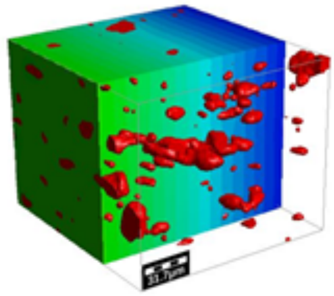
PHD POSITION

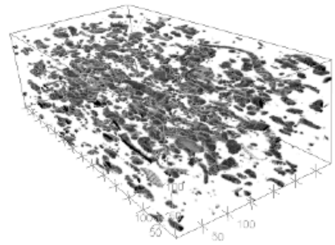
Contact: Sébastien GAUCEL
Valérie GUILLARD

Joint Research Unit : Agropolymers Engineering and Emerging Technologies

INRA, UMR 1208 IATE,
2 place Pierre Viala, Bât. 31
34000 Montpellier

Phone: 33 (0)4 99 61 21 51
E-mail: **sebastien.gaucel@inra.fr**
valerie.guillard@umontpellier.fr





Multi-scale modelling of mass transfer in bio-micro-composites.

For many years, environmental legislation, depletion of fossil resources as well as both industrial and consumer demand have led, in the field of food packaging, to the development of efficient solutions to produce new environmentally friendly materials, *i.e.* bio sourced and fully biodegradable in natural conditions. Biocomposites based on a biopolymer matrix and micrometric lignocellulosic fillers constitute an innovative and promising solution.

A reasoned design of food packaging materials based on a reverse engineering approach, requires the control of food degradation reactions. These reactions are strongly impacted by the moisture content and gas composition in the headspace and so rely on mass transfer phenomena, e.g. permeation of water vapour, O2 and CO2 between the atmosphere and the headspace.

The mathematical modelling of mass transfer is an inescapable tool in front of the diversity of the implied materials and the complexity of the food/packaging system. For that purpose, it is essential to represent and formalise the link between the structure and the mass transfer properties in a packaging material, which remains a bottleneck in the field of biocomposites.

The objective of the PhD is to bring new insights in the understanding of structure/mass transfer properties relationships in biocomposites, by focusing on the evaluation of pertinent quantitative structural parameters including the in situ (3D) filler dispersion state and the structure of the filler/matrix interphase, and on the study of their impact on mass transfer properties (gas and water vapour).

Recent advances allowed the characterisation of mass transfer at the scale of micrometric lignocellulosic particles (PhD V. Thoury). The next step, in charge of the applicant, will be the development of multi-scale mathematical models for predicting the influence of material structure on its mass transfer properties.

To achieve this goal, the 3D structure (obtained for example by TEM Tomo 3D) will be used as basis for numerical models of 3D mass transfers (using finite differences/volumes/elements methods). These models will allow testing hypotheses on the role of the interphase and will be confronted to experimental data. In parallel, simpler (3D or 2D) models will be developed, e.g. by approximating the geometry of the fillers (cylindrical shaped particles) in order to improve simulation speed and allow numerical exploration of a larger range of materials.

This PhD will benefit from H2020 GLOPACK project in which biocomposites materials will be developed and characterised.

Requirements

- ★ Good/excellent level of Master Degree or engineer in Applied Mathematics or Material Sc. or Process Engineering or other scientific domain with strong skills in numerical modelling.
- ★ Experience in MATLAB and COMSOL softwares will be a plus.
- ★ A scientific mind opened to applications, e.g. process/characterisation/use of bio-composites, will be welcome.
- ★ Demonstrated skills to effectively communicate in English and interact with other scientific partners.
- ★ Good ability to work within a team and be able of self-initiative.

Duration: 3 years. Expected starting date on 1st sept. 2018.

Location: Montpellier, south of France.

Net salary: about 1420 €/month.

Application deadline: Candidates must send their applications (cover letter and CV, list of publications if any and last academic marks report) **before June 15th 2018** to

sebastien.gaucel@inra.fr
valerie.guillard@umontpellier.fr