# Microstructural and Computational Fluid Dynamic (CFD) analyses of the Proton Exchange Membrane Fuel Cell (PEMFC) using the Lattice Boltzmann Method (LBM)

#### Industrial Partner: EH Group

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### Introduction:

Nowadays, depleting reserves of fossil fuels and their high output emissions have made alternative fuels a good topic for future studies. Herein, hydrogen is reported to be a suitable candidate, which can be utilized through proton exchange membrane fuel cells (PEMFC). As a result of the electrochemical reaction of hydrogen and oxygen, the output of PEMFC that can be used instead of internal combustion engines (ICE) is water, electricity, and heat. The gases diffuse through the gas diffusion layer (GDL), which is a porous medium inside the stack of PEMFC. Investigations have shown the positive effects of microporous layer (MPL), that can be attached to GDL to improve the microstructural properties and water/thermal management of the cell. Additionally, the characteristics of the catalyst layers (CLs) in the Membrane Electrode Assembly (MEA) such as Pt size and distribution and the rate of resulting electrochemical reactions in this layer is of interest to improve the performance and the efficiency of PEMFCs.

The goal of this master project is to use the Lattice Boltzmann Method (LBM) as an approach to perform Computational Fluid Dynamic (CFD) analysis to characterize the microstructure of the PEMFCs. In a typical CFD problem, commercial software such as ANSYS and COMSOL can be used to simulate the fluid behavior and to obtain the corresponding contours of velocity, pressure, density, temperature, etc. However, in the boundary of liquid, gas, and solid phases, the principal governing equations that are being used by the COMSOL and ANSYS such as momentum, mass, and energy are not verified, hence methods like LBM that use the kinetic energy to solve the fluid flow problems should be used.

## **Objectives:**

In this project, the real samples of the GDL, MPL, and MEA are being provided by the EH group. In the first step, the Scanning Electron Microscopy (SEM), Focused Ion Beam- Scanning Electron Microscopy (FIB-SEM) and Computational Tomography (CT) scan will be done by the co-supervisor, H. Pourrahmani, followed by segmentation and reconstruction of the three-dimensional images. A LBM code has been also developed as a part of this project that can be used in the Linux to characterize the obtained 3D images by microscope imaging.

The responsibilities of the applicant are as follows:

- Use the developed LBM code and the obtained images by H. Pourrahmani and analyze the fluid flow behavior inside the PEMFC by changing the operating conditions.
- Obtain the corresponding contours of the temperature, pressure, velocity, density, etc. with high quality to be used for publications.
- Provide the literature review of the current achievements in the field to be used in the publications.

Applicants familiar with the concepts of computational fluid dynamics (CFD) are welcomed to submit their resumes and due to the novelty of project possible publications are foreseen.

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