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Beyond Kozeny Carman - calculating hydrodynamic parameters with a two-scale approach

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An accurate quantitative description of the permeability and diffusion coefficient in a porous medium is essential for predictive transport modeling. Well-established relations such as the Kozeny-Carman equation and relations proposed by Buckingham, Penman, or Millington-Quirk, relate the scalar permeability and diffusion coefficient to the porous medium's porosity, respectively. To capture the porous medium's structure in more detail, further models include fitting parameters, geometric, or shape factors. Some models additionally account for the tortuosity, e.g. via Archie's law. A validation of such models has been carried out mainly via experiments relating the proposed description to a specific class of porous media (by means of parameter fitting).
Contrary to these approaches, upscaling methods directly enable calculating the full, potentially anisotropic permeability and effective diffusion tensor without any fitting parameters. As input only the geometric information in terms of a representative elementary volume is needed. To compute the permeability and diffusion-porosity relations, supplementary cell problems must be solved numerically for this volume and their (flux) solutions must be integrated. We apply this approach to provide easy to use quantitative relations that are based on representative single grain, platy, blocky, prismatic soil structures, porous networks, or random porous media. As a discretization method we use the Discontinuous Galerkin method on structured grids. To make the relations explicit, interpolation of the obtained data is used.
We furthermore compare the relations obtained with the well-established relations mentioned above and also with the well-known Voigt-Reiss or Hashin-Shtrikman bounds. We discuss the ranges of validity and comment on the role of tortuosity - porosity relations.