Postdoc position: numerical modeling of nanoparticle transport and deposition in porous media

Work environment, missions and activities:
You will be hosted at the "Mediterranean Environment and Modeling of Agro-Hydrosystems" (EMMAH), a joint research unit of INRAE and Avignon University located in Avignon, France.

The position is part of the project "Comprehensive Modelling of Nanoparticles Fate in Soils" (COMMON) funded by the French National Research Agency (ANR). It is led by Gustave Eiffel University, (Nantes), and gathers researchers from the ISCR (Rennes Institute of Chemical Sciences), the CEISAM (Interdisciplinary Chemistry: Synthesis, Analysis, Modelling, Nantes) and EMMAH.

The aim of the project is to develop a generic modeling framework to predict the mobility of nanoparticles (NPs) in soils with the ambition to go further than previous modeling approaches as e.g. the colloid filtration theory. To this end, the project combines transport experiments, at the column scale, in porous media of increasing complexity (sand, sand coated with goethite or humic acids) with state-of-the-art techniques to:

(i) determine not only the NP concentration in the column effluents but also their size distribution using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS),
(ii) provide molecular-level information on the interactions of NPs with environmental molecules and surfaces using nuclear magnetic resonance (NMR),
(iii) observe and quantify the transport and adsorption of NPs directly inside the porous media using time-resolved magnetic resonance imaging (MRI) and use these data to test the NP transport models to their very limits.

The columns experiments are being performed by two PhD student involved in the project (Nantes, Rennes). You will contribute to the project by **developing mechanistic models of transfer and deposition of NPs in the porous media of increasing complexity considered by the students.** You will **test these models** by comparing their outputs with the experimental data they gathered, in particular the MRI data, building on the approach developed by Lehoux et al., (2017).

The modeling work will be carried out in the Vsoil modeling platform developed by INRAE at EMMAH. It facilitates the implementation, coupling, use and sharing of numerical models representing physical, chemical and biological processes taking place in a soil profile. A number of modules representing matrix and macropore water transfer (Richards equation and kinematic wave models respectively), solute and colloid transfer (advection dispersion equation (ADE), mobile immobile model (MIM)) are available by default in the platform and will serve as the basis for the models you will build.

Depending on the experimental conditions—ionic strength, pH and concentration of the suspension, size and stabilization mechanisms of the NPs, characteristics of the sand surfaces—we expect different mechanisms of nanoparticles deposition onto the bare or coated sand surfaces. These include: deposition in the first and/or secondary minimum of the interaction potential, deposition of a monolayer (blocking) or of several layers (ripening) depending on the particle-particle interaction potential, homo-aggregation in solution that may lead to straining in the pore throats, diffusion through immobile zones of water—e.g., formed by clay aggregates or humic acids sorbed to the sand—before reaching the deposition sites. You will construct the model to consider these possibilities by modifying the modules already present in Vsoil.

Training and skills: You must hold a PhD in physics of colloidal systems or in transfer in porous media and must have skills in modeling including the ability to understand and make minor changes to the computer codes (Fortran, C++) and to use model-exploration tools (sensitivity analysis, parameter estimation). Previous experience with geochemistry would be a plus. The position requires good communications skills (interactions with the PhD students involved in the experimental work and their advisors). The working language is English : fluency is required, both spoken and written. Strong analytical and writing skills are a must.

Application process: To apply, email Eric Michel (eric.michel@inrae.fr) and Denis Courtier-Murias (denis.courtier-murias@univ-eiffel.fr). Applications should include a detailed résumé, a cover letter explaining your suitability for the position and contact information for referees.

Offer overview: 20-months fixed term contract, starting between January and March 2027. Gross salary starting from 3100€/month depending on previous experience.