A Growth Model for Porous Sedimentary Rocks

Sujata Tarafdar and Shashwati Roy

Condensed Matter Physics Research Centre
Physics Department
Jadavpur University
Calcutta-700032, INDIA.

Abstract
A growth model for porous sedimentary rocks is proposed, using a simple computer simulation algorithm. We generate the structure by ballistic deposition of particles with a bimodal size distribution. Porosity and specific surface area are calculated varying the proportion of small and larger particles. Permeability and it’s variation with porosity are studied. The fractal nature of the pore space is also discussed.

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\(^{1}\)E-mail: sujata@juphys.ernet.in
1 Introduction

Study of natural growth processes through models and computer simulation is useful and instructive. Successful computer models give an insight into how a simple sequence of steps governed by stochastic or other algorithms may generate a structure with very specific characteristics. The computer generated system can then be used to study other properties of interest.

A striking example is the diffusion limited aggregation or DLA model. DLA and it’s variation - the diffusion limited cluster-cluster aggregation (DLCA) can be used to generate patterns resembling growth of colloidal aggregates, bacterial colonies, corals, dielectric breakdown and many similar systems [1]. Another field where such growth models have been applied is the formation of rough surfaces [2].

An area where such studies are lacking is the formation process of porous sedimentary rocks. The study of sedimentary rocks is a very important field due to application in oil exploration, ground water flow problems, spread of pollutants and other such cases. The structure of sedimentary rocks show certain characteristic features which make them distinct from other porous materials - such as foams or aerogel [3]. However, there is still no simple model which simulates the growth process of sedimentary rocks.

The present work is an attempt in this direction. We use a simple ballistic deposition model on a square or cubic lattice with a bimodal particle size distribution. This generates a realistic rock structure with porosity varying according to the particle size distribution.

The paper is organised as follows; in the next section we briefly discuss the principal characteristics of sedimentary rock structure. In section 3 our model is presented and the details of the computer simulation are given in section 4. In the 5th section we present the results of our study and finally discuss the success and drawbacks of our approach.

2 Sedimentary rocks: Structure and properties

The sedimentary rocks originate from accumulation of small grains of sand or clay often together with organic material [4, 5]. Sedimentation takes place through the action of wind or water, and leads to a highly porous (50-80%) unconsolidated agglomerate. The sedimentation process is followed by compaction and diagenesis causing the unconsolidated mass to become a consolidated rock by flow of pore filling fluids accompanied by cementation, dissolution and other chemical processes. The resulting secondary porosity is usually less, but sometimes greater than the primary porosity.

Sedimentary rocks are divided into classes such as sandstones or limestones depending upon their composition. Our model has been developed with the sandstone structure in mind, however, it is quite general. The principal characteristics
of sedimentary rocks are as follows; 1. The solid phase and pore phase are both connected. 2. Porosities are usually in the range (5-25%). 3. Many studies report a fractal structure of the pore phase \[ \text{\cite{3}} \]. Adsorption studies report that the pore-solid interface is fractal, but this method gives no information whether the system is a volume fractal as well. But several scattering experiments indicate that the pore space is a volume fractal. 4. The electrical conductivity of brine filled porous sedimentary rocks and their permeability are found to follow two well known empirical laws, referred to as respectively Archie’s law and Darcy’s law \[ \text{\cite{6}} \].

Archie’s law is

\[
\sigma \propto \sigma_0 \phi_{\text{eff}}^m
\]

Here \( \sigma \) is the effective conductivity of the electrolyte filled rock, \( \sigma_0 \) is the conductivity of the electrolyte, \( m \) is a constant called the cementation exponent. Usually \( m \) has values between 1.3 and 4.0. For consolidated sandstones the value lies between 1.8 and 2.0. Normally \( \phi_{\text{eff}} \) means porosity of the connected pore space, i.e. excluding the isolated pores, however some authors give it a more restricted definition.

The permeability is defined by Darcy’s law

\[
J = \frac{K}{\mu} \nabla P
\]

Here \( J \) is the volumetric flow rate, \( K \) the permeability, \( \mu \) the viscosity of the fluid flowing through the porous medium and \( \nabla P \) the pressure gradient.

The permeability depends not only on the porosity, but also on other details of the pore structure \[ \text{\cite{7}} \]. Obviously, while a rock with no porosity will have zero permeability, two samples with same porosity may have very different permeabilities. Other relevant parameters characterising the permeability have been suggested as - the specific surface area, tortuosity and connectedness of the pore space. Definitions of the last two quantities are not very clear.

It is expected that a realistic model of a sedimentary rock will give a satisfactory description of the above properties.

3 The Model

Our work has two objectives – the proposed model should simulate the process of rock formation in a realistic way, and the final structure formed should be representative of a natural sedimentary rock.

The model has been developed in both two and three dimensional versions on a square and cubic lattice respectively with unit spacing. Sand particles are dropped onto a substrate from a definite height from a random horizontal position. If all particles are squares of unit size (or cubes in 3 dimension), obviously the whole space is filled up after a sufficient number of particles are allowed to deposit. The upper boundary may be highly uneven. If however, the particles to be deposited
include a fraction of particles of size larger than unity, we get a structure with voids left randomly. The rough upper boundary is cut off.

We find that a fraction $F \sim 0.01$ of larger particles can generate a significant porosity (about 8%), and the porosity increases with $F$. For $F = 1$, we get the maximum porosity permissible for a specific size and shape of the larger particle. The variation in porosity with $F$ gives a quite good logarithmic fit.

Let us discuss the two dimensional system first. For the larger sized particle, we tried out squares of dimension $2 \times 2$ and alternatively rectangles of dimension $2 \times 1$ with qualitatively similar results. Finally we confined our attention to the elongated larger grain version only, because real sand grains are reported to be ellipsoidal with the long axis approximately twice the shortest [5, 4]. The random structure generated is shown in the figures 1(a)-(c). We show three different porosity ranges for three values of $F$.

In the 3-dimensional version we choose $X$ - $Y$ plane horizontal, and the $Z$-axis to be vertical. The smaller grains are cubes of unit side, and the larger are rods with dimension $2 \times 1 \times 1$. Here the larger particles are allowed to settle ballistically with long axis parallel to either $X$ - or $Y$ - axis, with equal probability. A modified version allowing preferred orientation is also being tried.

This simple model simulates the action of gravity through vertical ballistic deposition. For the present we have not included the effects of drift or diffusion in the horizontal direction but this may be introduced in future work. We have studied the following features of the porous structure generated :-

1. The variation of average porosity with $F$ (the fraction of large particles).
   and the variation of porosity with sample size for a particular $F$.

2. The specific surface area of the pore-solid interface.

3. The fractal nature of the pore space generated and Archie’s law.

4. The permeability variation with porosity and specific surface area has been calculated using the Kozeny relation [8].

In the following section we give details of the computer simulation and the results obtained.

4 Computer Simulation

In our work the two-dimensional system has been generated upto size $600 \times 600$ and the three dimensional upto $150 \times 150 \times 150$. We first generate a linear (or square for three-dimensions) array of side $N_x$ which is solid i.e. all sites are occupied. An uneven layer is generated on top of this, by filling up certain sites randomly, other being left vacant. These two layers constitute the substrate.
Now the growth process by deposition starts. The site for deposition is chosen randomly at a height $N_z$ above the substrate ($N_z = N_x + 10$). The particle to be dropped is of size I (small) or II (elongated) with a probability $1 - F$ or $F$. Whether the particle is of size I or II is decided by a random number generator. The particle descends as long as the sites immediately below it are empty. It stops on encountering a filled site. Then the next particle drops. The process is continued until a square (or cube) of side $N_x$ is saturated, i.e. the porosity does not change further on adding more particles.

The structure generated in two-dimension is shown in figs 1 (a-c). We repeat the whole process for a large number of times $N_{av}$. We have averaged over 200-500 runs in two and 50-100 runs in three dimension.

4.1 Porosity and Fractal Nature

After generating the system of the largest possible size, the average porosity is calculated as (the number of pores) / (total number of sites) in boxes of gradually increasing size.

A typical porosity variation with size is shown in figure 2, here $F$ is constant. A constant porosity indicates a homogenous structure without any fractal characteristics. We find however, that the porosity first stabilises to an almost constant value for $N_x \sim 200$ in two and $N_x \sim 100$ in three dimensions. But for still larger sizes there is a slow but definite decrease in porosity. This shows that though the structure is homogenous for small sizes a fractality appears above a certain cutoff scale. This effect is more prominent for low porosities (i.e. small $F$). Our boxes are always smaller than $N_x$ to eliminate any end effects in the structure generated. In the subsequent discussion $P$ means the constant value of the porosity obtained, before it starts to fall.

We have estimated the fractal dimension using the relation

$$M(N) \sim N^{d_f}$$

(3)

Here $M$ is the number of pores in a box of size $N$ and $d_f$ is the fractal dimension of pore space. We find $d_f \geq 1.99$ in two and 2.99 in three dimensions initially but it deviates towards $d_f \approx 1.90$ in two and 2.89 in three dimensions as system size increases. The value of $d_f$ is lower for low porosities. Due to limited availability of computer facility we have not yet been able to generate larger sizes so as to give a converging value of the fractal dimension.

Porosity variation with $F$ is shown in figures 3 in three dimension. The curve obtained gives a good logarithmic fit. The maximum value of $P$ (for $F = 1$) is 0.50 in two and 0.63 in three dimensions. Figure-4 shows $\log M(N)$ plotted against $\log N$ for $F = 0.005$.  

5
4.2 Specific Surface Area

Pore dependent Properties of porous rocks depend not only on porosity but also on other characteristics of the pore structure, the easiest to calculate is the specific surface area – the interface area per unit mass (or volume).

We have calculated $S$ – the average pore-solid interface area per unit volume, in the structure generated. $S$ plays a crucial role in permeability of the rock.

The variation of $S$ with $P$ from our model is shown in Figure 5. As expected $S$ first increases with $P$ upto $P \approx 0.6$, after that the pores become so large that many of the vacant sites do not contribute to the interface and $S$ decreases. To get an idea of the connectivity of the pore structure we calculate $I = S/P$ this gives the average number of interfaces exposed per each pore site. For completely isolated pores the maximum value $I$ can have is 4 in two and 6 in three dimension. $I \leq 4$ is a necessary but not sufficient condition for connectedness in three dimension. We have calculated $I$ only in three dimension and find that $I$ remains close to 3, even for porosities near 4%. This indicates a high connectivity of the pore space. The variation of $I$ with $P$ is shown in figure-6. At $P \approx 0.2\%$ $I$ approaches 6, so pores definitely become isolated. The very sharp fall in $I$ between $P = 14\%$ to $P = 6\%$ seems to indicate that the connectivity threshold is in this region, but this must be verified.

5 Results and Discussion

We now discuss the results obtained and their relevance to the features of rock structures discussed earlier. $P$ for a given $F$ is taken as the constant value obtained for intermediate sizes (200 in two and 100 in three dimensions).

In two dimension the maximum porosity for $F = 1$ is 0.50. This is the percolation threshold for a square lattice in the random percolation (RP) problem \[^9\]. It is instructive to compare our model with RP. Here we have ensured the connectivity of the solid phase through our growth algorithm and obviously it is not possible to have both the pore and solid phases connected in two dimensions. But the diagrams generated in two dimension figs 1 show that a high degree of connectivity in pore space is present for large $F$, particularly in the vertical direction, i.e. pores are not isolated. There is an anisotropy in the structure generated in our model with pores elongated in the vertical direction. This shows up more clearly in the low porosity case. There is in fact some evidence of pores having higher aspect ratio in case of low porosity \[^10\]. There is also evidence of anisotropy of sedimentary rock structures, though there appears to be no systematic study \[^1\].

The three dimensional structure our model generates, cannot be shown in a two-dimensional figure, and it is not possible to see the connectivity directly. We have plans to make a complete study of the threshold porosity for connectedness and the pore size distribution. The percolation threshold for RP in three dimen-
sions is found to be $P_c \approx 25 - 30\%$, and for porosities in the range $P_c$ to $(1 - P_c)$ both pore and solid phases are connected. It will be of interest to see whether we get a connected pore space here for lower porosities.

Real rock structures are seen to be connected for very small porosities, in fact some authors speak of a zero percolation threshold [3]. At present we have calculated the porosity, specific surface area and permeability with interesting results.

5.1 Permeability

The permeability is an important property of a porous rock. It depends in a complicated manner on the structure of the pore space. $P$ and $S$ may be considered as the simplest parameters characterizing a pore space. To our knowledge no exact theory connecting the permeability with $P$ and $S$ or any other such parameter exists, for the case of such complicated multiply connected pore space as in our model.

We may however get a qualitative idea of permeability ($K$) behavior using the oversimplified Kozeny relation [8] which gives $K$ as

$$K \sim P^3/S^2$$  \hspace{1cm} (4)

In the case of a pore space consisting of a bundle of unconnected tubes.

Usually application of the Kozeny relation considers $P$ and $S$ as separate independently varying parameters. In our model, however, they are related both being obtained simultaneously as a function of $F$.

We omit the tortuosity factor appearing in Kozeny relation as a proportionality constant and consider only relative values of $K$ for different $F$ and plot it as a function of $P$.

The results are shown in figure -7. We find a very good exponential fit. This implies that

$$\log(K) \propto P$$

A large body of data for real rocks do show such a variation [3]. For sandstones from different sources log($K$) vs porosity shows on the average a quite clear linear variation. There is of course a considerable spread in the data for real rocks.

This may indicate that even in the case of such a complicated pore space, the Kozeny picture is not a very bad approximation as far as average flow properties are concerned. In determination of $K$ the values of $S$ and $P$ play more crucial roles than the connectivity, which is missing in Kozeny relation.

5.2 Conductivity

It has been shown that Archie’s law (eq 1) connecting the conductivity of brine-filled rocks with their porosity is valid for fractal pore spaces [12, 13, 14]. Though
we have not been able to conclusively demonstrate the fractal nature of the pore space generated by our model, we can make some conjectures from the results we have obtained.

For a fractal pore space, the cementation exponent depends on $d_f$ – the fractal dimension of the pore space and $d_w$ – the dimension of a random walk through the pore space as follows

$$m = 1 + (2 - d_w)/(d_f - d) \quad (5)$$

For $d_f$ close to 3 in three dimension, say 2.85–2.90 as indicated by our simulation we may assume a value of $d_w$ slightly larger than 2, say 2.1–2.2. With these values we get a range of m as 1.66 to 3, which is very realistic.

However, this results should be substantiated by an exact determination of $d_w$. Work on this problem is in progress.

In comparison to [12] and [14], where the rock is modelled as a deterministic fractal, the present model is more realistic being a statistical model.

6 Conclusions and Directions for Future Work

Let us review how far our growth model represents actual formation of sandstones. The first simplification is the assumption of cubic grains. In sanstones the grains do in fact have somewhat angular form [4], so this assumption is not worse than the more usual approximation of spherical grains. A consequence of the grains being cubic in our model is that the intergrain contact areas are large and flat, whereas the sandstones are reported to have tangential point contact between grains. This, however may take care partially of the compaction after deposition in our model, which we have otherwise ignored.

We have not considered the effect of restructuring of the pore space, after deposition through diagenesis. This may be taken up in future work. The elongated structure of the larger grains, which we have assumed, is realistic as mentioned earlier. We have also checked that square flat grains produce a higher porosity than $P_{\text{max}}$ in our 3-dimensional model.

One point to note is that the porosity we have calculated from our model is the total pore space per unit volume, not the effective porosity, which only considers the connected pore space. Calculation of the effective porosity is much more complicated, and we assume for the present that since the pore space is substantially connected the difference is not too much. In Archie’s law, some authors use the total porosity, and others the effective porosity.

Our calculation of pore space may also be modified by taking second nearest neighbor pores as connected. This would give a picture of pores connected by narrow throats as modelled by some authors [15].

The structure produced by our simulation algorithm has an anisotropy in the vertical direction. Pores are seen to elongated in the vertical direction, specially
for low porosities. We could not find any systematic data on anisotropy of pore structure in real rocks, but it is expected that due to the action of gravity an anisotropy should be present. The permeability data of some rocks show a marked anisotropy [6], which indicates anisotropy in the pore structure. The Kozeny theory does not take anisotropy into account since porosity and specific surface area are independent of direction. Experimental data shows the horizontal conductivity to be larger than the vertical in most cases, but the opposite trend is also seen sometimes.

In our model, connectivity appears to be larger in the vertical direction, inclusion of diagenesis in some form may increase the horizontal connectivity through flow of fluids.

Further modifications of this model are possible by including a horizontal drift or diffusion to simulate the effect of wind or water currents on the sedimentation process, in addition to the effect of gravity.

Comparing our model with the ballistic deposition model for surface growth [2], we note that our model introduces correlation between the adjacent growing columns, through incorporation of the larger sized particle.

In conclusion, we think the present model is a convenient starting point for study of the growth and structure of sedimentary rocks through simulation. Suitable modifications and further study of certain aspects of the present model are necessary, some of this work is already in progress.

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References

[1] T. Vicsek, Fractal Growth Phenomena, (World Scientific, Singapore), 1992.

[2] A Barabasi and H. E. Stanley, Fractal Concepts in Surface Growth, (World Scientific, Singapore), 1992.

[3] M. Sahimi, Rev. Mod. Phys., 65, 1393, 1993.

[4] F. J. Pettijohn, Sedimentary Rocks (CBS Publ., Delhi), 1984.

[5] G. V. Chillingarian, Compactional Diagenesis, pg. 57, in Sediment Diagenesis, ed. A. Parker and B. W. Sellwood, NATO ASI series C : 115, (D. Reidel Pub. Comp., Dordrecht), 1981.

[6] P. Wong, Physics Today, 24, December 1988.

[7] A. Scheidegger, The Physics of Flow Through Porous Media, (University of Toronto Press, Toronto), 1974.

[8] J. Kozeny, S.-Ber, Wiener Akad. Abst., IIa, 136, 271, 1927.

[9] D. Stauffer and A. Aharony, Introduction to Percolation Theory, 2nd ed., (Taylor and Francis, London), 1992. M. Sahimi, Applications of Percolation Theory, (Taylor and Francis, London), 1994.

[10] M. H. Cohen and M. P. Anderson in The Chemistry and Physics of Porous Media, ed. M. Tomkiewicz and P. N. Sen, (Pennington, New Jersey, The Electrochem Soc.), 1985.

[11] S. N. Davis, Porosity and Permeability of Natural Materials) pg. 53, in Flow Through Porous Media, ed. R. J. M. De Wiest (Acad., New York), 1969.

[12] S. Roy and S. Tarafdar, to be published in Phys. Rev. B, 1997.

[13] A. H. Thompson, A. J. Katz and C. E. Krohn, Adv. Phys. 36, 625 , (1987).

[14] J. F. Thovert, F. Wary and P. M. Adler, J. Appl. Phys., 68, 3872, 1990.

[15] J. Koplik and T. J. Lasseter, Soc. Model.Petr, Engg., p. 89, Feb 1985
Figure Captions

Figure 1(a)–(c) : Pore structure generated in 2-dimensions with (a) – $F = 0.2$, (b) – $F = 0.4$, and (c) – $F = 1.0$. Open squares represent pore sites.

Figure 2(a) : Porosity variation with sample size in 3-dimensional structure, for $F = 0.10$.

Figure 2(b) : Porosity variation with sample size in 3-dimensions for $F = 0.01$.

Figure 3 : Porosity variation with $F$ in 3-dimensions. Solid line shows logarithmic fit, and broken line shows simulation results.

Figure 4 : Log$[M(N)]$ plotted against Log$[N]$, the slope deviates from 3 for large N.

Figure 5 : Specific surface area versus porosity in 3-dimensions.

Figure 6 : (Surface area)/(no. of pore sites) versus porosity.

Figure 7 : Relative permeability ($K$) versus porosity. Solid line shows exponential fit, points are simulation results.