Pressure-Solution at Grain-to-Grain Contact: A New Model for Basin Modelling*

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Abstract

Pressure-solution reaction leads to closer packing of the granular rocks, resulting in a porosity decrease, but the mechanisms operating at the grain scale are not well understood, mainly because different mechano-chemical processes interact during deformation. Sandstones from the Brent reservoirs located in the Northern North Sea show pressure-solution features. We focused our work on the role of mass transfer in sandstone diagenesis, for which the present model of pressure-solution is developed.

Pressure-solution is driven by stress differences and its rate is affected by temperature, grain size, and fluid chemistry. The pressure-solution process comprises three kinetic steps: dissolution of the grain at stressed grain-to-grain contacts, diffusion to stress-free grain surface, and precipitation. The present treatment of pressure-solution idealizes the aggregate as a regular packing of truncated spheres, such that it is sufficient to consider a single spherical grain in contact with N identical neighbours. The grain is assumed to consist of a pure, isotropic solid substance that is soluble in the pore fluid. For conditions of temperature and pressure relevant for sedimentary basins, we show that the dissolution step is the slowest kinetic step, and therefore it controls the overall kinetics of pressure-solution. Another original feature of our model lies in the fact that the geometrical model comes from studies of metallurgy. This geometrical model permits to calculate the coordination number and the contact surface areas for each sphere as a function of the porosity.

The model is applied to the Brent reservoirs from the Northern North Sea. The inputs of the model are: (1) the temperature and the effective stress histories computed with TemisSuite Software, (2) the grain-size distribution of the reservoir unit. Then the model is used in post-processing of a basin-modelling calculation performed with TemisSuite. The computed porosities are in good agreement with the observed porosities.

References

de Boer, R.B., 1977, Pressure solution; theory and experiments: Tectonophysics, v. 39/1-3, p. 287-301.

de Boer, R.B., 1977, On the thermodynamics of pressure solution; interaction between chemical and mechanical forces: Geochimica et Cosmochimica Acta, v. 41/2, p. 249-256.

Dewers, T., and P.J. Ortoleva, 1990, Interaction of reaction, mass transport, and rock deformation during diagensis; mathematical modeling of intergranular pressure solution, stylolites, and differential compaction/cementation, *in* I.D. Meshri, and P.J. Ortoleva, (eds.), Prediction of reservoir quality through chemical modeling: AAPG Memoir 49, p. 147-160.

Gundersen, E., D.K. Dysthe, F. Renard, K. Bjorlyukke, and B. Jamtveit, 2002, Numerical modeling of pressure solution in sandstone, rate-limiting processes and the effect of clays, *in* S. de Meer, M.R. Drury, J.H.P. de Bresser, and G.M. Pennock, (eds.), Deformation mechanisms, rheology and tectonics; current status and future perspectives: Geological Society of London, Special Publications, v. 200, p. 41-60.

Lasaga, A.C., 1998, Kinetic theory in the Earth sciences: Princeton University Press, Princeton, New Jersey, 811 p.

Lehner, F.K., 1995, A model for intergranular pressure solution in open systems, *in* C.J. Spiers, and T. Takeshita, (eds.), Influence of fluids on deformation processes in rocks: Tectonophysics, v. 245/3-4, p. 153-170.

Nakashima, S., 1995, Diffusivity of ions in pore water as a quantitative basis for rock deformation rate estimates, *in* C.J. Spiers, and T. Takeshita, (eds.), Influence of fluids on deformation processes in rocks: Tectonophysics, v. 245/3-4, p. 185-203.

Paterson, M.S., 1973, Nonhydrostatic thermodynamics and its geologic applications: Reviews of Geophysics and Space Physics: v. 11/2, p. 355-389.

Renard, F., P. Ortoleva, and J.-P. Gratier, 1997, Pressure solution in sandstones; influence of clays and dependence on temperature and stress: Tectonophysics, v. 280/3-4, p. 257-266.

Robin, P.Y.F., 1978, Pressure solution at grain-to-grain contacts: Geochimica et Cosmochimica Acta, v. 42/9, p. 1383-1390.

Rutter, E.H., 1976, The kinetics of rock deformation by pressure solution: Philosophical Transactions of the Royal Society of London Series A Mathematical and Physical Sciences, v. 283/1312, p. 203-219.

Schneider, F., J.L. Potdevin, S. Wolf, and I. Faille, 1996, Mechanical and chemical compaction model for sedimentary basin simulators: Tectonophysics, v. 263/1-4, p. 307-317.

Weyl, P.K., 1959, Pressure solution and the force crystallization; a phenomenological theory: Journal of Geophysical Research, v. 64/11, p. 2001-2025.

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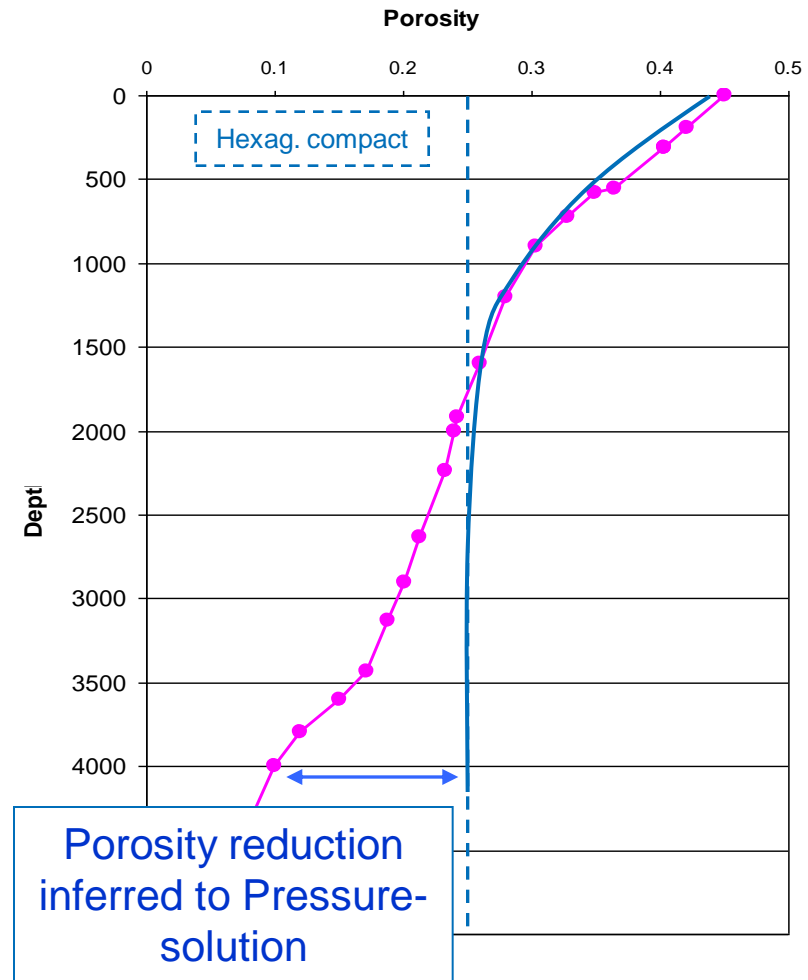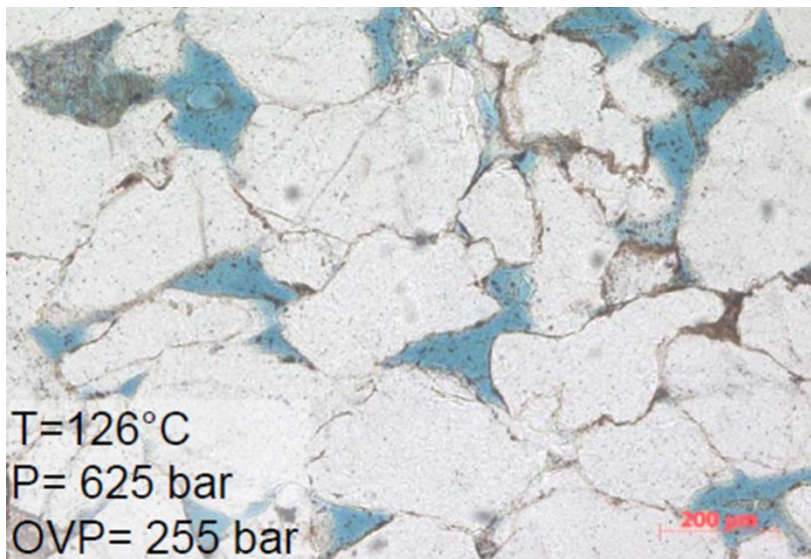
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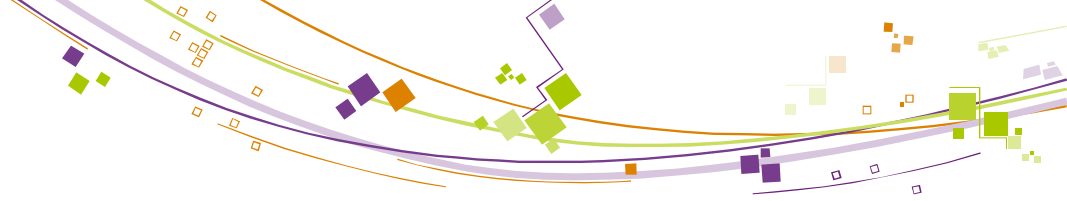
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Porosity evolution of sandstone reservoirs with burial

- **Mechanical compaction**
    - Grain organization
    - Porosity decreases down to 25%
- **For lower porosities, a new mechanism followed by quartz overgrowth**

T=126°C
P= 625 bar
OVP= 255 bar
200 µm

Porosity

Hexag. compact

Depth

Porosity reduction inferred to Pressure-solution

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Abundant Bibliography over the last 50 years

- Pressure solution creep is a temperature and stress dependent mechanism that modifies both grain size and rock porosity

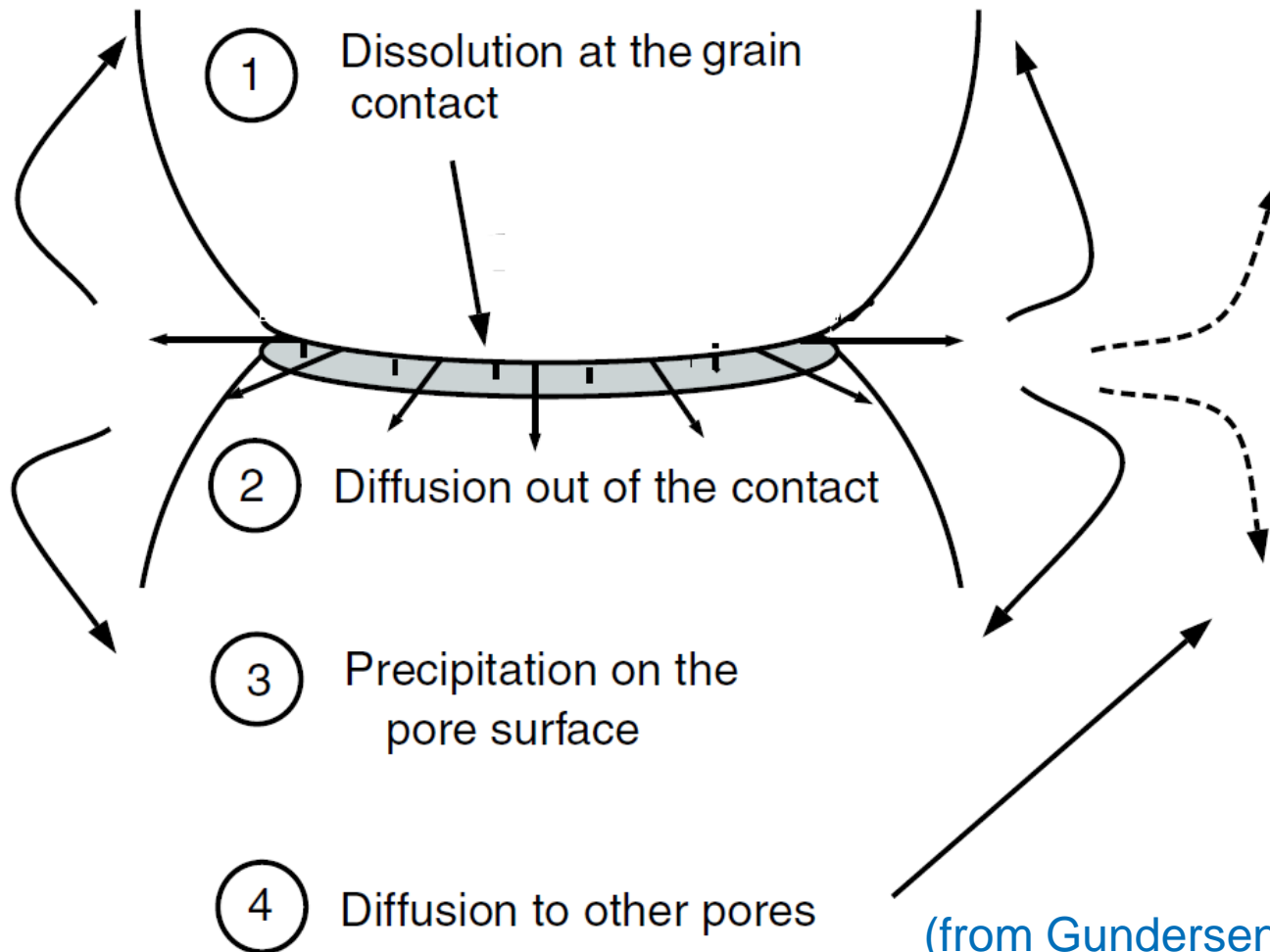| Grain scale	Macroscopic scale
Weyl (1959)	Schneider et al. (1996)
Rutter (1976)	
De Boer (1977)	
Dewers & Ortoleva (1990)	
Gundersen et al. (2002)	

Mechanisms operating at grain scales are not well understood, because several different mechanical-chemical processes interact during deformation

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A mechanism involving three kinetic steps

1. Dissolution at the grain contact
2. Diffusion out of the contact
3. Precipitation on the pore surface
4. Diffusion to other pores

(from Gundersen et al., 2002)

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Model description: Thermodynamic recalls

- The driving force for pressure-solution is the enhanced solubility at grain contacts due to the concentration of effective stress between grains.
  - the interaction between chemical and mechanical forces must be written according to thermodynamic principles

- several authors addressed to the issue (e.g. Paterson, 1973; De Boer, 1977; Robin, 1978; Lehner, 1995; ...)

$$\Delta a(\sigma) = a_{isotropic\_P} \left(\exp\left(\frac{(\sigma_n - P)\upsilon}{RT} \right) - 1 \right)$$

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Diffusion at grain-grain contact

- The path of mass transport by diffusion at grain-to-grain contacts is a critical factor in determining the rate-limiting step for pressure-solution.

- State of the art:
  - the rate of pressure-solution of quartz/mica aggregates is limited by the quartz-reaction kinetics at shallow (1–5 km) depth (Renard et al., 1997)
  - diffusion limited at greater depths (Rutter, 1976)
    - Misuse of electro-viscous model
  - Direct measurements of the diffusion coeff. (Nakashima, 1995)

$$\log D_e = \log(0.64 \times 10^{-9}) + 1.3 \log \Phi_{tot} \qquad \text{for micropore} > 25 \text{ nm}$$

$$\log D_e = \log(2.50 \times 10^{-9}) + 3.0 \log \Phi_{tot} \qquad \text{for nanopore} < 25 \text{ nm}$$
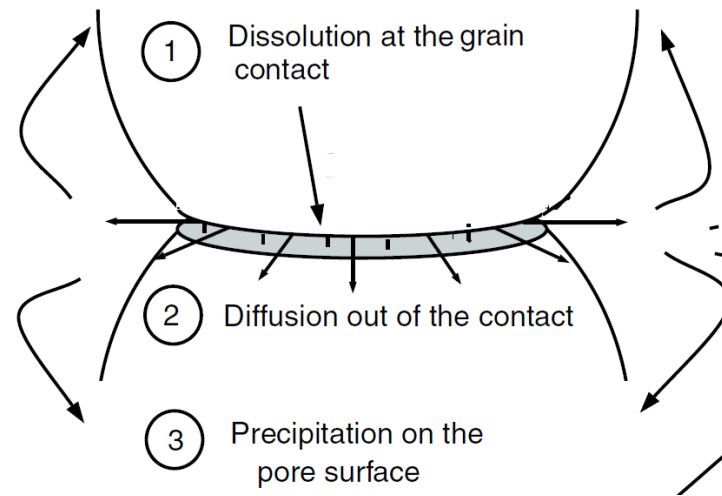
Kinetics of dissolution and precipitation of quartz

- Abundant literature, with approaches ranging from experimental studies to ab-initio calculations (Lasaga, 1998)
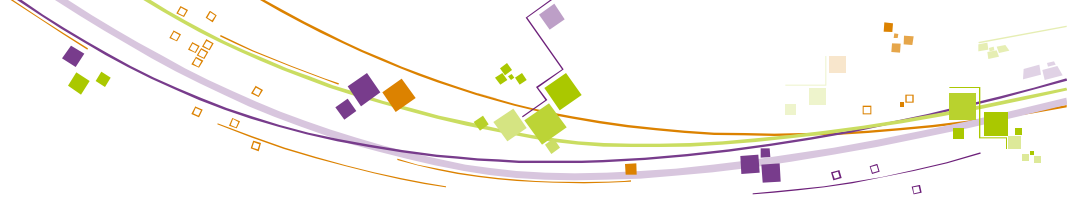
$$rate_{dissolution} = k_{Gislason}(T) S_{GrainContact}(1 - \Omega_{dissolution})$$

$$\Omega_{dissolution} = \frac{a_{H_4SiO_4}}{K_{eq\_contact}(T, \sigma_{eff})}$$

1. Dissolution at the grain contact

2. Diffusion out of the contact

3. Precipitation on the pore surface

$$SiO_{2(s)} + 2H_2O \underset{k_-}{\overset{k_+}{\rightleftharpoons}} H_4SiO_{4(aq)}$$
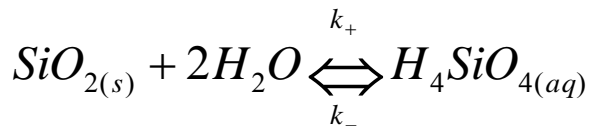
$$rate_{precipitation} = \frac{k_{Gislason}(T) \gamma_{H_4SiO_4}}{K_{eq}(T)} S_{FreeGrain}(1 - \Omega_{precipitation})$$

$$\Omega_{precipitation} = \frac{a_{H_4SiO_4}}{K_{eq}(T)}$$

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Geometrical model

- The geometric model plays a fundamental role in the overall description of pressure-solution mechanism:
    - it permits calculation of the surface area for kinetics processes
    - it permits calculation of how the effective stress is distributed between the particles
    - it permits statement of the relationships between the properties of porous medium and its micro-structure.

- Since Weyl (1959) up today, the pressure-solution models use regular packing models to describe the porous space

- Regular packing neglects the peculiarities arising from the fact that particle structure is never regular and changes continually during densification.

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Arzt's Model

- Hence as the average distance between particles decreases, the particles are pressed together and they create contact areas.

- During compaction the average number of contacts per particles (the so-called coordination number) will increase, implying that the forces acting on particle contacts diminish continuously because the external pressure is shared among an increasing number of contacts
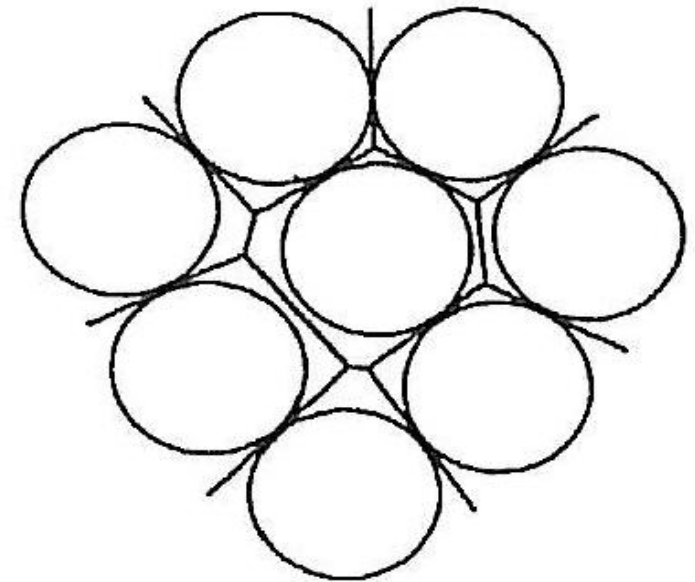
Characteristic times

- Comparison of the amount of dissolved quartz and of the amount of quartz transported by diffusion

  - Diffusion (Nakashima (1995))

    - for micropore (> à 25 nm)

      $$D\lambda = 5.5\text{x}10^{-14} \times 50\text{x}10^{-9} = 2.7\text{x}10^{-20} \text{ m}^3/\text{s}$$

    - for nanopore (< 25 nm)

      $$D\lambda \text{ ranging from } 9.7\text{x}10^{-23} \text{ m}^3/\text{s to } 2.9\text{x}10^{-24} \text{ m}^3/\text{s}$$

  - Dissolution rate

$$a_{Si}^{\ contact} \approx a_{Si}^{\ pore} = K_{eq}^{\ pore}(T) \qquad \Longrightarrow \qquad \Omega = \frac{K_{eq}^{\ pore}(T)}{K_{eq}^{\ contact}(T, \sigma_{eff})}$$

Temperature °C	Geometrical model	Rate of dissolution mol/m^2/s	Dissolved volume per second m^3/s
80	Arzt	$6\text{x}10^{-18}$	$7\text{x}10^{-30}$
80	Cubic	$4\text{x}10^{-17}$	$6\text{x}10^{-29}$
160	Arzt	$1.4\text{x}10^{-16}$	$2\text{x}10^{-28}$
160	Cubic	$1.7\text{x}10^{-15}$	$2.3\text{x}10^{-27}$

Characteristic times

$$\frac{rate_{dissolution}}{rate_{precipitaion}} = \frac{k_+}{k_-}\frac{S_{GrainContact}}{S_{FreeGrain}}\frac{\left(1-\Omega_{dissolution}\right)}{\left(1+\Omega_{precipitaion}\right)} << 1$$
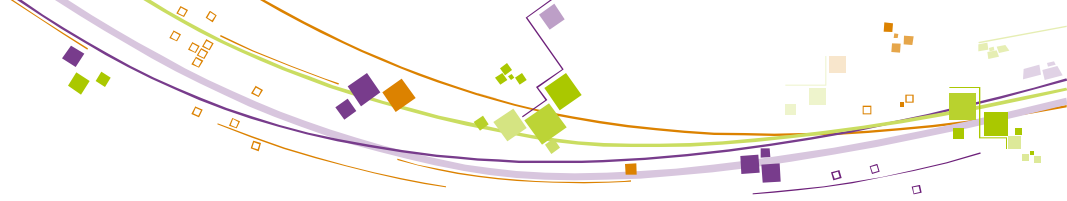
Since $\left(1-\Omega_{dissolution}\right)\approx 0.1$ With effective stress values for sedimentary basins

T = 80°C $\quad\left(1+\Omega_{precipitaion}\right)\approx\frac{k_+}{k_-}\frac{S_{GrainContact}}{S_{FreeGrain}}\left(1-\Omega_{dissolution}\right)\times\frac{1}{10^{-1}}\approx 6.10^{-4}\times 5.10^{-1}\times 10^{-1}\times\frac{1}{10^{-1}}\approx 3\times 10^{-4}$

T = 160°C $\quad\left(1+\Omega_{precipitaion}\right)\approx 2.10^{-3}\times 9.10^{-1}\times 10^{-1}\times\frac{1}{10^{-1}}\approx 2\times 10^{-3}$

If pore volume is 100 to 1000 times larger than the grain-to-grain contact volume, the assumption is verified

| Temperature	R_{grain}	Porosity	Z	Pore Vol.	Contact Surface Area/R^2	Film Thick.	Contact Vol.	Contact Vol. /PoreVol.
°C	µm	%	-	m^3	-	nm	m^3	-
80	50	25	8	2.6×10^{-13}	0.4	100	1.0×10^{-16}	3.0×10^{-3}
80	100	25	8	2.0×10^{-12}	0.4	100	4.0×10^{-16}	1.5×10^{-3}
160	50	5	12	5.9×10^{-14}	0.9	100	2.2×10^{-16}	4.5×10^{-2}
160	100	5	12	4.8×10^{-13}	0.9	100	9.0×10^{-16}	2.2×10^{-2}

Summary of the assumptions

- The kinetics of the phenomenon is controlled by:
  - effective stress
  - temperature
  - the number of contacts between grains (coordination number)

- The effective stress is used to calculate the solubility of quartz at the contact between the grains

- The kinetics of dissolution includes a term of deviation from equilibrium which is equal to the difference between the solubility at the contact and the solubility in the pore (only a function of temperature)

- The coordination number and the reactive surface are functions of porosity

- The kinetics of the phenomenon is controlled by the dissolution kinetics of quartz (the kinetics of precipitation and diffusion in the inter-grain are not considered)

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Algorithm description
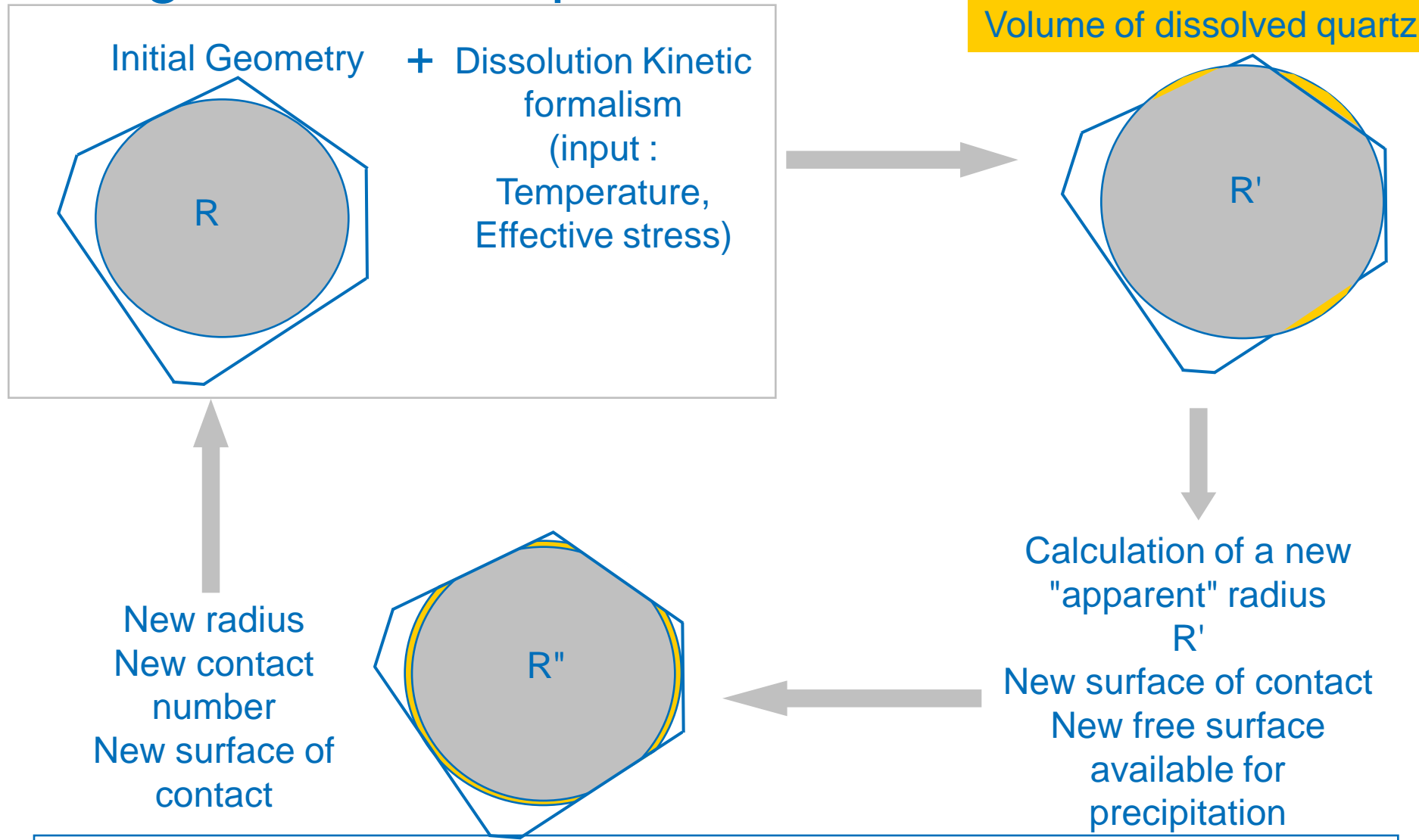
Initial Geometry **+** Dissolution Kinetic formalism
(input :
Temperature,
Effective stress)

R

R'
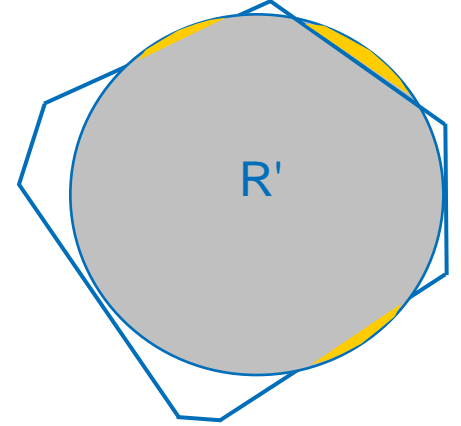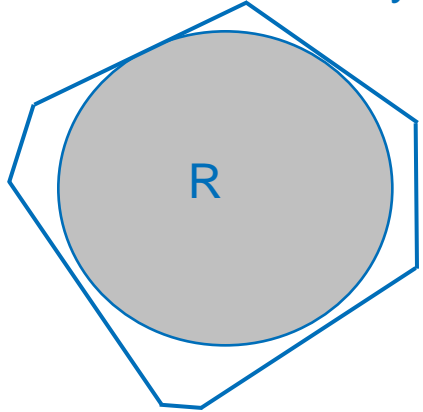
Calculation of a new "apparent" radius
R'
New surface of contact
New free surface available for precipitation

R"

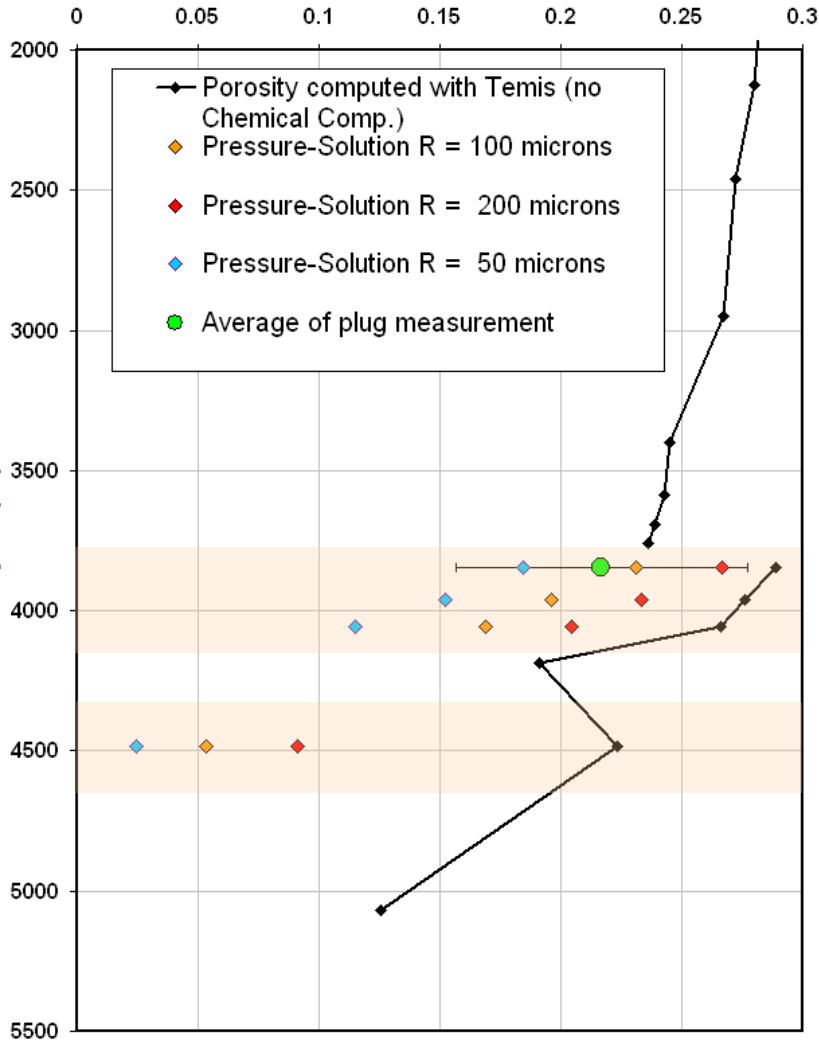New radius
New contact number
New surface of contact
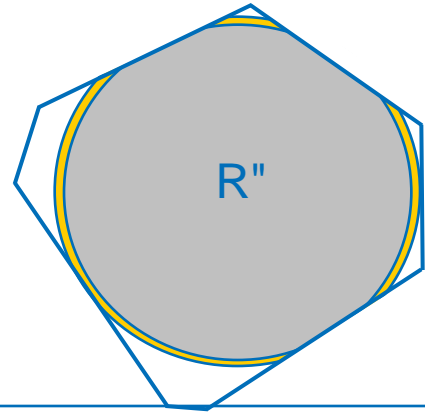
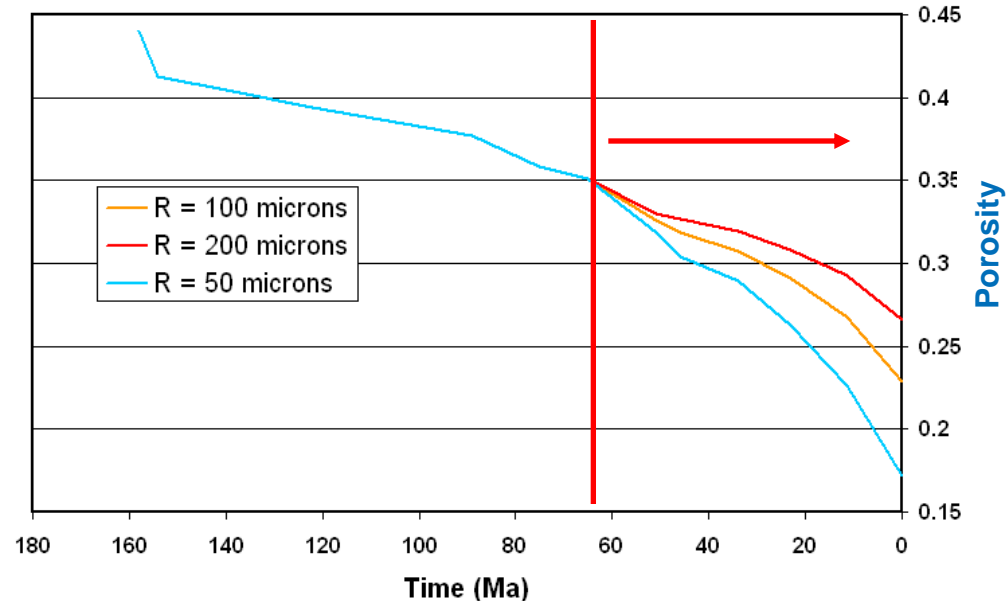The effective stress and temperature histories are provided by Temis computations

Case study: Northern North Sea

NNS dimensions

Area of interest

First well

In situ conditions
OP > 300 bar
T ~ 125°C

Thin-section point counting
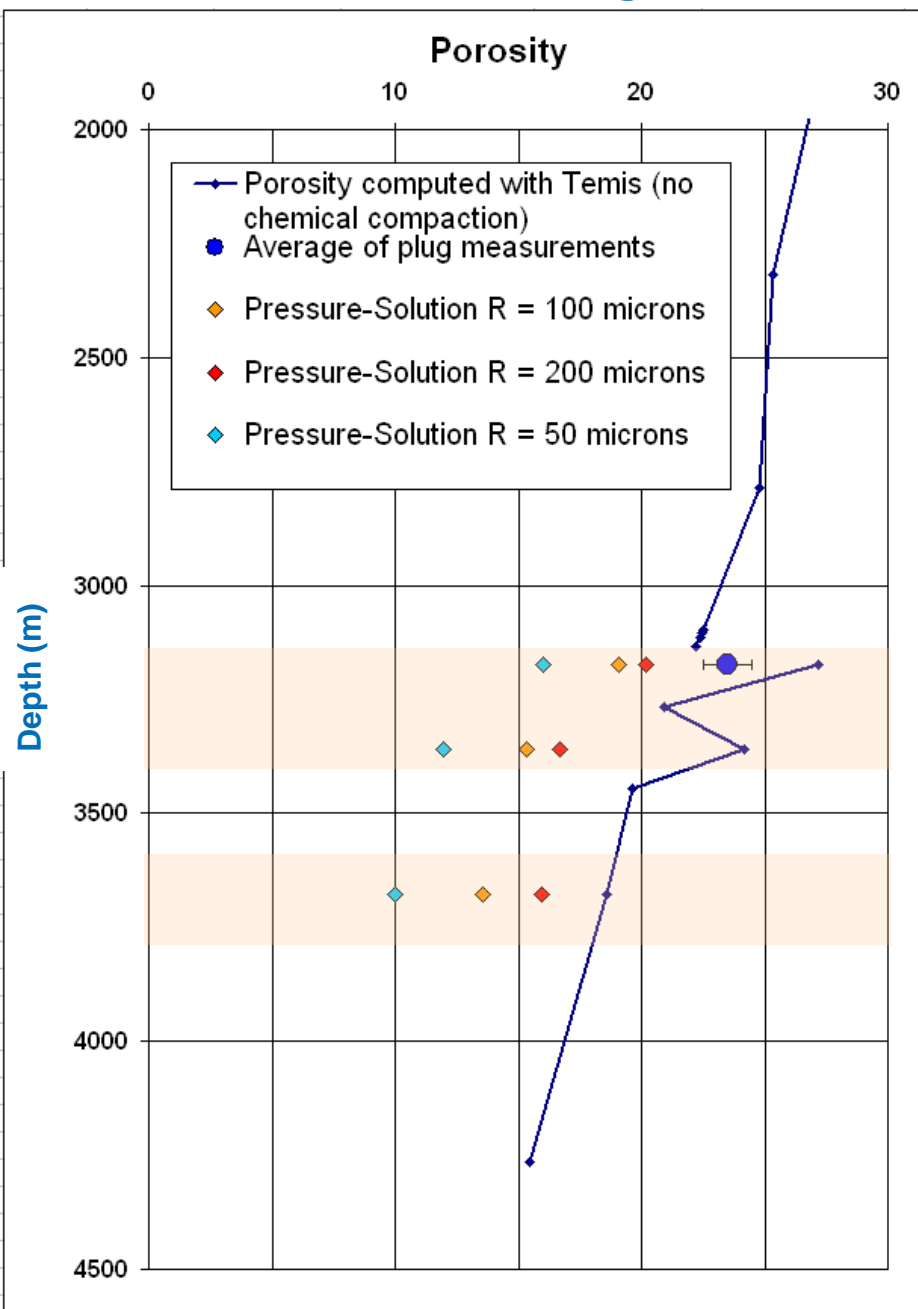R = 170 ± 25 microns

Second well
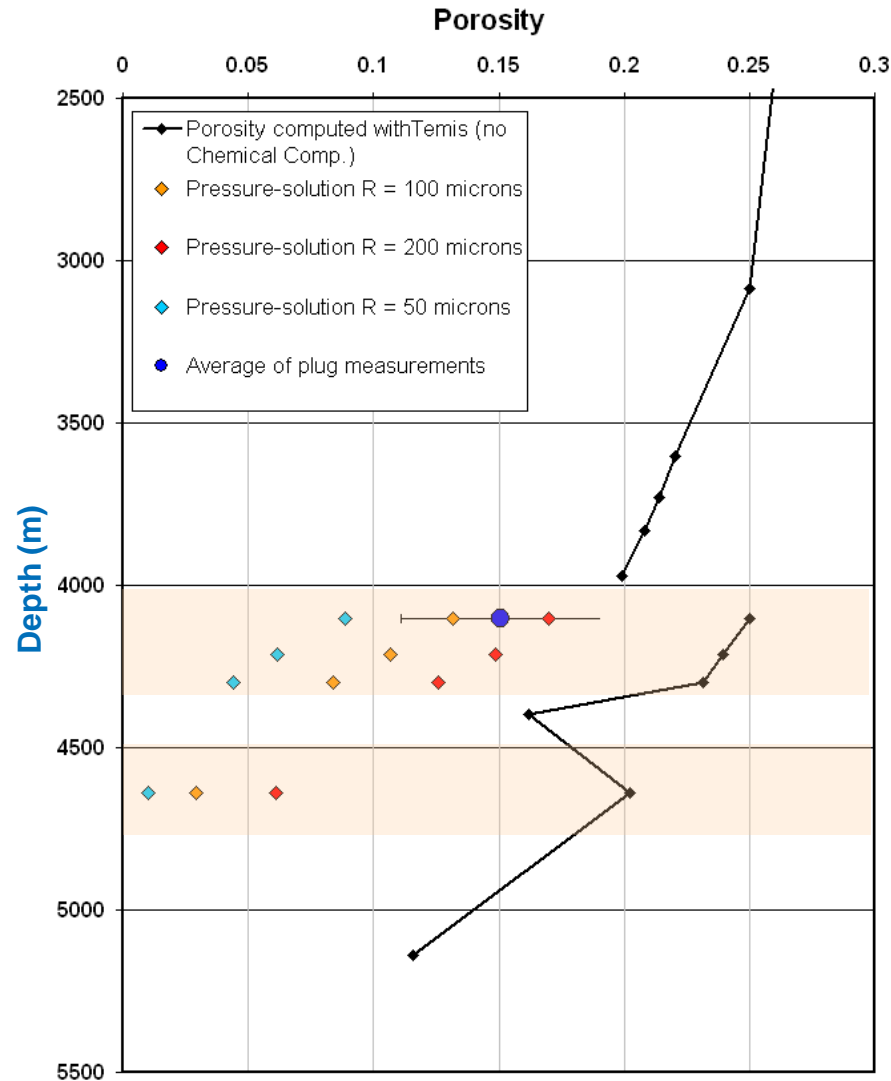
In situ conditions
OP > 350 bar
T ~ 145°C

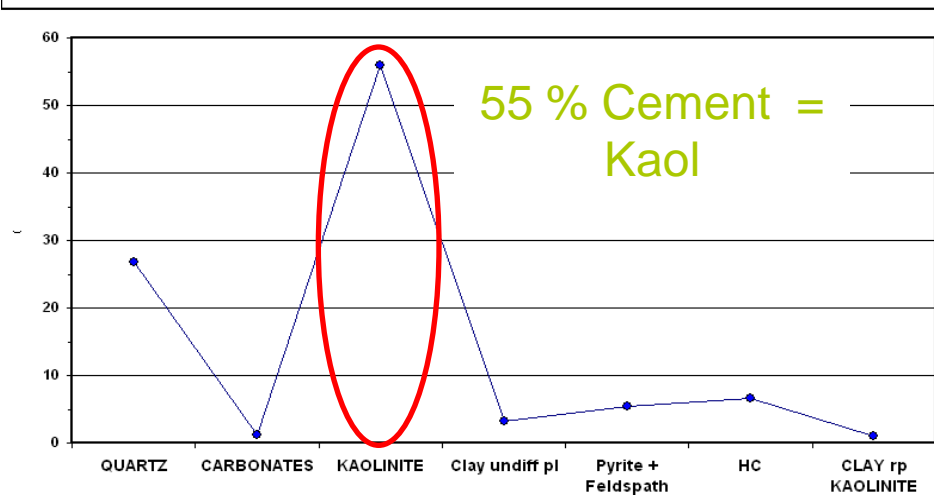Thin-section point counting
R = 210 ± 50 microns
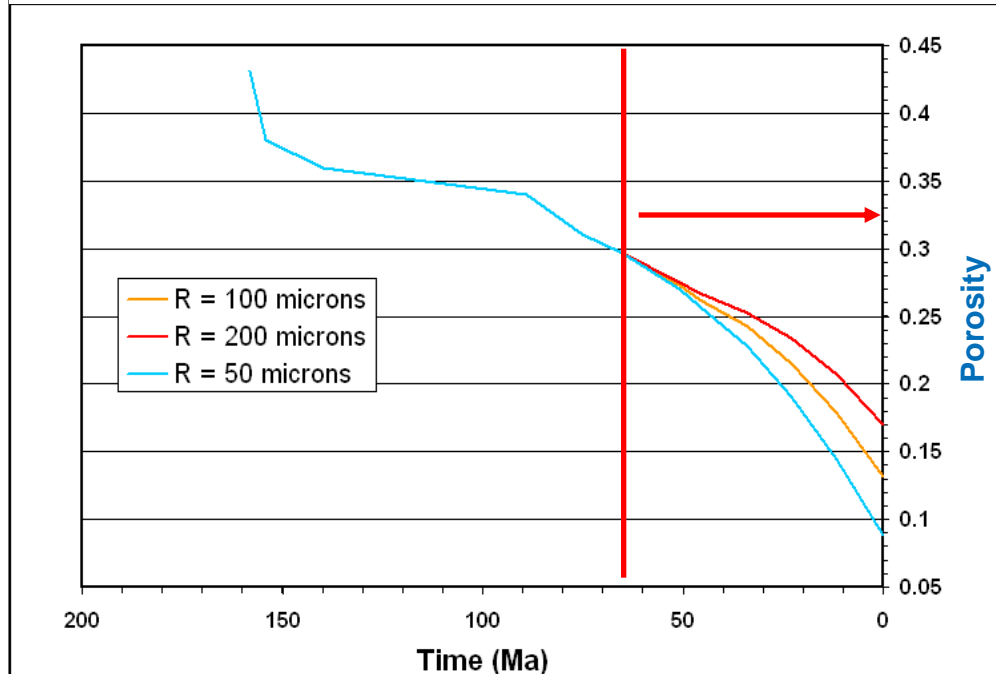
Example of disagreement

T ~ 110 °C / OP ~125 bar

- Calculations overestimate the porosity decrease
- Shaly cements have stopped the pressure-solution

85 % Qtz

10 % Kaol

55 % Cement = Kaol
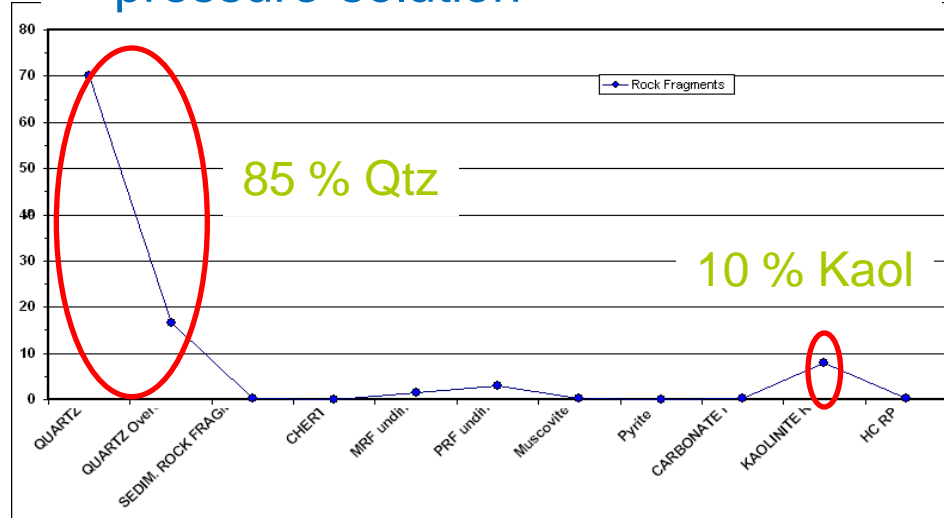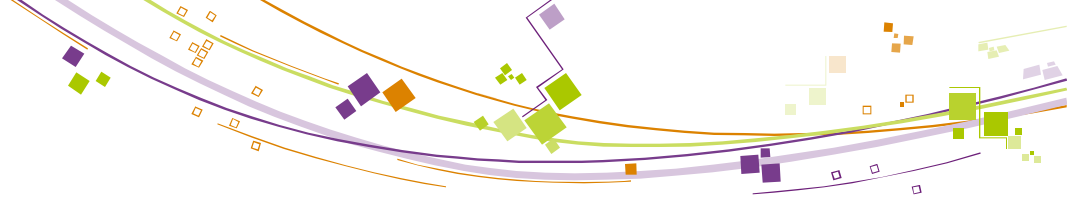
Conclusions

- **For clean sandstones the calculated porosity, over geological time scale, is in good agreement with the measured porosity**

- **The mean grain size is the only tunable parameter**

- **But… reservoirs are more complex**
  - **understand the effect of others cements**
  - **The effects of clay minerals are not obvious**
    - Are they inhibitors, or do they catalyze pressure-solution ?