Project: Open Circuit Voltage Modelling

ELEC8900-30-R-2021F Advanced Energy Storage Systems

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1. Introduction

As the electrification of vehicles and the widespread use of intelligent devices are booming, rechargeable batteries are in great demand. Among them, li-ion batteries (LIBs) are commonly used due to their high energy density and low memory effect [1]. Furthermore, LIBs have significant features such as long-life cycle, excellent charging or discharging efficiency, low self-discharge rate, and high reliability over a wide range of ambient temperatures [1].

As an important characteristic parameter of LIBs, the open circuit voltage (OCV) can be used to estimate the state of charge (SOC) of a battery, and to make the management of battery packs possible [2].

2. Problem Definition

The OCV-SOC characterization is a curve-fitting problem [3]. Firstly, different measurements of the {OCV, SOC} pairs are given, spanning the entire range of SOC; then, we need to perform the curve-fitting to accurately represent the OCV-SOC measurements, for which the parameters should be as few as possible [3]. As shown in Fig. 1, the OCV-SOC curve indicates that the OCV is a nonlinear function of SOC [1]. For a single LIB, the range is $\mathrm{OCV} = V_{\circ}(s) \in [3, 4.2]$ for $\mathrm{SOC} = s \in [0, 1]$ [4].

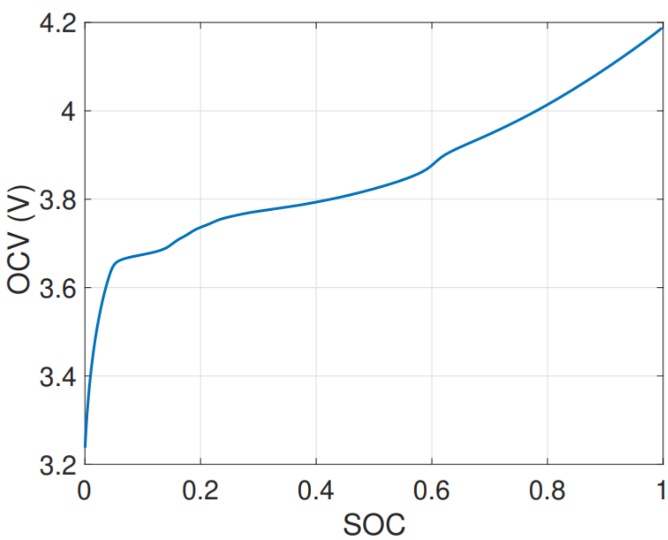

Fig. 1. OCV vs. SOC curve of a Li-ion battery [1].

In the following sections, four models for the suitable representation of OCV-SOC will be discussed, that is, Linear model, Polynomial model, Combined model, and Combined+3 model.

3. Solution Approach

3.1 Use Coulomb Counting for SOC Computation

The SOC at a given time which can be defined as:

$$s[k] \triangleq s \; at \; time \; k \tag{1}$$

Where the notation $\triangleq$ means “defined as”, that is, $s[k]$ indicates the value s at time k. To compute the true SOC at time k, we will use the Coulomb Counting equation:

$$s[k+1] = s[k] + \frac{\Delta_k i[k]}{3600\mathrm{C}_{\mathrm{batt}}} \tag{2}$$

Where Δ_k is the time difference between two measurements, $i[k]$ is the current through the battery, and $\mathrm{C}_{\mathrm{batt}}$ is the battery capacity in Ampere hour (Ah) [1].

However, there are five sources of errors that influence the Coulomb Counting approach [5]: current measurement error, current integration error, timing oscillator error, uncertainty of initial SOC, and uncertainty of the battery capacity. In [4], researchers use high precision measurement devices (such as Arbin testers) to collect OCV characterization data, this way, the best feature of this approach can be retained and errors can be reduced to a minimum [1].

3.2 SOC Scaling

When substituting $s = 0$ and $s = 1$ in equations that define the Combined model, Polynomial model, and Combined+3 model, may lead to numerical instability, as a result, the linear scaling approach will be used. As shown in Fig. 2, SOC domain $s \in [0, 1]$ is scaled to $s' \in [0 + \epsilon, 1 - \epsilon]$, this way, s' can not reach 0 or 1, therefore, computational stability can be ensured [1]. s' is defined as:

$$s' = (1 - 2\epsilon)s + \epsilon \tag{3}$$

Where $\epsilon = 0.175$ gives optimal results in Combined model and Combined+3 model [1].

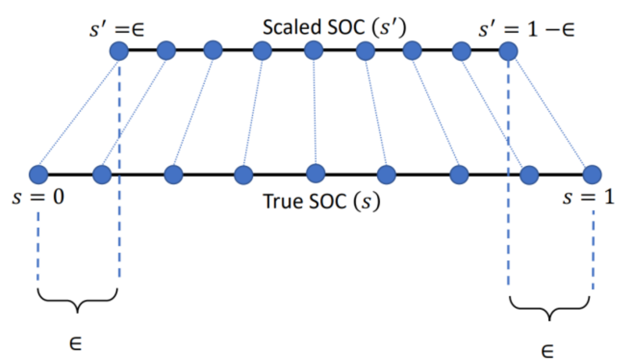

Fig. 2. Linear scaling [1].

3.3 Use Least Square Estimate to Obtain OCV-SOC Parameters

As shown in Fig. 3, the ECM is suitable only when very low current through the battery [1], thus, we can use this model to estimate OCV-SOC curve.

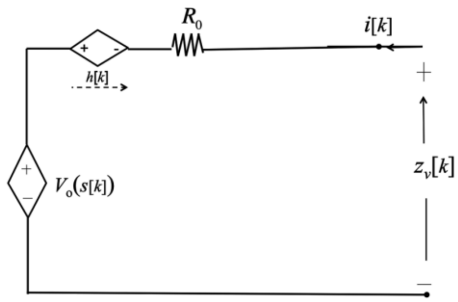

Fig. 3. ECM of a battery during slow charge/discharge [1].

The measured voltage across the battery terminals is expressed as [1]:

$$z_v[k] = v[k] + n_v[k] \tag{4}$$

Where $v[k]$ is the true voltage across the battery terminal, $n_v[k]$ is the voltage measurement noise which is modeled as white Gaussian with standard deviation σ_v [1]. When the battery is being charged/discharged, the terminal voltage can be expressed as [1]:

$$z_v[k] = V_\circ(s[k]) + h[k] + i[k]R_0 + n_v[k] \tag{5}$$

Where $V_\circ(s[k])$ is OCV at SOC $= s[k]$, $h[k]$ is the hysteresis which is a function of current and SOC of the battery [6]. The authors assume that the hysteresis is proportional to the current only when the OCV experiment is performed at a very low current [1, 3], i.e.,

$$h[k] \propto i[k] \tag{6}$$

Therefore, Eq. (5) can be written as [1]:

$$z_v[k] = V_\circ(s[k]) + i[k]R_{0,h} + n_v[k] \tag{7}$$

Where the effective resistance

$$R_{0,h} = R_0 + R_h \tag{8}$$

Where R_0 is the battery series resistance, and R_h is the constant-current hysteresis equivalent resistance.

The observation model in Eq. (7) can also be written in the vector notation form [1]:

$$z_v[k] = [\mathrm{p}_\circ(s[k])^T \quad i[k]] \begin{bmatrix} \mathrm{k}_\circ \\ R_{0,h} \end{bmatrix} + n_v[k] \tag{9}$$

Take the Combined+3 model as an example,

$$V_0(s) = k_0 + \frac{k_1}{s} + \frac{k_2}{s^2} + \frac{k_3}{s^3} + \frac{k_4}{s^4} + k_5 s + k_6 \ln(s) + k_7 \ln(1-s) \tag{10}$$

Therefore, in Eq. (9),

$$\mathrm{k}_{\circ} = [k_0 \quad k_1 \quad k_2 \quad k_3 \quad k_4 \quad k_5 \quad k_6 \quad k_7]^T \tag{11}$$

$$\mathrm{p}_{\circ}(s[k])^T = \left[1 \;\; \frac{1}{s[k]} \;\; \frac{1}{s^2[k]} \;\; \frac{1}{s^3[k]} \;\; \frac{1}{s^4[k]} \;\; s[k] \;\; \ln(s[k]) \;\; \ln(1 - s[k])\right] \tag{12}$$

Let's consider a batch of N voltage observations, Eq. (9) can be expressed as [1]:

$$\mathrm{v} = \mathrm{Pk} + \mathrm{n} \tag{13}$$

where

$$\mathrm{v} = \left[z_v[1] \quad z_v[2] \quad \dots \quad z_v[t_N]\right]^T \tag{14}$$

$$\mathrm{P} = \left[\mathrm{p}[1] \quad \mathrm{p}[2] \quad \dots \quad \mathrm{p}[t_N]\right]^T \tag{15}$$

$$\mathrm{n} = \left[n[1] \;\; n[2] \;\; \dots \;\; n[t_N]\right]^T \tag{16}$$

$$\mathrm{k} = [k_0 \quad k_1 \quad k_2 \quad k_3 \quad k_4 \quad k_5 \quad k_6 \quad k_7 \quad R_{0,h}]^T \tag{17}$$

The least square estimate of the parameter vector is given by:

$$\hat{\mathrm{k}} = (\mathrm{P}^T\mathrm{P})^{-1}\mathrm{P}^T\mathrm{v} \tag{18}$$

For a given SOC, the corresponding OCV estimate

$$\hat{V}_{\circ}(s) = \mathrm{p}_{\circ}(s)^T\hat{\mathrm{k}}_{\circ} \tag{19}$$

Where $\hat{\mathrm{k}}_{\circ}$ is a vector contains first 8 elements of $\hat{\mathrm{k}}$.

<u>Now, use the similar method to answer **Question 1**:</u>

Where $\mathrm{p}_{\circ}(s[k])^T$ and $\mathrm{k}_{\circ}$ in Eq. (9) will be expressed in different forms based on the following models.

A. Linear model

$$V_0(s) = a_0 + a_1 s \tag{20}$$

For this model, in Eq. (9), where

$$\mathrm{k}_{\circ} = [a_0 \quad a_1]^T \tag{21}$$

$$\mathrm{p}_{\circ}(s[k])^T = \left[1 \;\; s[k]\right] \tag{22}$$

Let's consider a batch of N voltage observations, Eq. (9) can be expressed as:

$$\mathrm{v} = \mathrm{Pk} + \mathrm{n} \tag{23}$$

where

$$\mathrm{v} = \left[z_v[1] \quad z_v[2] \quad \dots \quad z_v[N]\right]^T \tag{24}$$

$$\mathrm{P} = [\mathrm{p}[1]\ \ \mathrm{p}[2]\ \ \ldots\ \ \mathrm{p}[N]\ ]^T = \begin{bmatrix} 1 & s[1] & i[1] \\ 1 & s[2] & i[2] \\ \vdots & \vdots & \vdots \\ 1 & s[N] & i[N] \end{bmatrix} \tag{25}$$

$$\mathrm{n} = \left[n[1]\ \ n[2]\ \ \ldots\ \ n[\mathrm{N}]\right]^T \tag{26}$$

$$\mathrm{k} = [a_0\quad a_1\quad R_{0,h}]^T \tag{27}$$

The least square estimate of the parameter vector is given by:

$$\hat{\mathrm{k}} = (\mathrm{P}^T\mathrm{P})^{-1}\mathrm{P}^T\mathrm{v} \tag{28}$$

For a given SOC, the corresponding OCV estimate

$$\hat{V}_\circ(s) = \mathrm{p}_\circ(s)^T\hat{\mathrm{k}}_\circ \tag{29}$$

Where $\hat{\mathrm{k}}_\circ$ is a vector contains first 2 elements of $\hat{\mathrm{k}}$.

B. Polynomial model

$$V_0(s) = p_0 + p_1 s + \cdots + p_n s^n + p_{n+1}s^{-1} + \cdots + p_{n+m}s^{-m} \tag{30}$$

For this model, in Eq. (9), where

$$\mathrm{k}_\circ = [p_0\ \ p_1\ \ \cdots\ \ p_n\ \ p_{n+1}\ \cdots\ p_{n+m}]^T \tag{31}$$

$$\mathrm{p}_\circ(s[k])^T = \left[1\ \ s[k]\ \ \cdots\ \ s^n[k]\ \ \frac{1}{s[k]}\ \ \cdots\ \ \frac{1}{s^m[k]}\right] \tag{32}$$

Let's consider a batch of N voltage observations, Eq. (9) can be expressed as:

$$\mathrm{v} = \mathrm{Pk} + \mathrm{n} \tag{33}$$

where

$$\mathrm{v} = \left[z_v[1]\quad z_v[2]\quad \ldots\quad z_v[N]\right]^T \tag{34}$$

$$\mathrm{P} = [\mathrm{p}[1]\ \ \mathrm{p}[2]\ \ \ldots\ \ \mathrm{p}[N]\ ]^T = \begin{bmatrix} 1 & s[1] & \cdots & s^n[1] & \frac{1}{s[1]} & \cdots & \frac{1}{s^m[1]} & i[1] \\ 1 & s[2] & \cdots & s^n[2] & \frac{1}{s[2]} & \cdots & \frac{1}{s^m[2]} & i[2] \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & s[N] & \cdots & s^n[N] & \frac{1}{s[N]} & \cdots & \frac{1}{s^m[N]} & i[N] \end{bmatrix} \tag{35}$$

$$\mathrm{n} = \left[n[1]\ \ n[2]\ \ \ldots\ \ n[N]\right]^T \tag{36}$$

$$\mathrm{k} = [p_0 \;\; p_1 \;\; \cdots \;\; p_n \;\; p_{n+1} \;\; \cdots \;\; p_{n+m} \;\; R_{0,h}]^T \tag{37}$$

The least square estimate of the parameter vector is given by:

$$\hat{\mathrm{k}} = (\mathrm{P}^T\mathrm{P})^{-1}\mathrm{P}^T\mathrm{v} \tag{38}$$

For a given SOC, the corresponding OCV estimate

$$\hat{V}_{\circ}(s) = \mathrm{p}_{\circ}(s)^T\hat{\mathrm{k}}_{\circ} \tag{39}$$

Where $\hat{\mathrm{k}}_{\circ}$ is a vector contains first n+m+1 elements of $\hat{\mathrm{k}}$.

C. Combined model

$$V_0(s) = \kappa_0 + \kappa_1 s^{-1} + \kappa_2 s + \kappa_3 \ln(s) + \kappa_4 \ln(1-s) \tag{40}$$

For this model, in Eq. (9), where

$$\mathrm{k}_{\circ} = [k_0 \quad k_1 \quad k_2 \quad k_3 \quad k_4]^T \tag{41}$$

$$\mathrm{p}_{\circ}(s[k])^T = \left[1 \;\; \frac{1}{s[k]} \;\; s[k] \;\; ln(s[k]) \;\; ln\,(1-s[k])\right] \tag{42}$$

Let's consider a batch of N voltage observations, Eq. (9) can be expressed as:

$$\mathrm{v} = \mathrm{Pk} + \mathrm{n} \tag{43}$$

where

$$\mathrm{v} = \left[z_v[1] \quad z_v[2] \quad \ldots \quad z_v[N]\right]^T \tag{44}$$

$$\mathrm{P} = [\mathrm{p}[1] \;\; \mathrm{p}[2] \;\; \ldots \;\; \mathrm{p}[N]\,]^T = \begin{bmatrix} 1 & \frac{1}{s[1]} & s[1] & ln(s[1]) & ln\,(1-s[1]) & i[1] \\ 1 & \frac{1}{s[2]} & s[2] & ln(s[2]) & ln\,(1-s[2]) & i[2] \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \frac{1}{s[N]} & s[N] & ln(s[N]) & ln\,(1-s[N]) & i[N] \end{bmatrix} \tag{45}$$

$$\mathrm{n} = \left[n[1] \;\; n[2] \;\; \ldots \;\; n[N]\right]^T \tag{46}$$

$$\mathrm{k} = [k_0 \quad k_1 \quad k_2 \quad k_3 \quad k_4 \quad R_{0,h}]^T \tag{47}$$

The least square estimate of the parameter vector is given by:

$$\hat{\mathrm{k}} = (\mathrm{P}^T\mathrm{P})^{-1}\mathrm{P}^T\mathrm{v} \tag{48}$$

For a given SOC, the corresponding OCV estimate

$$\hat{V}_{\circ}(s) = \mathrm{p}_{\circ}(s)^T \hat{\mathrm{k}}_{\circ} \quad (49)$$

Where $\hat{\mathrm{k}}_{\circ}$ is a vector contains first 5 elements of $\hat{\mathrm{k}}$.

3.4 Modeling Error

The voltage modelling error is expressed as [1]:

$$\mathrm{e} = \mathrm{v} - \mathrm{P}\hat{\mathrm{k}} \quad (50)$$

Where v is true terminal voltage vector, P is parameter matrix as shown in Eq. (25), (35), and (45), and $\hat{\mathrm{k}}$ is the estimate of OCV-SOC parameter vector [1].

3.5 Evaluation of Fitting Accuracy

We use correlation coefficient R^2 to evaluate the accuracy of each of the four models, which can be expressed as:

$$R^2 = \frac{S_t - S_r}{S_t} \quad (51)$$

Where S_t is the total sum of squares around the mean and S_r is the sum of error squares, which can be expressed as:

$$S_t = \sum (v - \bar{v})^2 \quad (52)$$

$$S_r = \sum \left(v - \mathrm{P}\hat{\mathrm{k}}\right)^2 \quad (53)$$

Where v is the true terminal voltage vector, $\bar{v}$ is the mean of terminal voltage vector, P is parameter matrix, and $\hat{\mathrm{k}}$ is the estimate of OCV-SOC parameter vector [1].

4. Results and Discussions

The OCV-SOC parameters of the following four models will be obtained by using the data provided, as shown in Fig. 4.

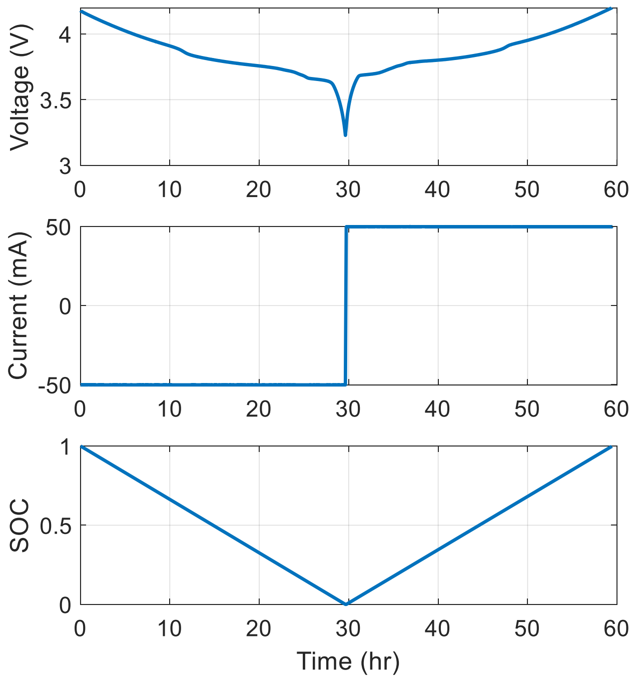

Fig. 4. Visualization of provided data.

4.1 Results of Question 2

See attachment 'AESS_Project_Q2_Q3.m' for Matlab Code.

A. Approach used to obtain the optimal polynomial order n and m

In Eq. (30), we assume the highest polynomial order n and m are 9 and 8, respectively; then, I use *for loop* in Matlab to perform the iterations. In each iteration, the polynomial model is tested with different order n and m; thus, we can find OCV-SOC parameters of the polynomial model formed by using LS estimate.

Then we calculate the correlation coefficient R^2 which is defined in Eq. (51). As shown in Fig. 5, each iteration will generate a new R^2 value, which indicates how accurate the chosen polynomial model fits the given data; this value will be stored in variable R_sq_polynomial; also, the polynomial order n and m with assigned value in each iteration will be stored in variable index_n_m. To determine the best fit model, we can find the highest R^2 in Matlab. Fig. 6 shows the code to find the optimal order n and m for the polynomial model, which indicates that the best fit occurred at 51st iteration, i.e., the optimal order n = 8, and m = 3.

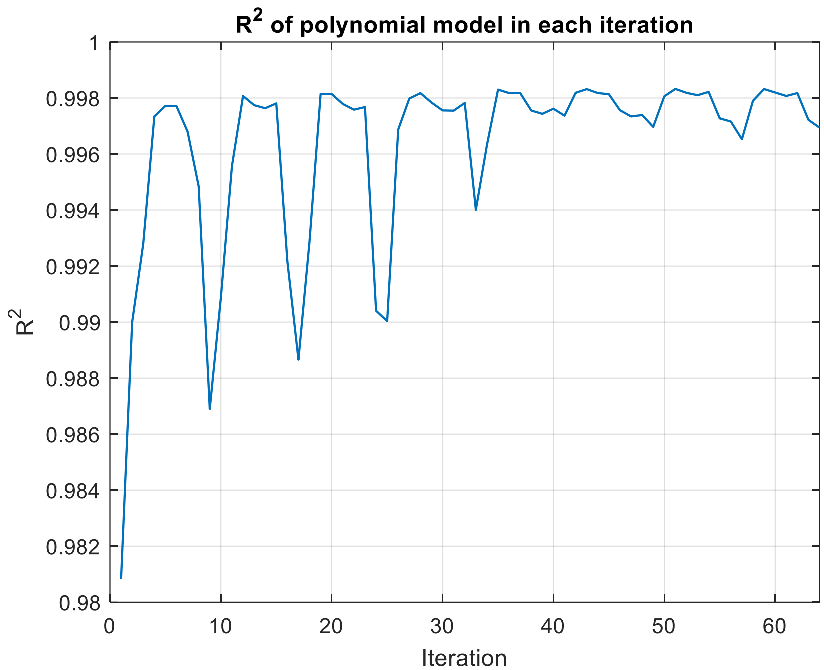

Fig. 5. The correlation coefficient R^2 of polynomial model in each iteration.

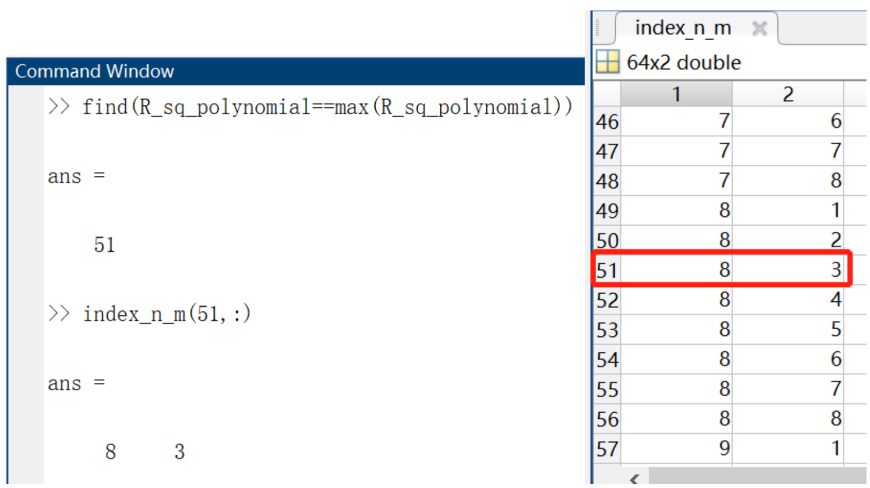

Fig. 6. Find the optimal polynomial order n and m in Matlab.

B. OCV-SOC parameters

```
Command Window
OCV-SOC parameters of Linear Model:
a0 = 3.585414  a1 = 0.544742

OCV-SOC parameters of Polynomial Model:
optimal degree n = 8  optimal order m = 3
p0 = 214.278312
p1 = -389.435542
p2 = 248.329823
p3 = 204.342101
p4 = -213.236972
p5 = -228.134174
p6 = 121.288391
p7 = 289.469987
p8 = -194.489240
p9 = -56.933565
p10 = 7.732293
p11 = -0.420650
```

```
Command Window
OCV-SOC parameters of Combined Model:
k0 = -1.041084
k1 = -0.809928
k2 = 7.128030
k3 = -4.534756
k4 = 0.318780

OCV-SOC parameters of Combined+3 Model:
k0 = -8.823921
k1 = 101.376889
k2 = -17.865896
k3 = 2.023786
k4 = -0.099720
k5 = -75.383464
k6 = 138.939551
k7 = -1.099040
```

C. Plot of OCV vs. SOC of all four approaches

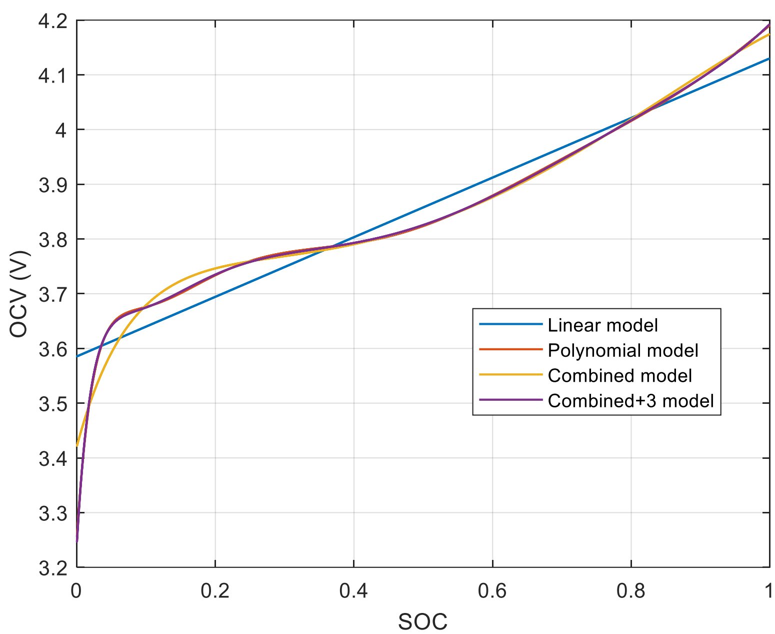

Fig. 7. OCV vs. SOC of each of four models.

D. Modeling error of each of four approaches

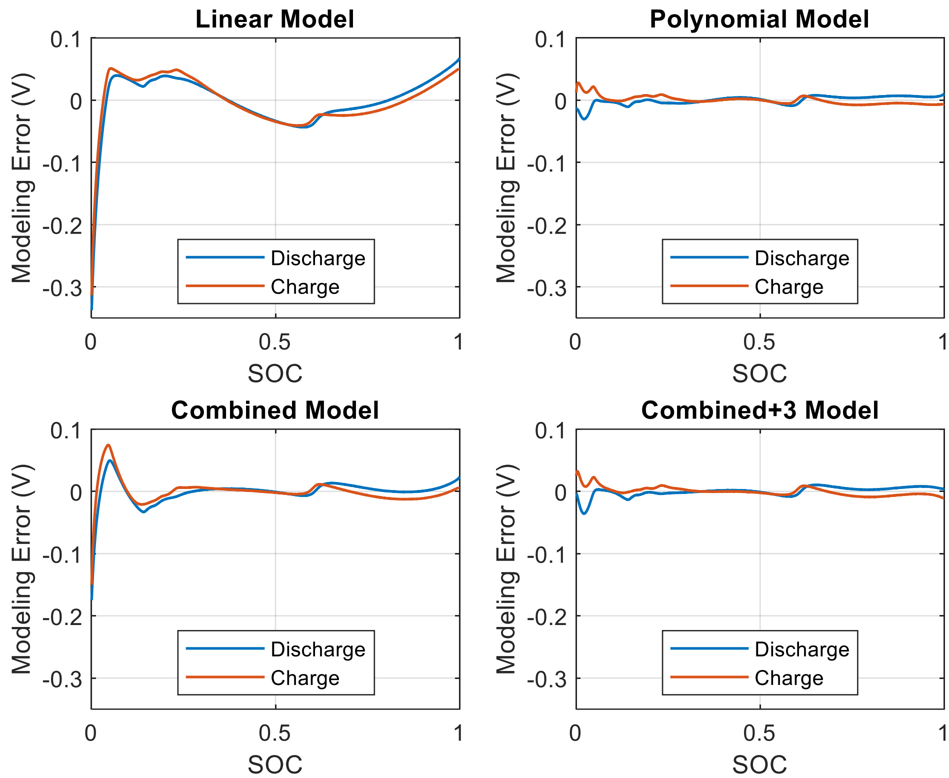

Fig. 8. Voltage modeling error of each of four models.

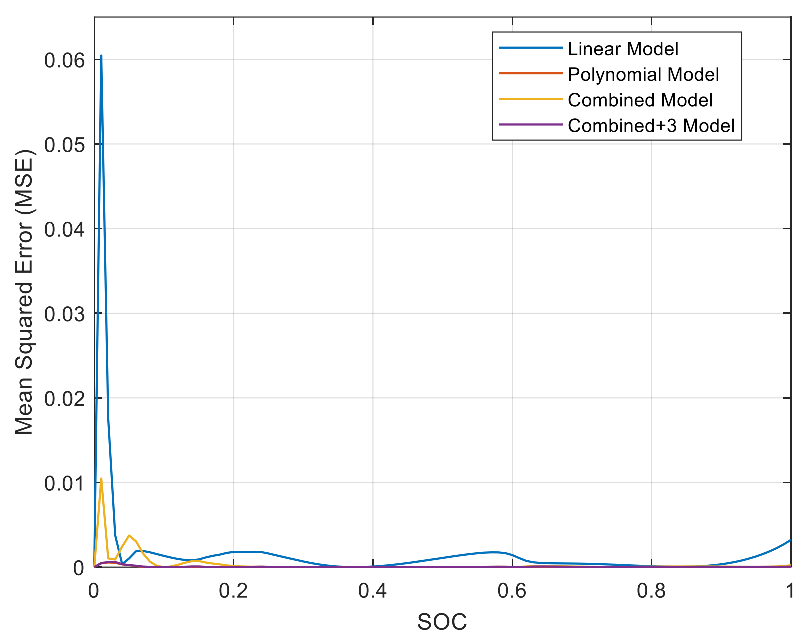

Fig. 9. MSE of each of four models.

4.2 Results of Question 3

See attachment 'AESS_Project_Q2_Q3.m' for Matlab Code.

As shown in Fig. 10, the most accurate model is polynomial model (n = 8, m = 3). The least accurate model is linear model.

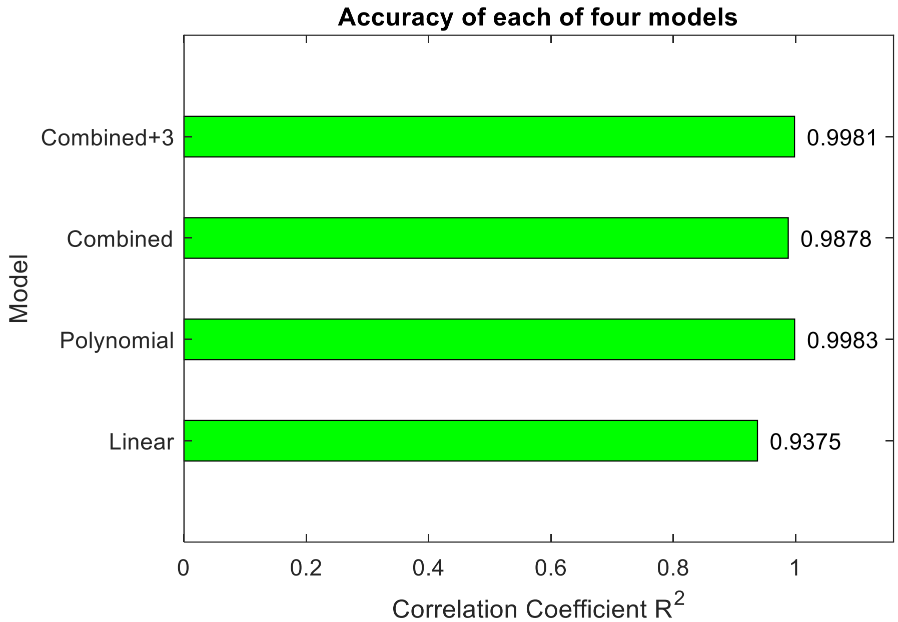

Fig. 10. Visualization of accuracy of each of four models.

4.3 Results of Question 5

When SOC is not given, we will use Coulomb Counting method shown in Eq. (2) to compute SOC. See attachment 'AESS_Project_Q5_new.m' for Matlab Code.

A. OCV-SOC parameters

```
Command Window
OCV-SOC parameters of Linear Model:
a0 = 3.584721   a1 = 0.544494

OCV-SOC parameters of Polynomial Model:
optimal degree n = 8  optimal order m = 3
p0 = 218.114197
p1 = -395.121969
p2 = 250.073510
p3 = 208.694945
p4 = -214.901035
p5 = -232.476109
p6 = 121.773323
p7 = 294.415446
p8 = -197.139942
p9 = -58.151231
p10 = 7.922118
p11 = -0.432336
```

```
Command Window
OCV-SOC parameters of Combined Model:
k0 = -1.090334
k1 = -0.822209
k2 = 7.200518
k3 = -4.592769
k4 = 0.323625

OCV-SOC parameters of Combined+3 Model:
k0 = -9.458357
k1 = 102.016900
k2 = -18.052462
k3 = 2.053336
k4 = -0.101598
k5 = -75.155482
k6 = 139.228033
k7 = -1.069760
fx >> |
```

B. Plot of OCV vs. SOC of all four approaches

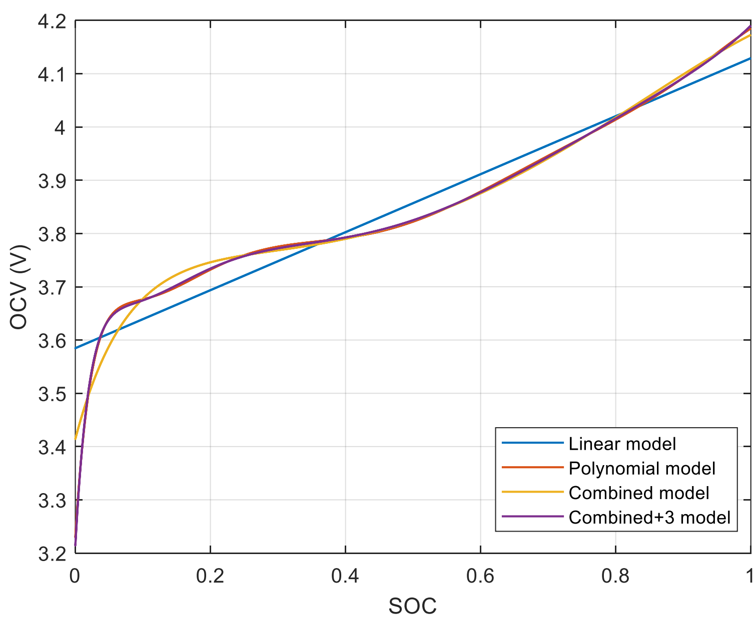

Fig. 11. OCV vs. SOC of each of four models without SOC provided.

C. Modeling error of each of four approaches

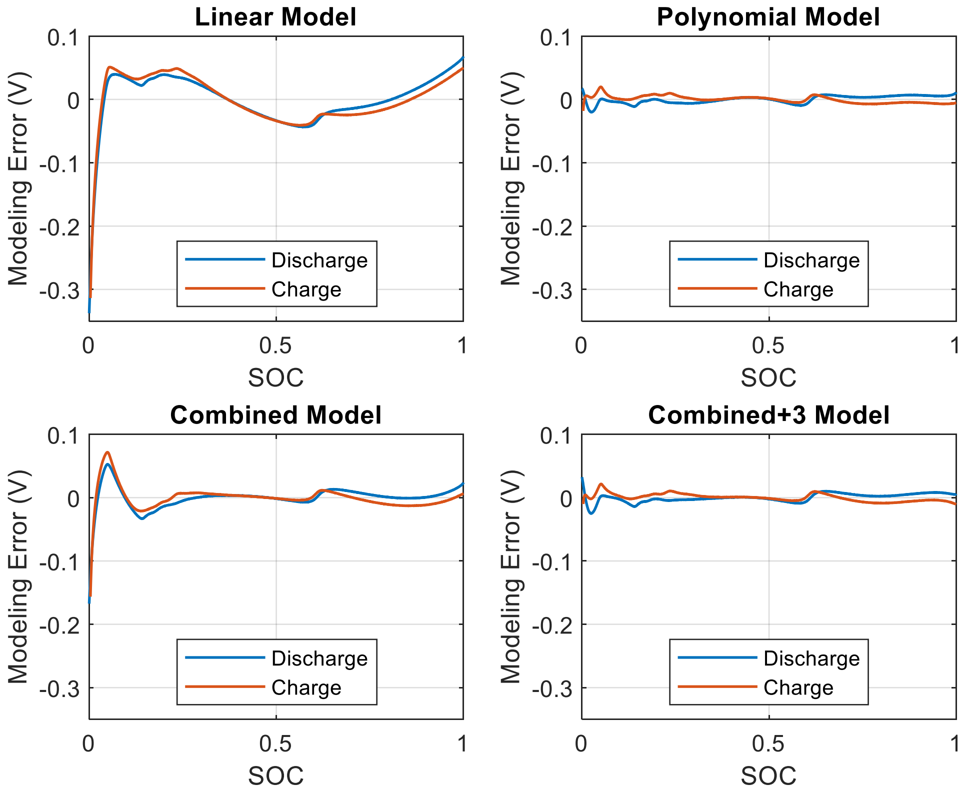

Fig. 12. Voltage modeling error of each of four models without SOC provided.

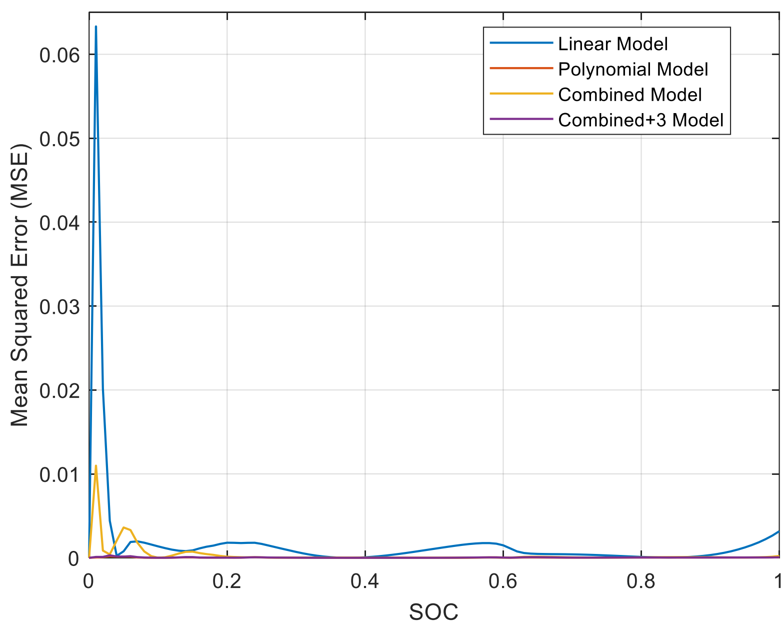

Fig. 13. MSE of each of four models without SOC provided.

4.4 Discussion (Question 4)

The advantages and disadvantages of each of four models are shown in Table 1.

Table 1. Comparison of different models

OCV-SOC Model	Pros	Cons
Linear	• Easier for modelling.	• Poor fitting accuracy.
Polynomial	• Better fitting effect. • The best fit is more accurate than Combined+3 model.	• Will increase the computation burden when the order is high. • May cause over-fitting.
Combined	• Acceptable accuracy can be achieved • Only a few OCV-SOC parameters needed.	• Less accurate compared to Combined+3 model • SOC values need to be scaled in case of numerical instability
Combined+3	• Higher accuracy can be achieved compared to Combined model	• Less accurate compared to Polynomial model • SOC values need to be scaled in case of numerical instability

5. Conclusion

By observing the fitting accuracy of each of four models, the Polynomial model seems to be the best choice for OCV-SOC characterization; however, if the order of the Polynomial model needs to be higher to ensure the fitting accuracy, the computation process will be slower; also, higher order means more parameters required, which in turn, makes this model more complicated; therefore, it is preferable to choose the Combined+3 model, which not only ensures an acceptable accuracy but also has a reasonable number of parameters.

References

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