Scaling Analysis of the Coupled Compaction, Kerogen Conversion, and Petroleum Expulsion During Geological Maturation*

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Abstract

Porosity rebound is associated with the kerogen conversion into hydrocarbons and the overpressure development in the coupled sedimentary compaction, kerogen conversion, sorption, and fluids expulsion processes. There are a large number of variables with uncertainties, which affect the porosity rebound. Uncertainty analysis to determine their sensitivity and importance via 3D basin-scale simulations is very time-consuming. To address this problem, we developed a simple but efficient model and performed scaling analysis to identify the relative importance of each mechanism/parameter. We then reduce the number of parameters to the most essential in controlling porosity rebound. The procedure is to first develop a unit cell model by considering elastic and inelastic deformation of solids, thermal expansion, primary and secondary cracking, sorption of hydrocarbon, and fluid expulsion. Inspectional analysis is then employed to obtain dimensionless equations as well as dimensionless numbers. The competing mechanisms for porosity rebound are represented by several dimensionless numbers. A two-level experimental design is then conducted to generate the combinations of all dimensionless numbers and corresponding scenarios. Through this research, we have reduced the variables from 53 physical parameters to 37 dimensionless numbers, out of which only 5 have the largest impact on porosity rebound. The ranking of the most important parameters associated with the dimensionless numbers follows: initial kerogen content, geothermal heating rate, compaction coefficient, fluid expulsion rate, and reaction rate. The results are verified against PetroMod simulations. We expect this work to provide useful guidelines in greatly simplifying analyses and simulations in basin modeling.

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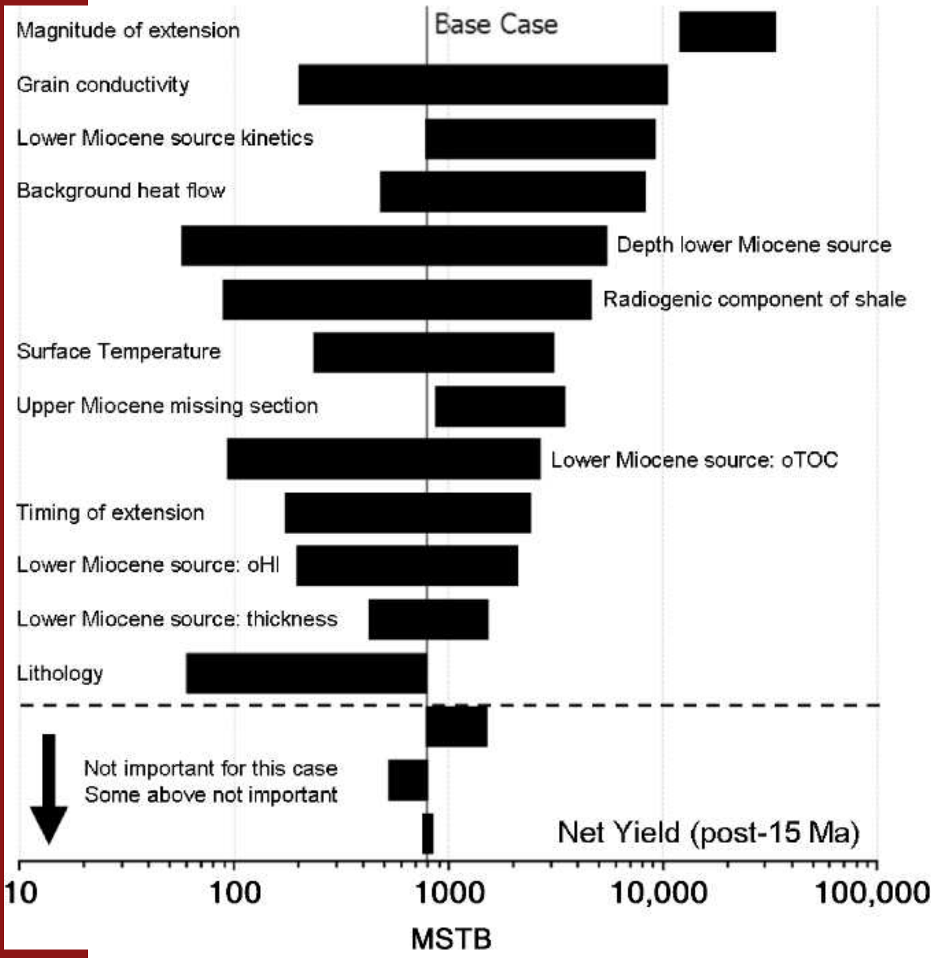
Outline

- Motivation
- Objective
- Model Development and Governing Equations
- Variations of Porosity and Volume Fraction of Hydrocarbons
- Dimensionless Groups and Their Relative Importance
- Comparisons with PetroMod
- Conclusions

Motivation



- How close is the base case to the **true case** in basin modeling?
- The uncertainty of each variable depends on **the chosen base case**.
- The uncertainty analysis is based on **individual variables, not processes or mechanisms**.

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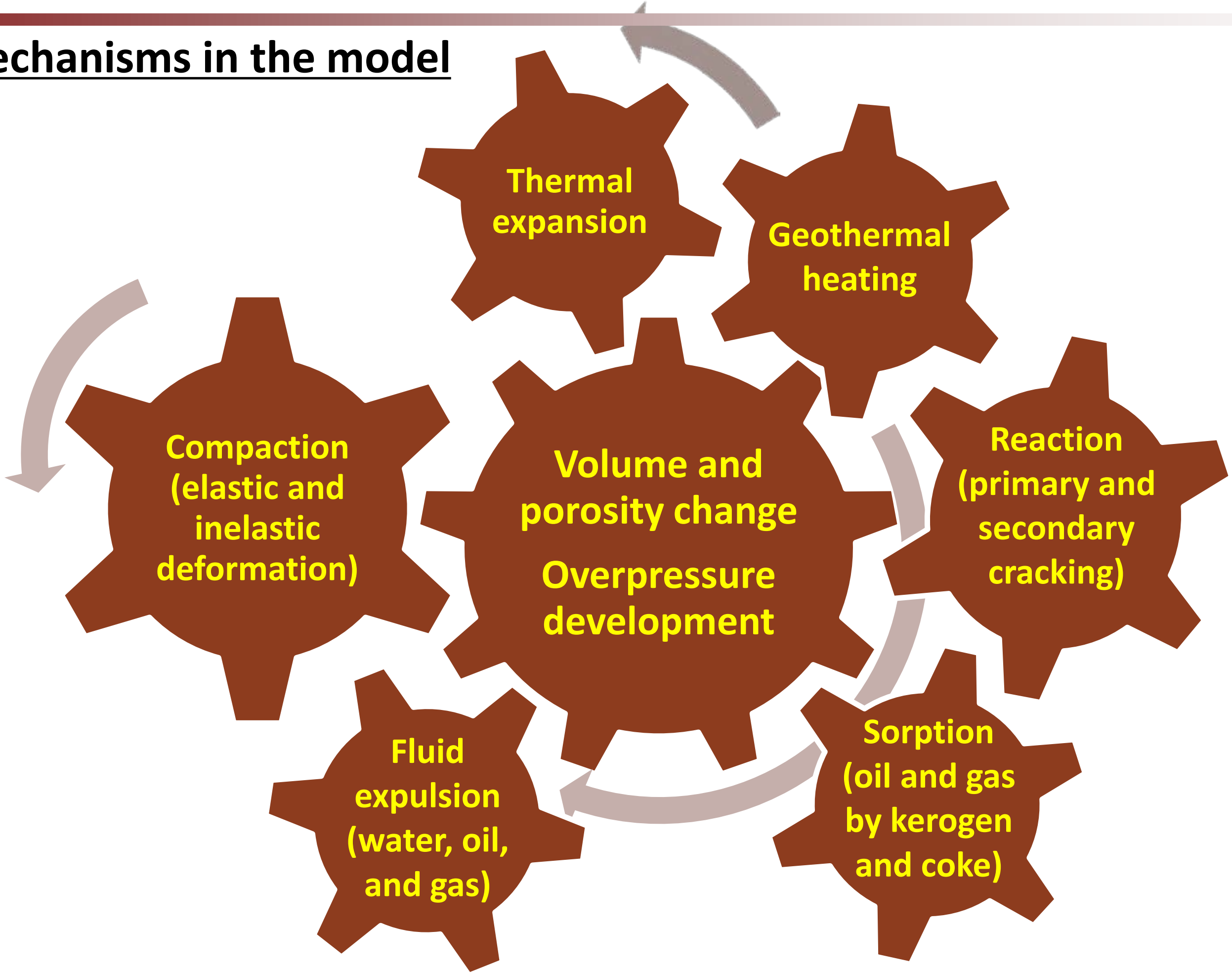
Objective

- Introduce the new concept of mechanism-based uncertainty analysis

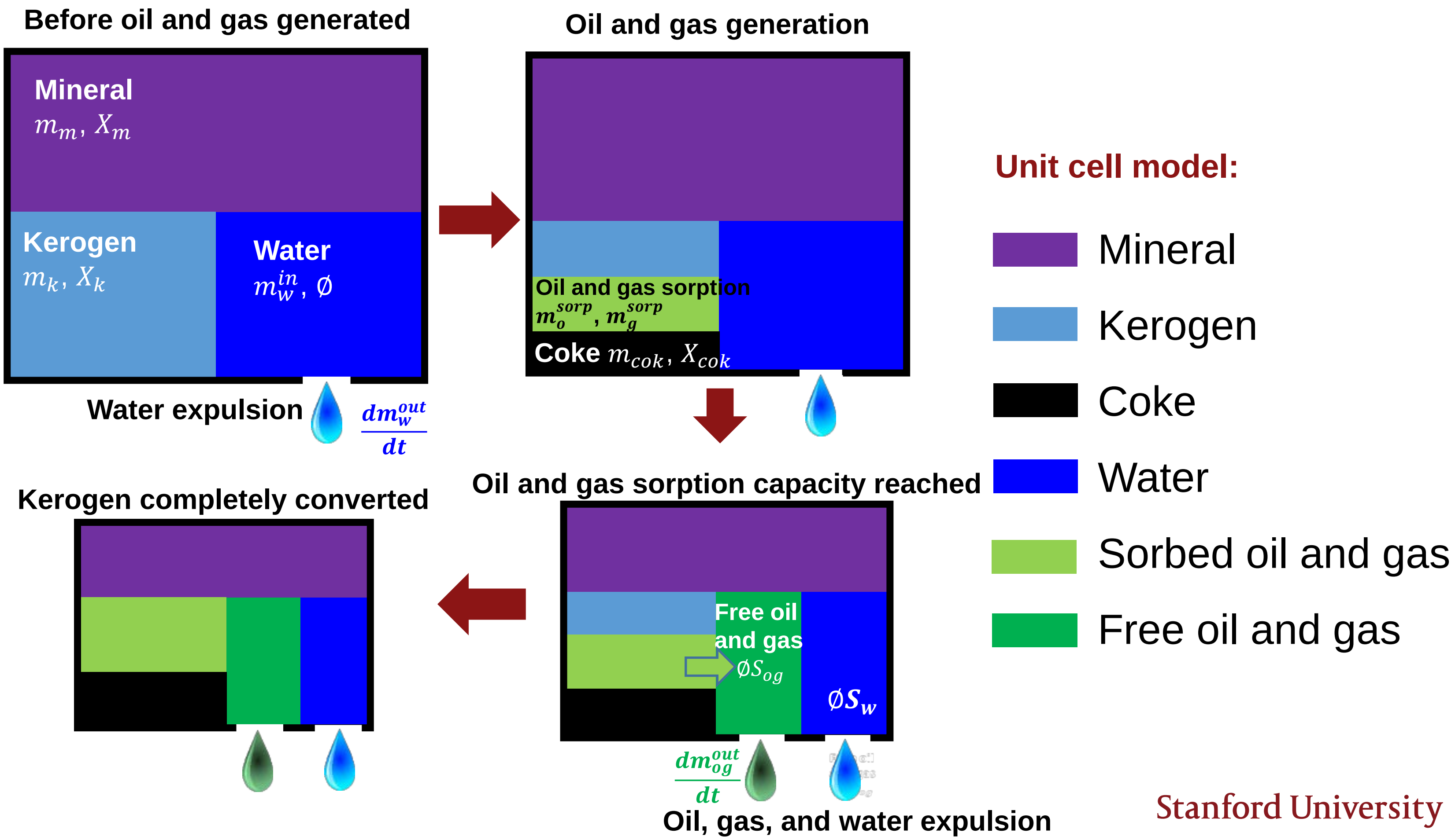
- Identify the relative importance of major mechanisms involved in porosity rebound during petroleum generation using scaling analysis

Model Development and Governing Equations

Main mechanisms in the model



Model Development and Governing Equations



Model Development and Governing Equations

Temperature change:

$$T = T_0 + \omega t \frac{dT}{dz} = T_0 + \omega t G_T$$

T_0: surface temperature; ω: constant deposition rate; G_T: geothermal gradient

Mass of water change:

$$m_w^0 = m_w^{in} + m_w^{out} \rightarrow \frac{dm_w^{in}}{dt} + \frac{dm_w^{out}}{dt} = 0$$ (water mass change is due to water expulsion)

Porosity change — Thermal expansion — Inelastic deformation

$$\frac{dm_w^{in}}{dt} = \frac{d(\rho_w V_b \emptyset S_w)}{dt} = F\left(\frac{d\emptyset}{dt}, \frac{dS_w}{dt}, \frac{dT}{dt}, \frac{dP_e}{dt}, \left[\frac{dV_b}{dt}\right]_{ie}\right)$$

Water saturation change — Compressibility

$$\frac{dm_w^{out}}{dt} = -\frac{C_{\Delta P}}{\mu_w} K(\phi) K_{rw}(S_w) \Delta P$$ (Darcy's type fluid expulsion)

Model Development and Governing Equations

Water saturation change:

Porosity — Water saturation — Overpressure — Inelastic deformation

$$S_w \frac{d\emptyset}{dt} + \emptyset \frac{dS_w}{dt} + \emptyset S_w(\beta_w + \beta_b)\frac{d\Delta P}{dt} + \frac{\emptyset S_w}{V_b}\left[\frac{dV_b}{dt}\right]_{ie}$$

$$= -\frac{C_{\Delta P}}{\mu_w} K(\phi) K_{rw}(S_w) \frac{\Delta P}{V_b}$$ ← Water expulsion

$$-\emptyset S_w(-\alpha_w + \alpha_b)\omega G_T$$ ← Thermal expansion

$$-\emptyset S_w[(\beta_w + \beta_b)\rho_w g\omega - \beta_b \rho_b g\omega]$$ ← Compressibility

$\Delta P = P_f - P_h$ (overpressure = pore pressure – hydrostatic pressure)

Model Development and Governing Equations

Primary Cracking:

Kerogen → f_{o1} Oil + f_{g1} Gas + f_{cok1} Coke

$$\left[\frac{dm_o}{dt}\right]_{generation} = -k_k m_k$$

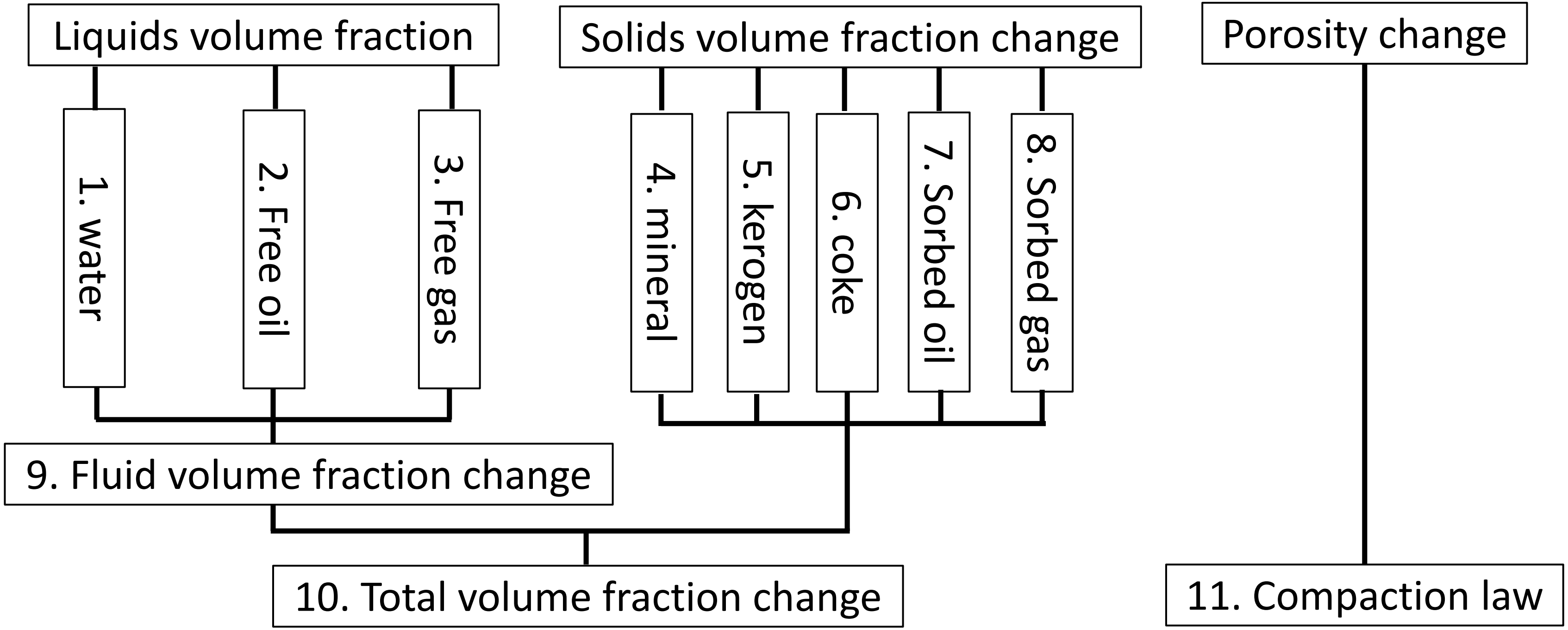
Secondary Cracking:

Oil → f_{g2} Gas + f_{cok2} Coke

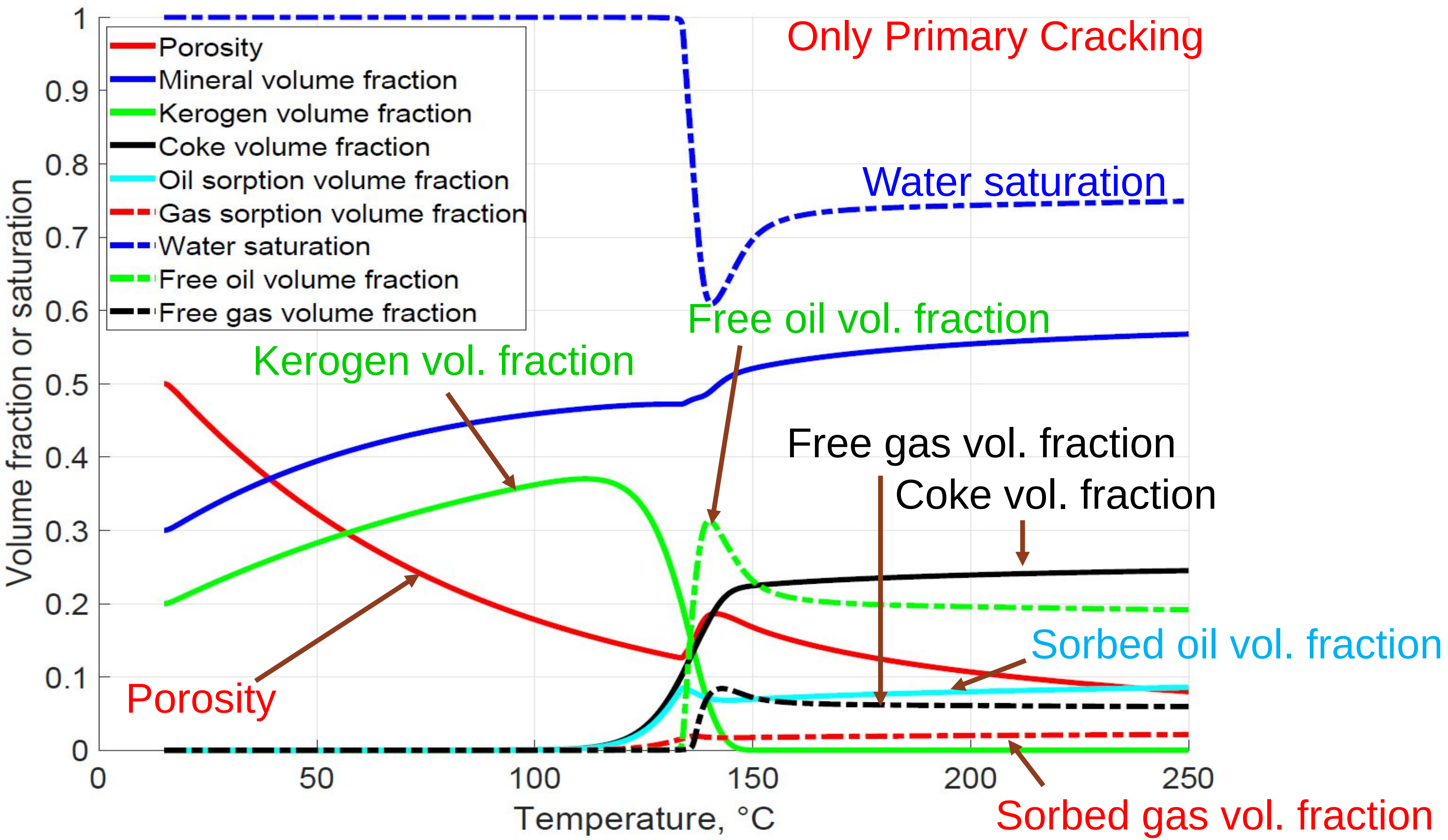
$$\left[\frac{dm_o}{dt}\right]_{cracking} = -k_o m_o$$

Only one component for oil and one component for gas

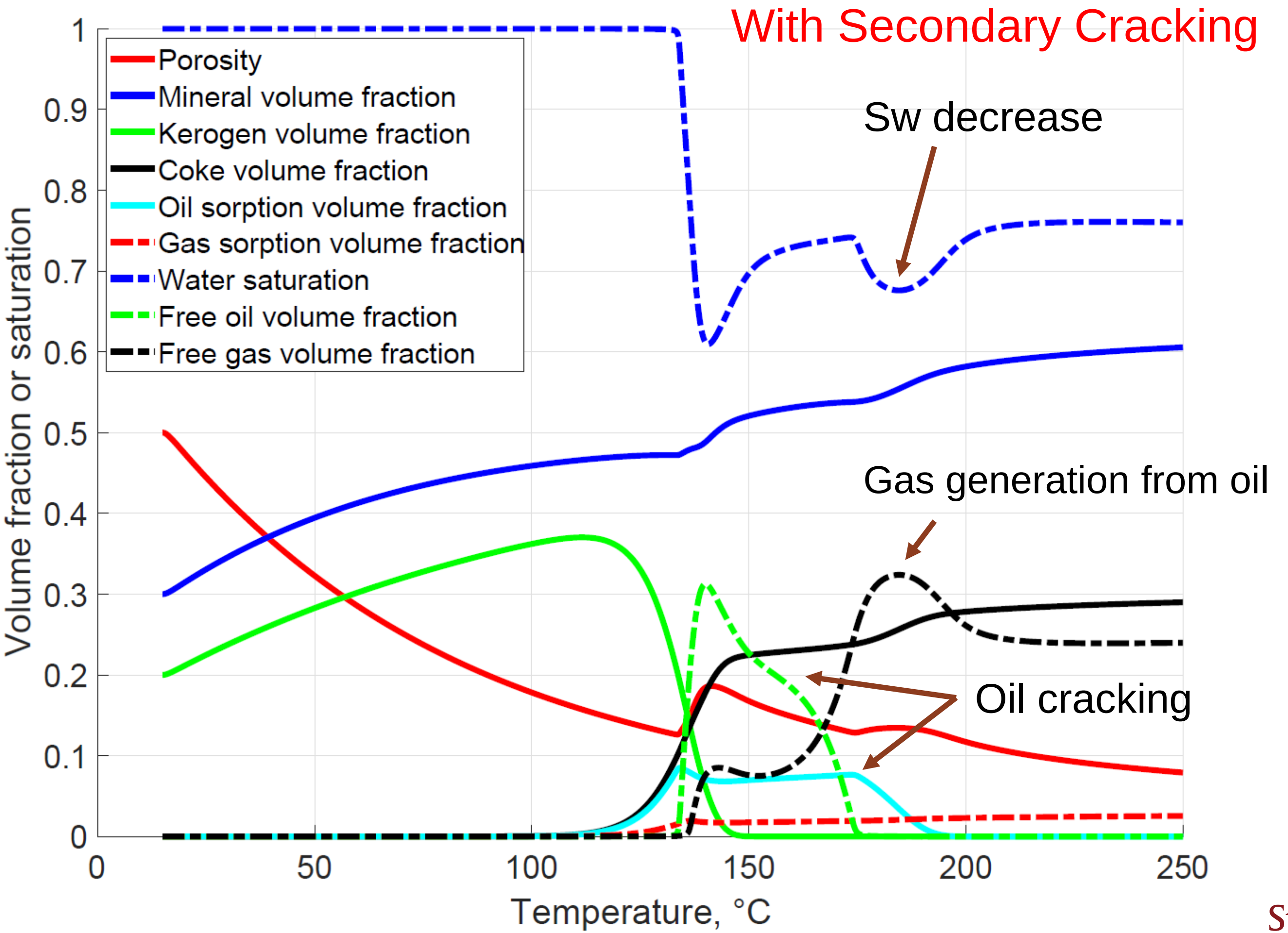
11 governing equations (ODEs) and 11 unknowns:



Variations of Porosity and Volume Fraction of Hydrocarbons



Variations of Porosity and Volume Fraction of Hydrocarbons



Dimensionless Groups and Their Relative Importance

(1) Empirical relations related: viscosity of water, oil, and gas

(2) Property related (mainly property ratios between different components)

Dimensionless thermal expansion coefficient:

$$D_6 = \frac{\alpha_w}{\alpha_m}, D_{23} = \frac{\alpha_k}{\alpha_m}, D_{24} = \frac{\alpha_{cok}}{\alpha_m}, D_{25} = \frac{\alpha_o^{sorp}}{\alpha_m}, D_{26} = \frac{\alpha_g^{sorp}}{\alpha_m}, D_{27} = \frac{\alpha_o^{sep}}{\alpha_m}, D_{28} = \frac{\alpha_g^{sep}}{\alpha_m}$$

Dimensionless compressibility coefficient:

$$D_4 = \frac{\beta_w}{\beta_m}, D_{16} = \frac{\beta_k}{\beta_m}, D_{17} = \frac{\beta_{cok}}{\beta_m}, D_{18} = \frac{\beta_o^{sorp}}{\beta_m}, D_{19} = \frac{\beta_g^{sorp}}{\beta_m}, D_{20} = \frac{\beta_o^{sep}}{\beta_m}, D_{21} = \frac{\beta_g^{sep}}{\beta_m}$$

Dimensionless density:

$$D_8 = \frac{\rho_w}{\Delta\rho}, D_{34} = \frac{\rho_k}{\rho_o^{sep}}, D_{35} = \frac{\rho_{cok}}{\rho_{og}}, D_{42} = \frac{\rho_o^{sep}}{\rho_o^{sep}}, D_{57} = \frac{\rho_k}{\rho_g^{sep}}, D_{71} = \frac{\rho_k}{\rho_g^{sorp}}$$

Dimensionless Groups and Their Relative Importance

(3) Coupled process related:

Compaction:

$$D_2 = \frac{C_m}{\beta_m}$$ Dimensionless compaction coefficient $\frac{\text{compaction coefficient}}{\text{rock elastic compressibility}}$

Reaction:

$$D_{43} = A_1\tau$$ Damkohler-like number $\frac{\text{compaction coefficient}}{\text{reference flow rate}}$

$$D_{44} = \frac{E_{a1}}{R\Delta T}$$ Arrhenius number $\frac{\text{activation energy}}{\text{potential energy}}$

Heating:

$$D_7 = \alpha_m \Delta T$$ Dimensionless thermal expansion coefficient

$$D_{31} = \frac{T_0}{\Delta T}$$ Reduced initial temperature $\frac{\text{surface temperature}}{\text{temperature difference}}$

Expulsion:

$$D_{13} = \frac{K_P^0 \tau}{\mu_w V_{b0} \beta_m}$$ Dimensionless expulsion rate $\frac{\text{water expulsion rate}}{\text{reference flow rate}}$

Dimensionless Groups and Their Relative Importance

53 physical/dimensional parameters

↓

52 **dependent** dimensionless groups

↓

37 **independent** dimensionless groups

↓

28 independent dimensionless groups of interest

Range (**dimensional**)

Min.	Max.
…	…
…	…

↓

Range (**dimensionless**)

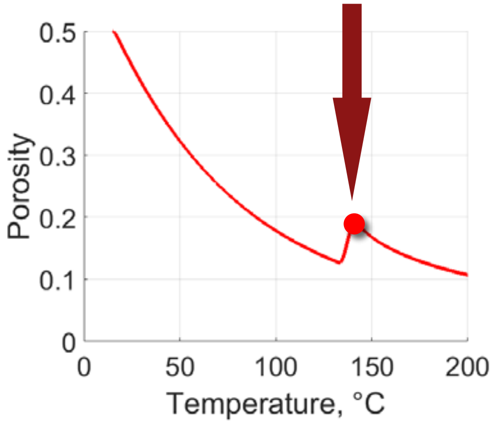
Min.	Max.
…	…
…	…

Dimensionless Groups and Their Relative Importance

Experimental Design - Two-level Factorial Design

$$y = \alpha_0 + \sum_{i=1}^{N=28} \alpha_i D_i$$

y : response (e.g. max. porosity during hydrocarbon generation)

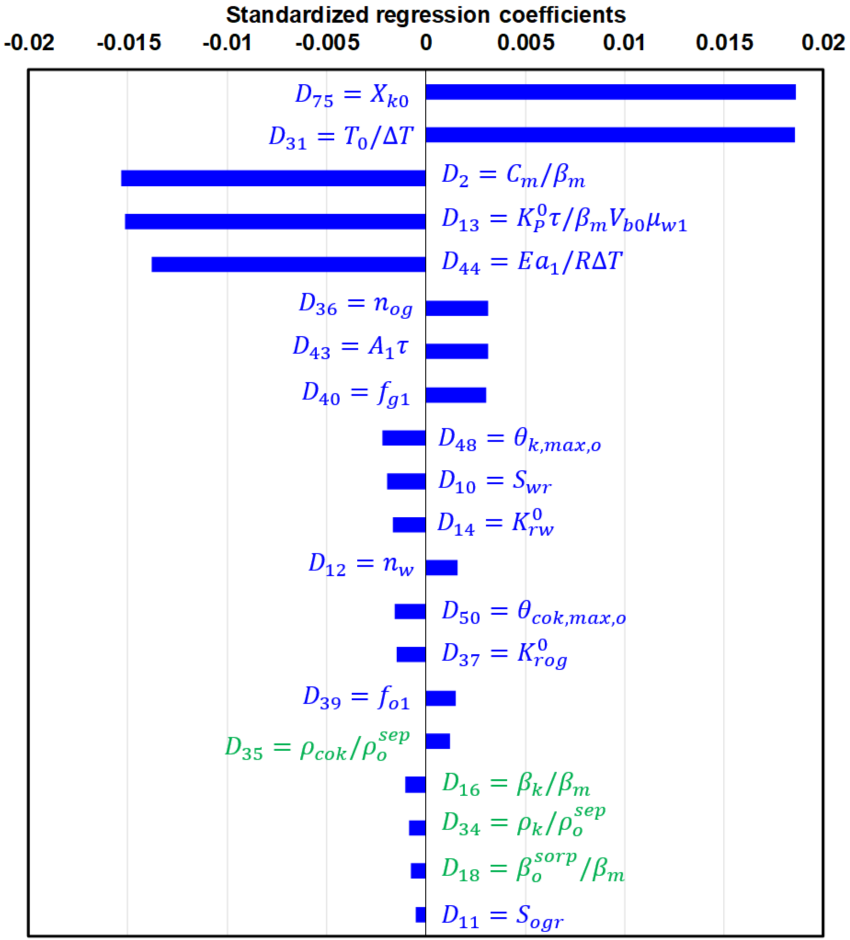


α_i: coefficient

D_i: dimensionless numbers

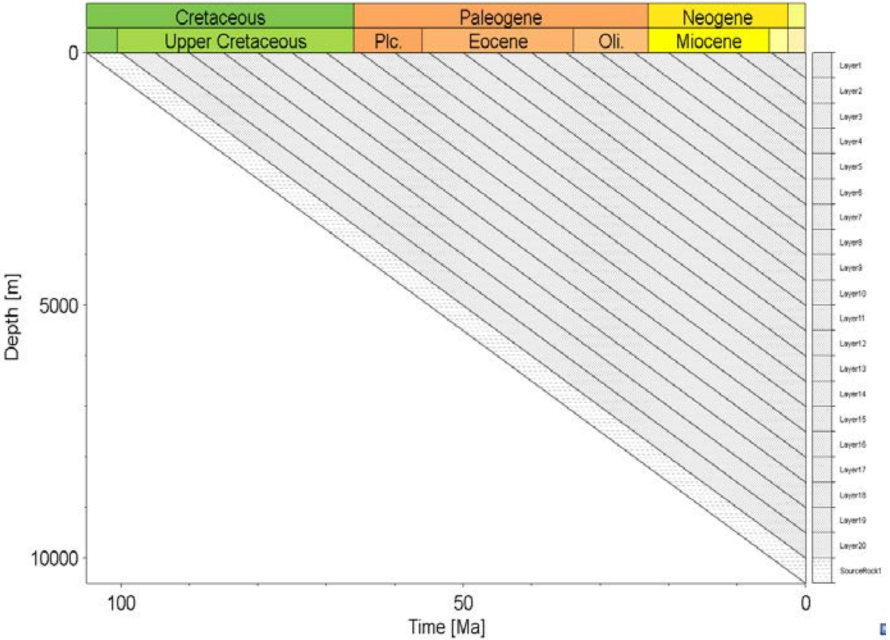
- Full two-level factorial design: 2^{28} runs
  - impossible to run all the cases
- Experimental design of IV resolution: at least $2^6 = 64$ runs
  - can identify the main effects, but not the interactive effects

Dimensionless Groups and Their Relative Importance



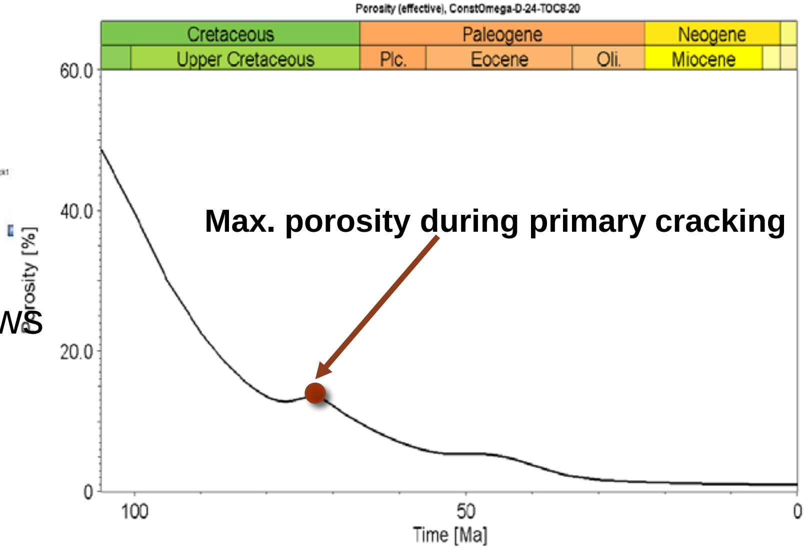
1. **initial kerogen content**
2. **reduced initial temperature**
3. **scaled compaction coefficient**
4. **fluid expulsion rate**
5. **Arrhenius number**
6. oil and gas relative permeability coefficient
7. Damkohler-like number
8. mass stoichiometric factor of gas
9. oil sorption capacity by kerogen
10. residual water saturation

Comparisons with PetroMod

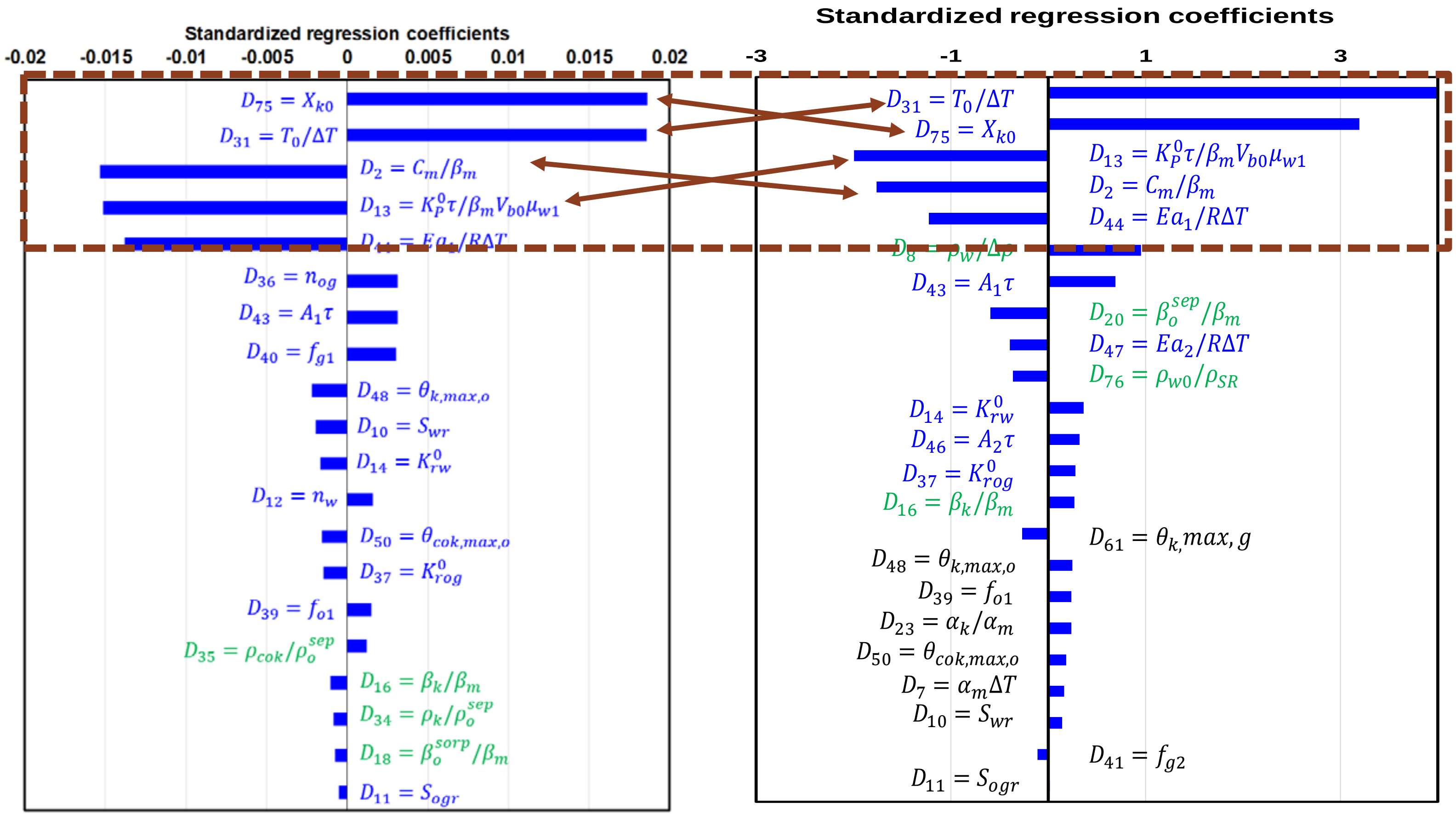


- ✓ PetroMod 1D model
- ✓ Constant deposition rate
- ✓ Initial porosity
- ✓ Density
- ✓ Compressibility
- ✓ Reaction
- ✓ …

- X 0D vs. 1D model
- X Constant geothermal gradient vs. heat flows
- X Two-phase vs. three-phase flows
- X Relative permeability
- X …



My model vs. PetroMod



Same 5 most important dimensionless groups but slightly different ranking

Conclusions

- New model is developed for the coupled compaction, kerogen conversion, and expulsion processes
- Major mechanisms and their corresponding dimensionless groups are identified and their relative importance is determined
- Mechanism-based uncertainty analysis concept is introduced

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  - Dr. Leslie Moogan

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