

Effective Physical Properties of Sandstones

J. Widjajakusuma¹ and R. Hilfer^{1,2}

¹*ICA-1, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart*

²*Institut für Physik, Universität Mainz, 55099 Mainz, Germany*

Abstract. In this paper we continue the investigation of the effective transport parameters of a digitized sample of Fontainebleau sandstone and three reconstruction models discussed previously in Biswal et. al., *Physica A* **273**, 452 (1999). The effective transport parameters are computed directly by solving the disordered Laplace equation via a finite-volume method. We find that the transport properties of two stochastic models differ significantly from the real sandstone. Moreover, the effective transport parameters are predicted by employing local porosity theory and various traditional mixing-laws (such as effective medium approximation or Maxwell-Garnet theory). The prediction of local porosity theory is in good agreement with the exact result.

Keywords: Porous materials, effective material parameters, self-consistent method, microstructure

1. Introduction

It is well-known that the overall mechanical and transport properties of porous materials depend strongly on the microstructure [1, 7–12, 19–22]. Because in general the exact microstructures of porous media are not known in detail, one often uses models for calculating the effective macroscopic properties. For detail see [1–3, 8–12] and references therein.

The objective of the present article is to continue the study of transport properties of digitized realistic porous media. Simultaneously, we are testing the validity of local porosity theory (LPT) [9, 11, 13]. Local porosity theory was employed successfully to distinguish the microstructures of various porous media [4, 13], and the mixing-law based on LPT was used to determine the effective transport parameters of porous media [12, 20, 22].

2. Effective transport parameters

For homogeneous and isotropic random media the effective parameter \bar{C} is defined through an ensemble average of the local constitutive

equation

$$\langle \mathbf{J}(\mathbf{r}) \rangle = -\bar{C} \langle \nabla U(\mathbf{r}) \rangle. \quad (1)$$

where $\mathbf{J}(\mathbf{r})$ is the local current and $\nabla U(\mathbf{r})$ is the local potential gradient. If one knows the exact microstructure of a porous medium, one can calculate $\mathbf{J}(\mathbf{r})$ and $\nabla U(\mathbf{r})$ numerically by solving the local continuity equation

$$\nabla \cdot \mathbf{J}(\mathbf{r}) = 0 \quad \mathbf{r} \in \mathbb{G} \quad (\mathbb{G} = \mathbb{P}, \mathbb{M}) \quad (2)$$

combined with the local constitutive equation

$$\mathbf{J}(\mathbf{r}) = -C(\mathbf{r}) \nabla U(\mathbf{r}) \quad (3)$$

and appropriate internal and external boundary conditions. In eq. (2) is $C(\mathbf{r}) = C_{\mathbb{P}} \chi_{\mathbb{P}}(\mathbf{r}) + C_{\mathbb{M}} \chi_{\mathbb{M}}(\mathbf{r})$, where $C_{\mathbb{P}}$ and $C_{\mathbb{M}}$ are material constants of pore space and matrix space, respectively. Eqs. (2) and (3) have been solved recently for a sample of Fontainebleau sandstone via finite-volume method [20, 22, 12]. After taking the average of $\mathbf{J}(\mathbf{r})$ and $\nabla U(\mathbf{r})$, and inserting the two averaged values in eq. (1) the effective conductivity \bar{C} can be directly obtained.

3. Local porosity theory

In practice, the exact microstructure of porous media is usually not known in detail. Therefore, only approximate effective transport parameters can be computed based on partial microgeometric knowledge, such as porosity, specific internal surface, connectedness or correlation lengths [9–13, 16, 20–22]. The partial microgeometric knowledge included into LPT is information about porosity and connectivity fluctuations of porous media in terms of *local porosity distribution* $\mu(\phi, L)$ and *local percolation probability* $\lambda(\phi, L)$. $\mu(\phi, L)$ is the probability density to find a local porosity ϕ within the cubic measurement cell of sidelength L and $\lambda(\phi, L)$ gives the fraction of percolating cells with prescribed local porosity ϕ .

The mixing-law based on local porosity theory reads [9, 11, 22]

$$\int_0^1 \mu(\phi, L) \left[\lambda(\phi, L) \frac{\bar{C}_{\mathbb{P}}(\phi) - \bar{C}_{\text{LPT}}}{\bar{C}_{\mathbb{P}}(\phi) + 2\bar{C}_{\text{LPT}}} + [1 - \lambda(\phi, L)] \frac{\bar{C}_{\mathbb{M}}(\phi) - \bar{C}_{\text{LPT}}}{\bar{C}_{\mathbb{M}}(\phi) + 2\bar{C}_{\text{LPT}}} \right] d\phi = 0, \quad (4)$$

where

$$\bar{C}_P = C_P \left(\frac{3C_M + 2\bar{\phi}(C_P - C_M)}{3C_P - \bar{\phi}(C_P - C_M)} \right) \quad (5)$$

$$\bar{C}_M = C_M \left(\frac{2C_M + C_P + 2\bar{\phi}(C_P - C_M)}{2C_M + C_P - \bar{\phi}(C_P - C_M)} \right). \quad (6)$$

The mixing-law based on LPT can be viewed as a generalization of the classical self-consistent approximation. In the limit $L \rightarrow 0$, Eq. (4) reduces to the classical effective medium approximation (EMA) [6]

$$\bar{\phi} \frac{C_P - C_{EMA}}{C_P + 2C_{EMA}} + (1 - \bar{\phi}) \frac{C_M - C_{EMA}}{C_M + 2C_{EMA}} = 0. \quad (7)$$

For $\mu(\phi, L) = \delta(\phi - \bar{\phi})$ and $\lambda(\phi, L) = 1$ we obtain the Maxwell-Garnett approximation with \mathbb{P} as the background phase (MGP)

$$\bar{C}_{MGP} = \bar{C}_P. \quad (8)$$

For $\mu(\phi, L) = \delta(\phi - \bar{\phi})$ and $\lambda(\phi, L) = 0$ Eq. (4) recovers the Maxwell-Garnett approximation with \mathbb{M} as background phase (MGM)

$$\bar{C}_{MGM} = \bar{C}_M. \quad (9)$$

For more detail see [11, 19].

4. Results and discussion

We apply now LPT to analyze quantitatively four different samples. The first sample is a digitized real Fontainebleau sandstone (EX), which is obtained by microtomographic imaging [3, 4]. The second sample is a diagenesis model (DM), which is obtained by imitating the natural sandstone-forming processes. As in the natural processes, the numerical modelling of DM is performed in three main steps: grain sedimentation, compaction and diagenesis described in detail in [2, 17]. The Gaussian field reconstruction model (GF) is generated in such a way that the two-point correlation function of this model is identical to a given reference correlation function by filtering Gaussian random variables. Here the reference correlation function is the correlation function of the real Fontainebleau sandstone G_{EX} . For further information see [1, 18]. The last model, denoted as SA, is reconstructed by employing a simulated annealing technique. This technique produces a configuration S_{SA} by minimizing the deviations between its correlation function G_{SA}

Table I. Overview of geometric properties of the Fontainebleau sandstone and its reconstruction models and their effective conductivity \bar{C} and standard deviation

	Samples			
	S_{EX}	S_{DM}	S_{GF}	S_{SA}
$\bar{\phi}$	0.1355	0.1356	0.1421	0.1354
\bar{C}	0.01880	0.01959	0.00234	0.00119
stand. dev.	± 0.00852	± 0.00942	± 0.00230	± 0.00234

and the reference correlation function G_{EX} . Besides the correlation function G another statistical property, which has to match with the reference statistical property, is porosity ϕ . The detailed description of the simulated annealing method can be found in [14, 23]. Note that we can choose other statistical properties, which should be equal to the prescribed reference properties, such as linear or spherical contact distributions [15].

We choose that the matrix space as nonconducting, i.e. $C_M = 0$, and pore space as conducting, i.e. $C_p = 1.0$ (dimensionless). The boundary conditions are chosen so that potential values were prescribed at two parallel faces of the cubic sample S (Dirichlet boundary condition), and the flux across the four remaining faces of S is set to zero (Neumann boundary condition).

The disorder average of fields $\langle \mathbf{J}(\mathbf{r}) \rangle$ and $\langle \nabla U(\mathbf{r}) \rangle$ are known to fluctuate strongly from one sample to another. To improve the statistics all of the samples were cut into eight pieces of dimension $128 \times 128 \times 128$. For each piece three values of \bar{C}_i were obtained from the exact solution corresponding to the application of the potential gradient in the x -, y - and z -direction. Then, the values of \bar{C} of samples are obtained by taking the arithmetic average of \bar{C}_i . The results are displayed in Table I. The standard deviations in Table I show that the fluctuations in \bar{C} are indeed rather strong. For ergodic geometries \bar{C} can be calculated directly from the exact solution for the full sample. For sample EX the exact transport coefficient for the full sample is $\bar{C}_x = 0.02046$ in the x -direction, $\bar{C}_y = 0.02193$ in the y -direction, and $\bar{C}_z = 0.01850$ in the z -direction [22]. All of these are seen to fall within one standard deviation of \bar{C} . The effective conductivity of the DM model matches quite closely to that of EX. The effective transport parameters \bar{C} of GF and SA differ strongly from \bar{C} of EX. This was already predicted in [4] on a pure connectivity analysis based on λ from LPT.

For LPT calculations we have to choose the sidelength L of the measurement cell \mathbb{K} . In the case of small L the local geometries become strongly correlated, and this is at variance with the basic assumption of weak or no correlations. On the other hand, for large L the assumption that the local geometry is sufficiently simple becomes invalid [11]. Hence, one expects that formula (4) will yield good results only for intermediate L . We use the so called percolation length L_p , which is defined through the condition

$$\left. \frac{d^2 p}{dL^2} \right|_{L=L_p} = 0 \quad (10)$$

assuming that it is unique. The idea behind this definition is that at the inflection point the function $p_3(L)$ changes most rapidly from its trivial value $p(0) = \bar{\phi}$ at small L to its equally trivial value $p(\infty) = 1$ at large L (assuming that the pore space percolates). For another choice of L see [11, 12, 20, 22]. At $L = L_p$ we find for the effective conductivity of EX the value $\bar{C}_{LPT} = 0.025115$ in good agreement with the exact result.

In contrast one has $C_{EMA} = 0$ for the effective medium approximation because the porosity $\bar{\phi}$ is below the percolation threshold $\bar{\phi}_c = 1/3$. Similarly, the result $\bar{C}_{MGM} = 0$ obtained by MGM-approximation underestimates the effective parameter \bar{C} of EX. On the other hand, $\bar{C}_{MGP} = 0.094606$ obtained from the MGP-approximation overestimates the exact result. These results reflect the nature of the approximations involved, because in both cases the inclusion phase is always dispersed in the background phase without having a connecting path. The functions μ and λ , which are used in LPT, provide more information about the underlying microgeometry than a single parameter $\bar{\phi}$, which are employed in the traditional mixing-laws (EMA, MGM, MGP). Therefore, the estimate of \bar{C}_{LPT} obtained by LPT seems to be better than those obtained by traditional mixing-laws.

Acknowledgements

We are deeply indebted to Dr. B. Biswal and C. Manwart for their close cooperation on many aspects of this work. We thank the Deutsche Forschungsgemeinschaft and the Graduiertenkolleg "Modellierung und Diskretisierungsmethoden für Kontinua und Strömungen" for financial support.

References

1. Adler, P. *Porous Media*. Boston: Butterworth-Heinemann, 1992.

2. Bakke, S. and Øren, P. 3-d pore-scale modeling of sandstones and flow simulations in pore networks. *SPE Journal*, **2**, 136, 1997.
3. Biswal, B., Manwart, C. and Hilfer, R. Three-dimensional local porosity analysis of porous media. *Physica A*, **225**, 221, 1998.
4. Biswal, B., Manwart, C., Hilfer, R., Bakke, S. and Øren, P. Quantitative analysis of experimental and synthetic microstructures for sedimentary rock. *Physica A*, **273**, 452, 1999.
5. Boger, F., Feder, J., Jøssang, T. and Hilfer, R. Microstructural sensitivity of local porosity distributions. *Physica A*, **187**, 55, 1992.
6. Bruggeman, D. A. G. Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen. I. Dielektrizitätskonstanten und Leitfähigkeiten der Mischkörper aus isotropen Substanzen. *Ann. Phys.*, **24**, 636, 1935.
7. Ehlers, W. Poröse Medien - ein kontinuummechanisches Modell auf der Basis der Mischungstheorie. Habilitationsschrift. Forschungsberichte aus dem Fachbereich Bauwesen der Universität-GH-Essen, Vol. 47, Essen, 1989.
8. Ehlers, W. Grundlegende Konzepte in der Theorie poröser Medien. *Technische Mechanik*, **16**, 63-76, 1996.
9. Hilfer, R. Geometric and dielectric characterization of porous media. *Phys. Rev. B*, **44**, 60, 1991.
10. Hilfer, R. Local porosity theory for electrical and hydrodynamical transport through porous media. *Physica A*, **194**, 406, 1993.
11. Hilfer, R. Transport and relaxation phenomena in porous media. *Adv. in Chem. Phys.*, **XCII**, 299, 1996.
12. Hilfer, R., Widjajakusuma, J. and Biswal, B. Dielectric relaxation in water saturated sedimentary rocks. *Granular Matter*, in print, 1999.
13. Hilfer, R. Local porosity theory and stochastic reconstruction for porous media. *in preparation*, 2000.
14. Manwart, C. and Hilfer, R. Reconstruction of random media using Monte Carlo methods. *Phys. Rev. E*, **59**, 5596, 1999.
15. Manwart, C., Torquato, S. and Hilfer, R. Stochastic reconstruction of sandstones. *preprint*, 1999.
16. Manwart, C., Widjajakusuma, J., Hilfer, R. and Ohser, J. Local specific surface distribution of sandstones. *in preparation*, 2000.
17. Øren, P., Bakke, S. and Arntzen, O. Extending predictive capabilities to network models. *SPE Journal*, p. SPE 38880, 1998.
18. Quiblier, J. A new three dimensional modeling technique for studying porous media. *J. Colloid Interface Sci.*, **98**, 84, 1984.
19. Sheng, P. *Introduction to Wave Scattering, Localization, and Mesoscopic Phenomena*. San Diego: Academic Press, 1995.
20. Widjajakusuma, J. Biswal, B. and Hilfer, R. Quantitative prediction of effective material properties of heterogeneous media. *Computational Materials Science*, **16**, 70, 1999.
21. Widjajakusuma, J., Manwart, C., Biswal, B. and Hilfer, R. Exact and approximate calculations for the Conductivity of Sandstones. *Physica A*, **270**, 325, 1999.
22. Widjajakusuma, J., Biswal, B. and Hilfer, R. Predicting transport parameters of heterogeneous media. *Preprint*, 1999.
23. Yeong, C. and Torquato, S. Reconstructing random media. *Phys. Rev. E*, **57**, 495, 1998.