

Computational Design of Electrochemical Engines for Hybrid Electric Vehicles

a report by

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Electrochemical (EC) engines, i.e. batteries and fuel cells, are an enabling technology for the successful deployment of fuel-efficient, environmentally responsible vehicles. A thorough understanding of an EC engine from the standpoint of performance, safety and longevity is important for successful application in hybrid electric vehicles (HEVs). Unfortunately, using experimental testing to evaluate battery and fuel cell characteristics and to obtain a performance that involves a myriad operating conditions and environments is a time-consuming and formidable task. Computer modelling and simulation that is based on the fundamental principles of electrochemistry and transport phenomena promise to reduce the number of trial-and-error iterations in EC engine design, scale-up and optimisation. In recent years, Penn State Electrochemical Engine Center (ECEC) has been devoted to the development of a general computational framework for EC engine design, based on computational fluid dynamics (CFDs), a technique that is widely used by the automotive industry for internal combustion engine studies. A family of CFD-based EC engine models has been developed, including those for valve-regulated lead-acid, nickel-metal hydride, Li-ion or Li-polymer batteries, proton exchange membrane fuel cells (PEMFCs) and direct methanol fuel cells (DMFCs). These models have demonstrated the following advantages of coupling first-principle modelling with experimentation.

- They provide a more complete understanding of the fundamental chemical and transport processes that occur inside a battery or fuel cell and thereby help to identify the key mechanisms and parameters governing cell performance.
- They permit 'what-if' parametric studies to establish guidelines for more rational and less costly experimental development efforts, particularly when destructive experiments are involved, such as abuse, thermal runaway and battery life-cycle tests.
- They accelerate EC engine development cycles by allowing engineers to evaluate many design alternatives prior to constructing a prototype cell and to establish a rational basis for design optimisation and innovation.

- They facilitate the unconventional integration and interfacing of EC engines with other concurrent power plants in hybrid vehicles, vehicle powertrains and auxiliary thermal and water management systems using high-fidelity engine simulators, rather than physical battery modules and fuel cell stacks.

Fuel Cell Engines

At the ECEC, the general CFD analysis tool was successfully applied to reformat/air PEMFC and DMFC to effectively establish design guidelines, modify existing designs, obviate the need for testing and evaluate concept feasibility. One such computational study involved analysing the effectiveness of an interdigitated flowfield (see *Figure 1*). In the interdigitated cathode, the end of the inlet flow channel is blocked to intentionally force flow under the current collecting rib, through the porous backing layer and into the adjacent exit channel, as shown by the predicted stream-traces for this design in *Figure 2*. This has the effect of delivering oxidant to the reacting cathode surface by forced convection rather than diffusion, thereby reducing concentration polarisation losses and enhancing water removal at high current densities, as shown in the predicted polarisation curve of *Figure 3*. The computer simulation showed that cell performance increases under high load conditions using the interdigitated design. It is up to the design engineer to determine whether the enhancement is great enough to justify the increased pumping requirements that are also predicted by the code. A decision about the feasibility of this design can be made without construction and trial-and-error testing.

In addition to basic design evaluation, insight into complex physico-chemical phenomena not yet experimentally measured can be gained with the use of a CFD-based fuel cell model. For example, in long, serpentine flow channels, there is often a significant pressure drop occurring between the inlet and the outlet. If this pressure drop exceeds that which is required to drive gas flow through the porous backing layer under adjacent ribs, the gaseous reactant will bypass the desired flow path. Only by using a three-dimensional fuel cell model can this effect be accurately predicted. Insight into this phenomenon, obtained

from CFD, can be used to determine design guidelines for flowfield path length, shoulder width and backing layer porosity for prototype construction.

CFD modelling is a useful tool for cell optimisation. A critical issue in DMFC performance is the phenomenon of methanol crossover through the electrolyte to the cathode by diffusion, convection and electro-osmotic drag. Diffusion normally dominates the methanol crossover process. Based on a CFD model, an optimal membrane thickness can be determined for a given set of operating conditions that will balance crossover losses with ohmic losses in the membrane for maximised performance. CFD-predicted output can be validated with highly instrumented experimental DMFC systems. Coupled with experimental testing of CFD-optimised designs, this provides a competitive edge and has effectively advanced several fuel cell designs. Design guidelines and modifications can be obtained by the design engineer early, reducing the development time and enhancing the fuel cell engine performance.

HEV Batteries

The CFD methodology has also been used with considerable success in modelling various battery systems, including the valve-regulated lead-acid, nickel metal hydride (Ni-MH), lithium thionyl chloride and Li-ion cells. These first-principles models describe important physicochemical processes in the cell, i.e. mass, charge, momentum and heat transfer, and kinetics and thermodynamics of reactions. They are based on experimentally measurable parameters. The CFD-based approach can include the momentum and heat transfer equations in general battery models. The main focus of these models has been to address the concerns of the electric vehicles and HEV industry. The models are based on a robust framework that ensures accurate predictions even under extremely transient operations, which are commonly encountered in HEV batteries. The approach that has been adopted is to combine theoretical predictions with experimental data on cells under both real-world and controlled conditions. The experimental data with

Figure 1: Schematic of a PEM Fuel Cell with Serpentine Anode and Interdigitated Cathode Analysed with CFD Tools

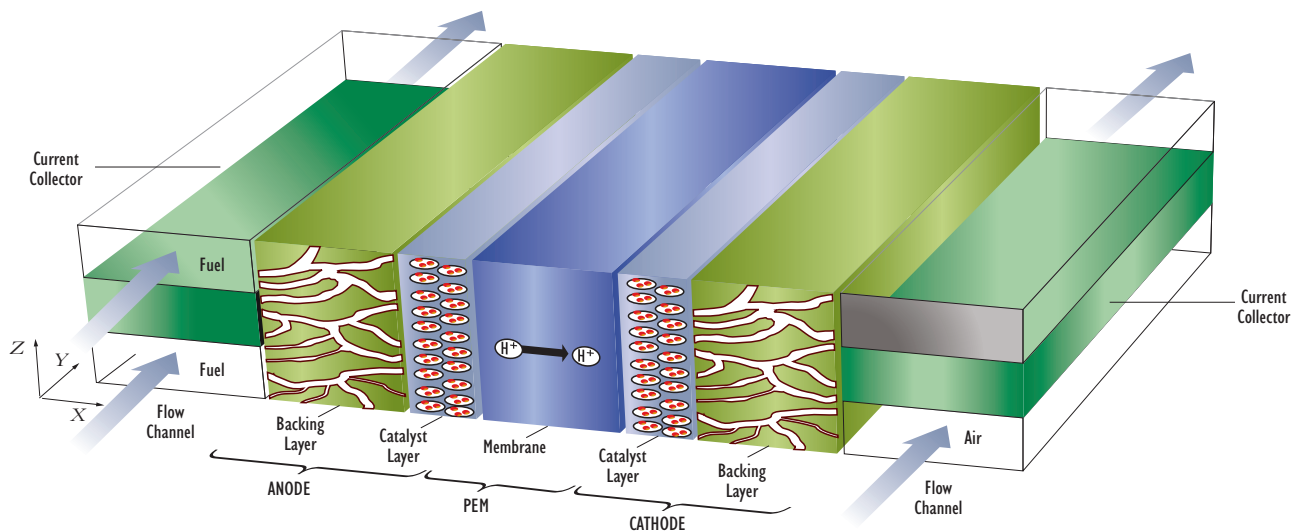


Figure 2: Predicted Cathode Stream-traces for a Reformate/Air PEM Fuel Cell with Interdigitated Cathode

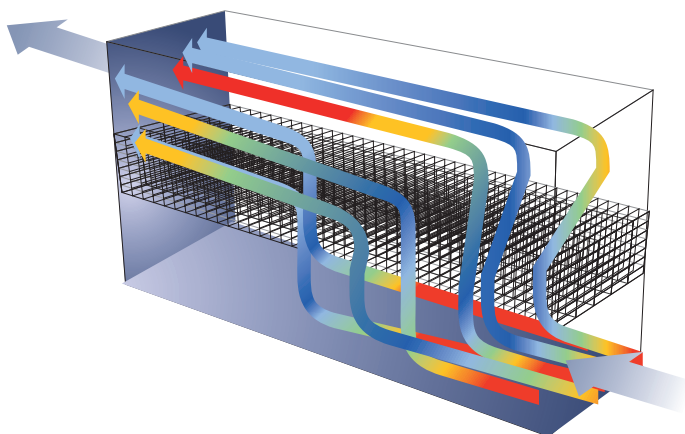


Figure 3: Polarisation Curves for a Reformate/Air PEM Fuel Cell with Interdigitated Cathode

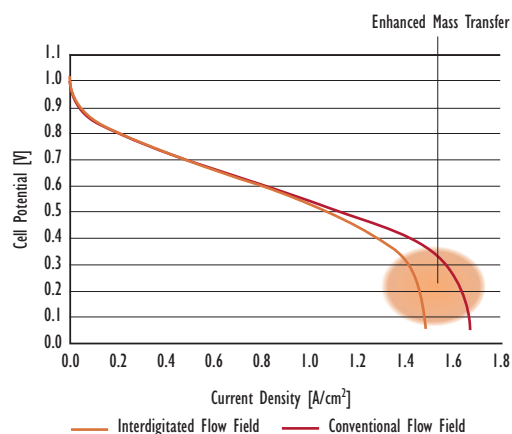
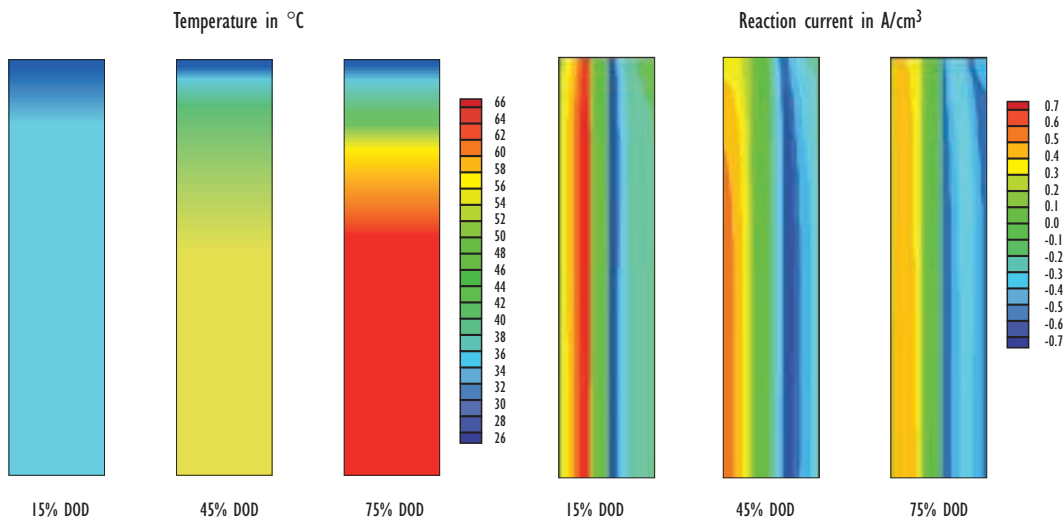


Figure 4: Temperature and Reaction Current Distributions During Various Depths-of-discharge in a Li-ion Cell



The heat is dissipated only from the tabs, which are located at the top of the cell.

which the models are compared to ensure accuracy is obtained either from a one-mile oval test track or a vehicle dynamometer facility. The model and experimental comparisons are used to refine the models and make them more robust. In addition, controlled laboratory-scale single cell experiments are also performed in order to extract parameters, which are fed back into the model. This iterative approach has been extremely successful, as shown by the model's ability to predict the behaviour of the Ni-MH battery.

In addition to predicting cell behaviour, the models are also useful for designing battery-charging and management systems to suit specific applications. For example, although Li-ion cells have high energy and power densities, they are a long way from being used in vehicles due to thermal stability and safety problems. Well-designed thermal-management systems would hasten the launch of this battery into the marketplace. The CFD-based models provide an excellent starting point for designing such systems. *Figure 4* shows the cell temperature and reaction rate contours during the discharge of a Li-ion cell. The significant increase in temperature (40°C) with discharge and the difference in temperature within the cell are seen clearly. These differences in temperature lead to differences in the EC behaviour, as can be seen from the reaction current contours. When many such cells are connected to each other in a pack, as would be used in a vehicle, these differences will result in significant imbalance. While some cells would be charged or discharged at a more rapid pace, others would be slow to respond, leading to safety concerns. Currently, a parallel computing approach is being used to explore the interaction between individual batteries in a pack with an emphasis on addressing the effect of cell imbalance. Such an approach should be fruitful in addressing issues that are critical to the design and operation of HEV batteries.

The models have been developed with the intention of aiding battery designers in designing new cells without the need for extensive experimentation, saving time and resources. To this end, the models are packaged with a user-friendly simulator with a wide range of flexible options. Modifications can easily be made to both the operating conditions and design parameters of batteries, and the results of the simulations are displayed in realtime through a graphical user interface post-processor. A typical simulation of real battery behaviour over many hours is completed in a couple of minutes using the simulator. The battery simulator is also available online (<http://mtrl1.me.psu.edu/>) on a secure server where battery manufacturers and car companies can come together to design advanced batteries for EV and HEV applications.

Summary

HEV and other automotive applications place an ever-increasing demand to develop advanced EC engines with high performance, low cost and excellent durability. Computer-aided design is indispensable in this development process and can dramatically reduce the expensive and time-consuming trial-and-error experimentation that is currently required. The complexity of EC engine simulation requires many interacting physicochemical submodels in order to be successful. Therefore, a fundamental understanding of the EC and transport processes occurring in these engines continues to be necessary. This can be best achieved through a combination of fundamental modelling and detailed diagnostics. In addition, further developments in computer hardware and numerical algorithms will eventually allow the use of CFD-based models in design, optimisation and control of complex EC engines, thereby significantly accelerating the commercial deployment of HEVs. ■