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Hydrogen Production Using an Anion-Exchange Membrane Water Electrolyzer: Mathematical and Bond Graph Modeling

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Abstract : Water electrolysis is one of the most advanced technologies for producing hydrogen and can be easily combined with electricity from different sources. Under the influence of electric current, water molecules can be split into oxygen and hydrogen. The production of hydrogen by water electrolysis favors the integration of renewable energy sources into the energy mix by compensating for their intermittence through the storage of the energy produced when production exceeds demand and its release during off-peak production periods. Among the various electrolysis technologies, anion exchange membrane (AEM) electrolyser cells are emerging as a reliable technology for water electrolysis. Modeling and simulation are effective tools to save time, money, and effort during the optimization of operating conditions and the investigation of the design. The modeling and simulation become even more important when dealing with multiphysics dynamic systems. One of those systems is the AEM electrolysis cell involving complex physico-chemical reactions. Once developed, models may be utilized to comprehend the mechanisms to control and detect flaws in the systems. Several modeling methods have been initiated by scientists. These methods can be separated into two main approaches, namely equation-based modeling and graph-based modeling. The former approach is less user-friendly and difficult to update as it is based on ordinary or partial differential equations to represent the systems. However, the latter approach is more user-friendly and allows a clear representation of physical phenomena. In this case, the system is depicted by connecting subsystems, so-called blocks, through ports based on their physical interactions, hence being suitable for multiphysics systems. Among the graphical modelling methods, the bond graph is receiving increasing attention as being domain-independent and relying on the energy exchange between the components of the system. At present, few studies have investigated the modelling of AEM systems. A mathematical model and a bond graph model were used in previous studies to model the electrolysis cell performance. In this study, experimental data from literature were simulated using OpenModelica using bond graphs and mathematical approaches. The polarization curves at different operating conditions obtained by both approaches were compared with experimental ones. It was stated that both models predicted satisfactorily the polarization curves with error margins lower than 2% for equation-based models and lower than 5% for the bond graph model. The activation polarization of hydrogen evolution reactions (HER) and oxygen evolution reactions (OER) were behind the voltage loss in the AEM electrolyzer, whereas ion conduction through the membrane resulted in the ohmic loss. Therefore, highly active electro-catalysts are required for both HER and OER while high-conductivity AEMs are needed for effectively lowering the ohmic losses. The bond graph simulation of the polarisation curve for operating conditions at various temperatures has illustrated that voltage increases with temperature owing to the technology of the membrane. Simulation of the polarisation curve can be tested virtually, hence resulting in reduced cost and time involved due to experimental testing and improved design optimization. Further improvements can be made by implementing the bond graph model in a real power-to-gas-to-power scenario.

Keywords : hydrogen production, anion-exchange membrane, electrolyzer, mathematical modeling, multiphysics modeling
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