JOB PROFILE

CNRS post-Doctoral Researcher in transport in porous media

PROJECT TITLE:

NUMERICAL INVESTIGATION OF THE FACTORS DRIVING ATTENUATION KINETICS OF NON-AQUEOUS-PHASE LIQUID (NAPL) SOURCE

DESCRIPTION

Petroleum hydrocarbons represent the most important contamination source of soils (37.22%). Light non-aqueous phase liquid (LNAPL) contaminants infiltrate through the unsaturated zone of the soil and migrate to the top of the aquifer before accumulating above it, forming a pure phase. The mechanism of transfer of pollution from soil to groundwater (through dissolution) is generally described by "local non-equilibrium" models (i.e. the concentrations measured in the groundwater are far from the thermodynamic equilibrium concentrations) governed by one (or more) mass transfer coefficients. The transient behavior of this parameter, which can be different for each of the constituents, remains very little studied (Brahma & Harmon, 2003; Shafieiyoun & Thomson, 2018) and is usually replaced by a constant and unique value (Soulaine et al., 2011). The variability in the relative solubility of the different constituents leads to a complex evolution of the composition of the dissolved pollution plume over time (Vasudevan et al., 2016). The overall objective of this work is to evaluate the factors influencing the mitigation of pollution sources through an evaluation of the impact of source composition and the presence of heterogeneities on the mass transfer models.

In a first step, we will investigate the case of multi-components pollutant sources. In order to clarify these phenomena and, in particular, the characteristic times associated with the mass exchange coefficients, we propose, starting from a NAPL phase with 2 then 3 components for which the diffusion within the NAPL phase is limiting, to study the evolution of the dissolution fluxes over time in order to characterize the variability of the mass transfer coefficients and hence, to evaluate the uncertainty around these parameters. The single-component case will be considered as reference solution. For this purpose, 2D and 3D simulations of pore-scale dissolution of NAPL on typical architectures of phase distribution (simple enough to allow a reasonable numerical approach: e.g., granular medium, periodic geometry of the soil porous matrix, presence of NAPL in the form of singletons or doublets) will be performed. We will assume that the solubility of each of the components is governed by Raoult's law so that the solubilities will evolve in a complex and coupled manner as a function of the molar fractions of the considered species, which are themselves time-dependent. The dissolved concentration fluxes for each of the organic components and their evolution over time will be calculated from these simulations in order to determine the evolution of the exchange coefficients and to link these behaviors to the hydrodynamic conditions (saturation, solubility, velocity) and to the geometry of the medium and the phase distribution.

In a second step, 3D macroscopic simulations of NAPL dissolution in heterogeneous media will be carried out by varying the operating conditions (i.e., Péclet and Damköhler numbers, the dimensionless numbers describing the preponderance of the attenuation mechanisms relative to each other). The configurations considered will range from stratified two-layer media to spatially correlated random media, more representative of the complexity of a real environment. Starting

from the equations describing the transport and dissolution of the organic phase at the Darcy scale, we will derive 1D macroscopic upscaled models using the volume averaging method (Ahmadi et al., 2001; Bahar et al., 2016). The evolution curves of dissolved contaminants predicted by the direct simulations will then be compared with the results from the 1D macroscopic model. The ultimate objective will be to study the different possible dissolution regimes as a function of hydrodynamic and reaction conditions and to propose typical attenuation models. A diagram identifying the different dissolution regimes and the associated models will then be proposed. We will first start from the single-constituent case before looking at the multi-components conditions using the mass transfer coefficients calculated previously.

SELECTION CRITERIA

The applicant must hold a PhD degree in fluid or computational mechanics, applied mathematics, reservoir engineering, hydrogeology or other relevant fields with, ideally, a strong track record on:

- *Scientific skills*: Expertise in flow and transport processes in porous media with a strong interest for numerical modelling is required. He or she may demonstrate fundamental knowledge of upscaling methods such as the volume averaging method. An experience in using commercial simulation software such as Comsol Multiphysics would be highly appreciated.
- *Communication skills*: Very good ability to write and transcribe results in English, autonomy in writing scientific articles, excellent written and oral communication skills, good aptitude and motivation for teamwork.

TERMS AND TENURE

This full time 12-months position will be funded by ADEME (GESIPOL call, QUASPER project). It will be located at **GeoRessources** laboratory of the **Université de Lorraine and CNRS in Nancy, France**. GeoRessources is a multi-disciplinary laboratory devoted to the study of geological resources, their exploration and exploitation, as well as their impact on society and the environment. The target start date for the position is March 2021**,** with some flexibility on the exact start date. The gross salary, will be around 2625€/month (net salary: 2150€) including social benefits and heath care. Travel expenses for conference participations are secured.

The successful applicant will be directly supervised by Dr. Fabrice Golfier (fabrice.golfier@univ-lorraine.fr) in collaboration with Dr. Anne Julie Tinet (anne-julie.tinet@univ-lorraine.fr), Dr. Constantin Oltéan (constantin.oltean@univ-lorraine.fr,) and Dr. Michel Quintard (michel.quintard@imft.fr, IMFT Toulouse) and will collaborate with the other partners of the project.

HOW TO APPLY

Applicants are requested to submit the following materials:

- A cover letter applying for the position
- Full CV and list of publications
- Two selected publications
- The names and contact information of two referees

Deadline for application is **15th December 2020**. Applicants will be interviewed by an ad hoc commission. Applications are only accepted through email.

REFERENCES

Ahmadi, A., Aigueperse A., Quintard M., 2001. Calculation of the effective properties describing active dispersion in porous media : from simple to complex unit cells. Advances in Water Resources 24, 423-438.

Bahar T.B., Golfier F., Oltéan C., Benioug M. 2016, An upscaled model for bio-enhanced NAPL Dissolution in porous media, Transport in Porous Media, 113(3) (2016) 653-693

Brahma P.P. Harmon T.C. 2003. The effect of multicomponent diffusion on NAPL dissolution from spherical ternary mixtures, Journal of Contaminant Hydrology, 67 (2003) 43-60.

Shafieiyoun S., Thomson N.R., 2018. The role of intra-NAPL diffusion on mass transfer from MGP residuals. Journal of Contaminant Hydrology 213 (2018) 49–61.

Soulaine C., Debenest G., Quintard M., 2011. Upscaling multi-component two-phase flow in porous media with partitioning coefficient. Chem Eng Sci 66 (2011) 6180–6192.

Vasudevan M., Johnston C.D., Bastow T.P., Lekmine G., Rayner J.L., Nambi I.M., Suresh Kumar G., Ravi Krishna R., Davis G.B., 2016, Effect of compositional heterogeneity on dissolution of non-ideal LNAPL mixtures, Journal of Contaminant Hydrology, 194(2016):10-16.