



# Computationally efficient approach for solving time dependent diffusion equation with discrete temporal convolution applied to granular particles of battery electrodes



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## HIGHLIGHTS

- Method for modelling spatial and temporal concentration distribution in a granule.
- Based on discrete convolution of the analytic solution of the step function problem.
- Capable of treating problems with arbitrary non a priori known boundary values.
- Shorter computational times at the same accuracy as finite volume and Padé methods.

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## ABSTRACT

The paper presents a computationally efficient method for solving the time dependent diffusion equation in a granule of the Li-ion battery's granular solid electrode. The method, called Discrete Temporal Convolution method (DTC), is based on a discrete temporal convolution of the analytical solution of the step function boundary value problem. This approach enables modelling concentration distribution in the granular particles for arbitrary time dependent exchange fluxes that do not need to be known a priori. It is demonstrated in the paper that the proposed method features faster computational times than finite volume/difference methods and Padé approximation at the same accuracy of the results. It is also demonstrated that all three addressed methods feature higher accuracy compared to the quasi-steady polynomial approaches when applied to simulate the current densities variations typical for mobile/automotive applications. The proposed approach can thus be considered as one of the key innovative methods enabling real-time capability of the multi particle electrochemical battery models featuring spatial and temporal resolved particle concentration profiles.

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## 1. Introduction

The development of lithium ion battery models emerged in early 90's [1,2]. Electrochemical models of the entire cell that are applied in a large variety of applications from the development to the control tasks, e.g. Refs. [3–8], rely on particle models in the electrodes. The transport of lithium ions into, within and out of electrode particles is generally governed by a complex diffusion mechanisms that include phenomena such as phase transition, surface tension, volume changes [9], hysteretic behaviour, particle

size and shape variation and other multi-particle effects [10]. However modelling of such complex phenomena comes at great computational costs, which is detrimental for applications where short computational times are needed. Furthermore comprehensive electrode models covering a wide range of operating conditions encountered in the real applications cannot include treatment of most of these phenomena due to a lack of sufficient experimental data needed for their parametrisation and inclusion in such electrode models [9,10]. Therefore the modelling of the diffusion in the electrode particles typically relies on two effective simplifications: the assumption of uniform spherical particles and the assumption of Fick's diffusion within the whole particle. These simplifications are particularly found in models aiming at fast computation, e.g. Refs. [3–8].

As lithium concentration at the surface of the granular particle

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influences the ion exchange flux and as calculation of this concentration generally requires a considerable CPU share in multi-particle models further enhancements of methods for solving Fick's diffusion are sought. Presently, several methods are used to predict the surface concentration: finite difference method [11], finite element method [11,12], polynomial approximation [6,13], differential quadrature [11], Duhamel's superposition method [13], diffusion length method [13], analytical methods [8,14,15], pseudo steady state methods [13,14,16,17], orthogonal collocation on finite elements [5] and Padé approximation state space method [4,18]. Results presented in Refs. [13,19] indicate that computational expenses of the models for calculating surface concentration of the particles significantly influence the computational expenses of the overall battery model as the evaluation of the particle surface concentration needs to be executed at every discretization point of the electrode.

In this paper a Discrete Temporal Convolution method (DTC) is presented and its results are compared against the results obtained with the following four common methods:

- 1 .Analytical method representing the exact solution in a case with a priori defined exchange flux;
- 2 .polynomial approximations representing very computationally fast methods; and
- 3 .finite volume/difference methods representing standard, i.e. benchmark, methods for solving time dependent diffusion equation.
- 4 Padé approximation state space method as an advanced computationally efficient method.

Finite volume/differences methods enable evaluation of spatial and temporal concentration profile by solving the time dependent diffusion equation numerically in both dimensions. As presented in Ref. [11] this type of method enables achieving high accuracy of the concentration profile resolution. However, within the field of real-time capable battery models, the computational expenses of finite volume/differences methods mostly limit their application to only the single particle models [11].

A Padé approximation state space method [4,18] offers faster computational times compared to finite volume/differences methods and will in the present study be used as a benchmark computationally efficient advanced method.

As a computationally much faster alternatives, approximation formulae are widely applied to evaluate the particle surface concentration [6]. The analyses done in this paper show that these approximation formulae return physically plausible results only for low frequency current variations, which is inherently related to their quasi-steady origin. Additionally, ref. [6] also disputes their accuracy when applied to cycles featuring high charging/discharging currents. These facts significantly limit their use in many applications, e.g. automotive. Deficiencies of the approximation formulae inherently arise from their approximation basis that does not consider physical governing mechanisms.

Alternatively, a fully analytical solution of the time dependent diffusion equation in spatial and temporal dimension is presented in Refs. [14,15]. This method is computationally efficient, however its deficiency in real hardware applications arises from the fact that a priori knowledge of the exchange flux, which must be given in an analytical form, is needed to evaluate the equation. Furthermore, Ref. [3,8] presents an approximate solution for the spherical diffusion equation that is fully derived and, similarly as in Refs. [14,15], benchmarked with an a priori (i.e.: constant [3,8] and sinusoidal [8]) molar flux of lithium ions at the particle surface in the radial direction.

This paper presents an approach for solving the time dependent

diffusion equation in the form of temporally convoluted analytical solutions of the step function boundary value problem. This approach efficiently tackles the shortcomings of the approaches analysed above and forms the basis for the method that:

- is capable of accurately solving for the spatial and temporal concentration profile as it is based on time dependent diffusion equation;
- features shorter computational times than finite volume/differences methods and Padé approximation state space method at the same accuracy of the results, which is to a large extent owed to its analytical solution in the spatial dimension;
- is capable of solving for arbitrary time dependent exchange fluxes that do not need to be known a priori as it relies on solution with discrete temporal convolution.

The proposed method thus opens ways for real-time capable multi particle electrochemical battery models featuring spatially and temporally resolved particle concentration profiles. Furthermore, the DTC's head principle of temporally convoluted analytical solutions of the step function boundary value problem can be extended to any geometry for which the eigen functions of the Laplace operator can be devised.

## 2. Theoretical framework

The core principle of the method presented in this paper is the analytically resolved spatial and temporal concentration distribution of ion concentration in one representative porous granule of the battery's granular solid electrode. The ion concentration distribution within the granule comes as a solution of time dependent diffusion equation with the boundary condition of given ion molar exchange flux in the radial direction defined at the granule surface. The diffusion equation obeying the Fick's law is assumed to apply to the whole granule. The modelled granule is assumed ideally spherical and small enough to assume uniform ion surface concentration and uniformly distributed ion exchange flux at the surface leading to the assumption of full spherical symmetry of the problem. For non-spherical and porous particles that do not feature very significant topology discrepancy compared to spherical geometry, it is reported in Ref. [20] that plausible results can be obtained for the particles of the same volume by applying model basis of the spherical particle and considering surface area difference between spherical particles and non-spherical and porous particles.

The temporal variation of ion exchange flux at the granule surface (i.e. the boundary condition of the diffusion problem) is treated discretely meaning that for the duration of the chosen computational time-step the influx at the surface is treated as constant and changes discretely only between time-steps. Thus, from the view point of the diffusion equation, the boundary condition is a parameter that varies as a step function. The value of this parameter does not need to be known for every time step prior to the start of simulation (a priori) but can be updated before every time-step by solving the electrochemical equation between time-steps. The diffusion equation reads:

$$\frac{\partial c(\vec{r}, t)}{\partial t} = D\nabla^2 c(\vec{r}, t), \quad (1)$$

where  $c$  is the ion concentration in granule and  $\vec{r}$  is the position vector. In spherical symmetry, with the coordinate origin at the centre point of the granule, this is expressed as:

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