NOVEL KINETIC CONCEPTS OF VITRINITE REFLECTANCE MODELLING AND PRIMARY KEROGEN CRACKING

Ulrich Berner, Statoil ASA, Norway

Introduction

Kinetic modelling of vitrinite reflectance equivalence values has become a standard approach in basin modelling to numerically simulate thermal maturity mainly using the EASY%Ro concept (Sweeney & Burnham 1990) with commercial software packages. Application in exploration suggest that EASY%Ro does not fully explain observed natural maturation trends and consequently attempts of improvement have been made (Berner et al. 1995; Ritter el al. 1996, Nielsen et al. 2015) which however are not fully applicable over a realistic range of geologically relevant heating rates (Figure 1).

Method development

To overcome significant modelling uncertainties a new kinetic concept (GeoChemVR) of thermal vitrinite alteration has been developed in which activation energies are related to specific frequency factors optimized to secure time-temperature stability at different heating rates. The range of activation energies is kept within physico-chemically relevant boundaries and tries to mimic geochemical changes of vitrinite alteration. The data set of Koch & Schellschmidt (2001) combines observed thermal maturities and measured maximum subsurface temperatures and has been used to calibrate stoichiometric conversion factors assigned to individual theoretical reactions of the new kinetic concept.

Results

The model can be used to simulate vitrinite alteration form about 0.2 to about 8 [%] covering the full range of stages from peat to meta-anthracite/graphite following the general observed natural data trends (Figure 1). The stability and validity of the model is demonstrated for heating rates between 1 [K my^{-1}] to 1 [K $100y^{-1}$]. It is also shown that a high time-step resolution is crucial to obtain realistic simulation results at geological heating rates.

Furthermore, two examples of simple kinetic concepts of primary cracking of Type II and III kerogens combined with the new vitrinite alteration kinetics demonstrate the relevance of the suggested approach of paired activation energy and frequency factors, and the significant advantage over previous concepts as they assure realistic time and temperature simulations in basin modelling.

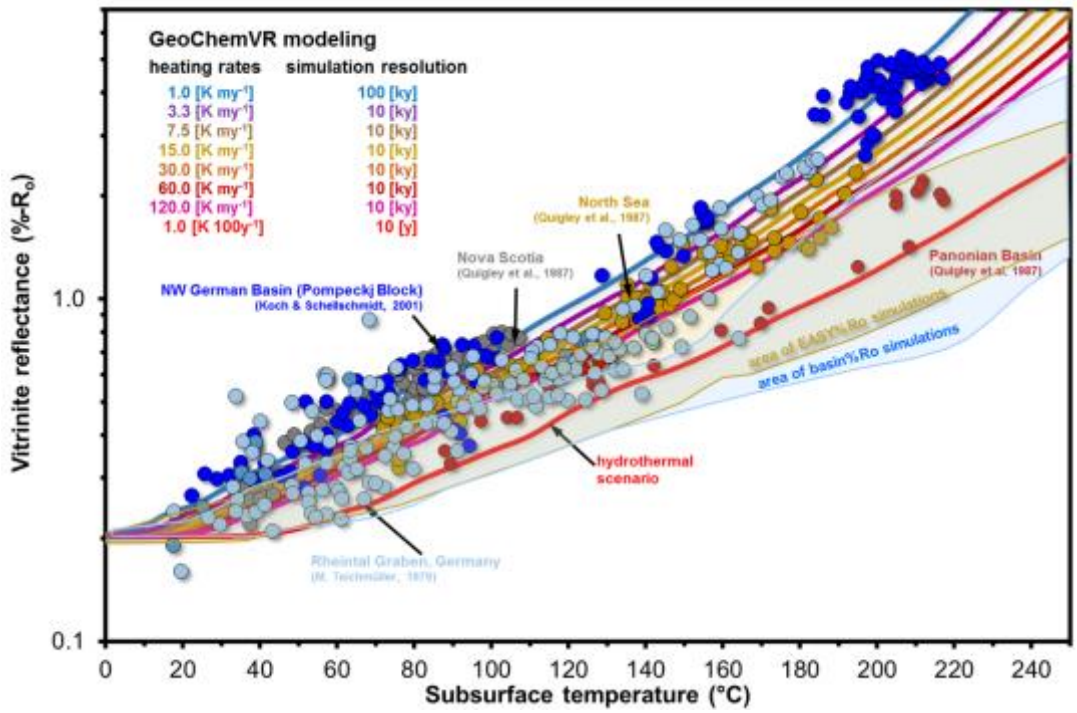

Figure 1 *Simulated vitrinite reflectance (colored lines) using the GeoChemVR concept at different geological heating rates and adequate time resolution in comparison with observations on subsurface temperature and measured vitrinite reflectance. Areas of EASY%Ro and basin%Ro simulations (heating rates from 1 [K/my] to 1 [K/100y]) are given as brown and blue shaded fields, respectively.*

References

Berner, U., Faber, E., Scheeder, G., & Panten, D. (1995): Primary cracking of algal and landplant kerogens: kinetic models of isotope variations in methane, ethane and propane. Chem. Geol. 126, 233 – 245.

Koch, J. & Schellschmidt, R. (2001): Zum Zusammenhang zwischen Inkohlung und Temperatur speziell der Kohlenbildung. Erdoel, Erdgas Kohle 117(4), 182 – 188.

Nielsen, S. B., Clausen O. R. & E. McGregor (2015): basin%Ro - A vitrinite reflectance model derived from basin and laboratory data. Basin Research (2015), 1 – 22.

Quigley, T.M., Mackenzie, A.S. & Gray, J.R. (1987): Kinetic theory of petroleum generation. In Doligez, B. (ed.): Migration of Hydrocarbons in Sedimentary Basins, 649 – 665 (Editions Technip.)

Ritter, U., Duddy, I., Mørk, A., Johansen, H. & Arne, D. (1996): Temperature and uplift history of Bjørnøya (Bear Island), Barents Sea. Petroleum Geoscience 2, 133 – 144.

Sweeney, J.J. & Burnham, A.K. (1990): Evaluation of a simple model of vitrinite reflectance based on chemical kinetics. AAPG Bull. 74 10., 1559 – 1570.

Teichmueller, M. (1979): Die Diagenese der kohligen Substanzen in den gesteinen des tertiaers und Mesozoikums des mittkeren Oberrhein-Grabens. Fortschr. Geol. Rheinld. u. Westf. 27, 19 – 49.