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Packing states of ideal reservoir sands: Insights from simulation of porosity reduction by grain rearrangement

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ABSTRACT

The question being tackled in this study is to which extent grain rearrangement contributes to porosity reduction in very well sorted quartzose sands (ideal reservoir sands). A numerical model, RAMPAGE (an acronym of random packing generator), has been developed to address this long-standing problem. RAMPAGE represents a synthesis of various algorithms designed to simulate packing of equal-sized spheres, which have been used to represent ideal solids, liquids, and gases, as well as natural porous media. The results of RAMPAGE simulations compare favourably to theoretical and experimental data from various disciplines and allow delineation of the field of gravitationally stable random packing of equal-sized spheres in the 2-D state space of porosity (P) versus mean coordination number (N). Three end-member packing states have been identified: random loose packing (RLP: $P=45.4\%$, $N=5.2$), random close packing (RCP: $P=36.3\%$, $N=7.0$), and bridged random close packing (Bridged RCP: $P=39.5\%$, $N=5.2$). Unlike previously proposed models, RAMPAGE can simulate the transition from RLP to any other point in the stability field. The RLP state is fully consistent with wet-packed porosities of synthetic sands with lognormal mass-size distributions reported in the literature. The much higher in-situ porosity values reported for modern (air-packed) sands are unlikely to be preserved at depth on geological time scales. Data on the relation between intergranular volume and burial depth indicate that the observed intergranular volume reduction in the upper ~800 m of the sediment column corresponds to the evolution of RLP to RCP, and is thus fully explained by non-destructive grain rearrangement.

1. Introduction

Prediction of the porosity of particulate materials is of interest in a broad range of research areas. Depending on the field of research, such materials may include detrital sediments, engineered systems of rock fragments used for construction, or industrial powders and pills (Cumberland and Crawford, 1987; German, 1989; Latham et al., 2002). The porosity of siliciclastic rocks is particularly relevant to hydrocarbon exploration and production, because it is related to permeability and provides information about the amount of hydrocarbons conceivably present in sandstone reservoirs. Exploitation of increasingly deeper reservoirs has prompted research into a wide range of diagenetic processes which modify the packing and porosity of sands after deposition. The properties of reservoir sandstones are determined by their burial history as well as by their initial conditions, i.e. texture, porosity, permeability, and framework mineral composition (Pittman and Larese, 1991; Primmer et al., 1997; Worden et al., 1997; Lander and Walderhaug, 1999; Rutter and Wanten, 2000; Milliken, 2001; Ajdukiewicz and Lander, 2010; Taylor et al., 2010).

Porosity reduction of quartzose sandstones is attributable to mechanical compaction, chemical compaction, and quartz cementation (Houseknecht, 1987; Wilson and McBride, 1988; Lundegard, 1992; Ehrenberg, 1995; Worden and Morad, 2000; Paxton et al., 2002; Worden and Burley, 2003; Cook et al., 2011). Non-destructive grain rearrangement is the principal mechanism of compaction in the shallow subsurface (Palmer and Barton, 1987; Ehrenberg, 1995). Rearrangement also contributes to chemical compaction at greater depths, in conjunction with processes that trigger small-scale movement of particles, such as removal of protruding corners from angular particles by pressure solution (Füchtbauer, 1967; Wilson and McBride, 1988; McBride et al., 1991). The importance of non-destructive grain rearrangement in the diagenetic evolution of sands depends largely on the timing of cementation, which prevents further mechanical compaction by "freezing" the particle pack (Paxton et al., 2002; Cook et al., 2011). During progressive burial, diagenetic processes such as ductile and brittle deformation, pressure solution, cementation, and wholesale dissolution of framework grains gradually become the overriding controls on porosity evolution (Lander and Walderhaug, 1999; Chuhan et al., 2002; Makowitz and Milliken, 2003; Sheldon et al., 2003; Chester et al., 2004).

Most efforts to predict porosity evolution during burial have been empirically driven (Houseknecht, 1987; Lundegard, 1992; Ramm,

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1992; Lander and Walderhaug, 1999), owing to the difficulty of constraining the large number of variables known to control diagenetic pathways (Giles, 1996; Primmer et al., 1997; Taylor et al., 2010). Borehole measurements have been used to construct porosity–depth curves, which in turn have led to a range of empirical equations that describe the relations between porosity and depth or overburden stress on a macroscopic scale (Baldwin and Butler, 1985; Scherer, 1987; Robinson and Gluyas, 1992; Gluyas and Cade, 1997; Bahr et al., 2001). Most of these empirical equations are of exponential form (Denny, 2002) and contain initial porosity as a parameter, which for well-sorted sands is generally taken to be in the range of 40% to 45%.

The contributions of individual processes to the overall compaction of sandstones cannot be quantified with the above (semi-)empirical approaches. The question addressed in this paper is to which extent non-destructive rearrangement of rigid grains contributes to compaction in ideal reservoir sands, i.e. relatively uncemented, (very) well sorted quartz arenites (cf. Paxton et al., 2002). The answer to this question may serve as a baseline for diagenetic models, because it allows closer delineation of the transition between non-destructive mechanical compaction on the one hand, and chemical compaction and/or brittle deformation on the other hand. A numerical model of grain rearrangement will be presented, which combines insights gained from simulation of particle packs in various branches of physics to represents ideal solids, liquids, and gases. The parameter space of random packings of equal-sized spheres will be explored, and modelling results will be compared to empirical and theoretical results obtained in other disciplines. Definition of the stability field of random packing arrangements of equal-sized spheres sheds new light on the intrinsic variability of initial porosity in natural sediments, and contributes towards quantification of the role of grain rearrangement in compaction.

2. Previous work: Packing data

2.1. Natural sediments

The large porosity variation of natural sediments at the time of deposition is controlled by their grain-size distributions, the wide range of natural grain shapes, and the depositional environment, all of which influence the mode of packing. The largest spread in porosity values has been recorded in aeolian (air-packed) surface sands. Fraser (1935) investigated porosity reduction by grain rearrangement by repeatedly tapping a cylinder containing moderately sorted coarse-grained beach sand. The experiments brought out clear differences between air-packed and water-packed sand. Porosity decreased from 47% to 38% in both cases, but much quicker for the air-packed sand. Pryor (1973) and Atkins and McBride (1992) measured in-situ porosities of medium to coarse-grained beach, dune, and river sands under (near) surface conditions. Initial porosities were found to range from 40% to 58%, with the highest values corresponding to air-packed sands. Oversized pores were present in sands from all environments. In contrast, Dickinson and Ward (1994) reported porosities of only 34% from well to moderately sorted aeolian sands in the Namib Desert.

A systematic investigation of porosities of artificially packed sands with φ-normal size distributions was carried out by Beard and Weyl (1973). They investigated the full range of sands from very well to very poorly sorted, with median sizes ranging from coarse to very fine. Their results show that sands which have been loosely packed in air have porosities which are inversely proportional to median size, ranging from 30% to 63%. The porosity of water-packed sands is much less sensitive to median grain size, but tends to be inversely proportional to the standard deviation of grain size and ranges from 24 to 43%. These observations are in line with the results of Palmer and Barton (1987), who showed that intergranular volume fractions (i.e. the sum of primary intergranular porosity, intergranular cement, and matrix fractions (Houseknecht, 1987)) of well-sorted fine-grained sands decrease from 44.4% at 20 m depth to 34.5% at 780 m depth.

2.2. Experimental packings

Relevant standards on experimental random packings and their analysis were set by Scott (1960, 1962), Bernal and Mason (1960), Scott and Kilgour (1969), Finney (1970), Onoda and Liniger (1990), and Aste et al. (2005, 2006). Most experimental packs were constructed by pouring a large number of spheres (n ranging from 1000 to 20,000) into a container, followed by shaking or tapping until no further reduction in volume was observed. The Finney pack consisting of 7994 ball bearings with a diameter of ¼ in (Bernal et al., 1970; Finney, 1970) is one of the largest and most accurately documented experimental random packs without notable boundary effects. The coordinates of 7935 spheres were made available for the purpose of this study (Finney, pers. comm.). Scott (1960) produced loose packing by tipping over the container and then slowly returning it to its original position. Onoda and Liniger (1990) generated loose packing of equal-sized glass spheres at the limit of zero gravity (neutral buoyancy) to examine the lower limit of packing density. Aste et al. (2005, 2006) extracted spatial statistics from a very large data set of random sphere packs ($n = 140{,}000$) by means of X-ray computed tomography.

2.3. Regular packings

Regular packing arrangements comprise rows and layers ordered in crystalline patterns. Basic regular packing types (cubic, orthorhombic, tetragonal–sphenoidal and rhombohedral) may be constructed from single layers with rows ordered at either 60° or 90°. Rhombohedral packing may be subdivided into two different arrangements, pyramidal and hexagonal, giving a total of five crystal lattices (e.g. Graton and Fraser, 1935; Cumberland and Crawford, 1987). A model consisting of 1000 spheres (10 layers of 10 rows of 10 spheres) was constructed for each regular packing. Because geometrical properties of crystal lattices are known exactly, these crystalline packings were used to determine the accuracy of packing statistics calculated from RAMPAGE simulations.

3. Packing models

3.1. Static models

Static models of particle packing are designed to produce a fixed packing arrangement, whereas dynamic models are capable of producing a sequence of packing arrangements. Static models have been used in the earth sciences to provide realistic boundary conditions for solving standing problems concerning flow through porous media, electrical conductivity, and mechanical strength of granular assemblages. Particle packs used in such petrophysical applications may be represented by a regular lattice (Bradley, 1980; Roberts and Schwartz, 1985), generated by stochastic methods (Quiblier, 1984; Adler et al., 1990; Liang et al., 1998; Yeong and Torquato, 1998a,b), or taken directly from experimental packs produced in the laboratory (Schwartz and Kimminau, 1987; Bryant et al., 1993; Cade et al., 1994).

The simplest approach to simulation of static particle packs is by sequential addition of particles to an initial configuration (Stillinger et al., 1964; Adams and Matheson, 1972; Bennett, 1972; Sadoc et al., 1973; Matheson, 1974; Frost et al., 1993; Tacher et al., 1997). A physically more realistic approach is to model sequential deposition of grains under the influence of gravity, by dropping particles from a random location and allowing them to roll until they settle on the bottom of a container or in a gravitationally stable position on three other spheres (Tory et al., 1968, 1973; Visscher and Bolsterli, 1972;