Basin Modelling and Diagenetic Effects of Groundwater Migration*

Xavier Guichet¹ and Sylvie Wolf²

Search and Discovery Article #40432 (2009)
Posted June 22, 2009

*Adapted from poster presentation at AAPG International Conference and Exhibition, Cape Town, South Africa, October 26-29, 2008

¹Geology-Geochemistry-Geophysics, IFP, Rueil-Malmaison, France (xavier.guichet@ifp.fr)
²Applied Mathematics, IFP, Rueil-Malmaison, France

Abstract

Our objective is to trace the volume of minerals that precipitate or dissolve in a sedimentary basin as groundwaters migrate along temperature and pressure gradients. In a sedimentary basin, temperature and pressure changes can occur in response to burial and exhumation or changes in heat flow. On the other hand, in a steady-state flow regime (T and P do not change with time), cementation only results from hydrologic mass transport. Our calculation is based on the assumption that minerals maintain local equilibrium with migrating groundwaters and their solubilities depend only on temperature and pressure. Thus every temperature and pressure change known by groundwater leads to a precipitation or a dissolution of the mineral in order to preserve local equilibrium. We developed a prototype based on Temis3D® Software, which is a coupled numerical simulation program that evaluates pore pressure, porosity, overburden and other petroleum parameters through time. Our prototype uses built-in solubility correlations to calculate solubilities of a large collection of minerals as a function of temperature and pressure. Finally the cementation or dissolution rate of a mineral is calculated in each cell of the basin model by solving a mass balance equation that describes transport of the dissolved mineral by advection. The prototype predicts cumulative volume changes of minerals following instantaneous rates of precipitation and dissolution and highlights area where cementation processes are expected to occur. Since our model does not take into account more complex geochemical factors that might control mineral precipitation or dissolution such as reaction kinetics or mixing fluids of differing composition, quantitative estimate of volume changes of minerals must be interpreted with caution.
References


Portier, S. and C. Rochelle, 2005, Modelling CO$_2$ solubility in pure water and NaCl-type waters from 0 to 300 degrees C and from 1 to 300 bar; application to the Utsira Formation at Sleipner in Geochemical aspects of CO$_2$ sequestration: Chemical Geology, v. 217/3-4, p. 187-199. DOI: 10.1016/j.chemgeo.2004.12.007


Our objective is to trace the volume of minerals that precipitate or dissolve in a sedimentary basin as groundwaters migrate along temperature and pressure gradients. In a sedimentary basin, temperature and pressure changes can occur in response to burial and exhumation or changes in heat flow. On the other hand, in a steady-state flow regime (T and P do not change with time), cementation only results from hydrologic mass transport. Our calculation is based on the assumption that minerals maintain local equilibrium with migrating groundwaters and their solubilities depend only on temperature and pressure. Thus every temperature and pressure change known by groundwater leads to a precipitation or a dissolution of the mineral in order to preserve local equilibrium. We developed a prototype based on Temis3D Software, which is a coupled numerical simulation program that evaluates pore pressure, porosity, overburden and other petroleum parameters through time. Our prototype uses built-in solubility correlations to calculate solubilities of a large collection of minerals as a function of temperature and pressure. Finally the cementation or dissolution rate of a mineral is calculated in each cell of the basin model by solving a mass balance equation that describes transport of the dissolved mineral by advection. Our prototype does not take into account more complex geochemical factors that might control mineral precipitation or dissolution such as reaction kinetics or mixing fluids of differing composition, quantitative estimate of volume changes of minerals must be interpreted with caution.

The first term on the right hand side of the equation account for cementation by groundwater advection. The second describes the effects of temperature and pressure changes, as might occur in response to burial and exhumation or changes in heat flow, on cementation. For a volume V of a basin strata having a constant porosity, the equation becomes:

\[ \frac{dV_i}{dt} = \nabla \cdot (\nabla \psi_i + \frac{\partial V_i}{\partial t}) \]

The last equation is equivalent to equation (13.3) of Bethke (2002).

### GEOFACIAL RECALL AND DATA

#### Calcite Solubility

The reaction of dissolution/precipitation of calcite can be written like a simple chemical equation:

\[ CaCO_3(s) + CO_2(g) + H_2O \leftrightarrow Ca^{2+} + 2HCO_3^- \]

All the species co-exist simultaneously and the concentrations of these ions are not independent but fixed by equilibrium between one another and any present solid phases:

\[

c_{CaCO_3} \leftrightarrow c_{Ca^{2+}} + c_{HCO_3^-} \cdot K_{Ca}
\]

\[

c_{CO_2} + c_{H_2O} \leftrightarrow c_{HCO_3^-} + c_{H^+} \cdot K_{H}
\]

\[

c_{HCO_3^-} + c_{H^+} \leftrightarrow c_{HCO_3^-} + 1/K_{K}
\]

For example neglecting activity coefficient and fugacity coefficient calcium concentration is linked with CO2 pressure by:

\[ [Ca^{2+}]^3 \sim \frac{K_{Ca}}{4c_{Ca} \cdot K_{H} \cdot P_{CO2}} \]

For basinal brines, effects of salinity modify considerably the solubility of calcite and cannot be neglected. Up to now, large discrepancies exist in the geochemical data, particularly for low temperatures (<100°C). We used the solubility function provided by Portier (2005) which can be applied for temperature range 0-300°C, salinity range 0-250 g/L and pressure range 1-100 bar.

#### Apparent Solubility Product of Quartz

The chemical reaction being modeled is of the form:

\[ SiO_2(\alpha) + 2 \cdot H_2O \leftrightarrow H_2SiO_4 \]

Several models for quartz solubility are available. Von Damm et al. (1991) provided a relationship calibrated for large ranges of temperature, pressure and salinity. More recently, Rimstidt (1997) gives a simple solubility function for temperature range 0-300°C:

\[
\log K = \frac{1107.12}{T} - 0.0254
\]
The Paris Basin is an intracratonic basin with up to 3 km of sedimentary infill deposited on top of Hercynian basement. Sediments range in age from Permian to Quaternary. There are two main permeable petroleum reservoir units in the central part of the Mesozoic of the Paris Basin; the Late Triassic fluvial sandstones (Keuper Formation) and the Middle Jurassic marine carbonates (Dogger Formation). Sandwiched between the Keuper sandstone and the Dogger carbonate are the Liassic (Early Jurassic) shales. These shales are the only major petroleum source rocks within the basin. The basin has experienced a simple burial history punctuated by periods of fairly rapid burial in the Early and Middle Jurassic and Late Cretaceous. Maximum burial occurred in the Oligocene, followed by uplift of variable extent during and following Alpine tectonism. There are several generations of faults within the Paris Basin some of which were inherited from the Palaeozoic basement and were still active in the Tertiary during Pyrenean and Alpine tectonism.

**Calcite Cementation in Dogger Aquifer**

Microthermometric data
70°C < Th < 90°C
Salinity and isotope data show that Dogger formation water contains 15% invasion Keuper water.
Cross formational flow of water occurred like upward flow along faults during the Tertiary
(Worden and Matray, 1995)

**Quartz Cementation in Keuper Aquifer**

Microthermometric data
90°C < Th < 125°C
(Guilhaumou, 1993)

We observe a good agreement between our simulations and microthermometric measurements for quartz overgrowth in Keuper aquifer.

For calcite cementation, simulations provide good localization of mineral reactions. However quantitative estimates of porosity variations are not obtained.

Permeability feedback results in a focusing of mineral reactions.

Our calculations are first step towards reactive transport modelling. Equilibrium assumption provides good results for basin scale simulations; however, estimate of volume changes of minerals rests on accurate solubility data.

Use of apparent solubility products accounts for the influence of salinity, CO2 pressure, and chemical interactions.

**Conclusion**

Salinity advection, equilibrium thermodynamics calculations for major cations and anions based on Gibbs free energy minimization.

**References**

Gonçalves et al., Bull. Soc. Geol. Française, 2003
Portier S., PhD (in French), Université Louis Pasteur, 2005
Von Damm et al., American Journal of Science, 291, 977-1007, 1991
Worden and Matray, Basin Research, 7, 53-66, 1995

Acknowledgements: IFP grants for Basin Modelling (D1489)