

Advanced modelling accelerates fuel cell development

ADVANCED PROCESS MODELLING IS HELPING TO CUT FUEL CELL COMPONENT AND SYSTEM DEVELOPMENT TIMES SIGNIFICANTLY, BY PROVIDING ACCURATE PREDICTIVE INFORMATION FOR DECISION SUPPORT.

Mark Matzopoulos

Fuel cell development companies are increasingly seeing advanced process modelling (APM) as a key tool for accelerating cell component and system development, and managing the associated risk. Modelling provides the ability to base important decisions on accurate numerical data, helping to reduce reliance on physical testing; and speeds up the screening of design alternatives, reduces risk and provides a much-welcomed mechanism to integrate R&D and engineering design activities more closely.

A major challenge in fuel cell design – and the reason that experimental techniques alone are inadequate – is that so many phenomena and interacting components need to be considered simultaneously. It is no use designing fuel or air flow channels without understanding how they interact with the chemical and electrochemical phenomena occurring in the electrolyte. Similarly it is pointless to design a fuel cell stack – with all its complex interactions – without considering the system within which it operates, and the dynamic load requirements to which it will be subjected during its operational life.

The benefits of modelling

A key benefit of modelling is that less successful designs or inappropriate materials can be screened out before proceeding to physical testing. This

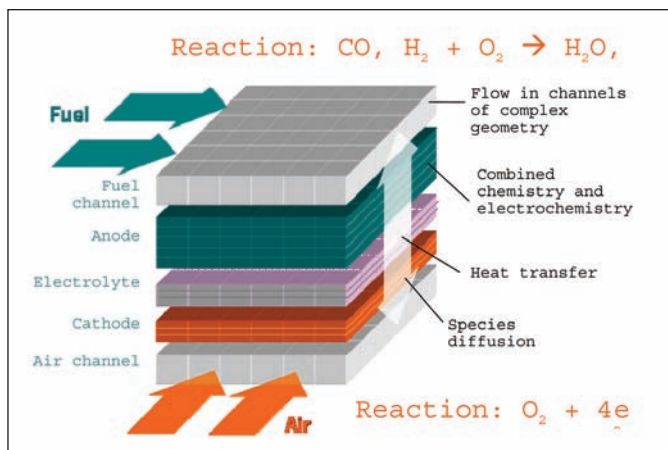


Figure 1: Phenomena that need to be considered simultaneously in modelling of a solid oxide fuel cell.

provides an immediate saving in time and money. One major developer of residential fuel cells claims a saving of US\$250,000-US\$500,000 every time the need to build and operate a test rig is eliminated.

Similarly, modelling helps to pinpoint the most important areas in which experimentation is required, thus eliminating unnecessary time-consuming and potentially costly experimentation.

Modelling also provides a valuable framework in which experimental data can be analysed using model-based data analysis techniques, as well as the wealth of information already within the model, to make sense of data in such a way that it can immediately be used to generate value. If performed in the correct way, such analyses are capable of providing a reliable quantitative measure of the risk involved in any design decision.

However the major benefit is that not only can the entire development process be accelerated, but design alternatives can easily and rapidly be investigated – in days rather than months – to come up with significantly improved designs. Once a validated model has been constructed it can be used to optimise virtually any aspect of component and system design and operation at a relatively small incremental cost.

An equally important “soft benefit” is that modelling provides a means to capture knowledge and understanding, and transfer this between the different groups involved in the development. Experience in the companies who have adopted a systematic approach to modelling shows that this provides significant scope for parallel, rather than sequential, working between different disciplines.

The most significant benefits are achieved by embarking on modelling early on in the development process. A reliable membrane model can be used for quantification of cell stack effects; a reliable cell-stack model can be used for control design and analysis of system dynamics, and so on. Not only is the time invested in model development repaid many times over, but a consistent basis is used for all stages of design.

Application areas

Modelling can be applied at virtually every stage of the fuel cell component and system development to help designers dealing with the challenges of

cost competitiveness, performance and reliability (*the box below provides some typical examples*).

What does modelling involve?

As can be expected, modelling such complex systems in order to produce accurate quantification is not a trivial task. However the techniques are well-established, and results can be achieved more quickly and with less effort than is commonly believed.

The key technology applied here is advanced process modelling (APM). Advanced process models have two attributes that make them capable of a very high degree of predictive accuracy, within a flexible framework.

The first is a detailed **first-principles representation** of all the fundamental physical and chemical phenomena that characterise the process, including the chemical and electrochemical reactions and interactions; the micro-scale diffusion of molecules across and within the layers; and the heat transfer across the layers and to the surroundings. This is constructed within a modelling framework, by noting the (relatively well-established) heat and material flow, reaction, diffusion, and geometry equations, and describing the interaction between elements in the process flowsheet. Typically such models are available in libraries and do not need to be constructed from scratch.

The second ingredient is **accurate model parameter information** – for example, reaction kinetic constants, heat transfer coefficients and other

material properties – derived from “real-world” laboratory, pilot or operating data. These are determined using the model, in conjunction with well-established mathematical optimisation-based parameter estimation techniques in a process known as model validation. The objective is to fit the most accurate possible model parameters from sets of experimental data.

It is the combination of these two that provides such models with a highly-accurate predictive capability over a wide range of design and operating conditions.

Hybrid modelling

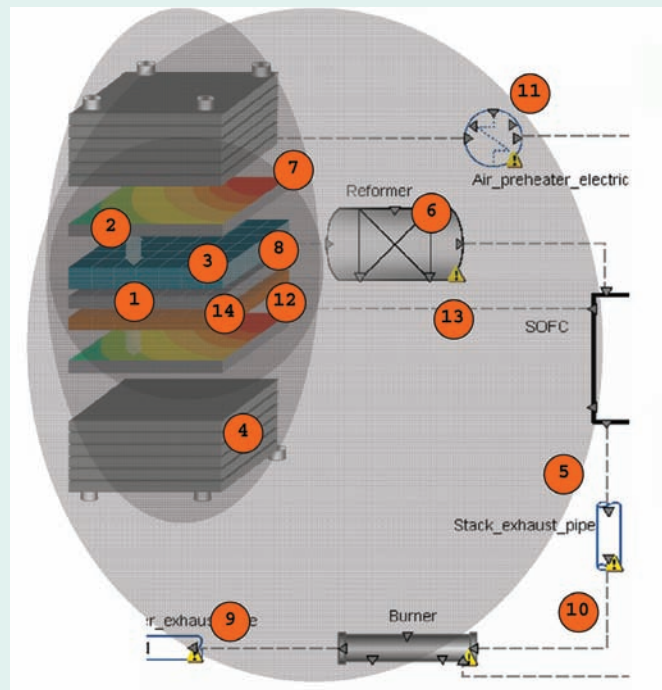
Modelling may involve a combination of more than one type of modelling system (software package) in order to handle the complex chemistry and electrochemistry (using, for example, **PSE's gPROMS**); flow channel hydrodynamics (**Fluent Inc.'s Fluent**); control analysis and design (**Mathworks MATLAB** and **Simulink**) and system flowsheeting and dynamics (**gPROMS** or **Aspen Technology's Aspen Plus** or **Hysys**). Such “hybrid simulation” or “co-simulation” is now well-established, and much of the recent work on hybrid simulation techniques has been pioneered in fuel cell applications because of their need to take into account complex interacting phenomena simultaneously.

Process optimisation vs. simulation

Once a fully-validated fuel cell model is available it can be used in conjunction with formal mathematical optimisation techniques to optimise many

What scenarios can modelling be used for?

- **1** Detailed analysis of the membrane physics, chemistry and electrochemistry – this is fundamental to understanding the operation of the cell and ultimately the fuel cell stack and system. What are the rate-limiting phenomena? Which parameters (for example, kinetic rate constants) have a critical impact on operation and therefore need to be determined as accurately as possible through further R&D?
- **2** Accurate determination of the flow channel architecture – is the current design effective? Are there areas that are starved of fuel or air? Are there significant temperature differences across the wafer? What sort of temperature differentials are seen when changing load rapidly? How will modifications to the flow channel patterns affect these?
- **3** Materials analysis, ranking and selection – given the temperature differentials determined above, which materials are likely to be able to withstand thousands of hours of operation? Which materials can be screened out immediately, thus saving lengthy and costly testing?
- **4** Heat transfer – how well does the stack dissipate heat under normal operating conditions? Are local hot spots generated during load changes, leading to early loss of effectiveness of areas of the cell?
- **5** Water and heat recovery – is the water recovery unit correctly sized? How does it interact with the rest of the tightly-integrated fuel cell flowsheet?
- **6** Fuel preparation system – what is the optimal reformed design? What is the optimal level of heat integration? How does the integrated system work under load changes?
- **7** Determine optimal operating conditions – what are the optimal feed concentrations for the maximum cell voltages for the required current densities?
- **8** Catalyst – is it possible to reduce the amount of platinum in the catalyst. What formulation minimises the production of carbon monoxide?
- **9** Water management (PEMFCs) – is hydration too fast or too slow during load changes?
- **10** Control scheme design / verification – what is the optimal control configuration required to maintain a steady ratio between reactant and oxygen, while balancing all the other system requirements? What are the optimal control parameter settings to ensure the required behaviour for a variety of typical operating scenarios? How do you manage temperature in the cell to avoid damage through thermal loading?
- **11** Investigate system interactions – fuel stack designs are often made on an



assumption of the performances of the system, and vice versa. Modelling allows an investigation of the interactions across the tightly-integrated fuel cell flowsheet;

- **12** Build-up of poisons – what is the likely build-up of destructive chemicals over the lifetime of the cell? What are the optimal operating conditions and strategies to avoid this?
- **13** Start-up – what is the optimal start-up policy to get to required production in the minimum time, while remaining within critical material and other operating constraints?
- **14** Durability – as with catalyst degradation in chemical reactors, advanced simulation can be used to simulate the ageing behaviour in cell materials and determine operating conditions – furnace temperature, current density and cell potential – that limit it. Time requirements can be reduced through modelling from thousands of hours of physical testing.

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different aspects of design and operation – and not just to simulate behaviour. Examples of a complex optimisation are “choose between one material from a selection of three that will minimise the temperature differential across the anode for a range of typical operating scenarios.” With a well-formulated predictive model, this question can be answered in a single run rather than many trial-and-error simulations coupled with physical testing.

Fuel cell modelling: from membrane to system

Modern modelling technology makes it possible to apply consistent modelling methods across all aspects of the fuel cell development and design process, from membrane to stack to system. It is now possible to cover the range of applications shown in the box (see page 45) with a single modelling platform. This is a significant improvement over the past, where the need to use different, incompatible environments for different applications led to inconsistency and time-consuming and error-prone rework.

The case studies below are based on PSE's experience of working with customers in the US, Europe and Japan in both the automotive and residential fuel cell sectors, and illustrate the potential for modelling applications at various stages of the development process. For consistency they are all SOFC processes; however the techniques apply equally to PEM and other designs.

Case study 1: membrane model

The detailed model of the anode-electrolyte-cathode “membrane” incorporates a fundamental understanding of electrochemistry, chemistry, materials, and heat and mass transfer in a form that can be easily understood, maintained, extended, used within broader stack or system flowsheets, or linked with other model components in hybrid simulations.

Typically the core of the model is three 1-dimensional spatially distributed models representing the anode, cathode and electrolyte respectively. The domains are distributed through the thickness of the elements. It is essential that highly accurate techniques are used to describe the multicomponent heat and mass transfer, as these are critical limiting factors that exert a major influence on the membrane's performance.

With the appropriate boundary conditions defined, the structure described here provides a convenient and flexible frame for describing important physical and chemical phenomena.

Model validation – from lab to reality.

As mentioned, once the fundamental first-principles model describing the essential phenomena has been constructed, it is validated against experimental data to determine key empirical parameters – reaction kinetic constants, heat transfer coefficients, electrolyte ionic conductivity parameters, internal current (leakage) parameters in this case – from experimental data.

The more accurate these parameters, the more accurate the model. The measure of inaccuracy in key parameters is a measure of the risk associated with using those values.

Model validation is performed using parameter estimation, which uses mathematical optimisation techniques to determine the best fit to the data based on the knowledge of the system that is contained in the model. In contrast to simulation, where the model is used to calculate outputs given inputs, here the goal is to calculate the most accurate parameter values possible from the information contained in the experimental data.

Risk analysis

Modelling packages such as PSE's *gPROMS* also provide model-based data analysis facilities that can determine the confidence levels for the parameters being fitted. This data can be used in formal mathematical analysis and quantification of the risk in any particular design.

By establishing which parameters carry the most risk, the confidence information can also be used to determine where to direct R&D spending most effectively. For example, if confidence intervals for the electrolyte ionic conductivity parameters are poor, and the model shows that this is a key design parameter, it is possible through modelling to quantify the potential consequences of useage with the current values. Design risk can be mitigated by focusing R&D effort on this particular area in order to improve the parameter confidence to acceptable levels.

Experiment design

At this stage modelling can also be used to design the experimental rig and experimental procedures for any subsequent experiments. Model-based experiment design can determine the optimal set of experiments (i.e. those requiring the minimum experimental time or cost, or other suitable objective function) to achieve a required parameter accuracy. This helps to integrate the R&D experimental programme with the engineering design, thus accelerating development and reducing resources, and potentially saving significant costs.

Typical results

Given composition and temperature of the feed and air channels and load resistance or voltage, the membrane model can be expected to calculate fuel consumption rate, water production rate, heat generation and electrical power generation.

Once such a membrane model is available, it can be executed in its own right to generate information on the membrane performance; combined with CFD models for flow channel design; or form the basis of a cell stack model for dynamic analysis of system performance.

Case study 2: fuel cell stack multi-scale modelling

In this example, a *gPROMS* advanced process model of the SOFC membrane is coupled to a Fluent Computational Fluid Dynamic (CFD) model of fuel and air flow channels, as shown schematically in *figure 2*.

This hybrid modelling approach is adopted to provide accurate hydrodynamic modelling of the flows in the complex gas channel geometries using all the power of CFD, while simultaneously taking into account the complex

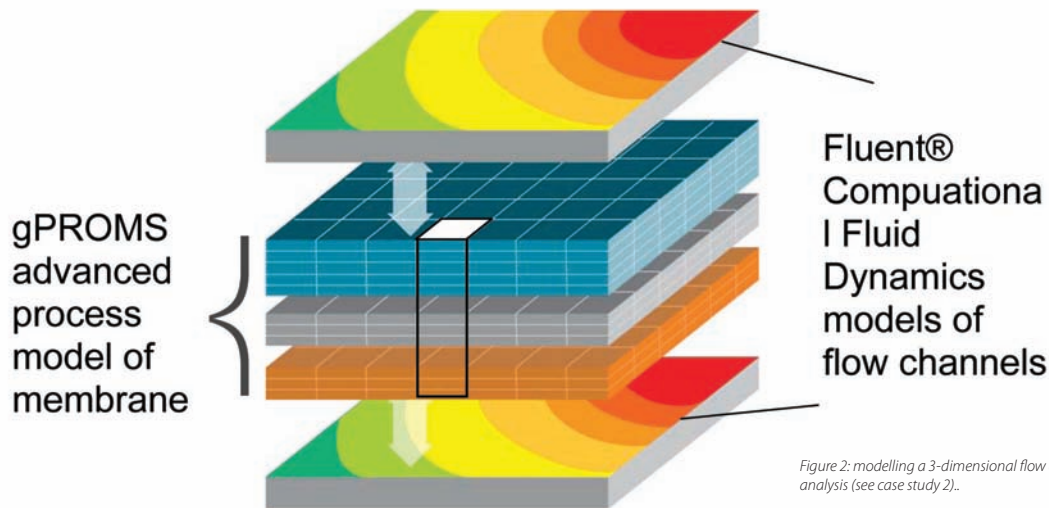


Figure 2: modelling a 3-dimensional flow channel temperature analysis (see case study 2).

chemical, electrochemical and diffusion effects occurring in the membrane. Modelling these two highly interdependent areas separately or sequentially would simply not produce the correct results.

The model is used to perform detailed hydrodynamic analysis, experiment with different flow channel designs, accurately quantify temperature profiles and species concentrations in the channels, and determine current densities across the fuel cell. This information is in turn used for decision support in material selection.

Changes to the channel design can be achieved simply by changing the CFD model of the flow channel geometry; all other calculation is taken care of automatically. This provides a means for rapidly assessing the effects of design changes in this key area of the stack design.

Typical results from this type of model are high-accuracy maps of key quantities – for example, temperature at various cross sections of the membrane, oxygen and fuel concentrations in the respective channels, and current density across the cell surface.

There are several significant benefits to the hybrid modelling approach: it removes the inconsistency that arises from solving the CFD model equations in a sequential manner, as is typically done in CFD-only applications; and by shifting the calculation from the CFD package can greatly reduce the time required for solving the entire model. In particular, all the knowledge captured in the membrane modelling stage (see case study 1) can be redeployed for detailed design purposes.

Information on the flow channel performance gained from executing the hybrid model can be incorporated into dynamic models for investigating the full stack and system performance.

Case study 3: dynamic system-level model of power plant

In practice, the highly-efficient transformation of chemical energy of fuel into electric energy offered by fuel cells can be fully realised only if the fuel cell is properly operated within a power plant system.

Thus it is important to be able to combine the fuel cell unit model with other component (device) and control system models to create a predictive dynamic model that is capable of simulating transient behaviour of the entire power plant under various load conditions. Typically this involves connecting the cell model with models of the fuel, air supply and exhaust systems, including their associated control systems.

With such a model it is possible not only to accurately simulate behaviour on startup, load change etc, but also possible to optimise various quantities to provide the optimal response within system constraints. Dynamic optimisation techniques can be used to determine, for example, the minimum

startup time while remaining within temperature constraints at critical points in the system.

Similar techniques can be used to determine the optimal sizes of equipment items (for example, reformer diameter) for anticipated load changes. These can be coupled with integer optimisation techniques that select the best process or control configuration from several alternatives. Optimisation allows all of these questions to be answered directly by the model rather than by time-consuming repeated simulation.

A key use for the dynamic model is to control system design. Using co-simulation techniques, with the appropriate software it is possible to use the process model directly within control design toolboxes such as *MATLAB* to design the control scheme. Once the system is designed, it is possible to test the response to any disturbance using the model, and to optimise preliminary control tuning parameters. In some cases it is possible to export the process in a form that can be used in hardware-in-the-loop testing.

Conclusions

The complexity of fuel cell systems mean that it is not possible to examine more than a tiny fraction of interaction-related performance issues using experimental techniques alone. However it is these interactions that will eventually determine whether the cell system is viable or not.

Modelling provides the framework in which it is possible to make decisions – having taken all the simultaneous interactions into account – and thus eliminate designs with deficiencies that might show up only after months of physical testing.

The key advantage of the approach described here is that it is possible to gain a detailed understanding of the fuel cell process based on accurate numerical data, and use this to rapidly refine the design using simulation and optimisation techniques. Not only does this mean that only the most promising design candidates need to proceed to physical testing – thus cutting out significant time and expense – it also means that many more design alternatives can be investigated within the same timeframe.

Increasingly the companies that deploy high-accuracy predictive modelling in a systematic fashion should help gain the advantage in the race to market with commercially viable designs.

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