



INTERNSHIP 2012

Lafarge Research Centre, research centre of Lafarge Group, world leader in construction materials present in 78 countries, is offering an internship within its laboratories.

«Company having signed an agreement in favour of employing disabled employees»

Topic

Coupled modeling of hydration of cement binders and durability of concrete – application to atmospheric carbonation

Details of the mission

Objective

The aim of the internship course is to validate a program that models the simultaneous phenomena of hydration, drying and durability of a wide range of cement-based materials. This **general modular model** analyzes coupled effects between mass transfer and chemical reactions in multiphase systems consisting of water, gas and minerals. The purpose of the internship is to **test** the different **numerical methods** used in FiPy, a python general solver for non-linear systems of partial differential equations. In particular the intern will compare a sequential iterative approach versus a fully coupled approach. For each approach, the intern will compare various time discretization schemes for the non-linear component diffusion matrix. Finally the intern will work on a method to analyze automatically the rate limiting step of the system. This method will be applied to the case of cement paste hydration, drying and carbonation.

Context

The **durability of concretes**, i.e. their capacity to withstand various aggressive environments, is key for long-lasting concrete structures. The expected service life of buildings and civil engineering structures ranges from several decades to more than a hundred years. Specific laboratory aging tests are available to estimate concrete durability but are generally time-consuming and costly. Modeling techniques can be used to complete or replace these laboratory tests in order to predict the potential durability of concretes

Motivation

The currently-developed models can describe the mineralogical alterations occurring in concretes due to their exposure to aggressive environments. Most of these models neglect some of the mechanism that may control the time space evolution of cement properties, such as gas advection, water vapor diffusion, and hydration reaction. These common assumptions prevent any **systematic analysis of competing mechanisms** and eventually the design of cement with optimized properties. Lafarge has



decided to tackle these issues by implementing a general and modular model for multi-phase, multi-component, multi-species system at variable pressure and temperature.

Skills & competencies

Strong interest for programming and numerical modelling. Strong abstract thinking capacities.

Core scientific knowledge:

- Non-linear algebraic equations, ordinary differential equations and partial differential equations
- Programming languages such as Fortran, C++ or Python
- Mass transfer in a porous medium (multiphase flow and ionic diffusion and gas diffusion),
- Thermodynamics of chemical equilibrium applied to inorganic systems composed of water, gas and minerals is a plus.

Education

Engineering, Master student.

Dates and length

6 months (starting February of March 2012)

Location

Lafarge Centre de Recherche, 95, rue du Montmurier, 38291 St-Quentin-Fallavier (France).
The site is located approximately 30 km East of Lyon city, with possible access by public transport.

Supervisor

Bruno HUET, Rémi BARBARULO

Send your CV and cover letter to rh.lcr@lafarge.com, indicating the reference **STAG-12-001**

