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Parameter estimation of an electrochemistry-based lithium-ion battery model

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HIGHLIGHTS

- Presenting a high-fidelity model of an electrochemistry Lithium-ion battery.
- Introducing a simulation scheme, robust in parameter estimation process.
- Applying homotopy optimization in parameter estimation of the battery model.
- Satisfying algebraic constraints during the optimization process.
- Updating initial conditions during optimization by the numerical algorithm.

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ABSTRACT

Parameters for an electrochemistry-based Lithium-ion battery model are estimated using the homotopy optimization approach. A high-fidelity model of the battery is presented based on chemical and electrical phenomena. Equations expressing the conservation of species and charge for the solid and electrolyte phases are combined with the kinetics of the electrodes to obtain a system of differential-algebraic equations (DAEs) governing the dynamic behavior of the battery. The presence of algebraic constraints in the governing dynamic equations makes the optimization problem challenging: a simulation is performed in each iteration of the optimization procedure to evaluate the objective function, and the initial conditions must be updated to satisfy the constraints as the parameter values change. The ε-embedding method is employed to convert the original DAEs into a singularly perturbed system of ordinary differential equations, which are then used to simulate the system efficiently. The proposed numerical procedure demonstrates excellent performance in the estimation of parameters for the Lithium-ion battery model, compared to direct methods that are either unstable or incapable of converging. The obtained results and estimated parameters demonstrate the efficacy of the proposed simulation approach and homotopy optimization procedure.

1. Introduction

Use of rechargeable batteries as electrochemical energy storage systems has gained a great deal of attention in many industrial fields. The automotive industry has benefitted substantially from battery technology, as it has enabled the manufacture of low-emission electric, hybrid electric, and plug-in hybrid electric vehicles [1–3]. Technologies for improving battery efficiency in vehicles have been of practical interest since the first electric cars were built in the mid-1800s. The optimization of automotive battery performance is facilitated by a physics-based model that represents the dynamic behavior of the battery, and can be used to predict its interaction with the vehicle and engine (e.g., in power management simulations). Additional practical aspects such as power, weight, longevity, safety, and cost define a broad research area in battery modeling and design.

Lithium-ion batteries are the most popular rechargeable battery units due to their low weight, low self-discharge rate, and high specific energy [4]. Electrochemical processes, together with thermal effects, are the key phenomena governing the dynamic behavior of batteries. Developing an accurate model of the

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Lithium-ion battery plays a pivotal role in control-oriented problems involving hybrid electric vehicles; however, high-fidelity models contain many parameters that must be estimated. Ideally, the battery model should be as detailed as possible while remaining capable of real-time performance, which is essential in the control-oriented design of automotive systems. Although more detailed models can be more accurate, the order and degree of nonlinearity of models based on fundamental physics can make them impractical for control design purposes. Spatial and temporal dependence in the governing equations of such models result in a system of partial differential equations (PDEs) that are coupled, stiff, highly nonlinear, and time-consuming to simulate.

Different types of physics-based battery modeling, from electrochemical-to circuit-based modeling schemes, have been studied in a comprehensive survey by Seaman et al. [5]. However, circuit-based models are not accurate enough in some control-oriented problems, which are essential in electric vehicle design. Estimating parameters of a detailed battery model can be challenging due to (1) a lack of physical significance for some parameters, especially in circuit-based models, and (2) difficulty in the experimental measurement of the parameters that are physically measurable. As a result, the practical design of battery models relies on *parameter estimation*, where unknown parameters in the governing dynamic equations are determined from experimental or simulated data. A *calibrated* and *validated* high-fidelity battery model is essential for our vehicle dynamics simulation work, including the design of power management strategies for hybrid electric vehicles [6,7]. The primary focus of this work is the model calibration phase. Although research on parameter estimation of Lithium-ion batteries has been primarily focused on equivalent circuit-based battery models [8–11], some work has used phenomenological battery models based on electrochemistry processes [12,13]. Forman et al. [12] used a genetic algorithm and Ramadesigan et al. [13] applied Gauss–Newton method, a Jacobian-based scheme, for the process of nonlinear optimization in their parameter estimation efforts, minimizing an objective function that represents the difference between the model outputs and their experimentally measured values. In general, finding a global minimum in the resulting optimization problem is the primary concern when estimating parameters. In this work, we use the homotopy optimization method [14,15], which is adept at finding global optima.

The remainder of this paper is organized as follows. In Section 2, we introduce the electrochemistry-based Lithium-ion battery model developed by Newman and Tiedemann [16] and Doyle et al. [17], which takes the form of PDEs. We also discuss the reduction procedure used by Dao et al. [4] to convert these PDEs into differential-algebraic equations (DAEs). The ε-embedding method, an efficient math-based algorithm, is introduced in Section 3 to solve the DAEs. Accordingly, we describe our procedure for numerical simulation. In Section 4, we present the homotopy optimization procedure, a global optimization scheme applied to parameter estimation in dynamic systems by Vyasarayani et al. [15,18]. The existence of algebraic constraint equations makes the optimization process more complicated in this application, since the initial conditions must be updated at each iteration in response to the changing parameter values. We then examine the application of homotopy optimization to estimating the parameters in the battery model in Section 5. Conclusions are discussed in Section 6.

2. Lithium-ion battery dynamic model

The electrochemical Lithium-ion battery model considered in this paper is derived using two main physical concepts: porous-electrode theory and concentrated solution theory [16,17]. As depicted in Fig. 1, the one-dimensional battery model is composed of positive and negative composite electrodes, the separator (an electrically non-conducting layer), and the electrolyte (a solvent containing a dissolved lithium salt that acts as an ionic conductor). Lithium ions travel parallel to the x axis between the positive and negative electrodes (also called the cathode and anode) through the electrolyte by way of diffusion and migration. The transport of lithium ions causes electrons to flow in the external circuit [19], thereby converting stored chemical energy into electrical energy. A thorough description of the charging and discharging processes in Lithium-ion batteries has been presented by Marcicki [20] and Dao et al. [4].

The focus of this work is the estimation of parameters in the equations governing the dynamics of the battery. The physical nature of these equations is discussed briefly; we refer to full explanations of the physics-based formulations in the literature. The battery equations are derived based on five electrochemical phenomena, described below. An inventory of all the battery parameters and their numerical values used in the simulation model is provided in Table A.1.

2.1. Species conservation for solid phase

According to the theory of porous electrodes, the lithium in a battery cell exists in two phases: the solid phase in the electrode material and the liquid phase in the electrolyte. As lithium ions (Li^+) intercalate into and out of the electrodes in the pseudo-dimension r (the direction normal to the surface of the electrodes, shown in Fig. 1), the diffusion equations for the solid phase are expressed in both the x-direction and the pseudo-dimension r [21]. Variations of lithium ion concentration in the solid phase can be expressed using Fick's laws of diffusion [17,22], assuming $c_{s,k} = c_{s,k}(x,r,t)$:

$$\frac{\partial c_{s,k}}{\partial t} = \frac{D_{s,k}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{s,k}}{\partial r}\right) \tag{1}$$

where $c_{s,k}$ and $D_{s,k}$ are, respectively, the concentration of lithium ions and the lithium ion diffusion constant coefficient associated with electrode k, assuming $k = p$ for the positive electrode and $k = n$ for the negative electrode. Associated with Eq. (1) are the following boundary conditions:

$$-D_{s,k}\frac{\partial c_{s,k}}{\partial r}\bigg|_{r=0} = 0 \text{ and } -D_{s,k}\frac{\partial c_{s,k}}{\partial r}\bigg|_{r=R_{s,k}} = J_k(x,t) \tag{2}$$

as well as the following initial condition:

$$c_{s,k}\big|_{t=0} = c_{s,k,0} \tag{3}$$

where $R_{s,k}$ and $J_k(x,t)$ are, respectively, the constant radius of intercalation and the pore-wall flux of lithium ions associated with electrode k.

Subramanian et al. [23] employed polynomial approximation and volume-average integration to derive equations for surface and average lithium ion concentrations. Introducing a three-variable polynomial function, together with volume-average integration for the original PDE and its derivative, Dao et al. [4] obtained two equivalent ordinary differential equations (ODEs) for the average