1
Preliminaries

1.1 Notation

Most problems in this book are solved in 1D along the vertical axis. It is natural to let the surface be at $z = 0$ and to have the z-axis pointing downwards, with positive z-coordinates for the subsurface. An advantage with this choice is that the acceleration of gravity is positive. A potential problem with the z-axis pointing downwards is that Fourier's law gives negative heat flow – heat that flows in the opposite direction to the positive z-axis. A simple solution to this problem is to drop the minus-sign in Fourier's law when the heat flow is computed in practical problems. There is a similar problem with Darcy's law, with the same simple solution. But Fourier's law and Darcy's law retain their minus signs when equations are derived. The full xyz-axis system is right-handed as shown in Figure 1.1b.

Vectors are written with lower case bold letters, as for instance, $\mathbf{v}$, $\mathbf{n}$ or as $\mathbf{n}^T = (n_1, \ldots n_2)$, where T denotes the transpose. Matrices are written with upper case bold letters, for instance like $\mathbf{A}$ and $\mathbf{R}$. The matrix elements are A_{ij} or R_{ij}, where the indices may be x, y and z for the respective spatial directions. Another example of a matrix is

$$\boldsymbol{K} = \begin{pmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{pmatrix}. \tag{1.1}$$

Scalar products can be written in several different ways depending on what is most convenient. Here are some examples:

$$\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y} = x_1 y_1 + x_2 y_2 + x_3 y_3 = \sum_{i=1}^{3} x_i y_i. \tag{1.2}$$

The second example shows the scalar product as a matrix product, where the vectors are written as row and column matrices. It is often convenient to write summations using what is called Einstein's summation convention, which says that summation is understood for every pair of equal indices. Here is an example: the scalar product

$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{3} x_i y_i \tag{1.3}$$

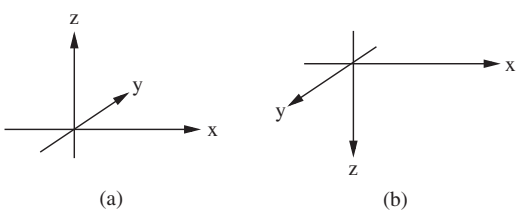


Figure 1.1. *(a) A right-handed coordinate system with the z-axis pointing upwards. (b) A right-handed coordinate system with the z-axis pointing downwards.*

is simply written as

$$\mathbf{x} \cdot \mathbf{y} = x_i y_i \tag{1.4}$$

when using Einstein's summation convention. Here is another example:

$$\sum_{j=1}^{3} \sigma_{ij} n_j = \sigma_{ij} n_j \tag{1.5}$$

which shows the summation over a pair of equal indices. The summation convention is often very useful, but it may lead to confusion. For instance, it implies that $K_{ii} = K_{11} + K_{22} + K_{33}$, which is the sum over the diagonal elements. If we want K_{ii} to denote one (single) diagonal element we have to state that explicitly. One pair of equal indices may be replaced by another pair of equal indices because there is a summation over them – for example $K_{ii} = K_{jj}$. There is never summation over x, y and z when they are used as indices. It is always possible to use these indices as numbers, where $x = 1$, $y = 2$ and $z = 3$. We therefore have that

$$\mathbf{n} = (n_x, n_y, n_z)^T \qquad \text{is the same as} \qquad \mathbf{n} = (n_1, n_2, n_3)^T. \tag{1.6}$$

An important point is the notation for dimensionless quantities. When depth z is scaled with a characteristic depth h it is written $\hat{z} = z/h$. A hat above a symbol denotes a dimensionless quantity. For example, dimensionless spatial coordinates, time and temperature are $\hat{x}$, $\hat{y}$, $\hat{z}$, $\hat{t}$ and $\hat{T}$.

1.2 Further reading

Riley *et al.* (1998) and Kreyszig (2006) are two comprehensive guides to mathematical methods for physics and engineering.

2
Properties of porous media

2.1 Porosity

Sediments and sedimentary rocks are porous media, and a porous medium is a solid with holes in it. The holes (pores) are normally connected and a fluid may flow through the pore space. The passage from one pore to another is through a pore throat, although there is not always a clear distinction between a pore and a pore throat. The way in which the pores are connected and the size of the pore throats control how permeable a porous medium is for fluid flow. The volume of the pore space controls its capacity to store fluid. Figure 2.1a shows an illustration of a porous medium made of a regular arrangement of spherical grains of equal size. It is a simple idealization of sediments and sedimentary rocks. A real rock has a much more complex pore space than the regular packing of spheres, as seen from the thin section in Figure 2.1b. It consists of grains of a variety of sizes, shapes and minerals. The pore space in rocks is also the result of a complex interplay of mechanical and chemical processes. The *porosity* is the volume fraction of void space of a porous medium, expressed as

$$\phi = \frac{V_p}{V_t} \tag{2.1}$$

where V_p is the volume of the void space and V_t is the total volume (of both solid and void) of the sample. An alternative way to measure the void space is to relate it to the solid volume of the rock rather than the total volume. This property, called the void ratio, is

$$e = \frac{V_p}{V_t - V_p} = \frac{\phi}{1 - \phi}. \tag{2.2}$$

The solid volume of the rock is the difference between the total volume V_t and the void volume V_p. Equation (2.2) can also be inverted to give an expression of the porosity as a function of the void ratio,

$$\phi = \frac{e}{e + 1}. \tag{2.3}$$

As we will see later it is often more convenient to work with the void ratio than the porosity.

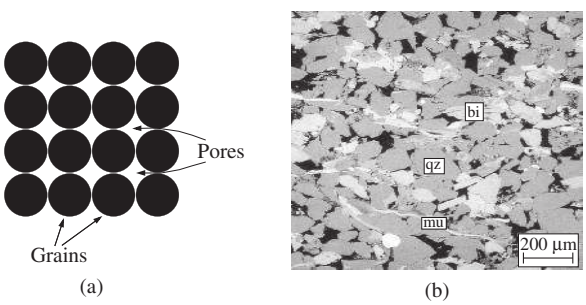


Figure 2.1. *(a) A regular porous medium made of grains of equal size. (b) A SEM image of a sandstone where the pore space is black and the quartz grains are gray. (qz = quartz, mu = muscovite and bi = biotite)*

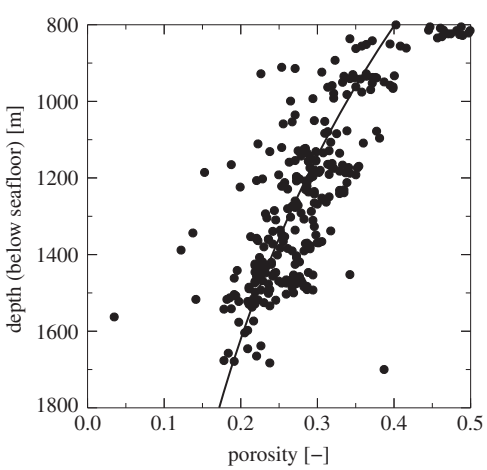


Figure 2.2. *Porosity of clays and silts as a function of depth. Data is from ODP site 1276, leg 210, see Sawyer and Fackler (2007). The porosity–depth trend is fitted with the function* $\phi(z) = 0.79\exp(-z/1180)$*, where z is the depth below seafloor in meters.*

It is not possible to obtain a meaningful porosity unless the bulk volume V_t contains a large number of grains. The porous medium is said to be *homogeneous* if the porosity is (almost) constant regardless of where in the medium the volume V_t is taken, and V_t is then called a representative elementary volume, REV. There are two types of porosity – connected and unconnected. It is only the volume of the connected pores that is normally included in the porosity. The term *effective porosity* is used to underline that only connected pores are included.

Sediments and rocks rarely are homogeneous. A characteristic feature of sediments and sedimentary rocks is their layered structure caused by deposition processes. Sedimentary rocks are therefore often strongly heterogeneous in the direction normal to the bedding plane. Figure 2.2 shows an example of clay and silt porosity in a 1000 m depth interval. This is a typical example of the large scatter often seen in sediment porosity, where there

Table 2.1. *Porosity–depth data for lithologies in the North Sea from Sclater and Christie (1980).*

Lithology	ϕ_0	z_0 [m]
Shale	0.63	1960
Sand	0.49	3703
Chalk	0.70	1408
Shaly sandstone	0.56	2464

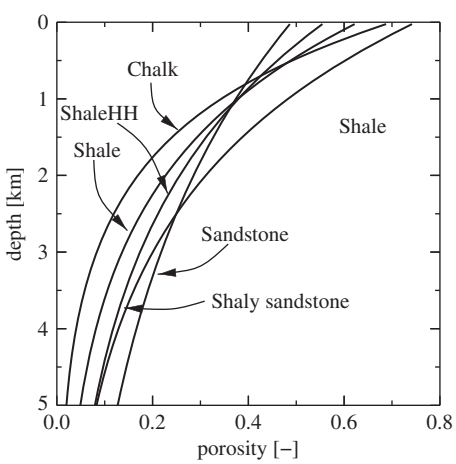


Figure 2.3. *Porosity–depth trends from Sclater and Christie (1980) and Helland-Hansen et al. (1988) (denoted HH).*

are considerable jumps in the porosity over short depth intervals. The porosity–depth trend in Figure 2.2 is fitted with the function

$$\phi(z) = \phi_0 \exp(-z/z_0) \tag{2.4}$$

where ϕ_0 is the surface porosity and z_0 is a depth that characterizes the compaction. The depth z is measured from the sediment surface. This porosity function was first applied by Athy (1930) to the porosity of sedimentary basins and has later been named the Athy function. Figure 2.3 shows the Athy function fitted against data for the lithologies shale, sandstone, chalk and shaly-sandstone from the North Sea. The parameters are obtained by Sclater and Christie (1980) and are listed in Table 2.1. Remember that these curves are smooth trends fitted against observations with a large scatter in the porosities. Another point is that the porosity varies from basin to basin depending on the deposition history and the temperature history. Fortunately, we rarely need to know the detailed porosity when dealing with compaction, subsidence or overpressure build-up on a basin

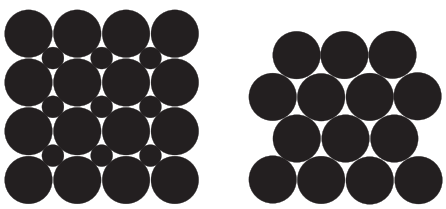


Figure 2.4. *Regular porous media. (a) Two grain sizes. (b) Rhombohedral packing.*

scale. We will meet the Athy porosity function later since it is a convenient function to work with.

Exercise 2.1 What is the porosity and the void ratio of a medium with exactly the same amount of void space as solid volume?

Exercise 2.2 Derive relationship (2.3).

Exercise 2.3 Calculate the porosity of the regular porous medium shown in Figure 2.1a, where all grains have equal size. Is the porosity dependent on the grain size (the radius)?

Exercise 2.4 Calculate the porosity of the porous medium shown in Figure 2.4. Notice that grains of different sizes allow for denser packing.

Exercise 2.5 The porosity of a dry rock sample can be measured from the increase in weight by filling the pore space by a wetting fluid. What is the porosity of a sample if its mass increases with Δm, when it is filled with a fluid of density ϱ, and it has the total volume V_t?

2.2 The correlation function and specific surface

A porous medium can specified by the *characteristic* function f defined as

$$f(\mathbf{x}) = \begin{cases} 0, & \text{when } \mathbf{x} \text{ is in a grain} \\ 1, & \text{when } \mathbf{x} \text{ is in the pore space} \end{cases} \tag{2.5}$$

where the porosity of the volume V is seen to be

$$\phi = \frac{1}{V} \int_V f(\mathbf{x})\, dV. \tag{2.6}$$

The characteristic function can be used to define the two-point correlation function

$$C(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{V} \int_V f(\mathbf{x} + \mathbf{r}_1) f(\mathbf{x} + \mathbf{r}_2)\, dV \tag{2.7}$$

which expresses how likely it is that the porous medium is void at position $\mathbf{r}_2$, when it is void at position $\mathbf{r}_1$. The medium is *statistically homogeneous* when the correlation function depends only on the distance $r = |\mathbf{r}_2 - \mathbf{r}_1|$ as

$$C(\mathbf{r}_1, \mathbf{r}_2) = C(\mathbf{r}_2 - \mathbf{r}_1) = C(r). \tag{2.8}$$

From the definition (2.7) it follows that the statistically homogeneous correlation function has the following properties:

$$C(0) = \phi \quad \text{and} \quad \lim_{r\to\infty} C(r) = \phi^2. \tag{2.9}$$

The latter relation assumes that the pore space is uncorrelated between any two positions separated by a "large" distance. An important reason for introducing the two-point correlation function is that it gives the surface area of the pore space per unit volume – *the specific surface area*. It is obtained from the two-point correlation function by the following simple relation (Berryman, 1987):

$$S = -4 \left.\frac{dC(r)}{dr}\right|_{r=0}. \tag{2.10}$$

This relation also holds for anisotropic porous media as shown in Note 2.1. The correlation function can be found experimentally for real porous media or exactly for simple models, and once it is obtained we will have the porosity from relation (2.9) and the specific surface area from relation (2.10).

Note 2.1 The derivation of the expression (2.10) follows Berryman (1987). We first introduce the angular average of the correlation function

$$\begin{aligned} C_a(r) &= \frac{1}{4\pi} \int C\Big(r\mathbf{n}_r(\theta,\varphi)\Big) \sin\theta \, d\theta \, d\varphi \\ &= \frac{1}{4\pi V} \iint_V f(\mathbf{x}) f(\mathbf{x} + r\mathbf{n}_r) \, dV \, \sin\theta \, d\theta \, d\varphi \\ &= \frac{1}{4\pi V} \iint_{V_p} f(\mathbf{x} + r\mathbf{n}_r) \, dV \, \sin\theta \, d\theta \, d\varphi \end{aligned} \tag{2.11}$$

where $\mathbf{n}_r(\theta, \varphi)$ is the unit vector in the direction of r. The integration of φ is from 0 to 2π, and the integration of θ is from 0 to π, see Figure 2.5. The last equality holds because

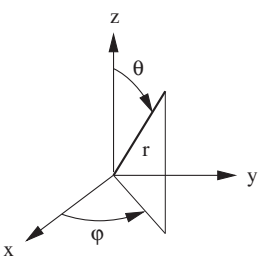


Figure 2.5. *A position in space is given by the spherical coordinates* (r, θ, φ). *The angles,* φ *from* 0 *to* 2π *and* θ *from* 0 *to* π, *parameterize the surface of sphere with radius* r.

$f(\mathbf{x}) = 1$ for $\mathbf{x}$ in the pore space V_p and otherwise 0. The derivative of the angular average of the correlation function is

$$\begin{aligned}
\frac{dC_a(r)}{dr} &= \frac{1}{4\pi V}\int\!\!\int_{V_p} \frac{\partial f(\mathbf{x}+r\mathbf{n}_r)}{\partial r}\, dV\ \sin\theta\, d\theta\, d\varphi \\
&= \frac{1}{4\pi V}\int\!\!\int_{V_p} \mathbf{n}_r \cdot \nabla f(\mathbf{x}+r\mathbf{n}_r)\, dV\ \sin\theta\, d\theta\, d\varphi \\
&= \frac{1}{4\pi V}\int\!\!\int_{V_p} \nabla \cdot \Big(\mathbf{n}_r\ f(\mathbf{x}+r\mathbf{n}_r)\Big)\, dV\ \sin\theta\, d\theta\, d\varphi \\
&= \frac{1}{4\pi V}\int\!\!\int_{A_p} \mathbf{n}\cdot\mathbf{n}_r\ f(\mathbf{x}+r\mathbf{n}_r)\, dA\ \sin\theta\, d\theta\, d\varphi. \qquad (2.12)
\end{aligned}$$

The volume integral is converted to a surface integral by means of the divergence theorem, and $\mathbf{n}$ is the outward unit vector of the surface A_p of the pore space. The coordinate system is now centered at $\mathbf{x}$ with $\mathbf{n} = \mathbf{n}_z$, which gives that $\mathbf{n}\cdot\mathbf{n}_r = \cos\theta$. The outward normal vector $\mathbf{n}$ of the surface of the pore space is pointing upwards, which means that the surface is locally in the xy-plane around $\mathbf{x}$. The solid is locally above the xy-plane and the pore space is locally below the xy-plane. The integral

$$\begin{aligned}
I &= \int_0^{2\pi}\int_0^{\pi} \sin\theta\, \mathbf{n}\cdot\mathbf{n}_r\ f(\mathbf{x}+r\mathbf{n}_r)\, d\theta\, d\varphi \\
&= 2\pi\int_0^{\pi} \sin\theta\ \cos\theta\ f(\mathbf{x}+r\mathbf{n}_r)\, d\theta \\
&= 2\pi\int_{\pi/2}^{\pi} \sin\theta\ \cos\theta\, d\theta \\
&= -\pi \qquad (2.13)
\end{aligned}$$

in the limit $r \to 0$. The function $f(\mathbf{x}+r\mathbf{n}_r)$ is then 0 for $\mathbf{n}_r(\theta,\varphi)$ pointing into the solid, with angles θ from 0 to $\pi/2$. Inserting the integral I into expression (2.12) gives that $dC/dr = -A_p/4V$, where A_p is the surface area of the pore space and the ratio A_p/V is the specific surface.

2.3 The penetrable grain model

The porosity and the characteristic function are not exactly known for other than some simple porous media. One example of such a porous medium is N randomly placed spherical grains of equal radius in a volume V. This model is called the penetrable grain model because the grains are allowed to overlap. A porous medium of penetrable spheres is shown in Figure 2.6a. The inverse of the penetrable sphere model, where solid and void are interchanged, is shown to the right. The inverse model is sometimes called a "Swiss cheese" model, because the pores are now overlapping spheres.

The porosity of the penetrable grain model is equal to the probability that a given point inside V is not overlapped by any of the N grains of volume V_g,

$$\phi = \left(1 - \frac{V_g}{V}\right)^N. \tag{2.14}$$

The probability that a point in V is overlapped by a single grain is V_g/V, when it is assumed that the grains are uniformly distributed. We can replace the volume V by the grain density $\varrho = N/V$, which is the number of grains per unit volume. The porosity is then

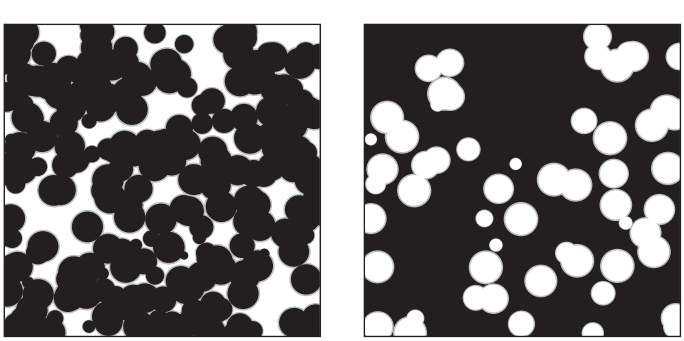
$$\phi = \left(1 - \frac{\varrho V_g}{N}\right)^N \tag{2.15}$$

which becomes

$$\phi = \exp(-\varrho V_g) \tag{2.16}$$

in the limit $N \to \infty$. (We have that $(1 + x/N)^N \to e^x$ when $N \to \infty$.) A porous medium of penetrable spheres of radius a has

$$V_g = (4/3)\pi a^3 \tag{2.17}$$



(a) (b)

Figure 2.6. *(a) Porous medium formed by overlapping spheres. (b) The inverse porous medium of the overlapping sphere model where the solid and the void are interchanged.*

and the porosity is

$$\phi = \exp\left(-\frac{4}{3}\varrho\pi a^3\right). \tag{2.18}$$

The pair correlation function $C(r)$ can be obtained in a similar way as the porosity. It is equal to the probability that two points separated by a distance r inside the volume V is not occupied by a pair of spheres. Using the number density ϱ and going to the limit of a large number of spheres gives

$$C(r) = \exp\left(-\varrho V_2(r)\right) \tag{2.19}$$

where V_2 is the volume of two overlapping spheres separated by a distance r. The volume V_2 is

$$V_2 = \frac{4\pi a^3}{3}\left[1 + \frac{3}{4}\left(\frac{r}{a}\right) - \frac{1}{16}\left(\frac{r}{a}\right)^3\right], \quad r < 2a \tag{2.20}$$

where the sphere radius is a. When $r \geq 2a$ the spheres do not overlap and we have that V_2 is the sum of the volumes of the two spheres,

$$V_2 = \frac{8\pi a^3}{3}, \quad r \geq 2a. \tag{2.21}$$

Relation (2.10) for the specific surface of the porous medium gives

$$S = -4\left.\frac{dC(r)}{dr}\right|_{r=0} = 4\pi a^2 \varrho\phi \tag{2.22}$$

where ϕ is the porosity given by (2.18).

We will later need an expression for the specific surface as a function of the porosity. This is for applications where the porosity is lost due to precipitation of minerals, and where the precipitation process is controlled by the available specific surface. Before we derive an expression for the specific surface as a function of the porosity, we will first find an expression for the volume of a grain as a function of the porosity. We have from (2.16) that

$$V_g(\phi) = V_0\frac{\ln\phi}{\ln\phi_0} \tag{2.23}$$

where the initial porosity ϕ_0 and the initial grain volume V_0 are used to eliminate the number density. From the volume of a grain (2.17) we obtain the following expression for the radius of a sphere as a function of the porosity:

$$a(\phi) = a_0\left(\frac{\ln\phi}{\ln\phi_0}\right)^{1/3}. \tag{2.24}$$

Finally, the specific surface (2.22) as a function of the porosity becomes

$$S(\phi) = -\frac{3\phi\ln\phi_0}{a_0}\left(\frac{\ln\phi}{\ln\phi_0}\right)^{2/3}. \tag{2.25}$$