Multi-scale modelling tools for fuel cell development

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Fuel cells inherently involve phenomena occurring over a wide range of length scales, from the molecular scale on electro-catalyst surfaces through various scales of porous media including catalyst layers, micro-porous layers porous transport layers, to gas supply channels within a cell and finally to the manifolds at the stack scale. In total, length scales spanning about 10 orders of magnitude are of interest to the fuel cell developer.

This talk will discuss various tools developed to represent phenomena occurring from the catalyst scale to the stack scale and methods for coupling information from the various scales. These tools include the ability to model arbitrary porous materials comprising multiple solid phases and to model transport phenomena and electrochemical reactions in these materials using both virtual porous media and experimentally determined geometries. At the next scale, full cell models are developed and are capable of modelling both beginning of life performance and selected degradation mechanisms. In particular, a new class of cell level models coupling traditional computational fluid dynamics with pore network models will be discussed. These models provide a more physically meaningful description of liquid water distributions in low temperature fuel cells. Finally, at the largest scale entire stack simulations are carried out and can be used to explore temperature composition and current distributions within a stack as well as stack manifold design.

The talk will highlight and present the open source software developed for these analyse and discuss the application of the tools to the design of better fuel cells.