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Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

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Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Dieter Prätzel-Wolters

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

An overview on the usage of some model reduction approaches for simulations of Li-ion transport in batteries

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Abstract

In this work, some model reduction approaches for performing simulations with a pseudo-2D model of Li-ion battery are presented. A full pseudo-2D model of processes in Li-ion batteries is presented following [3], and three methods to reduce the order of the full model are considered. These are: i) directly reduce the model order using proper orthogonal decomposition, ii) using fractional time step discretization in order to solve the equations in decoupled way, and iii) reformulation approaches for the diffusion in the solid phase. Combinations of above methods are also considered. Results from numerical simulations are presented, and the efficiency and the accuracy of the model reduction approaches are discussed.

1 Introduction

Secondary Li-ion batteries used for technical applications are based on porous insertion electrodes. In most of the technical applications the porous electrodes are random structures of active particles bound together by a mixture of polymeric binder and soot for enhancing the electrical conductivity of the electrode. During charging Li-ions are de-intercalated from the anode particles into the electrolyte and transported through the electrolyte to the porous cathode. There they are intercalated at the surface of the cathode particles and then transported via diffusion into the interior of particles. It is well understood that the microstructure (e.g. size and arrangement of the active particles in the porous electrodes) significantly influence the performance of the battery. Going beyond porous structures, it has even been shown that specifically designed electrodes, can achieve a much larger power density [9], but still a lot of research is needed in order to quantitatively evaluate the influence of 3D structures. Available 3D microscale models include mass transport in the electrolyte and in the solid particles, coupled with an equation for the potential [2, 1] and more generally also with an additional equation for the temperature [11]. Solving these models is only possible on cuts through the whole cell covering nevertheless the whole cathode anode direction [19, 5]. Simulations on the complete microstructure is not yet possible due to the tremendous CPU demand. One approach to overcome this problem at least for random porous electrodes pioneered by the group of J. Newman [13] is to model the electrodes as effective random one dimensional porous media characterized by a porosity [16, 6, 8, 14, 4, 15, 7]. Their effective transport properties are obtained by averaging the properties of electrolyte and the active particles. In addition the transport within the particles is modeled as diffusive transport in one effective particle per volume element coupled to the transport in the effective porous medium. The separator is also described as effective porous medium. Thus a pseudo-2D model (i.e. 1D+1D model) for the full battery cell is obtained. Three dimensional extensions (more exact 3D+1D models), which allow to simulate complex shaped electrodes are possible [21]. These macroscopic models are solved by some numerical method, e.g., finite difference, finite volume or finite elements. One (representative) spherical particle is located in each grid node (for FDM and FVM), or in each quadrature point (for FEM), and the macroscopic model is coupled to the model in the particle (see the text below for details). The solution of the coupled model (called also *full model* below in the text) requires solving diffusion equation for each particle in an extra pseudo-dimension, namely in the radius r. Consequently, the number of unknown variables in this 1D+1D model is large, thus still requiring significant computational time. To obtain models which can be solved in real time further approaches for reducing the demanded computational times have appeared in the literature. The goal of this paper is to present a computational study of the performance of three model reduction approaches, when applied to simulation of processes in Li-ion battery.

First, consider the approach which was earlier presented in [3]. It exploits reduced order method, ROM, which is based on proper orthogonal decomposition, POD. The Authors claimed that this method is efficient for the pseudo-2D model, and they provided some simulation results for test cases. However, the parameters (and thus regimes) for simulation of real processes sometimes differ from conditions considered in test cases, and therefore more studies are required for the case of real parameters.

Further on, reformulation methods were used to avoid solving the diffusion equation in the active particles, see, e.g. [13, 2, 20, 17, 12, 22, 18]. These methods are based on approximating the concentration in solid phase by some selected functions of r, followed by volume averaging. The basis functions are global (defined from 0 to R), but very few of them are used. The aim of the volume averaging is to avoid solving the diffusion equation in the active particles. Zhang and White [22] compared some of the reformulation methods and discussed their efficiency in solving test examples.

In this paper, we consider both of the above methods and apply them in order to reduce the model order of the pseudo-2D li-ion battery model. In the case of ROM based on POD, we select a basic set of parameters and perform full simulations. After that the solution is used to form so called transform basis. The latter are used to form reduced order model, and later on to simulate the processes for other sets of parameters. We also review most of the reformulation methods and consider combination of reformulation and ROM-POD approaches. Further on, we consider one new way to reduce the the complexity of the problem, namely a fractional time step discretization, allowing to solve for all the unknowns in a decoupled way. The dominated part of the unknowns can be solved in parallel, and the other part can be combined with ROM-POD to further increase the efficiency.

The rest of the paper is organized as follows. In section 2 we describe the full model and the discretization. In section 3, we discuss the algorithm of ROM based on POD and apply it to reduce the order of the full pseudo-2D model. In section 4, we present the fractional time step discretization and solve the full model in a decoupled way. In section 5, we review the reformulation methods and combine them with ROM. Conclusions are given in section 6.

2 Full pseudo 2D model

The sketch of a LiMnO2-carbon battery is shown in Figure 1. From left to right, the components of the battery are aluminum current collector, LiMnO2 positive electrode, separator, carbon negative electrode, and copper current collector. The governing equations and related expressions are summarized in Table 1 (see also [3]), and the parameters are given in Table 2.

For the discretization of the above model, cell centered finite volume method is adopted. The domain $(0, L_p + L_s + L_n)$ is divided into $N_p + N_s + N_n$ cells. Active particles are placed at the centers of those cells, which

Table 1: Governing equations and expressions

variable	equation	boundary conditions
c_s	$\frac{\partial c_s}{\partial t} = D_s \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial c_s}{\partial r})$	$-\frac{\partial c_s}{\partial r}\vert_{r=0} = 0,\ -\frac{\partial c_s}{\partial r}\vert_{r=R_{s,i}} = j_i$
c_e	$\epsilon_i \frac{\partial c_e}{\partial t} = D_{eff,i}\frac{\partial^2 c_e}{\partial x^2} + (1-t_+)a_i F j_i$	$-D_{eff,i}\frac{\partial c_e}{\partial x} = 0$
Φ_1	$\sigma_{eff,i}\frac{\partial^2 \Phi_1}{\partial x^2} = a_i F j_i$	$-\sigma_{eff,p}\frac{\partial \Phi_1}{\partial x} = I,\ \Phi_1\vert_{x=L_p+L_s+L_n} = 0$
Φ_2	$-\frac{\partial}{\partial x}(\kappa_{eff}\frac{\partial \Phi_2}{\partial x}) + \beta\frac{\partial}{\partial x}(\kappa_{eff}\frac{\partial lnc_e}{\partial x}) = a_i F j_i$	$-\kappa_{eff,i}\frac{\partial \Phi_2}{\partial x} = 0$
initial conditions	$c_{s,i}(r,0) = c_{s,i,0}$	$c_e(x,0) = c_0$
interface conditions		
$x = L_p$	$-D_{eff,p}\frac{\partial c_e}{\partial x} = -D_{eff,s}\frac{\partial c_e}{\partial x}$	$-\sigma_{eff,p}\frac{\partial \Phi_1}{\partial x} = 0 \quad -\kappa_{eff,p}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,s}\frac{\partial \Phi_2}{\partial x}$
$x = L_p + L_s$	$-D_{eff,s}\frac{\partial c_e}{\partial x} = -D_{eff,n}\frac{\partial c_e}{\partial x}$	$-\sigma_{eff,n}\frac{\partial \Phi_1}{\partial x} = 0 \quad -\kappa_{eff,s}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,n}\frac{\partial \Phi_2}{\partial x}$

expressions

$$U_p = 4.199 + 0.0566tanh(-14.555\theta_p + 8.609) - 0.0275[(0.998-\theta_p)^{-0.492} - 1.901] - 0.157exp(-0.0474\theta_p^8) + 0.81exp[-40(\theta_p - 0.134)]$$

$$U_n = -0.16 + 1.32exp(-3.0\theta_n) + 10.0exp(-2000.0\theta_n)),\ \theta_p = c_{s,p,surf}/c_{s,p,max},\ \theta_n = c_{s,n,surf}/c_{s,n,max}$$

$$j_i = 2k_m(c_{s,i,max} - c_{s,i,surf})^{0.5} c_{s,i,surf}^{0.5} c_e^{0.5} sinh(\frac{0.5F}{RT}(\Phi_1 - \Phi_2 - U_i)),\ \sigma_{eff,i} = \sigma_i(1-\epsilon_i-\epsilon_{f,i}),\ a_i = \frac{3}{R_{s,i}}(1-\epsilon_i-\epsilon_{f,i}),\ \text{i=p,n}$$

$$\kappa_{eff,i} = (4.1253\times10^{-2} + 5.007\times10^{-4}c - 4.7212\times10^{-7}c^2 + 1.5094\times10^{-10}c^3 - 1.6018\times10^{-14}c^4)\epsilon_i^{brugg_i},\ D_{eff,i} = D_e\epsilon_i^{brugg_i}, i = p,s,n$$

Table 2: Parameters

Parameter	Value	Unit	Parameter	Value	Unit
L_p	183	μm	$c_{s,p,max}$	22860	mol/m^3
L_s	52	μm	$c_{s,n,max}$	26390	mol/m^3
L_n	100	μm	$c_{s,p,0}$	3900	mol/m^3
$R_{s,p}$	8	μm	$c_{s,n,0}$	14870	mol/m^3
$R_{s,n}$	12.5	μm	σ_p	3.8	S/m
$D_{s,p}$	1.0×10^{-13}	m^2/s	σ_n	100	S/m
$D_{s,n}$	3.9×10^{-14}	m^2/s	$Brugg_p$	1.5	–
D_e	7.5×10^{-11}	m^2/s	$Brugg_s$	1.5	–
ϵ_p	0.444	–	$Brugg_n$	1.5	–
ϵ_s	1.0	–	k_p	2.334×10^{-11}	$mol/m^2s/(mol/m^3)^{1.5}$
ϵ_n	0.357	–	k_n	2.334×10^{-11}	$mol/m^2s/(mol/m^3)^{1.5}$
$\epsilon_{f,p}$	0.259	–	t_+	0.363	–
$\epsilon_{f,n}$	0.172	–	I	17.5(1C rate)	A/m^2
c_0	2000	mol/m^3	T	298	K

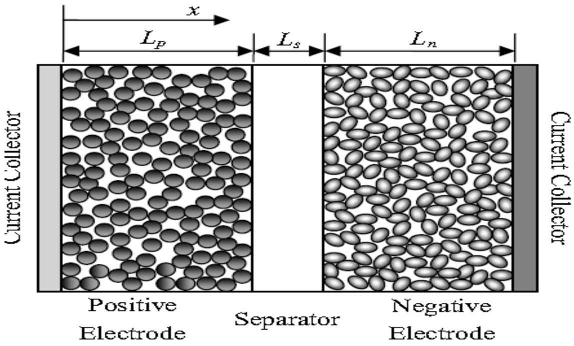

Figure 1: Schematic of a lithium battery

belong to the electrodes. The processes in the porous electrodes, described by macroscopic equations, are coupled via Butler-Volmer flux conditions on the surface of the particle to the processes in the particles, described by 1D model in spherical coordinates. This micro-macro coupling fits, for example, Heterogeneous Multiscale Method philosophy. Thus the pseudo-2D model assumes that the particles in the center of the grid cells (see Figure 2) are typical and represent all other particles in the cell. The active solid particles are considered to have spherical form, and it is further assumed that processes in r direction dominate, so that 1D model can be used in each particle. The radius r of each particle is divided into N_r control volumes (cells). N_r = 50 is used in simulations presented here. The (macroscopic) $x-$ regions of the positive electrode, of the separator, and of the negative electrode, are discretized into $N_p = 100$, $N_s = 70$, and $N_n = 100$ control volumes, respectively.

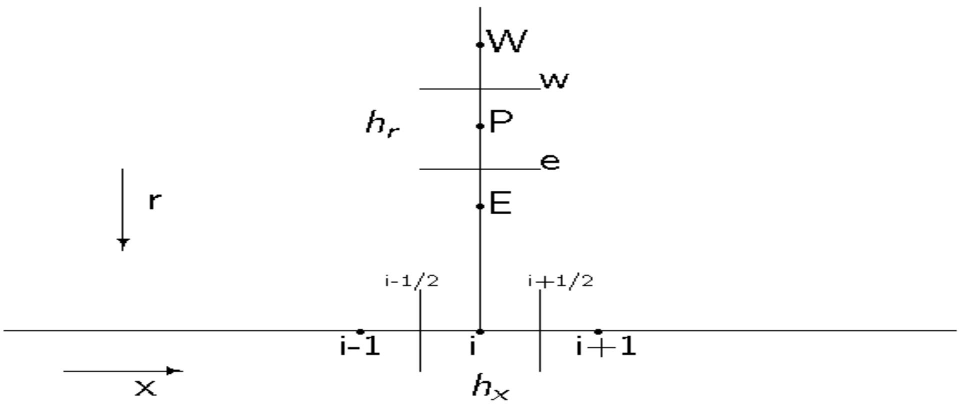

Figure 2: A typical volume in electrode

Thus, with the selected Ns, at every grid node of the macroscopic grid (x- coordinate), there are 54 unknowns. They are arranged in the following order: the first 50 unknowns correspond to the concentration of lithium ions in the respective particle, numbered from the center to the surface of particle. The 51th unknown stands for the concentration on the surface of the particle, the 52th unknown stands for the concentration in the electrolyte, the 53th stands for the potential in the solid phase, and the last one stands for the potential in the electrolyte. The respective 54 equations arising after the discretization are numbered from i_1 to i_{54} and they look as follows:

$$\begin{aligned}
\frac{dc_{s,P}}{dt} &= \frac{D_s}{r_P^2}\frac{r_e^2(c_{s,E}-c_{s,P})}{h_r^2} \qquad (i_1)\\
\frac{dc_{s,P}}{dt} &= \frac{D_s}{r_P^2}\frac{r_e^2(c_{s,E}-c_{s,P})-r_w^2(c_{s,P}-c_{s,W})}{h_r^2} \qquad (i_2)\cdots(i_{49})\\
\frac{dc_{s,P}}{dt} &= -\frac{r_e^2}{r_P^2 h_r}j-\frac{D_s}{r_P^2}\frac{r_w^2(c_{s,P}-c_{s,W})}{h_r^2} \qquad (i_{50})\\
c_{s,surf} &= \frac{-3h_r j+9D_s c_{s,50}-D_s c_{s,49}}{8D_s} \qquad (i_{51})\\
\epsilon\frac{dc_e}{dt} &= D_{eff}\frac{c_{e,i+1}-2c_{e,i}+c_{e,i-1}}{h_x^2}+(1-t_+)aj \qquad (i_{52})\\
aFj &= \sigma_{eff}\frac{\Phi_{1,i+1}-2\Phi_{1,i}+\Phi_{1,i-1}}{h_x^2} \qquad (i_{53})\\
aFj &= -\frac{\kappa_{eff,i+\frac{1}{2}}(\Phi_{2,i+1}-\Phi_{2,i})-\kappa_{eff,i-\frac{1}{2}}(\Phi_{2,i}-\Phi_{2,i-1})}{h_x^2}\\
&+\frac{\kappa_{\beta_{i+\frac{1}{2}}}(c_{e,i+1}-c_{e,i})-\kappa_{\beta_{i-\frac{1}{2}}}(c_{e,i}-c_{e,i-1})}{h_x^2} \qquad (i_{54})
\end{aligned} \tag{1}$$

Where $\kappa_\beta = \frac{\kappa_{eff}\beta}{c_e}$, $\kappa_{eff,i+\frac{1}{2}}$ is harmonic average of $\kappa_{eff,i+1}$ and $\kappa_{eff,i}$, means $\kappa_{eff,i+\frac{1}{2}} = \frac{2\kappa_{eff,i+1}\kappa_{eff,i}}{\kappa_{eff,i+1}+\kappa_{eff,i}}$, and similar to $\kappa_{eff,i-\frac{1}{2}}$, $\kappa_{\beta_{eff,i+\frac{1}{2}}}$ and $\kappa_{\beta_{eff,i-\frac{1}{2}}}$.

Remark 2.1 In the above discretization, j equal to j_p in positive electrode, zero in separator and j_n in negative electrode. For the surface concentration, as there is no governing equation for it in Table 1, we just interpolate it with the two nearest unknowns inside the particle, combined with the surface condition. For the nodes in the separator, only equations with numbers (i_{52}) and (i_{54}) are used, all other unknowns are assigned to be zeros.

Remark 2.2 For the treatment of interface conditions at $x = L_p$ (similarly at $x = L_p + L_s$), we use $-D_{eff,p}\frac{\partial c_e}{\partial x} = -D_{eff,s}\frac{\partial c_e}{\partial x} = -D_{eff,ps}\frac{c_{e,s}-c_{e,p}}{0.5(h_p+h_s)}$

and $-\kappa_{eff,p}\frac{\partial\Phi_2}{\partial x} = -\kappa_{eff,s}\frac{\partial\Phi_2}{\partial x} = -\kappa_{eff,ps}\frac{\Phi_{2,s}-\Phi_{2,p}}{0.5(h_p+h_s)}$, where $D_{eff,ps}$ is harmonic average of $D_{eff,p}$ and $D_{eff,s}$, and similar to $\kappa_{eff,ps}$.

For the time discretization, first order backward Euler is adopted. Uniform time step is used, and standard Newton-Raphsion method is applied to solve the obtained nonlinear system.

3 Reduced order model based POD

3.1 Method and algorithm

Let us denote the spatially discretized system of the full model(1) as

$$M_1\frac{d\mathbf{x}}{dt} = \mathbf{f}_1(t,\mathbf{x}) \tag{2}$$

Here M_1 is a $n_{full} \times n_{full}$ matrix, both $\mathbf{x}$ and $\mathbf{f}_1$ are $n_{full} \times 1$ vectors. The system order n_{full} is usually large (over 10,000 in our case). This is not just a system of ODEs, it is a large differential-algebraic system, DAE system, that is, M_1 has zero rows.

The idea of the reduced order method (see, e,g,[3, 10]) is as follows. Suppose that

$$\mathbf{x} = B\mathbf{y} \tag{3}$$

where B is a $n_{full} \times n_{rom}$ matrix and $\mathbf{y}$ is a $n_{rom} \times 1$ vector. Substitute (3) into (2) and multiply both sides by B^T. As a result we obtain the following reduced order system:

$$M\frac{d\mathbf{y}}{dt} = \mathbf{f}(t,\mathbf{y}) \tag{4}$$

where $M = B^T M_1 B$ is $n_{rom} \times n_{rom}$ matrix and $\mathbf{f}(t,\mathbf{y}) = B^T\mathbf{f}_1(t,B\mathbf{y})$ is a $n_{rom} \times 1$ vector.

The basis matrix B is the crucial ingredient of the above reduced order model. POD (proper orthogonal decomposition) [10] is often used to obtain B. The whole algorithm for the reduced order model is described below, see *Algorithm 1.*

Algorithm 1 Suppose $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{n_t}]$ is solutions at all n_t time steps for one case (base case).

(1) Do POD as $\mathbf{X}\mathbf{X}^T = \Phi\Lambda\Phi^T$

(2) Form transformation matrix B as: $B = \Phi(1:n_{rom})$

(3) Form reduced order system using the above B.

(4) Solve the reduced system in for the specified parameters, and use its solution to recover the solution of the full system by $\mathbf{x} = B\mathbf{y}$.

In the above algorithm, the number n_{rom} is determined as follows: choose the smallest n such that

$$\frac{\sum_{i=1}^{n_{rom}} \lambda_i}{\sum_{i=1}^{n_t} \lambda_i} > tol$$

where $\Lambda = diag(\lambda_1, \cdots, \lambda_{n_t})$, $\lambda_i \geq \lambda_{i+1}$ are the eigenvalues numbered in non-increasing order. The threshold $tol \in (0, 1)$, is often taken as $tol = 99.99\%$ or more close to 1. In act, the choice of the threshold depends on the accuracy required for solving the particular full problem.

Remark 3.1 The computed solution $\mathbf{X}$ is of size $n_p \times n_t$, where n_p is the number of unknowns at one time step and n_t is the number of time steps. Usually $n_p >> n_t$, and in this case we do POD as $\mathbf{X}^T\mathbf{X} = \Psi\Lambda\Psi^T$, $\Phi = \mathbf{X}\Psi$ and then normalize Φ.

Remark 3.2 We split the unknown variables into several groups, according to their meaning,

$$(c_{s,p}, c_{s,n}, c_{s,p,surf}, c_{s,n,surf}, \Phi_{1,p}, \Phi_{1,n}, c_e, \Phi_2)$$

, and after that perform POD and choose eigenvectors for each group. At the end we glue together the chosen eigenvectors from all the these groups in order to get the matrix B. The same approach is used, e.g., in [3].

Remark 3.3 Sometimes it is useful to include the initial value as one separate column in B, i.e.

$$B_1 = \Phi(1:n), \mathbf{p} = \mathbf{x}_0 - B_1^T B_1 \mathbf{x}_0, B = [\frac{\mathbf{p}}{||\mathbf{p}||}, B_1]$$

This will ensure that the obtained reduced order system is consistent with the given initial state.

3.2 Results and discussion

To test the efficiency of the presented ROM method, we consider three different examples here. In all the examples, the results obtained with ROM are compared with the solution of the full model.

(1) We choose the base case to be 1C discharge with the parameters given in Table 2, and change initial conditions $(c_e(x, 0) = 2500, c_{s,n}(r, 0) = 18870)$ as tested case. In this example, the base case and the tested case differ only in the values for the initial conditions. The full model solution and the ROM

solution of the tested case are compared in Figure 3. We can see that the ROM with only 27 eigenvectors (for comparison, the size of the full system is 14580) approximate the solution of the full model very well.

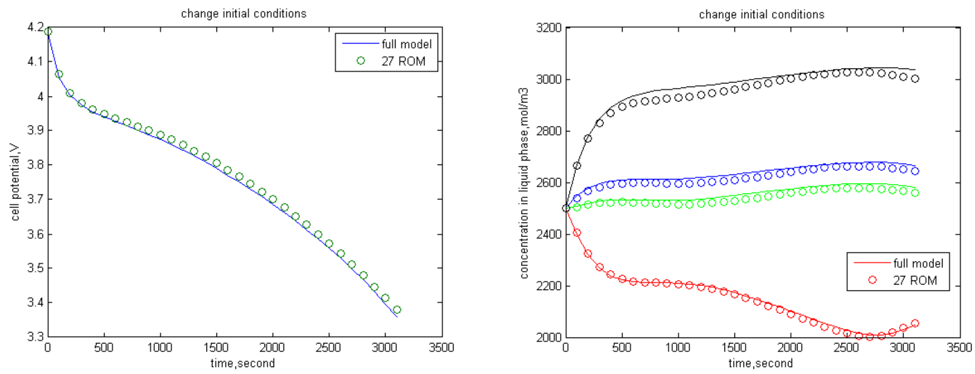

Figure 3: Change initial conditions *Left*: cell potential; *Right*: concentration at interfaces

(2) we choose the same base case as in the first example, but choose as tested case a problem with characterized by 10C discharge. All other parameters are the same as in the base case. For this example, as one can see on Figure 4, we need to choose for ROM solution more eigenvectors (than in the previous example) in order to achieve good accuracy.

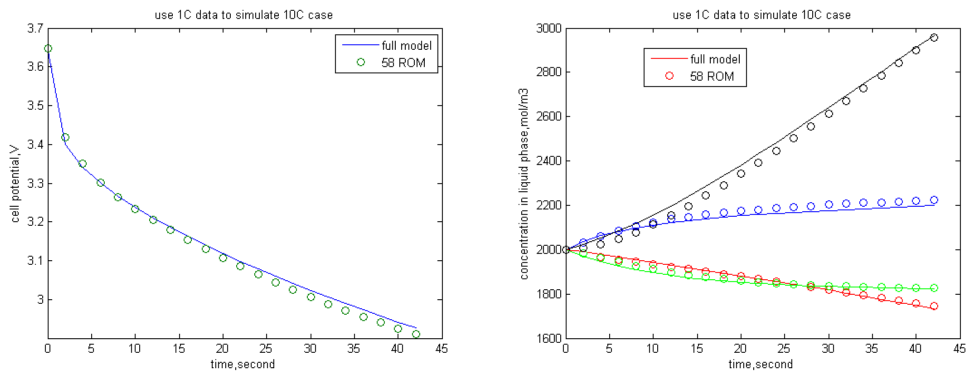

Figure 4: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

3)The third considered example corresponds to simulation of discharge-charge cycles. In one cycle, the battery is first discharged at 1C rate until the cell potential decrease to 3.0 V., followed by a 1C charge process up to 4.3 V, and at the last stage of the cycle the battery is charged at 4.3 V until the current decreases to 10 mA. In the simulations, we choose the solution of one cycle as a base solution, form reduced system and use the latter to simulate many cycles. The results in Figure 5 shows that the ROM with 105 eigenvectors works very well.

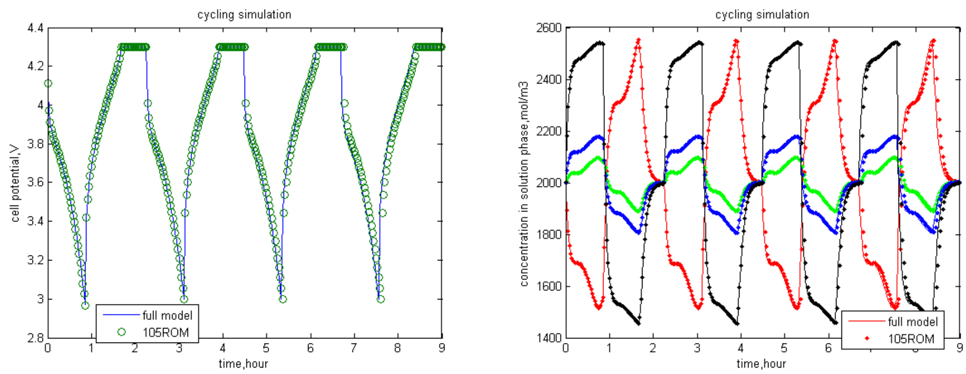

Figure 5: Cycling simulation *Left*: cell potential; *Right*: concentration at interfaces

4 Fractional time step discretization

4.1 Method description

Consider again the full model. When first order backward Euler is used for time discretization, the resulting discretized system at time t_{n+1} is written as follows

$$M\frac{\mathbf{x}^{n+1}-\mathbf{x}^{n}}{\triangle\ t} = f(\mathbf{x}^{n+1})$$

We divide all the unknowns into two classes, namely $\mathbf{x} = (\mathbf{x}_e, \mathbf{x}_p)$, where we choose $\mathbf{x}_p = (c_s, c_{s,surf})$ as concentration in the particles, and $\mathbf{x}_e = (c_e, \Phi_1, \Phi_2)$ to be collection of the remaining unknowns. With the new notations, the above Euler discretization can be rewritten as follows:

$$M_1\frac{\mathbf{x}_e^{n+1}-\mathbf{x}_e^{n}}{\triangle\ t} = f_1(\mathbf{x}_e^{n+1}, \mathbf{x}_p^{n+1}) \tag{5}$$

$$M_2\frac{\mathbf{x}_p^{n+1}-\mathbf{x}_p^{n}}{\triangle\ t} = f_2(\mathbf{x}_e^{n+1}, \mathbf{x}_p^{n+1}) \tag{6}$$

Fractional time step discretization can also be applied to the full system, thus obtaining a decoupled system. (Note, the questions about the theoretical study on the stability of this fractional time step discretization are not studied here. We can just note that our simulations show that it is worth to use this approach).

$$M_1 \frac{\mathbf{x}_e^{n+\frac{1}{2}} - \mathbf{x}_e^n}{\triangle\ t} = f_1(\mathbf{x}_e^{n+\frac{1}{2}}, \mathbf{x}_p^n) \tag{7}$$

$$M_2 \frac{\mathbf{x}_p^{n+1} - \mathbf{x}_p^n}{\triangle\ t} = f_2(\mathbf{x}_e^{n+\frac{1}{2}}, \mathbf{x}_p^{n+1}) \tag{8}$$

The above predictor-corrector discretization means that at each time step we first solve for $\mathbf{x}_e$ using the solution of $\mathbf{x}_p$ at the previous time, and after that solve for $\mathbf{x}_p$ at the new time step, using just computed $\mathbf{x}_e$.

Remark 4.1 Note that in this particular problem $\mathbf{x}_p$ contains much more unknowns compared to $\mathbf{x}_e$, and that one can solve the predictor step for each particle separately, as long as the values from the previous time step are used for $\mathbf{x}_e$. As a result, this decoupled solve works much faster than the coupled solve for the full model.

Remark 4.2 For the solve with respect to $\mathbf{x}_e$ at each time step, we can use the previous ROM method in order to reduce the order of this system. This combination of using decoupled solve (fractional time step discretization) and ROM, can further improve the efficiency.

4.2 Results and discussion

We test coupled and decoupled system in two cases: 1C discharge and 10C discharge. For decoupled system, we need some restrictions on the time step. If uniform time step is used, the time step need to satisfy $\triangle\ t < 70s$ for 1C case and $\triangle\ t < 7s$ for 10C case. If the time step satisfy these conditions, solving the decoupled system is much faster than solving the coupled system and, and the results obtained by the two approaches are very close. It should be noted that often very large time steps (even if allowed by the stability consideration) can not be used in the simulations, because this would lead to lose of accuracy. See Figure 6 and Figure 7 for details.

As pointed out in Remark 4.2, the above presented ROM approach presented can be used to solve for $\mathbf{x}_e$ at each time step. The results from such an approach for example 1 and example 2 are given in Figure 8 and Figure 9. It can be seen that in both cases the solution of the full model is approximated very well.

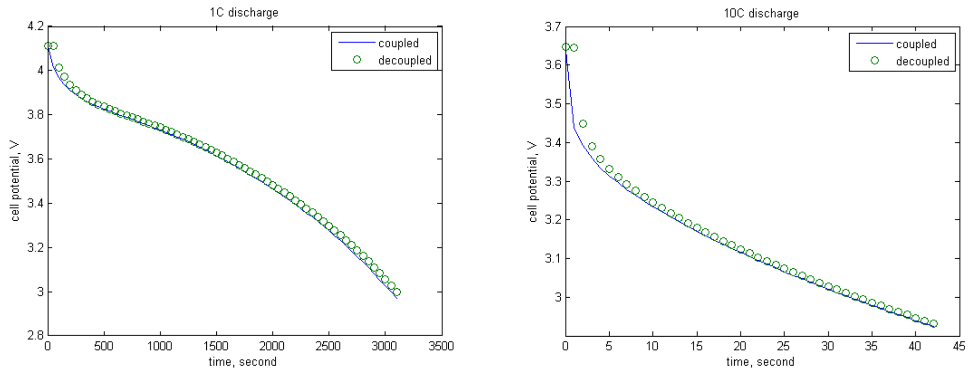

Figure 6: Cell potential. *Left*: 1C rate; *Right*: 10C rate.

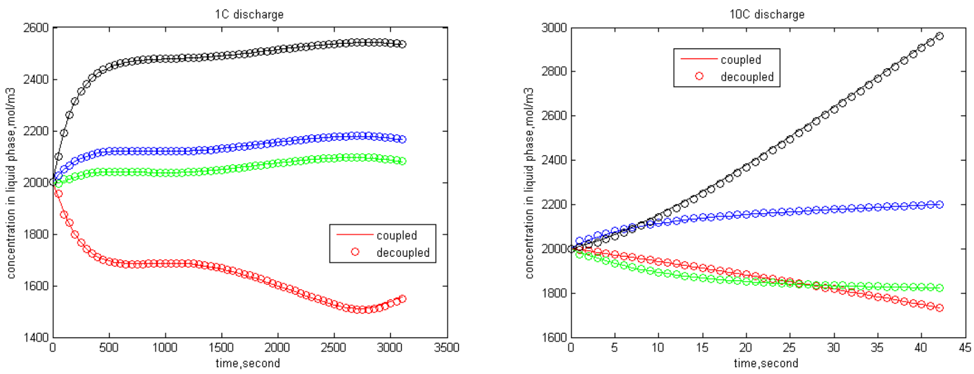

Figure 7: Concentration at interfaces. *Left*: 1C rate; *Right*: 10C rate.

5 Reformulation of particle diffusion

In the full model, most of unknowns come from the discretization of the following diffusion equation inside the particle

$$\frac{\partial c}{\partial t} - D_s \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial c}{\partial r}) = 0 \tag{9}$$

with boundary condition

$$D_s \frac{\partial c}{\partial r} = 0 \qquad at\ r = 0 \quad and\ for\ t \geq 0$$

$$D_s \frac{\partial c}{\partial r} = -j \qquad at\ r = R_p \quad and\ for\ t \geq 0$$

where j is the pore wall flux at the surface of particle and R_p is the radius of the particle. If we can avoid solving this equation, then the number of

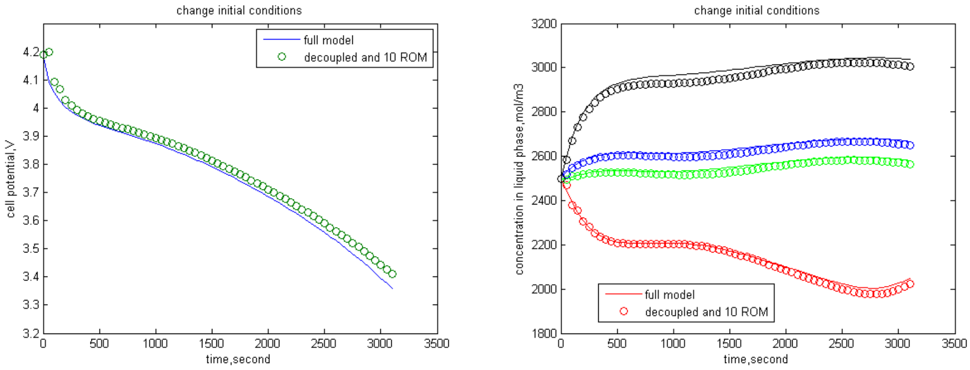

Figure 8: Change initial condition *Left*: cell potential; *Right*: concentration at interfaces

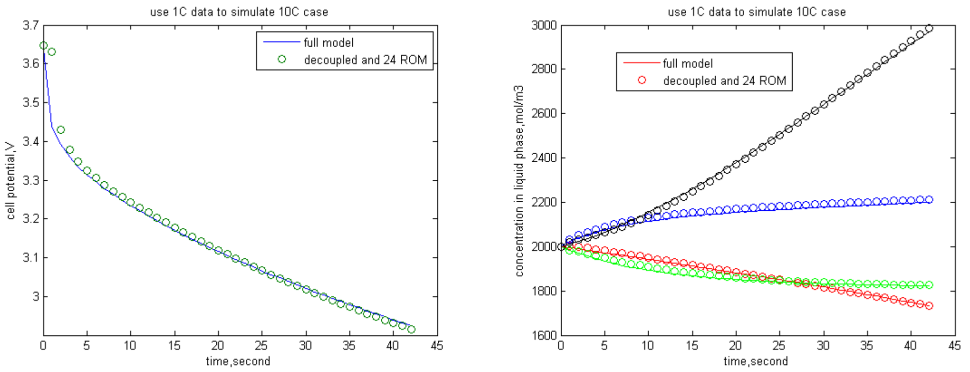

Figure 9: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

unknowns will decrease sharply. This is called Macro-Micro scale coupled simulation or reformulation of diffusion in solid phase. Below we will shortly review some of the existing methods in this area, will discuss their advantages and disadvantages, and will combine best of them with the above introduced ROM method.

5.1 Duhamel's superposition method

Duhamel's superposition method [13] was the first approximation method used in the porous electrode model. It relates the solution of a boundary value problem with time dependent boundary conditions to the solution of a similar problem with time-independent boundary conditions by means of a simple relation. The Duhamel superposition reformulation for the solid phase diffusion equation is

$$\frac{D_s}{R_p}\frac{\partial c_s}{dr}|_{r=R_p} = \sum_{k=0}^{n-2} \frac{c_{s,k+1} - c_{s,k}}{\triangle\ t} A_{n-k} + \frac{c_{s,n} - c_{s,n-1}}{\triangle\ t} A_1 \tag{10}$$

where

$$A_{n-k} = a[(n-k)\triangle\ t] - a[(n-k-1)\triangle\ t]$$

and

$$a(t) = \int_0^t \frac{\partial c_s}{\partial t}(R_p, \zeta)d\zeta$$

5.2 Low order polynomial method

Suppose the concentration inside the particle is the following quadratic polynomial

$$c(r,t) = a(t) + b(t)r^2$$

Define the volume averaged concentration by

$$\overline{c}(t) = \int_{r=0}^{R_p} 3r^2 c(r,t)dr$$

and surface concentration by

$$c_s(t) = c(R_p, t) = a(t) + b(t)R_p^2$$

then by averaging (9) and substituting the above expressions into the boundary condition, we can get the equations for these two variables as [17]

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{11}$$

$$\frac{D_s}{R_p}[c_s(t) - \overline{c}(t)] = -\frac{j}{5} \tag{12}$$

By the above definitions, at each node in x direction, we don't need to solve the concentration diffusion inside the particle (9), instead we solve (11) and (12). In this way, the simulation is pure 1D and for each node we only have 5 unknowns, that's volume averaged concentration $\overline{c}(t)$, surface concentration $c_s(t)$, electrolyte concentration $c_e(t)$, solid potential $\Phi_1(t)$ and electrolyte potential $\Phi_2(t)$.

5.3 High order polynomial method

Of course we can assume the concentration distribution in high order formulation as [17]

$$c(r,t) = a(t) + b(t)r^2 + d(t)r^4$$

Under this formulation, we need another unknown named volume averaged concentration flux as

$$\overline{q}(t) = \int_{r=0}^{R_p} 3r^2(\frac{d}{dr}c(r,t))dr$$

By averaging original equation (9) and its differential with r, combined with the boundary condition, we can get

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{13}$$

$$35\frac{D_s}{R_p}[c_s(t) - \overline{c}(t)] - 8D_s\overline{q}(t) = -j \tag{14}$$

$$\frac{d}{dt}\overline{q}(t) + 30\frac{D_s}{R_p^2}\overline{q}(t) + \frac{45}{2}\frac{j}{R_p^2} = 0 \tag{15}$$

In this way we have 6 unknowns for each node.

5.4 Diffusion length method

By assuming a parabolic concentration profile in the diffusion layer and using the volume average technique, [2] determined the diffusion length to be $l_s = R_p/5$ for spherical particles. The reformulation equations are:

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{16}$$

$$\frac{D_s}{l_s}[c_s(t) - \overline{c}(t)] = -j \tag{17}$$

5.5 Correct diffusion length method

Wang and Srinivasan [20] corrected the diffusion length method by empirically incorporating an intuitively expressed time dependent term into the diffusion length equations:

$$\frac{d}{dt}\bar{c}(t) + 3\frac{j}{R_p} = 0 \tag{18}$$

$$\frac{D_s}{l_s}[c_s(t) - \bar{c}(t)] = -j(1 - exp(-\frac{4}{3}\frac{\sqrt{D_s t}}{l_s})) \tag{19}$$

5.6 Pseudo steady state method

Liu [12] applied pseudo steady state (PSS) method, which is a form of a finite integral transform technique to eliminate the independent spatial variable r from the solid phase diffusion equation. For particle diffusion (9), the generalized PSS reformulation is:

$$\frac{d}{dt}\bar{c}(t) + 3\frac{j}{R_p} = 0 \tag{20}$$

$$\frac{D_s}{R_p}[c_s(t) - \bar{c}(t)] = -\frac{j}{5} + 2\sum_{m=1}^{N_q}\frac{\sqrt{1+\lambda_m^2}}{\lambda_m^2}(-1)^m sin(\lambda_m)(j - e^{-\lambda_m^2 D_s t/R_p^2} q_m) \tag{21}$$

$$\frac{dq_m}{dt} = \frac{\lambda_m^2 D_s}{R_p^2} e^{\lambda_m^2 D_s t/R_p^2} j, \quad m = 1 \cdots N_q \tag{22}$$

$$\lambda_m = tan(\lambda_m) \quad m = 1 \cdots N_q \tag{23}$$

5.7 Galerkin reformulation

Galerkin reformulation [18] is a modification of PSS method. By assuming

$$c(r,t) = a(t) + b(t)(r^2) + \sum_{m=1}^{N_q}\frac{d_m(t) sin(\lambda_m r)}{r}$$

and similar volume average technique, the reformulation is:

$$\frac{d}{dt}\bar{c}(t) + 3\frac{j}{R_p} = 0 \tag{24}$$

$$\frac{D_s}{R_p}[c_s(t) - \bar{c}(t)] = -\frac{j}{5} + 2j\sum_{m=1}^{N_q}\frac{1}{\lambda_m^2} - \frac{D_s}{R_p}\sum_{m=1}^{N_q}\lambda_m^2 sin(\lambda_m)Q_m \tag{25}$$

$$\frac{dQ_m}{dt} + \frac{D_s}{R_p^2}\lambda_m^2 Q_m - \frac{2}{R_p\lambda_m^2 sin(\lambda_m)}j = 0, \quad m = 1\cdots N_q \tag{26}$$

$$\lambda_m = tan(\lambda_m) \quad m = 1\cdots N_q \tag{27}$$

5.8 Results and discussion

It is reported in [22] that Duhamel's superposition method is more CPU time consuming than the full model, so we don't consider it here. PSS is numerically unstable as the values of the introduced there non-physical variables q_m are too large (10^{10} to 10^{50} for our test cases). Low order polynomial and diffusion length method are exactly the same, they work well for low current rate discharge but do not work for high discharge rate. For the test case here, as shown in Figure 10 and Figure 11, the correct diffusion length method and Galerkin reformulation with $N_q = 4$ work well for all the discharge rates.

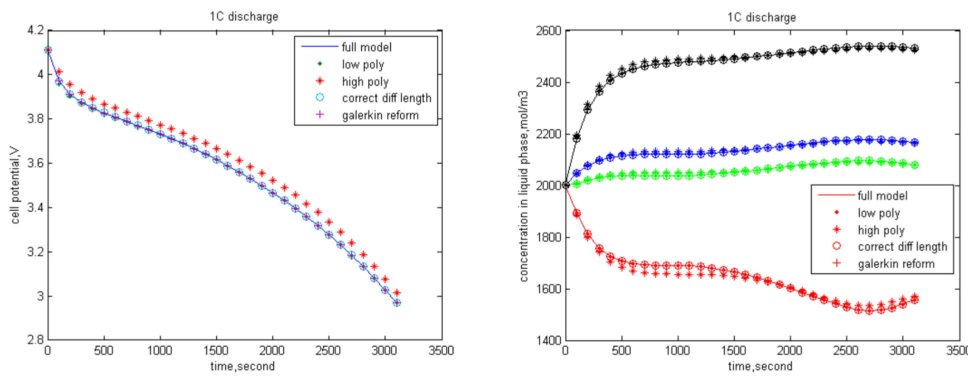

Figure 10: 1C discharge. *Left*: cell potential; *Right*: concentration.

The reformulated system for the particle can be combined with the above introduced ROM method to further reduce the system order. The results obtained with a combined use of ROM and the correct diffusion length method are given in Figure 12 and Figure 13.

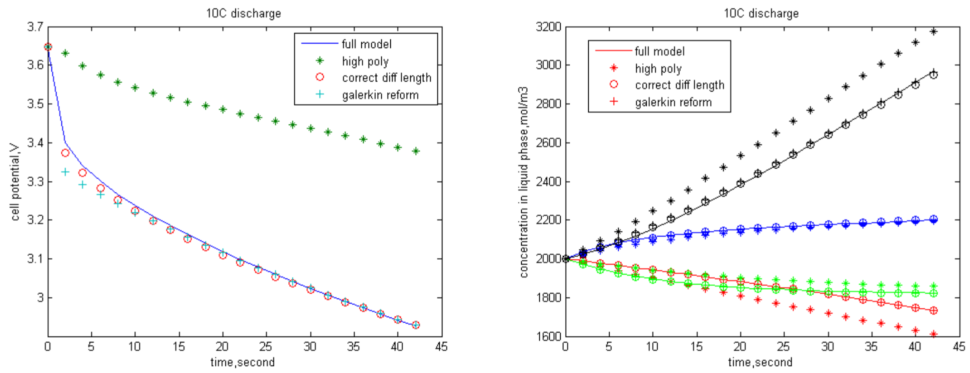

Figure 11: 10C discharge. *Left*: cell potential; *Right*: concentration.

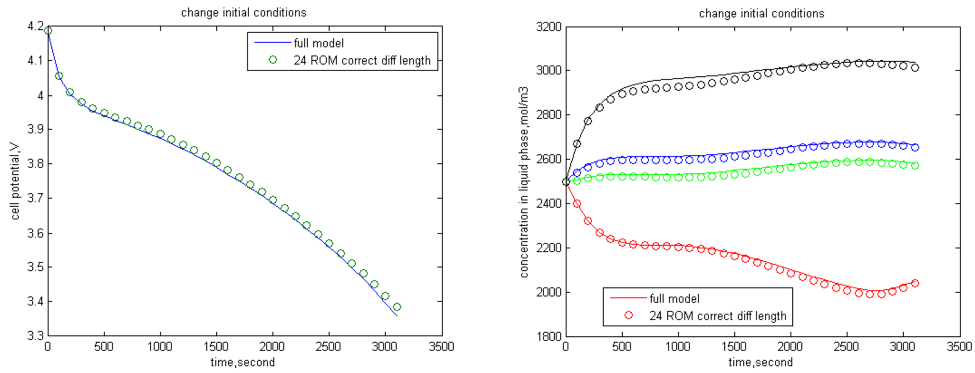

Figure 12: Change initial conditions *Left*: cell potential; *Right*: concentration at interfaces

6 Conclusion

The main goal of this paper is to discuss various model reduction approaches for simulation of Li-ion transport described by pseudo-2D model of the battery. For ROM based on POD, provided the solution for a basic case (i.e., for a basic set of parameters) is known, we can decompose this solution via POD, choose the dominating eigenvectors to form a reduced order model, ROM, and further use this ROM to compute approximate solutions of the pseudo 2D model for other sets of parameters. Furthermore, it was stated that a decoupled solve, with some minor restriction on time step, is much faster than a coupled solve for the full model, while preserving good accuracy. Finally, several approaches for the reformulation of diffusion in solid phase were discussed, and it was shown that the correct diffusion length method and Galerkin reformulation work well for the test cases considered here. We also show that both, the decoupled solve and the diffusion reformulation method,

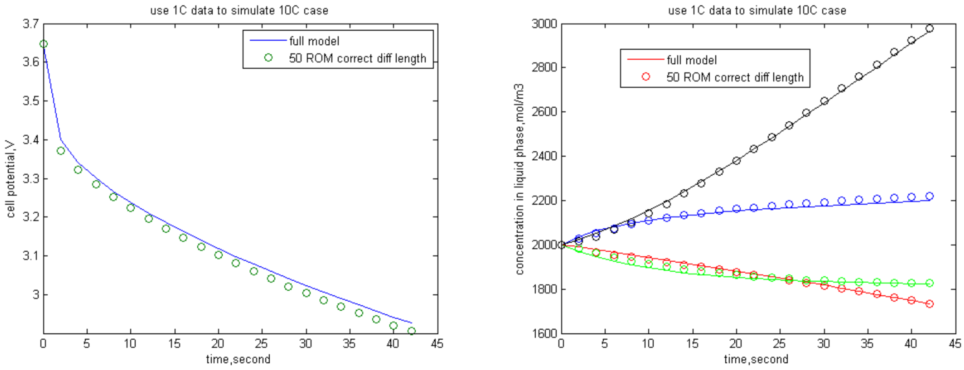

Figure 13: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

can be combined with ROM based on POD in order to further increase the computational efficiency.

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Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe werden sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Dieter Prätzel-Wolters

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

An overview on the usage of some model reduction approaches for simulations of Li-ion transport in batteries

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Abstract

In this work, some model reduction approaches for performing simulations with a pseudo-2D model of Li-ion battery are presented. A full pseudo-2D model of processes in Li-ion batteries is presented following [3], and three methods to reduce the order of the full model are considered. These are: i) directly reduce the model order using proper orthogonal decomposition, ii) using fractional time step discretization in order to solve the equations in decoupled way, and iii) reformulation approaches for the diffusion in the solid phase. Combinations of above methods are also considered. Results from numerical simulations are presented, and the efficiency and the accuracy of the model reduction approaches are discussed.

1 Introduction

Secondary Li-ion batteries used for technical applications are based on porous insertion electrodes. In most of the technical applications the porous electrodes are random structures of active particles bound together by a mixture of polymeric binder and soot for enhancing the electrical conductivity of the electrode. During charging Li-ions are de-intercalated from the anode particles into the electrolyte and transported through the electrolyte to the porous cathode. There they are intercalated at the surface of the cathode particles and then transported via diffusion into the interior of particles. It is well understood that the microstructure (e.g. size and arrangement of the active particles in the porous electrodes) significantly influence the performance of the battery. Going beyond porous structures, it has even been shown that specifically designed electrodes, can achieve a much larger power density [9], but still a lot of research is needed in order to quantitatively evaluate the influence of 3D structures. Available 3D microscale models include mass transport in the electrolyte and in the solid particles, coupled with an equation for the potential [2, 1] and more generally also with an additional equation for the temperature [11]. Solving these models is only possible on cuts through the whole cell covering nevertheless the whole cathode anode direction [19, 5]. Simulations on the complete microstructure is not yet possible due to the tremendous CPU demand. One approach to overcome this problem at least for random porous electrodes pioneered by the group of J. Newman [13] is to model the electrodes as effective random one dimensional porous media characterized by a porosity [16, 6, 8, 14, 4, 15, 7]. Their effective transport properties are obtained by averaging the properties of electrolyte and the active particles. In addition the transport within the particles is modeled as diffusive transport in one effective particle per volume element coupled to the transport in the effective porous medium. The separator is also described as effective porous medium. Thus a pseudo-2D model (i.e. 1D+1D model) for the full battery cell is obtained. Three dimensional extensions (more exact 3D+1D models), which allow to simulate complex shaped electrodes are possible [21]. These macroscopic models are solved by some numerical method, e.g., finite difference, finite volume or finite elements. One (representative) spherical particle is located in each grid node (for FDM and FVM), or in each quadrature point (for FEM), and the macroscopic model is coupled to the model in the particle (see the text below for details). The solution of the coupled model (called also *full model* below in the text) requires solving diffusion equation for each particle in an extra pseudo-dimension, namely in the radius r. Consequently, the number of unknown variables in this 1D+1D model is large, thus still requiring significant computational time. To obtain models which can be solved in real time further approaches for reducing the demanded computational times have appeared in the literature. The goal of this paper is to present a computational study of the performance of three model reduction approaches, when applied to simulation of processes in Li-ion battery.

First, consider the approach which was earlier presented in [3]. It exploits reduced order method, ROM, which is based on proper orthogonal decomposition, POD. The Authors claimed that this method is efficient for the pseudo-2D model, and they provided some simulation results for test cases. However, the parameters (and thus regimes) for simulation of real processes sometimes differ from conditions considered in test cases, and therefore more studies are required for the case of real parameters.

Further on, reformulation methods were used to avoid solving the diffusion equation in the active particles, see, e.g. [13, 2, 20, 17, 12, 22, 18]. These methods are based on approximating the concentration in solid phase by some selected functions of r, followed by volume averaging. The basis functions are global (defined from 0 to R), but very few of them are used. The aim of the volume averaging is to avoid solving the diffusion equation in the active particles. Zhang and White [22] compared some of the reformulation methods and discussed their efficiency in solving test examples.

In this paper, we consider both of the above methods and apply them in order to reduce the model order of the pseudo-2D li-ion battery model. In the case of ROM based on POD, we select a basic set of parameters and perform full simulations. After that the solution is used to form so called transform basis. The latter are used to form reduced order model, and later on to simulate the processes for other sets of parameters. We also review most of the reformulation methods and consider combination of reformulation and ROM-POD approaches. Further on, we consider one new way to reduce the the complexity of the problem, namely a fractional time step discretization, allowing to solve for all the unknowns in a decoupled way. The dominated part of the unknowns can be solved in parallel, and the other part can be combined with ROM-POD to further increase the efficiency.

The rest of the paper is organized as follows. In section 2 we describe the full model and the discretization. In section 3, we discuss the algorithm of ROM based on POD and apply it to reduce the order of the full pseudo-2D model. In section 4, we present the fractional time step discretization and solve the full model in a decoupled way. In section 5, we review the reformulation methods and combine them with ROM. Conclusions are given in section 6.

2 Full pseudo 2D model

The sketch of a LiMnO2-carbon battery is shown in Figure 1. From left to right, the components of the battery are aluminum current collector, LiMnO2 positive electrode, separator, carbon negative electrode, and copper current collector. The governing equations and related expressions are summarized in Table 1 (see also [3]), and the parameters are given in Table 2.

For the discretization of the above model, cell centered finite volume method is adopted. The domain $(0, L_p + L_s + L_n)$ is divided into $N_p + N_s + N_n$ cells. Active particles are placed at the centers of those cells, which

Table 1: Governing equations and expressions

variable	equation	boundary conditions
c_s	$\frac{\partial c_s}{\partial t} = D_s \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial c_s}{\partial r})$	$-\frac{\partial c_s}{\partial r}\vert_{r=0} = 0,\ -\frac{\partial c_s}{\partial r}\vert_{r=R_{s,i}} = j_i$
c_e	$\epsilon_i \frac{\partial c_e}{\partial t} = D_{eff,i}\frac{\partial^2 c_e}{\partial x^2} + (1-t_+)a_i F j_i$	$-D_{eff,i}\frac{\partial c_e}{\partial x} = 0$
Φ_1	$\sigma_{eff,i}\frac{\partial^2 \Phi_1}{\partial x^2} = a_i F j_i$	$-\sigma_{eff,p}\frac{\partial \Phi_1}{\partial x} = I,\ \Phi_1\vert_{x=L_p+L_s+L_n} = 0$
Φ_2	$-\frac{\partial}{\partial x}(\kappa_{eff}\frac{\partial \Phi_2}{\partial x}) + \beta \frac{\partial}{\partial x}(\kappa_{eff}\frac{\partial ln c_e}{\partial x}) = a_i F j_i$	$-\kappa_{eff,i}\frac{\partial \Phi_2}{\partial x} = 0$
initial conditions	$c_{s,i}(r,0) = c_{s,i,0}$	$c_e(x,0) = c_0$
interface conditions		
$x = L_p$	$-D_{eff,p}\frac{\partial c_e}{\partial x} = -D_{eff,s}\frac{\partial c_e}{\partial x}$	$-\sigma_{eff,p}\frac{\partial \Phi_1}{\partial x} = 0$ $-\kappa_{eff,p}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,s}\frac{\partial \Phi_2}{\partial x}$
$x = L_p + L_s$	$-D_{eff,s}\frac{\partial c_e}{\partial x} = -D_{eff,n}\frac{\partial c_e}{\partial x}$	$-\sigma_{eff,n}\frac{\partial \Phi_1}{\partial x} = 0$ $-\kappa_{eff,s}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,n}\frac{\partial \Phi_2}{\partial x}$

expressions

$$U_p = 4.199 + 0.0566 tanh(-14.555\theta_p + 8.609) - 0.0275[(0.998 - \theta_p)^{-0.492} - 1.901] - 0.157 exp(-0.0474\theta_p^8) + 0.81 exp[-40(\theta_p - 0.134)]$$

$$U_n = -0.16 + 1.32 exp(-3.0\theta_n) + 10.0 exp(-2000.0\theta_n)),\ \theta_p = c_{s,p,surf}/c_{s,p,max},\ \theta_n = c_{s,n,surf}/c_{s,n,max}$$

$$j_i = 2k_m(c_{s,i,max} - c_{s,i,surf})^{0.5} c_{s,i,surf}^{0.5} c_e^{0.5} sinh(\frac{0.5F}{RT}(\Phi_1 - \Phi_2 - U_i)),\ \sigma_{eff,i} = \sigma_i(1 - \epsilon_i - \epsilon_{f,i}),\ a_i = \frac{3}{R_{s,i}}(1 - \epsilon_i - \epsilon_{f,i}),\ \text{i=p,n}$$

$$\kappa_{eff,i} = (4.1253 \times 10^{-2} + 5.007 \times 10^{-4} c - 4.7212 \times 10^{-7} c^2 + 1.5094 \times 10^{-10} c^3 - 1.6018 \times 10^{-14} c^4)\epsilon_i^{brugg_i},\ D_{eff,i} = D_e \epsilon_i^{brugg_i},\ i = p, s, n$$

Table 2: Parameters

Parameter	Value	Unit	Parameter	Value	Unit
L_p	183	μm	$c_{s,p,max}$	22860	mol/m^3
L_s	52	μm	$c_{s,n,max}$	26390	mol/m^3
L_n	100	μm	$c_{s,p,0}$	3900	mol/m^3
$R_{s,p}$	8	μm	$c_{s,n,0}$	14870	mol/m^3
$R_{s,n}$	12.5	μm	σ_p	3.8	S/m
$D_{s,p}$	1.0×10^{-13}	m^2/s	σ_n	100	S/m
$D_{s,n}$	3.9×10^{-14}	m^2/s	$Brugg_p$	1.5	–
D_e	7.5×10^{-11}	m^2/s	$Brugg_s$	1.5	–
ϵ_p	0.444	–	$Brugg_n$	1.5	–
ϵ_s	1.0	–	k_p	2.334×10^{-11}	$mol/m^2s/(mol/m^3)^{1.5}$
ϵ_n	0.357	–	k_n	2.334×10^{-11}	$mol/m^2s/(mol/m^3)^{1.5}$
$\epsilon_{f,p}$	0.259	–	t_+	0.363	–
$\epsilon_{f,n}$	0.172	–	I	17.5(1C rate)	A/m^2
c_0	2000	mol/m^3	T	298	K

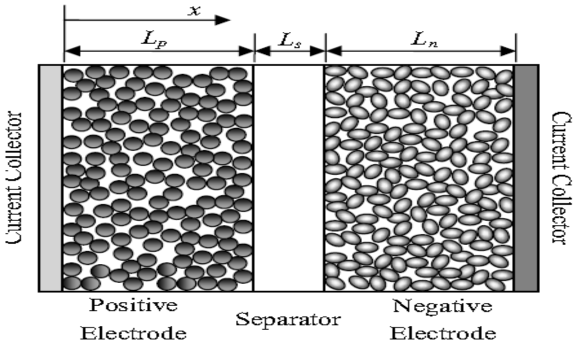

Figure 1: Schematic of a lithium battery

belong to the electrodes. The processes in the porous electrodes, described by macroscopic equations, are coupled via Butler-Volmer flux conditions on the surface of the particle to the processes in the particles, described by 1D model in spherical coordinates. This micro-macro coupling fits, for example, Heterogeneous Multiscale Method philosophy. Thus the pseudo-2D model assumes that the particles in the center of the grid cells (see Figure 2) are typical and represent all other particles in the cell. The active solid particles are considered to have spherical form, and it is further assumed that processes in r direction dominate, so that 1D model can be used in each particle. The radius r of each particle is divided into N_r control volumes (cells). N_r = 50 is used in simulations presented here. The (macroscopic) $x-$ regions of the positive electrode, of the separator, and of the negative electrode, are discretized into $N_p = 100$, $N_s = 70$, and $N_n = 100$ control volumes, respectively.

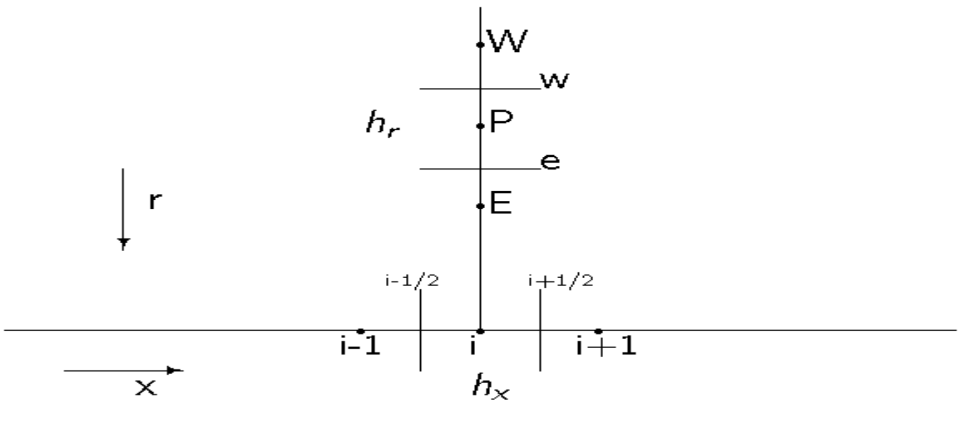

Figure 2: A typical volume in electrode

Thus, with the selected Ns, at every grid node of the macroscopic grid (x- coordinate), there are 54 unknowns. They are arranged in the following order: the first 50 unknowns correspond to the concentration of lithium ions in the respective particle, numbered from the center to the surface of particle. The 51th unknown stands for the concentration on the surface of the particle, the 52th unknown stands for the concentration in the electrolyte, the 53th stands for the potential in the solid phase, and the last one stands for the potential in the electrolyte. The respective 54 equations arising after the discretization are numbered from i_1 to i_{54} and they look as follows:

$$
\begin{aligned}
\frac{dc_{s,P}}{dt} &= \frac{D_s}{r_P^2}\frac{r_e^2(c_{s,E}-c_{s,P})}{h_r^2} \qquad (i_1) \\
\frac{dc_{s,P}}{dt} &= \frac{D_s}{r_P^2}\frac{r_e^2(c_{s,E}-c_{s,P})-r_w^2(c_{s,P}-c_{s,W})}{h_r^2} \qquad (i_2)\cdots(i_{49}) \\
\frac{dc_{s,P}}{dt} &= -\frac{r_e^2}{r_P^2 h_r}j-\frac{D_s}{r_P^2}\frac{r_w^2(c_{s,P}-c_{s,W})}{h_r^2} \qquad (i_{50}) \\
c_{s,surf} &= \frac{-3h_r j+9D_s c_{s,50}-D_s c_{s,49}}{8D_s} \qquad (i_{51}) \\
\epsilon\frac{dc_e}{dt} &= D_{eff}\frac{c_{e,i+1}-2c_{e,i}+c_{e,i-1}}{h_x^2}+(1-t_+)aj \qquad (i_{52}) \\
aFj &= \sigma_{eff}\frac{\Phi_{1,i+1}-2\Phi_{1,i}+\Phi_{1,i-1}}{h_x^2} \qquad (i_{53}) \\
aFj &= -\frac{\kappa_{eff,i+\frac{1}{2}}(\Phi_{2,i+1}-\Phi_{2,i})-\kappa_{eff,i-\frac{1}{2}}(\Phi_{2,i}-\Phi_{2,i-1})}{h_x^2} \\
&+ \frac{\kappa_{\beta_{i+\frac{1}{2}}}(c_{e,i+1}-c_{e,i})-\kappa_{\beta_{i-\frac{1}{2}}}(c_{e,i}-c_{e,i-1})}{h_x^2} \qquad (i_{54})
\end{aligned}
\tag{1}
$$

Where $\kappa_\beta = \frac{\kappa_{eff}\beta}{c_e}$, $\kappa_{eff,i+\frac{1}{2}}$ is harmonic average of $\kappa_{eff,i+1}$ and $\kappa_{eff,i}$, means $\kappa_{eff,i+\frac{1}{2}} = \frac{2\kappa_{eff,i+1}\kappa_{eff,i}}{\kappa_{eff,i+1}+\kappa_{eff,i}}$, and similar to $\kappa_{eff,i-\frac{1}{2}}$, $\kappa_{\beta_{eff,i+\frac{1}{2}}}$ and $\kappa_{\beta_{eff,i-\frac{1}{2}}}$.

Remark 2.1 In the above discretization, j equal to j_p in positive electrode, zero in separator and j_n in negative electrode. For the surface concentration, as there is no governing equation for it in Table 1, we just interpolate it with the two nearest unknowns inside the particle, combined with the surface condition. For the nodes in the separator, only equations with numbers (i_{52}) and (i_{54}) are used, all other unknowns are assigned to be zeros.

Remark 2.2 For the treatment of interface conditions at $x = L_p$ (similarly at $x = L_p + L_s$), we use $-D_{eff,p}\frac{\partial c_e}{\partial x} = -D_{eff,s}\frac{\partial c_e}{\partial x} = -D_{eff,ps}\frac{c_{e,s}-c_{e,p}}{0.5(h_p+h_s)}$

and $-\kappa_{eff,p}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,s}\frac{\partial \Phi_2}{\partial x} = -\kappa_{eff,ps}\frac{\Phi_{2,s}-\Phi_{2,p}}{0.5(h_p+h_s)}$, where $D_{eff,ps}$ is harmonic average of $D_{eff,p}$ and $D_{eff,s}$, and similar to $\kappa_{eff,ps}$.

For the time discretization, first order backward Euler is adopted. Uniform time step is used, and standard Newton-Raphsion method is applied to solve the obtained nonlinear system.

3 Reduced order model based POD

3.1 Method and algorithm

Let us denote the spatially discretized system of the full model(1) as

$$M_1 \frac{d\mathbf{x}}{dt} = \mathbf{f}_1(t, \mathbf{x}) \tag{2}$$

Here M_1 is a $n_{full} \times n_{full}$ matrix, both $\mathbf{x}$ and $\mathbf{f}_1$ are $n_{full} \times 1$ vectors. The system order n_{full} is usually large (over 10,000 in our case). This is not just a system of ODEs, it is a large differential-algebraic system, DAE system, that is, M_1 has zero rows.

The idea of the reduced order method (see, e,g,[3, 10]) is as follows. Suppose that

$$\mathbf{x} = B\mathbf{y} \tag{3}$$

where B is a $n_{full} \times n_{rom}$ matrix and $\mathbf{y}$ is a $n_{rom} \times 1$ vector. Substitute (3) into (2) and multiply both sides by B^T. As a result we obtain the following reduced order system:

$$M \frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y}) \tag{4}$$

where $M = B^T M_1 B$ is $n_{rom} \times n_{rom}$ matrix and $\mathbf{f}(t, \mathbf{y}) = B^T \mathbf{f}_1(t, B\mathbf{y})$ is a $n_{rom} \times 1$ vector.

The basis matrix B is the crucial ingredient of the above reduced order model. POD (proper orthogonal decomposition) [10] is often used to obtain B. The whole algorithm for the reduced order model is described below, see *Algorithm 1.*

Algorithm 1 Suppose $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{n_t}]$ is solutions at all n_t time steps for one case (base case).

(1) Do POD as $\mathbf{X}\mathbf{X}^T = \Phi\Lambda\Phi^T$

(2) Form transformation matrix B as: $B = \Phi(1 : n_{rom})$

(3) Form reduced order system using the above B.

(4) Solve the reduced system in for the specified parameters, and use its solution to recover the solution of the full system by $\mathbf{x} = B\mathbf{y}$.

In the above algorithm, the number n_{rom} is determined as follows: choose the smallest n such that

$$\frac{\sum_{i=1}^{n_{rom}} \lambda_i}{\sum_{i=1}^{n_t} \lambda_i} > tol$$

where $\Lambda = diag(\lambda_1, \cdots, \lambda_{n_t})$, $\lambda_i \geq \lambda_{i+1}$ are the eigenvalues numbered in non-increasing order. The threshold $tol \in (0, 1)$, is often taken as $tol = 99.99\%$ or more close to 1. In act, the choice of the threshold depends on the accuracy required for solving the particular full problem.

Remark 3.1 The computed solution $\mathbf{X}$ is of size $n_p \times n_t$, where n_p is the number of unknowns at one time step and n_t is the number of time steps. Usually $n_p >> n_t$, and in this case we do POD as $\mathbf{X}^T\mathbf{X} = \Psi\Lambda\Psi^T$, $\Phi = \mathbf{X}\Psi$ and then normalize Φ.

Remark 3.2 We split the unknown variables into several groups, according to their meaning,

$$(c_{s,p}, c_{s,n}, c_{s,p,surf}, c_{s,n,surf}, \Phi_{1,p}, \Phi_{1,n}, c_e, \Phi_2)$$

, and after that perform POD and choose eigenvectors for each group. At the end we glue together the chosen eigenvectors from all the these groups in order to get the matrix B. The same approach is used, e.g., in [3].

Remark 3.3 Sometimes it is useful to include the initial value as one separate column in B, i.e.

$$B_1 = \Phi(1:n), \mathbf{p} = \mathbf{x}_0 - B_1^T B_1 \mathbf{x}_0, B = [\frac{\mathbf{p}}{||\mathbf{p}||}, B_1]$$

This will ensure that the obtained reduced order system is consistent with the given initial state.

3.2 Results and discussion

To test the efficiency of the presented ROM method, we consider three different examples here. In all the examples, the results obtained with ROM are compared with the solution of the full model.

(1) We choose the base case to be 1C discharge with the parameters given in Table 2, and change initial conditions ($c_e(x, 0) = 2500, c_{s,n}(r, 0) = 18870$) as tested case. In this example, the base case and the tested case differ only in the values for the initial conditions. The full model solution and the ROM

solution of the tested case are compared in Figure 3. We can see that the ROM with only 27 eigenvectors (for comparison, the size of the full system is 14580) approximate the solution of the full model very well.

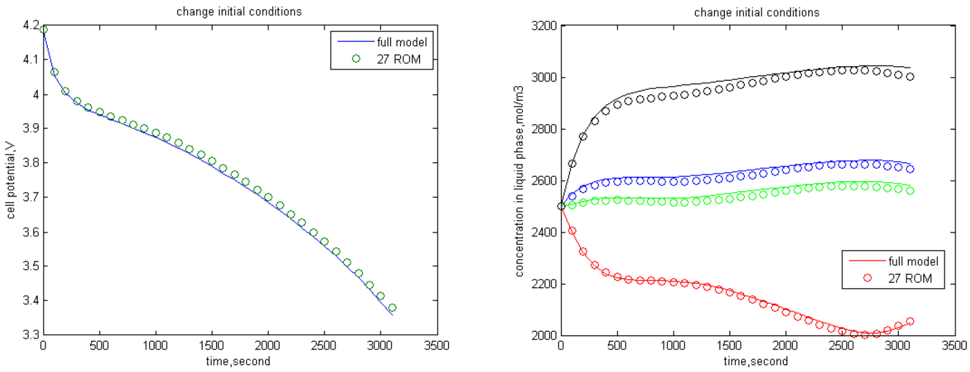

Figure 3: Change initial conditions *Left*: cell potential; *Right*: concentration at interfaces

(2) we choose the same base case as in the first example, but choose as tested case a problem with characterized by 10C discharge. All other parameters are the same as in the base case. For this example, as one can see on Figure 4, we need to choose for ROM solution more eigenvectors (than in the previous example) in order to achieve good accuracy.

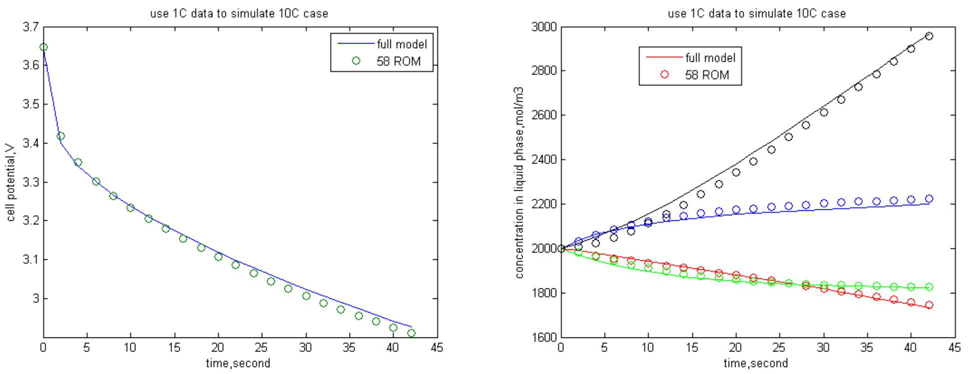

Figure 4: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

3)The third considered example corresponds to simulation of discharge-charge cycles. In one cycle, the battery is first discharged at 1C rate until the cell potential decrease to 3.0 V., followed by a 1C charge process up to 4.3 V, and at the last stage of the cycle the battery is charged at 4.3 V until the current decreases to 10 mA. In the simulations, we choose the solution of one cycle as a base solution, form reduced system and use the latter to simulate many cycles. The results in Figure 5 shows that the ROM with 105 eigenvectors works very well.

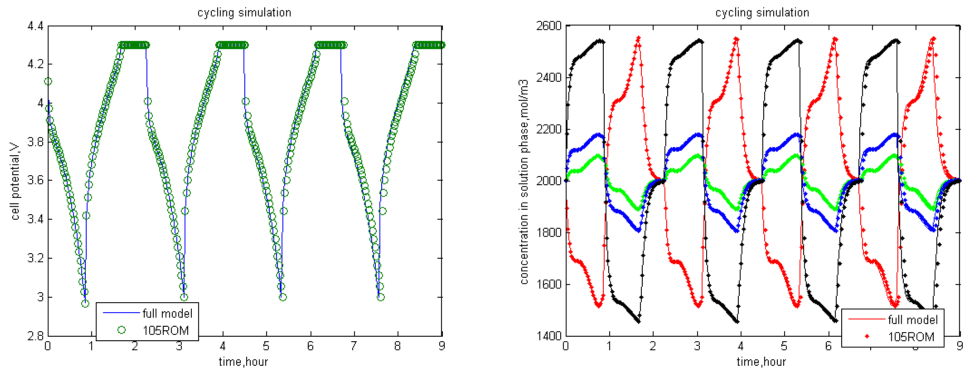

Figure 5: Cycling simulation *Left*: cell potential; *Right*: concentration at interfaces

4 Fractional time step discretization

4.1 Method description

Consider again the full model. When first order backward Euler is used for time discretization, the resulting discretized system at time t_{n+1} is written as follows

$$M\frac{\mathbf{x}^{n+1}-\mathbf{x}^{n}}{\triangle\ t}=f(\mathbf{x}^{n+1})$$

We divide all the unknowns into two classes, namely $\mathbf{x}=(\mathbf{x}_e,\mathbf{x}_p)$, where we choose $\mathbf{x}_p=(c_s,c_{s,surf})$ as concentration in the particles, and $\mathbf{x}_e=(c_e,\Phi_1,\Phi_2)$ to be collection of the remaining unknowns. With the new notations, the above Euler discretization can be rewritten as follows:

$$M_1\frac{\mathbf{x}_e^{n+1}-\mathbf{x}_e^{n}}{\triangle\ t}=f_1(\mathbf{x}_e^{n+1},\mathbf{x}_p^{n+1}) \tag{5}$$

$$M_2\frac{\mathbf{x}_p^{n+1}-\mathbf{x}_p^{n}}{\triangle\ t}=f_2(\mathbf{x}_e^{n+1},\mathbf{x}_p^{n+1}) \tag{6}$$

Fractional time step discretization can also be applied to the full system, thus obtaining a decoupled system. (Note, the questions about the theoretical study on the stability of this fractional time step discretization are not studied here. We can just note that our simulations show that it is worth to use this approach).

$$M_1 \frac{\mathbf{x}_e^{n+\frac{1}{2}} - \mathbf{x}_e^n}{\triangle\ t} = f_1(\mathbf{x}_e^{n+\frac{1}{2}}, \mathbf{x}_p^n) \tag{7}$$

$$M_2 \frac{\mathbf{x}_p^{n+1} - \mathbf{x}_p^n}{\triangle\ t} = f_2(\mathbf{x}_e^{n+\frac{1}{2}}, \mathbf{x}_p^{n+1}) \tag{8}$$

The above predictor-corrector discretization means that at each time step we first solve for $\mathbf{x}_e$ using the solution of $\mathbf{x}_p$ at the previous time, and after that solve for $\mathbf{x}_p$ at the new time step, using just computed $\mathbf{x}_e$.

Remark 4.1 Note that in this particular problem $\mathbf{x}_p$ contains much more unknowns compared to $\mathbf{x}_e$, and that one can solve the predictor step for each particle separately, as long as the values from the previous time step are used for $\mathbf{x}_e$. As a result, this decoupled solve works much faster than the coupled solve for the full model.

Remark 4.2 For the solve with respect to $\mathbf{x}_e$ at each time step, we can use the previous ROM method in order to reduce the order of this system. This combination of using decoupled solve (fractional time step discretization) and ROM, can further improve the efficiency.

4.2 Results and discussion

We test coupled and decoupled system in two cases: 1C discharge and 10C discharge. For decoupled system, we need some restrictions on the time step. If uniform time step is used, the time step need to satisfy $\triangle\ t < 70s$ for 1C case and $\triangle\ t < 7s$ for 10C case. If the time step satisfy these conditions, solving the decoupled system is much faster than solving the coupled system and, and the results obtained by the two approaches are very close. It should be noted that often very large time steps (even if allowed by the stability consideration) can not be used in the simulations, because this would lead to lose of accuracy. See Figure 6 and Figure 7 for details.

As pointed out in Remark 4.2, the above presented ROM approach presented can be used to solve for $\mathbf{x}_e$ at each time step. The results from such an approach for example 1 and example 2 are given in Figure 8 and Figure 9. It can be seen that in both cases the solution of the full model is approximated very well.

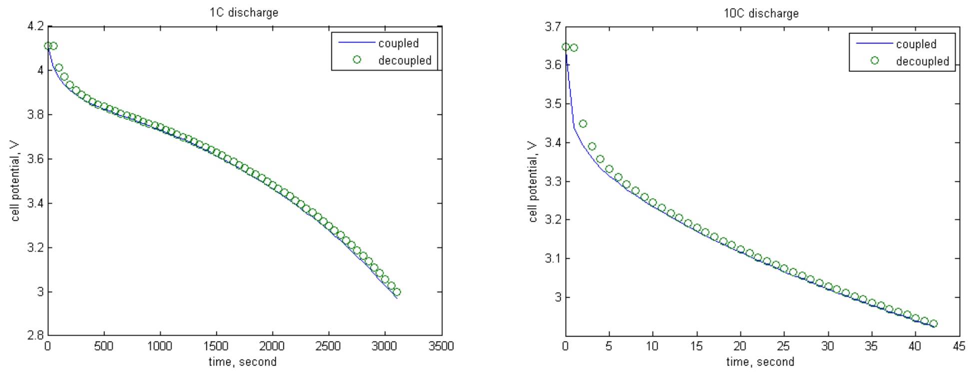

Figure 6: Cell potential. *Left*: 1C rate; *Right*: 10C rate.

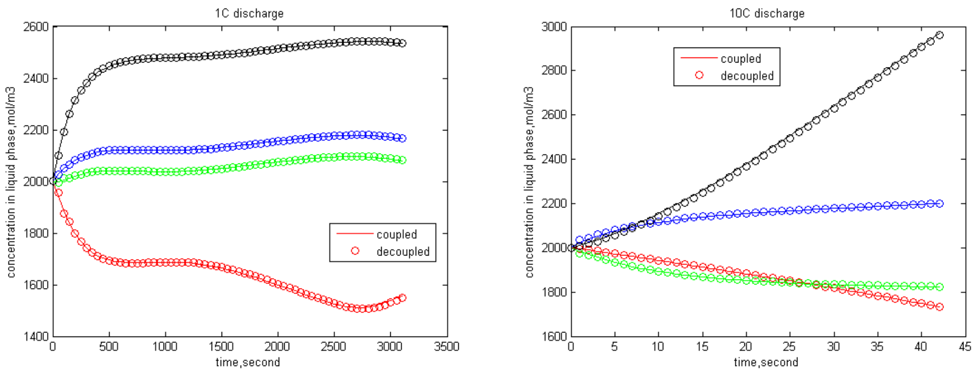

Figure 7: Concentration at interfaces. *Left*: 1C rate; *Right*: 10C rate.

5 Reformulation of particle diffusion

In the full model, most of unknowns come from the discretization of the following diffusion equation inside the particle

$$\frac{\partial c}{\partial t} - D_s \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial c}{\partial r}) = 0 \tag{9}$$

with boundary condition

$$D_s \frac{\partial c}{\partial r} = 0 \qquad at\ r = 0 \quad and\ for\ t \geq 0$$

$$D_s \frac{\partial c}{\partial r} = -j \qquad at\ r = R_p \quad and\ for\ t \geq 0$$

where j is the pore wall flux at the surface of particle and R_p is the radius of the particle. If we can avoid solving this equation, then the number of

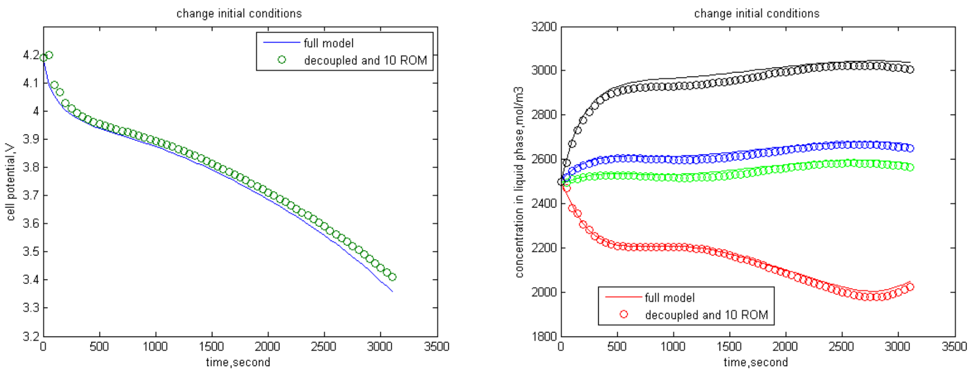

Figure 8: Change initial condition *Left*: cell potential; *Right*: concentration at interfaces

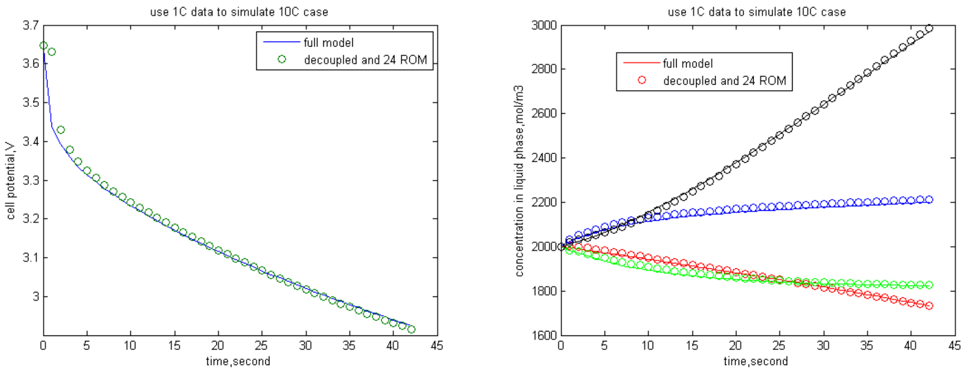

Figure 9: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

unknowns will decrease sharply. This is called Macro-Micro scale coupled simulation or reformulation of diffusion in solid phase. Below we will shortly review some of the existing methods in this area, will discuss their advantages and disadvantages, and will combine best of them with the above introduced ROM method.

5.1 Duhamel's superposition method

Duhamel's superposition method [13] was the first approximation method used in the porous electrode model. It relates the solution of a boundary value problem with time dependent boundary conditions to the solution of a similar problem with time-independent boundary conditions by means of a simple relation. The Duhamel superposition reformulation for the solid phase diffusion equation is

$$\frac{D_s}{R_p}\frac{\partial c_s}{dr}|_{r=R_p} = \sum_{k=0}^{n-2} \frac{c_{s,k+1} - c_{s,k}}{\triangle\ t} A_{n-k} + \frac{c_{s,n} - c_{s,n-1}}{\triangle\ t} A_1 \tag{10}$$

where

$$A_{n-k} = a[(n-k)\triangle\ t] - a[(n-k-1)\triangle\ t]$$

and

$$a(t) = \int_0^t \frac{\partial c_s}{\partial t}(R_p, \zeta) d\zeta$$

5.2 Low order polynomial method

Suppose the concentration inside the particle is the following quadratic polynomial

$$c(r,t) = a(t) + b(t)r^2$$

Define the volume averaged concentration by

$$\overline{c}(t) = \int_{r=0}^{R_p} 3r^2 c(r,t) dr$$

and surface concentration by

$$c_s(t) = c(R_p, t) = a(t) + b(t)R_p^2$$

then by averaging (9) and substituting the above expressions into the boundary condition, we can get the equations for these two variables as [17]

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{11}$$

$$\frac{D_s}{R_p}[c_s(t) - \overline{c}(t)] = -\frac{j}{5} \tag{12}$$

By the above definitions, at each node in x direction, we don't need to solve the concentration diffusion inside the particle (9), instead we solve (11) and (12). In this way, the simulation is pure 1D and for each node we only have 5 unknowns, that's volume averaged concentration $\overline{c}(t)$, surface concentration $c_s(t)$, electrolyte concentration $c_e(t)$, solid potential $\Phi_1(t)$ and electrolyte potential $\Phi_2(t)$.

5.3 High order polynomial method

Of course we can assume the concentration distribution in high order formulation as [17]

$$c(r,t) = a(t) + b(t)r^2 + d(t)r^4$$

Under this formulation, we need another unknown named volume averaged concentration flux as

$$\overline{q}(t) = \int_{r=0}^{R_p} 3r^2 (\frac{d}{dr} c(r,t)) dr$$

By averaging original equation (9) and its differential with r, combined with the boundary condition, we can get

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{13}$$

$$35\frac{D_s}{R_p}[c_s(t) - \overline{c}(t)] - 8D_s\overline{q}(t) = -j \tag{14}$$

$$\frac{d}{dt}\overline{q}(t) + 30\frac{D_s}{R_p^2}\overline{q}(t) + \frac{45}{2}\frac{j}{R_p^2} = 0 \tag{15}$$

In this way we have 6 unknowns for each node.

5.4 Diffusion length method

By assuming a parabolic concentration profile in the diffusion layer and using the volume average technique, [2] determined the diffusion length to be $l_s = R_p/5$ for spherical particles. The reformulation equations are:

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{16}$$

$$\frac{D_s}{l_s}[c_s(t) - \overline{c}(t)] = -j \tag{17}$$

5.5 Correct diffusion length method

Wang and Srinivasan [20] corrected the diffusion length method by empirically incorporating an intuitively expressed time dependent term into the diffusion length equations:

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{18}$$

$$\frac{D_s}{l_s}[c_s(t) - \overline{c}(t)] = -j(1 - exp(-\frac{4}{3}\frac{\sqrt{D_s t}}{l_s})) \tag{19}$$

5.6 Pseudo steady state method

Liu [12] applied pseudo steady state (PSS) method, which is a form of a finite integral transform technique to eliminate the independent spatial variable r from the solid phase diffusion equation. For particle diffusion (9), the generalized PSS reformulation is:

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{20}$$

$$\frac{D_s}{R_p}[c_s(t) - \overline{c}(t)] = -\frac{j}{5} + 2\sum_{m=1}^{N_q}\frac{\sqrt{1+\lambda_m^2}}{\lambda_m^2}(-1)^m sin(\lambda_m)(j - e^{-\lambda_m^2 D_s t/R_p^2}q_m) \tag{21}$$

$$\frac{dq_m}{dt} = \frac{\lambda_m^2 D_s}{R_p^2}e^{\lambda_m^2 D_s t/R_p^2}j, \quad m = 1 \cdots N_q \tag{22}$$

$$\lambda_m = tan(\lambda_m) \quad m = 1 \cdots N_q \tag{23}$$

5.7 Galerkin reformulation

Galerkin reformulation [18] is a modification of PSS method. By assuming

$$c(r,t) = a(t) + b(t)(r^2) + \sum_{m=1}^{N_q}\frac{d_m(t)sin(\lambda_m r)}{r}$$

and similar volume average technique, the reformulation is:

$$\frac{d}{dt}\overline{c}(t) + 3\frac{j}{R_p} = 0 \tag{24}$$

$$\frac{D_s}{R_p}[c_s(t) - \bar{c}(t)] = -\frac{j}{5} + 2j\sum_{m=1}^{N_q}\frac{1}{\lambda_m^2} - \frac{D_s}{R_p}\sum_{m=1}^{N_q}\lambda_m^2 sin(\lambda_m)Q_m \tag{25}$$

$$\frac{dQ_m}{dt} + \frac{D_s}{R_p^2}\lambda_m^2 Q_m - \frac{2}{R_p\lambda_m^2 sin(\lambda_m)}j = 0, \quad m = 1\cdots N_q \tag{26}$$

$$\lambda_m = tan(\lambda_m) \quad m = 1\cdots N_q \tag{27}$$

5.8 Results and discussion

It is reported in [22] that Duhamel's superposition method is more CPU time consuming than the full model, so we don't consider it here. PSS is numerically unstable as the values of the introduced there non-physical variables q_m are too large (10^{10} to 10^{50} for our test cases). Low order polynomial and diffusion length method are exactly the same, they work well for low current rate discharge but do not work for high discharge rate. For the test case here, as shown in Figure 10 and Figure 11, the correct diffusion length method and Galerkin reformulation with $N_q = 4$ work well for all the discharge rates.

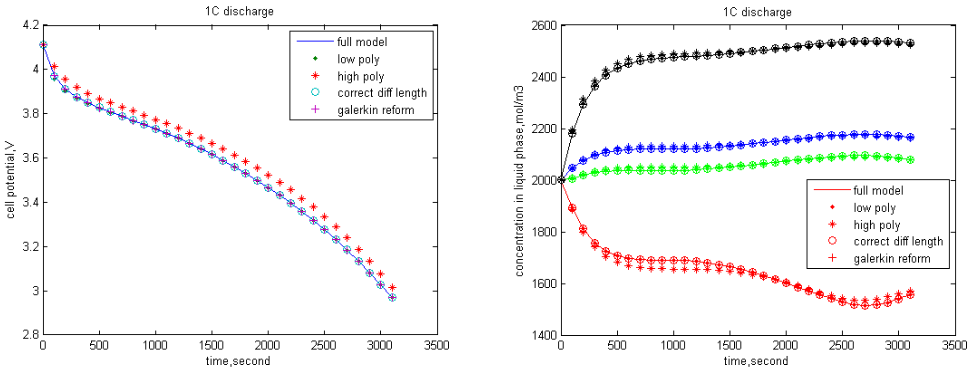

Figure 10: 1C discharge. *Left*: cell potential; *Right*: concentration.

The reformulated system for the particle can be combined with the above introduced ROM method to further reduce the system order. The results obtained with a combined use of ROM and the correct diffusion length method are given in Figure 12 and Figure 13.

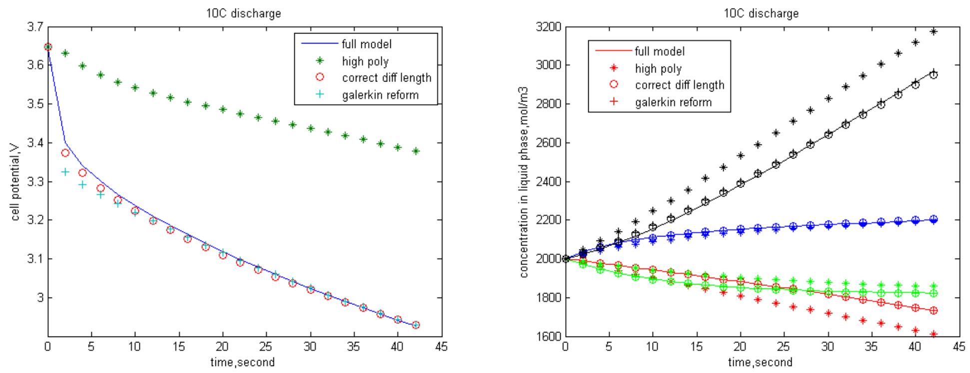

Figure 11: 10C discharge. *Left*: cell potential; *Right*: concentration.

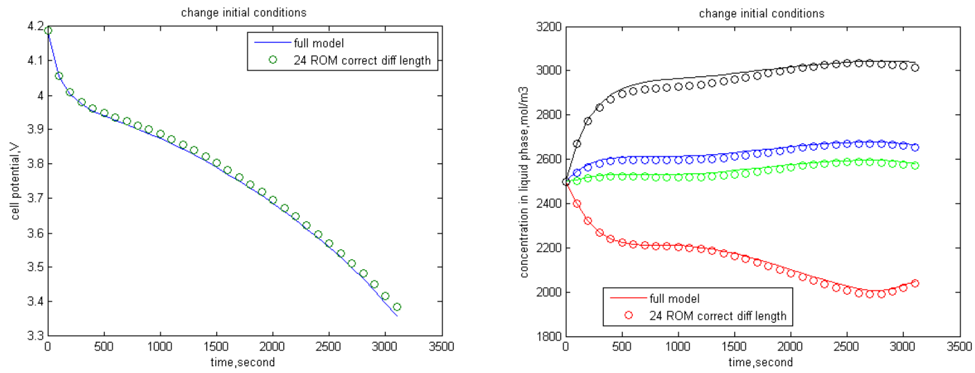

Figure 12: Change initial conditions *Left*: cell potential; *Right*: concentration at interfaces

6 Conclusion

The main goal of this paper is to discuss various model reduction approaches for simulation of Li-ion transport described by pseudo-2D model of the battery. For ROM based on POD, provided the solution for a basic case (i.e., for a basic set of parameters) is known, we can decompose this solution via POD, choose the dominating eigenvectors to form a reduced order model, ROM, and further use this ROM to compute approximate solutions of the pseudo 2D model for other sets of parameters. Furthermore, it was stated that a decoupled solve, with some minor restriction on time step, is much faster than a coupled solve for the full model, while preserving good accuracy. Finally, several approaches for the reformulation of diffusion in solid phase were discussed, and it was shown that the correct diffusion length method and Galerkin reformulation work well for the test cases considered here. We also show that both, the decoupled solve and the diffusion reformulation method,

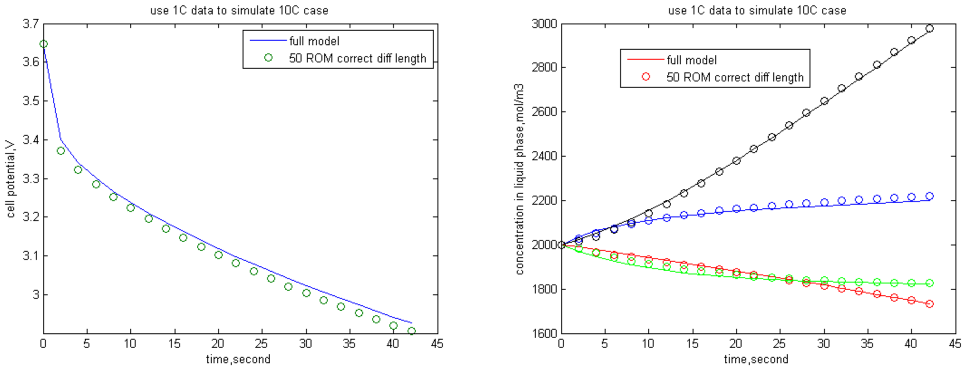

Figure 13: Change C rates *Left*: cell potential; *Right*: concentration at interfaces

can be combined with ROM based on POD in order to further increase the computational efficiency.

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