ΑΝΑΚΟΙΝΩΣΗ - ΠΡΟΣΚΛΗΣΗ

ΔΗΜΟΣΙΑ ΥΠΟΣΤΗΡΙΞΗ ΔΙΔΑΚΤΟΡΙΚΗΣ ΔΙΑΤΡΙΒΗΣ

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Προσκαλούμε τους μεταπτυχιακούς και προπτυχιακούς φοιτητές μας, τα μέλη Δ.Ε.Π., τους διδάσκοντες του Τμήματος και κάθε ενδιαφερόμενο, στη δημόσια υποστήριξη της Διδακτορικής Διατριβής του κ. Ανδρέα Τσιαντή με τίτλο:

«COMPUTATIONAL STUDY OF TRANSPORT PHENOMENA IN FLAKE FILLED COMPOSITE MATERIALS»

The aim of this thesis is to investigate how the effective diffusivity of flake filled polymeric membranes is altered by the presence and properties of flakes, such as their aspect ratio (α), volume fraction (φ), orientation (ϑ) and alignment relative to the direction of diffusion (ϑ + ε). We show that as a result of the dispersion of flakes in the polymeric matrix, materials with improved barrier properties are produced since the flake existence causes an increase in the distance travelled by the diffuse species through the membrane. This degree of difficulty is described by the Barrier Improvement Factor (*BIF*) and this coefficient is used to quantify the effect of the flake presence on the membrane barrier properties.

Besides the technological importance of this topic, an additional motivation for this investigation was the fact that the already proposed models have shown a small range of applicability and in general have limited success in providing a unifying framework for the description of the barrier properties of said materials. To address this issue we have carried out a comprehensive computational study and proposed and tested new theoretical models able to describe BIF for a range of flake concentrations and orientations.

The present thesis used 2D & 3D RVEs with periodic geometries and periodic boundary conditions that were created using a variety of computational tools including applications and algorithms that were written from scratch for the needs of this study. Subsequently with the created geometries we run simulations using the OpenFOAM toolbox in our laboratory cluster which was set up in the beginning of this thesis. With this combination of existing and new computational tools we managed to create a toolchain that enabled us to run thousands of simulations covering all the studied parameters in their full range and - in to our knowledge - the most comprehensive study in the literature so far. Also contrary to earlier studies the simulations were carried out in RVEs of realistic complexity, containing 1000's of individual flakes. We also check our results against the existing models described in the literature and we examine some common misconceptions and problems that exist in the field.