EVALUATION OF KINETIC UNCERTAINTY IN NUMERICAL MODELS OF PETROLEUM GENERATION

K.E. Peters¹, C.C. Walters², and P.J. Mankiewicz³

¹U.S. Geological Survey, 345 Middlefield Road, MS 969, Menlo Park, CA 94025-3561
²ExxonMobil Research & Engineering Co., 1545 Route 22 East, Annadale, NJ 08801-0998
³ExxonMobil Upstream Research Co., Box 2189, Houston TX 77252-2189

Oil-prone marine petroleum source rocks contain abundant type I or type II kerogen defined as having Rock-Eval pyrolysis hydrogen indices >600 or in the range 300-600 mg hydrocarbon/g total organic carbon (mg HC/g TOC), respectively. Samples from 29 marine source rocks worldwide that contain mainly type II kerogen (hydrogen index = 230-786 mg HC/g TOC) were subjected to open-system programmed pyrolysis to determine activation energy distributions for petroleum generation. Assuming a burial heating rate of 1°C/m.y. for each measured activation energy distribution, the calculated average temperature for 50% fractional conversion of the samples to petroleum is ~136°C ±7°C, but the range spans ~30°C (~121°-151°C).

Fifty-two outcrop samples of thermally immature Jurassic Oxford Clay Formation (Peterborough Member) were collected from five locations in the United Kingdom to determine natural variations of kinetic response for one source-rock unit. The samples contain mainly type I or type II kerogens (hydrogen index = 230-774 mg HC/g TOC) having activation energy distributions for conversion to petroleum centered at ~56 kcal/mol with an average frequency factor of ~3.5 x 10¹⁵ sec⁻¹. At a heating rate of 1°C/m.y., the calculated temperatures for 50% fractional conversion of the Oxford Clay kerogens to petroleum differ by as much as 23°C (127°-150°C).

The data indicate that kerogen type as defined by hydrogen index is not systematically linked to kinetic response and that "default" kinetics for the thermal decomposition of type I or type II kerogen can introduce unacceptable errors into numerical simulations. Furthermore, "custom" kinetics based on one or a few samples of thermally immature source rock may be inadequate to account for variations in organofacies within that stratigraphic interval. We propose three methods to evaluate the uncertainty contributed by kerogen kinetics to numerical simulations: (1) use the average kinetic distribution for

multiple samples of source rock and the standard deviation for each activation energy within that distribution, (2) when representative samples are available at different locations, use the source-rock kinetics determined at each location for that part of the study area, and (3) use a "weighted-average" method where kinetics for samples from different locations within the source-rock unit are combined by giving the activation energy distribution for each sample a weight proportional to its Rock-Eval pyrolysis S2 yield.