UNIVERSITÉ de POITIERS
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APPEL A CANDIDATURE

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CONTRAT : **01/11/2019 au 31/10/2020** Date limite de dépôt des candidatures : **01/10/2019 à 12h**	**Dénomination du poste** **E1E45 – Expert-e en calcul scientifique** **(Poste de catégorie A)**

Mission:

The postdoctoral intership is funded by the action 2 « Dynamique des contaminants » in the axis 3 « Chimie verte et préservation des ressources (eau, sol, biodiversité, carbone renouvelable) » of the ECONAT programme « gestion durable des ECOsystèmes et des ressources NATurelles » (CPER 2015 – 2020). One objective of the action 2 is to study the transport behavior of contaminants in fractured limestone structures of the catchment area of Charente. In this action 2, we propose to develop numerical models, based on the Monte Carlo approach, for estimating the maximum dilution index Emax in heterogeneous porous and fractured media.

Place of work:

He (or she) will be part of the HYDEE team (HYdrodynamique et Ecoulements Environnementaux) in the Fluids Thermal and Combustion department of the Institute Pprime, in the H2 building at the Futuroscope site (Postal address: Institut Pprime, CNRS – Université de Poitiers – ENSMA, SP2MI – Téléport 2, boulevard Marie et Pierre Curie, BP 30179, F86962 Futuroscopoe Chasseneuil Cedex). To carry out his (or her) mission successfully, the agent will be able to rely on the IT department (IT and scientific calculation unit) of the UP SP2MI site.

Context:

Studying the transport behavior of inert solutes through heterogeneous geological formations is important for many environmental and hydrogeological problems such as enhanced oil recovery, geothermal energy development, remediation of contaminated groundwater, and carbonate storage [Nowamooz *et al.*, 2013; Wang *et al.*, 2014]. During the transport of inert solutes in these same geological formations, two main mechanisms are involved: advection and molecular diffusion. These two basic mechanisms combine into dispersion. They are responsible for the mixing of inert solutes, combination of spreading and dilution that changes the size of inert solute clouds and the water volume occupied by the inert solutes [Dentz *et al.*, 2011; Herrera *et al.*, 2017].

This physical process can be quantified by the dilution index *E*, introduced by Kitanidis in 1994. In the past, it has been shown that the maximum dilution index *Emax* increases monotonically in steady Darcy flows through isotropic heterogeneous porous media [Kitanidis, 1994; Thierrin and Kitanidis, 1994]. Recent numerical simulations, based on the Monte Carlo approach, have allowed us to establish the relationship between the slope *a* of maximum dilution index *Emax* and the averaged positive second invariant *Qav* of deformation tensor ∇u [Beaudoin *et al.*, 2019]. The work proposed in this post doctoral internship, constitutes a development of these works.

<u>Work proposal:</u>

The first work of the young researcher is to complete the work by Beaudoin *et al.* on the estimation of the maximum dilution index *Emax* in steady Darcy flows through heterogeneous porous media [Beaudoin *et al.*, 2019]. The parameter study, performed by Beaudoin *et al.*, is incomplete. The young researcher will analyze the effect of pore scale dispersion on the maximum dilution index *Emax* from new 2D and 3D Monte Carlo numerical simulations. In the actual version of the numerical model, an exponential correlation function is used to characterize the log-normal distribution of the hydraulic conductivity. Other existing correlation functions will be implemented in the numerical model [Hsu, 2000; Gomez-Hernandez and Wen, 2018]. This will allow to study the effect of the nature of the hydraulic conductivity on the maximum dilution index Emax, always in steady Darcy flows through heterogeneous porous media.

The second work of the young researcher is to modify the actual version of the numerical model in order to simulate the flow of water and the transport of inert solutes through one single fracture. Two modifications will be made in the actual version of the numerical model. The first modification consists in setting up the flow simulation in the plane of the fracture as in the works by Plouraboue *et al.* (1998) or Zhang and Huan (2018). The Reynolds approximation will be applied to solve the flow. The aperture gradient will be assumed to be small enough in order to consider the flow in the fracture as a Poiseuille flow. Thus, the flow problem can be considered as 2D with the estimation of an aperture-averaged velocity field from the incompressibility condition and the Darcy law, with an hydraulic conductivity proportional to the aperture of the fracture. The generation of the fracture will be based on the work by Mourzenko *et al.* (1996 and 2016). The fracture will be bounded by two uncorrelated rough surfaces. The aperture of the fracture will be given by estimating the mean distance between the two surfaces. The roughness of each surface will be characterized by a random fluctuation with Gaussian or self-affine spatial auto-correlation function. The second modification consists in setting up the transport of inert particles in the plane of the fracture with a new trackering method allowing to take into account the Taylor-Aris dispersion without performing 3D numerical simulations. The difficulty is then to consider the deformation of particles induced by the velocity variations in the direction perpendicular to the plan of the fracture (Wang *et al.*, 2012; Wu *et al.*, 2017). The solution is to use the notion of moments. The moments make it possible to follow the form of particles during their transport in the fracture. The new numerical model will allow us to study the effect of the fracture aperture distribution on the transport of inert solutes (Stoff *et al.*, 2019).

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- P.A. Herrera, J.M. Cortinez and A.J. Valocchi, Lagrangian scheme to model subgrid scale mixing and spreading in heterogeneous porous media, Water Resources Research, 53 (2017), 3302–3318.
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- J. Thierrin and P.K. Kitanidis, Solute dilution at the Borden and Cape Cod groundwater tracer tests, Water Resources Research, 30 (1994), 2883–2890.
- Beaudoin, A. Dartois and S. Huberson, Analysis of the influence of averaged positive second invariant *Qav* of deformation tensor ∇u on the maximum dilution index *Emax* in steady Darcy flows through heterogeneous porous media, Advances in Water Resources, in press (2019).
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- K.C. Hsu, General first order expressions for solute transport in two and three dimensional randomly heterogeneous porous media, Geological Society of America, Special paper, 348 (2000).
- J.J. Gomez-Hernandez and X.H. Wen, To be or not to be multi-Gaussian ? A reflection on stochastic hydrogeology, Advances in Water Resources, 21 (2018), 47-61.
- F. Plouraboue, J.P. Hulin, S. Roux and J. Koplik, Numerical study of geometrical dispersion in self-affine rough fractures, Physical Review E, 58 (1998), 3334–3346.
- Y. Zhang and N. Huan, Numerical study on the shear-flow behavior and transport process in rough rock fractures, Compte Rendu Mecanique, 346 (2018), 877–886.
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- V.V. Mourzenko, J.F. Thovert and P.M. Adler, Conductivity and Transmissivity of a Single Fracture, Transport in Porous Media, 112 (2016).
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- Y. Wu, Q. Liu, A. Chan and H. Liu, Implementation of a time-domain random walk method into a discrete element method to simulate nuclide transport in fractured rock masses, Geofluids, 17 (2017).
- M. Stoll, F.M Huber, M. Trumm, F. Enzmann, D. Meinel, A. Wenka, E. Schill, T. Schäfer, Experimental and numerical investigations on the effect of fracture geometry and fracture aperture distribution on flow and solute transport in natural fractures, Journal of Contaminant Hydrology, 221 (2019), 82–97.

Main activities:

- Understand the numerical methods solving the problem of water flow and mass transport in high heterogeneous, porous or fractured, media: i.e. be able to describe them to other people or in a report.
- Implement these numerical methods in numerical models: i.e. write in C++ of libraries parallelized under mpi.
- Install and run these numerical models on supercomputers.
- Perform a validation of numerical models: i.e. define the benchmarks and apply them.
- Perform a physical, theoretical and/or applied study to improve the understanding of water flow and mass transport in high heterogeneous, porous or fractured, media.
- Organize the database and its accessibility: the database will be made up of numerical results obtained during the two previous steps.

Expected skills:

- PhD in Computer Sciences.
- Background in Applied Mathematics and Hydrogeology.
- Developments done in C++ and MPI, using available tools and software libraries.
- Autonomy.
- Ability to work in team.
- Written and oral expression in English and French.