PhD position at IFP Energies nouvelles (IFPEN)
in *physical and chemical science*

Transport of Pollutants in Porous Media: A Lattice Boltzmann Approach Accounting for Complex Adsorption Processes

When simulating the transport of pollutants in the subsurface or in the context of water remediation, special attention should be paid to the specific adsorption behavior of complex pollutants. These compounds, which are receiving increasing attention worldwide, include already identified as well as emerging pollutants (e.g. PFAS, nanoplastics, personal care products…). These molecules are characterized by physico-chemical behaviors at the fluid-solid interface that generally cannot be described using classical models (e.g. Henry, Langmuir). In turn, their specific interfacial behavior drastically influences the transport of these types of molecules. It is therefore necessary to develop and include a specific model for this kind of adsorption, based on experimental data, in the transport equations to obtain a physically consistent adsorption/transport behavior.

The objective of this thesis is to better understand the transport of complex pollutants in heterogeneous porous media. The thesis consists of a thermodynamic modeling part and a numerical part. First, we will adapt a thermodynamic adsorption formalism recently developed to pollutants characterized by non-classical adsorption isotherms. Then, the adsorption equilibrium and kinetics specific to each molecule will be implemented in an existing Lattice-Boltzmann code to simulate transport of this type of molecules first in simple geometries and then in heterogeneous porous media. In fine, the goal of this dual approach is to provide a rational framework to design and optimize water remediation processes taking into account the complex physical chemistry at play and its coupling with strong structural heterogeneities in porous media.

Keywords: Complex pollutants, adsorption, thermodynamics, transport in porous media

Academic supervisor	Dr. COASNE, Benoit, Laboratoire Interdisciplinaire de Physique, benoit.coasne@univ-grenoble-alpes.fr, https://benoitcoasne.github.io/ ORCID : 0000-0002-3933-9744
Doctoral School	Physics Doctoral School in Grenoble, https://doctorat.univ-grenoble-alpes.fr/ecoles-doctorales/ecole-doctorale-de-physique-668370.kjsp
IFPEN supervisor	Dr. BAUER, Daniela**,** Direction Sciences de la Terre et Technologies de l'Environnement, daniela.bauer@ifpen.fr
PhD location	IFP Energies nouvelles, Rueil-Malmaison
Duration and start date	3 years, starting in fourth quarter 2023
Employer	IFP Energies nouvelles, Rueil-Malmaison, France
Academic requirements	University Master degree physics, chemistry, or applied mathematics with background in physics, physical chemistry, applied mathematics
Language requirements	Fluency in French or English, willingness to learn French

To apply, please send your cover letter and CV to Benoit Coasne or Daniela Bauer.

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