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Thermal Battery Cell Models – Enabling Efficient and Hazard-Free Physical Thermal Testing of Battery Systems

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Abstract

The development and validation of battery thermal management systems conventionally deploys virtual simulations during most of the engineering cycle. Physical tests are performed where necessary, usually as end of line tests to meet specific norms and standards and are conducted almost exclusively with real battery cells. While being the most realistic approach, real cells pose numerous challenges and demand stringent safety measures due to their active cell chemistry, electrical voltage, and stored chemical energy.

Thermal Battery Cell Models (T-BCM) resemble actual battery cells and exhibit equivalent thermal behavior. However, unlike real battery cells, T-BCMs do not have the aforementioned potential hazards, as they are built from chemically inert materials without electrical potential.

This paper outlines the core motivation for substituting real battery cells in testing, defines a general system of objectives and derives an internal layout of a T-BCM. It then compares first simulations between a real reference cell and its T-BCM and selects appropriate and procurable materials to build the T-BCM. The investigation concludes by building the first prototype and by highlighting the shortcomings and potentials. Within all performed simulations, the inner temperature of the T-BCM differs no more than 1 K compared to the real battery cell. The main reason for this discrepancy is argued to be partly attributed to the simplified modeling approach, reducing the internal layer from 143 layers in the reference cell to 21 layers in the T-BCM. However, the predominant factor lies in the selected material aluminio-silicate, which exhibits an almost 30% lower volumetric heat capacity compared to the ideal design. Nevertheless, the proposed method promises great potential in testing due to the many benefits it can provide.

1 Motivation

When developing battery systems, battery thermal management is a major component of the development efforts. Not only does it ensure safe operation of the battery itself, but it also orchestrates the thermal interfacing with external systems. For automotive tractive batteries, this can entail shifting heat energy to or away from the battery, for example for (pre)conditioning in preparation for fast charging or heating the driver compartment respectively. These and many more battery internal as well as system-wide functions need validation [1] and knowledge generating testing during development.

1.1 Virtual simulations and physical testing

Conventionally, there are two approaches to work on validation tasks in battery thermal management system (BTMS) development. Until the very last stages of development, most tasks are mainly solved by extensive virtual simulations. There are many reasons for this reliance on computer aided methods. While in the early phases of development the shapes of many components may not yet be determined and are steadily iterated over, a flexible approach like virtual modelling is much faster than building physical prototypes. Especially for less detailed models like lumped thermal masses, simulations yield quick results [2]. However, the more complex and interconnected the simulated system becomes, potentially even multi-domain spanning, the longer the simulations take and the more intricate system knowledge for correct parametrization is required [3]. Additionally, tremendous expertise is necessary in modelling all components properly. In particular for battery cells, a thorough understanding of the inner workings of their chemistry, such as the dependencies between inner resistances, currents, state of charge and temperatures, but also processes like ageing is essential [3]. Lastly, the interpretation of the results presents a critical task in and of itself and a lot of experience is required to draw the correct conclusions. Without all this knowledge, trust in the outcomes of these simulations can diminish quickly.

On the other end of the spectrum, there is physical testing. Using real systems with real battery cells has the advantage of inherently relying on the underlying physics. Nevertheless, the exact final shape or at least a very close approximation is required. Also, physically building systems is a time and financial burden and variations cannot be easily tested, as new components need to be manufactured, making this whole approach inherently inflexible. Real battery cells add onto these challenges substantially, as they themselves pose severe risks, especially during thermal testing. Cells can go into thermal runaway, an event, where the inner structure of the cell breaks down and the cell heats itself uncontrollably, thereby potentially catching fire, venting toxic gases or exploding [4]. But also during thermally safe operation, there are potentially fatal electrical risks when handling high voltage systems. To handle these risks, expensive bespoke testing equipment needs to be available with inbuilt safety features and the ability to move vast amounts of electrical energy. Additionally, engineers need to be properly educated to work with the electrical and chemical hazards. Eventually, real battery cells also need to be charged, discharged, balanced and undergo ageing. All of these may alter their (thermal) properties, which of course is undesired behavior for reproducibility in testing. In conclusion, physical testing poses a cost-prohibitive and time-consuming challenge with high risks.

Most development teams therefore try to cut down physical testing as much as possible and try to rely on virtual simulations during the main development loops. Physical testing is deployed only where necessary, in particular for the final necessary (abuse) evaluations according to norms and standards like ECE R100 [5] or the transport norm UN T 38.3 [6], where physical tests are mandatory.

1.2 Mixed physical-virtual validation – the IPEK-X-in-the-loop framework

There exists an approach combining the advantages of both virtual and physical modelling. The IPEK-X-in-the-loop validation framework [7] perceives validation not as a binary choice between virtual and physical methods, but rather as a balanced integration of both worlds tailored to the specific requirements of a given validation task. Figure 1 shows an exemplary comparison between a physical and a virtual configuration, where the actual System in Development is shown on the left, whereas necessary Connected Systems are placed on the right. The vertical separation then delineates, which systems are implemented virtually or physically. The depicted validation task, which is kept throughout this publication, is from the view of an engineer, who aims to develop a new cooling unit for a battery module. The virtual approach (fig. 1a) could be a thermal simulation of the whole battery system including cells and all thermal interactions with the vehicle cooling system, all within one software. The physical configuration (fig. 1b) on the other hand might be a built battery system complete with the new cooling unit mounted on a test bench. Although a fully physical configuration, e.g. a driving vehicle on a test track with the new cooling unit integrated, is feasible in principle, it appears more viable to cut the system boundary to the virtual domain at the battery system enclosure on a test bench. Therefore, there are virtual components left within this configuration, but the battery system itself remains physical.

Inbetween these systems there often appears a so called Koppelsystem (ger. koppel – eng. coupling) [8]. A Koppelsystem is the virtual (KS_{vv}), physical (KS_{pp}), or mixed physical-virtual (KS_{vp}) manifestation of a

Koppelfunktion in the XiL architecture to overcome incompatibilities between models. These incompatibilities include:

- Incompatibility between inputs and outputs of different models.
- Spatial separation (e.g., greater distance between models or distributed in location).
- Relational reference (e.g. establishing temporal reference time synchronization).

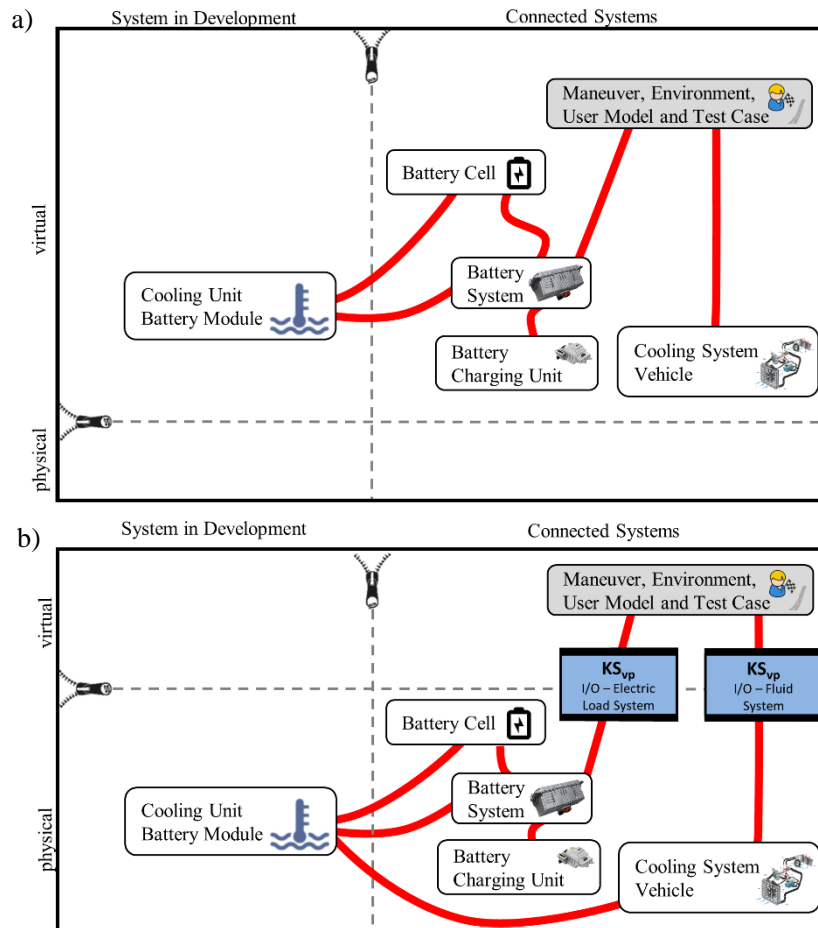


Figure 1: Virtual (a) vs. physical (b) validation configuration within the IPEK X-in-the-loop framework

Koppelfunktionen or Koppelsysteme sind nicht dazu gedacht, relevante Systemverhalten hinzuzufügen, sondern können selbst aus einem oder mehreren Modellen [9] bestehen. Das Koppelsystem als Implementierung der Koppelfunktion bringt bestimmte (falls bekannt) Eigenschaften (z.B. eine frequenzabhängige Übertragungsfunktion) mit, die einen unerwünschten und nicht vernachlässigbaren Einfluss auf das Systemverhalten haben können. Eine Kompensation dieses Einflusses oder eine Berücksichtigung bei der Ergebnisinterpretation kann notwendig sein.

1.3 Research Objective

Das Ziel dieser Arbeit ist es, die Vorteile von gemischter physikalischer virtueller Modellierung auf Basis des IPEK XiL-Ansatzes für die Entwicklung von BTMS zu nutzen. Insbesondere besteht das Ziel darin, ein Batteriezellenmodell zu entwickeln, das die Risiken des physischen Testens minimiert, während ein hohes Maß an Vertrauen in die Ergebnisse sowie die Expertise zur Nutzung des Modells auf einem handhabbaren Niveau beibehalten wird.

2 State of Research

Da rein virtuelle Simulationsansätze für das zuvor beschriebene Forschungsziel nicht geeignet sind und da virtuelle Simulationsmodelle für elektrische, thermische und mechanische Verhaltensweisen in der Literatur, gut dokumentiert und erforscht [10-12], wird in diesem Abschnitt nicht auf virtuelle Modelle eingegangen.

Instead, the focus is on physical or mixed thermal modelling methods, as they are rare and only scarcely researched at this point.

Only a small amount of known publications elaborates on modelling for various physical thermal testing tasks. The inner resolution of these models varies widely and they do not reflect all (typically orthotropic) thermal properties consistently or at all. They range from cutting out the inherent thermal behavior of the real battery cell and replacing it with a pure Koppelsystem (i.e. not adding relevant system behavior) in form of a simple heating element in the shape of a battery cell all the way to more sophisticated models, which try to capture the thermal behavior of battery cells more precisely.

An example of the former can be seen in the model by Eisele et al. [13, 14] (see Figure 2, connection to Maneuver, Environment, User Model and Test Case omitted) for validation tasks of a cooling unit for a battery module. They also use a mixed physical virtual modelling approach, but do deliberately not model the thermal behavior (volumetric heat capacity and orthotropic heat conductivity), as this was deemed not important for the validation tasks at hand.

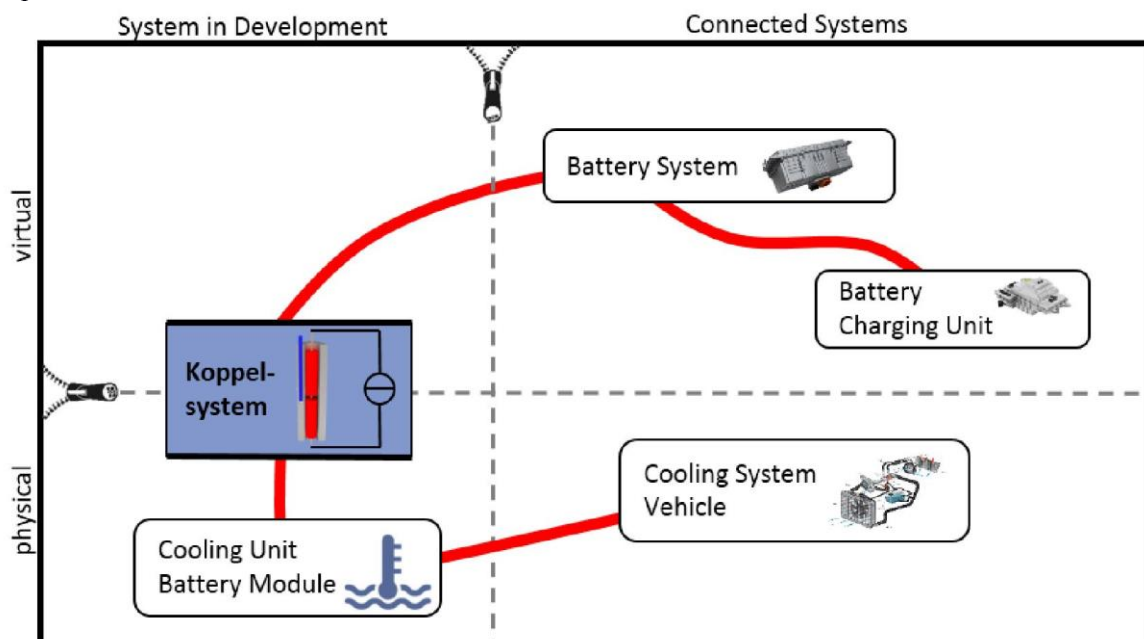


Figure 2: Mixed physical virtual validation configuration with a Koppelsystem replacing the battery cell [13]

A representation of the latter was described by Seegert et al. [15]. This publication hints at a more elaborate inner structure with good modelling precision but the inner layout itself is not clearly shown due to the involvement of industry partners. Li et al. [16] propose a cylindrical T-BCM and explore their thermal behavior in more depth. The structure of the cell is similar to Eisele's cell [13, 14], but more emphasis is placed on correct thermal behavior. Li's work shows the closest resemblance of what this work calls a T-BCM, in this case for cylindrical cells, where the transferability of the knowledge for pouch cells is limited due to a different inner structure.

Other authors are less concerned with the model itself, but rather go into detail about the validation tasks and take the physical model as a given component [17, 18].

While the general method presented in this paper is partly transferrable to all battery types, this research focusses on pouch cells only.

3 Method - Deriving the T-BCM

From the research shown in the last chapter, two conclusions can be made. Firstly, there is no concise definition of what a thermal battery cell model actually encompasses. Secondly, a possible inner layout remains unknown for pouch cells and needs to be defined.

3.1 The definition of a T-BCM

Within the scope of this publication, the definition is established as follows: A Thermal Battery Cell Model (T-BCM) captures the thermal properties of real battery cells. It is modelled with a mixed physical virtual approach including appropriate Koppelsystems between the two model sides. On the physical side, their shape and outer dimensions match the reference cell, but all hazardous active materials on the inside are replaced by chemically inert and electrical potential free materials such that the thermal properties of the T-BCM remain as unchanged as possible compared to the reference. The non-hazardous materials may be kept, which is especially meaningful for the outer pouch bag and/or the tabs, as these materials interface directly with the BTMS. The virtual model side contains the electrochemical properties and behaviors (not further investigated in this publication). The virtual model side supplies the calculated heat losses as an input for the physical model to generate the exact amount of heat energy within appropriate heating elements. The temperatures are then measured and serve as a feedback for the virtual model.

T-BCMs must allow for safe and efficient physical testing since all major drawbacks from real battery cells are absent. Additionally, T-BCM may open up new validation goals, such as examining the maximum stationary cooling capability of a specific solution, which, due to many dependencies i.e. on current, SoC, temperature and outer pressure of the heat losses during real battery operation, were infeasible or even impossible to obtain prior.

Specifically, they satisfy the following general system of objectives:

- Retaining the outer geometry (length, height and width) of the reference cell,
- (Optional, but advised) Maintaining the outer interface material (pouch bag and tabs),
- (Optional) Maintaining the inner inert materials (aluminium and copper collectors),
- Replacing all electrically and chemically active materials (porous electrodes, electrolyte and separator) by a single or multiple substitute layers and materials,
- Matching the orthotropic heat conductivities in- and through-plane as closely as possible with inert materials,
- Matching the volumetric heat capacity of the real battery cell,
- Adding heating elements and temperature sensing as Koppelsystems inside and / or outside the T-BCM, compensating them in modelling.

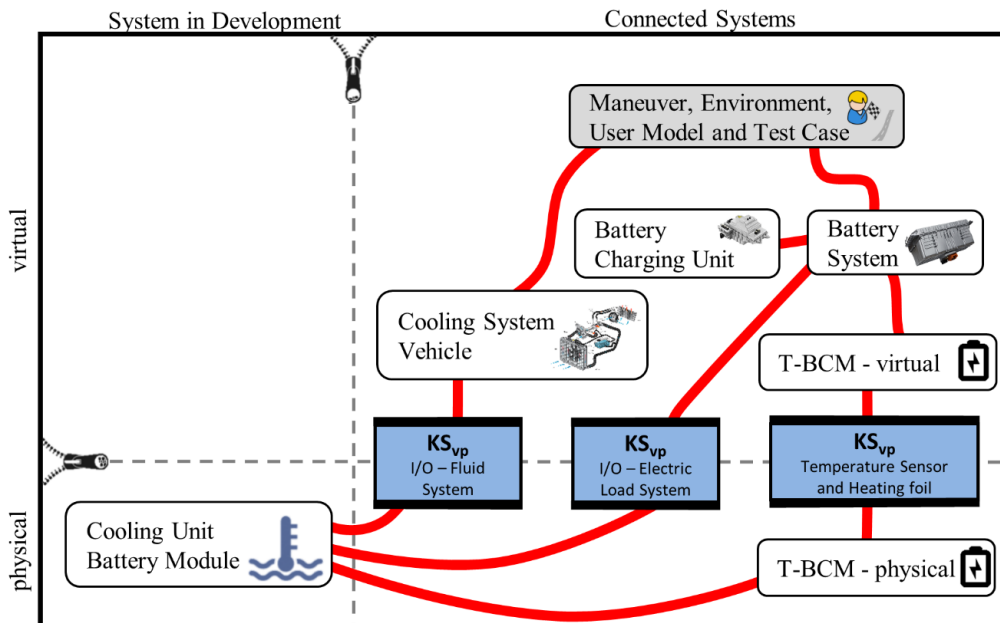


Figure 3: Mixed physical virtual validation configuration with a full T-BCM incl. Koppelsystem replacing the battery
 Figure 3 places the described T-BCM within the IPEK-XiL approach and highlights its three major components, the physical model, the virtual model and the Koppelsystems in between.

3.2 Inner Layout of a T-BCM with ideal substitute layer properties

To translate the system of objectives into an actual system of objects an ePLB C020 pouch cell by EiG was selected as the primary example and reference cell due to good thermal data coverage in literature [19]. Table 1 summarizes the relevant thermal properties.

Table 1: Thermal Properties of an ePLB C020 pouch cell by EiG (values adopted from [19])

	Material (-)	Number of layers N_i (-)	Thickness d_i (μm)	Volumetric heat capacity ρc_p ($\text{kJ}/\text{m}^3\text{K}$)	Heat conductivity k (W/mK)
Positive current collector	Al	17	21	2439.91	238
Negative current collector	Cu	18	12	3439.21	398
Separator (wet)	PP	36	25	2011.63	0.34
Positive electrode (wet)	NMC111	34	70	3676.65	1.58
Negative electrode (wet)	Graphite	36	79	2234.54	1.04
Pouch (case)	Polymer laminated Al	2	162	2185	: 55.1, \perp : 0.16
effective total value		143	7021	2740.03	: 25.35, \perp : 0.79

Before starting to develop the actual T-BCM, a baseline virtual thermal simulation model was established. A one-dimensional model with a lumped thermal mass per layer was set up in MATLAB and used to recreate the thermal behavior of the reference cell as closely as possible. Since the real battery cell was not procurable, the comparison was made between the new model and the values and graphs provided by literature [14]. As can be seen in Figure 4, the two simulations match very closely, so that the simulation performed by the authors could be used as a baseline.

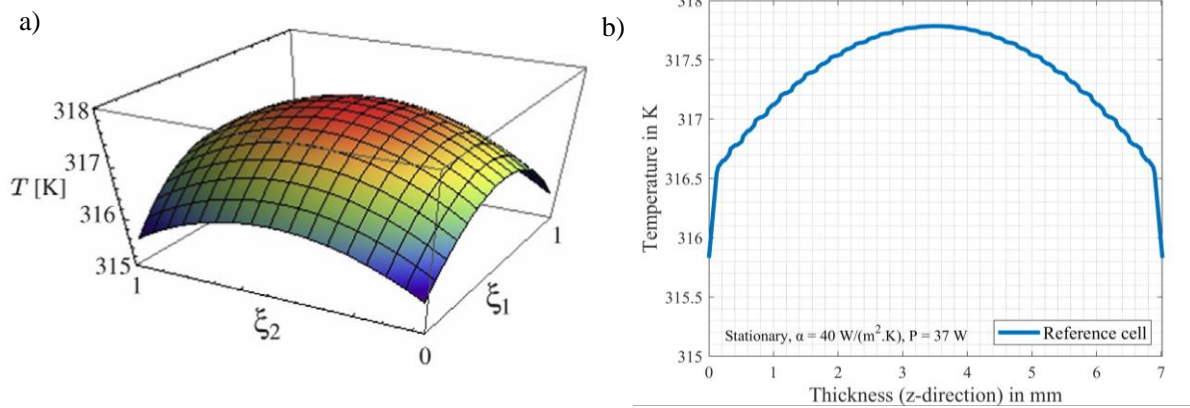


Figure 4: (a) Stationary two-dimensional temperature distribution, temperature drop over pouch bag not shown [19], (b) recreated one-dimensional simulation slice including the pouch bag at $\xi_1 = 0..1$ and $\xi_2 = 0.5$, both simulations use convective side cooling with 25 °C air at a convection heat transfer coefficient $\alpha = 40 \text{ W} / \text{m}^2\text{K}$ and an average power loss within the cell of $P = 37 \text{ W}$

From here, further virtual simulations were used to determine the optimal parameters of the T-BCM. As described in Section 3.1, one can keep the original inert materials, namely the pouch bag and both current collectors. However, the original thicknesses of the individual layers make for a difficult handling and assembly process. Therefore, by deploying stationary as well as transient simulations, the necessary number of layers was investigated. Naturally, the more layers were kept during simulation, the closer the approximation turned out. Figure 5 presents the simulation results conducted on the T-BCM model with varying layer counts, which are obtained under the same simulation conditions as illustrated in Figure 4. Even with a comparatively small layer count, the general temperature gradient could be closely approximated,

only showing up to 0.3 K absolute difference. As four substitute layers performed relatively worse than six or eight substitute layers whereas there was not much of a difference between six and eight layers, a substitute layer count of six was chosen as the best compromise between manufacturability and model precision. The pouch bag was kept with its original thickness, all other layers were increased in their thickness and the total layer count was reduced by almost factor 7. Table 2 shows the resulting ideal T-BCM composition, where the only difference to the reference cell stems from integer layer counts.

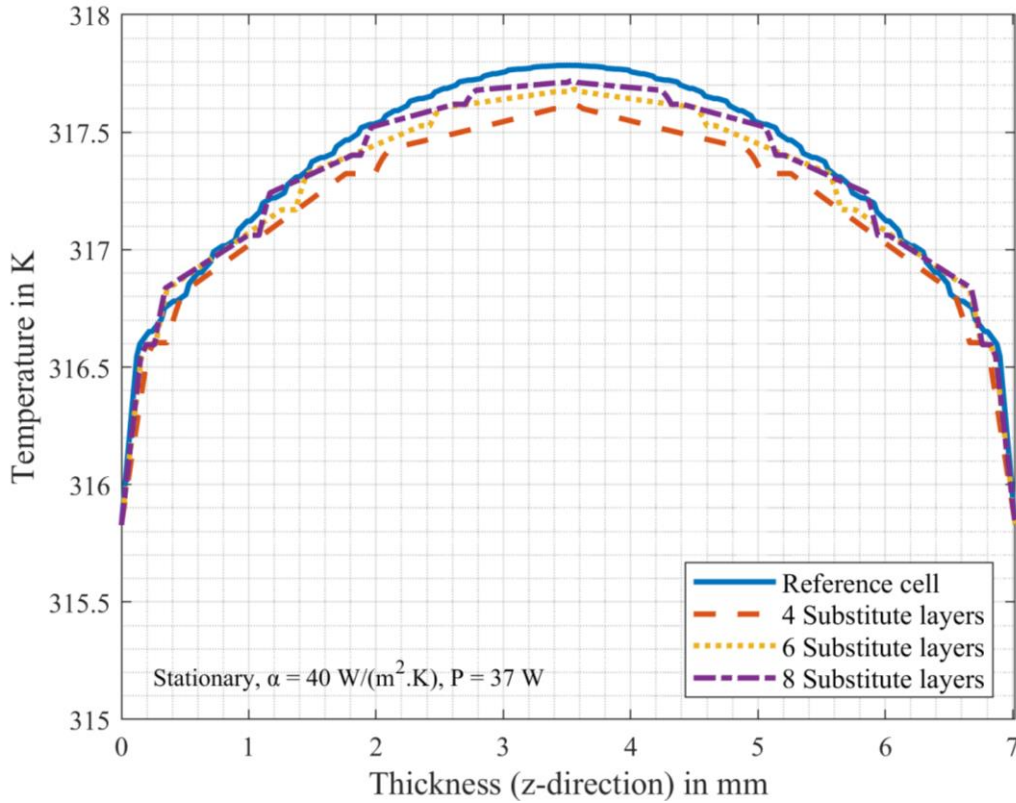


Figure 5: Simulation of inner temperature over cell z-direction for different layer counts of the T-BCM vs. reference cell

Table 2: Geometric and thermal properties of the ideal T-BCM

	Number of layers N_i (-)	Thickness d_i (μm)	Volumetric heat capacity ρc_p ($\text{kJ}/\text{m}^3\text{K}$)	Heat conductivity k (W/mK)
Ideal Substitution Layer	6	787	2943.96	: 1.157, \perp : 1.125
Aluminium	3	119	2439.91	238.00
Copper	4	54	3439.21	398.00
Pouch (case)	2	162	2185.00	: 55.1, \perp : 0.16
Heating Foil	7	200	2150.30	: 7.23, \perp : 0.52
effective total value	21	7019	2740.23	: 25.22, \perp : 0.79

The layers of the T-BCM follow the general layout of the reference cell with alternating current collectors and substitute layers in between. The number and position of heating foils was also investigated and a distribution was chosen with the best overall match to the reference cell. A mirrored distribution proved not

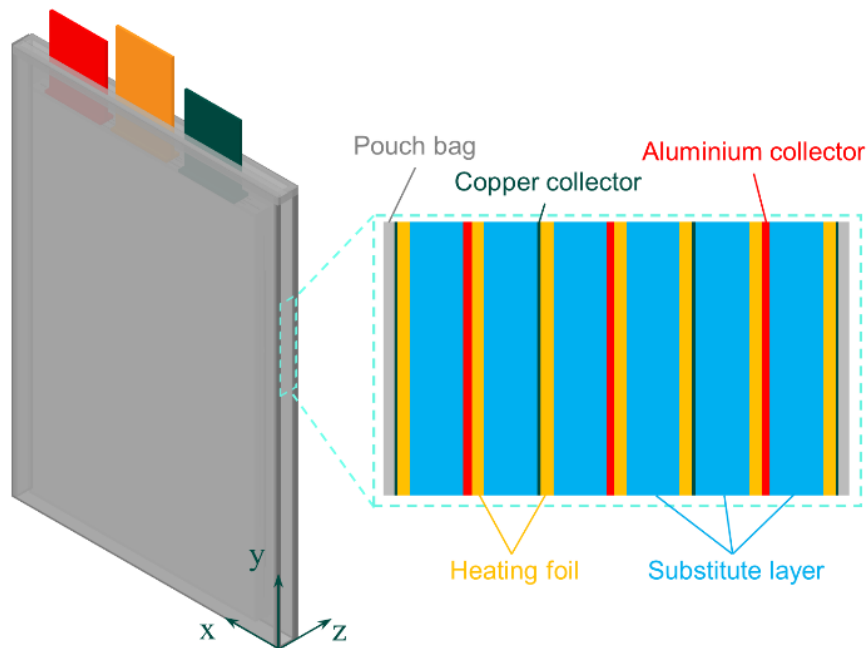


Figure 6: Inner layout of the designed T-BCM

optimal due to the concentrated heat generation or lack thereof at the center of the cell. Therefore, a configuration with the central heating foil only on one side of the central aluminium collector emerged as the best compromise. Figure 6 shows the final layout of the T-BCM.

4 A first prototype of a T-BCM

The ideal substitution layer detailed in table 2 shows very similar in-plane and through-plane heat conductivities. They are in the region of e.g. heat conductive plastics, but with a volumetric heat capacity between copper and aluminum. Matching all of these characteristics as closely as possible at the same time within a single procurable material was the key to success in actually building a T-BCM prototype.

Facilitating the materials database from Ansys Granta, a product originally developed by Mike Ashby and David Cebon, an analysis of available materials with matching properties was performed. This revealed, that three material groups come close. One of which was concrete, which was deemed unfeasible due to poor manufacturability and brittleness for thin layers. The other two material groups, ceramics & glasses as well as (reinforced) polymers (see Figure 7), while not ideal, were of greater interest, as manufacturing and procuring these materials was feasible. For an actual first prototype, an alumino-silicate glass with an isotropic heat conductivity of $k = 0,96 \text{ W}/(\text{mK})$ and a volumetric heat capacity $\rho c_p = 2032,8 \text{ kJ}/(\text{m}^3\text{K})$ was chosen. Both values were provided by the manufacturer of the glass sheets. While the total heat conductivity of the T-BCM was only slightly changed to $k = 0,77 \text{ W}/(\text{mK})$ (-2.73%), this material lowered the total volumetric heat capacity of the T-BCM significantly to $\rho c_p = 1952.23 \text{ kJ}/(\text{m}^3\text{K})$ (-28.76%) compared to the ideal T-BCM. With both the volumetric heat capacity as well as the heat conductivity below their optimal values, further simulations with the same boundary conditions were performed to assess the effect of these changes. They showed a maximum absolute deviation of temperature within 1 K compared to the reference cell, which is worse than the 0.3K obtained with ideal material parameters. All worst-case scenarios appeared within transient simulations during the heat up or cool down phase, where the effect of a changed volumetric heat capacity is most noticeable. As the simulation reached a stationary state, the influence of the volumetric heat capacity vanishes and the difference disappears.

A prototype using this material as its substitute layer was assembled as a proof of concept, see Figure 8. At the time of writing this article, no thorough tests have been performed with this prototype, as the testing infrastructure was under construction.

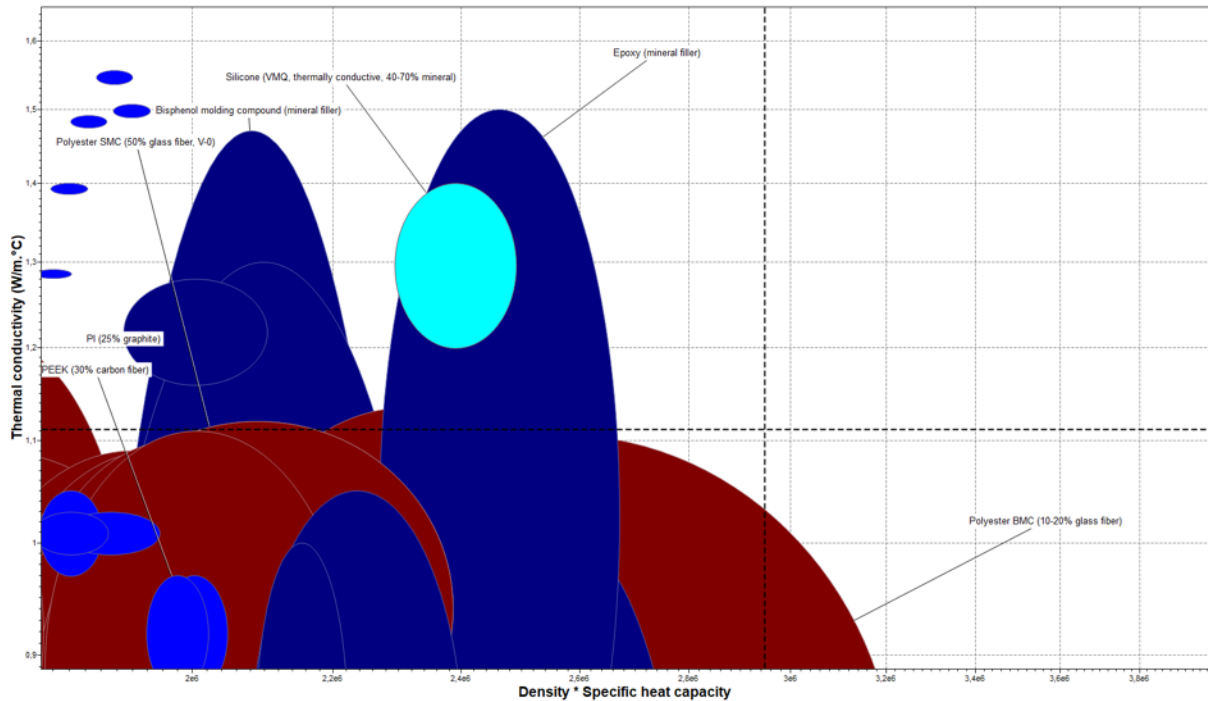


Figure 7: Materials overview of substitute layer candidates for polymers including reinforced plastics. The intersection of the two dashed lines shows the ideal material properties. The closest match was given by a polyester resin matrix with 10-20 % glass fibre.



Figure 8: First built prototype of a T-BCM

5 Summary and Future Outlook

This work outlines the very early progress in creating an efficient and hazard-free physical thermal testing environment for battery systems. This paper defines a first system of objectives for a T-BCM (Thermal Battery Cell Model), a field that has received very limited research attention to date. The Paper then proceeds to outline the actual design process and eventually presents the built prototype of a T-BCM. It addresses real world considerations, as ideal materials with perfect properties rarely exist. The resulting model consists only

out of chemically inert materials without any inherent hazards. It is designed from materials, that can be manufactured and/or procured.

The selected substitution material aluminio-silicate is not ideal and especially the high deviation in volumetric heat capacity might lead to considerable drift in T-BCM temperatures during longer test cycles, if not compensated accordingly. It is to be emphasized, that this shortcoming of the built T-BCM however does not come from a flaw in the design method itself, but rather from the final material selection. On the other hand, it needs to be added, that a T-BCM with ideal materials, which cannot be built due to the unavailability of these material, is of no real benefit to anyone, as it remains a purely theoretical construct. Therefore, a course of action is to refine the material selection, by investigating the group of polymers and composites in more depth, as they appear to come closer in thermal properties, but involve significantly more effort in procuring or manufacturing. Additionally, a test bench configuration is currently under construction and thorough examination of the T-BCM prototype and subsequent versions is imminent. To verify the modelling method, an inclusion of internal temperature measurement is also investigated in parallel. Additional work is required to verify the modelling approach, but the first steps seem promising and a clear path forward is laid out.

The motivation and vision were to aid the future engineer with development and validation tasks. The support generated by deploying the T-BCM instead of the conventional real battery cells shows different advantages. From the possibility to quickly test new iterations of cooling units for their temperature delta within the module without the need for elaborate safety equipment all the way to using the T-BCM for scoping out effects of new cell chemistries without required real cells there are numerous situations, where this new method provides tangible benefits.

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