Chapter 2 Fundamentals of Porous Structures

2.1 Introduction

The understanding of multiphase flow in porous media is of great importance in many fields such as hydrology, contaminant clean-up and petroleum engineering. Macroscopic properties—principally capillary pressure and relative permeability—are often needed when modelling flow and transport at the continuum scale, whether it is transport of non-aqueous phase liquids (NAPL) in contaminant clean-up or the production of oil during reservoir water flooding. These macroscopic properties are, however, difficult to obtain. It is possible to conduct physical experiments on samples of the reservoir, but this will only reflect one set of conditions. Furthermore, the scale of the reservoir itself is so much larger that a few experiments are unlikely to describe the variation likely to be present. Hence, there is a need to develop physically-based models that can predict multiphase flow and transport properties and their likely variation in a reservoir setting, based on readily available experimental data.

This chapter emphasizes the mathematical modelling of transport processes in porous media by the cell models, the digital reconstruction of the porous structure using the Lattice Boltzmann method and the stochastic modelling to obtain a realistic description of the porous structure.

2.2 Cell Models

Mathematical modeling of transport processes in porous media is a powerful tool employed whenever experimentation is either expensive or difficult due to the nature of the process. On the other hand, the realistic description of the porous structure significantly increases the complexity of the mathematics involved, due to the coupling between the physicochemical mechanisms and the geometrical complexity of the porous medium, thus requiring massive computational power. Given the poor

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Fig. 2.1 Schematic representation of sphere-in-cell model idealization (*a* and *b* denote the radii of the inner and outer spheres, respectively)

computational power available sixty years ago, along with the industry-driven increased necessity for research on porous media structure, in the late 1940s modeling aimed towards the achievement of analytical solutions. The conceptual idea behind this was the cell approach, where the medium is considered as an assemblage of unit cells gathered in a regular manner. Accordingly, it was widely accepted that the unit cell is the adequate representative of the whole medium, therefore processes occurring through the porous structure are described sufficiently by those occurring in the unit cell. As many industrial and technological applications are related with swarms of cylindrical or spherical grains (filtration, separation, fibers, etc.) and the analytical solution for the flow field around an isolated sphere was obtained by Stokes one hundred years ago, what was introduced in those days were the sphere-in-cell models, whose fundamental idea is schematically represented in Fig. 2.1.

Sphere-in-cell models are based on the representation of the overall solid mass of the swarm by a spherical or cylindrical solid body, which is embedded in a spherical or cylindrical liquid envelope, respectively. The boundary conditions imposed on the outer surface of the envelope is supposed to adequately represent the interactions with the other grains of the swarm. Obviously, the thickness of the surrounding fluid layer is adjusted so the ratio of the solid volume to the volume of the liquid envelope to represents exactly the solid volume fraction of the porous medium. The main advantage of these models is that an analytical expression for the stream function can be obtained demanding significantly less effort than that needed for numerical investigations. The spherical shape corresponds to a formulation which leads to axially symmetric flow that has a simple analytical solution of closed form, and can thus be used readily for heat and mass transport calculations. Although this analytical solution is actually an approximation of the real flow field in a complex porous structure, it was sufficient for the engineering applications raised until the early 1980s. On the other hand, the model has one disadvantage in that the outer envelope is not space filling, a difficulty which must be dealt with when a scale-up from the single unit cell to an assemblage of particles is necessary.

The first introduction of sphere-in-cell model was by Cunningham [18]. When considering particle sedimentation, Cunningham postulated that the movement of each spherical particle was allowed only within a concentric mass of fluid boundary. This model had problems in relating the size of the outer fluid sphere to the bed voidage (or particle concentration), therefore Uschida proposed at 1959 an improvement. He assumed that the porous medium is divided into numerous cubes and a particle is placed into the center of each cube. Although space filling, this approach failed to predict accurate flow field solutions due to discontinuities imposed internally by the cubic schema. Richardson and Zaki [59] developed a hexagonal cell model to predict the sedimentation velocity of uniform spheres under viscous flow conditions. In this model, two configurations were considered depending on the vertical particle arrangement. For the first, the distance between neighboring particles in the vertical direction was assumed to be equal to that in the horizontal direction, while the second configuration assumed that vertical neighboring particles are essentially in contact. Due, at least in part, to the oversimplification of the pressure gradient and questionable assumptions regarding the angles between the streamlines and the vertical axis, predictions of the sedimentation velocity from the two configurations were not applicable to a dilute concentration of particles. Happel [26] and Kuwabara [33] presented two independently devised sphere-in-cell models to address the flow problem in sphere packing. The major differences between these two models are in the boundary conditions imposed in the outer surface (A detailed description can be found in Chap. 3). Despite their fundamental differences, both models have been proved to yield very similar flow fields over a wide range of porosity values [67]. At the same time, using formulations analogous to those of spherical geometry, both Happel [26] and Kuwabara [33] also proposed cylinder-incell models that consider particles of cylindrical instead of spherical shape. These models were based on the cylindrical-cell model of Kawaguti [32] and found applications in modeling flow through fibrous mats and arrays of parallel fibers. Neale and Nader [45] proposed an important improvement over the aforementioned models. They considered that the basic spherical cell is embedded in an unbounded, continuous, homogeneous and isotropic permeable medium of the same porosity and permeability as those of particle swarm. To describe the flow through the porous surrounding, they used Brinkmans's equation [8]. A decade later, a new spherical cell model for predicting the bed expansion of a liquid-solid fluidized bed was presented by Moritomi et al. [43]. They assumed that Stokes' flow is valid for the fluid within the outer cell boundary while outside the cell the flow is approximated by a potential flow. However, prediction of the bed voidage did not agree well with their experimental data. Another use of Brinkman's equation in cell models is encountered Prasad et al. [54], which replaces the solid sphere of the sphere-in-cell model with a solid sphere surrounded by a concentric spherical shell of homogeneous and isotropic porous material. This model combines features of those developed by Happel and Kuwabara, and uses Brinkman's equation to describe the flow through the porous shell. The work of Prasad et al. is based on the work of Maslivah et al. [42] whose "solid-sphere-with-porous-shell" is embedded in an unbounded fluid instead of the fluid envelope presented by Prasad et al. [54].



Fig. 2.2 Schematic representation of sinusoidal cell concept

The models described above all considered either spherical or cylindrical grains, which corresponds to two-dimensional spherical geometry after some physical assumptions and mathematical manipulations. However, grain shape is closer to spheroidal than spherical for the majority of practical applications and this is a crucial limitation for model accuracy. Epstein and Masliyah [22] solved numerically the flow-field through clusters of spheroids under creeping flow conditions, whereas the analytical solution of Ammar and Hsieh [4] for Stokes flow inside an oblate hemispheroidal cap was the precursor for the work of Dassios et al. [19, 20]. The latter presented a complete spheroid-in-cell model, quite analogous to those of Happel and Kuwabara, and based on the introduced concept of "semi-separation", an analytical formulation for the stream-function under creeping flow conditions was obtained in terms of series expansions.

Depending on the application considered, several different non grain-type cell models have been proposed and used to simulate the usually complex porous structures. To model the transient behavior of deep-bed filtration systems, Payatakes et al. [50] and Tien et al. [68] proposed the representation of the granular medium by an ensemble of unit-bed elements (UBE), which was found to successfully describe the initial stages of the filtration process. Each UBE is constructed of a number of tube-type cells (collectors), sometimes surrounded by liquid envelopes [58]. Although the trend was to use straight capillaries for the sake of simplicity in the calculations, representation of the pore space by sinusoidal cells, as suggested by Payatakes et al. [51], seemed to produce results in good agreement with experimental observations. The fundamental idea of sinusoidal cells is schematically represented in Fig. 2.2.

The theoretical results of using UBEs for filtration simulations (Payatakes et al. [52]) were found to be in good agreement with experimental data, thus indicating that this simulator type could be used to provide an order-of-magnitude estimate on a truly predictive basis for filtration processes. Some years later, Chiang and Tien [12] used constricted tubes as collectors and employed the concept of UBE in their analysis. Unfortunately, this model cannot describe a complete filter cycle, as it does not deal with the problem of pore clogging and the simultaneous decrease



Fig. 2.3 Various unit cells

in permeability. Based on the UBE concept, Choo and Tien [14] presented another approach and assumed that each element contained a number of cylindrical tubes of various sizes. However, it was already known that the assumption of straight capillary tubes oversimplifies pore structure, leading to a substantial underestimation of the particle deposition rate in each cell [49].

Further to representation purposes, unit cells of various dimensions have been introduced and used for the study of diffusion, convection, dispersion and interfacial transport in homogeneous porous media [3, 17, 55–57]. Some of those unit cells are presented in Fig. 2.3.

2.3 Digital Reconstruction (Lattice Boltzmann Method) of the Porous Structure

Transport in porous media is a topic related to many technological and environmental applications. The accurate prediction of the transport coefficients in porous media is a challenging problem due to the complexity of transport mechanisms in fluid-solid systems and the difficulty in representing accurately the complicated and tortuous nature of a porous medium.

The digital reconstruction of porous materials is a relatively new, powerful methodology that enables the reliable representation of the complex biphasic structure induced by porosity. The significant advances in both experimental and numerical practices have allowed the development of reconstruction techniques, the most advantageous being (a) the statistical methods leading to the stochastic reconstruction of porous media in three dimensions based on statistical information obtained from one or several two dimensional images of thin sections of the actual material, and (b) the process-based methods, where the computational procedure tries to imitate the physical processes that commence during the formation of the medium. Although the latter seem to be closer to the physical system, they frequently exhibit severe computational requirements and hence are limited to the specific material considered in each case (Kainourgiakis et al. 31).

The Lattice Boltzmann method (LBM) constitutes a very powerful tool for the study of the hydrodynamical problem of fluid flow inside porous structures, mainly due to the simplified handling of the complicate boundary conditions, as well as, due to the efficiency of the method with regard to parallelization [63, 65]. Lattice Boltzmann method (LBM) is a mesoscopic approach for simulating computational fluid dynamics by solving a discretized Boltzmann equation [11, 60, 71]. An attractive feature of LBM is the ease of addressing complex boundary conditions by implementing very simple schemes. Numerous works have successfully applied LBM in modeling fluid flow in porous media and quantification of porous media permeability [10, 27, 48, 60]. LBM models fluids as particle distributions residing on a discrete lattice, propagating to their adjacent lattice nodes, and colliding with other particles to redistribute momentum.

Aharonov and Rothman [2] first used the Lattice Boltzmann method to simulate the flow of non-Newtonian fluids. Their pioneering work addresses two dimensional pipes and random media. They found that the flux is related to the driving force by a simple scaling law. Similar results were reported by Boek et al. [7]. Recently, Gabbanelli et al. [24] studied the flow of truncated power-law fluids in reentrant flow geometries and found a very good agreement between the results obtained by the Lattice Boltzmann method and those obtained by standard finite element methods, while Sullivan et al. [66] explored the relationship between lattice resolution and simulation accuracy as a function of the power-law index.

2.3.1 Porous Media Generation

Accurate numerical simulation of fluid flow in porous media requires detailed descriptions of porous media morphology, which should include geometric properties such as particle or pore shape and volume, and topological properties such as pore interconnectivity. In many cases, however, the type of model that can be employed is dependent on the modeling method, and more importantly, limited

computational resources. It is thus important to construct models that are able to closely mimic the heterogeneity of actual porous media, and at the same time are sufficiently efficient to allow simulation of flow and transport phenomena with reasonable computational effort. In this study, porous media are envisioned as a statistical distribution of non-overlapping circular disks representing soil particles distributed in a rectangular two-dimensional uniform continuum representing the pore space through which a fluid flows.

As first proposed by Gardner, particle size distributions in soil are often assumed to be lognormal in nature (Lerman [36]). Buchan noted that approximately one-half of the US Department of Agriculture textual classification triangle could be adequately modeled by a lognormal distribution. Since a standard lognormal distribution implies zero and infinity for the smallest and largest particle sizes, respectively, modified lognormal distributions were developed to constrain the upper and lower extremes of the particle size. Fredlund et al. [23] proposed a new model based on a unimodal mathematical function, which is believed to provide improved representations of particle size distributions relative to lognormal distributions. This model's ease of use, however, is limited by its employment of five fitting parameters; our study thus employs a modified lognormal distribution to describe particle size distribution, assuming that all particle sizes reside in a 95% confidence interval to eliminate extremely large or small particles.

Li et al. [37] modified the algorithm proposed by Yang et al. [72] for a three dimensional sphere packing, a two-step collective rearrangement technique to generate random porous media. In this work, the particles with size distributions following a modified lognormal distribution are generated until the required porosity is satisfied. The particles are then assigned to a two dimensional domain by assuming a uniform distribution of particle locations. Based on this initial, possibly overlapped configuration (i.e., one particle may overlap another particle), an iterative arrangement process is applied to achieve an overlap free condition. During each iterations the largest particle is selected for relocation if there is any overlap with another particle; if overlap occurs, its spatial location is adjusted until the overlap is removed, and then registered in the final non-overlap location. The procedure continues with the next largest particle, etc. until all particles are registered in their final non-overlap location. Periodic boundary conditions are maintained at all boundaries throughout the iteration process. Figure 2.4 provides an illustration of several of the generated random porous media employed in this study.

2.4 Stochastic Modeling

Most natural and biological phenomena, such as solute transport in porous media, exhibit variability which can not be modeled using deterministic approaches. There is evidence in natural phenomena to suggest that some observations cannot be explained using models which give deterministic solutions. Stochastic processes



Fig. 2.4 Example of generated porous media

have a rich repository of objects which can be used to express the randomness inherent in the system and the evolution of the system over time.

Transport processes are generally modeled by initial/boundary value problems for a partial differential equation (PDE) describing the local balance of the concentration fields. However, during probabilistic analysis of flow and transport properties in porous media, the uncertainties due to spatial heterogeneity of governing parameters will be often taken into account. The definition of the properties of porous media in space and time using the concept of random functions provides means for (1) studying the inherent heterogeneity, (2) evaluating the spatiotemporal variability of the properties, and (3) assessing the uncertainty associated with their estimated values.

For example, if a small control volume is considered, a mass balance on the solute, in one-dimension, without chemical reaction, leads to

$$\frac{\partial}{\partial x} \left(D_{\rm e} \frac{\partial C}{\partial x} - uC \right) = \frac{\partial C}{\partial t}$$
(2.1)

where D_e is the diffusion coefficient, *C* is the mean solute concentration, *u* is the interstitial velocity of fluid, and *t* the time. The velocity field u(x,t) and diffusion coefficients $D_e(x,t)$ instead account for the spatial heterogeneity of the porous media. Within the frame of Scheidegger's theory of dispersion in porous media the

components of the diffusion tensor are proportional with those of the velocity field [61]. The velocity field is modelled by the solution of flow equation. For instance, the stationary (in time) and divergence free flow through a saturated porous medium, is governed by Darcy and continuity equations

$$u_i = -\frac{K}{\varepsilon} \frac{\partial H}{\partial x_i}, \quad \sum_{i=1}^n \frac{\partial u_i}{\partial x_i}$$
(2.2)

where *K* is the isotropic hydraulic conductivity, ε is the porosity supposed to be constant and H is the hydraulic head. The solution of Eq. 2.2 describes flow through isotropic porous media.

For example, the hydraulic conductivity, K, as a function of x, it is convenient to use its logarithm $Y(x) = \ln K(x)$. This quantity can be inferred from field experiments consisting of pumping tests performed in observation wells. In most experimental settings the locations of the wells are chosen so that an optimum sampling of concentration during tracer tests is obtained. These results in a sparse and non-regular distribution of wells and, therefore interpolation techniques are used to estimate spatial correlations of Y(x). Based on experimentally inferred correlations, stochastic models are proposed. For example, it is assumed that Y is a statistically homogeneous in space random function, normal distributed with constant mean and exponential covariance function [13].

Consequently, Eq. 2.1 has random coefficients. The stochastic approach considers ensembles of solutions of (2.1), corresponding to the ensemble of K field realizations. Expectations and standard deviations of the concentration are computed as ensemble averages. In many applications an upscaled transport model with simpler structure (in general with constant coefficients) is used to describe the process at the desired observation scale. An observable transport process corresponds to a solution of (2.1) for a fixed realization of hydraulic conductivity. Therefore, to obtain realistic predictions, ergodicity assessments have to complete stochastic modelling. Ergodicity can be quantified, for instance, by root mean-square distances between single realization solutions and the output of the upscale model [64]. Technical issues related to the construction of the numerical solutions for PDEs of form (2.1) also provide arguments for a stochastic approach.

2.4.1 The Pore Space

The pore space description can be generated directly using X-ray microtomography (see [16]), where the rock is imaged at resolutions of around a few microns. This can be done due to the differences in X-ray absorption of rock matrix and void space. An example of a 3D image, of Fontainebleau sandstone, is shown in Fig. 2.5a along with a 2D cross section in Fig. 2.6a. This method has the advantage of directly reconstructing the pore space, but due to the specialized scanners required, it is not readily available and also very costly. It is, however,



Fig. 2.5 Comparison between different 3D voxel representations of a Fontainebleau sandstone [6], generated using different reconstruction techniques. The side length of each sample is 2.25 mm. a X-ray microtomography. b Object-based modelling. c Gaussian field technique. d Simulated annealing

very useful for validating numerical reconstruction techniques of the microstructure, described below.

Most stochastic reconstruction algorithms are based on threshold Gaussian field techniques [1]. These algorithms are based on porosity and two-point correlation functions, both of which can be readily obtained by image analysis of 2D thin sections. The technique is similar to that used in geostatistics. A continuous correlated field is generated using Fourier transform methods and threshold to retrieve the binary phases (pore space and matrix) with the correct porosity and correlation function, as sketched in Figs. 2.5c and 2.6c. This method can also be extended to include more phases, such as clays.

Realising that the earlier Gaussian based methods were not very good at reproducing the underlying particulate structures of the porous media, as evident from Fig. 2.6c, Yeong et al. [73] developed a stochastic method based on simulated annealing, later extended by Manwart et al. [40]. Rather than being restricted to one- and two-point correlation functions, the objective function used can be made to match additional quantities such as multi-point correlation functions,



Fig. 2.6 Comparison between different 2D cross-sections of a Fontainebleau sandstone [6], generated using different reconstruction techniques. The side length of each sample is 2.25 mm. **a** X-ray microtomography. **b** Object-based modelling. **c** Gaussian field technique. **d** Simulated annealing

lineal-path function or pore size distribution function to name a few. Since the method is based on moving pore-space voxels around to minimize the objective function, the correct porosity is always retained. They subsequently reconstructed a 3D Fontainebleau and Berea sandstones from 2D sections using an objective function based on both two-point correlation function and either lineal-path or pore size distribution function, Figs. 2.5d and 2.6d. The estimated percolation probability was closer to the reference than when only using the two-point correlation function, such as the local percolation probability, would most likely improve the reconstruction further, but that would also increase the computational cost of the method significantly.

Another technique is the use of object-based modelling whereby the actual rock-forming process is simulated. Packing algorithms for spheres are well established (see [1]) and algorithms for arbitrary shapes have also been presented by several authors [15, 34, 35, 53]. An algorithm that takes into account the whole rock-forming process where primary grain sedimentation is followed by compaction and diagenesis has been presented by Bakke and Øren [5] and later by Jin et al. [30]. A grain size distribution is determined from image analysis of thin sections. Grains are then randomly picked from this distribution during the sedimentation process. Compaction is modelled by moving the centre of each grain down in proportion to its original vertical position. Finally, diagenetic processes are modelled. Quartz overgrowth is modelled by increasing the radii of the grains, and clays are precipitated on quartz surfaces. The amount of diagenesis to include is also determined from thin section analysis. Though this reconstruction method does not guarantee that statistical geometrical parameters such as the two-point correlation functions are honoured, it is assumed that these will be adequately reproduced since the actual rock-forming process is simulated, Figs. 2.5b and 2.6b.

Biswal et al. [6] performed a quantitative comparison of three reconstruction methods (Gaussian field, simulated annealing and object-based) on a Fontainebleau sandstone, where the reference, containing 3,003 voxels, was obtained using microtomography. They found that the object-based technique reproduced the twopoint correlation function reasonably well. When comparing connectivity using local percolation probability it was clear that the object-based technique was far superior to the statistical techniques. This result agrees with analysis performed by other authors as Hilfer [28].

Recently several statistical reconstruction techniques have been suggested that try to improve on the deficiencies of the Gaussian field techniques, while not being as computationally demanding as simulated annealing. Thovert et al. [69] introduced a method that is a hybrid between the statistical and object-based methods. Their technique is statistical, using only porosity and two-point correlation function, but conditioned to an underlying granular structure, defined using a pore size distribution derived from the two-point correlation function. This is based on a Poissonian penetrable sphere model. They verified their method using a 3D Fontainebleau sample and reported good agreement with the reference, even for the percolation probability. Hilfer and Manswart [29] also developed a hybrid between statistical and object-based method. Initially a close packing of spheres is laid down. Matrix voxels are then randomly distributed in the pore space until a prescribed porosity is attained. The configuration of the added matrix voxels are then updated using simulated annealing, matching the two-point correlation function. They also verified their method using a 3D Fontainebleau sample and the local percolation probability was found to be significantly better than traditional simulated annealing though not quite as good as a traditional object-based method.

For many types of porous media it might, however, be difficult to define the structures that make up the matrix. In carbonate rocks post-depositional diagenesis often completely dominates the matrix structure (see [39]), making object-based techniques difficult to use. In field-scale reservoir characterization the same

problems are often experienced where there are multiple faces with distinctive connected geometries; for example, in fluvial reservoirs. Gaussian field techniques will not reproduce the channel connectivity whereas object-based methods rely on the faces geometries being easily parameterized. Strebelle [62] suggested a statistical algorithm in which the multiple-point statistics were inferred from exhaustive 2D training images of equivalent reservoir structures and then used to reconstruct the reservoir, adhering to any conditioning data. This method was applied successfully to both fluvial and more complex patterned reservoirs. The ability to reproduce any pattern makes this method highly attractive for reconstructing complex porous media like carbonates. Okabe et al. [46] have used this algorithm to reconstruct a 3D Fontainebleau sandstone from a 2D training image. Although the granular structure is not as well reproduced as in object-based methods, the local percolation probability is significantly better reproduced than that achieved by other statistical methods such as Gaussian field techniques.

2.4.2 Transport Properties

When estimating single phase transport properties like absolute permeability it is possible to conduct flow experiments directly on the 3D reconstructed sample. Many authors have reported good agreement with experimentally obtained values when solving the Stokes equation for single phase flow using finite difference methods (see [1, 29]) or the Lattice-Boltzmann method [41]. The importance of reproducing long-range connectivity in any reconstruction technique is clearly evident from calculations of absolute permeability. Whereas object-based methods reproduce permeability values within a few percentage points, traditional Gaussian field techniques and simulated annealing typically under-predict permeability by about a factor of ten for low porosity systems that are close to the percolation threshold [29, 41]. For higher porosity systems, the statistical methods generally perform somewhat better at reproducing the local percolation probability [40], with permeability predicted within a factor of about five (see [47]).

Even single phase simulations conducted directly on the 3D reconstructed sample are computationally very expensive. A common way to model both single and multiphase flow quickly on large systems is to represent complex porous media by an equivalent network of pores and connecting throats. Absolute permeability has been successfully predicted, as already mentioned, by Bryant et al. [9] using this method. Another approach is to skip the 3D reconstruction process and estimate absolute permeability directly from the 2D thin sections. Lock et al. [38] computed a distribution of fluid conductance's by recoding pore areas and perimeter lengths. From this a single effective conductance was found using effective medium theory, resulting in a direct estimate of absolute permeability. This approach was applied to a number of sandstone thin sections with predicted absolute permeability's generally within a factor of 2 of the measured values.

For multiphase flow it is possible to use Lattice-Boltzmann techniques (see [11, 25]) to solve the transport equations on the 3D reconstructed sample. Being computationally very demanding, their use in multiphase flow problems is, however, limited to relatively small systems. As a consequence their applications are more tailored towards understanding the fundamental physics of flow in complex systems rather than for quantitative predictions.

A whole range of empirical or semi-empirical methods for predicting relative permeability have suggested over the last five decades (see [21]). One of the most widely used is found by combining the model by van Genuchten [70], relating effective wetting saturation to capillary pressure, with the model for relative permeability by Mualem [44]. Empirical fitting parameters are found by matching the van Genuchten model to experimental capillary pressure. These parameters are subsequently used for the relative permeability predictions. However, what most of these models have in common is that they are only applicable for strongly water-wet data, and many of them also rely on difficult to define parameters such as tortuosity exponents.

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