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Fractal pore structure of sedimentary rocks: Simulation in 2-d using a relaxed bidisperse ballistic deposition model

Abhra Giri ^{a,b}, S. Tarafdar ^b, P. Gouze ^c, Tapati Dutta ^{a,b,*}

^a Physics Department, St. Xavier's College, Kolkata 700016, India

^b Condensed Matter Physics Research Centre, Physics Department, Jadavpur University, Kolkata 700032, India

^c Geosciences, Universite de Montpellier 2, Montpellier, France

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ABSTRACT

Several studies, both theoretical and experimental, show that sedimentary rocks have fractal pore-grain interface. The real rocks are 3-d structures with highly tortuous and often fractal pore spaces. Before attempting simulation of this daunting geometry, we present here, as a preliminary study, a simpler 2-d version. In this paper, a computer simulated 2-d sedimentary rock structure is generated by the relaxed bidisperse ballistic deposition model. Grains of two different sizes are dropped ballistically on a linear substrate. By changing the fraction of the two types of particles, the porosity of the rock structure can be tuned. The structure undergoes compaction through the relaxation of possible unstable overhangs. The micro structure of the pore space is investigated. The pore mass and the rock-pore interface show a fractal behaviour with the same fractal dimension indicating that the pore volume is a fractal. Our simulation results indicate that the process of compaction of grains during the deposition process seems to erase the dependency of the fractal dimension on the grain size distribution. The two point density correlation is measured for the pore space. It shows anisotropy which is an outcome of the growth rule. X-ray tomography of two-dimensional sections of real sedimentary rocks obtained from Mallorca Island is subjected to the same study and the results compared with those obtained from simulation. The simulation results agree qualitatively with the real rock sample. We also study diffusion on the pore space. Diffusion is found to be anomalous as is expected in fractal spaces. It also bears the signature of anisotropy of the structure. Diffusion studies on the real rock sample could not yield conclusive results as the system size is not large enough.

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1. Introduction

Several studies on sedimentary rocks (Katz and Thompson, 1985; Krohn, 1988a; Krohn, 1988b; Wong, 1987) have suggested that the pore system has a fractal nature. Though the pore–rock interface has been shown definitely to be a fractal, there is a controversy about whether the pore space is a volume fractal too. Not many measurements have been possible to probe the pore volume directly. The fractal nature of the pore phase if present, is possibly a consequence of the formation of the rocks by sedimentation and diagenesis of granular matter. All morphological changes that follow postdeposition of sediments in the process of formation of sedimentary rocks are collectively termed as diagenesis. The main features of diagenesis involve alteration of grain sizes and shapes, dissolution of grains and precipitation of cementing minerals in the interstitial spaces. The first stage of the process is compaction. Compaction occurs as the weight of the overlying material increases. Compaction

E-mail address: tapati_mithu@yahoo.com (T. Dutta).

forces the grains closer together, reducing pore space and eliminating some of the interstitial fluids. Porosity leads to inhomogeneities in the distribution of pressure because of the weight of super incumbent beds. The weight is carried on the relatively small areas of contact between the grains. This leads to dissolution at the points of contact and precipitation in the voids. If there are fluids that occupy the pore space, chemical reactions might occur within the solid framework. The porosity of the solid framework therefore decreases with time and with increasing depth. Other changes occur with the ageing of the deposit and still others when temperatures and pressures become high enough to induce more drastic morphological changes.

In an earlier work (Dutta and Tarafdar, 2003; Tarafdar and Roy, 1998), the authors had simulated a 3-d sedimentary rock structure using the bidisperse ballistic deposition model (BBDM) whose pore structure was investigated. The model mimics the deposition process of grains under gravity to generate the rock structure. Grains of two different sizes were taken to generate a porous structure. This model was extended under the 'relaxed bidisperse ballistic deposition model' (RBBDM) (Sadhukhan et al., 2007a), where the deposited grains were allowed to relax to mimic the process of compaction. The authors studied transport properties such as conductivity and

^{*} Corresponding author at: Physics Department, St. Xavier's College, Kolkata 700016, India. Tel.: +91 9330802208; fax: +91 33 2287 9966.

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permeability (Sadhukhan et al., 2007a, 2007b, 2008) on a 2dimensional version of the RBBDM. Since transport occurs through the pore space of the rock, the micro-structure of this pore space should be characterised and related to such rock properties. In this work we report the nature of pore volume, the rock-pore interface on our simulated structure whose porosity can be varied, using the RBBDM. We try to understand the effect of the relaxation of the grains that mimics the process of compaction in the simplest way, on the micro geometry of the pore space by comparing with our results obtained in Dutta and Tarafdar (2003).

In the following section we briefly discuss the RBBDM used for generating the sedimentary rock structure of varying porosity. The next section discusses our calculation of the two-point density correlation function done on the entire pore space of the generated rock structure. The results are compared with the values calculated on sections of real rock samples and those obtained from the BBDM (Dutta and Tarafdar, 2003). Following this, we check the nature of the connected pore space in the generated rock structure. In our earlier study (Dutta and Tarafdar, 2003) where the relaxation of the grains was not considered, we have shown that only the connected pore space was a fractal. If the entire pore space of the structure, i.e. connected as also the disconnected pore clusters is considered, the contribution from the disconnected pores masks any signature of a fractal nature if present. The pore space behaves like a homogeneous mass. However in this study where compaction is enabled through the grain relaxation, the entire pore space consisting of both connected and isolated pore clusters together, shows the same fractal nature as the connected pore space taken separately. This could indicate that diagenesis has an important role in the fractal nature often displayed by sedimentary rocks.

It is the connected pore cluster that is responsible for any transport through the sample. Transport of reactive fluids through porous rocks can lead to both dissolution of some of the minerals and precipitation of newer ones. These processes can create new conducting channels or block existing paths of flow and affect processes like subsurface storage, CO_2 sequestration, underground hydrocarbon production and study of risk assessment in underground flow. The rock–pore interface provides the substrate for all such reactions and plays an important role in all transport processes. The nature of the rock–pore interface is therefore checked for any fractal nature. The results are compared with those of the BBDM to study the role of compaction of grains. These results are also compared with the calculations done on two-dimensional sections of real sedimentary rocks for comparison.

We also study diffusion of a random walker in the connected pore space. A random walk through a fractal pore volume is expected to show anomalous behaviour. This is evident from our study and reinforces the fractal nature of the pore space.

Finally we conclude our investigation and share some of the future plans on this subject.

2. Model

The details of the BBDM and RBBDM are discussed in Dutta and Tarafdar (2003) and Sadhukhan et al. (2007a) respectively. Since the RBBDM is an extended version of the BBDM that included compaction of unstable overhangs, the basics of the RBBDM will be described briefly here for the sake of completeness. The porous structure is generated by ballistic deposition of grains of two different sizes. We drop square 1×1 and rectangular 2×1 grains on a square lattice. It is well known that natural sand grains are angular and elongated (Pettijohn, 1984), so the aspect ratio 2 is realistic. The squares are chosen with a probability p and rectangles with probability (1-p). With only square grains of size 1×1 , a compact solid structure would be generated. The presence of the longer grains leads to gaps in the structure. The porosity ϕ , defined as the vacant fraction

of the total volume (here area), depends on the value of p. For p =1, a compact rock structure with zero porosity is formed. As p is decreased, isolated pore 'clusters' start appearing and the porosity increases. For a specific value of p, the threshold value, a structure spanning cluster is generated. Thus the model has the potential of generating a structure with a connected rock phase that is needed for any stable structure and a tunable porosity. As the fraction of longer grains is increased, unstable overhangs can develop. A two-step overhang will topple over if possible, according to the rule of the simulation as shown in Fig. 1, leading to compaction. It has been shown in the BBDM (Dutta and Tarafdar, 2003) that in order to overcome substrate effects, a sufficient number of grains (depending on sample size) have to be deposited before the sample attains a constant porosity. Here, a 128×2000 size sample was generated, from which a 128×2000 sample was selected after the porosity had stabilised. The selected sample was chosen from below the deepest trough at the surface to eliminate surface effects. All simulations were carried out on this sample.

The elongated grains are deposited with their long axis horizontal and parallel to the *x* axis. The vertical direction is the direction of the *y*-axis and coincides with the direction of grain deposition. Sedimentary rocks usually have a porosity that rarely exceeds 0.5. Fig. 2a shows a section of the generated sample at maximum porosity with p = 0.0 and Fig. 2b shows a section of the sample at very low porosity for p = 0.97. At low porosities elongated and isolated pore clusters appear along the *y*-direction while the distribution of pores becomes more isotropic as porosity increases. The section now resembles sections of real rock as shown in Fig. 2c.

Analyses on real rock samples were done on X-ray tomography of sections of real Mondeville Limestone from the Paris Basin. The X-ray tomography of a two-dimensional section was first converted to a binary file. The graphical picture of Fig. 2c was then created from this binary file using MATLAB. The characterisation of the pore space of the real sample was done on this graphical file.

In our model, the presence of large grains introduces correlation between adjacent columns of grains on the square lattice. The toppling rule of the larger grains decreases the porosity somewhat. Therefore, as the fraction of large grains increase, the porosity increases and so does the isotropic nature of the sample.

Fig. 3 shows the variation of porosity with the fraction p of squares in the RBBDM. The porosity shows a maximum at p = 0 like the BBDM (Dutta and Tarafdar, 2003), however the quantitative value is lower in this case.

The final porosity in the RBBDM is decided by the competition between the correlation between grains and their compaction through toppling. The range of porosity covered by the RBBDM is 0.385 to 0.0. The value of porosity of the two-dimensional real rock sample was calculated to be 0.071, which is quite a low porosity value. From our RBBDM, this corresponds to a p = 0.97 thus establishing that the model has the potential to produce a structure with any given porosity.



Fig. 1. Toppling rule of the larger grains.

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