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A computationally efficient implementation of a full and reduced-order electrochemistry-based model for Li-ion batteries

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HIGHLIGHTS

- A computationally efficient implementation of the DFN model is proposed.
- Nonlinear model reduction is applied for the first time to the full nonlinear model.
- The implementation uses a particular numerical scheme based on Newton's method.
- This implementation is a step towards using the DFN model in real-time applications.

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ABSTRACT

Lithium-ion batteries are commonly employed in various applications owing to high energy density and long service life. Lithium-ion battery models are used for analysing batteries and enabling power control in applications. The Doyle-Fuller-Newman (DFN) model is a popular electrochemistry-based lithium-ion battery model which represents solid-state and electrolyte diffusion dynamics and accurately predicts the current/voltage response using a set of nonlinear partial differential equations. However, implementation of the full DFN model requires significant computation time. This paper proposes a computationally efficient implementation of the full DFN battery model, which is convenient for real-time applications. The proposed implementation is based on applying model order reduction to a spatial and temporal discretisation of the governing model equations. For model order reduction, we apply proper orthogonal decomposition and discrete empirical interpolation method, which leads to a set of reduced order nonlinear algebraic equations. These equations are solved using a particular numerical scheme, based on a damped Newton's method. In a simulation study, the computational efficiency of the proposed implementation is shown and the resulting accuracy is presented.

1. Introduction

Featured by high energy density and long service life, lithium-ion (Li-ion) batteries are used in various applications, such as consumer electronics, portable devices and (hybrid) electric vehicles. In order to properly analyse, design and control the batteries in the aforementioned applications, models of Li-ion batteries are needed. Among available battery models, the Doyle-Fuller-Newman (DFN) model is a popular one, see, e.g. [1,2], which describes solid-state and electrolyte diffusion dynamics and electric potentials (over space and time) and is governed by a set of nonlinear partial differential equations (PDEs). Solving the complete DFN model requires significant computation time, which precludes the DFN model to be used in real-time control and monitoring applications. These real-time application include state-of-charge or state-of-energy estimation [3–7], which requires estimates of the Li-ion concentration in solid and electrolyte phases, as well as optimal and fast charging of the battery [8–10]. These applications would benefit from having a computationally efficient electrochemistry-based battery model.

Several techniques have been proposed in the literature to address the highly complex DFN model. For instance, a single particle model has been employed to model the internal states of the Li-ion battery [11] and a simplified multi-particle model via linearisation has been proposed in [12]. These papers simplify the battery model by focussing on the solid phase diffusion, which is an important phenomenon in battery model, see, e.g. [13,14]. These solid-state diffusion dynamics

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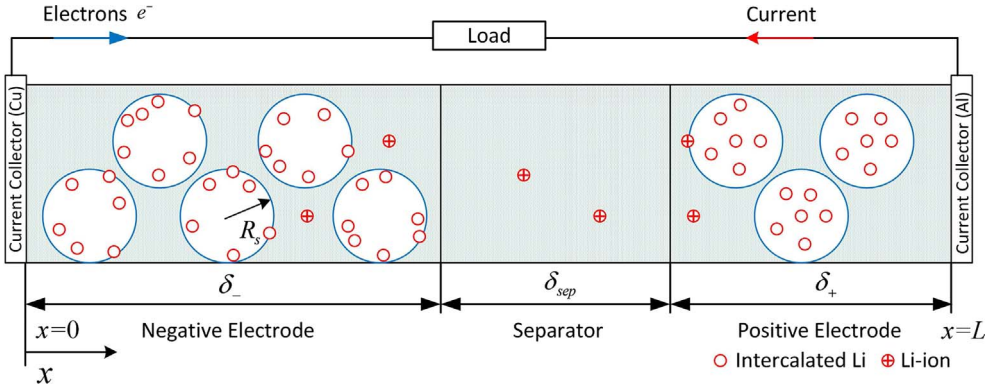

Fig. 1. Schematic of the Li-ion battery model during discharging.

can be simplified analytically, as was done in, e.g. [15,16], which considerably reduces the computational complexity.

Besides the simplifications, model order reduction techniques have been proposed for simplifying battery models. However, most of the existing papers in the literature use model order reduction techniques for (infinite-dimensional) linear systems to obtain reduced order battery models, such as Padé approximations [15,17], balanced truncations [18], or residue grouping [16], see [19] for an overview. Others use a Galerkin projection based on several Legendre polynomials [20], or a proper orthogonal decomposition (POD) [21]. Still, these latter two methods have only been applied to a linearised DFN model in [20,21]. Even though linearised models are valid for low (dis) charge currents, they become less accurate at higher currents. To summarize, the aforecited papers demonstrate model order reduction techniques for batteries on a priori simplified models (i.e., ones that only consider part of the dynamic behaviour, as discussed above) or even start from equivalent circuit models, see, e.g. [22].

In addition to the complexity of the modelling equations, the simulation time and required memory are affected by the particular numerical method for solving the DFN model equations [23]. Numerical methods have been studied in [16,24], while the computational performance of the suggested models has not been discussed. Furthermore, a computationally efficient implementation of the full DFN model has been proposed in [25]. However, [25] uses a simplification that was proposed in [16], which makes the model less accurate in comparison to the full DFN model. Moreover, [26] presents another computationally efficient implementation of the nonlinear Li-ion battery model, however it uses a simplification on the solid phase diffusion equations.

In this paper, we propose a computationally efficient implementation of the full DFN model. The proposed implementation is based on applying model order reduction to a discretisation of the infinite dimensional DFN model. The discretisation follows our previous work [27], where we have applied a spatial discretisation to convert the PDEs into a set of differential-algebraic equations (DAEs) and a temporal discretisation, based on a backward Euler method [28], to convert the entire model into a set of coupled nonlinear algebraic equations. To solve the discretised modelling equations, a computationally efficient numerical method is presented, based on a damped Newton's method, see, e.g. [29]. While it has been shown in [27] that the discretised DFN model already allows simulating the DFN model faster than real-time,[1] an accurate model implementation requires small step sizes in the discretisation, which still yields a very high-order model.

To reduce the order of the discretised DFN model, this paper proposes to apply model order reduction, which was not done in our previous work [27]. In particular, we apply a combination of POD [30] and discrete empirical interpolation method (DEIM) [31] to the full nonlinear DFN model, instead of applying it to a linearised or a priori simplified battery model, as was done in many of the aforecited papers. We employ the efficient implementation of [27] in the model order reduction and extend the simulation results of [27] to develop a suitable model, used for model order reduction. An extensive simulation study demonstrates that applying model order reduction leads to a lower-dimensional set of modelling equations, which requires less memory on an embedded real-time platform, have lower computational complexity and only have a minor loss of accuracy, when compared to the original DFN model implementation. Since the model order reduction has been applied to a electrochemistry-based model, which properly models the physical behaviour and internal states of the battery, these models are potentially interesting for real-time battery monitoring and control applications.

The rest of the paper is organized as follows. Section 2 outlines the DFN model. Then, a computational procedure is presented in Section 3 that implements the full DFN model. Section 4 introduces a model order reduction technique that simplifies the model and reduces the computation time and required memory. The simulation results of the full-order model implementation are given in Section 5, where computational performance analysis and model validation are discussed. Section 6 presents the simulation results of the reduced-order model implementation based on POD and DEIM that includes the snapshot and computational efficiency analysis. Finally, conclusions are drawn in Section 7.

2. Model of Lithium-ion batteries

The DFN model [1,2], considered in this paper, is a one-dimensional physics-based electrochemical model of a Li-ion battery. Fig. 1 shows the three different regions between the current collectors that determine the battery behaviour: the negative electrode, the separator and the positive electrode. During discharging, Li-ion de-intercalate from a solid-phase in the (porous) negative electrode, represented by spherical particles, and diffuse in a dissolved electrolyte phase through the separator towards the (porous) positive electrode, again represented by spherical particles, where they intercalate in the electrode. The reverse process occurs during charging. The DFN model is governed by a set of nonlinear PDEs that describe conservation of mass and charge in both the solid and electrolyte phases across the battery. A brief summary of the model is given below and the interested reader is referred to [1,2], or to [16] for a more control-oriented exposition of the model.

Li-ion concentration in the solid-phases c_s. The concentration of Li-ion in the solid-phases c_s in both electrodes (i.e., $x \in [0,\delta_-]$ for the negative electrode and $x \in [L-\delta_+,L]$ for the positive electrode, where δ_- and δ_+ are the thicknesses of negative electrode and positive electrode, respectively), derived from Fick's law of diffusion as a function of the radial coordinate inside the spherical particle $r \in [0,R_s]$ (where R_s is the radius of the spherical particles) and time $t \in \mathbb{R}^+$, is given by

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right), \tag{1a}$$

with boundary conditions

[1] Faster than real-time means that doing the simulation takes less time than the physical phenomena that are simulated take.