Title of the thesis: Study of mass transfers between fractures and the matrix containing them

Subject: The subject of this thesis is the understanding, modelling and numerical simulation of the transport of solutes, whether passive or reactive, in porous, permeable, heterogeneous and/or fractured media. The most immediate field of application is geological media, often with environmental concerns (sensitivity to contaminants, pollution clean-up), but geothermal energy also falls into this category if the solute is heat.

One of the most decisive aspects, and one that is difficult to take into account in modelling, concerns mass transfers between zones of strongly contrasting properties, and in particular between fractures (which constitute the preferential paths) and the matrix (which contains most of the possible accumulation volume, and is the site of possible sorptions and/or reactions).

When numerical simulation is based on an Eulerian approach such as the finite difference method, numerical difficulties may arise in taking into account rapid transient diffusive exchanges between matrix and fracture. One solution is to use a Lagrangian approach such as the particle method.

To test the particulate method, we will consider the case of a simple fracture with small variations in opening surrounded by a matrix in which there are only diffusive effects. The case of a simple fracture with a variable opening is particularly interesting, since changes in cross-section cause convective exchanges of solute between the fracture and the matrix. This effect has a strong impact (but different from the effect of diffusive exchange in the previous case) on macroscopic transport properties.

Initially, the numerical simulations will be carried out in 3D. They will provide numerical results for validating a reduced model made using the particle method. In the reduced model, only the fracture is represented by a surface with no thickness and with effective properties. This is the building block of DFN (Discrete Fracture Network) models used to represent a fractured medium on a global scale.

A method will be developed to take into account matrix diffusion at the fracture/matrix interface and Taylor Aris dispersion in the fracture. The hypothesis of modelling matrix diffusion at the fracture/matrix interface by a sorption mechanism will be studied. The Taylor Aris dispersion will be treated by modifying the particle method with the cutting method.

The reduced model constructed will be used to study diffusive exchanges between fracture and matrix. It will be possible to determine the time taken to establish the asymptotic regime, to formulate the homogenised model that then applies, and to determine its effective coefficients according to the parameters of the solute, the fracture and the matrix. The approach will also allow a complete description of the pre-asymptotic transient, starting from an arbitrary initial condition.

Keywords : Fractures, Solid matrix, Mass transfer, Taylor Aris dispersion, Particle method, Reduced model.

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