Project no.: **CT-2004-508341**

Project acronym: **PEMTOOL**

Project title: **Development of novel, efficient and validated software-based tools for PEM fuel cell component and stack designers**

Instrument **Co-operative Research Project**

Thematic Priority **Sustainable Energy Systems**

Final activity report

Period covered: from **31st May 2005** to **31st December 2007** Date of preparation: **January 2008**

Start date of project: **31st May 2005** Duration: **24 months** (extended to 31 months)

Project coordinator **Michael Vynnycky**
Project coordinator organisation **KTH**

1 Project execution

Objectives

The scientific and technical objectives of PEMTOOL are:

- **scientific:** to obtain an understanding of the interaction of the wide range of physical phenomena that occur in a PEM fuel cell, with a view to controlling that interaction in order to optimise the performance of the cell and arrangement of cells (stacks).
- **technical**: to develop a validated modelling tool that is able, quickly and efficiently, to predict this interaction and to guide its user towards the optimisation of cells and stacks.

The overall objective is that, at the end of the project, there should exist efficient and validated software tools that can be used by SMEs for optimising PEM fuel cell design. The specific measurable objectives are as follows:

1) to accelerate the development cycle, in terms of time, for PEM fuel cell product development by 50-60%;
2) to cut the cost of PEM fuel cell product development by 50-60%;
3) to improve PEM fuel cell performance by 30-50%.

Contractors involved:

Royal Institute of Technology in Stockholm	(KTH)
Cellkraft AB	(CEL)
Comsol AB	(COM)
Environment Park S.P.A.	(ENVI)
Hysytech S.R.L.	(HST)
Fundacion INASMET	(INASMET)
Volvo Technology Corporation	(VOL)

Work performed

In PEMTOOL:

- 3 SMEs (Cellkraft, Environment Park and Hysytech) whose core business involved the design and development of polymer electrolyte fuel cells (PEFCs) and one (Comsol) which develops numerical software, a potential capability of which is to act as modelling tool for assisting in the design of PEFCs, have made a list of specifications regarding primary issues of interest in PEFCs
- 2 RTD performers (KTH and INASMET) supply theoretical knowledge
- Theory is then programmed into Comsol's software, Comsol Multiphysics
- Cellkraft, Environment Park and Hysytech perform experiments on PEFCs, both to determine material input data necessary for modeling, and output necessary for model validation

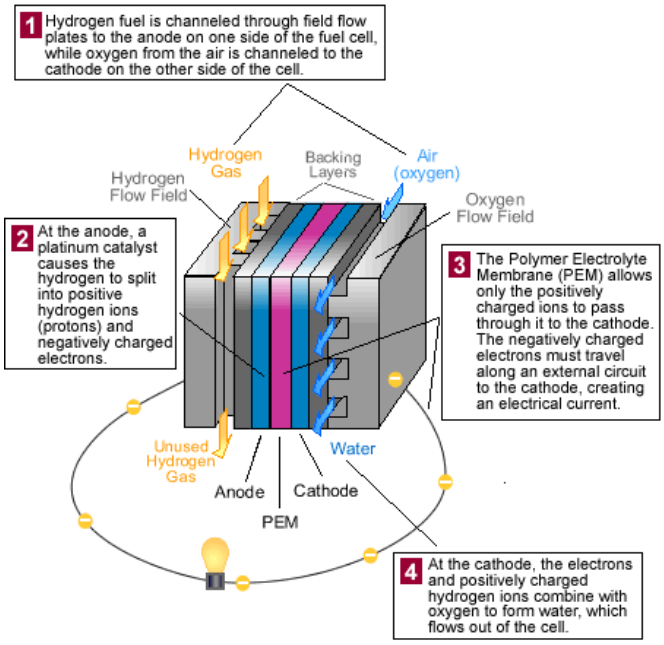

Figure 1: Schematic of the operation of a PEFC

- A large end-user (Volvo) performs experiments on a PEFC stack, which the validated models help to optimize.

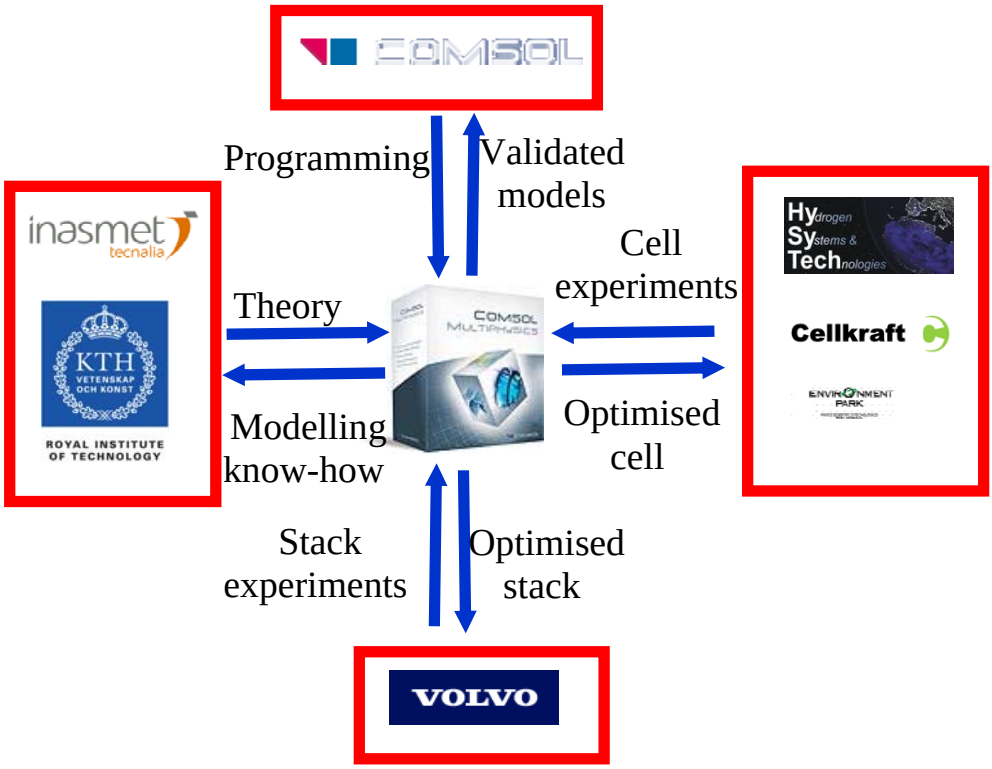

Figure 2: PEMTOOL work structure

The work structure, showing the interaction between SMEs, RTD performers and the large end-user is shown in Fig. 2 above.

Results achieved

- extensive set of experimental data of the performance of different PEFCs using the same components under different operating conditions

- derivation and analysis of theoretical models that encompass both the participating SMEs' specifications, as well as the latest literature
- implementation of models in commercially available software (Comsol Multiphysics)
- numerical solutions for both one- and two-phase flows for one- and two-dimensional models
- an up-to-date literature review of degradation mechanisms in PEFCs

It had been hoped that unambiguous validation of the model against the polarisation curve data of the PEFC used by one of the SMEs would be achieved. This was not achieved before the project ended; however, the experimental data has been retained and will form the basis of future Ph.D. projects.

Methodologies and approaches employed

The project uses a wide array of experimental techniques to determine the physical properties of PEFC components and their performance under actual operating conditions. In addition to standard techniques for measuring polarization curves, other techniques were developed for determining the structural mechanical properties of the porous gas diffusion layer, and a method for measuring the flow of water through a polymer electrolyte membrane. The results of these were used as input for mathematical modelling activities; derived models were implemented into finite-element software.

Project achievements relative to the state-of-the-art

The unique combination of experimental work, theoretical modelling, mathematical analysis and numerical simulation ensures that the work performed in PEMTOOL is state-of-the-art:

- the project takes account of the most recently available experimental and theoretical literature on PEFCs in relevant conference proceedings and journals, in order derive the necessary models.
- where appropriate, the physics within these models is developed further for the particular needs of the project, i.e. with respect to current density range, physical phenomena
- unlike in most previous models, mathematical analysis is conducted to enable systematic model reduction, which then leads to faster solution times
- the models are programmed in a state-of-the art finite-element multiphysics software package

Project impact on its industry/research sector

The project has increased the knowledge base in polymer electrolyte fuel cells both experimentally and theoretically at the university, research institute, the SMEs and the end-user that participated. From the industrial perspective, the availability of a tool to help predict good cell design from the point of e.g. good structural mechanical principles, is a significant step forward. From the research point of view, the gathering of accurate experimental results for the same components in different cells is perhaps unique, and should ensure that successful validation of the model will be forthcoming in the near future.

Logo

Website: https://www2.mech.kth.se/pemtool

2 Dissemination and use

Section 1 - Exploitable knowledge and its Use

Exploitable Knowledge (description)	**Exploitable product(s) or measure(s)**	**Sector(s)** of application	Timetable for commercial use	Patents or other IPR protection	**Owner** & Other Partner(s) involved
GDL characterisation technique	Standard method development for GDL and porous membrane	Industrial (fuel cells)	Short term	-	HST
PEFC reduced theoretical model	-	Academic, Industrial	-	-	KTH*
PEFC structure mechanics model	-	Academic, Industrial	-	-	INASMET*
PEFC numerical model	-	Academic, Industrial	-	-	COMSOL

*All IPR passes to SMEs.

Section 2 – Dissemination of knowledge

Planned/ actual dates	**Type**	**Type of audience**	**Countries addressed**	**Size of audience**	**Partner responsible /involved**
1.11.2005-	*Project website*	*General public*	**ANY**	*-*	*KTH*
26.6.2006	*Conference*	*Research*	**ANY**	*~30*	*KTH*
25.9.2006	*Conference*	*Research*	**ANY**	*~30*	*KTH*
21-26.1.2007	*Winter School*	*Research*	**ITALY**	*~30*	*HYS*
1.2.2007	*EU Brokerage event*	*Research*	**ANY**	*~200*	*KTH*
6-7.3.2007	*Conference*	*Research*	**ANY**	*~100*	*KTH*
30.5.2007	*Conference*	*Research,industry*	**SWEDEN**	*~100*	*KTH*
6-8.6.2007	*Conference*	*Research*	**ITALY**	*~200*	*ENVI*
15.6.2007	*Journal article*	*Research*	**ANY**	*-*	*KTH*

Details:

- Project website at www.pemtool.net (https://www2.mech.kth.se/pemtool from December 2007)
- *A reduced model for 3D heat and mass transport in PEFCs*, presented at 6th Euromech Fluid Mechanics Conference, Stockholm 26-30 June 2006 (authors: P. Yakubenko, G. Shugai & M. Vynnycky; presenter: P. Yakubenko)
- *Model of water transport processes for PEM in contact with water vapour*, presented at Nordic PEMFC 06, Stockholm 25-27 September 2006 (authors: G. Shugai, P.Yakubenko, P.Gode and M. Vynnycky; presenter: G. Shugai)
- *Presentation at a winter school on state of art & future of "Hydrogen & Fuel Cell Technologies" in Bardonecchia, Italy, 21-26 January 2007* (presenter: M. Antonini)
- Poster presentation at EU-sponsored FP7 Information & Brokerage Day on Hydrogen and Fuel Cells, 1 February 2007, Prague.

- *Towards segmented-cell validation of PEFC modelling*, presented at the 4th Symposium on Fuel Cell Modeling and Experimental Validation, 6-7 March 2007 in Aachen, Germany (presenter: M. Vynnycky)
- *Modelling the multiphysical heart of a polymer electrolyte fuel cell*, presented at the 2nd Nordic Conference on Fluid Dynamics in the Power Industry, 30 May 2007, Älvkarleby, Sweden (presenter: M. Vynnycky)
- *Research of a HySyLab internal standard procedure for single PEMFC*, presented at HySyDays – 2nd World Congress of Young Scientists on Hydrogen Energy Systems, 6-8 June 2007, Turin, Italy (authors: R. Cuccaro, A. Battaglia, M. Lucariello, A. Graizzaro; presenter: R. Cuccaro)
- *On the modelling of two-phase flow in the gas diffusion layer of a polymer electrolyte fuel cell*, Applied Mathematics and Computation **189** (2007) 1560-1575 (author: M. Vynnycky)

Section 3 - Publishable results

As of 31 December 2007, the consortium had published one peer-reviewed journal article and one article in conference proceedings:

1. Vynnycky, M., *On the modelling of two-phase flow in the gas diffusion layer of a polymer electrolyte fuel cell*, Applied Mathematics and Computation **189** (2007) 1560-1575.
2. Cuccaro, R., Battaglia, A., Lucariello, M. and Graizzaro, A., *Research of a HySyLab internal standard procedure for single PEMFC*, presented at HySyDays – 2nd World Congress of Young Scientists on Hydrogen Energy Systems, 6-8 June 2007, Turin, Italy.

The experimental and modelling results generated in the course of the project will lead to further publications (tentative titles):

3. Shugai, G., Yakubenko, P., Mellgren, N. and Vynnycky, M., *Asymptotically reduced modelling of PEFCs* (to be submitted to SIAM Journal on Applied Maths)
4. Vynnycky, M., *Further numerics of two-phase flow in the gas diffusion layer of a polymer electrolyte fuel cell* (to be submitted to Applied Mathematics and Computation)
5. Vynnycky, M., *Analysis of non-isothermal two-phase flow in the gas diffusion layer of a polymer electrolyte fuel cell* (to be submitted to Applied Mathematics and Computation).
6. Cellkraft & KTH, *Parameter extraction for PEFC modelling* (*spiral cell experiments and 1D model*): *one-phase conditions*, in preparation.
7. Vynnycky, M., *2D two-phase flow in GDLs*, in preparation.
8. Cellkraft & KTH, *Parameter extraction for PEFC modelling* (*spiral cell experiments and 1D model*): *two-phase conditions*, in preparation.
9. Volvo & KTH, *2D non-isothermal two-phase fuel cell model*, in preparation.
10. INASMET & KTH, *Structure mechanics in fuel cells*, in preparation.
11. Yakubenko, P., Shugai, G., Gode, P. and Vynnycky, M., *Model and experiments on a membrane* (to be submitted to J. Electrochem. Soc.)
12. Envipark & KTH, *Triple serpentine cell: modelling and experiment.*

The ordering 3-12 is an indication of how much further work is necessary to prepare the manuscripts for submission, i.e. how complete a potential manuscript already is; thus, in the case of lower numbers, most of the results have been obtained already, but need to be written up in appropriate form, whereas for the highest numbers, considerable further effort would be necessary, both in terms of writing and computation/experiment to complete the manuscript.