Integrated Multi-scale Hybrid Simulation of Transport Process in Proton Exchange Membrane Fuel Cell

정자훈*, 김홍찬, 한상필, 유황찬
LG화학 기술연구원 CRD 연구소
(jahjeong@lgchem.com*)

Integrated multi-scale hybrid scheme is applied to simulate transport process in proton exchange membrane fuel cell (PEMFC). Based on the PEMFC model reported by Um et al. (J. Electrochem. Soc. 147 (2000) 4485), species transport equations are derived and solved with the electrochemical kinetic equation called Butler-Volmer equation. For accurate and efficient computation, we use hybrid scheme: reactive domain computations are selectively activated by gPROMS, which provides not only an excellent modeling environment but also data communication interface with general CFD software of FLUENT to take charge of remainder domain computation. To verify our numerical procedure, we compare numerical prediction of the polarization curve with observation data from the 25cm2 unit cell experiment. Through this work, essential information on the transport process in PEMFC is brought out. Our efforts and initial success in numerical description of the transport process in PEMFC enhance its fundamental understanding and will eventually pave the road for full-scale, computer-aided fuel cell system design.