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Interactive Computer Aided Design of Electrochemical Systems

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ABSTRACT

The most popular and widely used rechargeable battery numerical model, the dualfoil, was developed in fortran by John Newman and coworkers[1-3], and enables the user to describe the time-dependent electrochemical transport of lithium and charge, through the application of concentrated solution theory in porous media. Such a model has enabled the design of many advanced lithium-ion batteries for hybrid and plug-in electric vehicles that can operate under high current densities. Historically, however, the dualfoil and other subsequently derived models are cumbersome and unwieldy when used, and offer limited flexibility regarding parameter variability, integration into more sophisticated numerical descriptions, coupling to multiscale formulations, or the simple visualization of generated data. The nature of dualfoil makes it difficult to use, and it does not allow for systematic parametric analyses, or direct integration into high performing, multiscale numerical frameworks. This work introduces a proof of concept for a flexible application programming interface, dualfoil.py, that enables hierarchical control over the dualfoil legacy code and visualization modules, and provides the user with the ability to rapidly set up complex, multiscale simulations. Furthermore, the program features a GUI-mode for single-run simulations, and a powerful text-mode for setting up large simulation queues. By making use of the object oriented nature of Python, dualfoil.py allows the user to generate, organize, and visualize the electrochemical responses from the battery. Cell potential, anode and cathode active material utilization, and power/energy densities of multiple battery scenarios are modeled and presented, demonstrating the iterative capability of dualfoil.py. This versatile program allows for users of any skill level to achieve robust results in a control oriented and rapidly deployable manner.

[1] Doyle, M., Fuller, T., and Newman, J. Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell. *J. Electrochem. Soc.* 1993, 140, 1526-1533.
[2] Doyle, M., Newman, J., Gozdz, A., Shmutz, C., and Tarascon J.-M. Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells. *J. Electrochem. Soc*. 1996, 143, 1890-1903.
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KEYWORDS

Rechargeable batteries, battery modeling, computational material science, multiscale models, computational material science