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BOOK OF ABSTRACTS

Transport models for risk assessment of natural and engineered nanoparticles in groundwater

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Nanosized particles of several materials, such as TiO_2, graphene, zero-valent iron, iron oxides, carbon nano-tubes, etc., are commonly used in industrial processes and for the manufacturing of commercial products. They can be released into the environment and, in particular, into groundwater throughout their entire life cycle, thus representing a potential risk for human health. Once released, nanoparticles can exhibit inherent toxicity, or play a role in enhancing the mobility of many contaminants, acting as a mobile solid phase which accelerates the transport of strongly sorbing contaminants (colloid-facilitated contaminant transport). It is therefore extremely important to develop approaches and tools suitable to predict the long-term fate of these emerging contaminants and the associated potential risk.

The quantification of the toxic and carcinogenic risk towards potential receptors requires the application of transport models for the evaluation of the nanoparticle concentration at the exposition point, C(poe). Nanoparticle transport in porous media is usually described by a modified advection-dispersion equation that takes into account the mass exchanges between liquid and solid phase due to physical and physico-chemical interactions. According to the degree of detail of the risk assessment procedure, C(poe) can be calculated via analytical formulations, Tier 2, or numerical tools, Tier 3.

In this work, NP-specific transport models are simplified and adapted to the analytical solutions commonly adopted in the conventional Tier 2 RBCA approach. The analytical solutions commonly used for the calculation of dissolved contaminant C(poe), are here extended to account for particle-porous-medium interaction. Moreover, the numerical tool MNM3D is proposed for the simulation of nanoparticle transport applied to Tier 3 risk assessment. MNM3D is a modified version of the well-known RT3D code, which implements numerical solutions to the NP transport equations porous media, accounting for the dependency of the attachment and detachment kinetic coefficients on transients in pore water ionic strength and velocity.

The analytical solutions and the numerical code MNM3D are here both applied to a synthetic case of release of silver nanoparticles and the results are compared. Finally the same release in a more complex hydrogeological scenario is simulated using the MNM3D code to highlight the effects of hydrochemical heterogeneities on the long term fate of nanoparticles in the environment.

References

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