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Improvement of accuracy of multi-scale models of Li-ion batteries by applying operator splitting techniques

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ABSTRACT

In this work operator splitting techniques have been applied successfully to improve the accuracy of multi-scale Lithium-ion (Li-ion) battery models. A slightly simplified Li-ion battery model is derived, which can be solved on one time scale and multiple time scales. Different operator splitting schemes combined with different approximations are compared with the non-splitted reference solution in terms of stability, accuracy and processor cost. It is shown, that the reverse Strang–Marchuk splitting combined with the implicit scheme to solve the diffusion operator and Newton method to approximate the non-linear source term can improve the accuracy of the commonly applied vertical (sequential) multi-scale models by almost 3 times without considerably increasing the processor cost.

1. Introduction

Li-ion batteries (LIB) are electric power sources which have been commercialized to energize portable devices in the 90s by Sony [1]. In recent years LIBs have become the key enabling technology to store sufficient amount of electricity for future electric vehicles (EV) with a desirable driving range. Despite the improved energy storage and power capability of EVs, the battery technology needs to be improved further. Product optimization needs the application of complex mathematical models which can couple diffusion, heat transfer, and migration at molecular level and in the same time explain current, potential, heat and concentration distribution at macroscopic-level.

The mathematical description of LIBs is based on a non-linear parabolic system of partial differential equations with non-linear source terms and couples physical and chemical phenomena from nano to cm scale. This broad length and time scales makes the LIB models difficult to solve. Since no general analytical solution has been derived, several numerical approaches are developed. Franco et al. concluded [2] that there is no single numerical mathematical model which can describe all the coupled phenomena, and suggested [2,3] the application of multi-scale modeling (also known as integrated multi-scale modeling). Multi-scale modeling is based upon the recognition that the types of physics occurring at small time and length scales are distinct from those occurring at longer time and length scales [4]. An effective and accurate multi-scale

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model, which couples continuum equations (diffusion, heat transfer, migration) describing current, potential, and concentration distributions with molecular-level events can be used not only to design and to control complex electrochemical system but also to simulate local materials failure events and their impact on global scale behavior (i.e., safety). Consequently, the performance (accuracy, processor cost etc.) of novel models capable to solve multi-scale problems need to be compared and investigated for possible improvement.

Multi-scale models can be vertical, such that the smaller scale physics models (which may be atomistic or microstructural) are embedded and run "inside" the larger size scale physics models (macrohomogeneous). Alternatively, multi-scale models can be horizontal [5], in such a way that the results of lower size scale simulations provide input parameters, e.g. kinetic constants or thermodynamic quantities, for the higher-scale simulations.

In spite of the broad application of multi-scale models, the numerical characteristics (stability, convergence, accuracy) of splitting and embedding the results of sub-problems at different length and time scale require further detailed studies.

Operator splitting techniques are commonly applied for solving complex systems. The main idea is to split the complex problem into a sequence of sub-problems with simpler structure. Hence, the approach of operator splitting and multi-scale modeling is similar in respect of splitting the complex problem to sub-problems. In case of multi-scale modeling they can split the complex multi-scale problem into simpler single scale sub-problems by solving each of the latter by the most appropriate numerical approximation. Several ways to split a complex system into simpler problems and to solve them on different time and length scales have been developed e.g. sequential splitting, symmetrical splitting or Strang–Marchuk (S–M) splitting [5–8]. These methods differ from each other in time discretization providing different computational benefits and drawbacks.

Faragó at al. [6] used sequential splitting method for air pollution modeling and also for the solution of the Maxwell equations including a source term [7]. In both cases accuracy and adaptability of the operator splitting were examined. Kriston et al. [8] applied sequential and symmetrical splitting methods for the simulation of the transient behavior of fuel cells. The applied partial differential system comprised only one dependent variable and two operators. In the case of LIB model, there are at least 3 dependent variables and 4 different operators, therefore they represent a more complex problem. Moreover none of the works [2,4–8] applied operator splitting for multi-scale modeling, and we are not aware of any work which applied operator splitting for multi-scale simulation of LIBs.

In this paper a novel approach for multi-scale modeling of LIBs is developed. Decoupling of the processes at different scales is realized by operator splitting techniques. The mathematical accuracy and processor cost of the developed multi-scale models are analyzed and compared. The results indicate that the accuracy of both of the horizontal and vertical multi-scale models can be substantially improved by an adequately constructed splitting scheme.

On one hand we recommend this paper to mathematicians who would like to start with the simulation of LIBs. On the other hand we detail the mathematical descriptions, algorithms, numerical methods and derivation of models for engineers and other scholarly readers.

1.1. Description of operator splitting

The mathematical model of a LIB can be described in the form of the following abstract Cauchy problem for $t \in [0, T]$ and $x \in [0, L]$

$$\begin{cases} \dfrac{\partial w(\cdot, t)}{\partial t} = \displaystyle\sum_{i=1}^{n} A_i w(\cdot, t) \\ w(\cdot, 0) = w_0(\cdot), \qquad \dfrac{\partial w(0, t)}{\partial x} = g_1(t), \qquad \dfrac{\partial w(L, t)}{\partial x} = g_2(t) \end{cases} \tag{1}$$

where $w : \mathbb{R} \times \mathbb{R} \to \Lambda$ is the Λ-valued unknown function for every fixed $t \in (0, T]$ and Λ denotes the possible states space, which is usually assumed to be a Banach space. Furthermore $w_0(x) \in \Lambda$ and $g_1(t), g_2(t) \in \Lambda$ define the initial and boundary conditions of the problem and operators $A_i : \Lambda \to \Lambda$ define the different sub-processes.

Operator splitting techniques were developed to find the solution of problem (1), when A_i consists of non-linear operator(s). Usually operators are splitted by the different mathematical structures (e.g. linear and non-linear part of the equation are grouped separately) or by the same partial differential operators (grouping different time and space derivatives together), but the splitting is arbitrary. Then the obtained simpler systems are discretized on potentially different meshes. One of the main advantages of operator splitting techniques is that different numerical schemes and discretizations with different length and time scales can be applied, selecting the most adequate one for a given sub-problem. The main drawback, however may be the loss of convergence and accuracy. Multi-scale models also split A_i in respect of the physical processes and solve them at different time and/or length scales, consequently they apply a sort of operator splitting technique. Vertical multi-scale models are most likely similar to a sequential splitting scheme, which is the most simple operator splitting technique.

In this work the separation of the linear and non-linear processes is applied for the splitting of operators. The effect of operator splitting methods (e.g. sequential, symmetrical, S–M), and numerical schemes (e.g. explicit, implicit) on the accuracy are analyzed in detail.