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Upscaling of the specific surface area for reactive transport modelling in fractured rock

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The impact of flow heterogeneity on chemical transport from single to multiple fractures, is investigated. The emphasis is on the dynamic nature of the specific surface area (SSA) due to heterogeneity of the flow, relative to a purely geometrical definition. It is shown how to account for SSA as a random variable in modelling multi-component reactions. The flow-dependent SSA is interpreted probabilistically, following inert tracer particles along individual fractures. Upscaling to a fracture network is proposed as a time-domain random walk based on the statistics of SSA for single fractures. Statistics of SSA are investigated for three correlation structures of transmissivity, one classical multi-gaussian, and two non-Gaussian. The coefficient of variation of single fracture SSA decreases monotonously with the distance over the fracture length; the CV of the upscaled SSA reduces further such that after ca 20 fractures it is under 0.1 for a disconnected field, and around 0.2 for connected and multi-gaussian fields. This implies that after 10-20 fractures, uncertainty in SSA is significantly reduced, justifying the use of an effective value. A conservative, lower bound for the dimensionless upscaled effective SSA was found to be 1, suitable for all heterogeneity structures, assuming the cubic hydraulic law applicable.