

## Numerical modelling of mixing in the flow through porous media

Conventionally, catalytic reactors contain catalytic pellets. Being convenient in production, catalytic pellets do not possess large surface area and exhibit few other unwanted properties. An EU FP7 project "Doped carbon nanostructures as metal-free catalysts" (FREECATS, http://cordis.europa.eu/projects/rcn/103070 en.html) is aimed at development of novel metal-free catalytic structures.

The silica carbide foams such as shown in the top photo will be covered with nano-fibres (SEM image) which in turn are doped with catalyst.

The aim of the current project is to model diffusion of a chemical when the fluid is being pumped through the foam. In particular, if a filament of a substance is entering the foam (top part of the figure below), it diffuses due to the flow splitting when passing through

the foam and exits as a set of wider time-delayed filaments (bottom part of the figure below). A model of randomised foam will be built using MATLAB and the filament diffusion will be described using random walk process. Simulation results will be compared with the experiment.



The project can be extended to a PhD programme on the modelling of catalytic reactions and heat transport in the system. The mini-project will be connected to Warwick Engineering work within the FREECATS project and the PhD will involve collaboration with Department of Chemical Engineering and Biotechnology, Cambridge.

More on the FREECATS project: http://www.alphagalileo.org/ViewItem.aspx?ItemId=11 9752&CultureCode=en http://www.scienceomega.com/article/375/eu-invests-4m-in-carbon-based-catalysis-research

Project supervisors:

Engineering: Petr Denissenko http://go.warwick.ac.uk/pdenissenko

Mathematics : Colm Connaughton http://www2.warwick.ac.uk/fac/sci/maths/people/staff /colm\_connaughton/