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# Evaluating PEM fuel cell system models

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#### Abstract

Many proton exchange membrane (PEM) fuel cell models have been reported in publications and some are available commercially. This paper helps users match their modeling needs with specific fuel cell models. The paper has three parts. First, it describes the model selection criteria for choosing a fuel cell model. Second, it applies these criteria to select state-of-the-art fuel cell models available in the literature and commercially. The advantages and disadvantages of commercial models are discussed. Third, the paper illustrates the process of choosing a fuel cell model with an example: the National Renewable Energy Laboratory's (NREL's) evaluation of two detailed stand-alone fuel cell system models. One is from Virginia Tech University, and the other is from Sweden's Royal Institute of Technology. Both models have been integrated into NREL's vehicle simulation model ADVISOR<sup>TM</sup> 2003 (Advanced Vehicle Simulator). © 2003 Elsevier B.V. All rights reserved.

Keywords: Fuel cell; Proton exchange membrane; Advanced vehicle simulator: fuel cell system modelling

# 1. Model selection criteria

Models play an important role in fuel cell development since they facilitate a better understanding of parameters affecting the performance of fuel cells and fuel cell systems. Before selecting a fuel cell model, it is of importance to take the time to clarify what the key features of the desired model are. Although vital for the result, these initial criteria often tend to be overlooked.

For instance, it is useful to state the simulation objective clearly so that linked issues of organizational resources, in terms of personnel, cost and time, can be taken into account. Also the "technical" constraints such as the issues to be addressed by simulation and the required level of details, the level of user knowledge and available information, need to be clarified and understood in order to make the best choice of fuel cell model. If the simulation objective is to provide a tool for education or detailed studies, the development and validation of a fuel cell model in-house is a useful way of gaining knowledge. Often, the development process tends to be costly and time consuming. For smaller projects or engineering applications with reduced resources, validated and reliable commercial fuel cell software may be an appropriate solution. Commercial software here is defined as software, or a module of already existing software, available publicly for

purchase or for free. (The word "model" will in the following text refer to both models found in literature and models in software.) Such software may include ready-to-use fuel cell models with the potential for user-defined modifications or a library of various fuel cell and system components for construction of a customer-adapted model. However, the indicated time-saving aspect of commercial software may not always be true since proper evaluation of demonstration kits of available software can be time consuming depending on the software usually comes with support from the software vendor or developer, the time required for specific software training and model modifications needs to be accounted for.

Thus, the optimal model choice differs for each application and user and the initial decisions are important to avoid costly changes later in the model evaluation process. Once the initial criteria have been set, details such as content and structure of the model should be considered. Table 1 summarizes the key features for model evaluation.

The first criterion in the table is *model approach*. It can be related to, among others, the *system boundary*, the third table item. The system boundary defines the area of interest of the model. It could be on the fundamental cell level including the electrodes and the membrane, the higher level with individual fuel cells assembled in a fuel cell stack, or the high fuel cell system level consisting of a fuel cell stack with its auxiliary system of compressor, pumps and so forth.

A theoretical (sometimes called "mechanistic") fuel cell model is based on electrochemical, thermodynamic and,

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Table 1 Key features of fuel cell models

Model approach (theoretical, semi-empirical)
State (steady-state, transient)
System boundary (fuel cell, stack, system)
Spatial dimension (zero to three dimensions)
Complexity/details (electrochemical,
thermodynamic, fluid dynamic relationships)
Time step (fixed, variable, real-time)
Speed
Accuracy
Flexibility
Source code (open, proprietary)
Graphical representation of model
Library of models, components and thermodynamic properties
Documentation
Validation

sometimes, fluid dynamic relationships, using basic, phenomenological equations such as the Nernst-Planck equation for species transport, the Stefan-Maxwell equation for gas-phase transport, and the Butler-Volmer equation for cell voltage. Depending on its focus, the model may provide details such as cell flow pattern, current density distribution, voltage and pressure drops in the fuel cell stack. If a tool for education or detailed studies is desired, a fuel cell model with a theoretical approach with flexibility in applications and operating conditions is recommended. Usual drawbacks of this type of model are that model development takes time and validation of the fuel cell stack details can be difficult to achieve. On the other hand, there are semi-empirical fuel cell models that are based on experimental data specific to each application and operating condition. As they typically do not provide as many details as theoretical models do and already, at least to some extent, are validated, they may provide a fast start into fuel cell modeling and a good basis for engineering applications. However, because the semi-empirical model is adapted for a specific application, it must be modified for new applications or operating conditions. There is no sharp distinction between theoretical and semi-empirical fuel cell models; for instance, a fuel cell system model may use a more theoretical approach to model the fuel cell and empirical maps of compressors and other devices in the system.

The *state* of the model, either steady-state or transient (or a special case, the quasi steady-state), may also be related to the system boundary. For example, the focus of the model could be on the cell or the system level, and the simulation objective could be for stationary or transportation fuel cell applications. Steady-state models, using one operating point in each step, are useful for sizing components in the system (e.g. heat exchanger area), calculating amounts of materials such as catalysts and parametric studies. Typically, laboratory fuel cells are operated at steady-state. Although the fuel cell responds immediately to variations in load, when integrated into a larger system (composed of compressor, humidifiers and so forth), the other system components will add to the response time. This is especially true if a reformer is included in the system. For use in a vehicle, a model should be dynamic to some degree to account for the important transients in a vehicular fuel cell system; for example, a fuel cell system efficiency calculated at steady-state would give only part of the picture. Transient models can be used for start-up and shutdown procedures, analysis of the influences of various components on flows during a drive cycle, and optimization of the response time on load changes.

Spatial dimension and complexity/details are also important criteria. A description of a fuel cell, with phenomena such as mass transport limitation taken into account, demands at least one dimension. From a fuel cell system perspective, zero-dimensional models using polarization curves can suffice for a system that is not designed to operate at or near the region of the limiting current. They can also be suitable for initial systems optimization. For a proper treatment of the thermal and water management, the model should contain not only electrochemical relationships but also thermodynamic and fluid dynamic equations. Heat transfer equations and mass and energy balances are important for providing an appropriate picture of all processes in the fuel cell and the fuel cell system.

Other criteria related to software include time step (e.g. the ability to use fixed, variable and/or real time steps), speed, accuracy, flexibility and source code. The graphical representation of the model, library of thermodynamic properties and system components, and documentation of the model are features of the finished model. Using fuel cell software with a thermodynamic property library or fuel cell system software with various system component blocks to choose from can provide a benchmark test for a proprietary fuel cell model. Regarding the source code, model input specifications can be complex or the code inflexible, making it difficult to use or alter the code for an application. The user must know the algorithms and/or the simplifications of the model in detail to be able to fully understand and use the model. Ideally, the model should have an open source code with no masked sub-systems. However, this information is often proprietary; a more realistic way to learn about the model is by a well-written manual and tutorial and practical support from the software developer.

Finally, the *validation* of a model is important because a model must be validated to some degree to be a useful and credible tool. Appropriate data are needed for validation. With limited resources, this can be difficult because most data cannot be found in the open literature. Although data from an entire fuel cell system are usually proprietary, data from single fuel cell system components, such as fuel cell stack and compressor, are easier to acquire. Therefore, a way to deal with lack of data is to develop more limited, well-defined sub-system models, validate them separately or in groups and then assemble them for implementation in a larger fuel cell system model.

# 2. Review of fuel cell models

# 2.1. Fuel cell models in literature and modeling in-house

During the past 10 years, several PEM fuel cell models, from simple zero-dimensional to complex three-dimensional models, have been described in the open literature. Many universities, national laboratories and companies have developed their own fuel cell models, all with different modeling approaches and levels of detail [1-31]. Most models are theoretically based, detailed and complex, trying to account for phenomena in fuel cells. The models normally focus on one aspect or region of the fuel cell only. This is unsatisfactory to a user who wants to acquire a more comprehensive fuel cell model, leaving the user the work of assembling and linking several models into a larger model. Some models are semi-empirical, trying to provide a general voltage-current relationship. However, these relationships tend to be specific to one particular fuel cell stack with no real physical justification. The coefficients in the voltage-current equation have to be re-evaluated for each new fuel cell configuration. This limits this type of model as a predictive tool. Fuel cell system models usually use a simplified approach to the electrochemical aspects such as electrode kinetics and mass transport limitation in the fuel cell. These models are generally semi-empirical, with additional thermodynamic and fluid dynamic relationships for the auxiliary system. Table 2 provides an example of the features of some literature models covered for this paper.

# 2.2. Commercial fuel cell software

Re-creating and validating models from the literature can be time consuming, making ready-to-use models an attractive option when time is limited. A few commercial fuel cell models and additional software modules are available, e.g. Emmeskay, ADVISOR<sup>TM</sup> 2002 from the National Renewable Energy Laboratory, General Computational Toolkit (GCTool) from Argonne National Laboratory (ANL), the fuel cell modules in Easy 5 from Ricardo and FEMLAB from COMSOL [32–37]. More commercial models are being developed, especially multi-dimensional models. For example, Ansoft Corporation and Synopsys (formerly Avant!) will make PEM fuel cell system models available in the near future, and Fluent and CD adapco Group will soon release CFD PEM fuel cell packages [38,39].

Fig. 1 shows a selection of fuel cell models available in literature and commercially. The figure provides a systematic overview of the collected fuel cell models. If a more detailed and complex fuel cell model is desired, the user should look on the upper half of the figure. If the user is looking for a fuel cell system model, the box defined by the "0-D" and "Semi-empirical" axis labels is a good starting point.

Table 3 gives a more detailed view of the commercial fuel cell models described below. The information about the upcoming fuel cell modules from Fluent and CD Adapco Group (shown in Fig. 1) is not sufficient for this more detailed comparison. Therefore, the two models are not included in Table 3. Details of the software features shown in Table 3 were found in vendor information, demonstration kits, software manuals and so forth. Information about the models varies greatly and changes over time. The details in Table 3 should therefore be seen as the state-of-the-art as of the time this paper was written.

The Emmeskay fuel cell model is a zero-dimensional fuel cell stack software package. The model is based on the MathWorks graphical simulation code Simulink. It can run fixed and variable time steps and can run in a real time mode. The fuel cell stack in this model is modeled as a "black box", using a MATLAB S-function to link to a compiled proprietary source code. It features details such as water transport across the membrane, water condensation and evaporation, and transfer of the heat generated due to

Table 2

An example of features of some literature fuel cell models covered for this paper	er
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Models	State <sup>a</sup>	System boundary Studied phenomena			
Theoretical approach					
Springer et al. [1]	SS	Fuel cell	Water transport		
Bernardi and Verbrugge [2]	SS	Catalyst layer	Cell polarization, water transport and catalyst utilization		
Fuller and Newman [3]	SS	Fuel cell	Heat and water management and fuel utilization		
Nguyen and White [4]	SS	Gas channels	Heat and water management		
Yi and Nguyen [11]	SS	Fuel cell	Heat and water management, species transport		
Dannenberg et al. [21]	SS	Fuel cell, along-the-channel	Heat and water management		
You and Liu [28]	SS	Cathode catalyst layer	Transport and flow in gas channels and gas diffusers		
Boettner et al. [31]	SS	Fuel cell system	System and system component performance and control strategies		
Semi-empirical approach					
Kim et al. [5]	SS	Fuel cell	Empirical cell polarization equation		
Amphlett et al. [7]	TR	Fuel cell stack	Heat management		
Mann et al. [20]	SS	Fuel cell Generic model			

<sup>a</sup> SS: steady-state; TR: transient.



Fig. 1. An overview of fuel cell models available in literature and commercially.

L31 Boettner et al., 2002 (ref. 31)

reaction. One special advantage of this model is that it includes pressure dynamics. The cathode and anode pressures are controlled via a PI-controller that controls the cathode and anode outlet mass flow rates. The cathode outlet temperature is also controlled via a PI-controller that regulates the coolant mass flow. Having the feature of pressure dynamics enables evaluation of different fuel cell system control

C7 Star-CD fuel cell package

strategies. However, little information on the calculation details of the fuel cell is available because they are property to Emmeskay.

Two empirically based steady-state fuel cell system models are integrated into NREL's publicly released vehicle analysis software ADVISOR<sup>TM</sup> 2002. ADVISOR<sup>TM</sup> is written in MathWorks MATLAB and Simulink. One model Table 3

An overview of some commercial fuel cell software (the assessment of the models refers to the specific fuel cell modules of the software packages)

Model	Emmeskay	ADVISOR <sup>TM</sup> 2002	GCTool	Easy5	FEMLAB
Origin	Emmeskay	NREL	ANL	Ricardo	COMSOL
Dimension	0	0	0	0	2
State					
Transient	+	_	+	+	+
Steady-state	_	+	+	+	+
System boundary					
Cell	_	+	_	_	+
Stack	+	_	_	+	_
System	_	+	+	+	_
Approach					
Theoretical	+	_	_	+	+
Semi-empirical	-	+	+	-	_
Fixed and variable time step option	+	+	_	+	N/A
Complexity					
Cell/stack	Medium	Low	Medium/high	Medium	High
System	N/A	Medium	Medium/high	Medium/high	N/A
Graphical representation	+	+	_	+	+
Library	_	+	+	+	+
Documentation	_	+	+	+	+

N/A = not available.

simply simulates the fuel cell system via maps with characteristic system efficiency as a function of system net power output. An assumption is that the fuel cell system can provide a specified net power while consuming a set amount of fuel independent of the complexity of the system.

The second ADVISOR<sup>TM</sup> 2002 fuel cell system model has a similar approach except that its fuel cell performance is based on a polarization curve, the associated fuel use per cell, and the number of individual cells within the stack. The auxiliary system (e.g. compressor, fuel pump, and cooling fans) can be specified separately from the fuel cell stack and is composed of component maps. The system efficiency/power maps and polarization curves included in the public release, specific for fuel cell stacks of a certain size and power output, were provided by ANL and UTC Fuel Cells (formerly IFC).

One drawback of the two ADVISOR<sup>TM</sup> 2002 models is that thermal and water management is not included. The heat interaction between the fuel cell system and the rest of the vehicle cannot be displayed. Furthermore, sub-models of system components such as reformer and compressor are not included. The two models are displayed as "ADVISOR<sup>TM</sup> 2002" in Table 3. A third fuel cell system model, GCTool from ANL, is included in ADVISOR<sup>TM</sup> 2002 as a co-simulation option. Depending on the user's specific interests, any one of these three models can be used in ADVISOR<sup>TM</sup> to represent the fuel cell interaction with the rest of the vehicle.

GCTool was one of the first fuel cell software packages publicly available. Developed and maintained by ANL, it is a sequential model programmed in a C-based language. It contains models of different types of fuel cells and system components such as reformers, condensers, pumps and nozzles. The user designs system configurations of various component models, which are interconnected by defined flows. Steady-state and dynamic simulations can be performed. GCTool has its own thermodynamic property library, which was one of its major advantages when first released. The GCTool software package includes a manual and examples of how to use the software.

The fuel cell package in Easy5 of Ricardo is similar to GCTool. Both GCTool and Easy5 are block-based fuel cell system simulation software packages, although Easy5 displays information for each block in a more accessible way. Like GCTool, Easy5 has a database containing various system components displayed as blocks that can be arranged in multiple ways. The database includes system components such as fuel cell stack, reformer, gas clean-up and electric and control devices. It also contains thermal and fluid systems models. An advantage of Easy5 is the capability for systems optimization and component sizing. However, in contrast to GCTool, it does not include a thermodynamic property library.

A more detailed fuel cell model is provided in the Chemical Engineering Module of FEMLAB. FEMLAB uses the MathWorks simulation code MATLAB. Here, the PEM fuel cell is a steady-state two-dimensional model. For even more detailed studies, three-dimensional models of individual cell components (e.g. the cathode) are also available. The Chemical Engineering Module offers detailed modeling, including heat and mass transfer phenomena in the fuel cell. One benefit of this package is the post-processing and visualization of the results. It is accompanied by a manual and tutorial.

#### 3. Choosing fuel cell models: an NREL example

#### 3.1. NREL's model selection

As previously discussed, the three existing fuel cell system models in ADVISOR<sup>TM</sup> 2002 provide tools for evaluating fuel cell vehicles. However, NREL decided that fuel cell system models with more flexibility and details were needed. NREL's simulation objective was to provide a tool for more detailed studies such as parametric studies, component sizing and optimization. With a robust stand-alone fuel cell system model, system parameters such as cell temperature, cell pressure and stoichiometric coefficients for the anode and cathode flows can be optimized.

The aim was also to integrate the fuel cell system model into ADVISOR<sup>TM</sup> so that effects of the auxiliary system on the fuel cell system power output and on the rest of the fuel cell vehicle are taken into account. Hence, integrating the model into ADVISOR<sup>TM</sup> enables the results to be displayed in a vehicle context (e.g. fuel economy, vehicle mass, acceleration, grade tests and multiple drive cycles).

One of NREL's constraints was time (limited to about 6 months); this made ready-to-use models attractive. Both discrete and continuous analysis of the system was anticipated. Among the issues to be addressed by simulation were thermal and water management and start-up requirements. In addition to using the criteria discussed in the Model Selection Criteria section of this paper, NREL wanted a model based on MATLAB/Simulink to facilitate implementation into ADVISOR<sup>TM</sup>.

## 3.2. Comparison of two fuel cell system models

NREL decided to evaluate two models that were recently made available: the Virginia Tech (VT) model and the Royal Institute of Technology (KTH) model. The two fuel cell system models share similar features. They are zero-dimensional models based on MATLAB/Simulink and have open source codes. They combine empirical component data maps with theoretical models to predict performance and thermal and water management. In Fig. 1, the two models would be located in the lower left box of the matrix (semi-empirical, zero-dimensional).

### 3.3. VT fuel cell system model

The VT fuel cell system model (Fig. 2), developed by Virginia Tech in collaboration with NREL, consists of a fuel cell model and an auxiliary system model [40]. It is a transient, semi-empirical model that accounts for the thermal management and water balance in the system. The fuel cell model is a polarization curve based on a specific fuel cell stack available to VT. Its compressor model uses maps with data from Opcon Autorotor [41].

The model is designed for incorporation into ADVISOR<sup>TM</sup> 2003. The goals of the model are to provide hot- and cold-start effects on vehicle fuel economy, power limitations due to temperature, and a water balance for reactant humidification. The following are examples of the model's inputs (constants and parameters):

- number of cells and active cell area;
- stoichiometric coefficients of anode and cathode inlet flows;
- air compressor and pump characteristics;
- minimum cell voltage and current density;
- maximum coolant temperature;
- constants: open circuit voltage, heat capacities, molecular weights, density and specific heat ratio of air, lower heating value of hydrogen and so forth;



Fig. 2. The VT fuel cell system model [40].



Fig. 3. An example of output of the VT fuel cell system model: the system efficiency as a function of the system net power and fuel cell system operating temperature.

- initial conditions: temperatures of the ambient air, reservoir, radiator, cathode outlet, compressor outlet, humidifier outlet, inlet coolant ambient pressure and humidity minimum coolant mass flow rate;
- condenser percentage recovery.

Outputs of the VT model are net power output from the fuel cell system and system characteristics. The system characteristics include auxiliary system power requirements (e.g. air compressor, condenser fan, and coolant pump), mass flows at various points, heat losses, water generation, water balance, cell voltage and current. An example of the impact of the fuel cell system operating temperature on the system efficiency is shown in Fig. 3.

An example of the fuel cell system in a vehicle context is provided in Fig. 4, where the output from the VT fuel cell system model integrated into ADVISOR<sup>TM</sup> 2003 is displayed. The figure shows an efficiency comparison between hot- and cold-start modes on a highway drive cycle. There is a clear cold-start penalty, shown as lower system efficiency and as longer time for reaching the fuel cell operating temperature. (This particular drive cycle normally runs with hot start.)

#### 3.4. KTH fuel cell system model

The KTH fuel cell system model (Fig. 5) shares similar features with the VT model. It is a semi-empirical model with thermal and water management [42]. However, the KTH model is a steady-state model. Furthermore, the fuel cell stack component of the model is theoretical, partly based on work by Springer et al. [1] and accounts for phase changes of the water in the fuel cell stack. The model's theoretical approach allows for stack definition, i.e. calculation of the number of cells based on the required maximum power output of the system. With assumptions of active area and stoichiometric coefficients of hydrogen and air, it could be used for any fuel cell stack, giving the model a significant flexibility.

The auxiliary system includes a hydrogen tank and power demand calculations for individual pumps and fans. It also contains maps with compressor data from Opcon Autorotor. The system allows hydrogen to be re-circulated and allows for the water produced in the stack to be condensed and used in the humidifiers. Heat produced in the fuel cell stack is transferred to a cooling loop. The model also accounts for frictional losses found in lines, elbows and filters.

Inputs for the KTH model are similar to those for the VT model. Examples of unique features include the purge percentage (the amount of the anode exhaust to be removed from the system) and pipe diameter and length.

The model outputs are the net fuel cell system power, the stack definition and system characteristics such as mass flow of the reactants, product, inert material and coolant, heat developed in the stack, individual auxiliary parasitic loads, water balance of the fuel cell system (including humidifiers and condensers), and the efficiency of the fuel cell and system.



Fig. 4. An example of output from the VT fuel cell system model integrated into ADVISOR<sup>TM</sup> 2003: the system efficiency comparison between hot and cold start modes on the US EPA Highway drive cycle.



Fig. 5. The KTH fuel cell system [42].

An example of the results of the KTH fuel cell system model integrated into ADVISOR<sup>TM</sup> 2003 is provided in Fig. 6. A small fuel cell vehicle of about 1000 kg using the fuel cell system power output of 48 kW and 43% at peak



Fig. 6. An example of the KTH fuel cell system model integrated into ADVISOR<sup>TM</sup> 2003 using the US EPA Highway drive cycle to simulate the load of a small fuel cell vehicle.

load is simulated using the US EPA Highway drive cycle. The upper diagram shows the drive cycle speed specification and vehicle speed in miles per hour (mph). The three diagrams below display the impact of the auxiliary system on the net fuel cell system power output. The first of these diagrams displays net system power achieved during the cycle. The diagram below shows the variation of the auxiliary system power demand, including those of the compressor, pumps, and fans. The major component of the auxiliary system power load is that of the compressor, and its power demand is also shown in the diagram. The variation in the fuel usage during the drive cycle is shown in the diagram at the bottom of the figure.

# 4. Discussion

Table 4 compares the VT and KTH fuel cell system models. Although they have similar features (e.g. dimension, system boundary and environment), there are distinct differences. For instance, the fuel cell model approach of the KTH model departs from the VT model in the details of the electrochemistry. The KTH model has a more theoretical and more general approach. The VT model has more details on heat transfer, whereas the KTH model has fluid dynamic details. One option in the future is to combine the more detailed thermal models of the VT model with the detailed fuel cell model of the KTH model to provide an optimal fuel cell system model that accounts for heat transfer over

Table 4Comparison of the VT and KTH models

Model	VT	KTH				
Origin	Virginia Tech	Royal Institute of Technology, Sweden				
Dimension	0	0				
State						
Transient	+	_				
Steady-state	—	+				
System boundary	_	_				
Stack	+	+				
System	+	+				
Approach—overall						
Theoretical	-	-				
Semi-empirical	+	+				
Approach-fuel cell						
Theoretical	_	+				
Semi-empirical	+	_				
Complexity						
Cell/stack	Medium Medium/high	Medium/high Medium/high				
System	Medium/mgn	Wedum/mgn				
Thermodynamics and fluid dynamics	+	+				
Environment	MATLAB/Simulink	MATLAB/Simulink				
Speed in the UDDS cycle (1369 s)						
<1/90 real time (15 s)	+	-				
<1/30 real time (45 s)	-	+				
Fixed and variable time step option	+	+				
Flexibility	+	+				
Graphical representation	+	+				
Documentation	+	+				

system boundaries. The combination of the VT and KTH fuel cell system models could form a valuable tool for future parametric and optimization studies.

Both models are fast as stand-alone models. When integrated into ADVISOR<sup>TM</sup> 2003, the solution speed is lowered to in the order of 1/30th real time. The UDDS drive cycle serves here as basis for comparison. Real time matches the drive cycle that is about 20 min long. The VT model is somewhat faster than the KTH model. This is due to the architecture differences of the models; the VT model has a Simulink block structure whereas the KTH model is based on MATLAB m-functions.

Neither of the models have the option to run either at fixed or variable time steps. They both run at fixed time step, facilitating integration of the models into ADVISOR<sup>TM</sup> 2003, which runs at fixed time step. A newly developed variable/fixed time step model at NREL will enable integration of models running at variable time steps.

Because the source code is open, the VT and the KTH models are very flexible, enabling easy integration of new blocks and features into the models. Another feature making

understanding the systems easy is the fact that the models are based on Simulink with graphical blocks and flow interconnects. The documentation of the models, available in papers and theses, will also facilitate the use of the models.

None of the models have yet been validated as a whole. With data for system components such as the compressor and the fuel cell stack in the VT model and the compressor in the KTH model, the models could be seen as only partly validated. It is, however, NREL's intention to validate the models with data of other system components in the near future.

## 5. Conclusion

The choice of whether to develop a proprietary fuel cell model or acquire ready-to-use software depends on the simulation purpose and constraints such as time and cost. This paper presents and discusses a list of key fuel cell model features and a way of systematically classifying fuel cell models to facilitate evaluation of appropriate fuel cell models for a specific application.

Fuel cell models from the literature are classified into groups such as state, dimension and model approach. Fuel cell software packages that are, or soon will be, available are also classified and discussed. Finally, a more detailed evaluation of two fuel cell system models is presented and discussed. In combination, the VT and KTH fuel cell system models form a valuable tool for parametric and optimization studies. Separately, they function well when integrated into ADVISOR<sup>TM</sup> 2003. In future work, NREL intends to validate the two fuel cell system models with data of various system components.

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#### References

- [1] T. Springer, et al., J. Electrochem. Soc. 138 (1991) 2334.
- [2] D. Bernardi, M. Verbrugge, J. Electrochem. Soc. 139 (1992) 2477.
- [3] T. Fuller, J. Newman, J. Electrochem. Soc. 140 (1993) 1218.
- [4] T. Nguyen, R. White, J. Electrochem. Soc. 140 (1993) 2178.
- [5] J. Kim, et al., J. Electrochem. Soc. 142 (1995) 2670.
- [6] K. Weisbrod, et al., Proc. Electrochem. Soc. 95-23 (1995) 152.
- [7] J. Amphlett, et al., J. Power Sour. 61 (1996) 183.
- [8] D. Thirumulai, R. White, J. Electrochem. Soc. 144 (1997) 1717.
- [9] M. Wöhr, et al., Int. J. Hydrogen Energy 23 (3) (1997) 213.
- [10] K. Broka (Dannenberg), P. Ekdunge, J. Appl. Electrochem. 27 (1997)
- 281. [11] J. Yi, T. Nguygen, J. Electrochem. Soc. 145 (1998) 1149.
- [12] D. Xue, Z. Dong, J. Power Sour. 76 (1998) 69.
- [13] V. Gurau, et al., AIChE J. 44 (11) (1998) 2410.

- [14] M. Eikerling, A. Kornyshev, J. Electroanal. Chem. 453 (1998) 89.
- [15] M. Virji, et al., J. Power Sour. 71 (1998) 337.
- [16] J. Lee, T. Lalk, J. Power Sour. 73 (1998) 229.
- [17] J. Yi, T. Nguyen, J. Electrochem. Soc. 146 (1) (1999) 38.
- [18] G. Squadrito, et al., J. Appl. Electrochem. 29 (1999) 1449.
- [19] S. Um, et al., J. Electrochem. Soc. 147 (2000) 4485.
- [20] R. Mann, et al., J. Power Sour. 86 (2000) 173.
- [21] K. Dannenberg, et al., J. Appl. Electrochem. 30 (2000) 1377.
- [22] V. Gurau, et al., J. Electrochem. Soc. 147 (2000) 2468.
- [23] R. Cownden, et al., Int. J. Hydrogen Energy 26 (2001) 615.
- [24] J. Hamelin, et al., Int. J. Hydrogen Energy 26 (2001) 625.
- [25] B. Eaton et al. in: Proceedings of the ASME, International Mechanical Engineering Congress Exposition, 2001.
- [26] G. Maggio, et al., J. Power Sour. 101 (2001) 275.
- [27] A. Kulikovsky, Fuel Cells 1 (2001) 162.
- [28] L. You, H. Liu, Int. J. Heat Mass Transfer 45 (2002) 2277.
- [29] T. Berning, et al., J. Power Sour. 106 (2002) 284.
- [30] L. Pisani, et al., J. Power Sour. 108 (2002) 192.
- [31] D. Boettner, et al., Trans. ASME 124 (2002) 20.
- [32] Emmeskay Documentation, for more information www.emmeskay. com.

- [33] K. Wipke, et al., IEEE Trans. Vehic. Technol.: Hybrid Elec, Vehic. 48 (6) (1999) 1751–1761.
- [34] T. Markel, et al., J. Power Sour. 110 (2002) 255.
- [35] Argonne National Laboratory, General Computational Toolkit (GC-Tool) Documentation, for more information www.transportation. anl.gov/modeling.
- [36] COMSOL, FEMLAB Documentation, for more information www.comsol.com/products/chem.
- [37] Ricardo (Easy5 fuel cell module) Documentation, for more information www.ricardo.com.
- [38] Fluent Documentation, for more information www.fluent.com.
- [39] CD Adapco Group (Star-CD) Documentation, for more information www.cd-adapco.com.
- [40] S. Gurski, Cold start effects on performance and efficiency for vehicle fuel cell system, MSc Thesis, Virginia Polytechnic Institute and State University, 2002.
- [41] G. Kulp, D. Nelson, in: Proceedings of the SAE, 2001-FTT-63 (2001).
- [42] K. Johansson (Haraldsson), Modelling of a proton exchange membrane fuel cell system for automotive applications, Licentiate of Engineering Thesis, Royal Institute of Technology, Stockholm, Sweden, 2001.