot 10^{-5}T^4 + 3.5686 \cdot 10^{-8}T^5 - 4.1208 \cdot 10^{-11}T^6) \quad (\text{T in } ^\circ\text{C})$$

- 4. Forsterite and Fayalite Functions:** Special temperature dependent functions are available for crustal materials. These functions are also valid for very high temperatures.

Forsterite $c_r = 1.55 \cdot 10^{-3} (238.64 - 2001.3 \frac{1}{\sqrt{T}} - 11.624 \cdot 10^7 T^{-3}) \quad (\text{T in K})$

Fayalite $c_r = 1.55 \cdot 10^{-3} (248.93 - 1923.9 \frac{1}{\sqrt{T}} - 13.910 \cdot 10^7 T^{-3})$

- Mixing:** Rock specific heat capacity values are always averaged arithmetically for mixtures of lithotypes. Bulk values of specific heat capacity are obtained by arithmetic averaging.

Models for Thermal Conductivity

The following models describe temperature dependent thermal conductivities for rocks (λ_r):

1. Sekiguchi Model (Default): This very general equation can be applied to any mineral, lithology, kerogen and coal.

$$\lambda_r = 1.84 + 358 \cdot (1.0227 \lambda_{20} - 1.882) \left(\frac{1}{T} - 0.00068 \right) \quad (T \text{ in K})$$

(K. Sekiguchi: A method for determining terrestrial heat flow in oil basinal areas. In Cermk, L. Rybach, and D.S. Chapman, editors, Terrestrial Heat Flow Studies and Structure of the Lithosphere, volume 103 of Tectonophysics, pages 67-79, 1984)

Claystones experience changes in their anisotropy factor during compaction based on the orientation of the grains. This effect is described with one additional parameter: the depositional anisotropy factor. The general anisotropy factor is then considered as a limit for completely compacted sediments (porosity=0).

(D.W. Waples and H. Tiersgaard: Changes in matrix thermal conductivity of clays and claystones as a function of compaction. Petroleum Geoscience, 8:365-370, 2002)

2. Multipoint Model: A multipoint curve is given for thermal conductivities vs. temperatures in an interval between the minimum and maximum temperature. Outside the interval the curve is continued with a constant value.

3. Felsic, Mafic, Olivine Functions: Special temperature dependent functions are available for crustal materials. These functions are also valid for very high temperatures.

Olivine

Felsic Rocks

Mafic Rocks

$$\lambda_r = 0.0023 \cdot (T_c - 226.84) + \frac{1}{(0.0005T_c + 0.221)}$$

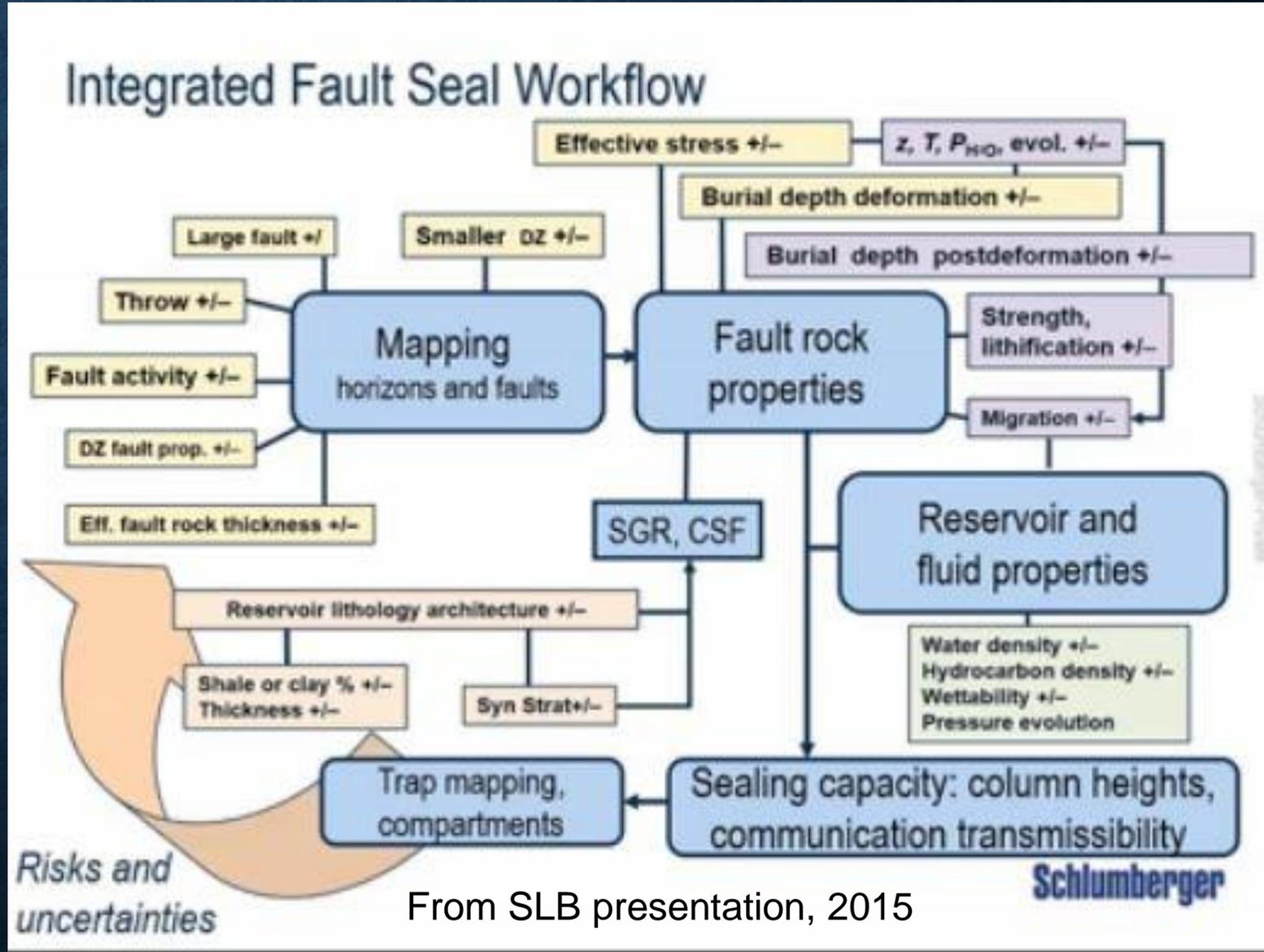
$$\lambda_r = 0.64 + \frac{807}{(T_c + 350)}$$

$$\lambda_r = 1.18 + \frac{474}{(T_c + 350)} \quad (T_c \text{ in } ^\circ\text{C})$$

Anisotropy: All the above model function describe the vertical values (λ_v). Horizontal values (λ_h) are defined with the anisotropy factor a : $\lambda_h = a \cdot \lambda_v$

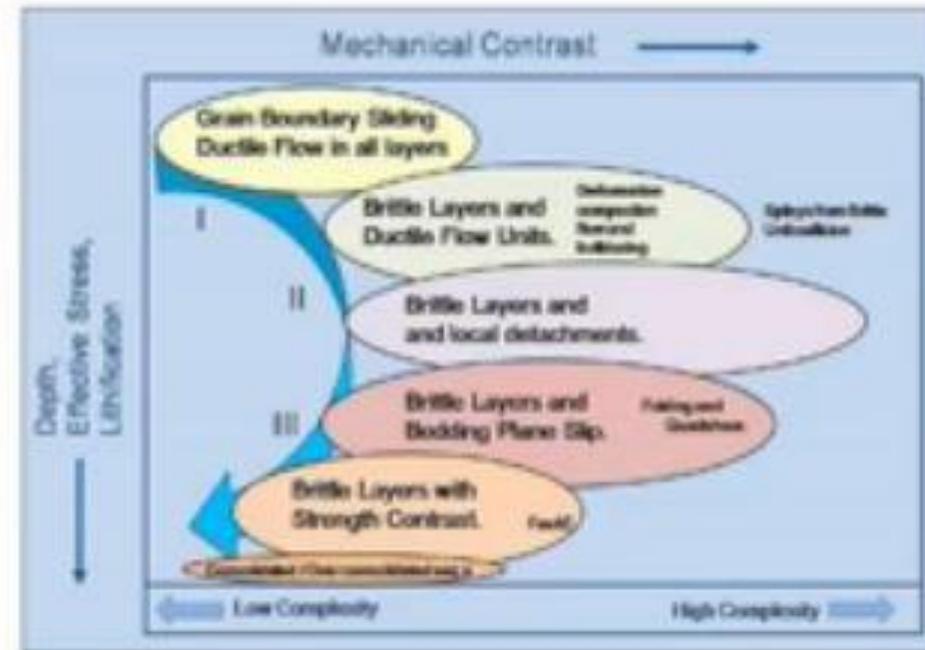
Mixing: Rock thermal conductivities are mixed geometrically for homogeneous mixtures of the lithotypes. In layered mixtures the horizontal values are mixed arithmetically and the vertical values are mixed harmonically. The bulk thermal conductivity is obtained by geometrically averaging the rock matrix and pore values.

PSM: AN AID TO FLOW MODELING ALONG FAULTS



PSM: AN AID TO FLOW MODELING ALONG FAULTS

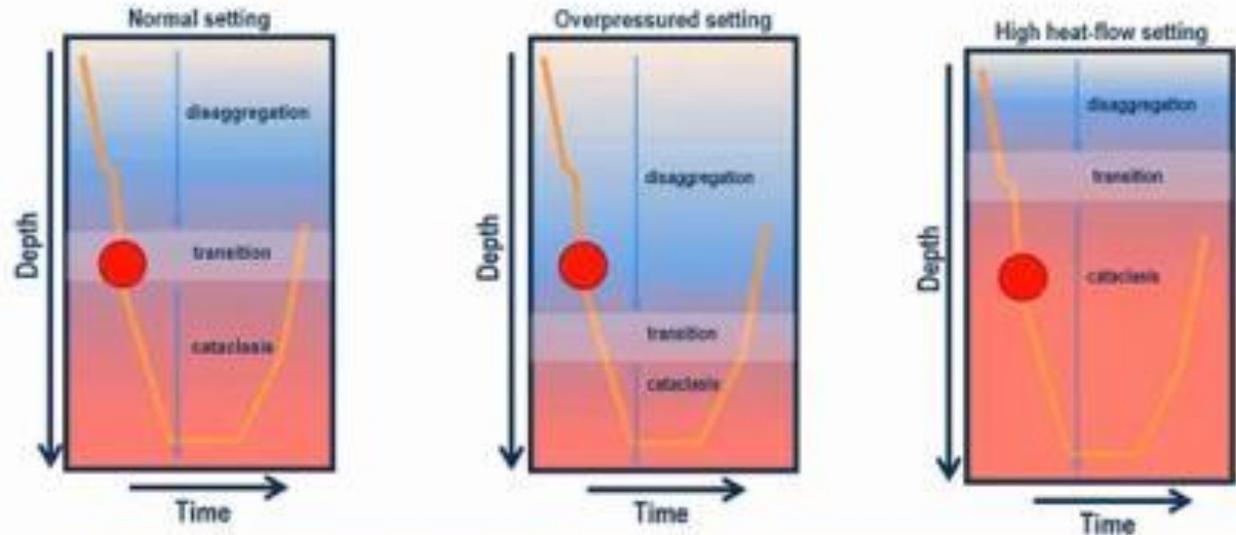
Fault Mechanism Diagram



- Fault complexity increases with mechanical contrast but changes with mean effective stress or geohistory.
- These concepts improve prediction of fault zone architecture, fault rock algorithms, and cross-fault flow resistance.

PSM: AN AID TO FLOW MODELING ALONG FAULTS

Local Calibration and Impact of Burial History



- The deformation to deformation is influenced by the burial history and basin evolution.
- Controls on deformation process.
 - Rocks at the same depth of burial may have undergone very different pressure and temperature conditions, changing the deformation mechanisms.
- Local calibrations required to capture the impact of local geohistory.

SPERREVIK FAULT MODEL

- Similar lithological scenario to FWU (shales and sandstone)
- Similar max burial depths (3000m's)
- Most customizable inputs

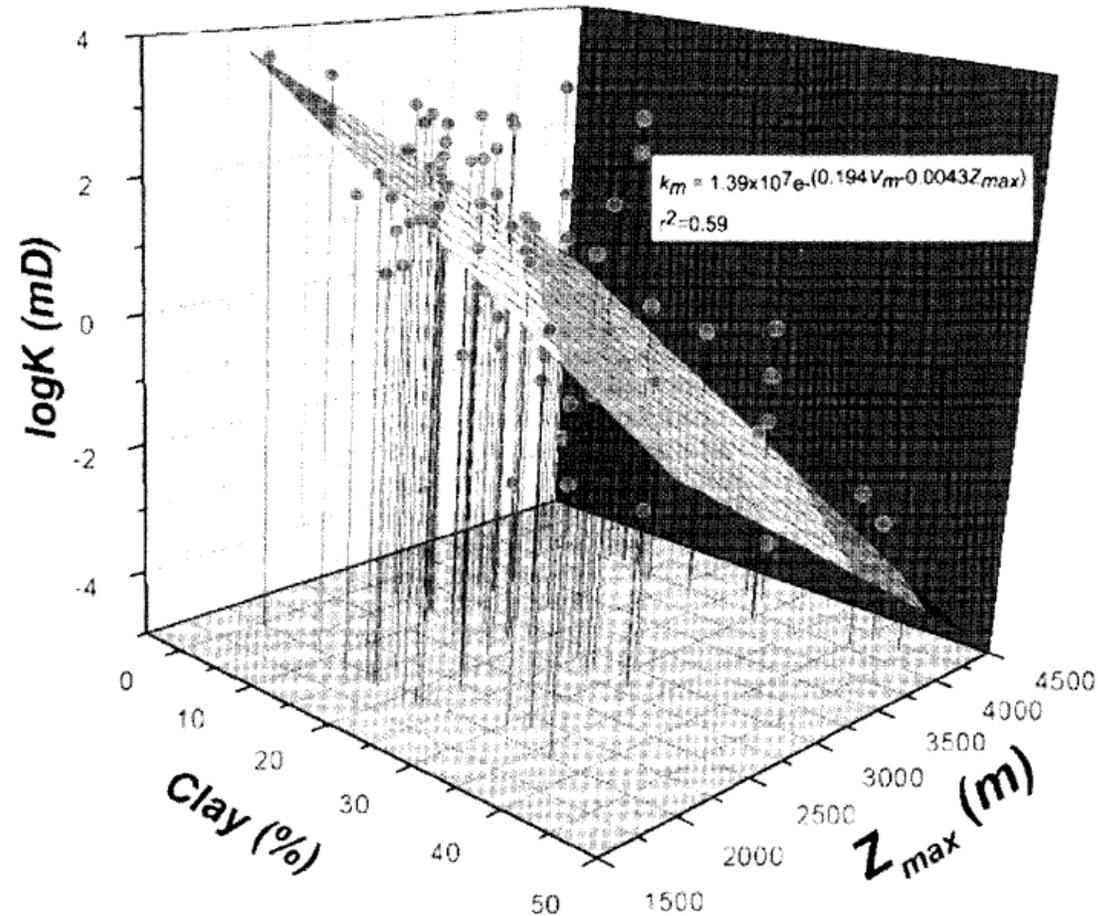


Fig. 3. 3D plot showing the relationship between measured clay content, permeability, and maximum burial depth for host rocks. The plane represents the exponential least squares regression (Eq. 4).

From Sperrevik et al. (2002)

13-10A: 1D MODEL PRIMARY INPUTS

Model Parameters:

Cell Size: 8m

Max Time Step: 10Ma

EOS: Peng Robinson

Layer	Top (m)	Base (m)	Thick (m)	Eroded (m)	Depo From (m)	Depo to (Ma)	Eroded From (Ma)	Eroded to (Ma)	Lithology	PSE	TOC	Kinetic	HI
Permian/Ceno	0	619	619	1000	270	50	50	30	Sandstone (subarkose, clay rich)	Overburden Rock			
Red Cave	619	722	103		275	270			Siltstone (organic lean)	Overburden Rock			
Wellington	722	1002	280		280	275			Sandstone (typical)	Overburden Rock			
Wolfcampian	1002	1498	496		299	280			Dolomite (typical)	Overburden Rock			
Virgilian	1498	1746	248		303	299			Shale (typical)	Overburden Rock			
Missourian	1746	1879	133		304	303			Shale (typical)	Overburden Rock			
Kansas City	1879	2010	131		305	304			Limestone (shaly)	Overburden Rock			
Marmaton	2010	2082	72		305.3	305			Limestone (shaly)	Seal Rock			
Cherokee	2082	2384	302		310	305.3			Shale (typical)	Seal Rock			
Thirteen Finger	2384	2421	37		311	310			Limestone (shaly)	Source Rock	9.18	Lewan(2002)_TII (WoodSh)	295.3
Upper Morrow Shale	2421	2433	12		313.7	311			Shale (organic rich, typical)	Source Rock	3.62	Lewan(2002)_TII (WoodSh)	116
Morrow B	2433	2441	8		314	313.7			Sandstone (subarkose, typical)	Reservoir Rock			
Lower Morrow Shale	2441	2624	183	15	324	314.5	314.5	314	Shale (organic rich, typical)	Source Rock	1.1	Lewan(2002)_TII (WoodSh)	10
Mississippian	2624	2745	121	150	354	330	330	324	Limestone (organic rich - typical)	Underburden Rock			
Woodford	2745	2758	13		369	354			Shale (organic rich, typical)	Source Rock	1.5	Lewan(2002)_TII (WoodSh)	300
Cambrian-Devonian	2758	3670	912		542	369			Limestone (organic rich - typical)	Underburden Rock			
Basement	3670	4670	1000		1500	542			Granite (> 1000 Ma old)	Underburden Rock			

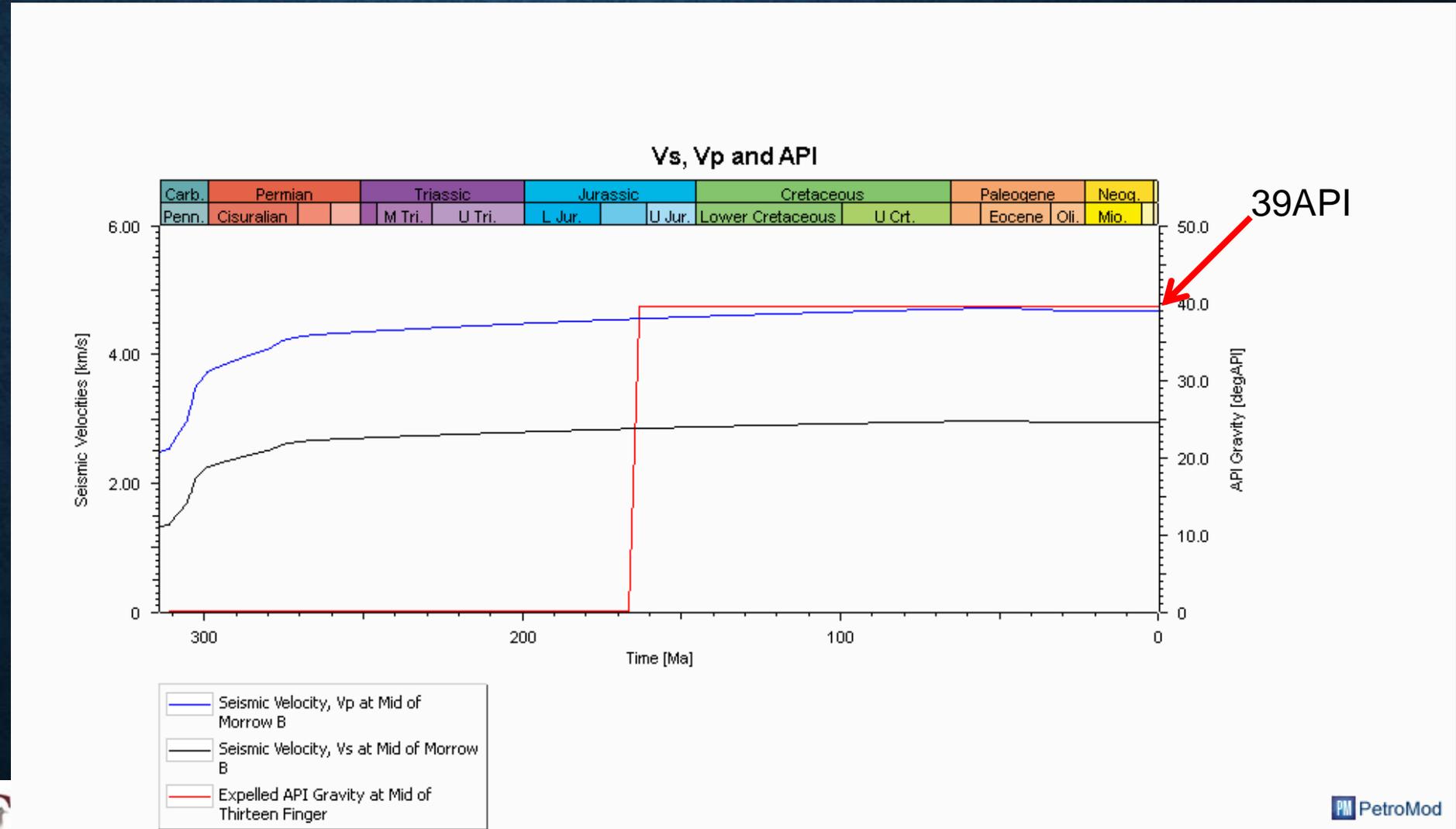
ADVANCED PREDICTIONS

Fluid and Seismic Properties

- FWU oil samples are 38API

- Bulk Kinetic model used for 1D (1 component)

- Compositional Kinetic model will be used for 2D (4 Components)



PRESSURE CONUNDRUM

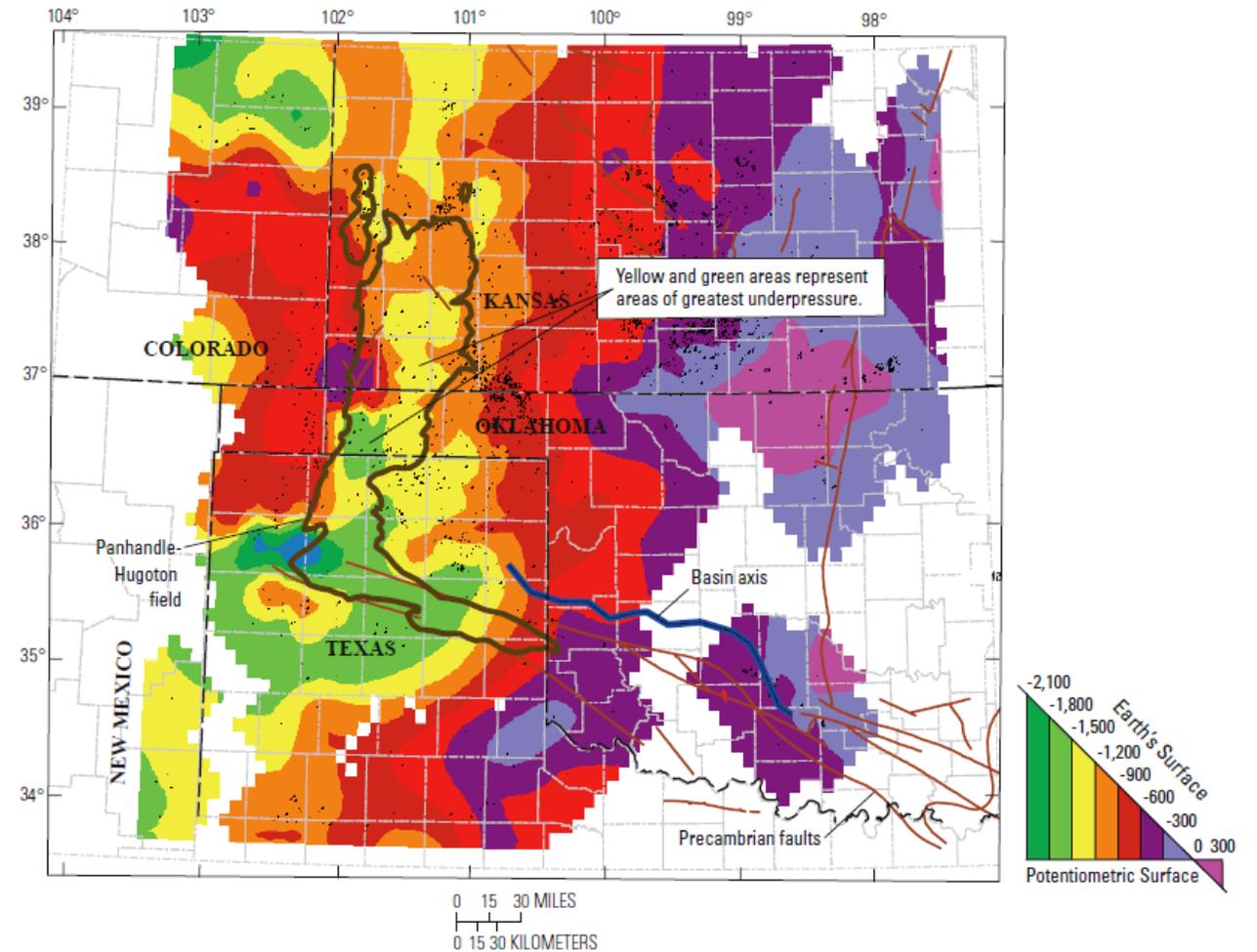
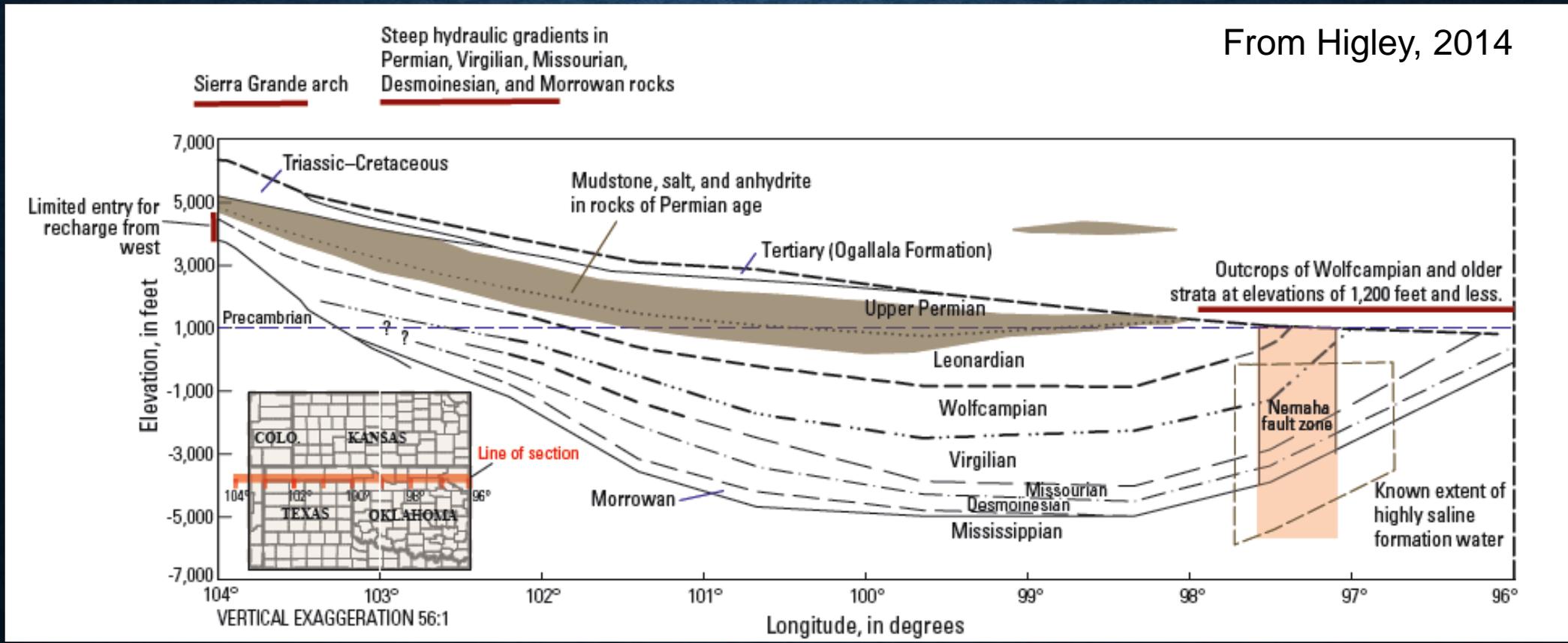


Figure 14. Map with contours showing separation between the potentiometric surface in Permian rocks and land surface elevation, in feet. For example, the yellow areas show where the potentiometric surface lies -1,500 to -1,800 ft below surface elevation. The underpressured Hugoton-Panhandle gas field lies in a trough of maximum separation between the potentiometric surface and surface elevation.

From Higley, 2014

CROSS SECTION FOR HYDROLOGIC REGIME

From Higley, 2014



PRESSURE CONUNDRUM

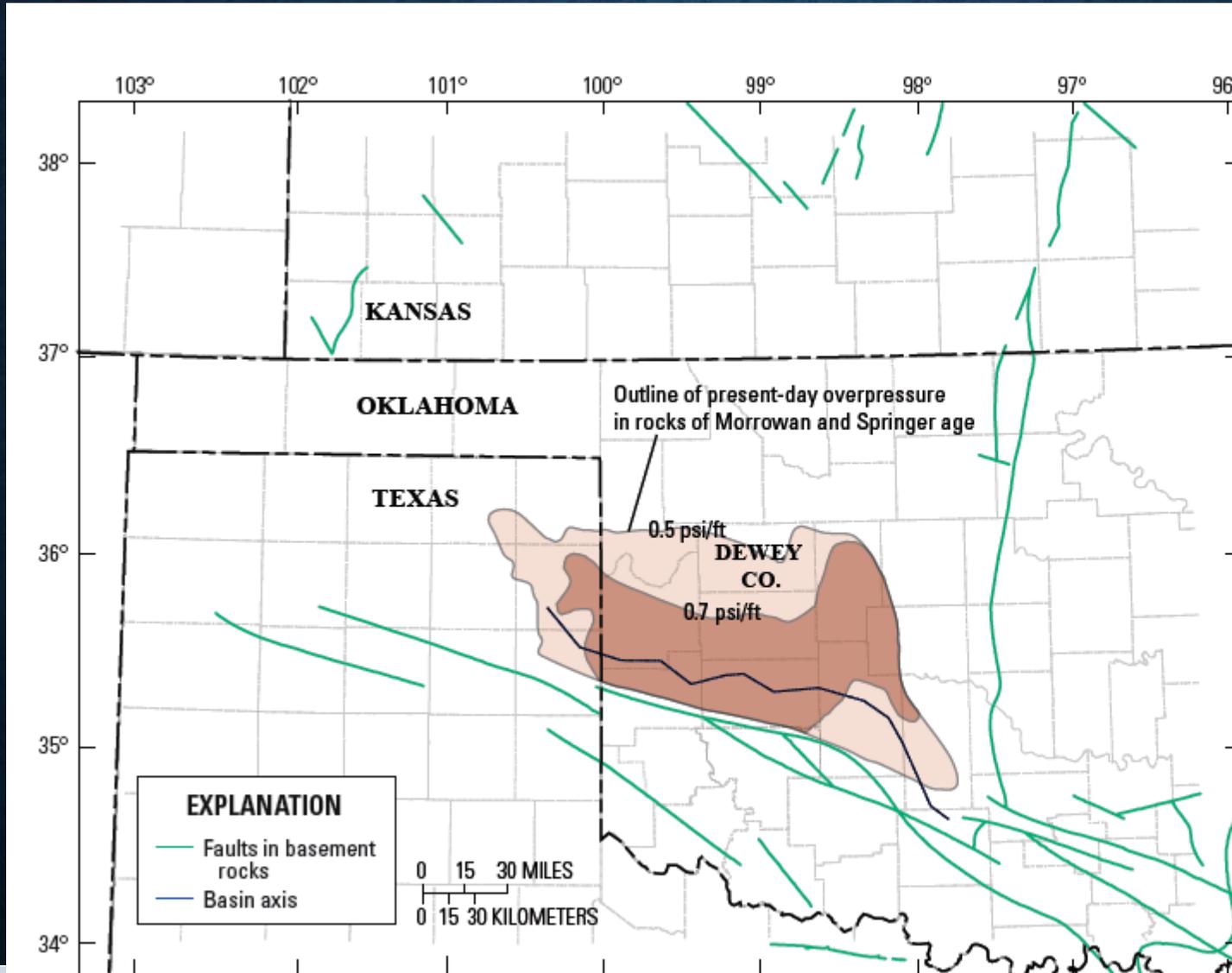


Figure 7. Map showing outline of present-day overpressure in rocks of Morrowan and Springer age, based on data from Al-Shaieb and others (1994a) and augmented by pressure data from IHS Energy (2009). Contour lines and shading represent the ratio of pressure to depth in pounds per square inch per foot (psi/ft).