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A Comparison Between Different Discretization Techniques for the Doyle-Fuller-Newman Li+ Battery Model

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Abstract : Since its proposal, the Doyle-Fuller-Newman (DFN) lithium-ion battery model has gained popularity in the electrochemical field. In fact, this model provides the user with theoretical support for designing the lithium-ion battery parameters, such as the material particle or the diffusion coefficient adjustment direction. However, the model is mathematically complex as it is composed of several partial differential equations (PDEs) such as Fick's law of diffusion, the MacInnes and Ohm's equations, among other phenomena. Thus, to efficiently use the model in a time-domain simulation environment, the selection of the discretization technique is of a pivotal importance. There are several numerical methods available in the literature that can be used to carry out this task. In this study, a comparison between the explicit Euler, Crank-Nicolson, and Chebyshev discretization methods is proposed. These three methods are compared in terms of accuracy, stability, and computational times. Firstly, the explicit Euler discretization technique is analyzed. This method is straightforward to implement and is computationally fast. In this work, the accuracy of the method and its stability properties are shown for the electrolyte diffusion partial differential equation. Subsequently, the Crank-Nicolson method is considered. It represents a combination of the implicit and explicit Euler methods that has the advantage of being of the second order in time and is intrinsically stable, thus overcoming the disadvantages of the simpler Euler explicit method. As shown in the full paper, the Crank-Nicolson method provides accurate results when applied to the DFN model. Its stability does not depend on the integration time step, thus it is feasible for both short- and long-term tests. This last remark is particularly important as this discretization technique would allow the user to implement parameter estimation and optimization techniques such as system or genetic parameter identification methods using this model. Finally, the Chebyshev discretization technique is implemented in the DFN model. This discretization method features swift convergence properties and, as other spectral methods used to solve differential equations, achieves the same accuracy with a smaller number of discretization nodes. However, as shown in the literature, these methods are not suitable for handling sharp gradients, which are common during the first instants of the charge and discharge phases of the battery. The numerical results obtained and presented in this study aim to provide the guidelines on how to select the adequate discretization technique for the DFN model according to the type of application to be performed, highlighting the pros and cons of the three methods. Specifically, the non-eligibility of the simple Euler method for longterm tests will be presented. Afterwards, the Crank-Nicolson and the Chebyshev discretization methods will be compared in terms of accuracy and computational times under a wide range of battery operating scenarios. These include both long-term simulations for aging tests, and short- and mid-term battery charge/discharge cycles, typically relevant in battery applications like grid primary frequency and inertia control and electrical vehicle breaking and acceleration.

Keywords : Doyle-Fuller-Newman battery model, partial differential equations, discretization, numerical methods
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