

# Hydrogen Energy Systems: Development of Modelling Tools and Applications

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**Abstract:** This paper deals with the modelling and optimisation of a series of typical hydrogen systems. The systems models have been developed on the TRNSYS<sup>1</sup> platform. The mathematical models and the methodology used for analysis are described in this paper, as well as the validation of the models. An application on an island in Norway is also presented.

## 1. Introduction

The so-called hydrogen economy and the energy systems associated with it are often presented as the means to solve both global warming and depletion of fossil fuel resources. However, the technology is still immature and the performance of prototype hydrogen systems is often disappointing when compared to conventional alternatives. This poor performance can often be attributed to poor design of the system and controls, coupled with ad-hoc selection of components. However, analysis using computer models can help to improve the situation, leading to more robust hydrogen demonstration system designs, and move what is a research field towards technical and commercial viability.

The University of Strathclyde in Glasgow and SgurrEnergy, an engineering consultancy specialising in renewable energy in Glasgow, have been working in collaboration for two years on developing generic computer models suitable for the analysis and optimisation of hydrogen system designs. These systems models make use of a suite of hydrogen component models developed by Institute for Energy Technology in Norway.

## 2. Hydrogen components models

### PV generator

The model of the PV generator is based on an equivalent circuit of a one-diode as shown in Fig. 1. The relationship between the operation current  $I$  and the operation voltage  $U$  of the equivalent circuit can be expressed by:

$$I = I_L - I_D - I_{sh} = I_L - I_0 \left\{ \exp\left(\frac{U + IR_s}{a}\right) - 1 \right\} - \frac{U + IR_s}{R_{sh}}$$

with  $I_L$  the light current (A),  $I_D$  the diode current (A),  $I_{sh}$  the shunt current (A),  $I_0$  the diode reverse current (A),  $R_s$  and  $R_{sh}$  the series and shunt resistance ( $\Omega$ ),  $a$  the curve fitting parameter.

Fig. 2. shows typical current-voltage and power-voltages characteristics for a PV generator.

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<sup>1</sup> TRaNsient SYstem Simulation program: <http://sel.me.wisc.edu/trnsys/>

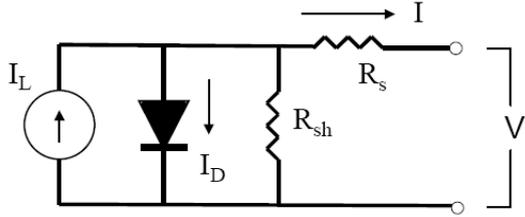


Fig. 1. The equivalent electrical circuit for the PV cell

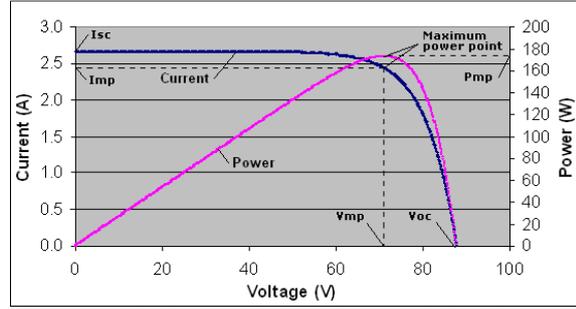


Fig. 2. Typical I-U and P-U characteristics for a PV generator

### Power conditioning equipments

Power conditioning equipments are used to operate the electrolyser and the fuel cell. The model is based on empirical efficiency curves and an expression for the power loss is:

$$P_{loss} = P_{in} - P_{out} = P_0 + \left( \frac{U_S}{U_{out}} \right) P_{out} + \left( \frac{R_i}{U_{out}^2} \right) P_{out}^2$$

where  $U_S$  is the set point voltage (V) and  $R_i$  is the internal resistance ( $\Omega$ ). With respect to the nominal power  $P_{nom}$  of the power conditioner, the previous equation can be expressed as:

$$\frac{P_{in}}{P_{nom}} = \frac{P_0}{P_{nom}} + \left( 1 + \frac{U_S}{U_{out}} \right) \cdot \frac{P_{out}}{P_{nom}} + \frac{R_{ipn}}{U_{out}^2} \cdot P_{nom} \cdot \left( \frac{P_{out}}{P_{nom}} \right)^2$$

### Electrolyser

The model for the high pressure alkaline electrolyser shown in Fig. 3 is based on a combination of thermodynamics, heat transfer and empirical electrochemical equations. The electrochemical model is based on a temperature dependent I-U curve for a given pressure (Fig. 4) and a Faraday efficiency curve independent of temperature and pressure.

The electrode kinetics of an electrolyser cell is modelled using empirical I-U relationships. Overvoltages and ohmic resistance play an important role in the modelling of the I-U curve:

$$U = U_{rev} + \frac{r_1 + r_2 T}{A} I + (s_1 + s_2 T + s_3 T^2) \times \log \left( \frac{t_1 + t_2 / T + t_3 / T^2}{A} I + 1 \right)$$

being  $U$  the operation cell voltage (V),  $U_{rev}$  the reversible cell voltage (V),  $r_i$  the parameters for the ohmic resistance of electrolyte ( $\Omega$ ),  $s_i$  and  $t_i$  the parameters for the overvoltage on the electrodes,  $A$  the electrode area ( $m^2$ ),  $T$  the temperature of the electrolyte ( $^{\circ}C$ ) and  $I$  the current through the cell (A).

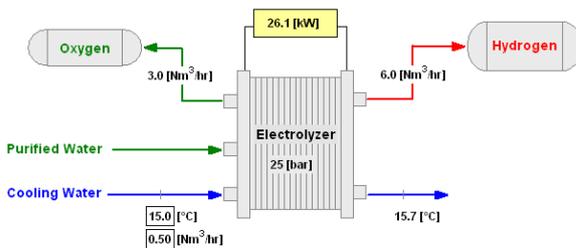


Fig. 3. Scheme of a high pressure alkaline electrolyser

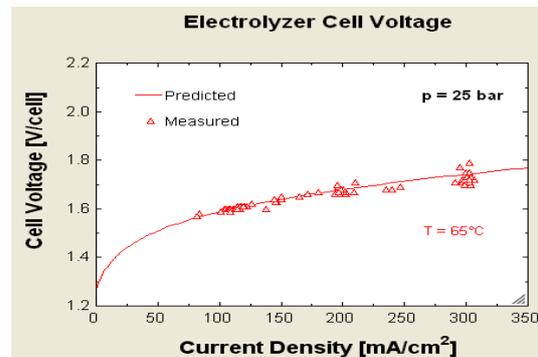


Fig. 4. Typical I-U curve for an electrolyser

### Proton-Exchange Membrane Fuel Cell

The PEMFC model shown in Fig. 5 is largely mechanistic, with very theoretical basis.

The performance of a fuel cell is represented by its output voltage. The voltage of the single cell is calculated as:

$$U_{cell} = E + \eta_{act} + \eta_{ohmic}$$

where  $E$  is the thermodynamic potential,  $\eta_{act}$  is the anode and cathode activation overvoltage (the voltage loss associated with the electrodes), and  $\eta_{ohmic}$  is the ohmic overvoltage (the losses associated with the proton conductivity of the solid polymer electrolyte and electronic internal resistances).

$E$  is defined through the Nernst equation:

$$E = 1.23 - 0.00085 \cdot (T_{stack} - 298) + 0.0000431 \cdot T_{stack} \cdot \ln(p_{H_2} \cdot p_{O_2}^{0.5})$$

$\eta_{act}$  is based on the theoretical equations from kinetic, thermodynamic and electrochemistry fundamentals:

$$\eta_{act} = -0.95 + 0.00243 \cdot T_{stack} + 0.000192 \cdot T_{stack} \cdot \ln(A_{PEM}) - 0.000192 \cdot T_{stack} \cdot \ln(I_{FC}) + 0.000076 \cdot T_{stack} \cdot \ln(c_{O_2})$$

Finally,  $\eta_{ohmic}$  is totally empirical, based on temperature and current experimental data:

$$\eta_{ohmic} = \frac{-I_{FC} \cdot t_{PEM}}{A_{PEM}} \cdot \frac{8}{\exp\left(3.6 \cdot \left(\frac{T_{stack} - 353}{T_{stack}}\right)\right)} \cdot \left(1 + 1.64 \cdot \frac{I_{FC}}{A_{PEM}} + \gamma \cdot \left(\frac{I_{FC}}{A_{PEM}}\right)^3\right)$$

Fig. 6 shows the cell voltage variation as a function of the current.

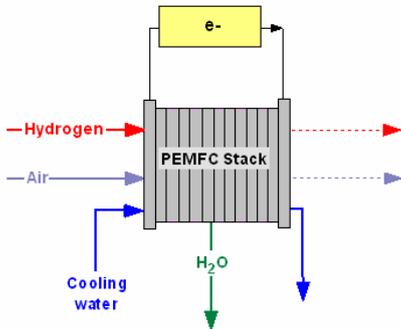


Fig. 5. Scheme of an PEM fuel cell

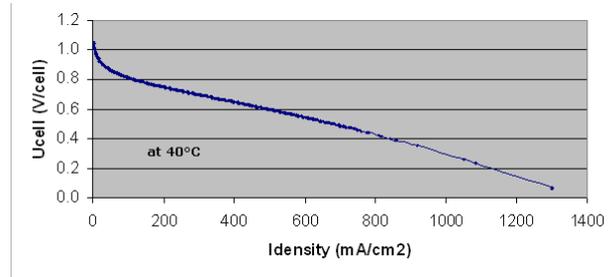


Fig. 6. Typical current-voltage curve for a PEMFC

### Compressor

The compressor model is based on a two-stage polytropic compression process with intercooling. The total compression work for the process is given by:

$$W_{comp} = \dot{n}_{gas} \frac{(W_1 + W_2)}{\eta_{comp}}$$

$$\text{with } W_1 = \frac{nRT}{n-1} \left[ 1 - \left( \frac{p_x}{P_1} \right)^{\frac{n-1}{n}} \right] \text{ and } W_2 = \frac{nRT}{n-1} \left[ 1 - \left( \frac{p_2}{P_x} \right)^{\frac{n-1}{n}} \right]$$

being  $\dot{n}_{gas}$  the gas flow ( $\text{mol} \cdot \text{s}^{-1}$ ),  $W_1$  and  $W_2$  the polytropic works ( $\text{J} \cdot \text{mol}^{-1}$ ),  $\eta_{comp}$  the compressor efficiency,  $n$  the polytropic coefficient,  $R$  the universal gas constant ( $8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ),  $T$  the inlet gas temperature (K) and  $p_i$  the pressure values (Pa).

### Gas storage

The compressed gas storage model calculates the pressure in the tank based on either the ideal gas law or van der Waals equation of state for real gases.

According to the ideal gas law, the pressure of a gas storage tank is given by:

$$p = \frac{n \cdot R \cdot T_{gas}}{V}$$

For real gases, the Van der Waals equation of state indicates that the pressure of gas stored in a tank is:

$$p = \frac{n \cdot R \cdot T_{gas}}{V - n \cdot b} - a \cdot \frac{n^2}{V^2}$$

$$\text{with } a = \frac{27 \cdot R^2 \cdot T_{cr}^2}{64 \cdot p_{cr}} \text{ and } b = \frac{R \cdot T_{cr}}{8 \cdot p_{cr}}$$

where  $T_{cr}$  is the critical temperature (K) and  $p_{cr}$  the critical pressure (Pa) of the gas.

### 3. Validation of the models

The models described previously have been successfully validated using a combination of analytical tests and empirical comparisons. The analytic tests included the use of typical curves found in the literature and other energy systems modelling tools.

Fig. 7 and 8 show the current-voltage curve and the power curve obtained from the simulation of the Flagsol (KFA) 150 cell module at different temperatures. Fig. 9 presents the current-voltage curve of the same module at different solar radiation levels. At standard test conditions (25°C and 1000 W/m<sup>2</sup> of solar radiation), the simulation indicates a 173.18 W maximum power point. Fig. 10 presents the effect of temperature on the simulated performance of the PHOEBUS alkaline electrolyser. Finally, the effect of temperature on the performance of a typical PEM fuel cell is simulated on Fig. 11 and 12.

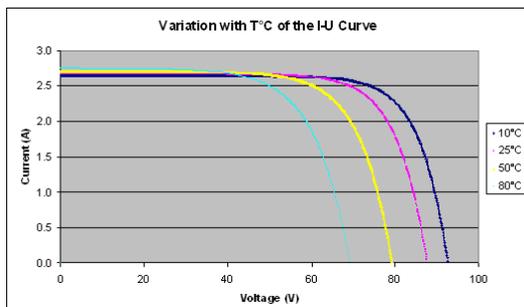


Fig. 7. PV current at different temperatures

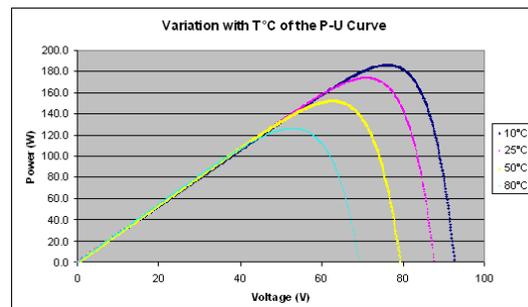


Fig. 8. PV power at different temperatures

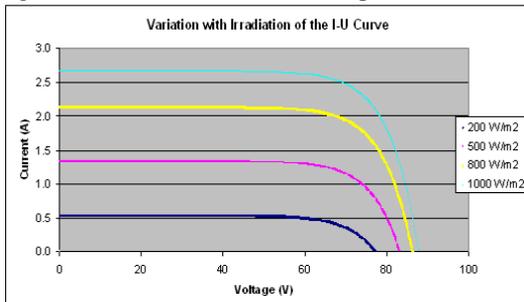


Fig. 9. PV current at different irradiation levels

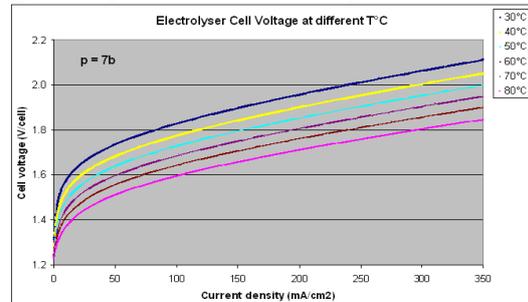


Fig. 10. Temperature dependence of an electrolyser

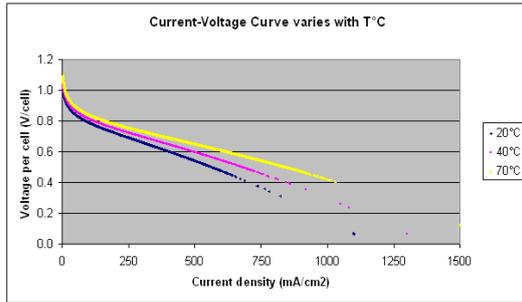


Fig. 11. PEMFC voltage at different temperatures

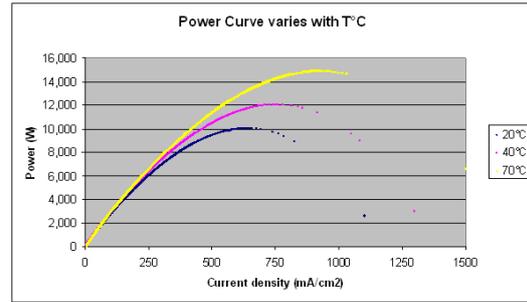


Fig. 12. PEMFC power at different temperatures

All these results are typical and verify the results available in the literature. They prove that the components models are accurate and that simulating hydrogen systems with TRNSYS provides reliable results.

#### 4. Model Development and methodology

Models of four generic hydrogen systems based on the components models previously presented have been developed on the TRNSYS platform. The models cover the broad spectrum of prototype hydrogen demonstration systems emerging around the world. These are:

- a stand-alone power system
- low power application
- filling station
- energy buffering system for large scale renewables

TRNSYS can be particularly tricky to use. To make the models easier to use, TRNSED applications have also been designed. TRNSED is a customised interface that presents a simplified view of the TRNSYS file with only a few selected parameters available to users.

A cost-benefit analysis model has been included to analyse the economic performance of the systems. The total net present cost of the system and the levelized cost of energy are calculated.

The model also includes an optimisation method to optimise the technical and economic performance of the systems modelled.

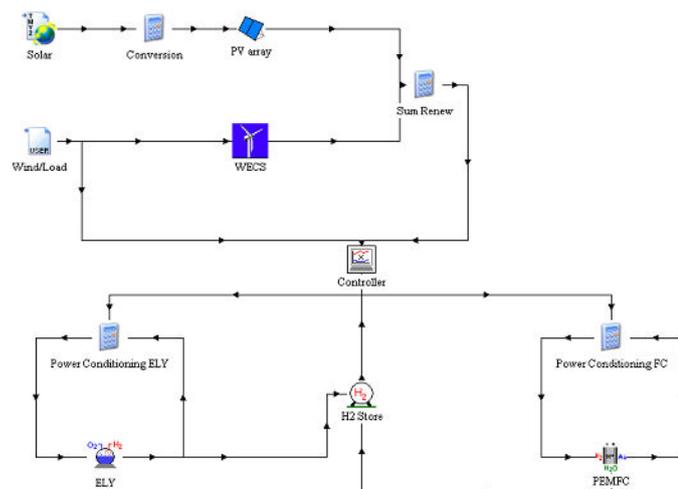


Fig. 13. TRNSYS model of a Stand-Alone Power System

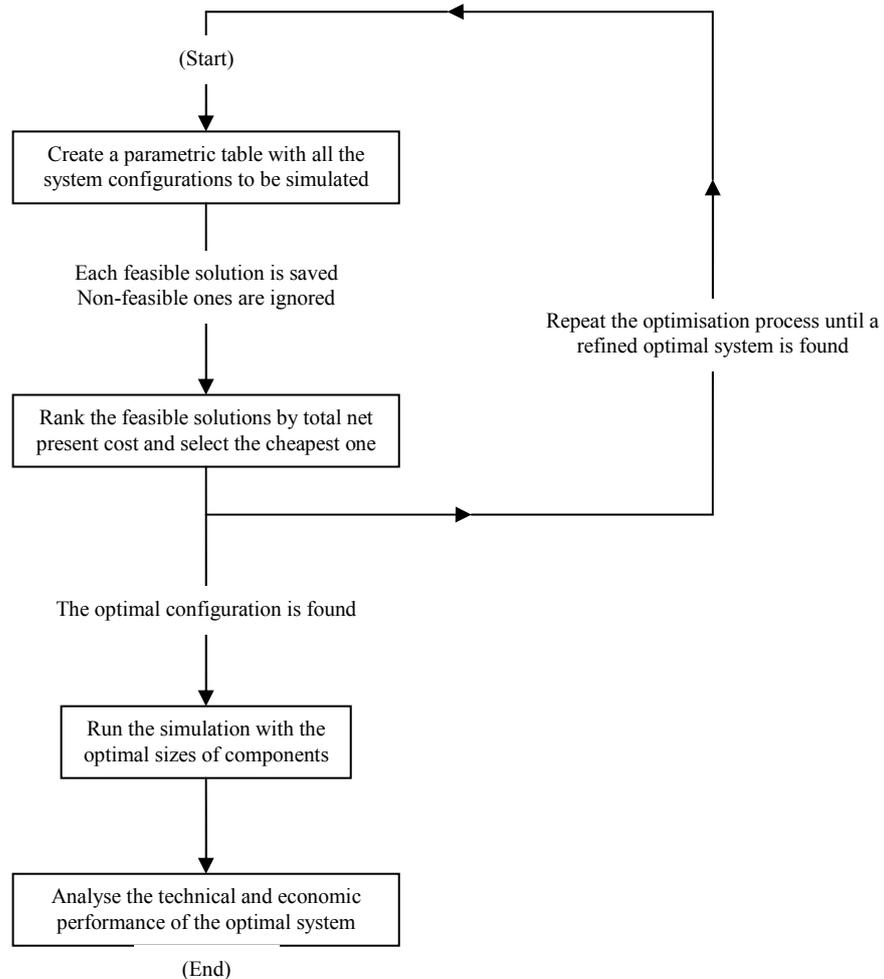


Fig. 14. Flow chart of the optimisation process

## 5. Applications

The models have also been successfully applied to the analysis of two real systems: the HARI Project in Loughborough, UK and the Utsira Project in Norway.

Utsira is a small island community located approximately 18 kilometres off the west coast of Norway. The Utsira project is the world's first full-scale stand-alone renewable energy system where the energy balance is provided by wind and stored hydrogen.

*To be completed....*

The application of the models improved confidence in their predictions and capabilities and also highlighted problems in the design and operation of the real and prospective systems including: poor control strategies, poor sizing of system components and mismatches of energy supply and demand.

## 6. References

*TRNSYS 16, Volume 5, Mathematical Reference.* University of Wisconsin-Madison, 2006