Postdoc position – Upscaling mass and charge transport in the porous separator of lithium-ion batteries

Important information

We are looking for someone with a strong background in physics, mechanics or applied mathematics. Knowledge on transport in porous media and upscaling methods, such as homogenization or volume averaging, would also be greatly appreciated.

- Dates: Two-year postdoc position, starting date in fall 2022.
- Location: Institut de Mécanique des Fluides de Toulouse (IMFT), Toulouse, France.
- Salary: Calculated from profile & experience. Up to about 50k euros gross / year.
- Supervisors: IMFT (Yohan Davit, Olivier Liot), CIRIMAT (Céline Merlet), TotalEnergies (Romain de Loubens)

Context and scientific project

Lithium-ion batteries (LIB) are the primary energy storage technology for modern portable electronic devices such as laptop computers, tablets and mobile phones. They are also supporting the development of renewable energies that require stationary storage and are at the core of the transition towards electric vehicles. LIBs will remain the dominant technology for the foreseeable future, with an enormous increase in demand. Improving the performance and safety of LIBs is therefore an important research area. Besides its role in understanding fundamental mechanisms, modeling of LIBs is key in defining robust state observers, such as the state of charge, that can be used for safe control in the battery management system. Modeling is also helpful in assessing ageing or in optimizing the operating conditions and the battery cell design. The so-called "Porous Electrode Theory" introduced in the 1970's is the current state of the art in modeling LIBs at cell level. It consists in 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).

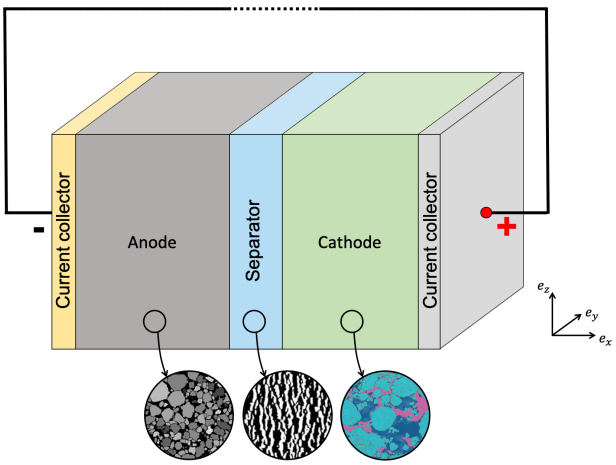

Fig. 1: Schematic view of a LIB cell

Our goal is to develop new models of LIBs that can exploit advances in sub-micron scale imaging and high-performance computing (HPC). To do so, we will work on direct upscaling of transport equations in the different LIB components (Figure 1), the positive electrode, the separator and the negative electrode. The idea is to obtain average formulations involving effective parameters that can be directly calculated through resolution of closure problems over representative geometries based upon real images of battery structures. The project will start with both a postdoctoral position and a PhD studentship. The postdoctoral researcher will focus on upscaling for the separator. 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). In the liquid electrolyte filling the pores of the separator, electrolyte concentration c_e and ionic potential φ_e satisfy the following mass and charge conservation

equations,

$$\frac{\partial c_e}{\partial t} = -\nabla \cdot \mathbf{N}_e = \nabla \cdot \left(D_e \nabla c_e - \frac{t_+^0}{F} \mathbf{i}_e \right), \tag{1}$$

$$0 = -\nabla \cdot \mathbf{i}_e = \nabla \cdot \left(\kappa_e \nabla \varphi_e - \frac{2RT(1-t_+^0)}{F} \kappa_e \nabla \ln c_e \right). \tag{2}$$

The right-hand side of the mass conservation equation contains the contributions of diffusion and electric migration to the total ionic flux, $\mathbf{N}_e$. D_e is a concentration-dependent inter-diffusion coefficient, t_+^0 is the dimensionless and concentration-dependent Li^+ transference number, and F is Faraday's constant. The divergence-free current density $\mathbf{i}_e$ satisfies a modified Ohm's law where κ_e is a concentration-dependent ionic conductivity. The ionic potential is defined as $\varphi_e = \Phi_e + \mu_e/F$, where Φ_e and μ_e denote the electric and chemical potentials of the electrolyte, respectively.

The postdoctoral researcher will

1. use upscaling methods to derive average transport for the coupled, non-linear system of mass and charge conservation equations, Eqs. 1 and 2.
2. use HPC direct numerical simulations (DNS) of mass and charge conservation at pore-scale to aid in determining adequate hypotheses for upscaling. TotalEnergies is developing a code for this purpose and will provide support to train and assist the postdoc.
3. compare the results of the average formulation with that of DNS in simple model geometries.
4. calculate effective parameters for real separator geometries. The images will be be provided by Saft and TotalEnergies. The code for solving the closure problem will be developed in collaboration with TotalEnergies.

Contacts

If you are interested, please send a resume to the following addresses and use "postdoc_LIB_application" as the title of your e-mail.

- Yohan Davit, yohan.davit@imft.fr
- Romain de Loubens, romain.de-loubens@totalenergies.com