





PhD thesis offer (funded under an industrial agreement: thèse CIFRE) – click here to read this offer in PDF online Evaluation of functional barriers for the generalized use of recycled plastic materials for food contact

### **PLACES OF WORK**

<sup>1</sup>INRAe, Université Paris-Saclay, UMR 0782 SayFood «*Paris-Saclay Food and Bioproduct Engineering Research Unit* » (formerly UMR 1145 GENIAL) – AgroParisTech site de Massy, 1 rue des Olympiades, 91300 Massy, France.

<sup>2</sup>Centre technique Industriel de la Plasturgie et des Composites de Clermont Ferrand – Biopole Clermont-Limagne - 2 rue Michel Renaud - 63360 Saint Beauzire, France.

# WORK DESCRIPTION

**Context**. Context. European and national environmental protection policies have scheduled the phasing out of singleuse plastics, including for food use. Because plastic materials are widely used for non-sustainable applications such as packaging (36% of applications, with an average lifespan of 6 months), food packaging accounts for 50% of plastic waste. Reusing plastic materials for the same use is sensible, but it can only be considered for food contact within a stringent framework defined by Regulation (EC) No. 282/2008. The main hazard comes from secondary contamination of wastes and possible harmful practices before entering the recycling loop. The packaging may have been mixed with materials that are not suitable for food contact or diverted from its original purpose, for example, to clean paintbrushes. Currently, only recycled polyethylene terephthalate (rPET) is authorized for food contact by the European Food Safety Authority (EFSA). Other polymer matrices (polyolefins, polyamides and possibly polyvinyls) and other materials (paper and cardboard) could be authorized for direct contact with food if the absence of carcinogenic and reprotoxic molecules is demonstrated and if the risk of transfer of substances to food is below the acceptable thresholds previously defined by the EFSA. The risk of contamination of food (drinks, ready meals, etc.) by recycled materials can be reduced if a barrier layer, called functional, because not absolute, separates the recycled material from the food.

**Goal of the thesis**. The objective of the thesis is the characterization of the barrier properties to organic contaminants ( breakdown products of polymers and additives, solvents, pesticide substances...) of different types of organic (virgin polymer) or mineral (silica deposit or amorphous carbon) functional barriers that do not hinder the subsequent recycling of the material. The final objective is to develop a predictive approach to the risk of contamination that takes into account the history of the material and the food. The conclusions of this work will support the future evolution of European regulations. **Research hypotheses**. The concepts of permeability of polymers and vacuum deposits are well known for gases but insufficiently characterized for organic molecules. Two effects are sought: the diffusion barrier effect (delay of contamination) and the low chemical affinity for the layer in contact. In the case of thermoplastic polymers, semicrystalline polar polymers such as EVOH (ethylene vinyl alcohol) are the best candidates to reduce the transfer of hydrophobic aromatic and/or oligomeric substances. However, our previous works have shown that the selectivity of the functional barriers varied significantly between the processing conditions (melt) and the end-use conditions (semicrystalline rubbery or glassy), and was lost with the plasticizing action of the food moisture or during the thermal processing of food [1, 2]. The solubility barrier concept is also sensitive to local moisture and is highly dependent on the migrant [3]. Despite the apparent complexity of the coupling between heat and mass transfer [4, 5], diffusion and mutual sorption of several substances, all these phenomena can be described in 1D or 3D using the multiple approaches already developed by INRAe [6-8]. On the other hand, the effects of aging (physical or chemical) and the application to mineral barriers have been little studied in the literature.

**Proposed approach and methodology**. The thermodynamic properties of sorption (water, model organic solutes reproducing contaminants and food constituents), diffusion (binary or mutual) and their activation by temperature will be studied simultaneously using (i) devoted experiments (sorption and cosorption microbalance, diffusion and permeation cells) and (ii) molecular dynamics simulations (all-atom or coarse-grained) to ensure the extrapolation of results to a wide range of conditions and migrants. The complete approach will be integrated into the FMECAengine open source project (https://github.com/ovitrac/FMECAengine) and its extensions to allow rapid scaling of functional barriers with the conditions of use (possibly variable) of the considered recycled materials (plastics, cardboard, etc.). Experimental validation could be envisaged for some typical applications.

Keywords. polymer science, mass transfer, modeling, analytical chemistry, risk assessment, food safety

# **PROFILE & CONTACT**

**Profile sought.** General engineering degree or master 2 in process engineering, physical chemistry of polymers or physical chemistry. Skills in analytical chemistry, numerical analysis, modeling, and programming will be appreciated.

**Funding** : The PhD student will be enrolled (3 years contract) as an engineer by the Industrial Technical for Plastics and Composites (IPC) under the research CIFRE agreement (<u>https://www.enseignementsup-recherche.gouv.fr/cid22130/les-cifre.html</u>) between IPC et the French National Institute for Agriculture, Food et Environment (INRAE).

Contact. Please send a CV, cover letter, and a summary of previous research work.

- Olivier Vitrac, Researcher INRAe, Habilitation in Chemical Engineering, ORCID: 0000-0001-7787-5962, E-mail : <u>olivier.vitrac@agroparistech.fr</u>.
- Jacques Thébault, Director or IPC Clermont-Ferrand. E-mail : jacques.thebault@ct-ipc.com.

Doctoral School. ABIES (Université Paris-Saclay) - suggested disciplines

- Food processing sciences, sanitary security and risk, animal health and public health,
- Engineering sciences applied to living matter and the environment.

# **INDUSTRIAL PARTNER**

**Presentation of the industrial partner.** IPC (Centre Technique Industriel de la Plasturgie et des Composites) is a branch technical center under governmental supervision. It currently employs nearly 130 people on five sites in France. The Clermont-Ferrand site is dedicated to packaging, with two areas of development: safety in contact with materials and environmental impact. The proposed thesis is part of a multi-year development program entitled DIS30 (Intelligent and Safe Sustainable Plastics by 2030) supported by the Auvergne region, Rhône-Alpes. Website : <u>https://ct-ipc.com/</u>

**Collaborations.** The research work is part of a framework agreement with four laboratories and technical centers on the suitability of recycled materials for food contact: IPC, INRAe/AgroParisTech, the French national reference laboratory for metrology and testing (LNE, UMT SafeMat, Trappes, Dr. P.M. Nguyen), the technical center for the conservation of agricultural products (the CTCPA packaging laboratory, Bourg-en-Bresse, Dr. P. Dole).

### REFERENCES

[1] Fang X, Domenek S, Ducruet V, Refregiers M, Vitrac O. Diffusion of Aromatic Solutes in Aliphatic Polymers above Glass Transition Temperature. *Macromolecules*. 2013;**46**:874-88 <u>https://doi.org/10.1021/ma3022103</u>.

[2] Zhu Y, Welle F, Vitrac O. A blob model to parameterize polymer hole free volumes and solute diffusion. *Soft-Matter*. 2019;**15**:8912-32 <u>https://doi.org/10.1039/C9SM01556F</u>.

[3] Nguyen P-M, Guiga W, Dkhissi A, Vitrac O. Off-lattice Flory-Huggins approximations for the tailored calculation of activity coefficients of organic solutes in random and block copolymers. *Industrial & Engineering Chemistry Research*. 2017;**56**:774-87 <a href="https://doi.org/10.1021/acs.iecr.6b03683">https://doi.org/10.1021/acs.iecr.6b03683</a>.

[4] Dole P, Voulzatis Y, Vitrac O, Reynier A, Hankemeier T, Aucejo S, Feigenbaum A. Modelling of migration from multilayers and functional barriers: Estimation of parameters. *Food Additives and Contaminants*. 2006;**23**:1038-52 <u>https://doi.org/10.1080/02652030600658003</u>.

[5] Feigenbaum A, Dole P, Aucejo S, Dainelli D, Garcia CDC, Hankemeier T, N'Gono Y, Papaspyrides CD, Paseiro P, Pastorelli S, Pavlidou S, Pennarun PY, Saillard P, Vidal L, Vitrac O, Voulzatis Y. Functional barriers: Properties and evaluation. *Food Additives and Contaminants*. 2005;**22**:956-67 <u>https://doi.org/10.1080/02652030500227776</u>.

[6] Nguyen P-M, Goujon A, Sauvegrain P, Vitrac O. A Computer-Aided Methodology to Design Safe Food Packaging and Related Systems. *AIChE Journal*. 2013;**59**:1183-212 <u>https://doi.org/10.1002/aic.14056</u>.

[7] Vitrac O, Hayert M. Risk assessment of migration from packaging materials into foodstuffs. *AIChE Journal*. 2005;**51**:1080-95 <u>https://doi.org/10.1002/aic.10462</u>.

[8] Zhu Y, Guillemat B, Vitrac O. Rational Design of Packaging: Toward Safer and Ecodesigned Food Packaging Systems. *Frontiers in Chemistry*. 2019;**7** <u>https://doi.org/10.3389/fchem.2019.00349</u>.

