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Investigating the effects of initial concentration and population distribution on the transport of aggregating nanoparticles in porous media

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In order to investigate the migration of nanoparticles in porous media, the model developed by Katzourakis and Chrysikopoulos (2021) is applied to simulate the transport of aggregating nanoparticles under various initial conditions. In the aforementioned model, nanoparticles may collide with each other and form larger particle structures with different mobility and reactivity characteristics. Individual particles as well as aggregates can be found suspended in aqueous phase or attached, reversibly and/or irreversibly, on the solid matrix. The aggregation process modelled after the Smoluchowski population balanced equation (PBE), is coupled with the conventional advection-dispersion-attachment (ADA) equation to form a system of coupled equations that govern the transport of aggregating nanoparticles. Particle collisions are expected to increase exponentially with increasing initial number of injected particles (N_0). Therefore, substantially pronounced aggregation is expected when N_0 is increased. Similarly, the initial particle diameter distribution of the injected particles is expected to affect the average size of aggregates and in turn influence their mobility in a porous medium. Several model simulations were performed with different N_0 and particle diameter distributions. The results indicated the strong importance of taking into account the initial particle concentration and realistic particle diameter population distribution into consideration.