

# Predicting Hydrocarbon Composition in Unconventional Reservoirs with a Compositional Generation/Expulsion Model\*

Daniel (Xinyu) Xia<sup>1</sup>, John M. Guthrie<sup>2</sup>, Caroline Burke<sup>2</sup>, Steven Crews<sup>2</sup>, and Yongchun Tang<sup>3</sup>

Search and Discovery Article #80397 (2014)\*\*

Posted August 18, 2014

\*Adapted from oral presentation given at 2014 AAPG Annual Convention and Exhibition, Houston, Texas, April 6-9, 2014

\*\*AAPG©2014 Serial rights given by author. For all other rights contact author directly.

<sup>1</sup>Hess, Houston, Texas, US ([xxia@hess.com](mailto:xxia@hess.com))

<sup>2</sup>Hess, Houston, Texas, US

<sup>3</sup>PEER Institute, Covina, California, US

## Abstract

Estimation of hydrocarbon compositions (GOR, CGR, and gas wetness) is critical to appraise unconventional reserves and to determine the production strategy. Unfortunately, estimation from basin modeling is challenging because it relies on a detailed and accurate description of hydrocarbon generation and migration processes. Based on state of the art knowledge obtained by recent exploration and production in shale plays, we have developed a practical model to predict the hydrocarbon compositions in shale plays. In this model, we applied a compositional reaction network for hydrocarbon generation. The compositions include specific gas components (methane, ethane, propane, butane, and pentane isomers), light oil (C6-C14 hydrocarbons), and heavy oil (C15+ hydrocarbons, resin, and asphaltene). The precursor fraction of these components and the kinetic parameters of precursor cracking are calibrated by the laboratorial high-pressure pyrolysis of the source rock in closed reactors. The retained and expelled hydrocarbon amounts are modeled by coupling the hydrocarbon generation and expulsion processes. The generated/cracked amount of hydrocarbons and their precursors are calculated from the retained precursor amount and temperature-dependent kinetic parameters. Hydrocarbon expulsion occurs when the retained hydrocarbon exceeds the storage capacity. The storage capacity is determined by pore volume, surface area, fluid density, and adsorption affinities; whereas the fluid density is determined by fluid composition, pressure, and temperature. Thermal history, pore volume, and pressure history are modeled separately as input. The expulsion of oil and gas is assumed to be through microfractures as Darcy flow. Resin and asphaltene components have such a high viscosity that they can only migrate when dissolved in oil. This mechanism brings about the compositional fractionation in oil during expulsion. The concentrations of mobile species in the instantaneous expelled fluid are proportional to the concentrations in the residual fluid. Retained hydrocarbons crack with increasing maturity (secondary cracking). Field data indicates that secondary cracking under geological conditions is self-accelerated, and the products are more enriched with methane than the laboratorial products. The model results are consistent with the production data from different shale plays, and provide details to help understand production behavior of tight reservoirs.

## **Selected References**

- Ewing, T.E., 2006, Mississippian Barnett Shale, Fort Worth basin, north-central Texas: Gas-shale play with multi-trillion cubic foot potential: AAPG Bulletin, v. 90/6, p. 963-966.
- McNeil, R.I, and W.O. BeMent, 1996, Thermal Stability of Hydrocarbons: Laboratory Criteria and Field Examples: Energy Fuels, v. 10/1, p. 60-67.
- Pollastro, R.M., D.M. Jarvie, R.J. Hill, and C.W. Adams, 2007, Geologic framework of the Mississippian Barnett Shale, Barnett – Paleozoic total petroleum system, Bend Arch–Fort Worth Basin, Texas: AAPG Bulletin, v. 91/4, p. 405–436.
- Tang, Y., and D. Xia, 2011, Quantitative Assessment of Shale Gas Potential Based on Its Special Generation and Accumulation Processes: AAPG, Search and Discovery Article #40819.
- Xia, D., 2014, Kinetics of gaseous hydrocarbon generation with constraints of natural gas composition from the Barnett Shale: Organic Geochemistry, DOI: 10.1016/j.orggeochem.2014.02.009.
- Xia, D., J. Chen, R. Braun, and Y. Tang, 2012, Improving Hydrocarbon Resource and Fluid Property Prediction with a Coupled Generation/Expulsion Model: AAPG, Search and Discovery Article #40958.
- Xia, D., and Y. Tang, 2010, Carbon Isotope Composition as an Indicator to Assess Oil-Cracking and Reforming Gas Contribution to Shale Resource Plays: AAPG Hedberg Convention, Search and discovery Article #90122.
- Zumberge, J., K. Ferworn, and S. Brown, 2012, Isotopic reversal (“rollover”) in shale gases produced from the Mississippian Barnett and Fayetteville formations: Marine and Petroleum Geology, v. 31/1, p. 43-52.



---

# Predicting Hydrocarbon Composition in Unconventional Reservoirs with a Compositional Generation/Expulsion Model

---

Daniel Xia, John Guthrie,  
Caroline Burke, Steve Crews (Hess Corporation),  
and Yongchun Tang (PEER Institute)

[xxia@hess.com](mailto:xxia@hess.com)

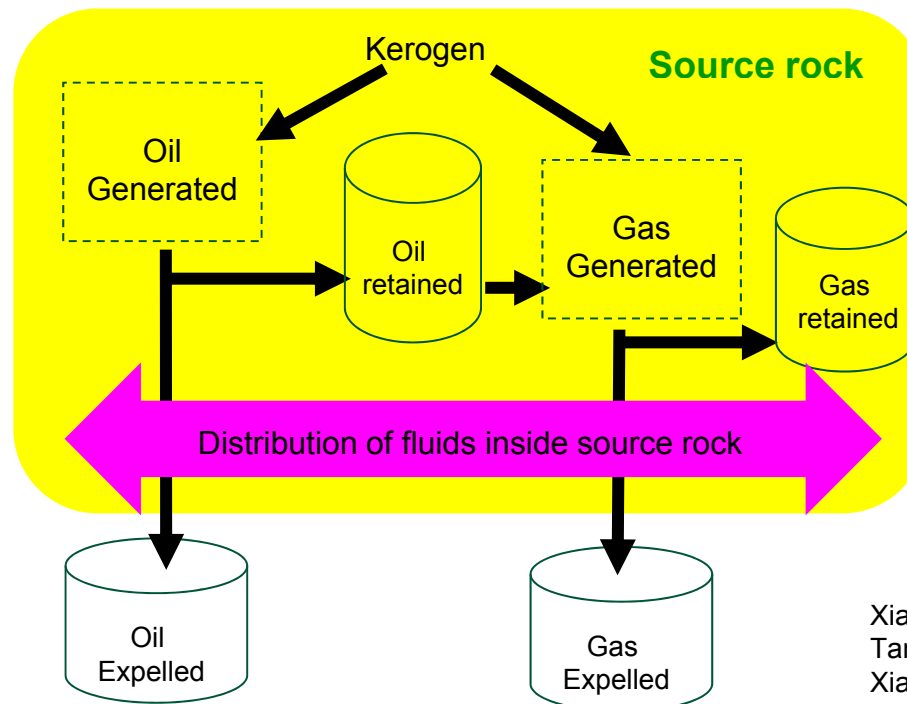


- To improve the estimation on hydrocarbon composition in unconventional resources
  - Gas-to-Oil ratio (GOR)
  - Gas composition (wetness or BTU)
- To optimize hydrocarbon generation parameters for basin modeling
  - Minimize the uncertainties (esp. in gas window)

# Scope of this work

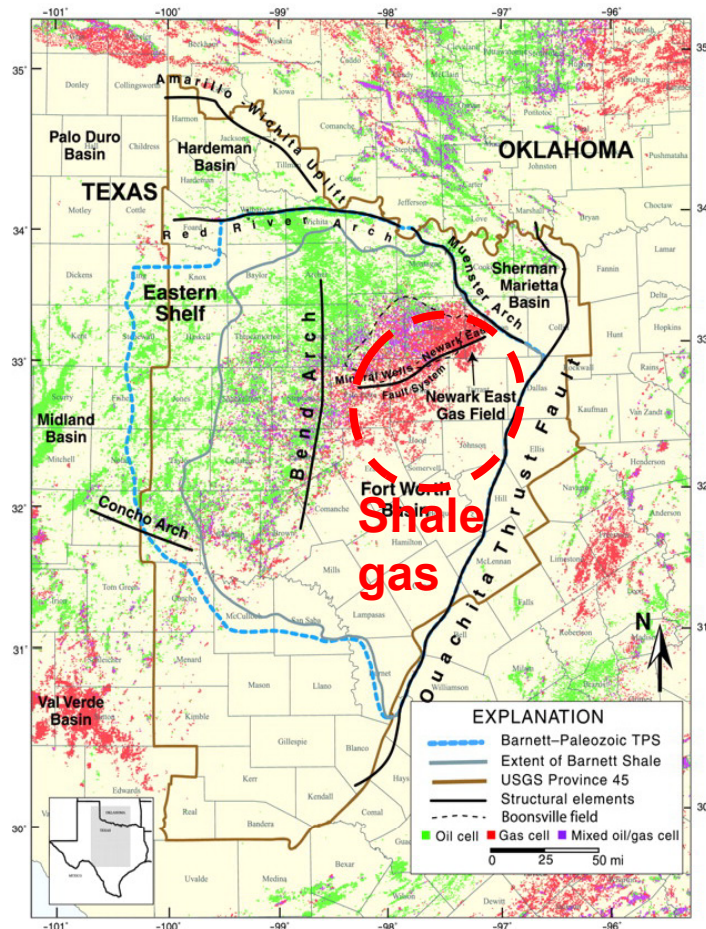


- Application of constraints from field data
  - RockEval HI with respect to  $R_o$ :  
Residual hydrocarbon generating potential  $\leftrightarrow$  source rock thermal maturity
  - GOR & gas wetness with respect to  $R_o$ :  
Oil/gas composition  $\leftrightarrow$  source rock thermal maturity
- Detailed generation / expulsion processes

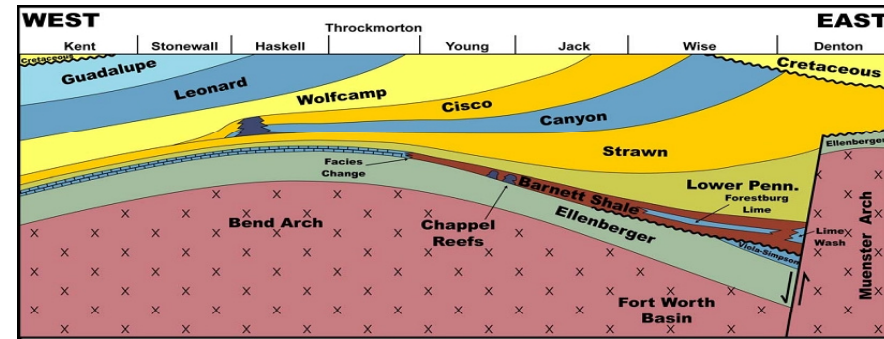


Xia and Tang, AAPG Hedberg Convention 2010  
Tang and Xia, AAPG Convention 2011  
Xia et al., AAPG Convention 2012

# Using the Barnett Shale as the example



Pollastro et al., AAPG Bull., 2007

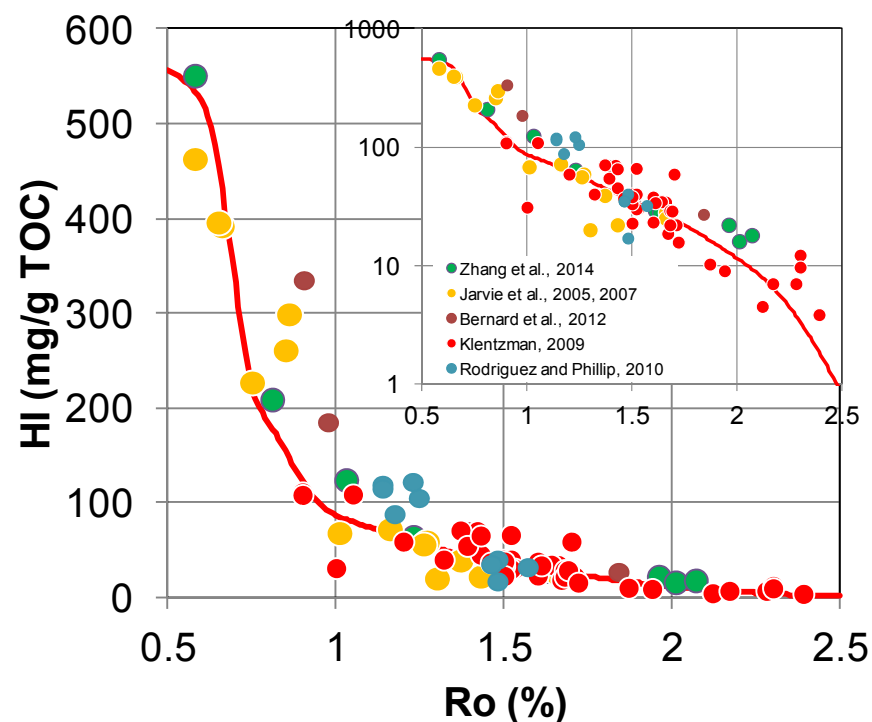


- Abundant published data
  - Burial history (Ewing, 2006)
  - GOR, composition of produced gas  
(Zhao et al., AAPG Bull. 2007; Klentzman, Master thesis of Baylor, 2009 ; Zumberge et al., Marine & Petroleum Geology 2012)
  - Source rock thermal maturity (Klentzman, 2009)
  - RockEval results  
(Jarvie et al. AAPG Bull. 2007; Rodriguez & Philip, AAPG Bull. 2010; Benard et al. Organic Geochemistry 2012; Zhang et al. 2014 in preparation)

# Constraints from HI



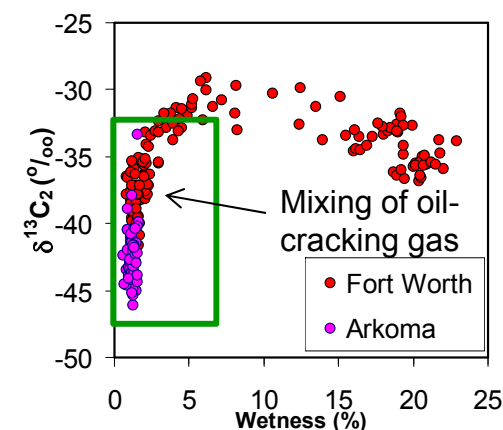
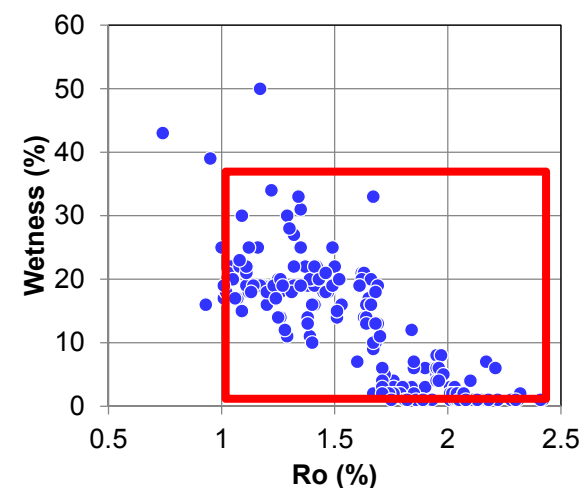
- Kerogen hydrocarbon potential depleted at  $R_o$  1.5 % - 2.0 %
  - Retained gas of  $R_o > 2.0\%$  is mainly products of early maturity stage, or from oil-cracking
- Relation largely independent of hydrocarbon migration
- Constraining kinetics of primary cracking
  - If  $A = 10^{13} \text{ s}^{-1}$ , then  $E = 49.5 - 59.5 \text{ kcal/mol}$  (bulk kinetics)



# Constraints from gas composition



- Wetness > 20% at low maturity
  - $\delta^{13}\text{C}$  of ethane and propane in the early wet gas much more positive than oil-cracking gas
    - Wet gas is mainly the early product of kerogen/bitumen, not from oil
    - Constraining the kinetics of methane and ethane generating from kerogen
- Rapid wetness drop at  $R_o$  1.5 – 2%: mechanism?
  - Most convenient answer – cracking of ethane and propane, but not supported by isotopic data
    - Ethane and propane are stable in source rock till  $R_o \sim 2\%$
  - The mechanism is flushing wet gas with dry gas



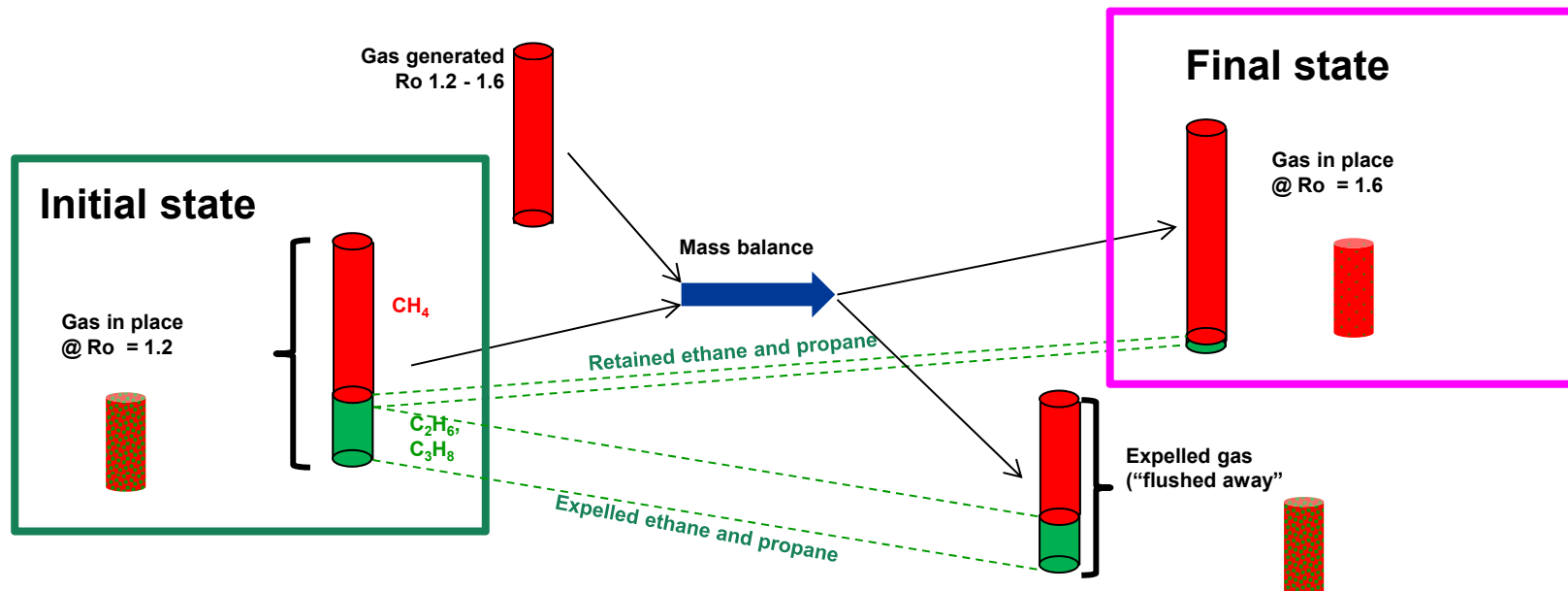
After Zumberge et al., Mar. Petrol. Geol. 2012



# Flushing the wet gas: rigorous constraint to retained oil amount



- Enough dry gas is required to flush the wet gas



- To decrease wetness from 20% to 2% at constant GIP, required methane generation amount is at least

$$\ln(20/2) = 2.3 \text{ times of original GIP}$$

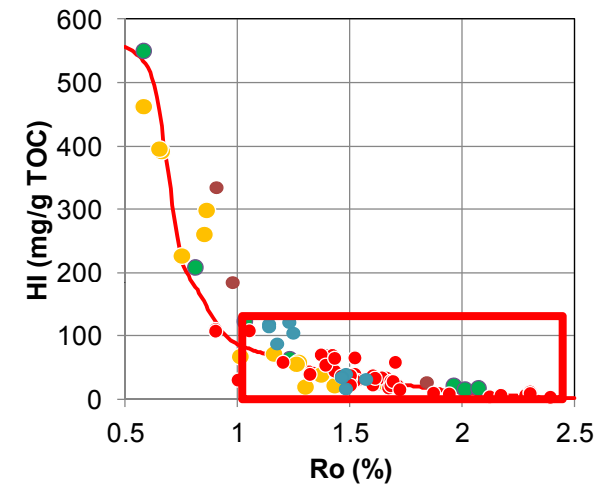
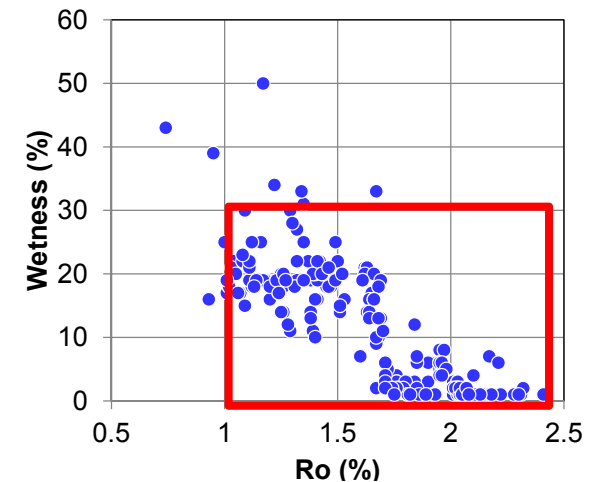
# Flushing the wet gas: rigorous constraint to retained oil (ctn'd)



- But kerogen HI depleted, cannot generate so much late gas
  - Methane in late gas is mainly from oil cracking
  - Oil cracking product is dominantly methane
    - Different from lab pyrolysis
    - Mechanism:  
oil attached to solid kerogen preferentially cleaves methyl groups (generating methane)

(McNeil and BeMent, Energy Fuels 1996)

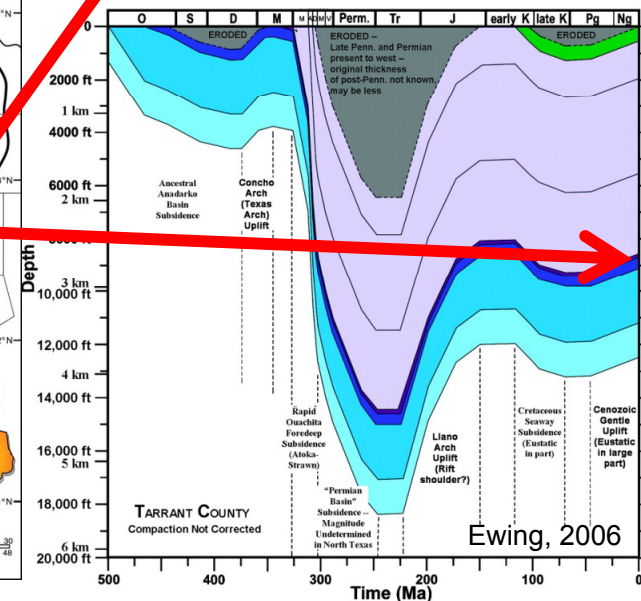
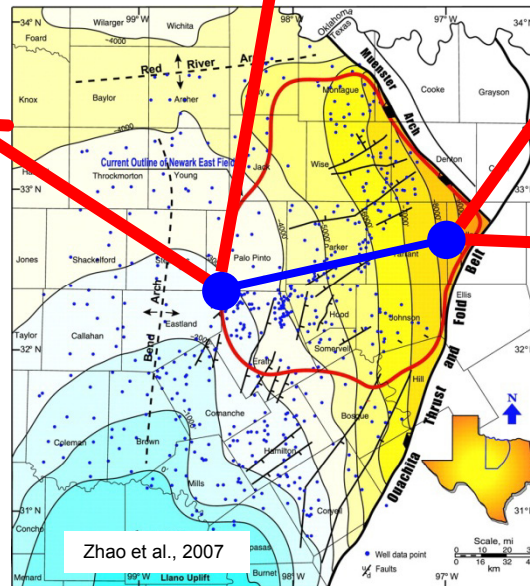
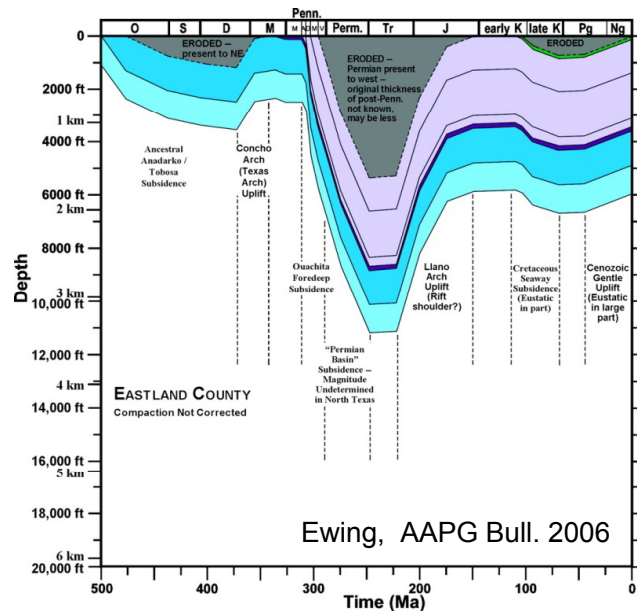
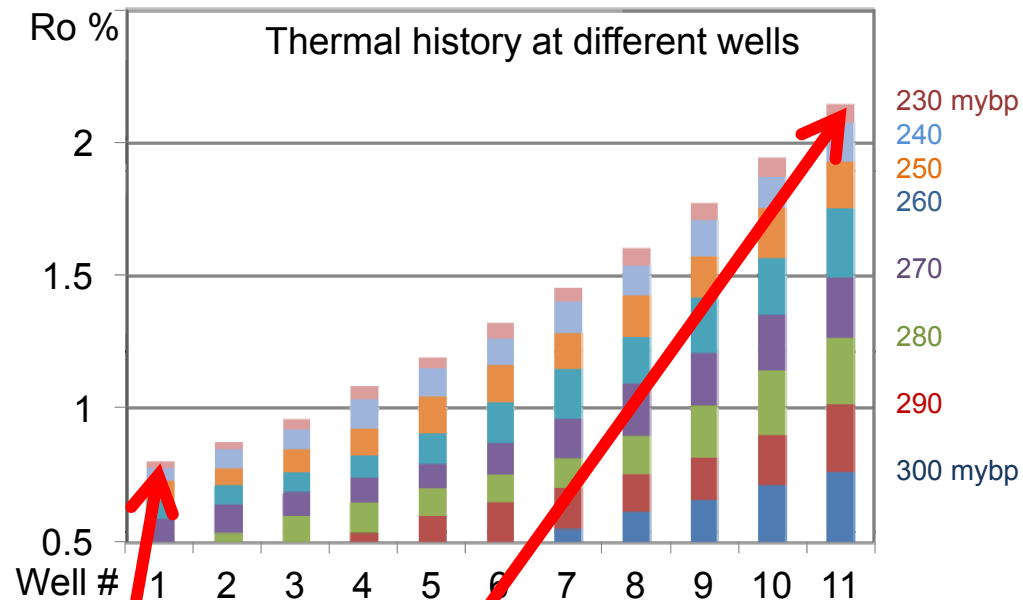
- Oil cracking peak:  $R_o$  1.5 – 2%
  - Accompanied by rapid increase of GOR



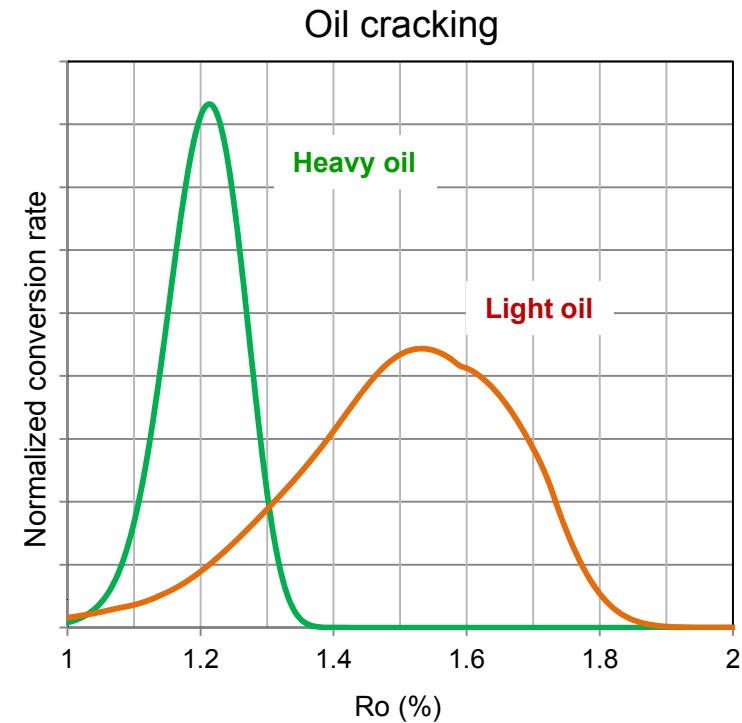
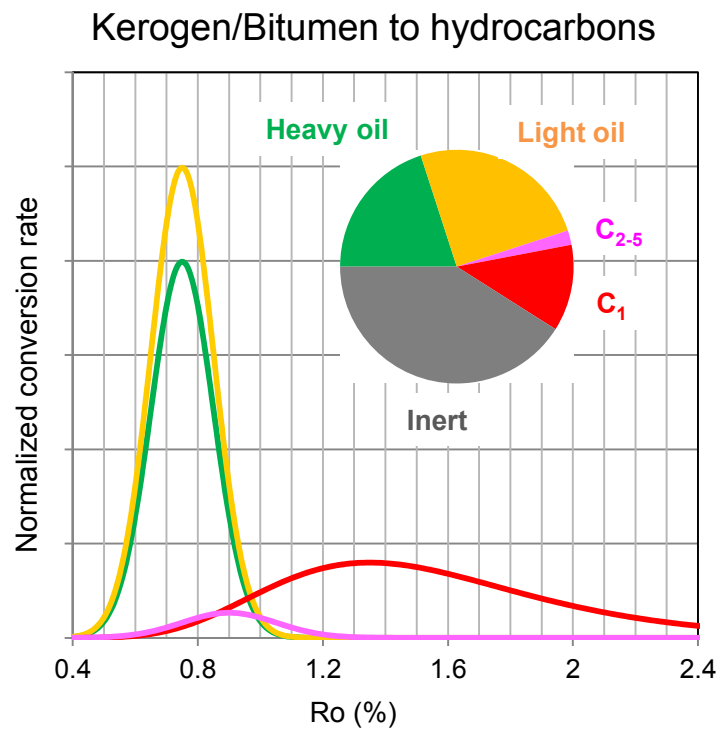
# Optimizing the model



- Eleven pseudo wells
- General parameters
  - Current depth 1,100-2,700 m
  - Current maturity:  $R_o$  0.8-2.2%
  - Initial TOC = 4%
  - Initial HI = 570 mg HC/g TOC
  - Inorganic porosity 4%
  - Organic porosity calculated from densities of oil/gas/kerogen/coke



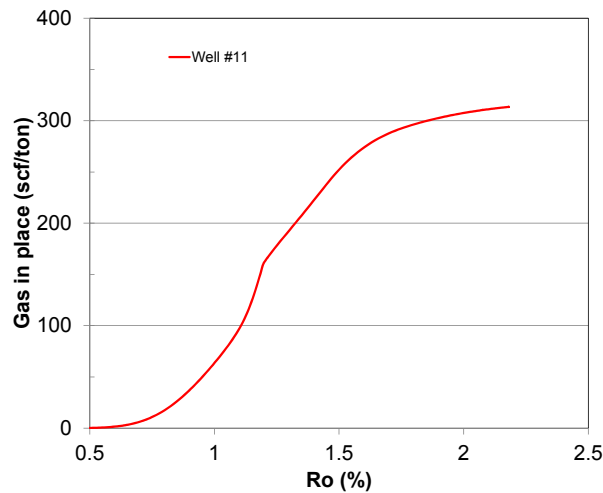
# Constrained and optimized kinetics and precursor ratios



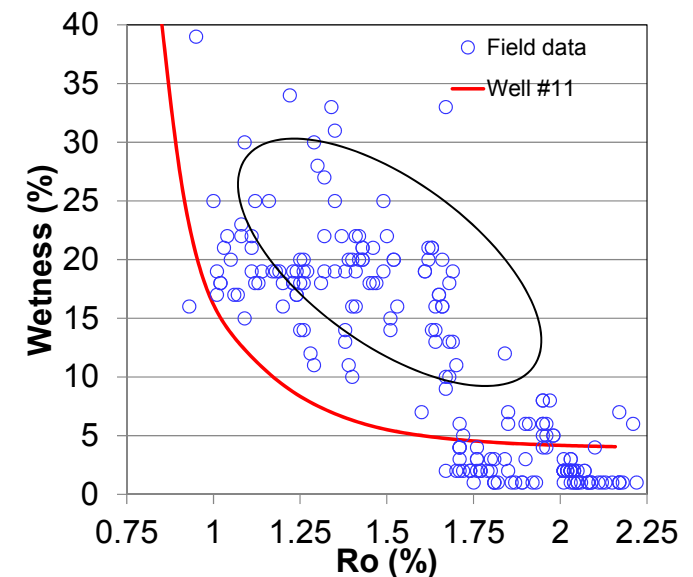
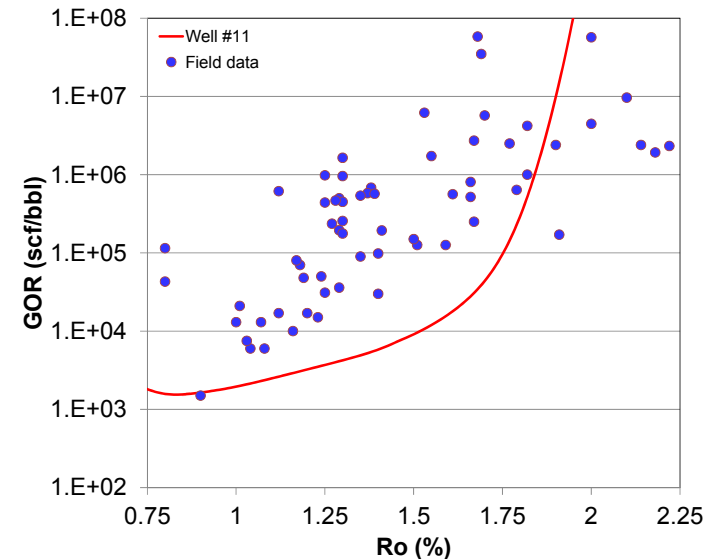
# Modeling results of the well with highest thermal maturity



- GIP: easiest to model – controlled by storage



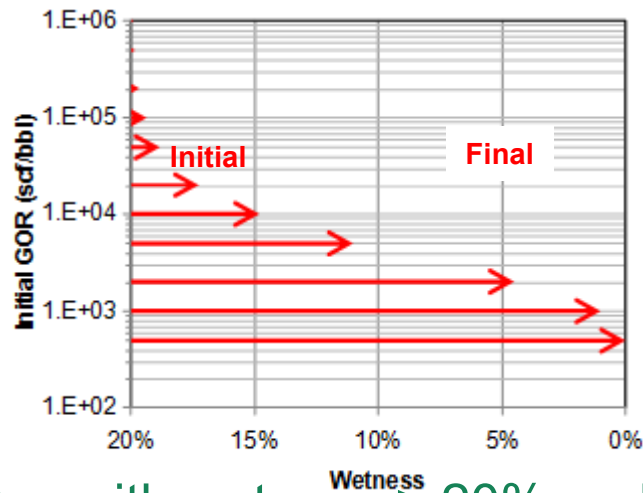
- GOR:
  - calculated < produced
  - May be contributed to retrograde condensation
- Critical inconsistency: wetness vs. thermal maturity



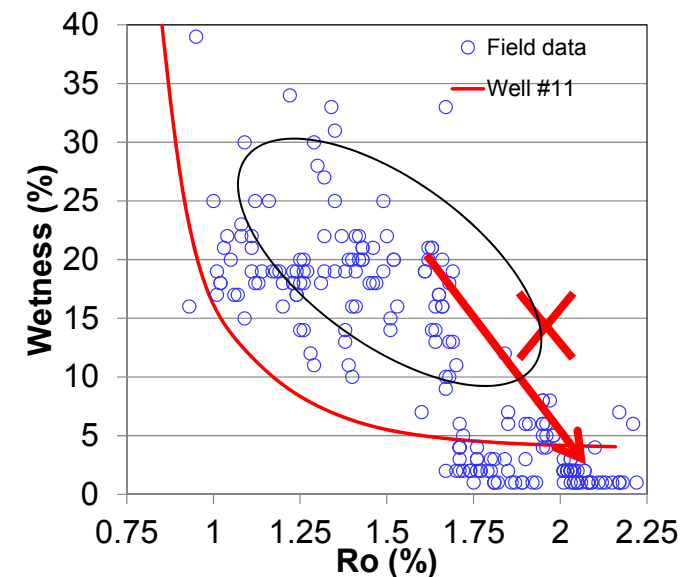
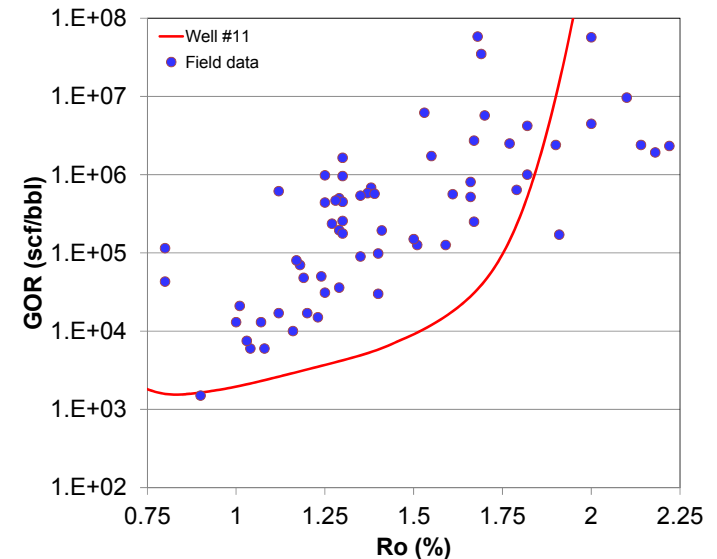
# Mass balance: why we cannot fit the data



- Lower GOR evolves to drier gas



- Gas with wetness > 20% and GOR > 10<sup>4</sup> scf/bbl cannot evolve to dry gas (without C<sub>2</sub> and C<sub>3</sub> cracking)
  - These gases are not on normal thermal maturity path
  - Special reservoir history involved

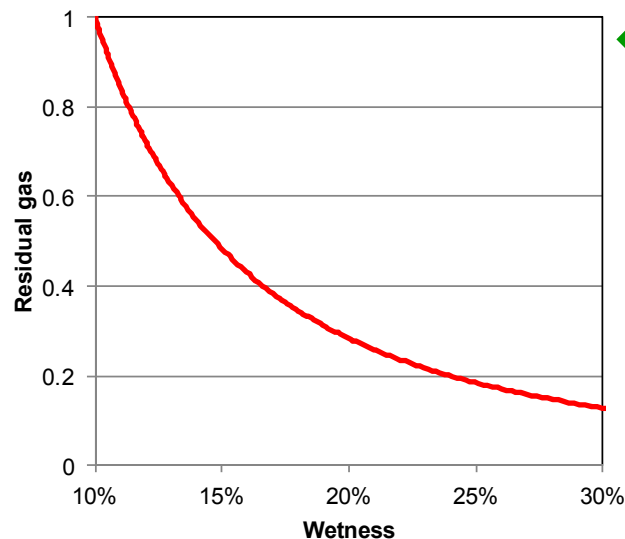
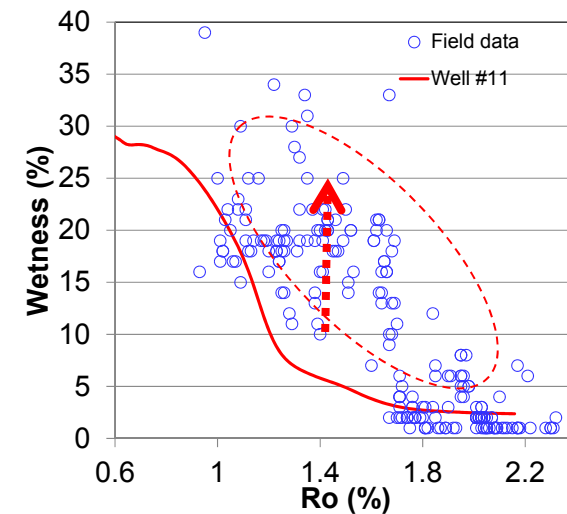


# Evolving of wet gas unlikely due to preferable lose of methane



- No dramatic solubility (or diffusivity) difference between methane and ethane
  - Solubility of  $\text{CH}_4$  :  $\text{C}_2\text{H}_6$  = 2.5 : 1 in formation water
  - If wetness is increases from 10% to 30%, then 87% gas removed by water

(inconsistent to production and water saturation data)



Suppose initial GIP  
= 300 scf/ton

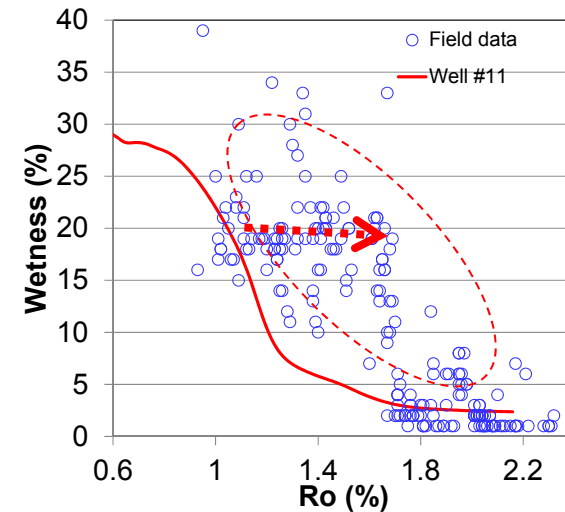
Then final GIP  
= 40 scf/ton

# Local accumulation of early gas may account for high wetness



- Reason:
  - Wet gas is mainly the early product of kerogen/bitumen (discussed above)
- To have wet gas at high maturity:

The early wet gas should be separated from oil, so that it is not diluted (or “flushed”) by the late dry gas

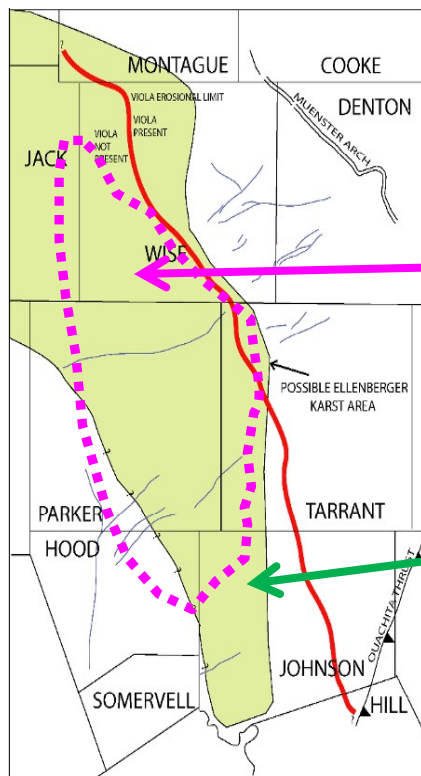




# Possible factors for separating wet gas from oil



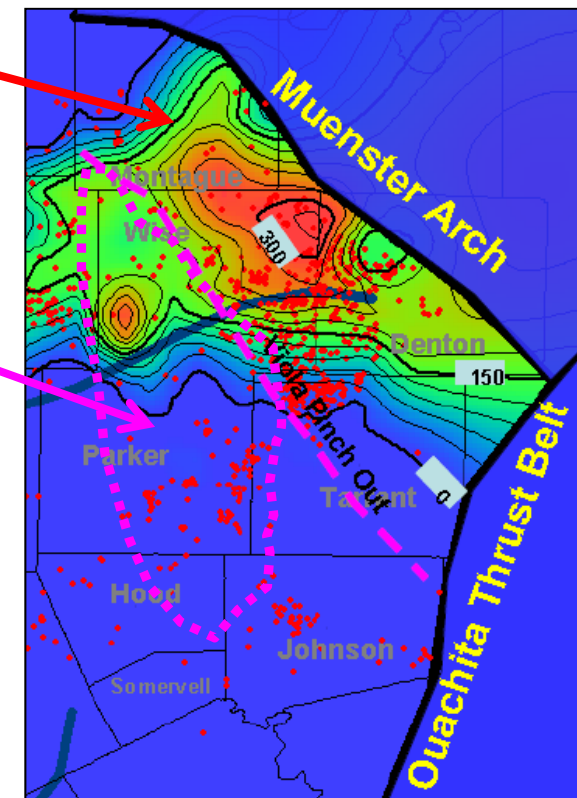
- Heterogeneity in pore system and on organic surfaces
- Migration through faults
- Storage in Ellenberger Karst area
- Separation of Forestburg limestone



**Forestburg limestone**  
(Tian, 2010)

**Wet gas inconsistent to thermal maturity**  
(Klentzman, 2009)

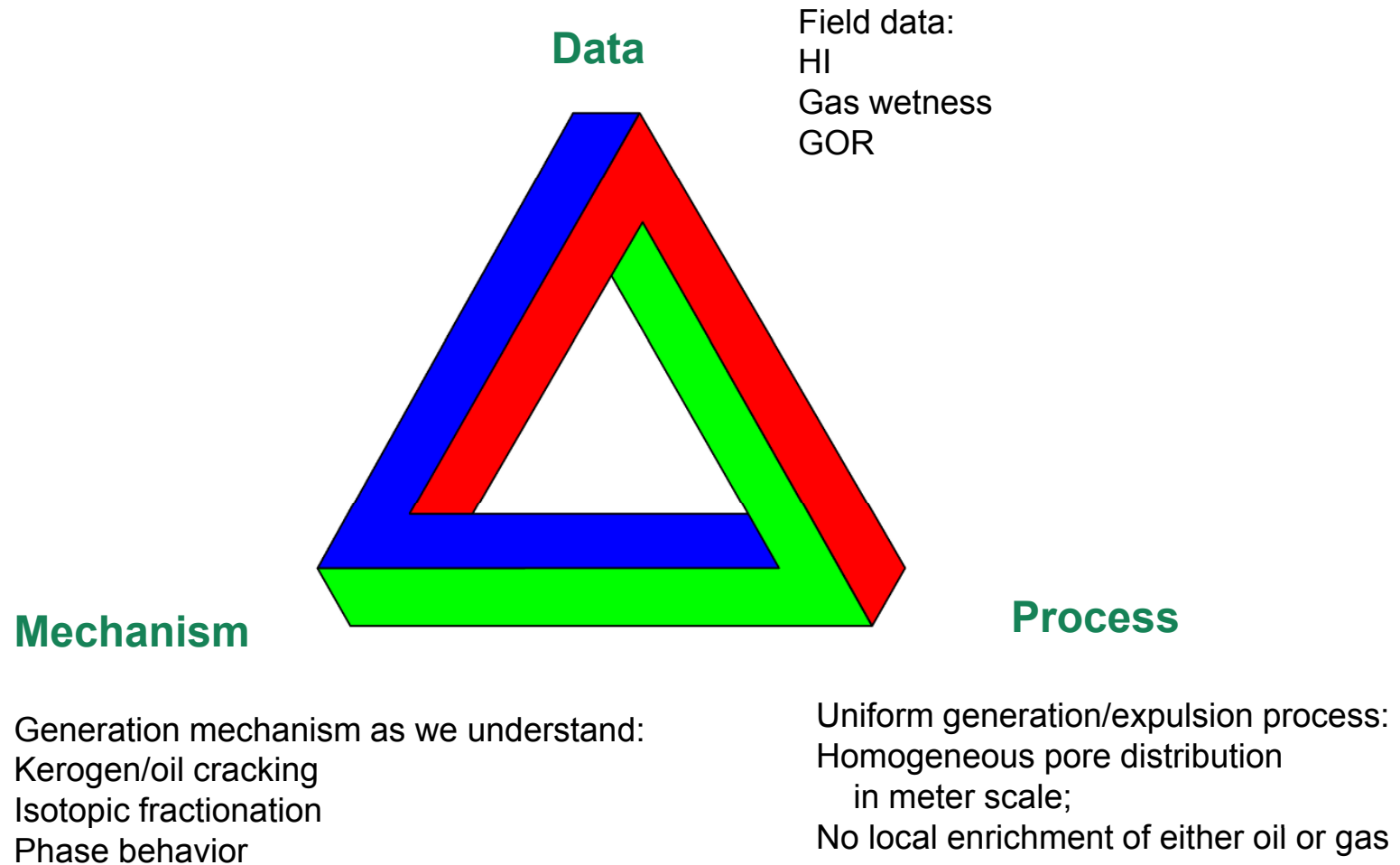
**Ellenberger Karst area**  
(Givens and Zhao)



# Composition trilemma



- Pick only two of the three!



# Conclusions

---



- Field data (HI and gas composition) of shale plays provide rigorous constraints to model hydrocarbon generation
- There are still significant unknowns in hydrocarbon generation/expulsion processes
  - Different from lab pyrolysis
  - Different from much of the current models
- Hydrocarbon composition in shale not merely controlled by thermal maturity, or by a uniform generation/expulsion process
  - Geological factors should be taken into account
    - Heterogeneity of storage and migration path
    - Heterogeneity of accumulation/dissipation of oil/gas

# Acknowledgement

---



- Discussion with
  - Jie Huang, Ellie Chuparova, Rick Requejo, Neil Fishman and Ted Dolman (Hess)
  - Zhiyong He (Zetaware)
  - Tongwei Zhang (University of Texas, Austin)
- Support of Hess's management



---

**Thanks for your attention!**

---