

Modelling and Numerical Simulation

Introduction

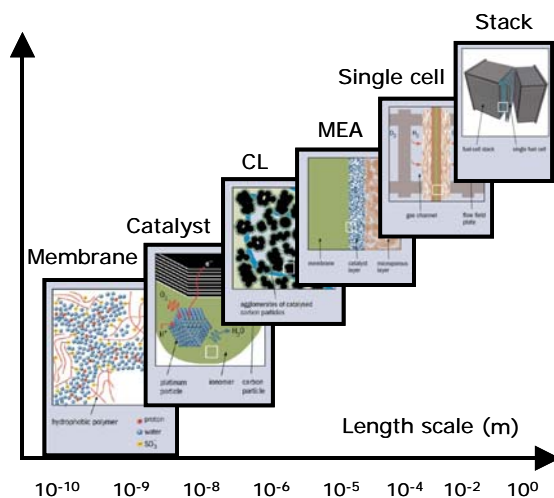
As a key core competency of NRC-IFCI, the Modelling Group provides Canadian clean energy sectors with fundamental knowledge and technologies in energy conversion devices and systems through modelling and simulation. The application of these scientific and technical areas encompasses fuel cell electrodes and stacks, battery electrodes, heat exchangers, combustors, wood-product and bio-mass processing.

Through partnership with IFCI's experimental teams, universities (SFU, UBC, UVic, UAlberta and UWaterloo) and industry (Ballard, AFCC, Hydrogenics, Hyteon, Tekion, Nissan), this group has established a distinguished, world-class reputation in fundamental understanding of microstructure formation and mass transport phenomena of Proton Exchange Membrane (PEM) fuel cell electrodes, stack design, and optimization.

In addition, the group plays a key role in harmonizing fundamental research with the needs of other surging renewable energy industries such as batteries and super-capacitors. Strategic research directions explore the optimization of device performance through modelling and the design of new advanced materials and breakthroughs in engineering.

Core Competency

The Modelling Group has a number of core members with expertise in computational chemistry, physical chemistry, computational fluid dynamics, computational solid mechanics, and applied mathematics.



Multi-scale approach in PEMFC modelling

CL: Catalyst layer

MEA: Membrane Electrode Assembly

At the micro level, our expertise includes high throughput screening of materials through first-principle computer simulations, as well as the computer-based rational design of advanced electrocatalyst materials. Specifications of current fuel cell technologies drive material selection. At the same time, materials are under constant revision as further research continues to define promising directions and restrictions.

At the nano- to meso-scale, our activities comprise research in solid and fluid mechanics, physical modelling of electro-chemical phenomena including mass and energy transfer, and microstructure formation and changes.

Computational Fluid Dynamics (CFD) and computational solid mechanics techniques

provide valuable insight into fuel and oxidant flow throughout the system and failure modes at the individual cell and stack level, constituting a tool for the optimization of their design and performance.

At the component level, techniques such as mass and energy balance are used to optimize the design of the operational device.

At the integrated system level, the Group utilizes process modelling to perform "what-if" analysis of integrated energy systems such as hydrogen fuelling stations and hydrogen-assisted renewable power systems.

Our codes help to establish the relations among structure, properties and performance, predicting material architectures and operating conditions that optimize fuel cell operation.

modelling R&D services and shared computing facilities within all industrial R&D projects at IFCI.

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Aussi disponible en français



Computational Resources

IFCI's ongoing industrial and collaborative modelling projects, both at the national and international levels, focus on large-scale calculations of microstructure formation and characterization, performance optimization and diagnostics. Our high-performance computing cluster features 320 fast-interconnected processors offering versatile and reliable