Modeling of 2-MW co-generative PEM fuel cell for hydrogen recovering from Chlorine industry

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The chlorine industrial production process is energy-intensive in terms of heat and electricity and generates a relevant amount of hydrogen as byproduct; consequently, it is particularly interesting for cogeneration and energy integration by means of fuel cells. The *DEMCOPEM-2MW* European Project is meant to design and build a demonstrative 2MW PEM fuel cell power plant coupled with a chlor-alkali process in China, aiming at covering about 20% of the industrial process consumptions based on the use of waste hydrogen. Scale-up of stationary fuel cell plants is an ongoing process with many open challenges. Therefore, in the framework of the project, a model is developed in order to evaluate the plant expected performances and optimize operational strategies on plant lifetime.

The simulation is built in Aspen PLUS® environment, using available thermodynamics libraries and standard process components and developing customized components for electrochemical and electronic devices. The general modeling approach was described in a previous work [1], while here the model is refined and applied to the 2 MW plant in view of operational optimization and lifetime performances evaluation. Calibration and validation of the model are performed against data from (i) a 70 kW PEM stack installation operating in AkzoNobel's plant in Delfzijl [2], where Nedstack PEM fuel cell stacks of the same class used in the projected plant are being tested; and from (ii) a 1 MW PEM plant operated in Lillo (Belgium), developed by Nedstack and MTSA with a layout similar to the design of *DEMCOPEM-2MW* plant.

Fuel cell modeling

The system model is focused on system analysis and employs a specific customized lumped model of the PEM stacks. The fuel cell model calculates mass and energy balances, using regressed polarization curves based on the expression [3]:

$$V(i, x_H, x_O) = A + B\ln\left(\frac{x_{H2}}{x_{H2,st}}\right) + C\ln\left(\frac{x_{O2}}{x_{O2,st}}\right) + Di + E\ln\left(\frac{i}{i_0}+1\right) + F\ln\left(1-\frac{i}{i_L}\right) \qquad (1)$$

where the cell voltage is calculated as a function of the ratio to stoichiometry of reactants molar fractions x and current density i. In order to take into account the increasing impact of reactants excess on polarization during lifetime, i_0 and i_L parameters are expressed as linear functions of stoichiometry. Two set of parameters were regressed, one on BOL (beginning of life) data and the other on EOL (end of life); intermediate conditions are evaluated through linear interpolation, at constant average decay of the cells for each working condition [2]. The model shows errors below 1% (BOL) and 3% (EOL) towards experimental data. The real PEM fuel cell is structured in groups of stacks in series and in parallel, in order to reach the desired total power and voltage. The model allows introducing differences for each single stack (e.g. different polarization curves), which are however neglected in this preliminary evaluation.

System modeling

Figure 1 shows the plant layout; the model considers all main auxiliaries, including saturators, heat exchangers, blowers, pumps. Blowers performance curves and lumped characteristics of heat exchangers are included in order to evaluate the impact of part load operation. Reactants excess to stoichiometry and fuel cell power are the independent parameters; consequently, the model estimates the flows entering the system, the cooling requirements and the recovered heat through mass and energy balances of each component. Results include the overall efficiency, auxiliaries consumption, pressure drops and components operating conditions which can be evaluated at nominal or

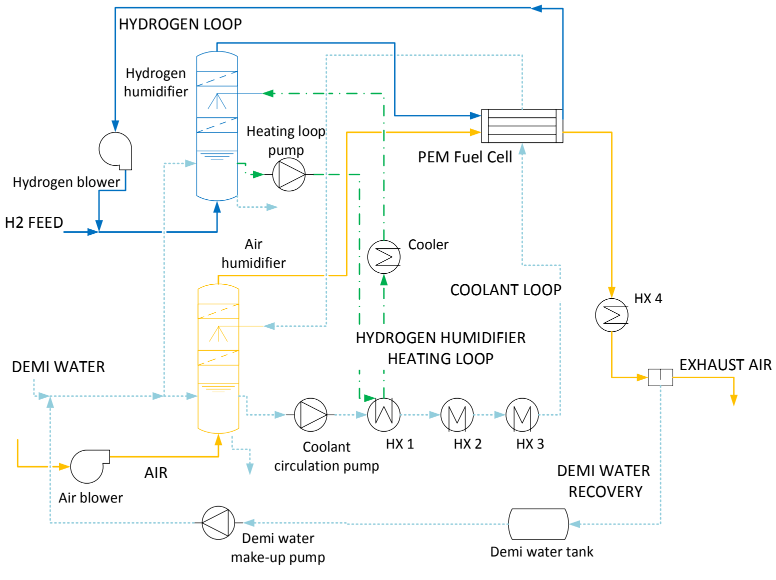

Figure 1. Simplified plant layout.

different conditions. In figure 2, the energy balance of the system for a given air utilization factor is evaluated at BOL and EOL, considering the same DC electric output. Auxiliaries consumption is about 4% of the total hydrogen energy input. Electrical efficiency reduction due to cell voltage decay causes an increase of hydrogen consumption and of the absolute values of the losses, reducing also the thermal recovery efficiency.

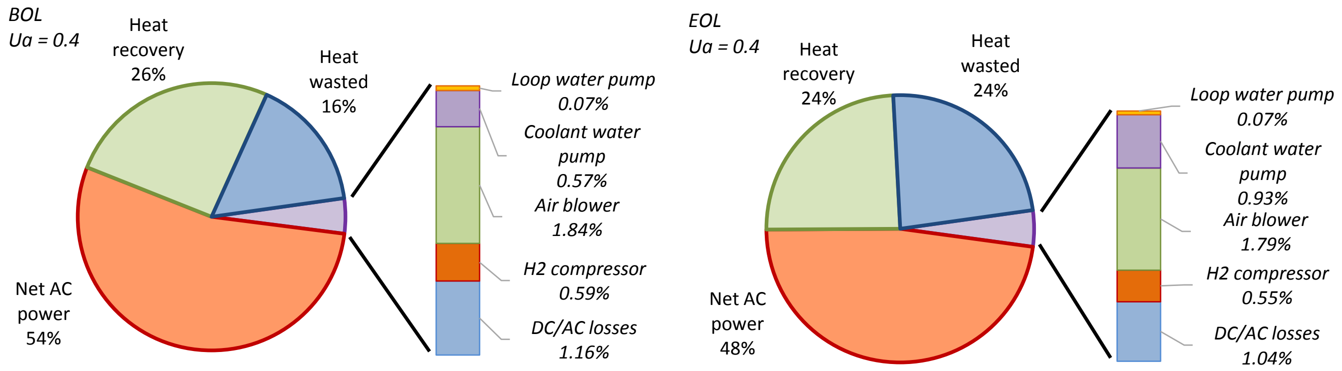

Figure 2. Comparison of energy balance of the plant at BOL and EOL (U_a = 0.4) at constant gross DC power production

Figure 3 shows the evolution vs. time of system efficiency, electric and thermal power for an exemplifying condition. Different operating conditions are investigated in order to improve the operational strategy and evaluate the impact of fuel cell decay on the global performances.

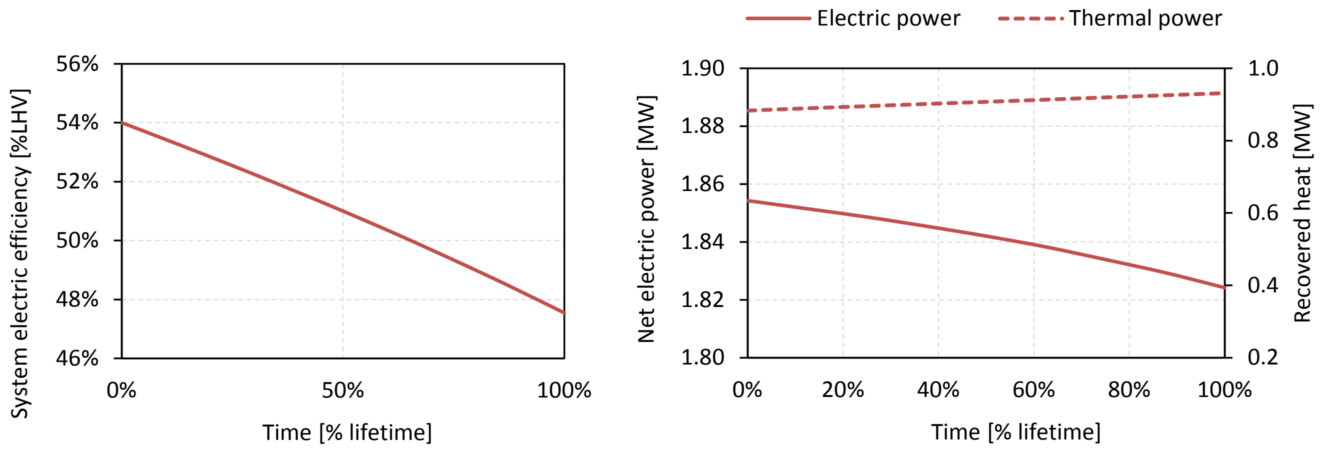

Figure 3. System efficiency, net electric AC power and thermal recovery during lifetime (U_a = 0.4)

The model allows to investigate alternative layouts. For instance, removing hydrogen recirculation and burning excess hydrogen in a boiler would allow generating more heat; this solution could be attractive for plant applications requiring high temperature heat, moving the heat-to-electricity ratio from 0.5 up to nearly 2; electric efficiency drops to about 28%, but total energy recovery increases up to 97%. More generally, the discussed model allows optimizing the plant operation strategies and evaluating the deviations of real plant behavior from theoretical conditions (e.g. supporting in fault detection); over the lifetime of DEMCOPEM project, data from the demonstrative plant will be collected and compared with model results.

Aknowledgements

This work is developed in the framework of the FP7-FCH-JU project "DEMCOPEM-2MW", cofounded by the FCH JU under grant agreement n° 621256.

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