

# **Predicting TOC, Organic Porosity and Gas Retention Distribution in a Shale-Gas System Using Petroleum Basin Modelling\***

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Search and Discovery Article #40973 (2012)\*\*  
Posted July 16, 2012

\*Adapted from oral presentation at AAPG Annual Convention and Exhibition, Long Beach, California, April 22-25, 2012

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## **Abstract**

Natural gas can be stored as a condensed phase on shale matrix and organic materials or as conventional free gas in porous spaces (Lu et al., 1995). During the last decade, gas shale has been considered as important unconventional reservoirs in which part of the gas is stored in adsorbed state (Ross and Bustin, 2007). Several processes control fractionation and indeed retention mechanisms of gas hydrocarbons as the relative solubility of petroleum compounds in kerogen (Ritter, 2003), the gas adsorption on mineral surfaces (Brothers et al., 1991), in organic matter (Lamberson and Busting, 1993) or in nanopores of vitrinite (Ritter and Grover, 2005). In addition, several studies have paid attention to the distribution of pore system structures to further elucidate the gas storage process in these gas shales (Loucks et al., 2009).

Most nanopores in these rocks are linked to the thermal cracking of the organic matter and are observed as intraparticle organic pores. This organic contribution to the shale porosity is a good candidate for "in situ" gas storage. Gas retention can be likely controlled by the evolution of TOC in the source rock. In this work, a method is proposed to calculate, at the basin scale, the evolution of TOC, organic porosity and gas retention capacity through time and space in shale gas. Application is done on a 3D basin model of the Barnett Shale in Texas, calibrated for thermal maturity on Rock-Eval and vitrinite reflectance data. In order to predict the evolution of TOC within shale, an organic carbon balance was derived from a compositional kinetic approach containing 18 classes (Behar et al.,

2008). Also, gas adsorption potential on organic material was calculated using a modified-Langmuir model implemented within the basin simulator which takes into account temperature and remaining TOC. To reproduce the present-day average TOC distribution, an initial TOC map was determined by inversion of 3D calculations. Original TOC from 5% to 8% were consistent with observed TOC and maturity stages. Accordingly, organic matter cracking would be at the origin of more than half of the total shale porosity in mature zones. Applying the modified-Langmuir law, most retained gas in the Barnett Shale is concentrated in mature areas ranging from 40 to 100 kg/m<sup>2</sup>. Under these conditions, the Barnett Shale can generate more late gas by secondary cracking and simultaneously these generated gases can likely be retained in these higher maturities zones.

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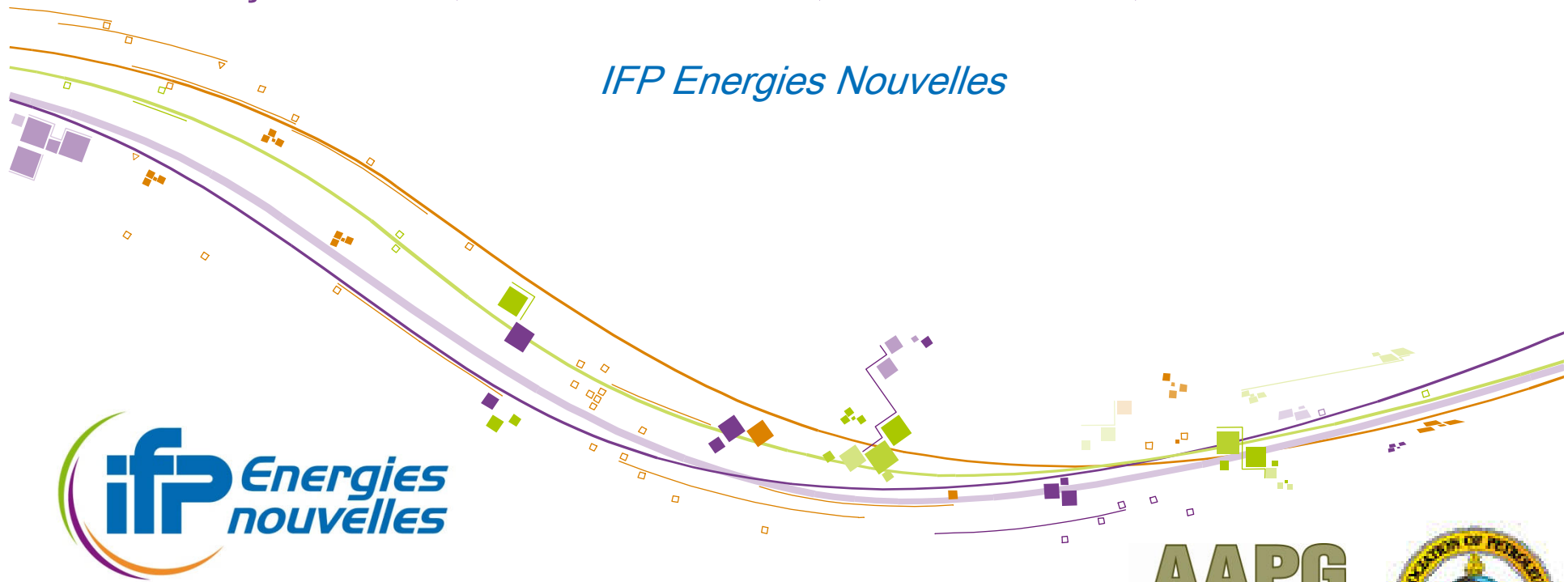
Ritter, U., and A. Grover, 2005, Adsorption of petroleum compounds in vitrinite; implications for petroleum expulsion from coal: International Journal of Coal Geology, v. 62/3, p. 183-191.

Ross, D.J.K., and R. M. Bustin, 2009, The importance of shale composition and pore structure upon gas storage potential of shale gas reservoirs: Marine and Petroleum Geology, v. 26/6, p. 916-927.

# Predicting TOC, Organic Porosity and Gas Retention Distribution in a Shale-Gas System using Petroleum Basin Modeling

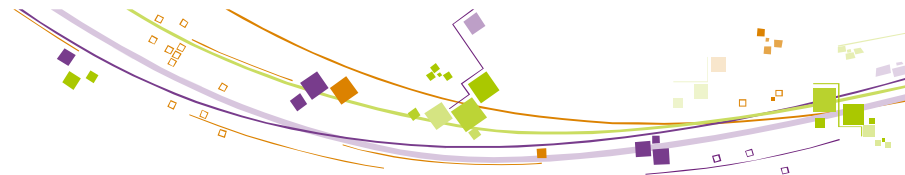
Maria-Fernanda Romero-Sarmiento, Mathieu Ducros, Bernard Carpentier, François Lorient, Sébastien Rohais, Isabelle Moretti, Alain-Yves Huc

*IFP Energies Nouvelles*



Long Beach AAPG / ACE 2012





# The Shale Gas balance

## ■ Net gas in place:

*Available gas play at time  $t = f$*

Gas Generation  
Storage Capacity  
Expelled gas

## ■ Stored Gas

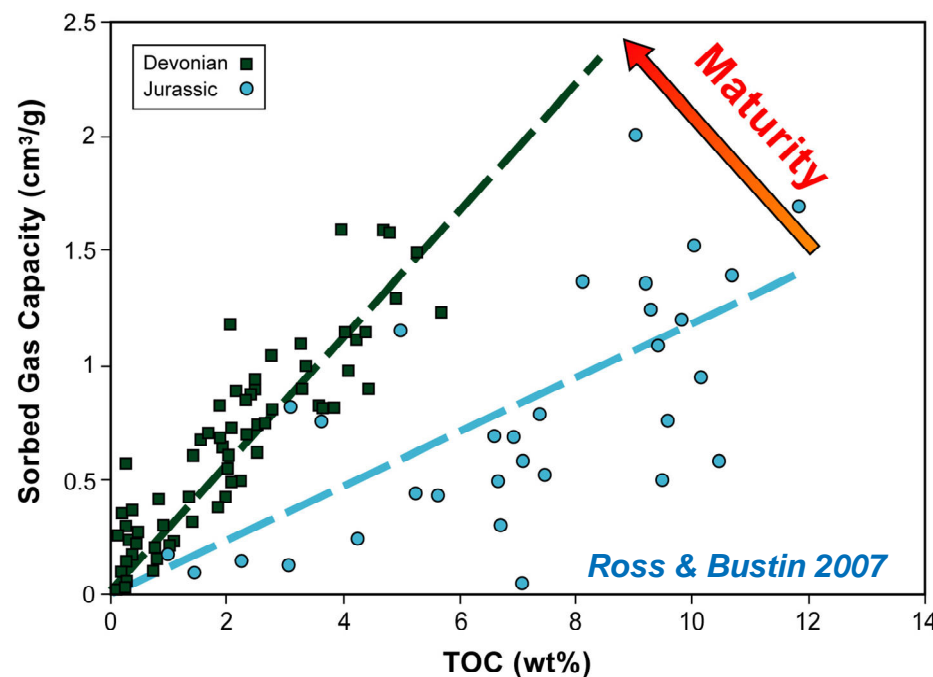
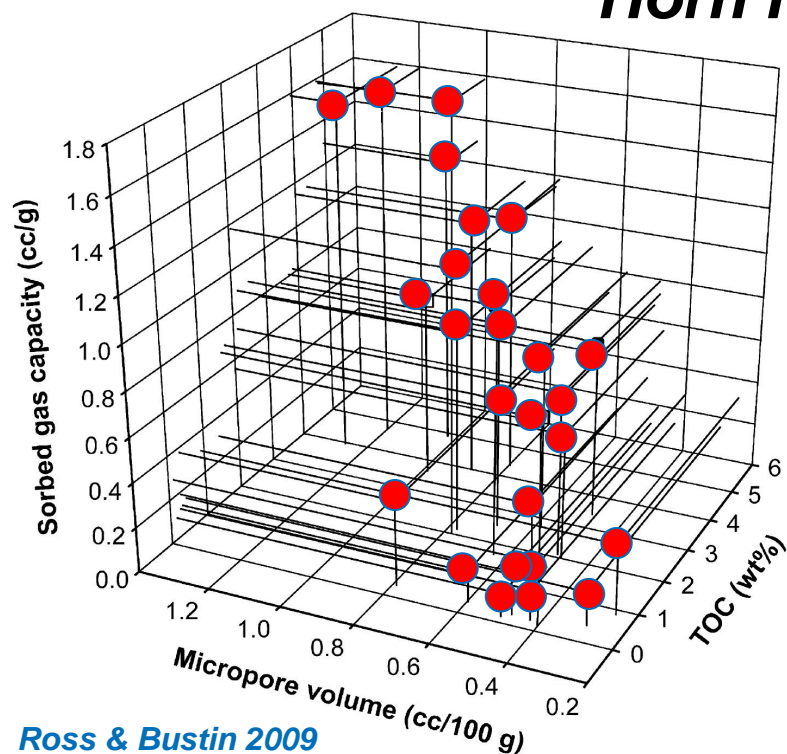
- Free
- Dissolved
- Adsorbed

- Porosity
- Micro-fractures



Special attention has been recently dragged on the instrumental role of the kerogen itself on the amount of gas stored in shale

## *Horn River Basin, British Columbia*

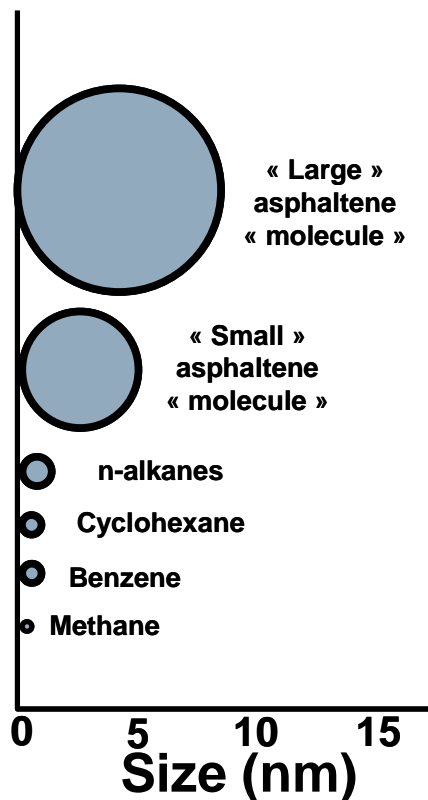
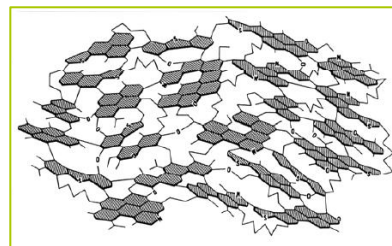
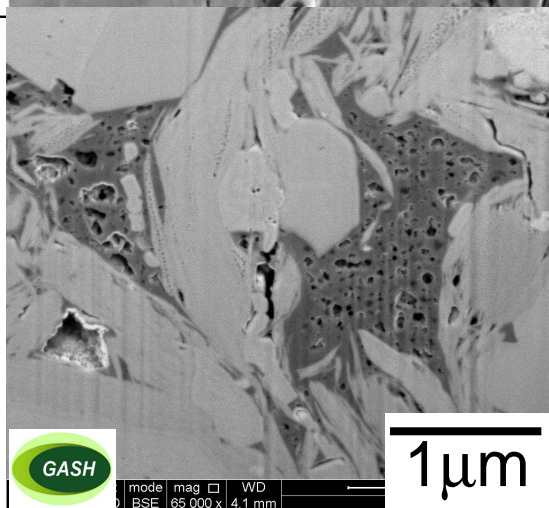
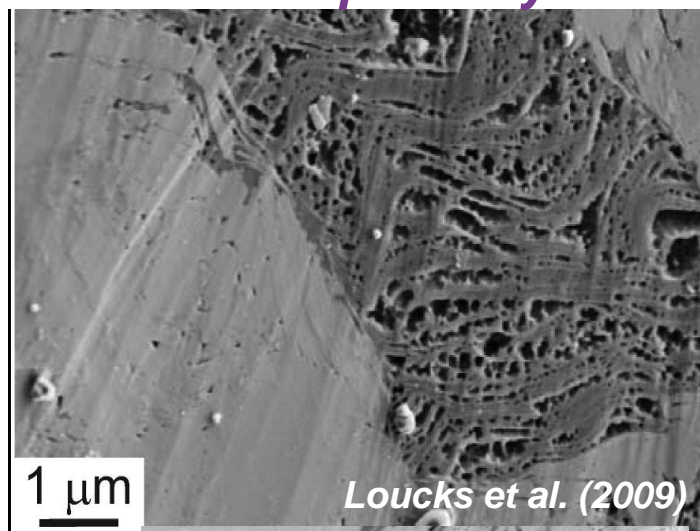




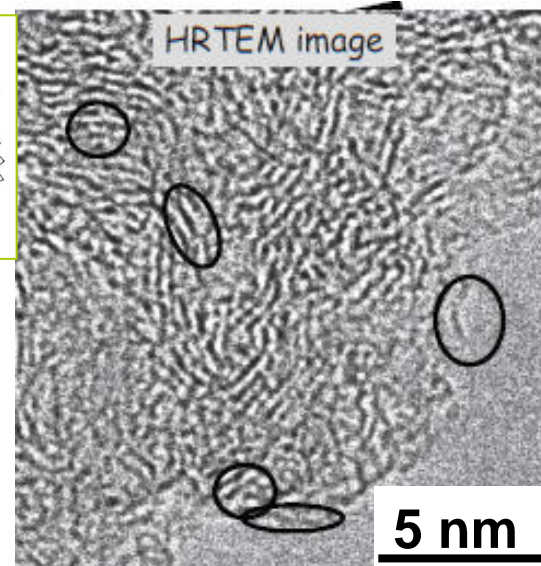
# Organic Porosity potentially occurs as micro- and nano-porosity likely fitted to accommodate HC

*Kerogen micro-porosity*

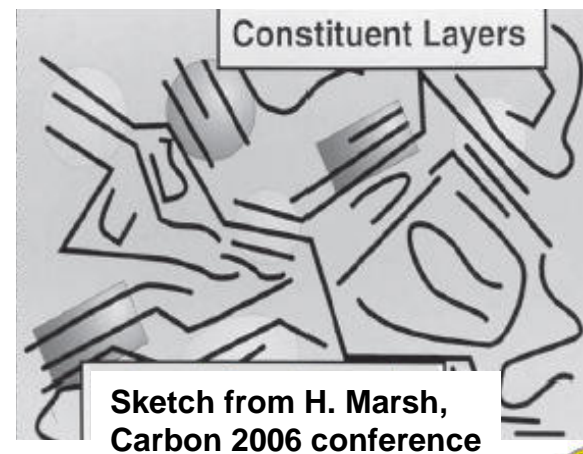
« *Loucks' porosity* »



*Kerogen nano-porosity*



Formation La Luna – Venezuela (Image 2011)  
After Rouzeaud & Romero-Sarmiento (work in progress)



# Focus on the HC associated with the Kerogen, more specifically on CH<sub>4</sub> adsorption modeling; with application to Lower Barnett shale, Fort Worth Basin

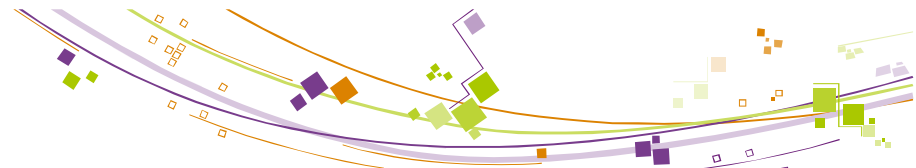
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The presented approach involves a specific module fully coupled to an integrated basin model

The module relies on:

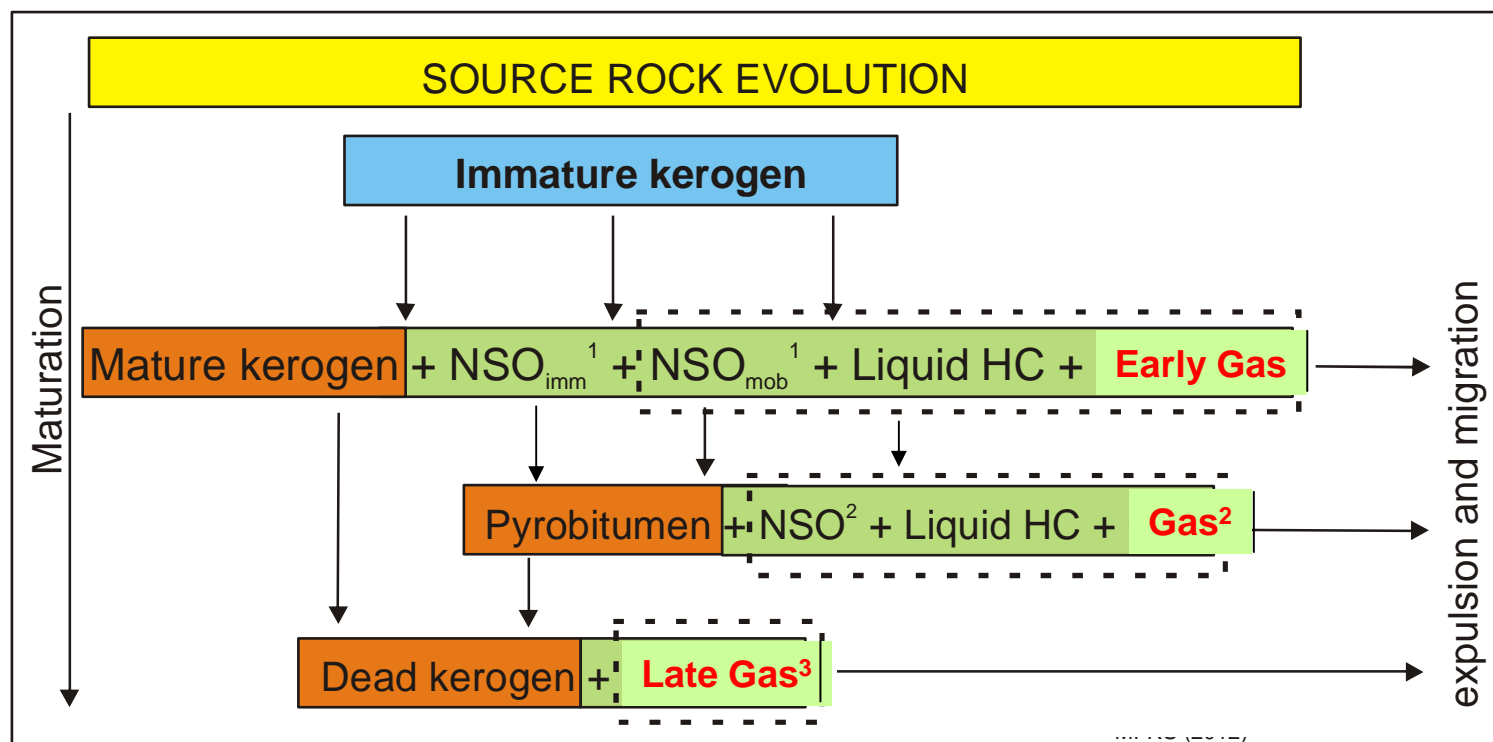
- The generation of CH<sub>4</sub> and the formation of organic porosity, derived from a new compositional model (Behar and Jarvie, *in press*)
- The back-calculation of the initial TOC of the SR
- A Langmuir derived formalism accounting for the maximum adsorption capacity of the remaining TOC in the thermally matured SR



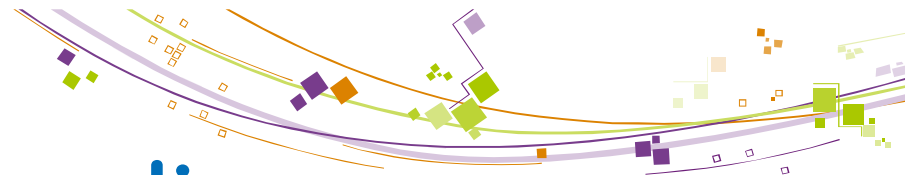


# Generation of $\text{CH}_4$ and of Organic Porosity

Gas generation and Computation of Carbon mass balance  
( Kerogen C loss  $\rightarrow$  organic  $\phi$  ), are derived from a new 19 fractions  
compositional thermal maturation modeling  
(Behar and Jarvie, *in press*).



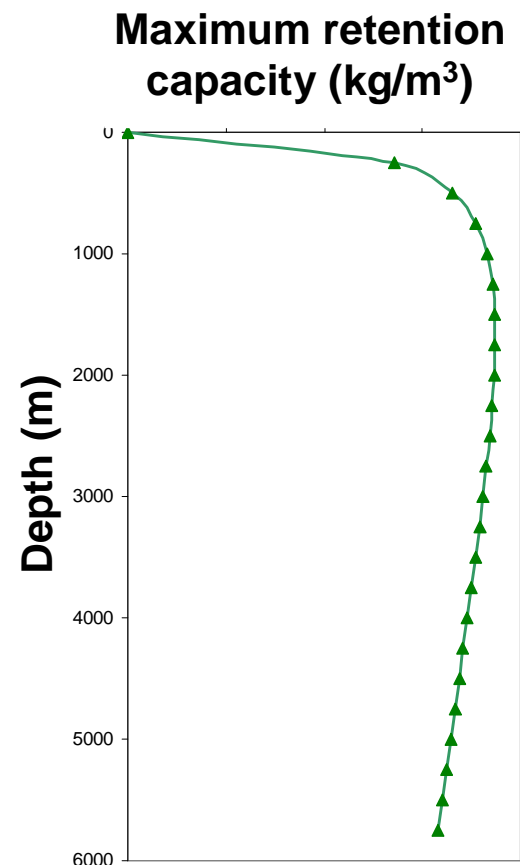
*simplified from Behar & Jarvie (in press)*



# Gas adsorption formalism

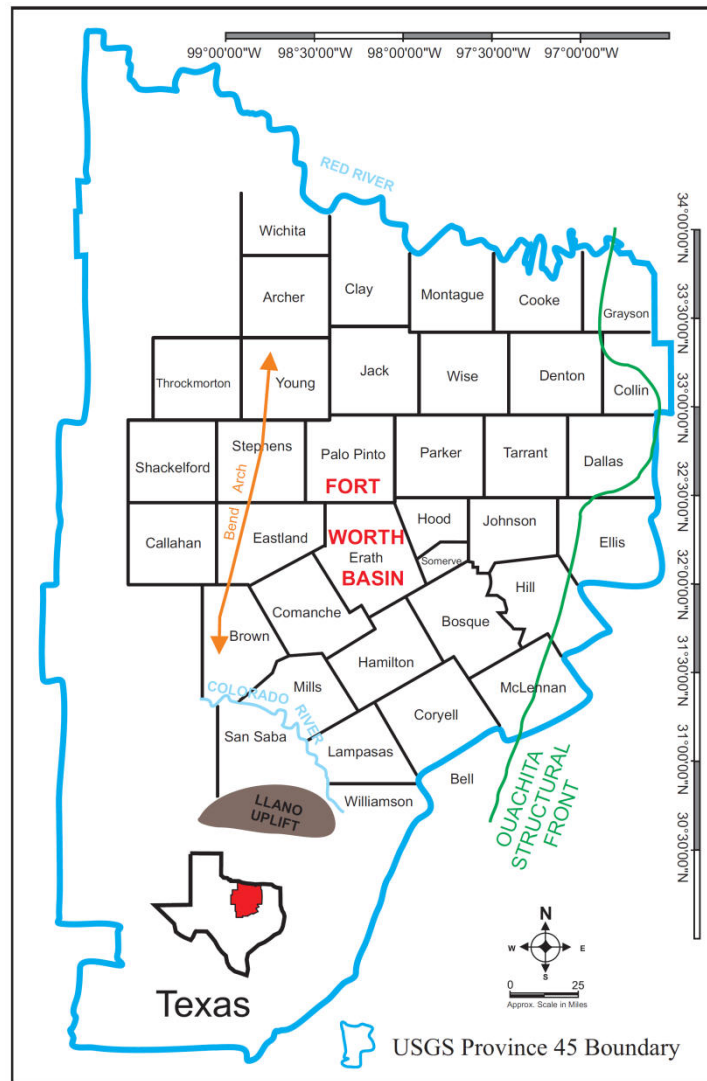
■ Approach accounting for gas adsorption on organic matter:

- "Langmuir-based" adsorption
- Maximum retention capacity  
=  $f(P, T, \text{Remaining TOC})$
- Accounting on HC composition (herein applied to  $\text{CH}_4$ )



# Application to Lower Barnett Shale Unit

## Fort Worth Basin



(a) SYSTEM, SERIES & AGE (Ma)		STAGE	GROUP or FORMATION
CRETACEOUS	LOWER	~95	COMANCHEAN
		~120	
PERMIAN		251.0 ± 0.4	OCHOAN - GUADALUPIAN
		270.6 ± 0.7	LEONARDIAN
		284.4 ± 0.7	WOLFCAMPIAN
		299.0 ± 0.8	VIRGILIAN
PENNSYLVANIAN		303.4 ± 0.9	CISCO GROUP
			MISSOURIAN
		307.2 ± 1.0	
			DESMOINESIAN
		311.7 ± 1.1	
MISSISSIPPIAN			ATOKAN
			MORROWAN
		318.1 ± 1.3	CHESTERIAN - MERAMECIAN
		328.3 ± 1.6	OSAGEAN
ORDOVICIAN	U	~453	
	M	~460	
	L	~477	
		~479	
CAMBRIAN	UP	488.3 ± 1.7	
		~499	
GRANITE - DIORITE - METASEDIMENTS			

■ Inverted foreland

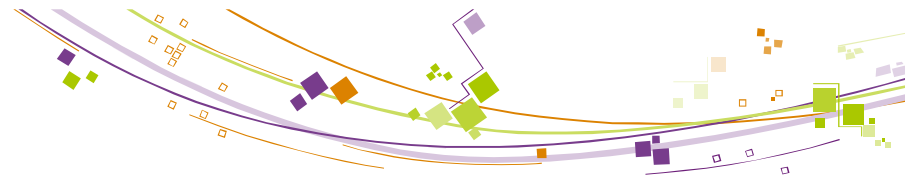
■ Max Burial: Permian

■ Erosion: late Permian to Cretaceous

■ Source Rock: Upper Barnett Shale

→ Lower Barnett Shale

*modified from Pollastro (2003)*



# Measured Present-Day Average TOC Distribution

*...from data available in the literature.....*

a present-day TOC map:

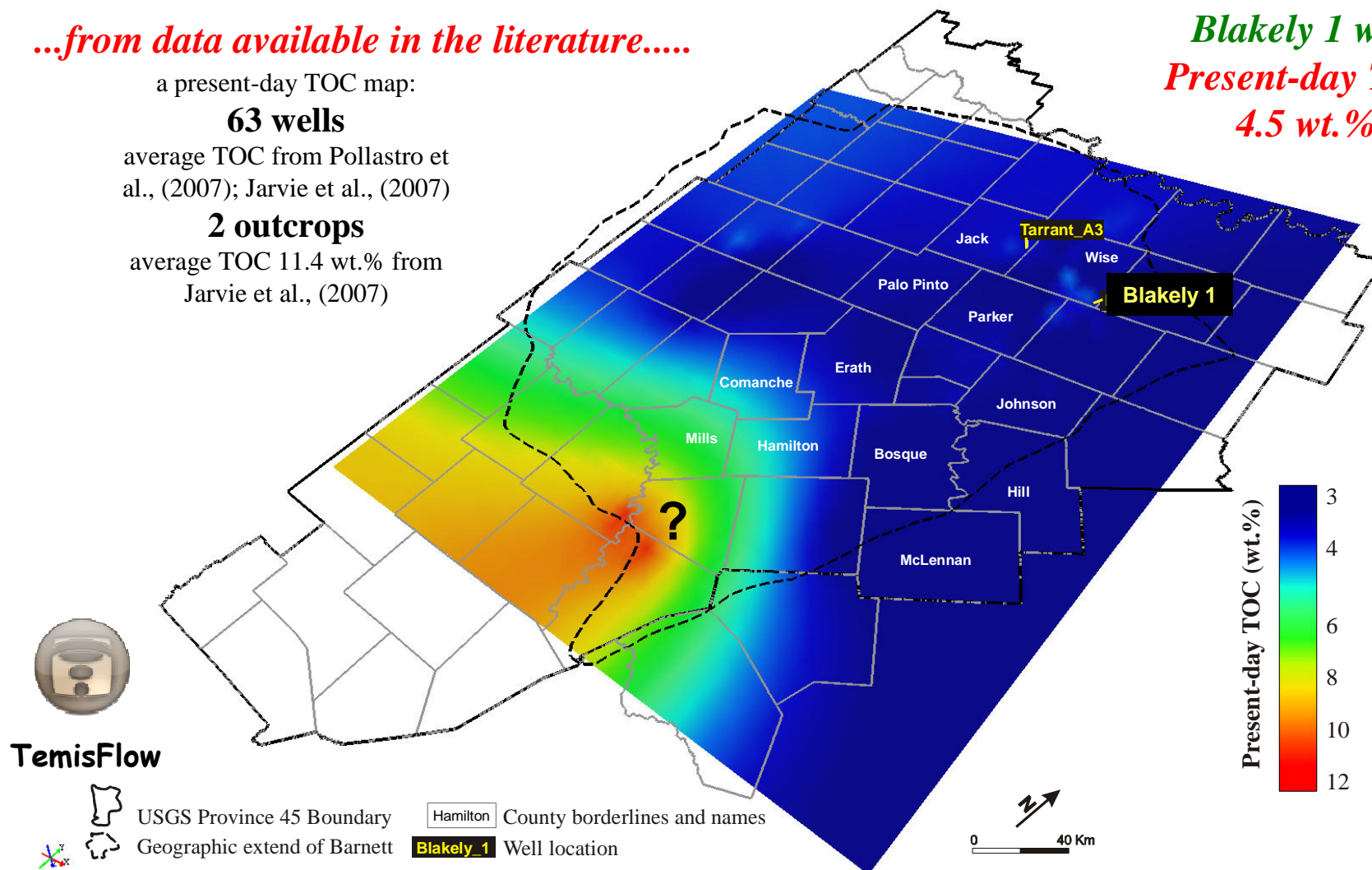
**63 wells**

average TOC from Pollastro et al., (2007); Jarvie et al., (2007)

**2 outcrops**

average TOC 11.4 wt.% from Jarvie et al., (2007)

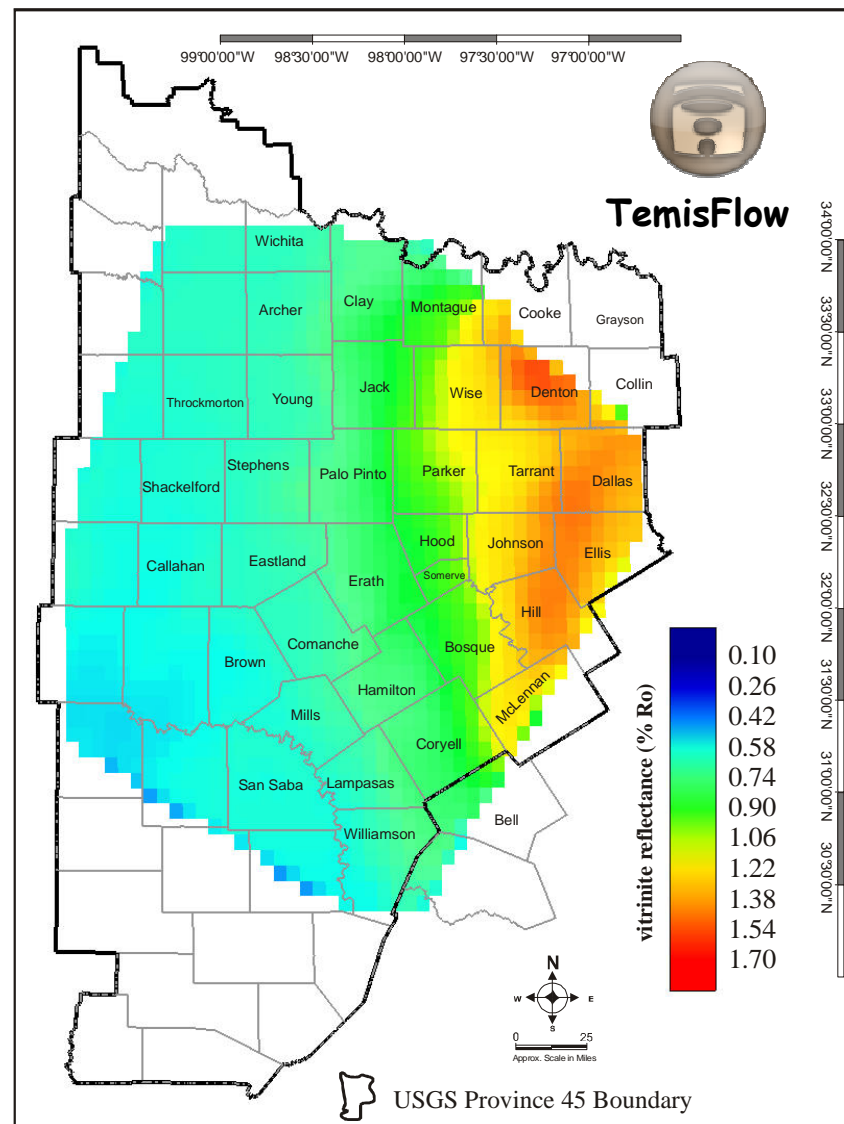
*Blakely 1 well*  
*Present-day TOC*  
*4.5 wt. %*





# Thermal Maturity (%Ro, TR), 3D Model outputs

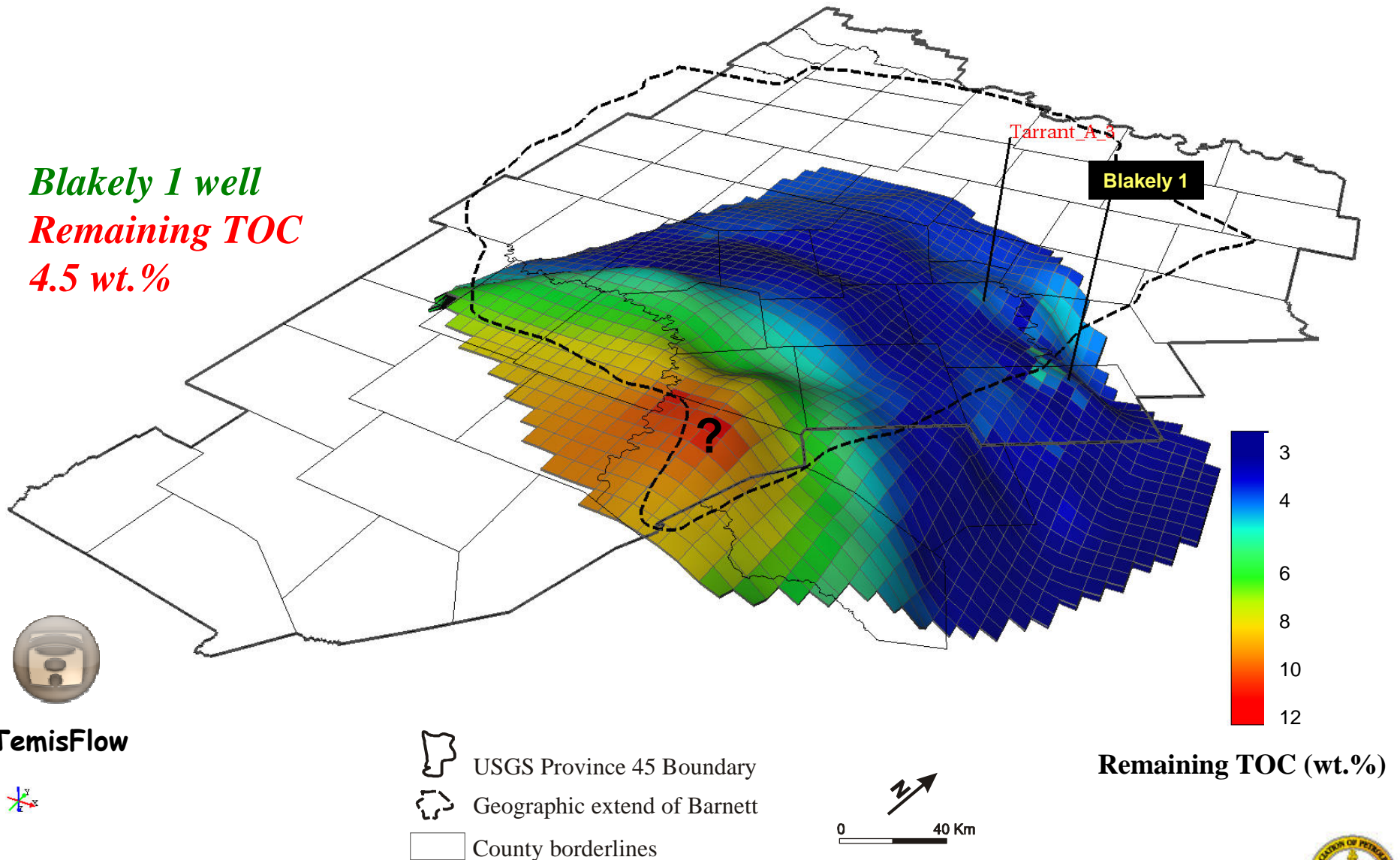
Calculation based on  
specific kinetic and  
stoichiometric parameters  
determined for the  
Barnett Kerogen





# Remaining TOC distribution in the Lower Barnett Shale

*Blakely 1 well*  
*Remaining TOC*  
*4.5 wt. %*



**TemisFlow**

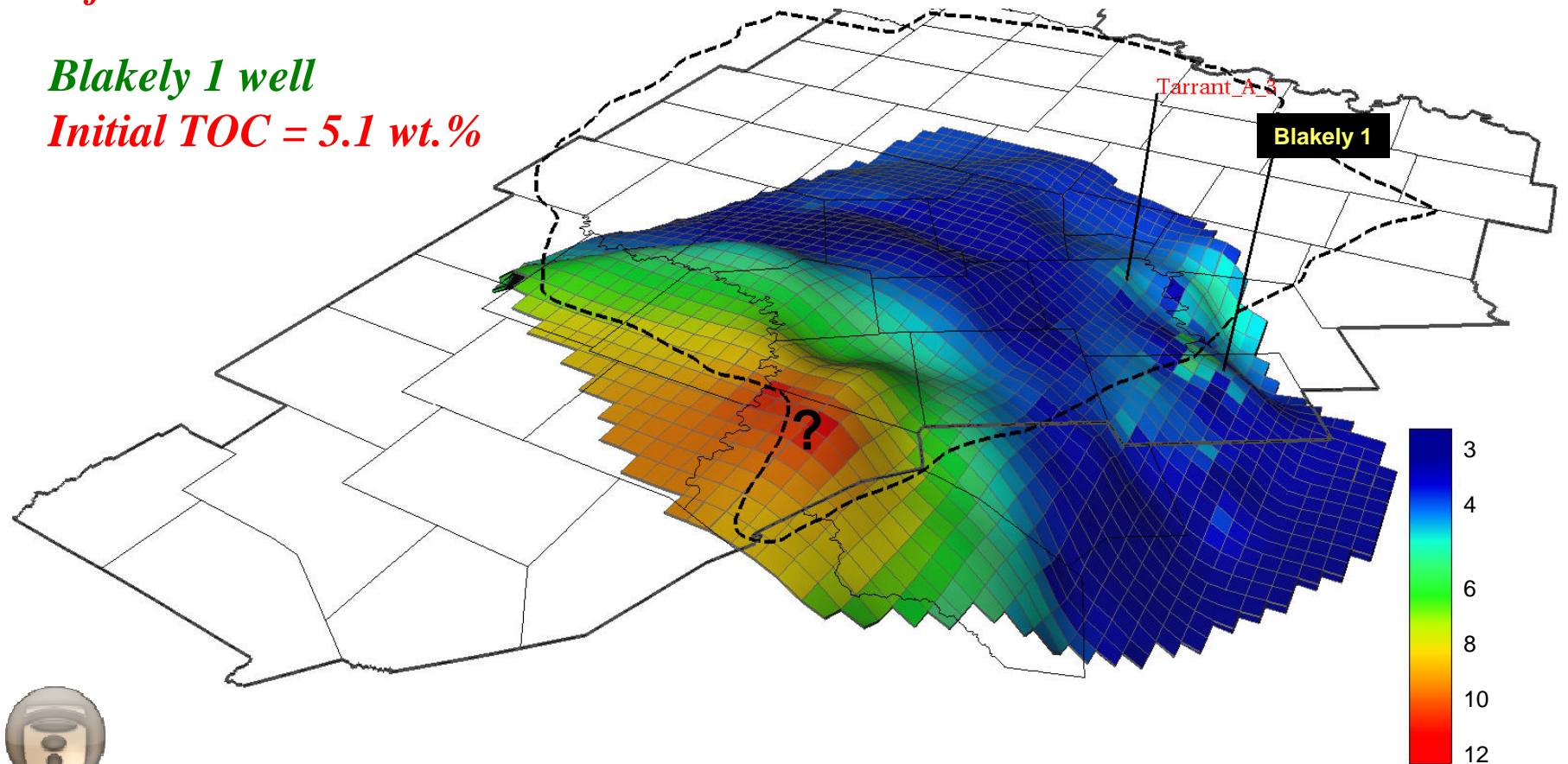


# Initial TOC distribution in the Lower Barnett Shale

*... from basin simulations...*

*Blakely 1 well*

*Initial TOC = 5.1 wt. %*



**TemisFlow**



USGS Province 45 Boundary

Geographic extent of Barnett

County borderlines



**Initial TOC (wt.%)**

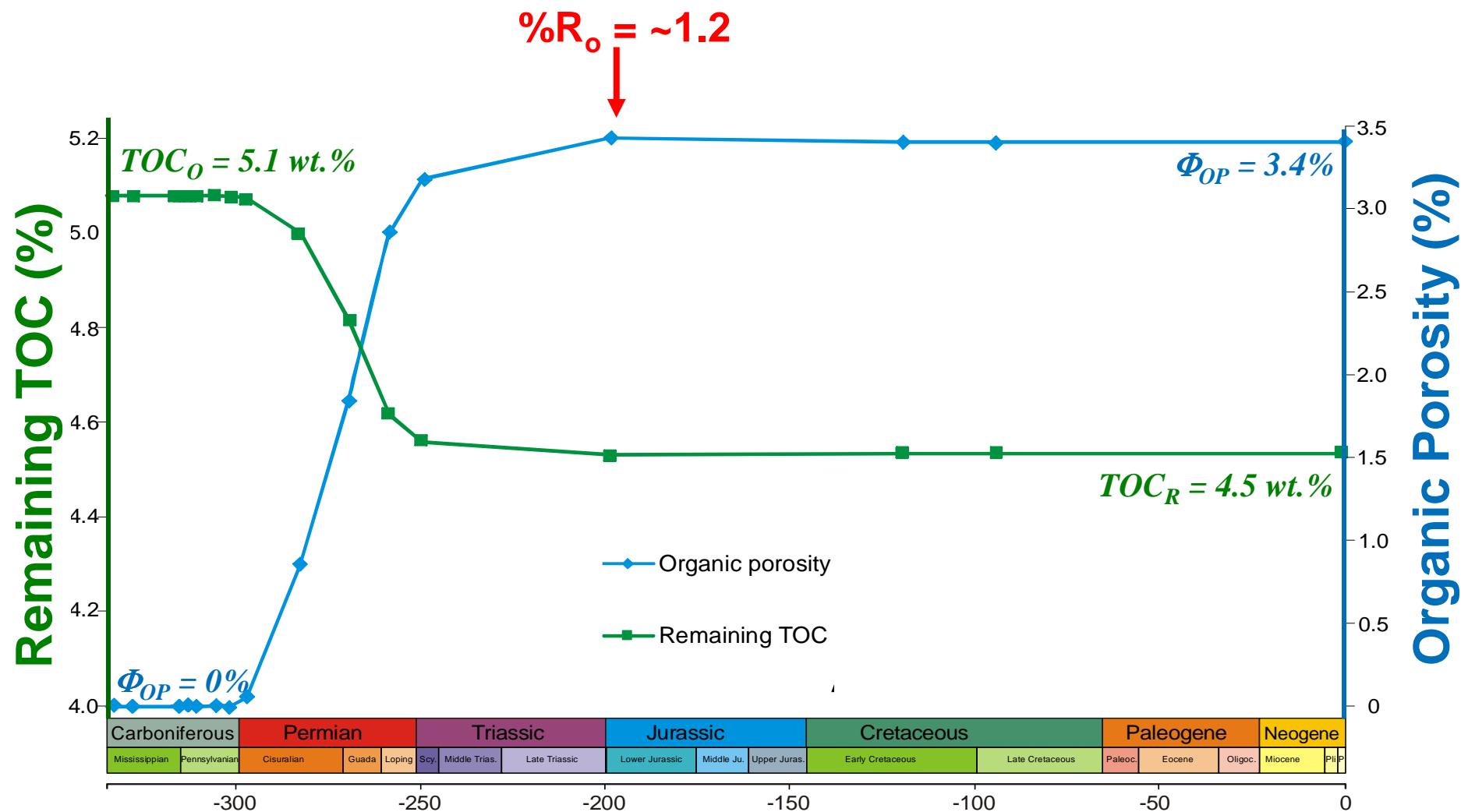


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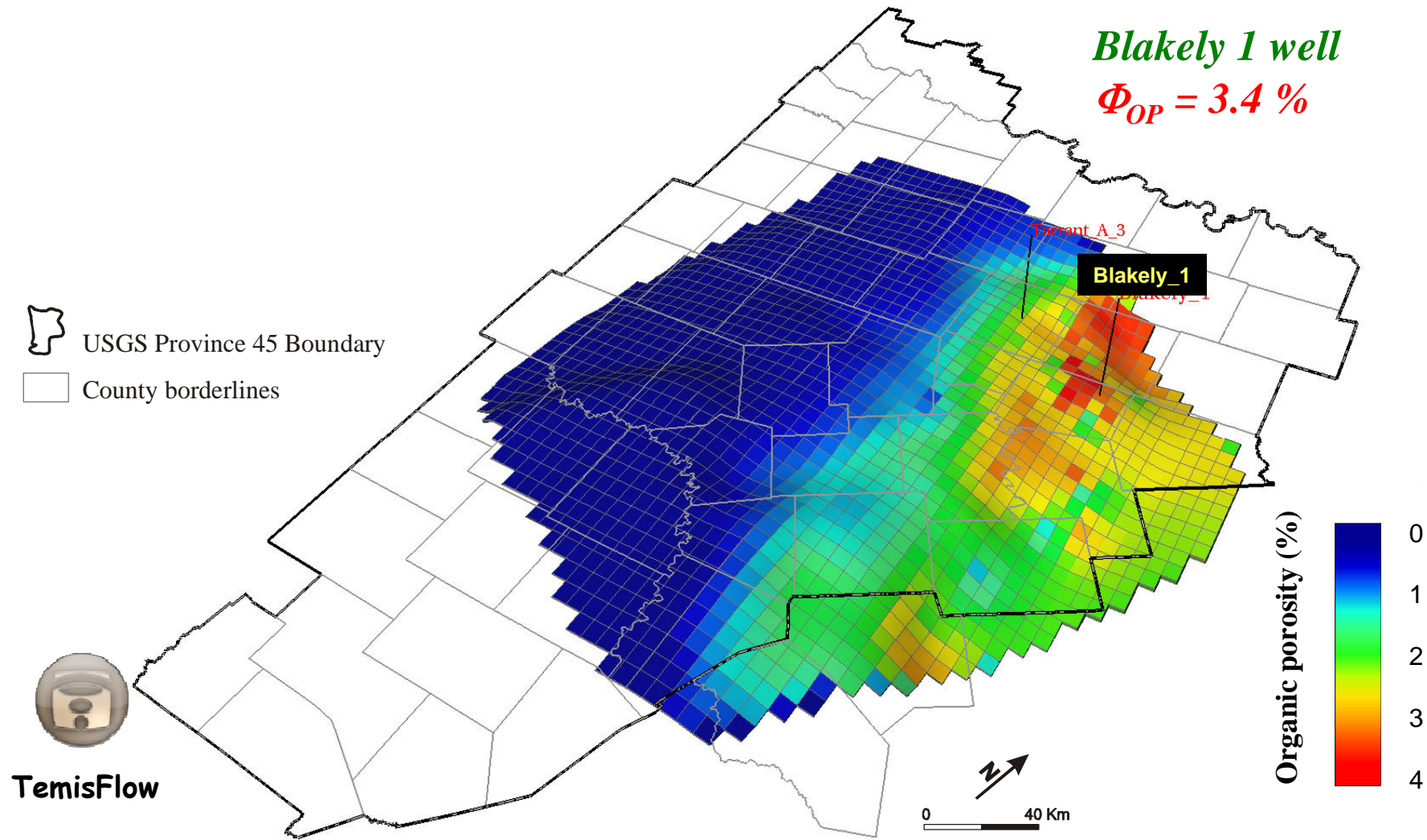




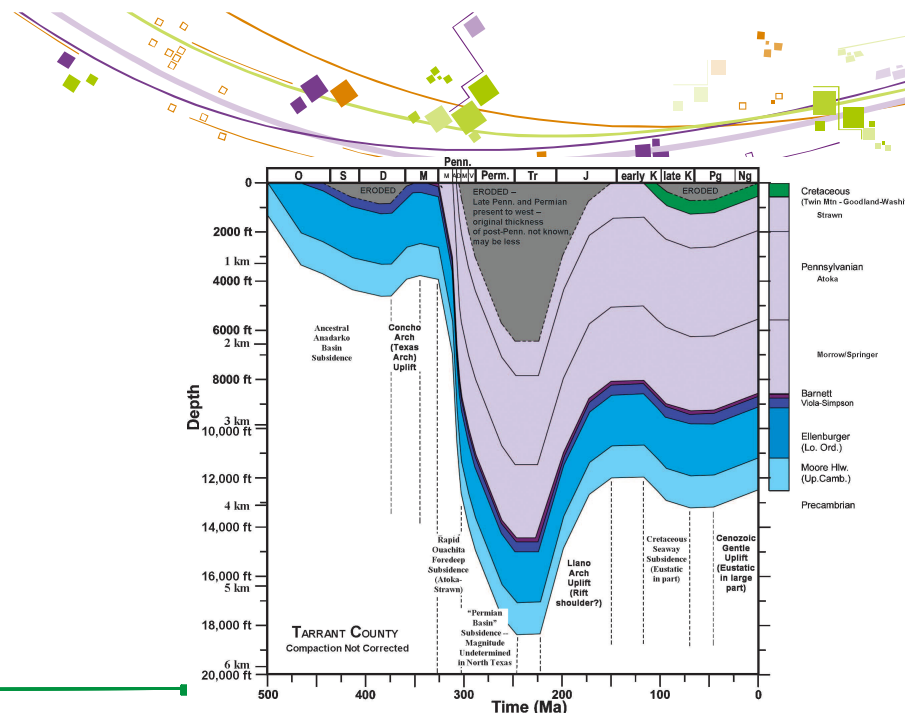
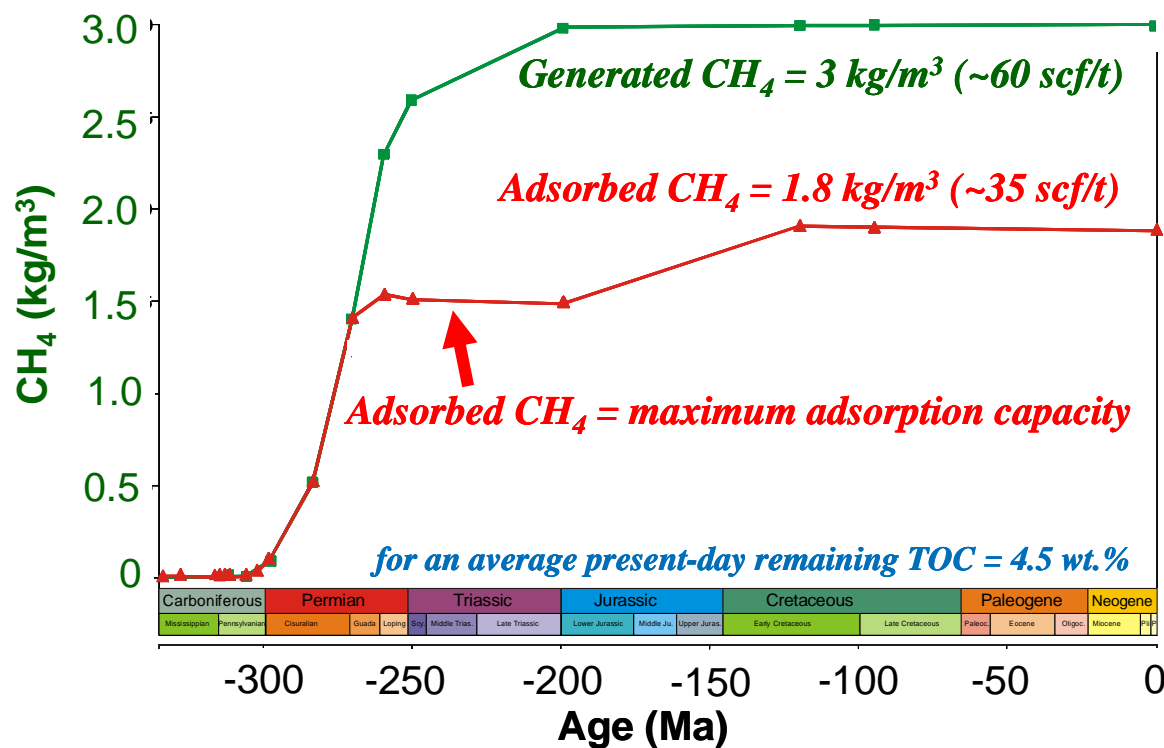
# Mature zone of the Lower Barnett Shale unit Blakely 1 well



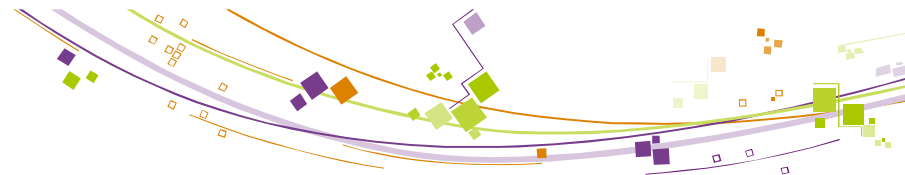
# Computed organic porosity in the Lower Barnett Shale



# Mature zone of the Lower Barnett Shale unit e.g. Blakely 1 well



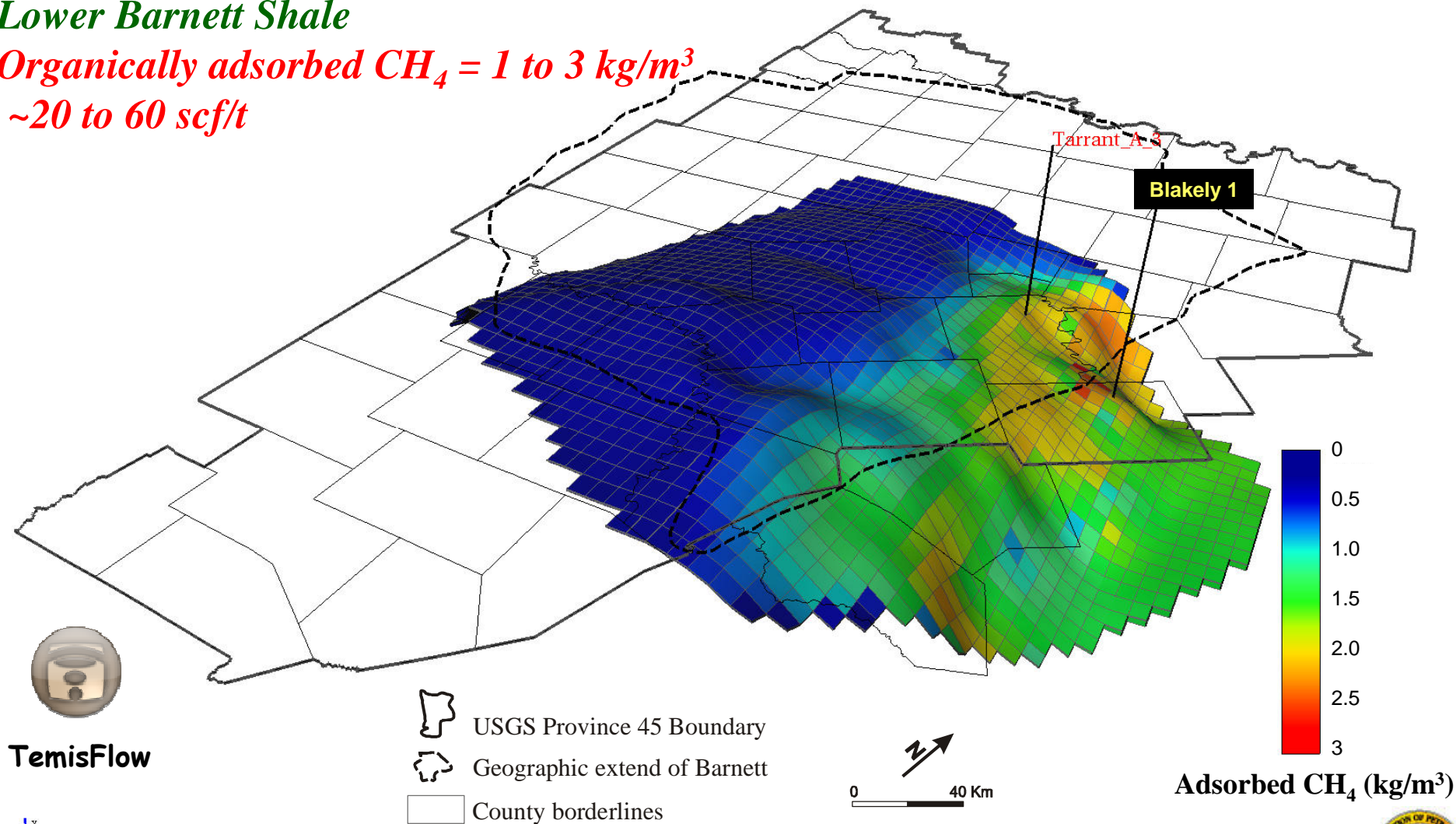
Ewing 2006



# Computed amount of CH<sub>4</sub> adsorbed on Organic Matter

*Lower Barnett Shale*

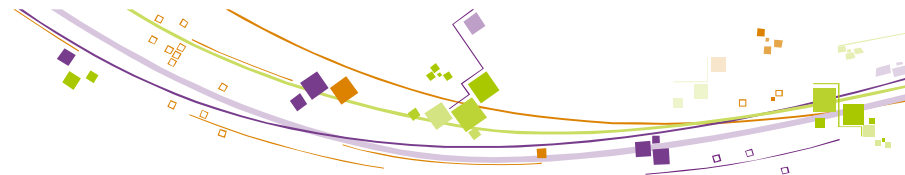
*Organically adsorbed CH<sub>4</sub> = 1 to 3 kg/m<sup>3</sup>  
~20 to 60 scf/t*



**TemisFlow**



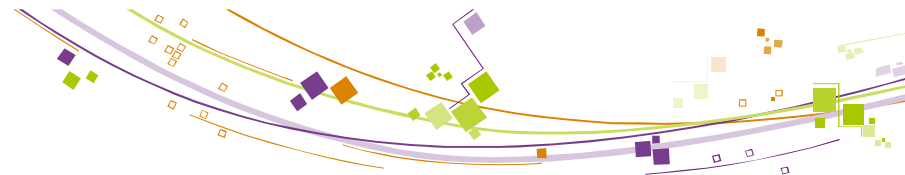




## Conclusions

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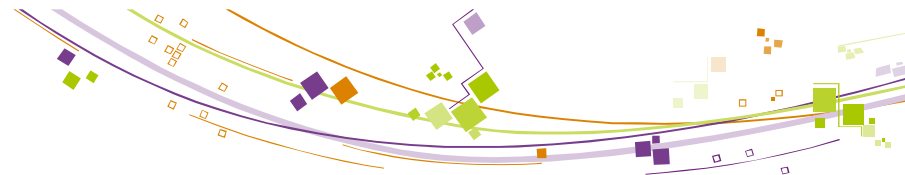
- In the perspective to assessing shale gas prospects, a method is proposed to model the evolution of TOC, organic porosity and gas adsorption potential associated with kerogen moieties.
- The approach results in a specific numerical module fully coupled to an integrated basin model.
- The methodology has been applied to the Lower Carboniferous (Mississippian) Lower Barnett unit in the Fort Worth Basin.




## Conclusions

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- The modelling exercise provides a map of initial TOC, performed thanks to an inversion procedure and accounting for the specific reactivity of the considered Kerogen.
- The computed data honour the current measured remaining TOC distribution as well as the maturity map of the Barnett shale.
- According to the model, the thermal cracking of organics creates an organic porosity up to 4% in mature areas.
- In mature areas of the basin, the part of the gas which is adsorbed on organics in the Lower Barnett Shale is suggested to range between 1 to 3 kg/m<sup>3</sup>.



## Acknowledgements

The construction of the initial 3D model of the Fort Worth  
has been done through the  consortium.



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