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Investigating the effect of triple-phase boundary in zinc-air cathodes utilizing pore network modeling approach

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Zinc-air flow batteries are energy storage devices that have started to receive attention due to their high energy density, and zinc metal being particularly appealing since it's safe and cost effective. Increasing the performance of these electrochemical devices and their useful life will have a substantial economic and operational impact on the development of energy storage projects. Different factors affect these devices'performance including the structure of their porous air electrode and the transport phenomena within the catalyst layer (CL) where the oxygen reduction reaction (ORR) occurs. The ORR takes place at the interface of three phases: catalyst (solid), electrolyte (liquid), and oxygen (gas), the so-called triple phase boundary (TPB). The extent and distribution of the TPB and the electrolyte invasion pattern throughout the CL affect the transport of reactive species and subsequently the performance of air electrode. Therefore, understanding these parameters is a crucial step towards designing and optimizing the CL structure. To investigate the CL porous structure and the TPB at pore scale, a rigorous pore-scale modeling tool is required. Pore network modeling (PNM) is suitable for such investigations due to its low computational cost compared to other modeling options such as continuum-based models, and direct numerical simulations; and more importantly PNMs can easily capture the detailed information on the electrolyte invasion and TPB extent at pore-scale.

In this work a mathematical framework was developed for PNM of the transport phenomena in the CL of the air electrode. The effects of electrolyte invasion pattern, CL's pore size distribution, and TPB extent on the performance of the air electrode were investigated. The PNM results show that in low to intermediate electrolyte saturation (0.1-0.7) as the electrolyte invasion in the CL proceeds, the TPB extent increases and the electrode performance in terms of peak power increases accordingly. In contrast, at saturations greater than 0.7, further invasion by the electrolyte results in reducing the TPB length and reducing its performance in terms of the generated power.

In practice it is possible to alter the electrolyte invasion pattern and the TPB extent by changing the electrode structure. This idea was explored by changing the pore size distribution of the CL in the PNM. The results showed that a narrow pore size distribution provides a higher performance at low saturations whereas a wide pore size distribution provides a higher performance at higher saturations. Although the developed mathematical framework was implemented on synthetic cubic pore network models, it can be applied on extracted networks for other CL samples.

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Time Block Preference

Time Block C (18:00-21:00 CET)

Participation

Unsure

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