38th International Electric Vehicle Symposium and Exhibition (EVS38) Göteborg, Sweden, June 15-18, 2025

Battery digital twin for real time operation of an electric vehicle

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Executive Summary

Digital twins have found applications in diverse industrial applications from power plants to refineries. The use of AI/ML to process and build models has provided a powerful technique to supplement and enhance reduced order models (ROM) for real time prediction and optimization of physical equipment. A reduced order model for temperature prediction in a battery pack and machine learning models for state of health (SoH) and remaining useful life (RUL) are described. The temperatures inside the pack are predicted using a lumped capacitance model coupled with a forced convection model and a cell electro-thermal model. The thermal model is validated with a high-fidelity computational fluid dynamics (CFD) model. The ML model for SoH and RUL prediction is validated with publicly available cell data.

Keywords: battery management system, network thermal model, state of health, remaining useful life, reduced order model

1 Introduction

Batteries form an important component of green energy and sustainability as they store the energy from renewable sources like wind and solar and are used in electricity grids and electric vehicles. For electric vehicles, Lithium-ion batteries are preferred due to their high energy density and flat voltage output over a large state of charge range (SoC). Several cells are assembled in a module and several modules are used together in an automobile for providing the required voltage and current. These cells are placed closely to each other due to space constraints in a vehicle [2]. Lithium-ion batteries are flammable because metallic lithium is combustible and can catch fire when heated beyond a certain temperature. This is commonly termed thermal runaway [3]. This typically happens when the cells are overcharged when the voltage of the cell exceeds a certain limit. Cells also generate heat due to ohmic losses during charging and discharging, and due to reversible heat generation while charging. Additionally, the capacity of the cell to hold charge decreases as the reversible Lithium ions undergo certain irreversible side reactions. The rate of capacity degradation increases with increasing operating temperature of the cells.

To prevent thermal runaway and to control the temperature rise in the pack, different cooling mechanisms are employed. For electric vehicles, forced convection cooling using liquid coolants is preferred because of the greater thermal mass of the coolant. Since heat transfer between the cells and the coolant is not uniform, cell capacity decreases differentially and requires cells that have degraded more be cutoff earlier compared to other cells while charging. This is done through a mechanism called cell balancing. Battery management systems are commonly used to control the behavior of the pack by cutting off supply during charging and discharging to maintain the health of the pack. However, this is based on a limited number of temperature measurements and it becomes difficult to identify the exact location of thermal runaway. Since cell performance and its health are strongly dependent on its temperature, it is important to monitor temperature distribution of the coolant within the pack. As it not possible to install many temperature sensors within a battery pack, digital twin of a batter pack with soft sensors based on first principles or machine learning would be of great utility to monitor, optimize and control the performance and health of a battery pack.

Modeling the temperature distribution in the cells and capacity degradation of the cells from first principles is computationally expensive, and alternate fast running models are required. The present work is to address two issues in battery digital twin. 1. Predicting the temperature of cells in a battery pack using lumped capacitance models including two-state thermal models for cells with equivalent circuit thermal-electric models for cell behavior. 2. A fast running memory efficient data-based model for capacity degradation and remaining useful life prediction using past charging-discharging behavior. The description for the thermal model and data-based SoH model are given and the results from the two models are presented.

2 Battery Pack Model

2.1 Geometry of the battery pack

A schematic of the battery pack is shown in
Figure *1*. A serpentine configuration with a straight non-wavy cooling channel next to the cell column is considered. The cell and the channel are thermally connected using an elastomer assembly, also shown in Figure *1*. For the sake of demonstration, the battery pack is assumed to be similar to that of a module in Tesla EV pack [2]. The module consists of 240 cylindrical cells that are arranged in a 10×24 configuration. A non-staggered configuration with the center of the cells in a straight line between two adjacent rows is considered. The cylindrical cell modeled is A123 cell with capacity of 2.3 Ah [1], [9]. A glycol-water mixture of 50-50 based on volume is taken as the coolant. The depth of the channel is assumed to be the same as the height of the cell. The thickness of the elastomer varies from 14 mm to 28 mm and width of the channel is assumed to be 4 mm.

2.2 Equivalent circuit model

The cell is modelled assuming a 1R - 2RC model [9]. The terminal voltage of a cell is calculated as

$$V_T = V_{OCV} - V_{R_1C_1} - V_{R_1C_2} \quad (1)$$

where V_{OCV} is open circuit voltage of the cell, $V_{R_1C_1}$ and $V_{R_2C_2}$are voltage drops across the RC pairs. The change in SoC in a cell with time is given by:

$$\frac{dSoC}{dt} = -\frac{1}{C_{bat}} I \quad (2)$$

where C_{bat} is capacity of the cell and I is current.

The voltages across the two RC pairs are given by:

$$\frac{dV_{R_1C_1}}{dt} = \frac{1}{R_1C_1} V_{R_1C1} + \frac{1}{C_1}\mathrm{I} \quad (3)$$

$$\frac{dV_{R_1C_2}}{dt} = \frac{1}{R_2C_2} V_{R_2C_2} + \frac{1}{C_2}\mathrm{I} \quad (4)$$

The rate of generation of heat in the cell Q is calculated as:

$$Q = I^2 R_s + \frac{V_{R_1C_1}^2}{R_1} + \frac{V_{R_2C_2}^2}{R_2} \tag{5}$$

R_1, R_2, C_1, C_2 and R_s are calculated using the following equations:

$$R_{il} = (R_{0_{i1l}} + a_{1il}SoC + a_{2il}SoC^2)e^{\frac{T_{ref_{R_{il}}}}{T_{in}-T_{shift_{R_{il}}}}} \tag{6}$$

$$\mathrm{i} = \begin{cases} 1, & \text{for } \mathrm{R}_1 \\ 2, & \text{for } \mathrm{R}_2 \end{cases}, \qquad \mathrm{l} = \begin{cases} \mathrm{c}, & \text{for charge} \\ \mathrm{d}, & \text{for discharge} \end{cases}$$

$$C_{i1} = C_{0il} + C_{1il}SoC + C_{2il}SoC^2 + (C_{3il} + C_{4il}SoC + C_{5i}SoC^2)T_{in} \tag{7}$$

$$\mathrm{i} = \begin{cases} 1, & \text{for } \mathrm{R}_1 \\ 2, & \text{for } \mathrm{R}_2 \end{cases}, \qquad \mathrm{l} = \begin{cases} \mathrm{c}, & \text{for charge} \\ \mathrm{d}, & \text{for discharge} \end{cases}$$

$$R_{is} = R_{0_l} + a_{1l}T_{in} + a_{2l}T_{in}^2$$

$$\mathrm{l} = \begin{cases} \mathrm{c}, & \text{for charge} \\ \mathrm{d}, & \text{for discharge} \end{cases}$$

Here R_1, R_2, C_1, *and* C_2 are resistances and capacitances of the electrode-electrolyte interface and R_s is resistance of the electrolyte. V_{R_1C1} and $V_{R_2C_2}$ are voltage drops across the two RC circuits. T_{in} is the maximum temperature in the cell core, *I* is the t current in the cell, and SoC is state of charge of the cell. All other quantities are assumed to be constant and fitted using vehicle battery data.

2.3 Battery Pack Thermal Model

A two-state thermal model with a cell core temperature and shell temperature is adapted from [9].

$$C_c \frac{dT_{in}}{dt} = Q + \frac{T_s - T_{in}}{R_c} \tag{8}$$

$$C_s \frac{dT_s}{dt} = \frac{T_f - T_s}{R_u} - \frac{T_s - T_{in}}{R_c} \tag{9}$$

where C_c and C_s are thermal masses of the cell core and shell, respectively, T_{in} is the maximum temperature seen at the cell core, Q is heat generation in the cell, T_s is shell temperature of the cell, T_f is free stream fluid temperature, and R_u and R_c are thermal resistances between cell core and shell and between shell and fluid, respectively.

The heat transfer from the cell to coolant channel is facilitated by an elastomer. The two-state thermal model is extended to include the elastomer shown in
Figure *1* and the model is solved for calculating the surface temperature of the elastomer next to the coolant channel instead of the shell temperature. The lumped resistances of the shell-elastomer assembly are obtained by carrying out detailed CFD simulations using the individual elastomer-cell assembly. The free stream

temperature T_f is replaced by mean fluid temperature in the channel for these simulations.

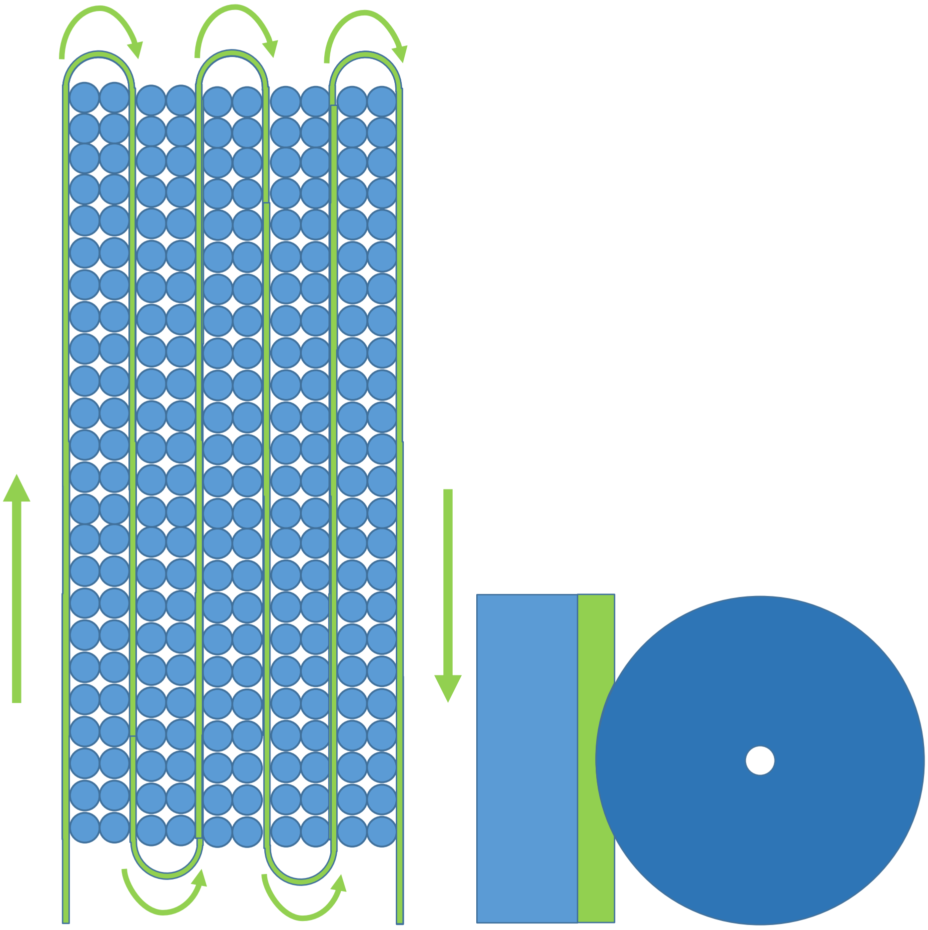

Figure 1: Schematic of the cell assembly and an individual cell with elastomer shown in green convection channel

2.4 Fluid-side Heat Transfer

The coolant channel is divided into elements along the direction of flow with the element length matching diameter of the cell next to it. A lumped parameter model of the coolant channel is used with the outlet temperature, with mean temperature of the coolant element used for heat transfer with the cell element adjacent to it. The heat balance for the coolant element is solved algebraically with input and output temperatures along with heat addition from the cells adjacent to it. The surface elastomer temperature *Ts* and the fluid temperature T_f are coupled using the heat transfer coefficient calculated from (10).

The coolant flow regime is in the laminar regime with Reynolds number in the order of 100s. For the conditions encountered, the development of thermal boundary layer is delayed due to high Prandtl number of the fluid while the laminar boundary layer develops much quicker. In this scenario, the velocity and pressure do not change after the flow develops. Hence, the problem becomes linear with respect to the temperature. The convolution method developed by Graetz for arbitrary wall temperatures applies to current operating conditions [8]. In the original method the technique requires heat flux at certain point be the function of temperature histories upstream of that location.

To simplify the Shah correlation that models the developing boundary layer is used in place of Graetz solution and convolution is applied to first few cells downstream of the inlet. The equation is given by

$$Nu_{Dh} = \begin{cases} 1.233(x^*)^{-\frac{1}{3}} + 0.4, & x^* \leq 0.001 \\ 7.541 + 6.874(10^3 x^*)^{-0.488}\, exp(-245x^*), & x^* > 0.001 \end{cases} \quad (10)$$

here x^* is the non-dimensional distance from the inlet, calculated as x/D_hRePr where x is distance from the inlet along the fluid path, Re is the Reynolds number based on average velocity, D_h is hydraulic diameter, and Pr is the Prandtl number of the flow, Nu_{Dh} is the local Nusselt number. The cell temperature is assumed to be uniform along its height. Since convective heat transfer dominates among other mechanisms, heat transfer on the sides of the cell, top and bottom are ignored. The cells don't exchange heat with each other due to their circular geometry. Axial conduction along the length of the elastomer is ignored in the fluid flow direction.

The equations for SoC, V_1, V_2, T_{in}, and T_s are solved for each cell, and so for the full model, 240×5 equations are solved. These equations are coupled with convective side heat balance, with one convection element adjacent to cell-elastomer element shown in Figure *1*.

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3 State of Health (SoH) & Remaining Useful Life (RUL) Models

The State of Health (SoH) and Remaining Useful Life (RUL) of batteries are crucial metrics in cell management systems, particularly for applications involving electric vehicles, renewable energy storage, and consumer electronics. SoH represents the current capacity or performance of a cell relative to its original, ideal state—typically expressed as a value between 0 and 1, or as a percentage. RUL, on the other hand, refers to the estimated time or usage cycles remaining before the cell becomes unusable or reaches a predefined performance threshold.

Accurately estimating SoH and predicting RUL helps ensure safety, maximize performance, plan timely maintenance, and reduce costs. Our work presents a robust, data-driven approach to model SoH and predict RUL using a machine learning algorithm.

3.1 State of Health Estimation Method

To estimate cell SoH, we use beta regression, a statistical modeling technique particularly effective for outcomes that lie within a bounded interval — such as SoH values that always fall between 0 and 1.

Beta regression is built upon the beta distribution [5], which is flexible and capable of modeling a wide variety of curve shapes (symmetric, skewed, etc.) depending on the data. This makes it ideal for representing cell health, which show nonlinear or asymmetric behavior over time.

For modeling, dataset provided by NASA using 'randomized battery usage' is used [4]. In this case, the cell is charged and discharged with randomly selected current values for a short duration. Such a cycle is termed as a random walk (RW) cycle. Reference cycle is carried out after several RW cycles to measure the cell capacity and to observe the cell degradation over time

The published data was generated under 7 different charging/discharging conditions. Four similar cells were used for each test condition. All three states of the cell, that is, charging, discharging and rest were realized in a random manner. Further, there were reference cycles in between, where for several 500 or 1500 random cycles the cell capacity is measured. Details of these tests are summarized in [4].

Before training the beta regression model on this data, feature engineering is performed to extract useful features. These features capture subtle patterns and relationships with SoH. We propose the following extracted features for prediction of SoH and RUL:

1. Mean Cumulative Charging Load (MCCL): As the name suggests, this feature is related to the cumulative value of total input charge into the cell over time at any given instance of time. It is defined as the ratio of total charge input (Qch) to the cell to total charging time since inception ($T_{opn_{ch}}$) till given instance of time 't'.

$$hLcum = \frac{Q_{ch}}{T_{opn_{ch}}} \tag{11}$$

It is useful in explaining the general trend of cell degradation as shown in Figure 2.

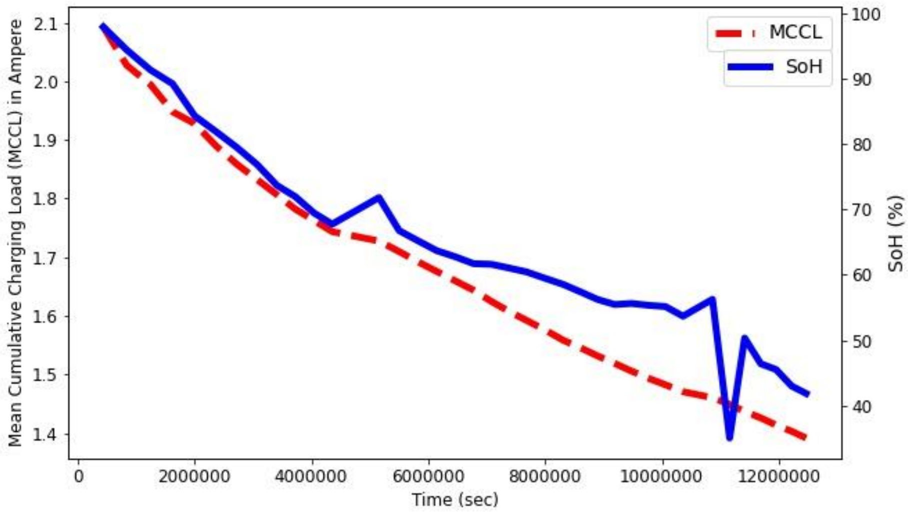

Figure 2: Relation between SoH and Mean Cumulative Charging Load (MCCL)

2. Cumulative Elapsed Time Ratio [$ETRatio$]: After an idle period in cell operation, the cell capacity increase. This phenomenon is called 'capacity regeneration'. Capacity regeneration can be observed after a long rest period as can be seen in Figure 3 where prolonged rest period is getting captured in terms of cumulative elapsed time ratio as a sudden spike in the ETRatio (due to random rest period for small time this ratio is seen increasing value, but spike can be seen in the ratio after unusual, prolonged rest). It is defined as the ratio of total rest period (time when cell is not charging or discharging), T_{rest}, to total absolute time since the inception of new cell, T_{abs}.

$$ETRatio = \frac{Trest}{Tabs} \tag{12}$$

Or

$$ETRatio = \frac{Tabs - Topn}{T_{abs}} \tag{12}$$

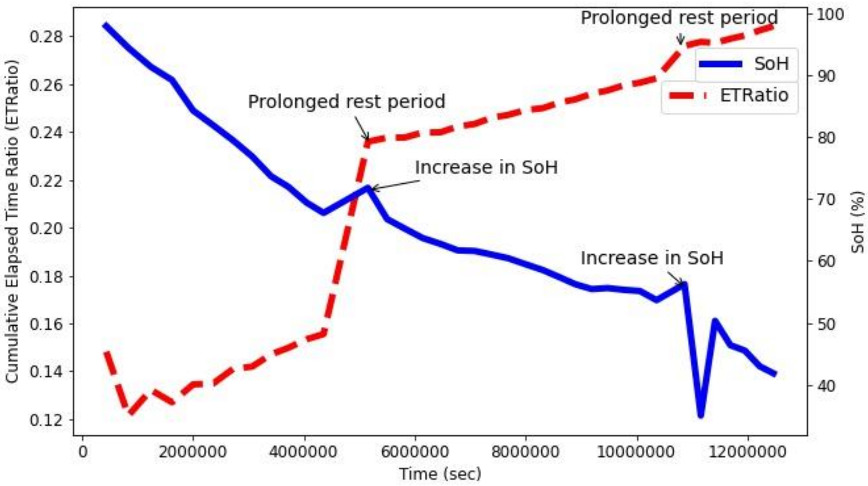

Figure 3: Effect of Elapsed Time Ratio on SoH

Elapsed Time Ratio gives insights on cell usage in terms of the percent of time the cell is rested over a given period of its life.

3.2 RUL Prediction Method

To predict the Remaining Useful Life (RUL) of the cell, we extend the approach above using the previously constructed features and the trained SoH model.

First, values of the engineered features into future time steps re forecasted using Gaussian process regression [11], [12]. These future feature values are then fed to the trained beta regression model to generate predicted SoH values for those future points in time. These predicted SoH values for the future time steps are compared with the predefined threshold value. Once the predicted SoH falls below this threshold, it is considered as the end of useful life. The corresponding time gives us the RUL.

4 Results

4.1 Thermal network model

4.1.1 Validation with CFD results

Before the model was used in the 240-cell battery pack, it was tested on a reduced 72 cell battery pack with two convection passes to minimize computational cost. Ansys Fluent^{TM} software was used to run simulations. To simplify the model, a constant resistance of 0.01 ohms was used for the cells. The current profile used is urban assault cycle (UAC) taken from [9]. The mesh count used in the CFD runs was around 140,000. A user defined function (UDF) was integrated to model cyclotropic thermal conductivity of the A123 cell. The shell of the A123 cell is modeled using the shell conduction model available with Ansys Fluent.

The model parameters are estimated as functions of cell state of charge, cell core temperature and charge or discharge conditions for the 2 RC circuits. Electrolyte resistance is treated a function of cell core temperature and charge discharge condition. The open circuit voltage of the cell V_{OCV} is a function of the state of charge of the cell. The model is first validated with experimental data from [9] before being used in the battery pack.

The results are presented for a water-glycol mixture with average velocity of 0.1 m/s. This corresponds to a Reynolds number of 300.
Figure 4 shows the comparison between CFD and reduced order model runs. The temperature rise in the cell core is reported for 5 cells, with the total cell index *i* calculated as $j\times24+72\times k$, here *j* is row number. For two rows, it is 0 and 1 counted from left to right, and *k* is column number of the cells counted from the bottom,

varying from 0 to 23. The maximum error in the simulation was around 7% for the cell close to the outlet, at the total cell index *i*=48.

4.1.2 **Full Battery Stack Simulations**

After validating the model with CFD for simplified two pass runs with constant resistance, the full battery stack consisting of 240 cells is modeled using the equivalent circuit model and 2- state thermal model. The same conditions used for the CFD validation are used for the full stack run with UAC cycle with glycol as coolant with velocity of 0.1 m/s. Equations for state of charge (SoC), voltage across RC circuits, V_1, V_2, temperature in cell core T_{in} and on elastomer surface T_s surface are solved. The heat source is a function of cell resistance R_1, R_2, and R_s. The initial temperature of the cells and the inlet coolant temperature is set as 20 C. The results are provided in Figure 5.

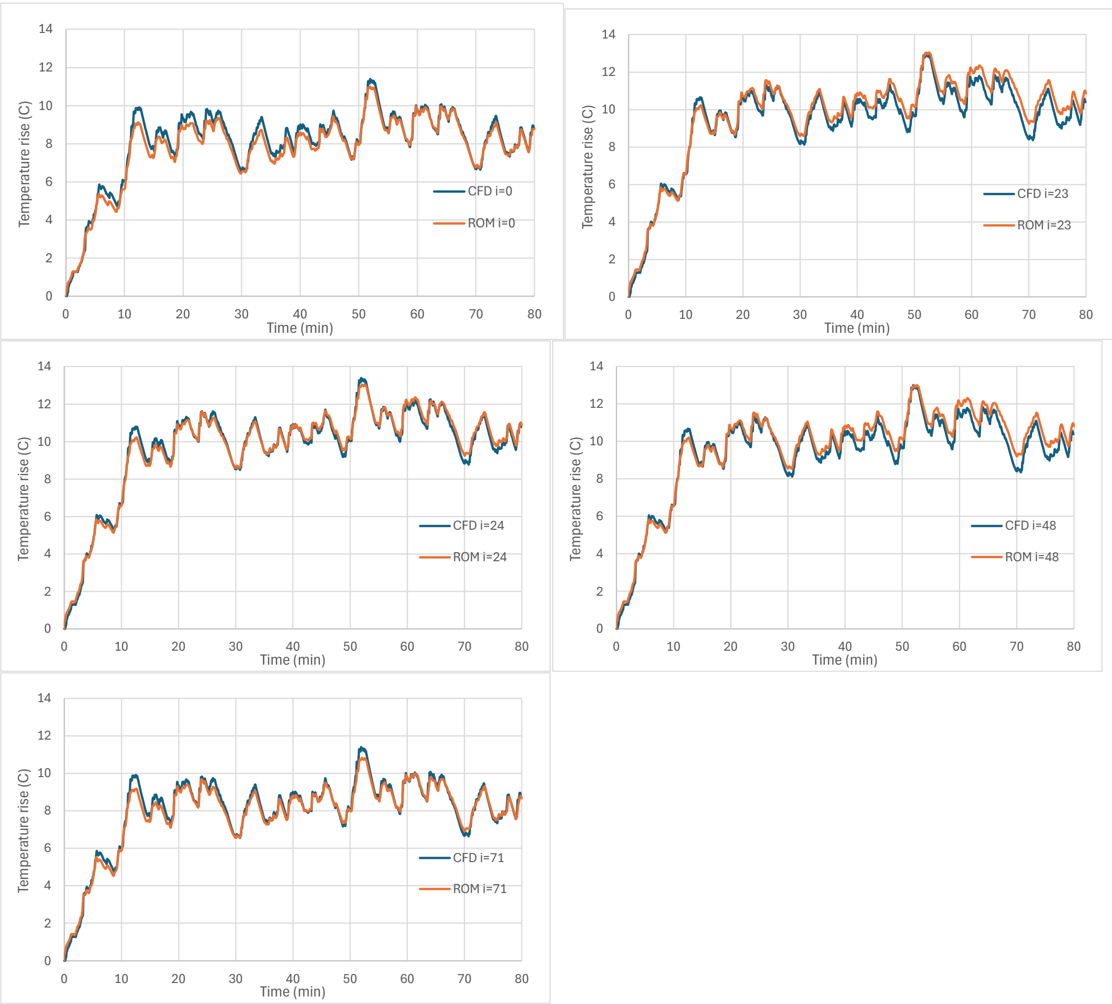

Figure 4: Temperature rise history of selected cells: Comparison of CFD and Reduced Order models for UAC profile assuming constant cell resistance

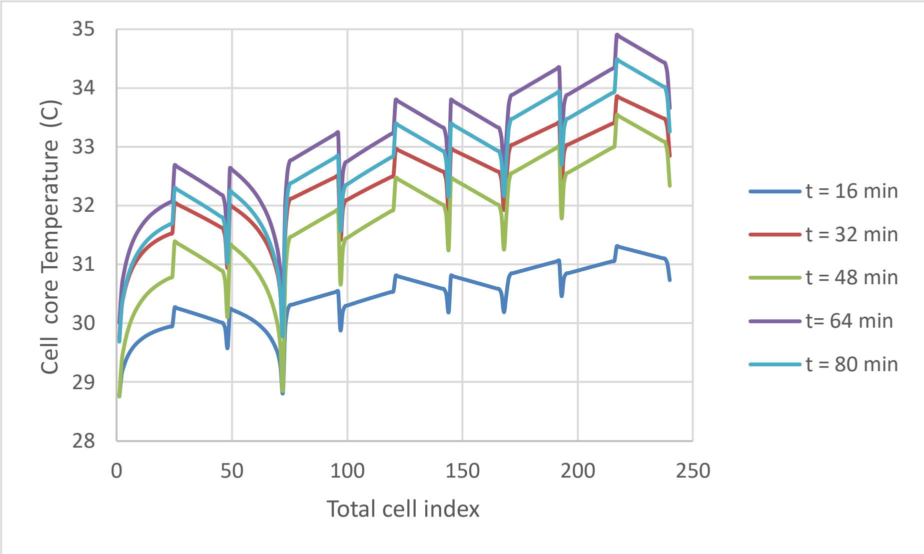

Figure 5: Cell core temperature profiles for 240 cell assembly at different times predicted using the ROM with UAC

The total cell index defined in the previous section is used here. The jumps in the temperature are due the numbering of the cells, as the first column of cells counted from bottom to top ends, the second column starts at bottom and since the coolant fluid in second pass flows from top to bottom, the cell with total index 24 has higher temperature compared to cell with total index of 48. The overall temperature variation in the assembly is around 6 C.

4.2 State of Health and Remaining Useful Life Prediction

The SoH in Table 2 accurately the beta regression model compares with other commonly used models. The results indicate that the model captures the degradation trend effectively, even across diverse usage profiles as seen in Figure 6

Table 3 shows predicted RUL values alongside ground truth RUL the predictions closely match the actual end-of-life points, highlighting the strength of the method in forward-looking battery management. Some key findings include the beta regression model computed prediction accuracy across various cell types and degradation patterns. Feature forecasting added a valuable time dimension, enabling smooth RUL estimations. The model adapts well to noisy and incomplete data, due to its statistical nature and use of engineered features.

In conclusion, the proposed method provides a powerful framework for estimating cell SoH and predicting RUL. This approach is scalable, interpretable, and suited for real-time deployment in smart battery systems.

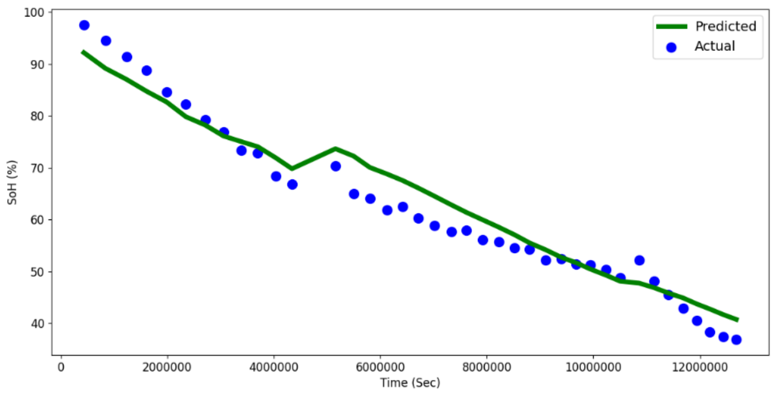

Figure 6: Comparison of predicted SoH with measured SoH for test battery cell RW9

Table 1: Summary of NASA randomized battery dataset

Dataset title	Battery Code	Reference Charge Description	Random Walk Charge Description
Battery Uniform Distribution Charge Discharge DataSet 2Post	RW9, RW10, RW11, RW12	CC charge with 2A till 4.2 V, then CV charge till current drops to 0.01A	Random CC charge with f0.75A, 1.5A, 2.25A, 3A, 3.75A, 4.5Ag. Till battery voltage reaches to 4.2V, or 5 minutes has passed.
1. Battery Uniform Distribution Discharge Room Temp DataSet 2Post	RW3, RW4, RW5, RW6	CC charge with 2A till 4.2 V, then CV charge till current drops to 0.01A	CC charge with 2A till 4.2 V, then CV charge till current drops predefined threshold
2. Battery Uniform Distribution Variable Charge Room Temp DataSet 2Post	RW1, RW2, RW7, RW8	CC charge with 2A till 4.2 V, then CV charge till current drops to 0.01A	Battery is charged for constant interval of time randomly for 0.5 hours, 1 hours, 1.5 hours, 2 hours, 2.5 hours, or charge until full. Additionally, batteries are charged at a 2A current (in CC and then in CV) until either the battery reaches max voltage 4.2V or the charging time exceeds the allotted interval.
3. RW Skewed High 40C DataSet 2Post, 4. RW Skewed High Room Temp DataSet 2Post, 5. RW Skewed Low 40C DataSet 2Post, 6. RW Skewed Low Room Temp DataSet 2Post	RW13-RW28	CC charge with 2A till 4.2 V, then CV charge till current drops to 0.01A	CC charge with 2A till 4.2 V, then CV charge till current drops predefined threshold

Table 2: Comparison of R^2 obtained with different algorithms for battery SoH model

Battery Pack Name	R^2			
	Gamma Regression	Beta Regression	GPR (Matérn Kernel)	Linear Regression
Battery Uniform Distribution Charge Discharge DataSet 2Post	0.825	0.86	0.891	0.873
Battery Uniform Distribution Discharge Room Temp DataSet 2Pos	0.723	0.673	0.771	0.721
Battery Uniform Distribution Variable Charge Room Temp DataSet 2Post	0.873	0.874	0.869	0.879
RW Skewed High 40C DataSet 2Post	0.8	0.7	0.167	0.732
RW Skewed High Room Temp DataSet 2Post	0.75	0.93	0.907	0.859
RW Skewed Low 40C DataSet 2Post	0.736	0.823	0.512	0.757
RW Skewed Low Room Temp DataSet 2Post	0.933	0.947	0.914	0.97
Groupwise Average	0.806	0.830	0.719	0.827

Table 3: Battery RUL model prediction results

Battery Pack Name	Battery Cell No.	Actual life (days)	Predicted End of Life (days)			Comment
			30% Training	50% Training	70% Training	
Battery Uniform Distribution Charge Discharge DataSet 2Post	RW10	145	75	110	117	
Battery Uniform Distribution Discharge Room Temp DataSet 2Pos	RW5	152	109	118	134	
Battery Uniform Distribution Variable Charge Room Temp DataSet 2Post	RW7	148	134	126	148	
RW Skewed High 40C DataSet 2Post	RW27	92	NA	NA	NA	Data within the dataset are insufficient for RUL prediction
RW Skewed High Room Temp DataSet 2Post	RW20	91	NA	NA	NA	Data within the dataset are insufficient for RUL prediction
RW Skewed Low 40C DataSet 2Post	RW21	188	NA	NA	NA	Data within the dataset are insufficient for RUL prediction
RW Skewed Low Room Temp DataSet 2Post	RW14	203	174	160	160	
		$RMSE_{norm}$	0.291	0.209	0.155	

Conclusions

Models are important components of a digital twin system. Two important models for prediction and optimization of battery pack life in electric vehicles, a network thermal model that provides accurate temperature distribution in a battery pack and a feature-based State of Health and Remaining useful Life model for battery capacity degradation are presented in this work. The models were tested with rigorous CFD simulations or with publicly available experimental data. These models will be incorporated as part of a digital twin system of a battery pack for real-time monitoring, optimization and control subsequently.

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Acknowledgements

The authors thank the management of TCS for the financial support and permission to publish this work, and Dr. Harrick Vin, and Dr. Sachin Lodha for their encouragement and support.

Presenter Biography

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Saurabh Desai works as a researcher in TCS research. He has a master's in statistics and a bachelor's in mechanical engineering. He is working on data-based modeling of battery management systems and in digital twins in general. His main interests are in data science and optimization.

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