PhD position
Multiscale modeling of lithium-ion batteries based on high-resolution 3D images of porous electrode and separator microstructures

Important information

We are looking for someone with a strong background in applied mathematics and a degree in either applied Mathematics, Physics, Engineering, or Chemistry. More specific knowledge on object-oriented C++ programming, high-performance computing, porous media and/or the physics of transport phenomena would also be greatly appreciated.

- o **Dates**　　　　Three-year PhD position with a flexible starting date in early 2022
- o **Location**　　　Institut de Mécanique des Fluides de Toulouse (IMFT), Toulouse, FR
- o **Salary**　　　　About 32 k€ gross / year
- o **Supervisors**　IMFT (Yohan Davit, Olivier Liot), CIRIMAT (Céline Merlet)
  　　　　　　　　　TOTAL/TotalEnergies (Romain de Loubens)

Context and motivations

Physical modeling of rechargeable lithium-ion batteries (LIB) is a high-impact research area, which has repercussion not only on the fundamental understanding of LIB mechanisms, but also on control and design applications. In particular, the development of high-fidelity multiscale models represents the main challenge for the computational design of next-generation LIB technologies and for the construction of more robust state observers via model reduction techniques.

The current state of the art in the modeling of LIBs at cell level is given by the so-called "Porous Electrode Theory" introduced in the 1970's. It is a mixed formulation, where transport equations are averaged for the electrolyte phase and the exchange flux between phases is modeled by locally solving the microscale transport equation in the active material (solid phase), which is often represented by spherical particles. Along with simplifications of the porous electrode microstructure, this formulation relies on the timescale separation of the different transport mechanisms, hence it can lead to inaccurate predictions notably in fast-charging scenarios.

In the past two decades, the "Direct Numerical Simulation" (DNS) of porous electrode microstructures has gained significant attention, with the development of sub-micron scale imaging devices and the rapid evolution of high-performance computing facilities. Such DNS relies on micro-continuum models of mass and charge transport in the electrolyte and solid phases, with electrochemical reactions at the solid-electrolyte interface. Depending on the nature of materials and the operating conditions, additional effects can be modeled, such as the Li plating/stripping reaction that is likely to occur in the anode at high charging rate.

DNS models can be applied on "representative" sub-volumes of electrodes and separator, but their application at the scale of LIB cells is currently not feasible due to performance limitations. In practice, the number of charge/discharge cycles that can be simulated is also limited, so that DNS is mostly used to evaluate performances at the beginning of life. In spite of these limitations, it remains a very powerful tool to investigate the microscale physics of battery cells.

Scientific objectives

Exploiting the possibility of accurate simulations at the microscale, this research work will focus on the development of volume-averaged or homogenized multiscale models, starting from the governing equations at the microscale. The main objective will be to derive a macroscale formulation

of transport and electrochemistry, where effective properties are rigorously calculated by DNS on real imaged structures. Due to the emphasis of this project on fast charging applications, the multiscale modeling of Li plating/stripping will also need to be addressed.

This work will benefit from experimental data provided by SAFT and Total, including high-resolution images of electrode and separator samples, measurements of material and microstructure properties, and in operando data of Li distribution.

To clarify the discussion, a simplified representation of a LIB cell is provided in Figure 1. It consists of three porous regions that are supposed to be entirely filled by the liquid electrolyte:

- The anode layer of thickness ~100 μm is usually composed of graphite particles (size distribution: 1 to 20 μm) and polymer binder additives.
- The cathode layer of thickness ~100 μm is composed of metal oxide particles (size distribution: 1 to 20 μm) and/or phosphate-based particles (size distribution: 50 to 200 nm), as well as carbon black and polymer binder additives.
- The separator is a mesoporous polymer membrane of ~20 μm thickness, composed of polyethylene (PE) and polypropylene (PP) in a three-layer structure (PP/PE/PP).

The initial focus of this research work will be on the upscaling of the microscale governing equations in the separator region, which is conceptually simpler to model. For the development of multiscale models in the anode and cathode regions, specific issues will be addressed, such as non-equilibrium effects, Li plating or double-porosity structures.

In general, indications on the directions to take will be obtained from DNS results, available experimental data, and theoretical analysis of the relevant equations. Macroscale models will be proposed following this quantitative analysis. Techniques and numerical tools will be developed to estimate the effective transport properties incorporating as much information as possible from the real imaged structures.
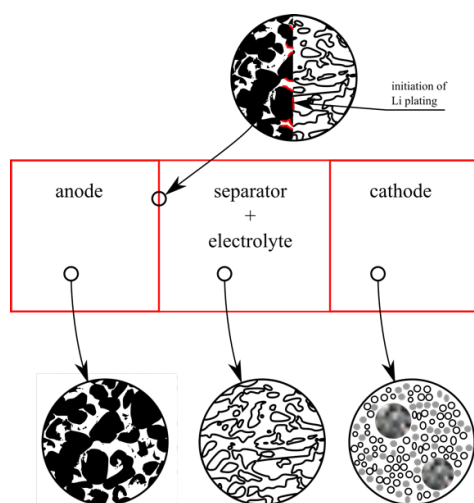

Figure 1: Schematic view of a LIB cell (not at scale, and current collectors not represented)

Contacts

Please send a resume, a motivation letter and your most recent grades/rankings at the following addresses. Please use PhD_LIB_application as the title of your e-mail.

Yohan Davit	yohan.davit@imft.fr
Olivier Liot	olivier.liot@imft.fr
Céline Merlet	merlet@chimie.ups-tlse.fr
Romain de Loubens	romain.de-loubens@totalenergies.com