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Optimal Design of Battery Storage Systems for RES Using Simulation Methods

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Abstract: The use of battery storage systems (BSS) is an increasingly common topic in the context of the operation of various types of renewable energy sources (RES). One of the applications may be to solve the problem of energy-free operation of small hydropower plants, where quite specific requirements are placed on the design of the BSS. In the context of optimal BSS design for a given application, this paper discusses the computer analysis capabilities that are essential in the design and performance verification phase of a BSS. The paper presents the possibilities of simulation methods in the field of electrical analysis of cell current load during charging and discharging processes, thermal analysis related to the selection of a suitable cooling system with respect to the operating mode of the battery system.

Keywords: Battery storage system, renewable energy sources, lithium-ion battery, battery thermal management system, optimization, CFD simulation

1 Introduction

During the operation of renewable energy sources (RES) various situations arise when energy storage is required, at least for a short period of time. For example, when using solar energy, its availability during 24 hours a day needs to be dealt, where battery storage system (BSS) is an ideal solution. In the operation of a small hydropower plants the power grid may fail for various reasons. This means a sudden disconnection of the electric generator. The relieved turbine (no load from the generator) is then spun up to runaway speed and has to be shut down in an emergency. This is so-called energy-free operation and it is an undesirable condition where the structure is overstressed. In some locations, such outages happen more frequently and can last from a few minutes to several hours. The energy-free operation problem can be solved by using a battery storage system - the battery modules will be charging at the time of disconnection from the grid. Such a BSS is ideal for the use of "second-life" batteries. These are lithium-ion batteries retired from use in electric vehicles, which are reused in industry after the regeneration process.

BSSs are composed of battery packs, which are made up of an array of lithium-ion cells. Lithium-ion batteries (LIB) store a certain amount of electrical energy and generate a significant amount of heat during the charging and discharging processes. The heat generated by lithium-ion batteries is divided into two main components, the heat generated by reversible reactions q_{re} and the heat generated by irreversible reactions q_{irr}. The heat generated by

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irreversible reactions is directly related to the discharge rate of the batteries, i.e. the amount of so-called irreversible heat is higher the higher the discharge rate, while the amount of heat generated by reversible reactions is predominant at lower discharge rates. The total heat generated by the battery can be determined by equation (1) [1].

$$q_{tot} = q_{re} + q_{irr} \tag{1}$$

The reversible heat generation is related to the entropy change during charging and discharging due to the intercalation and deintercalation processes at the electrodes. The entropy changes at the electrodes depend on the electrode materials and the state of charge. The state of charge (SOC) is known to be a factor that has a large influence on reversible heat generation. The calculation of the amount of heat generated by reversible reactions is described in equations (2) and (3) [1]:

$$q_{re} = S_{(a,i)} j_{(loc,i)} \frac{T\Delta S}{n \cdot F} \tag{2}$$

$$\Delta S = n \cdot F \frac{\delta U_i}{\delta T} \tag{3}$$

where $S_{a,i}$ is the specific surface area (m^{-1}), $j_{loc,i}$ is the local current density (Am^{-2}), ΔS is the entropic change, U_i is the breakdown voltage, which describes the equilibrium potential of the electrodes as a function of SOC, F is the Faraday constant $(F = 96487 Cmol^{-1}), n$ is the number of electron moles [1].

Irreversible heat generation is divided into two categories, Joule heat generation, which occurs due to the internal resistance of the battery, and polarization heat generation due to the electrochemical reaction that occurs during the charging and discharging process. The irreversible heat is calculated according to equation (4) [1].

$$q_{irr} = q_p + q_j \tag{4}$$

The generation of polarization heat is calculated according to the following equation (5).

$$q_p = S_{(a,i)} \cdot j_{(loc,i)} \left(\varphi_{(1,i)} - \varphi_{(2,i)} - U_i\right) \tag{5}$$

U_i is the breakdown voltage, which describes the equilibrium potential of the electrodes as a function of SOC. Since temperature influences the battery discharge process, it is necessary to include the so-called Taylor expansion at the reference temperature in the equation (6) [1].

$$U_i = U_{ref,i} + \left(T - T_{ref}\right) \frac{dU_i}{dT} \tag{6}$$

Joule heat generation in battery cells is based on three different factors, the resistance of the material, the movement of ions through the electrolyte and the heat generated through the collector. Joule heat can be calculated using equation (7) [1].

$$q_j = I^2 R \tag{7}$$

where I is the discharge current and R is the internal resistance of the cell. The above equation shows that the magnitude of the discharge current affects the amount of heat generated quadratically [1].

2 Problems in LIB operation

During the charging and discharging processes of LIB batteries, a certain amount of heat is generated due to electrochemical reactions. If the generated heat is not transferred properly, conditions unfavourable to LIB batteries may occur.

2.1 Impact of high temperatures

Due to the high temperature of the cell, loss of capacitance and reduction of operating voltage may occur. A large amount of heat is generated at elevated operating values, such as a cell operating at a high discharge rate. Capacity loss occurs when the active material inside the battery is converted to inactive material. Due to raised temperatures, the internal impedance of the cell will increase, which will reduce the operating voltage at different discharge rates. The capacity of a lithium-ion cell depends on the cell temperature. LIB have an optimum operating temperature range set by the manufacturers, usually 15-35 °C. Operating battery cells outside this range can have several negative effects on capacity and lifetime (Fig. 1.) [2].

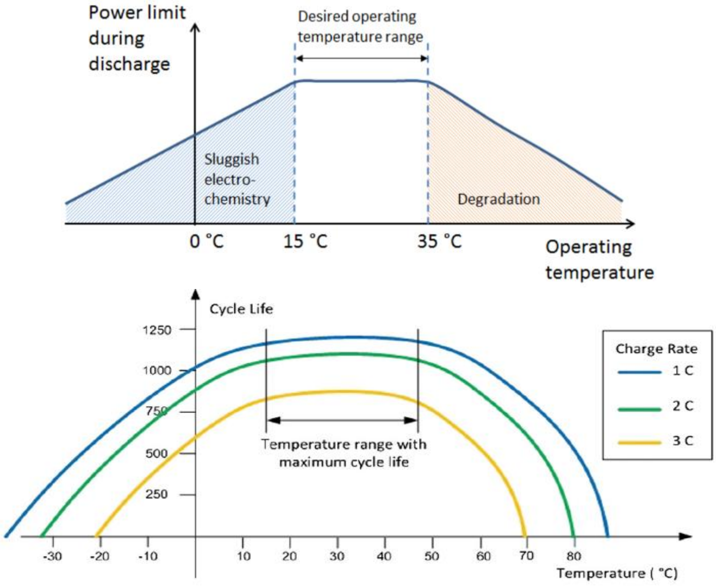

Fig. 1. Optimal operating temperature of the cell in terms of its performance during the discharge process (up) and in terms of lifetime at different discharge currents (down) [1].

2.2 Thermal Runaway (TR)

TR of lithium-ion cells can be initiated for various reasons such as internal short circuit, overheating, overcharging or over-discharging. These reasons cause the temperature of the cells to rise further and trigger chemical reactions that lead to even faster temperature rise of the cells. TR is a sequence of reactions that results in irreversible damage to the battery cell or its surroundings; a violent exothermic reaction can end in an explosion and a fire that is difficult to extinguish (Fig. 2.) [2].

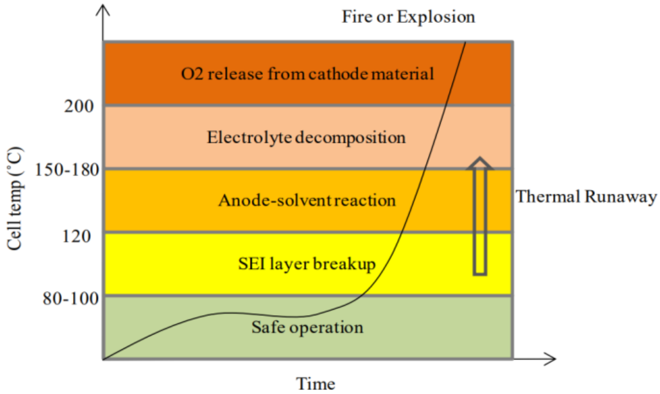

Fig. 2. Thermal Runaway [2].

2.3 Temperature maldistribution

If the charging or discharging rate is increased, more heat will be generated in the cells. If this heat is not properly dissipated, it will concentrate inside the battery cells. In addition, heat transfer by convection takes place only on the outer surfaces of the battery units. This will result in uneven temperature distribution inside the battery packs. As mentioned in the previous section, the performance of a cell is dependent on its temperature. This means that sustained inappropriate temperature distribution will lead to variability in capacity between cells. This will create a chain reaction where cells with a suitable operating temperature are forced to deliver higher power to compensate for cells with lower power, which in itself leads again to an increase in the temperature of the more stressed cells. In addition, lithium cells have a low tolerance to overcharging, so the total capacity of the batteries when charged is limited to the cell with the lowest power output. In principle, it states that the max. allowable temperature variation between cells in a battery module should be less than 5 °C [2]. Based on the above problems, it is necessary to ensure sufficient cooling of the battery system. Due to the large number of cooling system concepts and the resulting cooling system parameters, the cooling design of the BSS needs to be solved at the conceptual and design stage.

3 LIB cooling options

Several types of different cooling system concepts are used to cool the BSS (Fig. 3.).

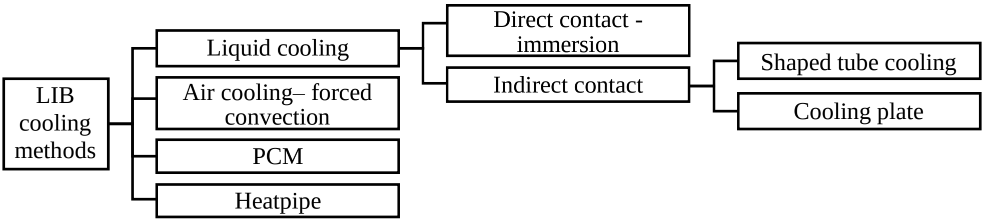

Fig. 3. Cooling systems used for LIB batteries.

3.1 Liquid cooling with direct contact

In this method, the coolant is "forced" to flow through the battery module and dissipate the heat generated, as shown schematically in Fig. 4. If the battery module is directly immersed in the coolant, the coolant must have dielectric properties. The heated fluid is then cooled by a heat exchanger. This method is preferable to forced air cooling due to the higher heat capacity and thermal conductivity of the coolant. There is no need for an additional cooling system to dissipate heat even at high discharge or charge rates (C-rate) [3], [6].

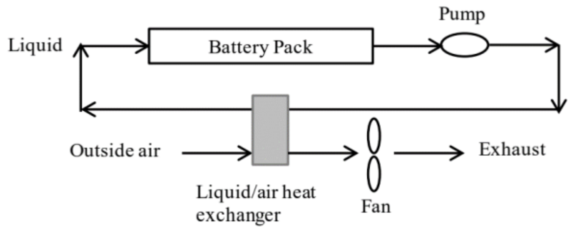

Fig. 4. Liquid cooling system with direct contact [2].

3.2 Liquid cooling with indirect contact with a shaped tube

In this indirect cooling method, ethylene glycol most often acts as the cooling medium. Between the individual battery cells, a shaped tube is placed. The heat from the battery is transferred into the tube material and then by convection into the coolant. Many automotive companies use a method of indirect cooling using so-called shape tubes. The coolant is cooled back either by a compressor cooling circuit or by a heat exchanger [3], [6].

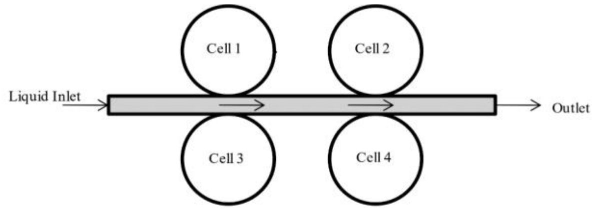

Fig. 5. Liquid cooling system with indirect contact - shaped tube [2].

3.3 Liquid cooling with indirect contact with the cooling plate

In this method of cooling the battery cells, a plate with coolant flowing from one end of the battery pack to the other is placed under the battery in the case of cylindrical cells (Fig. 6.). The heat from the battery is transferred to the plate material, then the coolant in the plate channels removes heat due to convection. The cooling method shows poor performance in terms of temperature distribution within a single cell (applies exclusively to cylindrical cells). However, the temperature distribution within the battery module is relatively uniform. Many automotive companies use this method of cooling batteries by means of so-called cooling plates, but mainly for flat or prismatic cells, where the contact area between the cell and the exchanger plate is many times larger compared to the cylindrical cell type [3], [6].

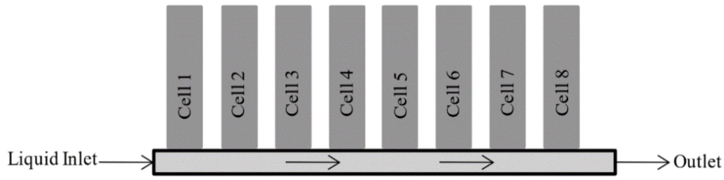

Fig. 6. Liquid cooling system with indirect contact - cooling plate [2].

3.4 Air cooling with forced convection

In this method, air is forced to flow through the battery pack and dissipate the heat generated, as shown in Fig. 7. The air cooling system is mostly used in hybrid cars such as the Toyota Prius and Nissan Leaf. The air-cooled battery cooling system is widely used due to its simple design, high reliability and low acquisition cost. However, the low heat capacity and low thermal conductivity of air may not be suitable for high performance applications.

For forced convection, a fan or blower is required to extract the heated air to the outside and draw in the cold air. Due to the lower thermal capacity and conductivity, higher temperature differences may occur between the individual cells in the battery module. As a disadvantage, it is also necessary to mention a certain noise level of the air-cooled system [3], [4], [5].

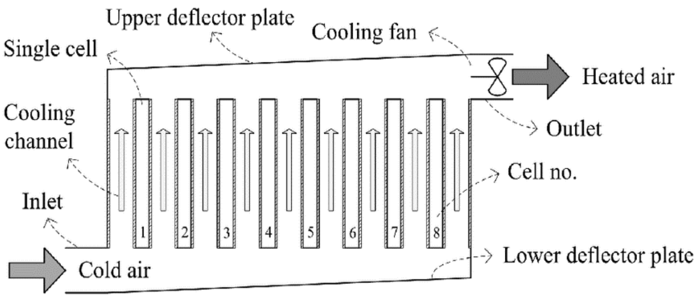

Fig. 7. Air cooling system - forced convection [5].

3.5 Heatpipe cooling system

Heatpipe is a self-acting device designed for heat transfer, combining the principles of thermal conduction and phase transition for efficient heat transfer between two solid surface interfaces. The main parts of the Heatpipe device are: the evaporator side (hot side), the condenser side (cold side), the porous material and the working fluid. The body is usually copper or aluminium. The operating temperature range is approximately 25° to 150 °C. Based on the application, the working fluid is suitably selected, typically water, acetone or liquid butane is used. The heatpipe is usually placed between the battery cells as shown in Fig. 8. The hot side of the Heatpipe is attached to the battery from which it extracts heat. The other (cold) side of the Heatpipe is placed outside the battery so that it can be cooled. The working fluid removes heat on the battery side (hot side) while evaporating. Due to the increase in static pressure, the vapour passes to the cold side where it condenses. The condensate leaks spontaneously back to the hot side through the porous material, due to its own viscosity, pressure differences and possible gravity [5], [7], [8].

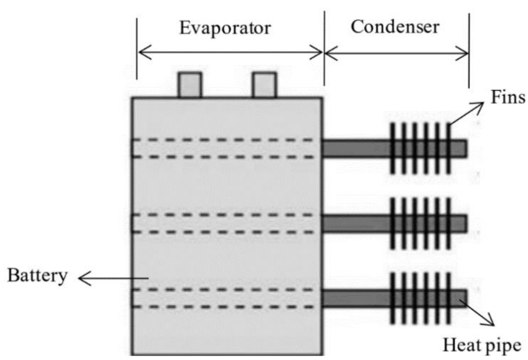

Fig. 8. Heatpipe cooling system [2].

3.6 PCM cooling

PCM is a material that accumulates or transfers heat through a phase change process from one state to another at a specific temperature. Phase change materials used for cooling are divided into organic (paraffin wax), inorganic and eutectic compounds. PCM materials are often mixed with graphite powder, metal foam and carbon fibre to improve the thermal conductivity of the resulting composite. This cooling system often requires an additional system to remove heat from the PCM material [7], [8].

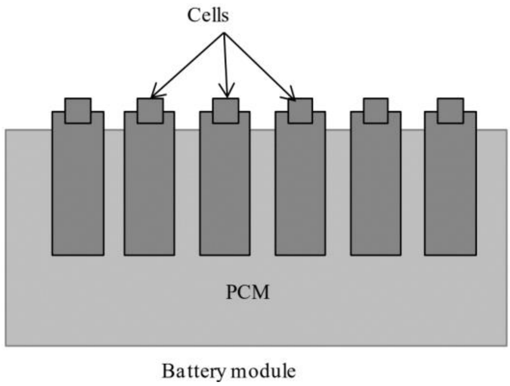

Fig. 9. PCM cooling system [2].

Both the suitability of the individual systems must be assessed in terms of operation, design and other requirements, and the specific cooling system must be optimised (in terms of geometry, shape, dimensions, etc.). The above tasks can be solved with the application of CFD methods. In general, it can be stated that CFD simulation of a BSS can be used to calculate the temperature of cells and other components of the battery pack and to assess the safety of operation with respect to the maximum temperature. The importance of CFD methods in BSS design can be divided into several groups:

1. deciding or assessing the suitability of specific types of cooling systems,
2. selection of suitable materials for construction,
3. sizing, i.e. shape and dimension optimization of the battery system.

A properly constructed and tuned CFD model should be characterised by or take into account the following attributes:

1. Geometry of the whole pack (multiple packs with which the coolant flow channels).
2. Heat generation inside the battery cells (due to electrochemical reactions, Joule heat, etc.) during charging/discharging.
3. Conduction of heat through the solid walls of cells, modules, packs, etc.
4. Heat transfer between solid walls and coolant.
5. Coolant flow and heat transfer in coolant.
6. Heat transfer to the surroundings.
7. Results should include coolant flow rate distributions and temperature distributions throughout the pack space (evolution over time to be calculated).

4 Numerical modelling capabilities of LIB cells in ANSYS Fluent

ANSYS Fluent has implemented several different methods for simulating physical processes in LIB batteries (including cooling modelling). Since cooling simulations of battery modules are a rather challenging, essentially multi-physics task, the CFD setup will be built sequentially from the simplest cases (heat transfer on the surface of a single cell without modelling coolant flow) to complex tasks (cooling of the whole pack with coolant flow). Some approaches for modelling heat generation in cells or for modelling electro-thermal phenomena (Conjugate Heat Transfer, Ciruit Networ Method, Multi Scale Multi-Dimensional approach) as well as some sub-models related to the modelling of electro-chemical phenomena (Equivalent Circuit Model, NTGK model, etc.) will be tested step by step. Several ways of defining boundary conditions (mainly related to the calculation of heat transfer to the surroundings) will also be tested. Experimentally determined discharge characteristics will be applied in the calculations.

The aim will be to firstly debug the different approaches to CFD simulation and then (based on comparison with experimental results) to select the optimal approach for modelling the above phenomena. The final simulation model will be used to calculate the heat transfer and temperature distribution on the surface of the batteries or the cooled battery system during battery discharge. At the same time it will serve as a tool for the development of the cooling device of the developed battery system and for the shape-dimensional optimization of some structural parts of the system. A detailed description and individual electro-thermal models and electro-chemical sub-models and their equations can be found in literature sources [9], [10] and [11].

5 Numerical modelling options – summary

The following Tables 1, 2 and 3 provide examples of the basics of setting up a CFD for a proper battery solution from an electrical, thermal and cooling perspective.

Table 1. CFD simulation on a single battery cell (least complex approach).

Access to simulation	**Calculation of 1 battery cell**		
	Conjugate Heat Transfer Model (CHT)	Circuit Network + Equivalent Circuit Model	MSMD + Equivalent Circuit Model
Simulated physical processes	Heat generation (fixed heat output), Joule heat generation in the passive zone, heat conduction through the solid cell material, heat transfer by convection to the surroundings	Heat generation (ECM method - takes into account electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, heat transfer by convection to the surroundings	Heat generation (ECM method - takes into account electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, heat transfer by convection to the surroundings
Equations describing given processes	Energy equation, "User scalar 0"	Energy equation, ECM equations	Energy equation, ECM equations
Outputs monitored	Temperature of the cell	Temperature of the cell	Temperature of the cell

Table 2. CFD simulation on multiple connected battery cells.

Access to simulation	**Calculation of multiple connected battery cells**			
	Circuit Network + Equivalent Circuit Model	Circuit Network + NTGK Model	Circuit Network + Equivalent Circuit Model + Coolant Flow	Circuit Network + NTGK Model + Coolant Flow

Simulated physical processes	Heat generation (ECM method - takes into account electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through a solid cell material, heat transfer by convection to the surroundings	Heat generation (NTGK method - takes into account the electro-chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, heat transfer by convection to the surroundings, capacity drop as a function of temperature	Heat generation (ECM method - takes into account the electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, coolant flow with turbulen-ce, heat transfer by convection into the coolant, heat transfer in the coolant and ambient heat transfer	Heat generation (NTGK method - takes into account the electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, coolant flow with turbulence, heat transfer by convection into the coolant, heat transfer in the coolant and ambient heat transfer
Equations describing given processes	Energy equation, ECM equations	Energy equation, NTGK equation	Continuity equation, N-S equations, turbulence model equations, energy equation, ECM equations	Continuity equation, N-S equations, turbulence model equations, energy equation, NTGK equations
Outputs monitored	Temperature of the cell	Temperature of the cell	Temperature of the cell	Temperature of the cell

Table 3. CFD simulation on the whole battery module (pack).

Access to simulation	**Calculation of the whole module (pack)**	
	Circuit Network + Equivalent Circuit Model + Coolant Flow	Circuit Network + NTGK Model + Coolant Flow
Simulated physical processes	Heat generation (ECM method - takes into account the electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, coolant flow with turbulence, heat transfer by convection into the coolant, heat transfer in the coolant and ambient heat transfer	Heat generation (NTGK method - takes into account the electrical - chemical reactions), Joule heat generation in the passive zone, heat conduction through the solid cell material, coolant flow with turbulence, heat transfer by convection into the coolant, heat transfer in the coolant and ambient heat transfer
Equations describing given processes	Continuity equation, N-S equations, turbulence model equations, energy equation, ECM equations	Continuity equation, N-S equations, turbulence model equations, energy equation, NTGK equations
Monitored outcomes	Temperature of the cell	Temperature of the cell

6 Conclusion

The paper describes a CFD approach to optimize the proposed BSS cooling system, which will be verified in the near future on a physical model of the battery module from which the BSS is formed, as high agreement between simulation and measurement results is a prerequisite. Initially, the simulations of the electrochemical processes that take place in the cells in the context of heat generation will be debugged, under different discharge and charging conditions. Subsequently, the numerical model will be extended to include the battery module and the cooling system, possibly a part of it, resulting in a rather complex multiphysics numerical model. For the CFD calculations, ANSYS Fluent simulation software will be used. The results of the research will later be applied for the complex design of the cooling system, which is a key part of the BSS.

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