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Three Dimensional Thermal Modeling of Li-Ion Battery Pack based on Multiphysics and Calorimetric Measurement

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***Abstract*— A three-dimensional multiphysics-based thermal model of a battery pack is presented. The model is intended to demonstrate the cooling mechanism inside the battery pack. Heat transfer (HT) and computational fluid dynamics (CFD) physics are coupled for both time-dependent and steady-state simulation. Inside the battery cells in the pack a lumped value of heat generation (HG), that works as a volumetric heat source, is used. The measured HG stems from the cell level isothermal calorimeter experiment. The batteries inside the pack stay in the same initial thermal state in the simulation case. The pack is simulated to find the temperature gradient over the pack surfaces. Moreover, the temperature evolution results are simulated. It is demonstrated that the developed pack model can provide the thermal spatio-temporal behaviour with great detail. The result helps to understand the thermal behavior of the cells inside a battery pack.**

Keywords— Battery Pack Model, Multiphysics model, surface temperature, temporal and spatial distribution, Isothermal Calorimeter, LTO, thermal management

I. INTRODUCTION

Different operating conditions inside the battery pack invoke different thermal performances. It is due to temperature dependence of heat generation. The thermodynamics of lithium-ion cells are complicated by the presence of liquid electrolyte mixtures as well as single-phase and multiphase solids. Heat generation may result from mixing and phase change, as well as the main electrochemical reactions [1, 2]. Reliable prediction of temperature profiles of individual cells of a battery system as a whole requires first of all accurate and precise measurement of the total heat generation rate. So an isothermal calorimeter can be used for the purpose [3, 4]. Accordingly, measurements of temperature rise and heat dissipation of the battery cells inside the pack are essential. In general, temperature affects several aspects of a battery for instance: operation of the electrochemical system, round trip efficiency, charge acceptance, power and energy capability, reliability, life and life cycle cost, etc. Ref. [5, 6] reported that, although the capacity increases as the operating temperature is raised, the degree of capacity fade also increases, so poor performance is observed at both low and high operating temperature. Also, excessive or uneven temperature rise in a system or pack reduces its cycle life significantly [7]. There are two main problems caused by temperature. The first is that the high temperature during charge and discharge will lead to the possibility that temperatures will exceed permissible levels and decrease the battery performance. Another is that the uneven temperature distribution in the battery pack will lead to a localised deterioration. Thereof, temperature uniformity, within a cell and from cell to cell, is important to achieve the best performance assuring maximum cycle life of cell, pack and system [8]. To circumvent all the problems related to temperature gradient, battery thermal management system (BTMS) can play a significant role to enhance the fidelity of the battery system. BTMS attempts to guarantee that all the cells to retain the same temperature during use. More specifically, the temperatures are kept close to the optimum temperature. Because deviation from this optimal temperature can speed up the accelerated ageing of the cells, the forced cooling is needed in between the cells. It requires a medium to reject the heat produced. It is necessary that proper cooling is secured to prevent the failures in the battery pack. It is a well-established fact that an accurate thermal pack model is a very useful tool to ensure good thermal management. Though the various aspects of performance required from a battery cell regarding power and energy can be assessed experimentally, yet the modelling scheme is used as a complimentary framework. It adds the value of the experimental data since battery modelling is used to explore various thermal and cooling limitations and variations. Using the model, it is possible to develop a BTMS with appropriate specifications and configurations, and it helps to design proper battery system. Numerous modelling methods and techniques are available in the literature to model the non-uniformity of the pack temperature. Moreover, the effectiveness and limitations of these methods are concisely discussed from the thermal behaviour of the investigated cells in different review literature [9, 10].

Knowledge of the multidisciplinary science and engineering is required to model the thermal dynamics of the battery pack. Moreover, there exists a countless amount of configuration of the underlying system and cooling process in both cell and pack setting. So, from a general thermal research point of view, it is a necessity that the modelling method should be coherent and general enough to handle a wide variety of thermal problems inside the battery pack.

In this research, there is an attempt to trace the thermal gradients inside the battery pack using multi-physics finite element modelling (FEM) technique. Section II presents the methodology for this investigation while Section III presents the detailed model. It includes the electro-thermal modelling of the cell, packs specification and configuration as well as underlying theoretical considerations, hypotheses, the mathematical equation framework, FEM modelling steps for instance employed tools and meshing recommendations. The pack model consists of a 3D model that couples the steady state and time dependent heat transfer problem of the battery with the forced convection problem within the heat transfer fluid air inside the pack. The simulation result of the spatio-temporal modelling of the surface temperature is presented in Section IV. It includes the experimental parameterization of the model. The simulation is performed with a focus on the HG and temperature distribution over the surface of the battery cell that has an exposure of cooling fluid air. Then, thermal model predictions are presented and compared with various operating conditions. In the end, the conclusions of the research are presented in Section V.

II. METHODOLOGY

The studied battery pack is made of eight large-size pouch lithium titanate (LTO) cells having the 13Ah nominal capacity. The target is to develop an electro-thermal pack model including cooling phenomena. It integrates the main design parameters of the battery pack (cell dimensions, materials, and corresponding physical parameters, pack dimensions and configurations) and relevant physics (such as heat transfer (HT) and computational fluid dynamics (CFD)). Primarily, the modelling of the pack is composed of three stages. Those are pre-processing, solution of the model, and post-processing stages respectively.

At the pre-processing stage, the battery cell and pack geometry are analysed extensively and generated for further investigation using CAD tools (refer to Fig. 1). The relevant physics dependent parameter values and corresponding operational settings are inserted as an input parameter (refer to TABLE I.). The next is to stipulate relevant physics to the corresponding geometric domains as required.

The research includes steady state and the time-dependent thermal problem of the battery pack. It is solved numerically by considering the heat generation in the battery cell as a bulk heat source. The amount of heat generation (inside LTO cell corresponding to the current rate) is measured by an isothermal calorimeter. All of the cells have the same characteristics. The battery cells in the pack have direct exposure to a uniform and isotropic cooling medium, air, coming from a defined direction. However, the cells inside the pack have anisotropic properties. The initial temperature state between the inlet section of the battery pack remains stable and constant. So, a uniform defined initial temperature is imposed on the corresponding boundaries. When the battery is operational, it suddenly releases a finite and constant quantity of heat energy in the homogeneous cooling fluid air. There is an unobstructed propagation of the heat energy in the longitudinal (x), lateral (y) and normal (z) directions. After that, other essential boundary conditions are introduced. In the next step, it is needed to combine with the laminar fluid flow of the system to integrate the fluid flow with the current heat transfer phenomena. After accomplishing this, the whole domain is broken down into a suitable mesh for resolving through finite element method (FEM) technique using proper meshing, discretization and solver selection steps. The final result is the determination of temperature distribution and the amount of heat generation of the battery cell under both charge and discharge operating conditions. In the post-processing stage, the results are crosschecked with a series of associated outputs i.e. heat generation measurement and surface temperatures of the battery cell.

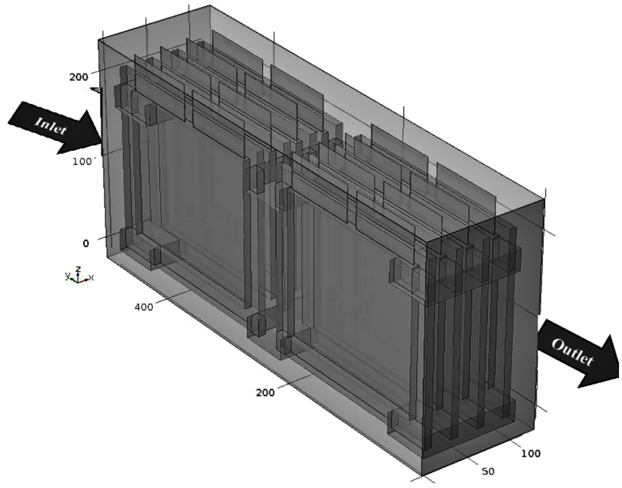

Fig. 1. The pack geometry. The air flows in at inlet portion of the long side of the battery pack, splits into many flows streams as it flows up the passages between the cells and then recombines and flows out the outlet of the battery pack.

III. MODEL

A. *Parameters and Physical Properties*

The battery pack module is composed of eight battery cells having a case, a positive and negative electrode as well as holder casing as presented in [11]. The next step is to introduce and to define the suitable physical properties of the materials of the pack in the different domains of the model (associated with the corresponding pack geometry). The underlying physics of the 3D battery pack model is heat transfer and CFD. Moreover, there are a set of parameters that include the battery materials properties, the external environment, and other influencing conditions as shown in TABLE I. The other relevant electrical and physical properties used in the model are provided in TABLE I. In a steady-state solution to a 3D model, parameters can vary only as a function of position in space (x), space (y), and space (z) coordinates, while in case of time dependent solution there is an addition of time dependence. There is an air flow from one side of the battery, and there is only one outlet available to pass through this air.

Type	Name	Value	Origin of the value
Geometrical Parameters	Outer Rectangle Length of cell	222 [mm]	Measured
	Outer Rectangle Width of cell	214 [mm]	Measured
	Inner Rectangle Length of cell	182 [mm]	Measured
	Inner Rectangle Width of cell	172 [mm]	Measured
	Thin layer thickness	0.5e-3 [m]	Measured
	Thickness of the Battery	7.7 [mm]	Measured
	Thickness of the Electrode Conductor	0.5 [mm]	Measured
	Lateral Distance among the cells	30 [mm]	Measured
	Axial Distance among the cells	250 [mm]	Measured
	Width of the Holder	20 [mm]	Measured
	Depth of the Holder	70 [mm]	Measured
	Height of the Holder	25 [mm]	Measured
	Elevation of the holder on longitudinal Direction	-5 [mm]	Measured
	Elevation of the holder on lateral Direction	-5 [mm]	Measured
	Elevation of the holder on normal Direction	-5 [mm]	Measured
	Fluid Width of the outer domain Box	40 [mm]	Measured
	Fluid Depth of the outer domain Box	250 [mm]	Measured
	Fluid Height of the outer domain Box	260 [mm]	Measured
	Clearance of the longitudinal edge of the outer domain fluidbox	-15 [mm]	Measured
	Clearance of the lateral edge of the outer domain fluidbox	-15 [mm]	Measured
	Clearance of the normal edge of the outer domain fluidbox	-15 [mm]	Measured
Pack Parameters	Number of cells in a row	4	Measured
	Number of cells in a column	2	Measured
Battery electrode Physical	Positive Electrode Width	82 [mm]	Measured
	Positive Electrode Length	42 [mm]	Measured
	Negative Electrode Width	82 [mm]	Measured
	Positive Electrode Length	42 [mm]	Measured
Battery Physical Parameters	Density of Battery	2700 [kg/(m^3)]	Reference [12]
	Heat Capacity of Battery	860 [J/(kg*K)]	Reference [12]
	Heat Source Magnitude	1536 [mW]	As Measured in calorimeter
	Thermal Conductivity in longitudinal direction	30 [$Wm^{-1}K^{-1}$]	Reference [12]
	Thermal Conductivity in lateral direction	30 [$Wm^{-1}K^{-1}$]	Reference [12]
	Thermal Conductivity in normal direction	0.16 [$Wm^{-1}K^{-1}$]	Reference [12]
Battery case Physical Parameters	Case Heat capacity at constant pressure	678 [J/(kg*K)]	Multiphysics Library
	Case Density	2320 [kg/(m^3)]	Multiphysics Library
	Case Thermal Conductivity	155 [$Wm^{-1}K^{-1}$]	Multiphysics Library

TABLE I. PARAMETER LIST USED FOR THE THREE-DIMENSIONAL MODELLING OF THE BATTERY CELL(NEGATIVE VALUE MEANS EXTRUDING OUT OF SURFACE)

Type	Name	Value	Origin of the value
Holder casing Physical Parameters	Holder Casing Heat capacity at constant pressure	893 [J/(kg*K)]	Multiphysics Library
	Holder Casing Density	2730 [kg/(m^3)]	Multiphysics Library
	Holder Casing Thermal Conductivity	155 [$Wm^{-1}K^{-1}$]	Multiphysics Library
Positive Electrode Physical Parameters	Positive Electrode Heat capacity at constant pressure	385 [J/(kg*K)]	Multiphysics Library
	Positive Electrode Density	8700 [kg/(m^3)]	Multiphysics Library
	Holder Casing Thermal Conductivity	400 [$Wm^{-1}K^{-1}$]	Multiphysics Library
Negative Electrode Physical Parameters	Negative Electrode Heat capacity at constant pressure	900 [J/(kg*K)]	Multiphysics Library
	Negative Electrode Density	238 [kg/(m^3)]	Multiphysics Library
	Negative Electrode Thermal Conductivity	2700 [$Wm^{-1}K^{-1}$]	Multiphysics Library
Air Physical Parameters	Air Heat capacity at constant pressure	1005 [J/(kg*K)]	Multiphysics Library
	Air Density	1.125 [kg/(m^3)]	Multiphysics Library
	Air Thermal Conductivity	0.0271 [$Wm^{-1}K^{-1}$]	Multiphysics Library
Environmental Parameters	Pressure	1 [atm]	Assumed
	Maximum Velocity	1 [m/s]	Assumed
	Initial Temperature	27+273.16 [K]	Measured
	External Temperature	27+273.16 [K]	Measured

B. Assumptions and Boundary conditions

The coupled boundary conditions as provided satisfy the continuity of temperature at the boundary line for the interface between battery cell surface, airflow channels and associated peripherals. It is accomplished by the coupling of the conductive heat transport toward the cell array surface with corresponding heat transport by convection by the surrounding domains. The same coupling is defined for both terminals on the Li-ion cell. This model only considers transport of heat by conduction inside the battery and forced convection for the cooling medium air. This is a simplification of the thermal effects inside a pack setting, for instance, other heat sources can be present such as heat emitted from cabin heating system, heat generation from power electronics and peripherals, etc. [13, 14].

The following additional significant assumptions are used to reach a solution. Those are categorised according to physics:

1) Heat Transfer Assumptions

The thermal properties of the fluid and battery pack elements are homogeneous. So those remain constant unless stated otherwise. There is negligible radiative energy transfer, and it is not accounted for. Forced convection is the dominant process for heat transfer from the battery terminal surfaces. An average specific heat for the cell is employed in the simulation in steady state and time dependent situation as the approximation of real life measurement. It is assumed that the battery cells inside the pack are a non-uniform and anisotropic medium with different thermal conductivity in each coordinate direction as shown in TABLE I.

In this study, different values for the volumetric heat generation are considered as measured by a calorimeter for the battery cell. These are the only heat generation sources that come from the Li-ion cells. The generated heat of the cells is spatially uniform inside the battery domain.

C. CFD Assumptions

The flow of incompressible heat transfer fluid air is assumed as laminar flow. The normal stress at the inlet of the system is determined from the flow conditions at the entrance to a fictitious channel of length one meter appended to the boundary.

D. Mathematical description of the model

The thermal pack model is developed by setting up a generic energy balance equation that accounts for accumulated, conducted and generated local heats of the battery cell array and the cooling process of the cooling medium air as described by [13-16].

Thermal models describe the thermal behavior regarding heating of the battery cells inside the pack and those are built on the energy conservation of the whole system as follows in Eqn. (1)

$$\rho C_p \frac{\partial T}{\partial t} = k\nabla^2 T + Q \qquad (1)$$

where, T —temperature of the system domain, ρ—density of the system component, C_p—specific heat capacity, k — thermal conductivity and Q — the heat generation amount having a volumetric heat source.

In this modelling framework, the macroscopic geometrical unit of the pack is the battery cell. This battery cell is divided primarily into three domains: electrode, tab (positive and negative) and casing (Refer to [11]). As different domains are made up of different material attributes are associated with corresponding physics. Thus, Equations for the three respective domains are presented in Eqn. (1).

The CFD equations are presented in Eqn.(2) and Eqn.(3):

$$\frac{\partial u}{\partial t} + \rho(u.\nabla)u = \nabla.(-\mathrm{pI} + \mu(\nabla u + (\nabla u)^T)) \qquad (2)$$

$$\rho\nabla.(u) = 0, \qquad (3)$$

where

ρ is the density.

u is the velocity vector.

The finite element method (FEM) is employed in this study to discretize the governing equations. Depending on the level of the modelling, these modelling equations are applied to the separate domains of the battery pack.

E. Meshing, Discretization, and Solver selection

To achieve the appropriate results from a simulation, it is required to accomplish the diverse type of procedures as required for FEM, for instance, mesh generation, discretization, and selection of proper solvers. To address these issues, Comsol® Multiphysics™ software environment is used. Boundary layers are employed since there is a high-velocity gradient at the interface between the battery pack surface and the cooling medium and it is important for the heat transfer calculation between the pack and the cooling medium air. A swept mesh is employed. Mesh sweeping operates on the 3D pack domain by first meshing a source face of the battery. Then it sweeps the resulting pack surface mesh through the domain to an opposite destination surface. All the surfaces that encompass the planes of the battery pack are classified as either source surfaces or a destination surface or linking surfaces. The linking surfaces of the battery are the faces that connect the source and destination surfaces. So, the sources for the swept mesh consist of several surfaces. Additionally, for solving the governing equations, the geometric multigrid solver is employed. It accelerates the convergence of the iterative solver by solving the FEM problem on a series of meshes rather than a single one. The multigrid algorithm starts with the initial physics controlled mesh and automatically builds a series of coarser meshes. The process is repeated until the coarsest mesh leads to a low enough number of degrees of freedom to reach in the desired solution using the direct solver.

IV. Results and discussion

A. Temperature Spatial Distribution and Influence of the Cooling

The numerical results of the three-dimensional battery pack model can exhibit the heating behavior inside a pack with a good resolution. Fig. 2 illustrates the distributions of the temperature over the pack. The non-uniform heat generation and propagation are observed. At the end of the 4C discharges, the highest temperatures are reached (Fig. 2 and Fig. 3). It is due to the increase in the heat generation inside the cells. At the end of the discharge, it indicates lower temperatures (around 27°C) at the front near the inlet and higher temperatures (around 43°C) at the rear of the module (Fig. 2 and Fig. 3). Therefore, the figure emphasises the need for a sufficient inlet air velocity for a proper thermal management of the cells located in the module. Therefore, thermal management is vital to avoid large temperature gradients surrounding the cells. This is especially important during the high C-rate discharge and charge condition of the module. Since those certainly, exhibit higher gradient and high amount of heat generation. Then the temperature gradient within this particular cell increases with higher current. The rationale of the phenomena is that the temperature gradient causes portions of the cell to generate more current (electrochemically reaction rate is increased). This causes these hotter sections to increase further in temperature for the adjacent cells inside a pack. So this positive current temperature feedback can be countered by airflow that flows from the inlet. The impact of the cell-to-cell temperature balance within packs can be found.

On the contrary to the empirical modelling approaches, the presented physics-based pack model can provide detailed information for the states of a battery due to the inherent detail level. Even if the high rate charging takes place only for a short part of the life time of a battery inside the pack, the developed thermal gradients imposed can be lowered with the right selection of carrier fluid velocity to keep the thermal states in a controllable manner. Higher gradient scenarios can be avoided by taking preventive action increasing safety and reliability in the desired application.

B. Time-dependent result

A time-dependent model is constructed using the same methodology to investigate transient behaviour. The model is simulated for 4C discharge case, and the initial thermal states are same as the steady state case. The temporal battery temperature distribution of the battery pack is revealed in Fig. 4. Variations in temperature profiles are observed during continuous discharge at 4C current rate. When heat is generated inside the battery pack, internal temperature gradients will necessarily develop with time.

Considering cooling the battery with air, an ambient maximum temperature levels around the battery of around 34-35°C is likely in this current rate with the given cooling. Hence, the battery temperature is manageable with higher velocity. Fig. 4 shows modelled spatio-temporal temperature profiles. Deploying the given model along with the associated parameters coupled with the relevant physics some insight of the thermal gradient evolution is found. Subsequently, a proper cooling mechanism can help to avoid unwanted temperature state condition.

The result of the multiphysics simulation research may enable the battery producers and application developers to simulate the thermal condition without building the prototype, so it helps to save both money and time. Moreover,it helps to determine the answer whether given battery system is employed with enough cooling for the desired application. Evaluating thermal management of batteries in the light of the developed modelling framework will lead to the verifiable and decisive conclusion that the method of cooling and different configurations of the battery pack that provides the best performance. Since it provides the improved understanding of heat distribution inside a battery cell surface, the result can be used to determine the best possible or optimal cooling requirement for a battery system.

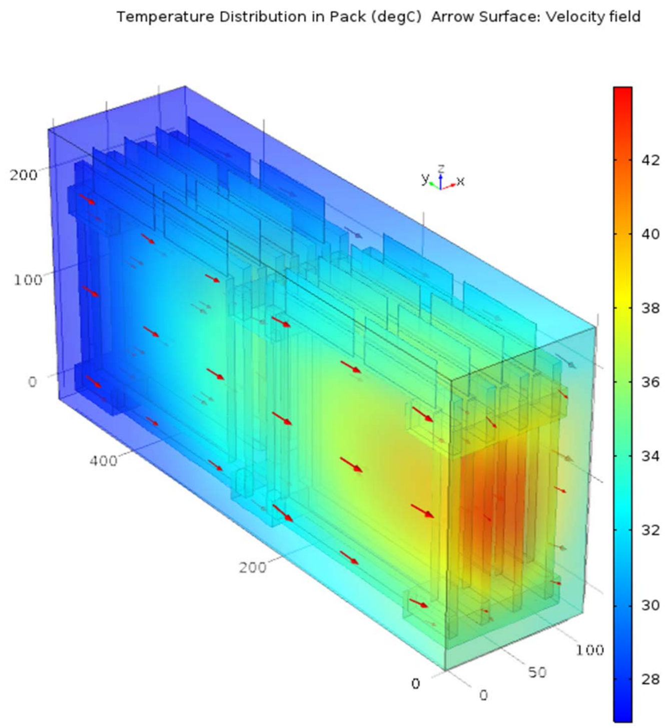

Fig. 2. The temperature distribution of the pack on 4C charge and discharge. There is a visible cooling effect near inlet due to the cooling fluid flow (showing less temperature) and the opposite is true near the outlet.

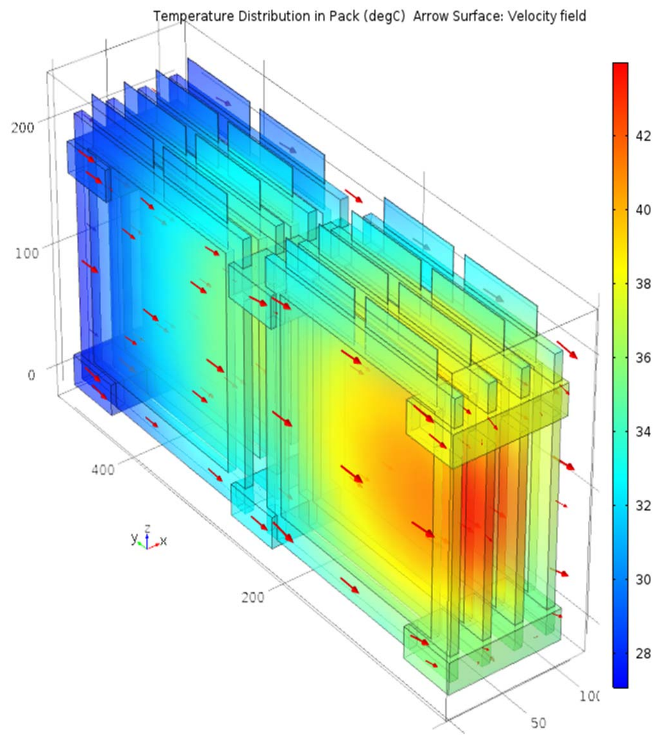

Fig. 3. The close up look on the temperature gradient of the cells.

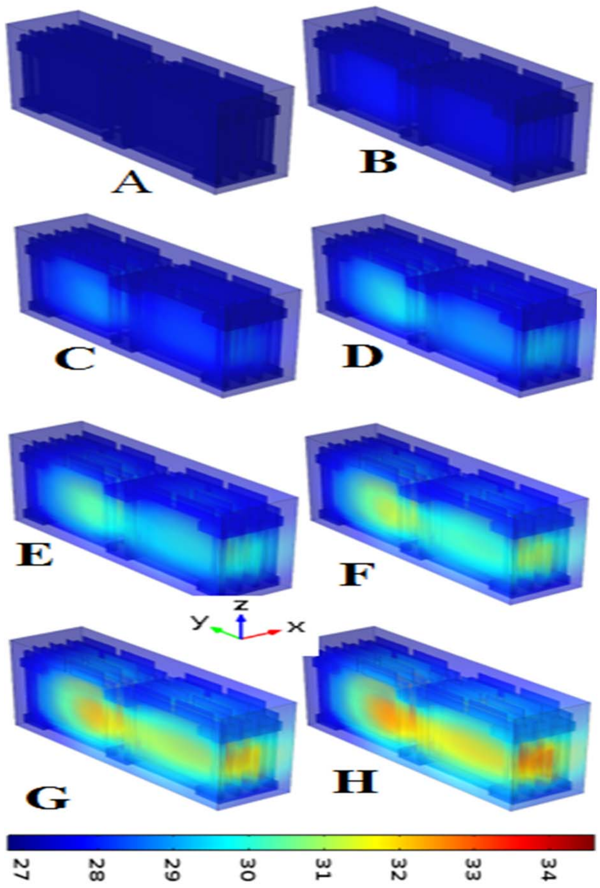

Fig. 4. Transient simulation results of the battery pack with a cell with 4C discharge in alphabetic caption order.There is a significant temperature gradient with the time evolution.[A]0 sec [B]1 min 52 Sec [C] 3 min 44 Sec [D] 5 min 36 Sec [E] 7 min 28 Sec [F] 9 min 20 Sec [G] 11 min 20 Sec [H] 15 min .

V. CONCLUSION AND FUTURE WORK

The investigation has successfully detected the impacts of the cell-to-cell temperature gradients within packs. It can show the impact of heat generation, eventually to track the temperature gradient among the battery cells inside the pack. The modelling method provides the spatial temperature distribution over the surfaces of the battery pack. Besides the time-dependent model provides the temperature evolution over the surface of the pack. Moreover, it gives the significant confirmation of the well-known fact that the thermal performance and the dissipation measures can provide a proper thermal management design inside a battery pack. The temperature gradient within a particular cell increases with higher current. This temperature gradient causes portions of the cell to generate more current, which causes these hotter sections to increase further in temperature for the adjacent cells inside the pack. So this positive current temperature feedback can be countered by appropriate cooling mechanism. The modelling of the pack can be considered as a building block or a unit for a battery system inside an electric vehicle.

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