With industrial parternship

PhD Offer

Multiscale simulation of mechanical fracture and mixing in foods

Hosting Institution: University Paris-Saclay, INRAe, UMR 0782 Paris SayFood between INRAe and AgroParisTech (formerly UMR 1145 Food Processing and Engineering), group Modeling and Engineering through Calculations.

Address: (before moving to the new campus of Paris-Saclay): AgroParisTech - 1 rue des Olympiades - 91300 Massy, France

Contact: Dr. Olivier Vitrac, Researcher | E-mail: olivier.vitrac@agroparistech.fr | https://orcid.org/0000-0001-7787-5962 | Please send a CV and a motivation letter.

Summary: INRAe (French National Research Institute for Agriculture Food and Environment) is enrolling a Ph.D. student (3-year contract) to develop a simulation framework to describe the mechanics of rupture and dissolution across the scales in foods. This work is part of an important collaborative project (2 Ph.Ds) with the industry aiming to lay the foundations of a reverse approach to control oral perception from controlled fractures and dissolution kinetics. The work will be carried out in UMR 0782 within an interdisciplinary group specialized in multiscale modeling in food from the molecular scale (nm) to the process scale (m). Targeted length scales are between 10^{-7} m and 10^{-2} m.

PROJECT DESCRIPTION

The project aims to develop a mesh-free computing framework to simulate mechanical fracture and dissolution in various food products based on the concepts of soft-matter physics. Dissipative Particle Dynamics (DPD) [1] and Smoothed Particle Hydrodynamics (SPH) [2] are the two simulation methods considered. In the last decade, they have been linked to bridge hydrodynamics simulations with the mesoscale, where thermal fluctuations are significant. DPD can be parameterized from atomistic simulations (bottom-up approach), but this strategy remains impractical for complex foods (multiconstituent and highly structured materials). SPH and SDPD (Smoothed Dissipative Particle Dynamics) are more appropriated because only the macroscopic properties of the fluid (density, viscosity) and the solid (elasticity, plasticity, toughness) are used as inputs (top-down approach). The project will explore and extend the capabilities of these two methods to study the mechanical problems associated with oral processing, where both dissolution and fracture play an essential role. Finally, the consequence of food destructuration on mass transfer can later be simulated by Langevin Dynamics [3].

Most of the developments will be performed with LAMMPS. Pre- and post-treatment will be implemented in Python using various packages. The framework will be progressively validated

by comparing simulations with experimental results at the microscopic scale already published and produced in the course of the project (contribution of the 2nd Ph.D.).

A multidisciplinary and international group (in the EU and the US) will support the Ph.D. student. English is mandatory and will be used as the main working language.

QUALIFICATION

- You are highly motivated to work at the boundary between continuum mechanics and mesoscale simulation.
- You have an engineering degree, a master's degree, or equivalent (obtained within four years) in Mechanics / Physics / Physico-Chemistry / Nanosciences / Microfluidics / Chemical Engineering with an excellent theoretical background.
- You have practical experience in parallel computing with good programming skills.
- Good knowledge about solid and fluid mechanics
- You have strong communication and presentation skills in English (verbal and written)
- You enjoy working independently and overcoming scientific obstacles with an optimist aptitude.

APPLICATION

Send your application by e-mail to olivier.vitrac@agroparistech.fr, including CV, with names and addresses of two referees and a motivation letter.

REFERENCES

[1] Espanol P, Warren PB. Perspective: Dissipative particle dynamics. J Chem Phys. 2017;146:150901 https://doi.org/10.1063/1.4979514.

[2] Violeau D, Rogers BD. Smoothed particle hydrodynamics (SPH) for free-surface flows: past, present and future. *Journal of Hydraulic Research*. 2016;54:1-26 https://doi.org/10.1080/00221686.2015.1119209.

[3] Vitrac, O., Hayert, M. Modeling in food across the scales: towards a universal mass transfer simulator of small molecules in food. *SN Appl. Sci.* 2020;2**,** 1509. https://doi.org/10.1007/s42452-020-03272-2.