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Improved stochastic pore network generation algorithms for porous media

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Pore-scale modeling and simulation are widely applied to investigate transport phenomena in porous media. Because the applicability of direct methods, like lattice Boltzmann and particle-based methods, remains restricted due to their high computational cost, pore network modeling (PNM) has emerged as one of the most efficient and effective approaches for practical applications. However, the direct extraction of a full pore network (PN) from 3D pore structure images is often infeasible for materials with wider pore size distributions, owing to the inherent conflict between image resolution and field of view. Therefore, achieving representative and reliable PNs often necessitates both scale-extension (expanding small actual networks to large virtual networks) and scale-integration (merging multiple single-scale PNs as extracted from single 3D images).

Given the stochastic nature of pore structures in porous media, scale-extension and scale-integration are typically accomplished through stochastic PN generation. After extracting the template PN from a 3D image, its geometrical and topological features are translated into statistical information, which is then used to generate the desired PN at arbitrary size. The generated PN is statistically equivalent to the extracted PN, by retaining its key geometric and topologic characteristics. In this study, three existing geometry replica algorithms (G_1 to G_3) from the literature are implemented, along with the proposed improved G_4. G_4 targets the porosity-weighted pore radius distribution and also employs stratified random sampling to determine geometric PN parameters. These parameters are obtained through a Gaussian multivariate copula that integrates marginal probability distributions with joint correlations. Additionally, two improved topology replica algorithms T_1 and T_2 are put forward. T1 uses a quasi-random low-discrepancy Sobol sequence to determine the location of the pore bodies, while T2 examines the ranges of neighboring pores considered for pore body connection.

These stochastic algorithms are evaluated by comparing simulated unsaturated hygric properties of generated PNs with those of the extracted PNs. Ten PNs are generated for each algorithm to ensure robust results, and a PN-based hygric property simulator is employed to attain the moisture retention and permeability curves, as storage and transport property respectively. The resulting curves are first assessed visually for qualitative comparison, which is followed up by a quantitative evaluation using four deviation indices. To demonstrate the exhaustive effectiveness and adaptability of the improved algorithms, PNs from four porous materials, with varying degrees of complexity, are applied: Ketton carbonate, sintered glass, Berea sandstone and ceramic brick.

The results reveal that the combination of G_4 and T_2.3 –where the number of neighboring pores considered for connections is five times the maximal coordination number of the extracted PN –highly enhances the reliability of the generated PNs. Compared to the basic geometry and topology replica algorithms, the deviation indices are relatively reduced by an average of 67% to 98%. These improved stochastic algorithms for single-scale PNs also pave the way for generating full-scale PNs of porous materials with exceptionally wide pore size ranges. Future research can build on these algorithms to generate such full-scale PNs using multiple 3D image sets with different resolutions.

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