## Current and voltage efficiency of high pressure PEM water electrolyzers

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In terms of energy storage, the pressurization of hydrogen is a useful task in order to enhance the energy density of the gas [1]. Thus, a direct electrochemical compression during water electrolysis is considered as a convenient and effective way to produce and compress hydrogen [2,3]. During polymer electrolyte membrane (PEM) water electrolysis, both hydrogen and oxygen produced gases can permeate through the membrane [4-6], a phenomenon commonly referred to as crossover. The crossover of gases will directly affect the overall efficiency, partial load range, purity of the product gases and safety due to the mixing of hydrogen and oxygen [5,6]. These negative aspects will be also more severe when operating at high pressures [5,6], despite the low gas permeability of proton exchange membranes and the concomitant gas purity being identified in literature as a big advantage of PEM electrolysis compared to alkaline electrolysis [2].

In this work, we have simulated the influence of cathodic hydrogen pressure on the purity of produced oxygen as a function of the membrane thickness. The simulated outcome was afterwards compared to the in-situ measurements obtained from a standard PEM electrolysis cell. For the simulation, the proton conductivity, permeability and solubility coefficients found in literature [4] for commercially available Nafion<sup>®</sup> membranes were assumed. With this study, we quantified higher hydrogen crossover rates towards thinner membranes that finally reduce the current efficiency. Conversely, thicker membranes result in a reduced voltage efficiency, which has also been estimated. This study provides an accessible computational tool, where an optimization of the membrane thickness for cell efficiency, with respect to the applied hydrogen pressure, is obtained. Figure 1 shows results of the simulated losses, in which a temperature of 80°C and absolute cathodic pressures of 1bar and 30bar were respectively applied. The losses due to electrochemical compression, crossover and ohmic resistance of the membrane were included and normalized to the reversible voltage of 1.23V for the electrochemical decomposition of water at standard conditions. At low current densities losses due to crossover dominate, while at higher current densities this contribution is overwhelmed by the ohmic losses.

In addition, the efficiencies of both subsequent and direct electrochemical compression of the produced hydrogen are computationally compared. From these results we estimated the compressor efficiencies required to compensate losses due to crossover at higher pressures.

The presented simulation for the gas crossover and efficiency can potentially be employed for the water electrolysis in alkaline media, as well as the electrolysis of other substances such as sodium chloride. To utilize the model for other systems, ionic conductivity, permeation and solubility coefficients of the considered species must be adapted to fit the model in question. Concluding, a model estimating the gas crossover and ohmic resistance of Nafion<sup>®</sup> membranes and the corresponding losses was developed, in order to optimize the membrane thickness in dependence of the cathodic pressure.



**Figure 1:** Loss due to electrochemical compression, crossover and ohmic resistance of the membrane in dependence of the current density at 80°C for various membrane thicknesses and cathodic pressures of 1bar (top) and 30bar (bottom).

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