Derivation of dispersion coefficients in large random arrays of spheres and cylinders

A. Jourak⁵, V. Frishfelds⁶, J.G.I. Hellström⁵ and T.S. Lundström⁵

Direct pore-scale computations of longitudinal and transversal dispersion coefficients in random two-dimensional (2D) and three-dimensional (3D) porous systems consisting of up to $2 \times 10^4$ solid particles (spheres or cylinders) are performed. The system is divided into different-sized particles using modified Voronoi diagrams so that none of the Voronoi surfaces cross the particles. The relationship between the variation of the stream function and averaged vorticity is obtained by sampling local configurations of particles to CFD data. Then the whole flow pattern is obtained minimizing the dissipation rate of energy¹. The configuration of particles is obtained by a large number of random dispositions of particles until a homogeneous random structure is acquired.

Longitudinal dispersion coefficient is calculated by fitting the solution of one-dimensional advection-dispersion equation to the resulting effluent curve. Transversal dispersion coefficient is derived by calculating the extension of concentration from a wall with fixed concentration parallel to main flow field, see Fig. 1. It was found that the 2D system requires substantially more particles to obtain consistent results than the 3D system. Also the transverse dispersion is more pronounced for the system of cylinders².

The results are compared with numerous experimental 3D data with almost perfect fit. However, there is a lack of 2D experimental data for the system of cylinders.

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² Jourak et al., *AIChE* (in review).

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Figure 1: (a) Longitudinal dispersion in a system of spheres. (b) Transverse dispersion in a system of cylinders.