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Extended summary

Knowledge-based approaches to support the design and development of the electrochemical storage systems

Scuola di Dottorato di Ricerca in Scienze dell'Ingegneria
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Abstract.

The need to shorten the "time-to-market" is the prerogative of all companies that operate in different industry sectors, in order to carve out a profitable position in the market against competitors. The design process has focused primarily on reducing costs, reducing production times, without decreasing the quality of the product. Nowadays also the environmental aspects play a key role and is an important factor for the success of the products on the market , in fact, a growing environmental awareness is developing among consumers . From these considerations it comes to light the need to study and develop a knowledge-based approach able to assist designers during the lifetime of the product , analysing the aspects related to performance, cost and environmental aspects.

Therefore one of the most important problems is to be able to decrease the cost and time of passage between idea and market launch; therefore have available technologies, able to predict the actual behaviour of the various systems, determines a considerable advantage in terms of economic and organizational links.

The challenge for Italian engineering companies is to sell quality products while continuing to develop innovative solutions quickly, and keeping costs low . To meet this challenge, companies need to invest more and more in the design process to ensure the future of the company with dedicated strategies for innovation and technology.

The objectives of this work can be summarized as the definition of a new design approach , based on knowledge which can provide new tools for the analysis and assessment of the performance of products in different application scenarios.

The work focuses on the analysis of next generation storage systems consisting of lithium-ion batteries used both in automotive and stationary applications . You can still apply the methodology described also working with other application cases . With regard to the design of battery packs , the work represents a first step in the definition and design of the lithium-ion storage systems battery . In particular , within this thesis the state of the main storage systems has been analysed , our attention is on lithium-ion technology and their main usage problems . A deep analysis was performed for the determination of the heat generated by the individual lithium batteries during their operation . The research results have been applied to small-scale production customization, both of electric vehicles, and energy storage systems for homes.

Keywords: Electrochemical storage systems, Lithium-ion batteries, Electric Vehicles, Cooling system, Modelling.

1 Problem statement and objectives

One of the “20-20-20” targets [1] is the reduction in EU greenhouse gas emissions of at least 20% below 1990 levels by 2020. This EU objective has to be achieved through a package of measures which also includes transportation. In this scenario, Fully Electric Vehicles (FEV) receive a lot of attention and are seen as a suitable path to reduce the dependency on oil, decrease CO2 emissions and allow driving with zero local emissions in city centres.

However, while the Hybrid Electric Vehicles (HEV) market is growing in accordance with the coming of several new models in the years 2012-2013 (from small-cars to executive ones) by large car manufactures, the FEV market is still a niche market which really concerns light urban commercial vehicles and mini-cars with an autonomy of approximately around 100km/day. The lack of mass diffusion of pure electric vehicles depends on limited battery autonomy and high costs in comparison with other types of vehicles. This particular situation gives the opportunity for many small-medium sized vehicle manufacturers and their suppliers to gain market share developing customized solutions for mobility.
Electric and hybrid electric vehicles (EV and HEV) today represent the best solution in the transport sector to reduce oil dependence, greenhouse gas emissions and the emission of pollutants.

Rechargeable lithium-ion battery storage systems are the most suitable for automotive applications due to the high specific energy and high energy density compared to other types of electrochemical storage. For example, nickel-metal hydride (NiMH) batteries, which have dominated the HEV market, have a nominal specific energy and energy density of 75 Wh kg-1 and 240 Wh L-1, respectively.
In contrast, lithium-ion batteries can achieve 150 Wh kg-1 and 400 Wh L-1 [2], i.e., nearly two times the specific energy and energy density of NiMH batteries. If we compare the lithium battery systems with lead-acid storage systems we get to have specific energies and capacity of nearly 5 times higher than for lithium.
Although lithium ion batteries are rapidly displacing NiMH and nickel-cadmium secondary batteries for portable and hand-held devices, they have not yet been widely introduced in automotive products. The main barriers to the deployment of large fleets of vehicles on public roads equipped with lithium-ion batteries continue to be safety and cost (related to cycle and calendar life) [3] and thermal problems that develop around the battery.

Since the recent introduction of HEV fleets, the industry trend is toward larger batteries required for plug-in hybrids, extended-range hybrids, and all-electric vehicles. These larger battery designs impose greater pressure on the need to lower costs and improve safety.
The generation of heat in the battery is directly proportional to the power required by the vehicle itself. The manufacturers of cells provide the range within which the battery can operate the battery to avoid security problems and a deterioration of the battery.

The single lithium-ion battery cannot supply power, capacity and voltage requirements in various applications, it is necessary to group them into packages in order to obtain the desired performance. Consider that in an electric vehicle, using an elementary cell of capacity 150 ah, you may have parcels that contain about 100 cells.

2 Research planning and activities

The necessity of packing Li-ion battery cells is due to the impossibility to achieve high energy density with classical single module batteries for engine propulsion in automotive use. As previously mentioned a battery pack is a set of single cells array where a correct connection of many modules guarantees the required values of current and voltage for the final specific application. Current is constant for all modules while resulting battery voltage adds up according to the number of cells [4].
The main parameters in order to design the battery pack are: the operative conditions of the target application, the choice of cells type and number, the modules location and, finally, the evaluation of heat reactions. Even if cell definition is the core of design, the modules layout has an important weight on final performance. Currently, manufacturers of automotive batteries follow different approaches to Li-ion battery pack design. As cited before an important difference is due to the target number of produced batteries. The traditional design approach, commonly used in many SMEs, is based on the experience of engineers supported by CAD systems and trial-and-error procedures.
Designers use basic calculation tools to analyze and elaborate new solutions. The engineer calculates the electrical layout configuration, determines the geometrical shapes and defines the cooling system size. Then, the corresponding physical prototype is manufactured and physical tests give him/her the performance quality. Possible design errors require time expensive iterations and time to market stretches. The main activities are repetitive tasks and designers are limited to using their own experience on past project data (such as empirical tables, drawings, reports and feedback).
Computer Aided Engineering (CAE) systems can be successfully used to investigate the performance of virtual products without using physical prototypes [5]. Such numerical methods are also adopted to evaluate the heat generation of a Li-ion cell. This second approach is complementary to the traditional one and introduces numerical analysis of the electrochemical reactions. Many commercial tools based on Finite Elements Methods (FEM) offer advanced functions to predict cell performance and CFD solvers to verify the convective cooling air-flow [5]. Several researchers propose a solver of cell behavior by analysis of an equivalent electrical model, the calculation of generated heat by internal resistance and the cooling performance evaluation by thermal resistance and convective heat exchanged coefficient [6]. The main disadvantage of these last methodologies is that they need a complete cell characterization. The lack of specific tools to support the rapid definition of whole battery pack layout can imply time consuming activities. The inputs of the CFD analysis are the electrical and thermal data of a single cell then it is extended on a virtual model of the complete battery. A determined geometry is required before generating of a mesh to solve the flow field around each array of cells. A deep connection between the CFD solver and parametric variables of CAD system is necessary to increase company productivity simplifying the iterative optimization process. Ghosh [7] showed many good results using this kind of tool, however they require large computing resources to simulate the cooling effect.
The adoption of only thermo fluid dynamic analysis is limited to completely support the battery design process because the packs have to also guarantee properties such as high density energy, little weight, compact dimensions and the possibility of a second life in a new application.
One of the last innovative methods proposed in literature is based on the FOSTER network. Starting from the initial cell characterization and the FEM analysis of a single module

of cells, a network comparison predicts flow cooling behavior and superficial cell temperature at different current rates [8]. Computing time is reduced but very high competencies are necessary to build the FOSTER network. The single cell characterization considers the linear model of generated and transferred heat and final temperatures are the weighted sum of the contribution of each cell. The various cells compose a matrix from which it is possible to resolve by operation of convolution and integrals to evaluate heat generation.
In all cases by implementing virtual prototyping technologies based on FEM tools, specific knowledge is required for a correct interpretation of the results and the outputs of CAE systems must be matched with experimental tests in order to draw correct results. The integration between CAD technology and simplified specific analysis tools can facilitate the design process by respecting time and cost constraints.
The Figure 1 describes the framework of the proposed knowledge-based design approach. The powertrain specifications such as nominal power and dimensional constraints are the input data to define the energy storage system. The configuration tool is represented by a user interface to choose the main battery pack characteristics (cell type, number of cells, air-cooling mass rate, distances, etc.) and it drives the design parameters calculation through accessing the formalized knowledge base. Then geometrical modelling is the phase which uses the calculated parameters to instantiate specific customized battery models (templates) and to automatically generate a simplified CAD model. Finally this virtual model can be evaluated by using the analysis tools. The dashed area of Figure 15 contains the KBE application (Knowledge Base, database and templates).
Specifically, the first steps of research have been focused on the implementation of a method to support the cooling design of customized battery packs for the powertrain. One important factor is the energy balance extended to the average volume of a single cell. Several experimental tests have been analyzed to elaborate the physical constants, such as heat capacity, and the electrochemical parameters, such as the average gradient of open circuit potential at different temperatures and state of charge. A lot of knowledge has been extracted from the experimental measurements and from the theory of physical phenomena.

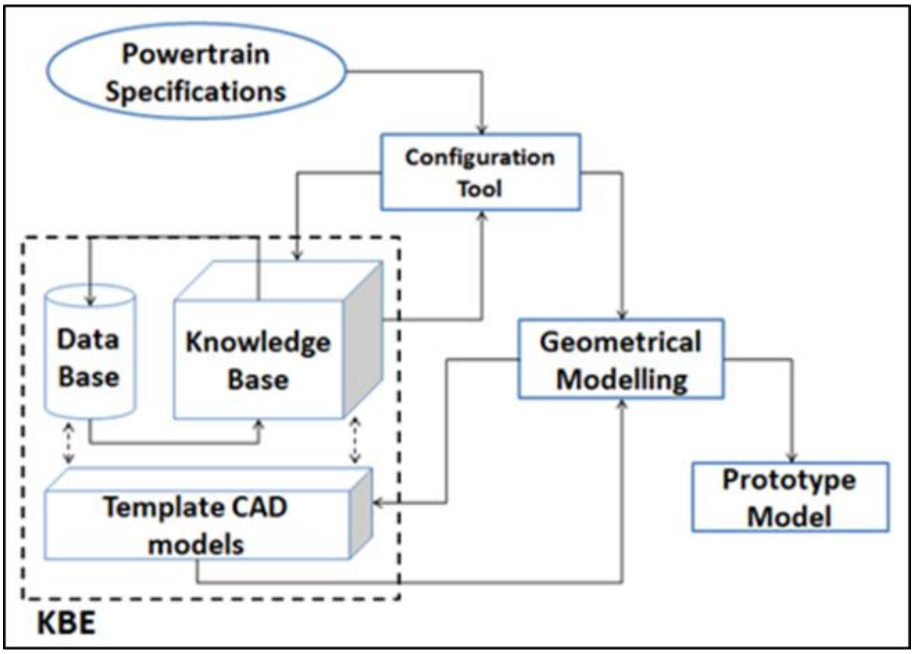

Figure 1 Methodology approach of a Knowledge Based System for Battery Pack Design

3 Analysis and discussion of main results

This section presents the methodology studied to support the cooling system design for a Li-Ion battery pack. A knowledge based framework has been developed interacting with classic tools such as database, test bench and CAD/FEM software. In Figure 2 a block diagram about input and output data of a battery design process using a KBE application is reported.

The most important parameters are the electric motor details (such as voltage, nominal power, max power and torque). Another set of parameters is the collection of battery requirements (such as autonomy, cycles of charge). A third group of parameters considers the vehicle requirements (max vehicle weight, use

destination and operative condition). The operative condition concerns the powertrain type (hybrid or full electric vehicle), climatic conditions (temperature, moisture, etc.), and vehicle size class (mini car, small car, medium car, luxury car, sport car, minivan, etc.).

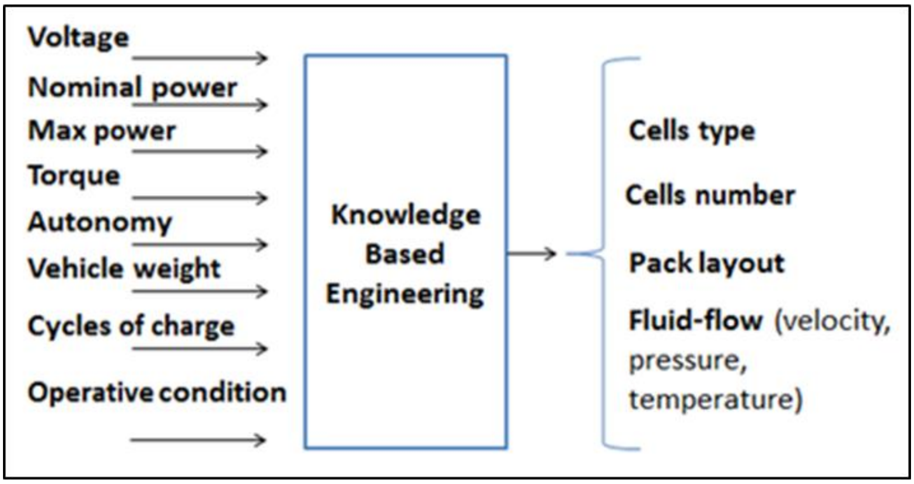

Figure 2 Input and Output of KBE application for customized battery pack design

The system outputs are the geometrical modelling of pack layout, the choice of cells type and number and the definition of physical variables of fluid flow. However, our research aims to create interaction between each block differently. The output becomes the input for another.

The design knowledge about the Li-ion battery has been studied with an appropriate modular approach to obtain the main knowledge domains useful to plan the product configuration process.

Different levels of knowledge domains have been identified: electrical, material, thermo fluid dynamic, geometrical, normative, performance and second life. Each level of knowledge is interconnected with the other ones, so the complete battery pack configuration is based on a relationship network between the different domains. Each level has a collection of rules to determine the right links Figure 3. The description of the seven main different sets of the analyzed knowledge domains are reported below.

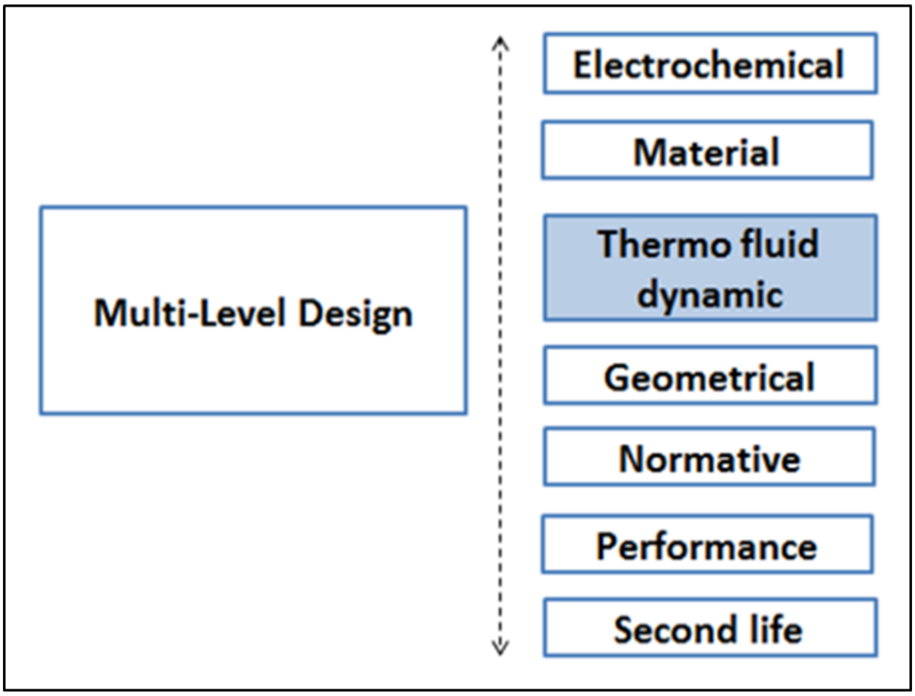

Figure 3 Knowledge levels on battery pack design

Electrochemical domain

An automotive Li-ion battery pack is a package of more cells used for the production and storage of electrical energy by chemical reactions. In these rechargeable batteries, lithium ions move from the negative electrode to the positive electrode during discharge, and back when charging. The electrochemical knowledge of cell is required to evaluate the final battery behavior as health, generate power, current discharge rates, etc. Main variables are nominal voltages, nominal capacity, specific energy, charge condition, discharge condition and operative condition.

Material domain

Knowledge about material is complex in the area of electrochemical and polymeric Li-ion battery, however, the material compound of a single Li-ion cell can be considered as a single block of material with its specific properties and characteristics. Cell materials must be properly formalized and classified on a specific collection.

Thermo fluid dynamic domain

This domain contains rules to evaluate the electrochemical heat generated and the cooling performance of a fluid flow. Thermal behavior depends on electrochemical parameters such as current, voltage and SOC. Fluid dynamics laws ensure the calculation of convective heat dissipation of a battery pack. Knowledge needed is almost all explicit and related to professional handbooks.

Geometrical domain

This knowledge manages geometrical data along with expertise rules. Main data are represented by: boundary space, single-cell geometry and dimensions, cells distance, spatial arrangement of cells on ordered arrays, etc. Rules to define geometrical design values are related to the thermal domain and to the cooling requirements.

While the thermo fluid dynamic domain fixes the fluid flow and its heat transfer properties, the geometrical knowledge is the competence of a technical designer who exploits his experience to optimize the battery pack performance by a correct lay-out. So elicitation activities to gather information and then formalization processes of this knowledge domain in geometric formulas and rules are difficult.

Normative domain

The Standards and normative provide rules to guarantee a safe installation and operation of the battery pack. This kind of knowledge comes both during parts choice but also as verification of the obtained configuration. The normative often presents purely analytical knowledge, based on constraints, which is stored on official publications. This knowledge is normally readily available, but technical meetings have been useful to comprehend rules and laws in the specific design context. Normative knowledge can be regarded as fixed and unavoidable. When opposite requirements emerge other domains indications must accommodate to meet the particular request of normative.

Performance domain

This aspect is a synthesis of conceptualization, system modelling, experimentation and expertise. Empirical and theoretical approaches mix to estimate battery pack performance. Total performance is evaluated in terms of installed cells and thermal dissipation. This knowledge has been formalized through diagrams, tables, formulas and corrective factors. Main parameters are: current rates, specific energy, cycles of life, et.

Second life domain

Currently study of second life application is a sustainable target of European electrical vehicles development to guarantee less environmental impact. The aim of second life is to find new applications for the batteries after they have outlived their usefulness for powering vehicles; for example partly depleted batteries could be used as backup power supplies for electricity outages, another application could be the storing of renewable energy. Knowledge about these applications is important to elaborate the second life planning at the beginning phase of battery designing in order to ensure a sustainable production.

As Figure 4 shows, the KBE module groups the phase of the Test Cycles Configuration, First Analytical Thermal Analysis and Pack Layout Configuration. These phases are mainly based on battery know-how; so rules, data and formulas are implemented to guide the designer on the thermal evaluations of the issue. The three levels of KBE have to relate with the classical test bench and engineering tools in order to reach a valid virtual prototype and reduce the project development lead-time.

This approach to work has been applied to the design and optimization of electrochemical storage systems for motor vehicles, but the same approach can be used to support the design of any system of accumulation needed in other applications, such as UPS, smart home, etc.

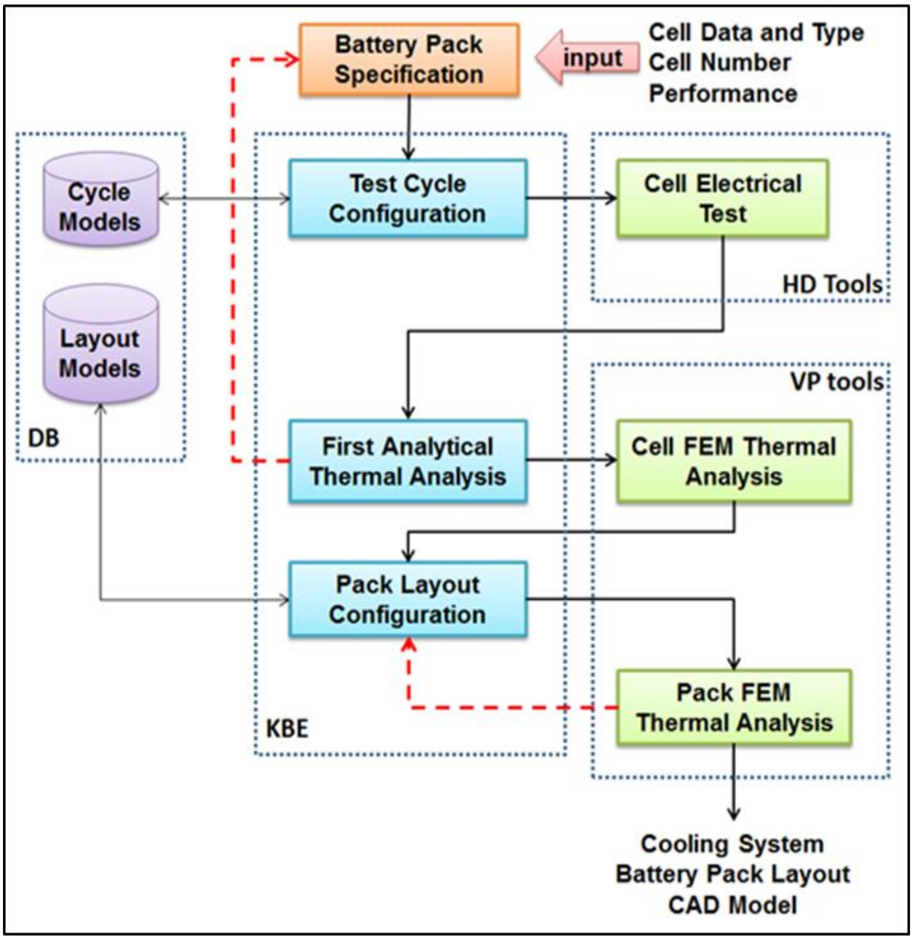

Figure 4 The scheme of proposed methodology

As validation of the proposed methodology is reported the result of a simulation of a module of a battery pack composed of 59 cylindrical cells used for the power supply of an electric vehicle light.

This simulation reproduces the thermal load, constituted of 4 repeated ECE R15 driving cycles. In particular, the temperature distribution in Figure 5 The temperature map on the middle section with air cooling at 20°C and 100 m3/h volumetric flow regards the middle section of selected battery module.

The starting temperature analyzed is 20°C and the air cooling flow is at the same temperature during the simulation. Using this setup, the maximum cell temperature, simulated after a driving cycle of 780 sec, is 22.05 °C (Figure 5), while the minimum value is 20.74 °C (with a gap of 1,31 °C).

On the other hand, in Figure 6 The temperature map on the middle section with air cooling at 20°C and 50 m3/h volumetric flow the simulation report with a different air cooling condition is shown. The air intake elaborated by compact fan wheels has a volumetric flow of 50 m3/h . This second analysis aims to investigate the influence of air flow rate on the cooling performance, in order to evaluate the battery cooling with virtual prototyping tools

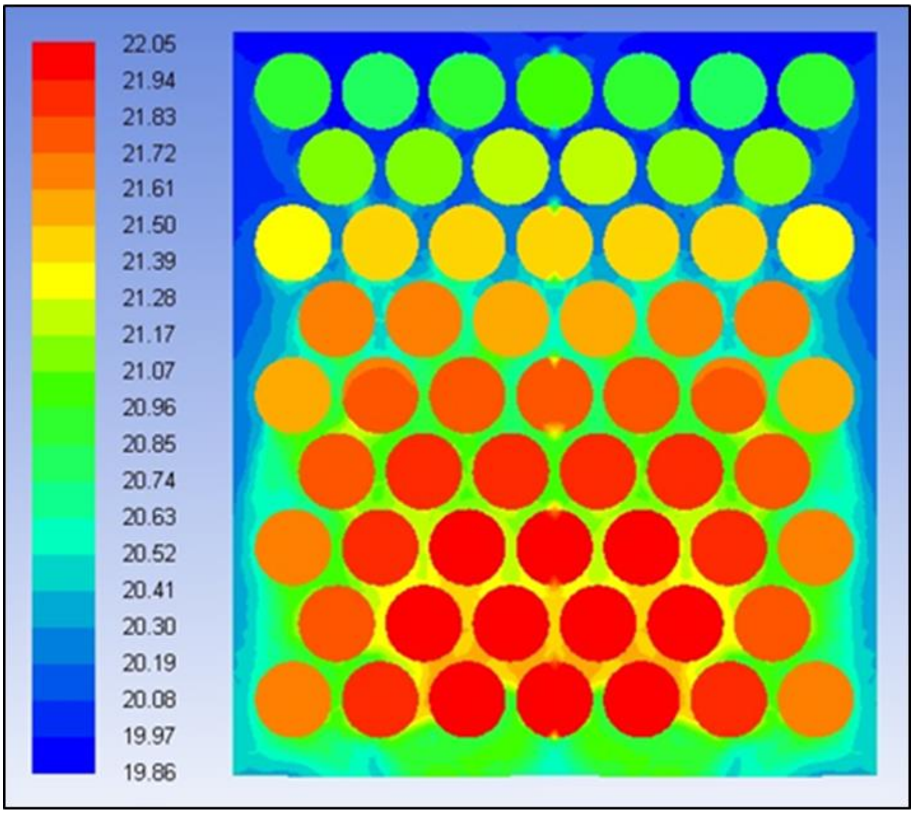

Figure 5 The temperature map on the middle section with air cooling at 20°C and 100 m3/h volumetric flow

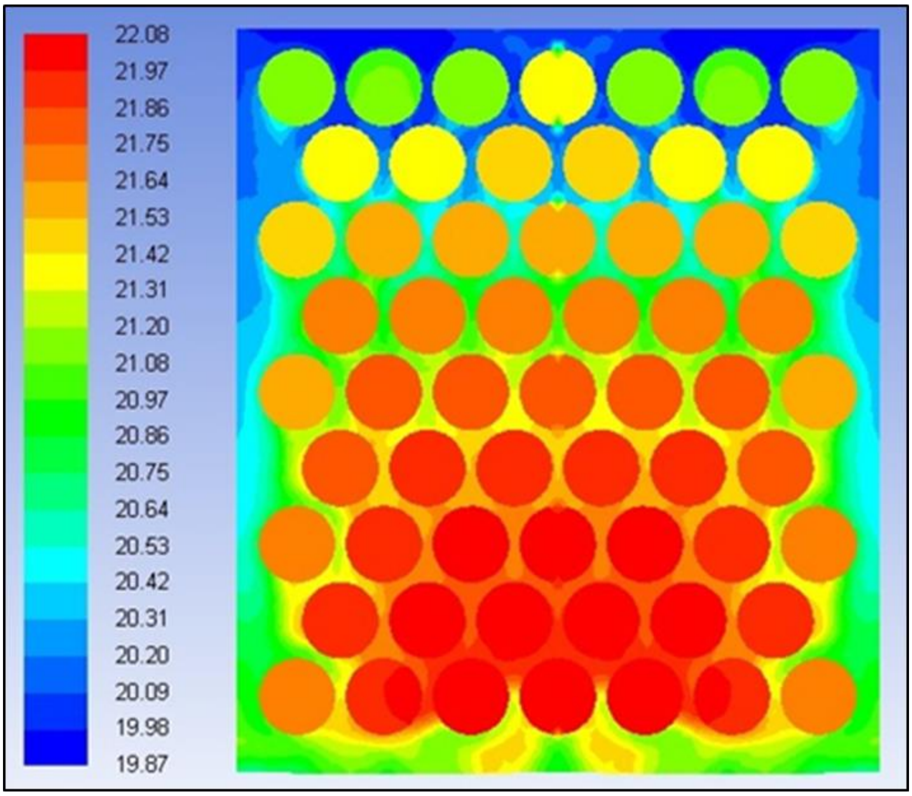

Figure 6 The temperature map on the middle section with air cooling at 20°C and 50 m3/h volumetric flow

4 Conclusions

The work carried out in this thesis aims to propose a new methodology of work, able to support the designer during the implementation phases of the product.

Through the application of knowledge and the input data of the specific problem we are able, through a specific workflow to arrive quickly and without the construction of numerous physical prototypes to the achievement of the required product.
All of this minimizes the construction of physical prototypes and allows innovative, high performance products to be brought to market in a short time.
Moreover, this approach to work is very useful for small and medium-sized enterprises, which are able to cope with the design and construction of small amounts of different types of product.

The methodology has been applied to the design of cooling systems for electric and hybrid vehicles. An analytical model has been validated, which allows you to know the maximum surface temperature reached by the cell in any working condition, without necessarily having advanced knowledge about the chemistry of the battery.

Through FEM modeling techniques it has been possible to analyze not only the single cell, but also the temperatures reached inside the battery pack and study a cooling system for the present case.

In order to validate the analytic model different cells of varying size, shape and chemistry have been tested. In all cases the results are considered satisfactory, as the deviation between actual values and values calculated analytically was always less than 5%.
Regarding the battery pack a hybrid vehicle used for the collection of waste in an urban area has been considered. As a result, in this case the battery pack, analysed by the proposed methodology, is functioning in its real application.
Looking at the presumed growth of the market for cars with electric drive, this method can find more and more applications in business realities.
Future developments will manage an introduction of a charge / discharge able to subject different currents to individual cells of the package, in order to make the temperature reached more uniform.

The methodology can be extended by adding tools to evaluate the environmental impacts of chemical storage systems throughout the life cycle. This analysis may be useful during the process of choosing between one type of battery compared to another.

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