

3.1.11**Application of pyrolysis methods to multi-component modelling**

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(david.j.curry@exxonmobil.com)**THEME 3:
Volatiles of the Earth****Session 3.1:
Petroleum geochemistry and migration**

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This session offers a unique forum for a multi-disciplinary discussion on geochemical processes associated with the generation, migration and alteration of oil and gas. Papers are invited which address any of the topics: 1) Interaction of Petroleum with the Subsurface and Subsea Biosphere: Deep biosphere electron donors and acceptors; Petroleum and biogeochemistry of subsea hydrocarbon vents; Formation of biogenic gas; Biodegradation. 2) Tracing Sources, Sinks and Fluxes of Petroleum and associated basin fluids: Biogeochemical and biodegradation markers; Novel isotopic applications (e.g. ^2H , ^{14}C); Identifying early gas formation; Compositional kinetics; Phase behaviour. 3) Water as a Reactant and Transport Medium: Role of water in petroleum generation; Effects of water interaction during migration; Biodegradation products in formation waters. 4) Geochemistry of Unconventional Gas Resources: Shale gas; Coal Bed Methane; Basin-Centred Gas. Interdisciplinary studies are highly encouraged.

As petroleum exploration moves into increasingly demanding environments, enhanced basin modelling capabilities are needed to help mitigate the increased risk and cost. These enhanced capabilities include the use of multi-component hydrocarbon generation, expulsion, and cracking models to predict fluid volumes, types, and properties. Pyrolysis methods (both open and closed) are used to calibrate these models and determine the appropriate input parameters for different geologic conditions. However, closed-system pyrolysis only approximates natural generation and open-system pyrolysis, while providing data on compositions, yields, and kinetics, does not simulate natural maturation processes. Consequently pyrolysis data are not directly applicable to modelling natural generation and must be interpreted in a geologic context to insure that laboratory artifacts are not carried through into geological models. In closed pyrolysis the secondary cracking of products (particularly aliphatic components) frequently begins prior to the end of petroleum generation. Consequently, although closed pyrolysis can be used to determine the bulk compositions of the non-polar fractions prior to the onset of secondary cracking, the assessment of maximum potential yields requires a combination of closed and open system data. In addition, since the generation of cyclohexanes is suppressed and generation of one-ring aromatics is favored at laboratory conditions relative to natural systems, detailed compositions (e.g., yields of saturates and aromatics) need to be adjusted using data from natural systems. The generation, cracking, and expulsion of polar components also vary between geologic and laboratory conditions, with significantly higher concentrations of polar fractions observed in expelled pyrolysates compared to reservoir oils. Because of the overlap of generation and cracking reactions, closed pyrolysis is not always effective for determining generation kinetics of different components. Calibration of the extent of generation or cracking to different maturity indicators also varies significantly between laboratory and geologic conditions. Coals are particularly challenging since they have high concentrations of functional groups and demonstrate a degree of auto-reactivity at relatively low levels of heating. Consequently, there can be significant differences in the petroleum generation from coals under laboratory versus geological conditions. Pyrolysis techniques are powerful and precise methods to calibrate and parameterize multi-component models. However, closed and open-systems pyrolysis data must be interpreted in the geologic context and integrated with the expulsion and cracking elements of these model to insure full applicability.