Parametric Study of the Hydrogen Fuel Cell Electrochemical Model

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Markku Ohenoja

Department of Process and Environmental Engineering

Control Engineering Laboratory

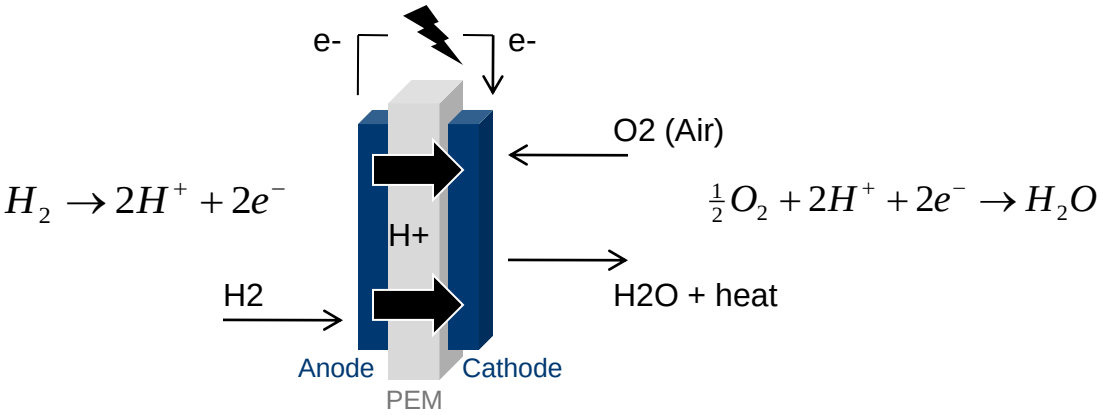
Background

- Hydrogen production for fuel cells by bioethanol reforming (REFORMH2)
- Simulation and optimization of the process chain:

- Dynamic model for hydrogen fed fuel cell (→ PEMFC)

PEMFC?

= Polymer Electrolyte Membrane Fuel Cell



- Maximum output voltage ≈ 1 Volt
- Fuel cell stacks include dozens of FCs
- Suitable applications:
    - Batteries
    - Transportation
    - Localised power generation

PEMFC

+ Low operating temperature and pressure
+ Fast response times on load changes
+ High efficiency comparing to heat engines
+ Pollution-free
+ Flexibility

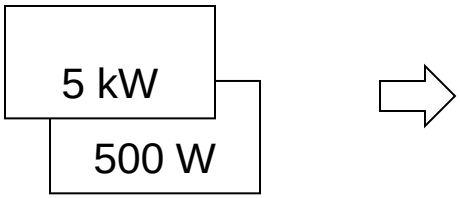
- Catalyst costs
- Low tolerance of impurities
- Distribution of hydrogen (→ Direct Alcohol Fuel Cells)

Progress of the research

- Modelling of two different scale fuel cell systems
  - 5kW stack: 35 fuel cells, maximum load current 300A, cooling system
  - 500W stack: 48 fuel cells, maximum load current is limited to 25A, no internal cooling
- Parameter fitting for the two electrochemical models
  - Model 1 has 7 tuneable parameters
  - Model 2 has 3 tuneable weighting factors
- Sensitivity analysis for Model 1

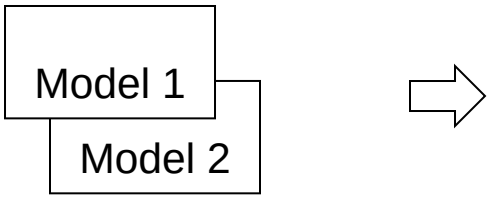
Modelling

Stack models



Dynamic performance
Electrochem. module
Heat balance
Mass balance

Electrochemical models



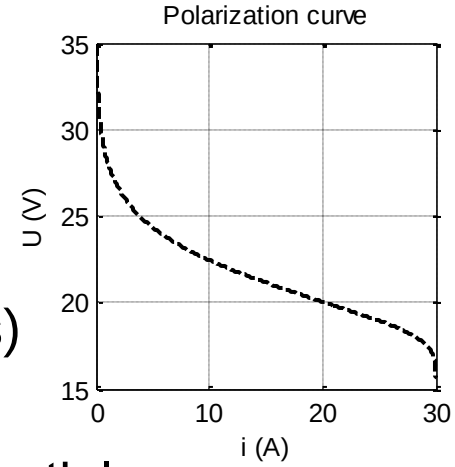
Internal potential
Activation overpotential
Concentration overpotential
Ohmic overpotential

Parameter identification

- Different fuel cell stacks were simulated by changing the properties and operation conditions:

Stack:	N	A (cm^2)	l (cm)	I_{max} (A)	T (K)	P_{H2} (atm)	P_{O2} (atm)
SR-12	48	62,5	0,0025	42	323	1,47628	0,2095
BCS	32	64	0,0178	30,016	333	1	0,2095
Ballard	35	50,6	0,0178	75,9	343	1	1
250W	24	27	0,0127	23,22	343-353	1-3*	1-5*

Parameter fitting



- Parameter fitting was based on voltage-current characteristics (polarization curves)
- Model 1 has seven tuneable parameters
  - ξ1, ξ2, ξ3, ξ4 for activation overpotential
  - Rc, λ for ohmic overpotential
  - B for concentration overpotential
- Model 2 has one weighting factor (Kact, Kohm, Kconc) for each overpotential term

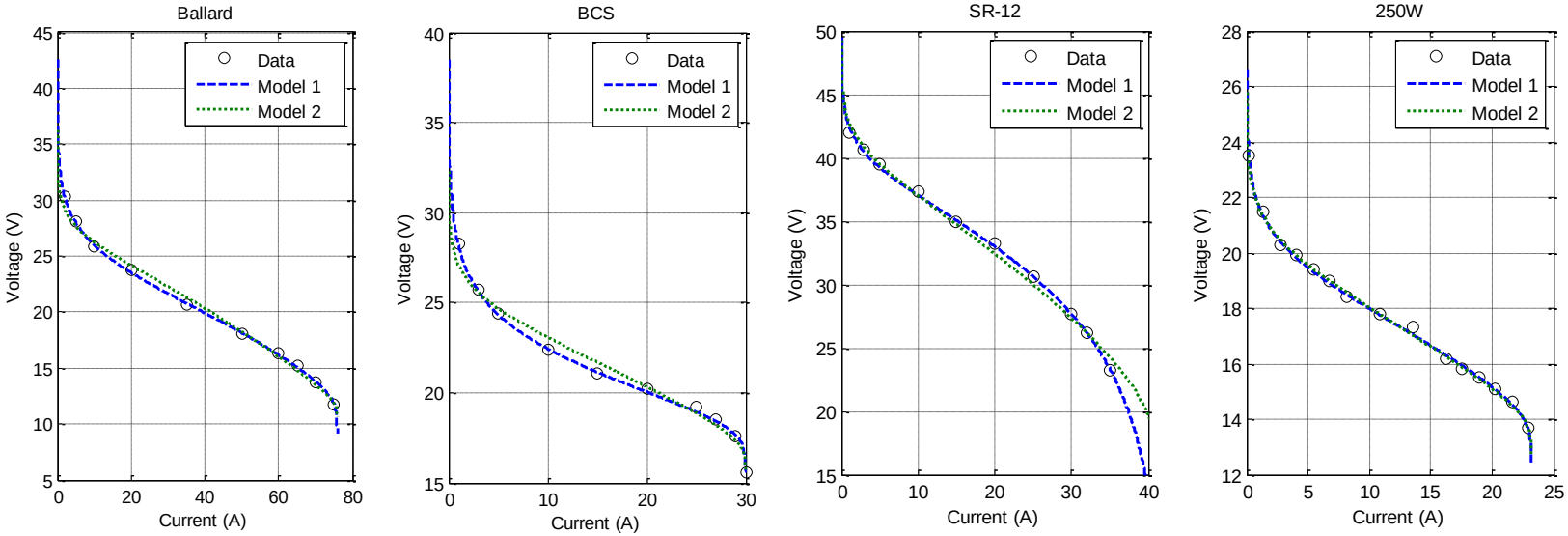
```
% Model 1
Enernst=1.229-0.85e-3*(T-298.15)+4.3085e-5*T*log(Ph2.*Po2.^0.5);
Vact=-(xi1+xi2*T+xi3*T.*log(i)+xi4*T*log(Co2));
Vohm=i.*(Rm+Rc);
Vcon=-B*log(1-i./imax);
V1=N.*(Enernst-Vact-Vohm-Vcon);
```

```
% Model 2
Enernst=1.229-0.85e-3*(T-298.15)+4.3085e-5*T*log(Ph2.*Po2.^0.5);
Vact=Kact*(0.9514*1.0284-2.2e-3*T+T*0.4*1.87e-4.*log(i));
Vohm=-Kohm*(-0.0158+3.8e-5*T-3.0e-5.*i).*i;
Vcon=-Kconc*4.3085E-5*T*log(1-i./imax);
V2=N.*(Enernst-Vact-Vohm-Vcon);
```

Parameter fitting

- Parameter fitting was done with the Genetic Algorithms optimization method
    - GA are stochastic method which mimic the evolution in the nature
    - The population consisting of chromosomes improves towards a better solution
    - Chromosomes include the parameters to be optimized
    - Crossover and mutation operations, elitism
- Objective function was SSE between the simulated values and measured values
- Optimization was repeated 500 times

Results



Model 1

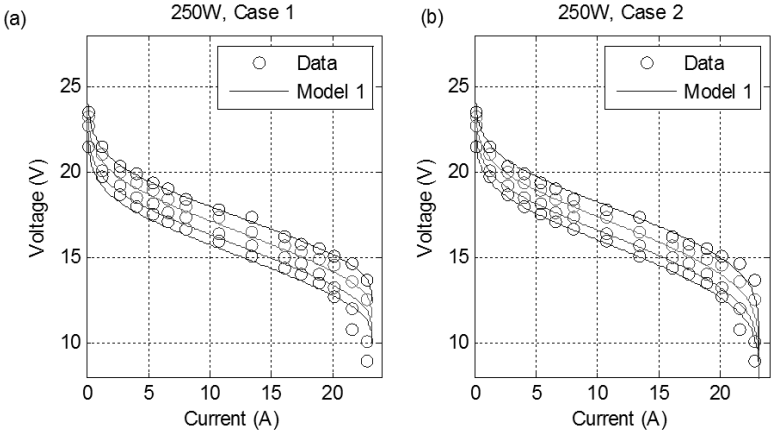
	Minimum	ξ_1	$\xi_2 \cdot 10^{-3}$	$\xi_3 \cdot 10^{-4}$	$\xi_4 \cdot 10^{-5}$	B	λ	$R_c \cdot 10^{-4}$
Ballard	0,0918	-0,8922	2,9497	-1,9077	8,2096	0,0156	22,3209	1,6872
BCS	0,1040	-1,1044	3,6177	-2,0805	7,8346	0,0146	23,9823	1,0207
SR-12	0,4475	-0,9151	3,0500	-0,9565	7,6636	0,1541	17,2415	1,0523
250W	0,1679	-1,1048	3,3081	-1,2246	6,8258	0,0138	11,9561	4,7566

Model 2

	Minimum	K_{act}	K_{ohm}	K_{conc}
Ballard	2,4432	1,4529	0,8892	0,4473
BCS	2,6729	1,3688	1,3656	0,7201
SR-12	3,0958	1,1319	1,3805	2,9989
250W	0,2931	1,3706	2,1446	0,7464

Results

- Validation of the results is impossible for the three fuel cells with only one data set (curve) available
- Validation for the fuel cell with four datasets shows that optimization should contain more than one dataset

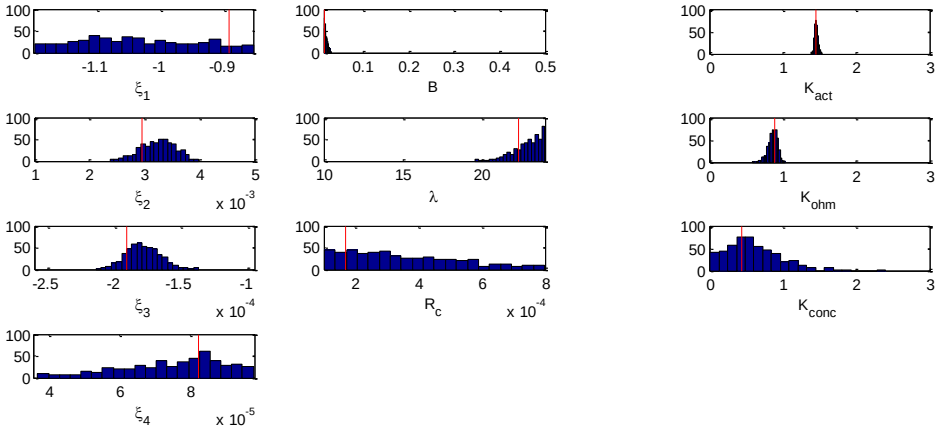


	SSE
Range 1	8,4854
Range 2	16,2746
Mo et al. 2006	16,6082

- Optimization with two datasets gives promising results comparing optimization results presented in literature

Results

- Statistically Model 2 gives a better confidence on the parameter values



- Model 1 needs some further examination, it seems that the parameter ξ1 is dominating the search

Results

- Parameter sensitivity for Model 1 was examined with normalized sensitivity function

Sensitivy indices

	ξ1	ξ2	ξ3	ξ4	B	λ	Rc
BCS	**1,6555**	**1,8058**	0,26613	**0,60649**	0,023917	0,064062	0,0024529
250W	**1,7726**	**1,7998**	0,14237	**0,51845**	0,062756	0,097838	0,0028261

- Parameters ξ2 and ξ1 are the most sensitive in Model 1 with quite equal sensitivity indices
- The results are in good conformance with the literature

Importance of the parameter

	ξ1	ξ2	ξ3	ξ4	B	λ	Rc
NSC	2	1	4	3	6	5	7
Correa et al.	1	-	3	2	5	4	6

Summary

- Two PEM fuel cell stack models including electrochemical model, energy balance and mass transfer
- Both electrochemical models can be tuned, Model 1 is more accurate
- Genetic algorithms can be used directly for parameter identification
- Identification should be based on several datasets
- Parameters ξ2 and ξ1 are the most sensitive in Model 1