Dr. Lorenzo Fusi
Department of Mathematics "Ulisse Dini"
University of Florence, Italy
Viale Morgagni 67/a – 50134 Firenze

PROBLEM: Neutralization of acid wastewaters

The proposed problem concerns the process of neutralization of an acid solution by means of a reactant material. The main practical application is acid mine drainage remediation (AMD), i.e. the treatment of acidic streams from abandoned mines. The aim of the model is to give qualitative and quantitative information that can be useful in designing systems of reactive cartridges to be used for treating acid waste-water of mining plants.
The mathematical model must take into account the reaction kinetics (e.g. CaCO3 in HCl) and the evolution of the reacting surface, predicting how much time it takes to increase the pH of the solution of a fixed amount.
The problem can be set up by writing molar mass balance and the reaction kinetics, which in the case of CaCO3 and HCL can be safely considered of the first order. Through a proper adimensionalization of the system we observe that different temporal scales arise, accordingly to wether we are selecting the consumption, reaction of convective time scales.
Within the context of mixture theory the system can be modelled as a porous medium where the the main physical variables are the liquid/solid volume fractions and the concentration of ions [H+]. Due to the complexity of the problem we will assume that the flux is given (we do not conisder Darcy's law). The solid structure is modelled as if composed by solid spheres of different diameters. The assumption of a saturated porous media can be made if we assume that all the pores are filled by acid waters. The problem will be studied in cylindrical geometry (which is the one of some neutralizing cartridges) assuming that the main variables do not depend on the radial coordinates (1D setting).

Scheme of the work to be done

1) Introduction of the problem. Kinematic description, mass balance laws and reaction kinetics.
2) Scaling of the problem and simplifications.
3) Analysis of the approximated problems and numerical simulations
4) Discussion on possible extesions of the model (including diffusion, Darcy's effects etc)

Mathematical Background:

Partial differential equation, multi-scale models, asymptotic expansion.