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Title : COMPUTATIONAL MODELLING OF MASS TRANSPORT AND DYNAMIC SIMULATION OF A HIGH PRESSURE POLYMER ELECTROLYTE MEMBRANE ELECTROLYSER

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Hydrogen as a fuel source is acclaimed as a new energy carrier of the future. It is one of the potential solutions to the current energy and environmental pollution crises due to its carbon-free and environmentally friendly characteristics. Hydrogen is primarily used in the chemical industry, but in the future, hydrogen will become a significant fuel for a fuel cell system and combustion cycles that produce fewer greenhouse gases than competing fossil systems. The Polymer Electrolyte Membrane Electrolyser (PEME) is essentially inverted Polymer Electrolyte Membrane Fuel Cells (PEMFC), where, instead of generating electricity by harnessing the reaction potential of hydrogen and oxygen to form water, it instead consumes energy to split water into hydrogen and oxygen. One of the benefits of the PEME over many other forms of hydrogen generation is that it is simpler and generates no harmful by-products other than pure oxygen. In addition, it is also capable of producing hydrogen gas at high pressure, thus facilitating storage. In the PEME, gases and water permeate the membrane, leading to the presence of hydrogen on the oxygen side and vice versa, referred to as gas cross-over. Extensive mixing of the product gases could produce explosive conditions. The research presented in this thesis contributes to the modelling and understanding of the steady state and dynamic behaviour of the PEME. The focus of this research is to provide a numerical model of a single cell PEME that can assist in improving the current level of understanding of this system. Parametric analysis of a PEME cell was performed to understand the effect of the operating parameters of this system on its performance. This study includes the development of numerical models of electrochemical and mass transport phenomenon of gas cross-over on the PEME. Mass transfer using Fickian diffusion is implemented in the model. In addition to solving a phenomenological transport equation for the gas cross-over membrane, the model takes into consideration the dynamics in the polymer electrolyte membrane. It uses the mathematical model to simulate the effects of membrane thickness, current density and operating pressure of the anode and cathode chambers on the mass transport phenomenon and operating voltage. The simulations show that higher membrane thickness increases the operating voltage of the PEME. A Simulink model was developed as a dynamic model of a PEME, based on an analytical and mechanistic approach to computing the dynamic voltage–current characteristics. A time-dependent, isothermal model of the PEME was developed and implemented using an electrochemical and thermodynamic model. The dynamic model of the PEME system can be used as a tool to improve the design for large-scale PEME systems, especially when integrated with renewable energy system models, such as, solar, wind energy etc, to estimate operating parameters and optimize the sustainable energy system. The main conclusion of this work is that the simulation method of the PEME cell study, under various conditions, could be used to successfully create correlations and perceptions between those topologies for the overall performance of the PEME cell. The operational performance of the PEME cell does not only depend on component efficiency but also on the system design and consumption behaviour.