

Influence of pore fluid chemistry on the state of stress in sedimentary basins

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ABSTRACT

In order to accommodate growth of a grain, an equivalent volume of the surrounding material must be removed by deformation, displacement, or diffusion. Under certain conditions of stress, fluid pressure, and pore fluid saturation, the process known as pressure solution can occur in reverse, the grains moving apart as solute diffuses into the grain contacts and precipitates there. In this paper the horizontal stress required to prevent lateral spreading of a rock due to reverse pressure solution is shown to be equal to the fluid pressure, plus an extra term dependent on the saturation level of the pore fluid. Results of numerical modeling suggest that the contribution of this term can be significant, equivalent to the horizontal stress required to resist expansion due to overpressure. Such interaction between chemistry and stress may have significant consequences for the stress state within sedimentary basins.

Keywords: pressure solution, horizontal stress, numerical modeling, compaction.

INTRODUCTION

Thermodynamic principles predict a relationship between stress and chemistry, such that solubility increases with the stress acting on a solid-fluid interface (Gibbs, 1906). This relationship has been invoked to explain the phenomenon of pressure solution (Elliott, 1973; Rutter, 1976; Weyl, 1959), in which grains dissolve preferentially along their mutual contacts and the solute diffuses into the adjacent pore space due to the inhomogeneous distribution of stress over grain surfaces. Dissolution along grain contacts causes the grains to move toward one another; however, if the pore fluid is oversaturated with respect to the grains, solute may diffuse into the grain contacts and precipitate there, causing the grains to move apart (Weyl, 1959). This concept, which is sometimes referred to as the “force of crystallization,” has been more widely discussed in the context of metamorphism (Spry, 1969). For example, porphyroblast growth must be accompanied by deformation or displacement of the surrounding matrix, if the reaction involves a net volume change. The term “force of crystallization” is, in detail, inappropriate to describe this phenomenon, because the growing crystal does not exert a net force on, or change the stress field in, its surroundings. However, stress and chemistry are linked: e.g., if the boundary conditions are such that the volume of the system is fixed, the stress field must be modified in order to allow the porphyroblast-forming reaction to proceed. In this paper we investigate this concept in the context of a sandstone undergoing

pressure solution, using the theory of Lehner (1995) to show how pore fluid chemistry can influence the stress state in sedimentary basins.

THEORETICAL ANALYSIS

Pressure solution is a three-stage process involving: (1) dissolution along grain contacts; (2) diffusion of dissolved material through the grain contact to the pore fluid; and (3) removal of solute from the pore fluid by advective and diffusive transport, and precipitation on the free faces of grains (i.e., cementation). Under appropriate conditions of stress, fluid pressure, and pore fluid composition, this process may occur in reverse, with solute diffusing into the grain contacts and precipitating there.

The strain rate due to pressure solution can be described by a viscous flow law, such as that of Lehner (1995):

$$\dot{\epsilon}_n = -\frac{k_{gb}\bar{V}}{b_n(1 + \Gamma_n)RT} \times \left[(\bar{\sigma}_n - P) - \frac{RT}{\bar{V}} \frac{\Delta C}{C_0} \right]; \quad (1)$$

$$\Gamma_n = \frac{a_n^2 \rho_s k_{gb} \bar{V}}{8 \rho_f C_0 D_{gb} \delta}, \quad (2)$$

where k_{gb} is the rate constant for dissolution (or precipitation) in the grain contacts, \bar{V} is the molar volume of the solid, b is the distance between adjacent grain centers, R is the gas constant, T is temperature, $(\bar{\sigma}_n - P)$ is the component of the local effective stress acting

normal to the grain contacts (compressive stress positive), C_0 is the equilibrium concentration of the dissolved mineral in the pore fluid, ΔC is the difference between the actual concentration and the equilibrium concentration, a is the radius of the grain contacts, ρ_s and ρ_f are the densities of solid and pore fluid, respectively, D_{gb} is the grain contact diffusion coefficient, and δ is the thickness of the grain contact fluid layer. Subscript n denotes the direction of strain; e.g., for vertical strain, it refers to the vertical component of stress acting on horizontal grain contacts. The supersaturation term, ΔC , is dictated by the rate at which solute is added to or removed from the pore fluid, which in turn depends on the rates of grain contact dissolution, advective and/or diffusive transport in the pore fluid, and cementation. The magnitude of the local effective stress $(\bar{\sigma}_n - P)$ depends on the macroscopic effective stress $(\bar{\sigma}_n - P)$, and on the area of the grain contacts, which increases over time during pressure solution and cementation. The relationship between local and macroscopic stresses is given by equation 30 of Lehner (1995).

The term inside the brackets in equation 1 represents the driving force for pressure solution, comprising contributions from the effective stress and the concentration of solute in the pore fluid. If the supersaturation (ΔC) is small or negative, a compressive effective stress leads to dissolution along the grain contacts, causing the grains to move closer together (negative strain rate). Conversely, if ΔC is large (pore fluid oversaturated with the dis-

solved mineral), it may counteract the effective stress and allow solute to diffuse into the grain contacts, where it precipitates as the grains move apart.

Consider a vertical column of sand undergoing porosity reduction due to pressure solution and cementation. As the sand compacts, pore fluid is squeezed out and moves upward through the column. The column is assumed to form part of a larger body of sand that is constrained laterally; i.e., it is undergoing uniaxial strain, with no movement of solid or pore fluid in the horizontal direction. The vertical effective stress is a function of the weight of overburden and pore fluid pressure, P . The horizontal stress can be derived by substituting $\dot{\epsilon}_h = 0$ into equation 1, leading to the following relationship between horizontal stress and supersaturation:

$$\bar{\sigma}_h = P + \frac{RT}{V} \frac{\Delta C}{C_0} \quad (3)$$

Equation 3 predicts that, in the absence of supersaturation in the pore fluid ($\Delta C = 0$), the horizontal stress must be equal to the pore fluid pressure in order to prevent lateral expansion of the sediment. However, if the pore fluid is oversaturated ($\Delta C > 0$), a larger stress is required to resist lateral expansion. Conversely, if the pore fluid is undersaturated ($\Delta C < 0$), the required stress will be smaller than the fluid pressure.

NUMERICAL MODELING

A numerical model of pressure solution, cementation, and compaction-driven fluid flow has been developed, and is used here to investigate the interactions between stress, fluid pressure, and chemistry. The model describes the porosity evolution of a one-dimensional column of quartz sand undergoing pressure solution. As the sand compacts, the pore fluid is squeezed out and moves upward through the column. Dissolved silica is added to the pore fluid by dissolution along grain contacts, is removed by precipitation on the free faces of the grains (i.e., cementation), and is transported in the pore fluid by diffusion and advection.

The model is based on the flow law of Lehner (1995) (equations 1 and 2 herein), coupled with statements of conservation of mass and momentum, equations describing the relationships and evolution of textural parameters (e.g., grain size, reactive surface area, grain contact area), and equations for the dependence of certain parameters on pressure and temperature (e.g., fluid density and viscosity). The resulting system of partial differential equations is solved by the finite difference method, using a differential-algebraic equation

solver developed by Enviros QuantiSci of Abingdon, Oxfordshire, in 1998.

The model allows certain parameters to be varied, such as the thickness and diffusion coefficient of the grain contact fluid layer, the grain contact dissolution/precipitation rate, and the rate constant for precipitation on the free faces of grains. Estimates of the values of these parameters span several orders of magnitude; summaries of the relevant literature can be found in Dove and Rimstidt (1994) and Gundersen et al. (2002). Here we have chosen values of these parameters that yield a geologically reasonable rate of porosity reduction, and illustrate the interaction between stress, fluid pressure, and chemistry that is the subject of this paper. The values of the parameters are as follows: (1) $\delta = 10$ nm, $D_{gb} = 10^{-3}D$, where D is the diffusion coefficient in the pore fluid; (2) $k_{gb} = k$ or $k_{gb} = 10^{-6}k$, where k is the rate constant for dissolution of quartz (Dove, 1994); and (3) $k_{ff}S = 10^{-6}kS$, where k_{ff} is the rate constant for precipitation of quartz on the free faces of grains, and S is the reactive surface area.

This combination of parameters represents quartz grains coated with impurities (e.g., clays or micas), as is often the case in sandstones that have undergone pressure solution. The presence of impurities ensures a fast rate of diffusion in the grain contacts (represented by δD_{gb} ; Renard et al., 1997; Renard and Ortoleva, 1997), but inhibits precipitation on the pore walls, hence the small value of $k_{ff}S$ (McBride, 1989). The effect of impurities on the grain contact dissolution rate is contentious; some studies suggest that clays enhance the dissolution rate, possibly due to a local enhancement of pH (Bjørkum, 1996; Oelkers et al., 1996; Thomson, 1959), while others suggest inhibition of dissolution due to release of Al^{3+} from mica surfaces (Niemeijer and Spiers, 2002). These two cases are represented by $k_{gb} = k$ and $k_{gb} = 10^{-6}k$, respectively.

The model was used to investigate the evolution of porosity, fluid pressure, pore fluid composition, and stress over 200 m.y. in a 4 km column of quartz sand with an initial porosity of 40%. The results are illustrated for the cases of slow and fast dissolution ($k_{gb} = 10^{-6}k$ and $k_{gb} = k$) in Figures 1A–1E and 2A–2E, respectively. In both cases, the porosity decreases smoothly with depth until a minimum value ($<1\%$) is reached, beyond which no further porosity reduction occurs (Figs. 1A and 2A). This corresponds to the position at which the fluid pressure gradient changes from approximately hydrostatic to approximately lithostatic (Figs. 1B and 2B), and occurs when the permeability becomes too small to allow the pore fluid to escape fast enough to maintain normal pore pressure. In the over-

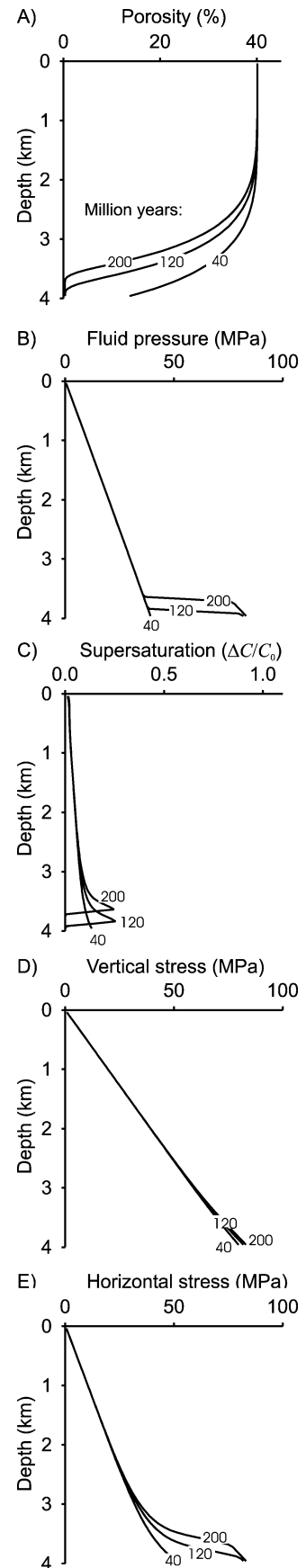


Figure 1. Evolution of parameters during pressure solution with slow dissolution and slow precipitation.

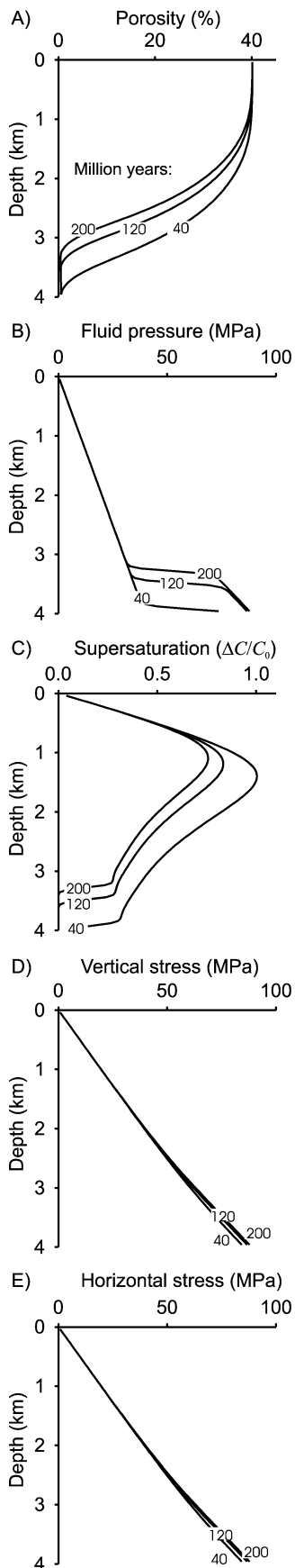


Figure 2. Evolution of parameters during pressure solution with fast dissolution and slow precipitation.

pressured region, the concentration of dissolved silica in the pore fluid is approximately equal to the equilibrium concentration (Figs. 1C and 2C). Above this, where pressure solution is still taking place, the pore fluid is oversaturated. The level of oversaturation is greater in the fast dissolution case (Fig. 2C) because solute is being added to the pore fluid rapidly by dissolution and diffusion out of the grain contacts, but cannot be removed so rapidly because of the low precipitation rate. Conversely, where the dissolution rate is slow (Fig. 1C), the rate of precipitation almost keeps pace with the rate of addition of solute. Advective and diffusive transport in the pore fluid has virtually no effect on the distribution of solute in the pore fluid.

The effects of fluid pressure and supersaturation on the horizontal stress can be seen in Figures 1E and 2E. In the slow dissolution case, the horizontal stress is approximately equal to the fluid pressure, with slight enhancement due to the low level of oversaturation. In the fast dissolution case, the horizontal stress is approximately equal to the vertical stress throughout the column (Fig. 2D). In the overpressured region this is due to the fluid pressure, and in the normally pressured region it is due to supersaturation of the pore fluid. Note that the stresses shown in Figures 1D–1E and 2D–2E are components of the macroscopic stress, $\bar{\sigma}$; plots of the local stress, $\tilde{\sigma}$, show similar patterns, but the behavior is complicated by the textural evolution of the rock, specifically the grain contact area. It is the macroscopic stress that is important on the basin scale, hence this parameter was chosen for the purposes of illustration.

DISCUSSION

Two assumptions that are implicit in the model deserve further consideration. First, the model assumes a stable, simple cubic arrangement of grains, in which mechanical compaction does not occur. The occurrence of mechanical compaction would increase the horizontal stress that is required to resist lateral expansion. However, significant mechanical compaction is generally limited to depths shallower than ~ 1 km (Giles, 1997; Wilson and Stanton, 1994), so the effect of this process on horizontal stress would not greatly influence the results presented in this paper.

Second, we have ignored the effects of processes driven by local variations in surface energy, such as neck growth. Neck growth involves precipitation around the periphery of grain contacts, thus it may cause a decrease in the rate of reverse pressure solution by (1) removing some of the solute, and (2) increasing the length of the grain contact diffusion pathway. Therefore, the operation of this process

would lead to a reduction in the horizontal stress that is required to resist lateral expansion relative to that predicted by our model. However, the effect of surface energy on chemical potential is generally small, relative to that of effective stress and pore fluid supersaturation (Wheeler, 1991), and so the driving force for neck growth will also be small. Thus, it is unlikely that neck growth would have a significant impact on our results.

It is interesting to consider the predictions made in this paper in the light of independent estimates of the stress state within the crust. Any model in which the horizontal strain rate depends on effective stress, like the one presented here, will predict a relationship between horizontal stress and overpressure. The anticipated relationship exists, horizontal stresses typically being largest in overpressured regions of basins (Engelder and Fischer, 1994, and references therein). However, stress fields that are close to lithostatic (horizontal stress = vertical stress = overburden pressure) occur widely (Jaeger and Cook, 1976; McGarr, 1988), and overpressure cannot be the explanation in all cases. A number of explanations have been offered, such as residual stress associated with uplift and erosion, local variations in stress due to variations in lithology (so called “structural stress”), or the long-term response of the crust to inelastic deformation (Jaeger and Cook, 1976; Bjørlykke and Høeg, 1997). Our analysis suggests that stress enhancement due to supersaturation of pore fluids should be added to this list. Here we have shown that supersaturation can arise in a sandstone undergoing pressure solution. In reality, the concentration of solute in the pore fluid is also influenced by other diagenetic reactions, such as illitization and feldspar breakdown. Thus, diagenesis may have significant implications for the stress state in sedimentary basins. Whether this effect encompasses the entire basin, or just small parts of it, will depend on the length scale of diagenetic variability. This in turn depends on the sedimentological and structural characteristics of the basin, and could range from a few centimeters to several kilometers. However, the aim of this paper was not to resolve the stress state for the entire crust or even for entire basins: rather, we have shown that pore fluid chemistry can have a significant effect on the stress state within basins, and so the interaction between stress and chemistry should not be ignored.

CONCLUSION

It has been shown that the tendency for grains to move apart, due to precipitation in the grain contacts from an oversaturated solution, can have significant consequences for

the horizontal stress in sedimentary basins. In a laterally constrained sediment undergoing pressure solution, the horizontal stress must be equal to the pore fluid pressure, plus an extra term due to the concentration of solute in the pore fluid. This extra term can be significant, the same order of magnitude as the stress enhancement associated with overpressure. The effects of grain growth have previously been recognized on a small scale in the context of metamorphism, but the analysis presented here suggests that this phenomenon may have consequences on a larger scale within sedimentary basins.

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