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Comparison of two optimization approaches in an electrochemical reaction-diffusion system from an entropy generation perspective

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As the use of electrochemical energy devices, such as rechargeable batteries and fuel cells increases in many fields, from stationary power generation to transportation and heavy-duty applications, it is imperative to further improve them to make them cost-effective compared to conventional systems [1]. The search for the best composition for porous electrodes of these technologies has been the interest of many researchers over the past decades. Recently, some studies, such as [2, 3], have focused on the use of topology optimization techniques in designing the electrode structure. While such studies provide beneficial techniques for innovative electrode design at the application level, fundamental understandings of the physicochemical mechanisms that improve system performance are strongly needed. This study fills this research gap by linking an optimization problem to the concept of entropy generation.

This study aims to investigate the optimal structure of an electrochemical reaction-diffusion (ERD) system. It is assumed that the proposed porous reactor consists of three material constituents, including a solid phase, a proton-conducting polymer (ionomer), and voids. Such a system is analogous to the catalyst layer of a polymer electrolyte membrane fuel cell. However, the method used in this study can be employed for any other type of electrochemical device with some slight modifications. A reactant species diffuses into this ERD system through the pores as it oxidizes in the presence of the solid phase. The solid phase and ionomer phase are responsible for discharging the generated electrons and positive ions, respectively. Two topology optimization strategies are used to find the optimal spatial distribution of constituent materials. In the first approach, the goal is to maximize the overall reaction rate in the system. In the second strategy, an attempt is made to minimize the losses of the system while keeping the overall reaction rate constant. An entropy generation model is developed based on the concept of non-equilibrium thermodynamics. The change in entropy production rate during the two optimization processes is evaluated and compared. The results show that both optimization approaches lead to a complex tree-root-like structure. Such a structure facilitates the delivery of reactant species to entire parts of the ERD system, thus reducing mass transport limitations. In addition, the findings of this study indicate that the entropy production rate increases with the increment of the total electrochemical reaction rate. This is associated with the increase of inevitable entropy production in a maximization approach. On the other hand, the minimization approach leads to lower entropy production, which is consistent with the minimization of entropy generation [4].

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Participation

In-Person

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Primary authors: Mr ALIZADEH, Mehrzad (Department of Mechanical Engineering, Graduate School of Engineering, Osaka University, Suita, 565-0871, Osaka, Japan); Dr CHAROEN-AMORNKITT, Patcharawat (Electrochemical Energy Storage and Conversion Laboratory, Department of Mechanical Engineering, Faculty of Engineering, King Mongkut's University of Technology Thonburi, 126 Pracha Uthit Rd., Bang Mod, Thung Khru, Bangkok, 10140, Thailand); Dr SUZUKI, Takahiro (Department of Mechanical Engineering, Graduate School of Engineering, Osaka University, Suita, 565-0871, Osaka, Japan); Prof. TSUSHIMA, Shohji (Department of Mechanical Engineering, Graduate School of Engineering, Osaka University, Suita, 565-0871, Osaka, Japan)

Presenter: Mr ALIZADEH, Mehrzad (Department of Mechanical Engineering, Graduate School of Engineering, Osaka University, Suita, 565-0871, Osaka, Japan)

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