BATTERIES EUROPE
TASK FORCE “Safety”

Definition of Safety Key Performance Indicators (KPIs)

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1 Introduction

Through the continuous decrease of production costs and performance improvements, the lithium-ion batteries (LIB) sector is currently knowing a significant expansion. LIBs represent a key technology in the EU's efforts to achieve GHG emissions reductions. This perspective will impose the augmentation of the number of batteries in use. Therefore, their production will need to be increased by involving European industries as well as ensuring sustainability. For LIB deployment over the coming years to be successful, EU political incentives will need to be followed with the consumer acceptance. This acceptance is conditional to various factors: price, performance, sustainability, but also safety. All those factors are considered in the Strategic Research Agenda (SRA)[1] published in 2021 by Batteries Europe. Safety is dealt within a dedicated position paper[2], establishing the R&I actions to be taken over the whole value chain of LIB to ensure their safe development and adoption in the EU ecosystem. These directions were considered by BEPA (Batteries Europe Partnership) and the European Commission (EC) when writing the Horizon Europe research calls on the subject funded by the EU member states. One of the recommendations was concerning the necessity to use Safety Key Performance Indicators (KPI) as references for guidance to fairly compare the safety level of current and future battery technologies. This recommendation could not be followed because, contrary to cost or performance, few, and very specific safety KPIs are currently in use (eg: EUCAR level[3] and UL9540), because of the difficulty of quantification and scale to be applied. To fill this gap, the Batteries Europe Safety Task Force, composed of experts from the academic and industry sectors, started a reflection to be the first step toward the definition of Safety KPIs that can be used as a reference and guidance for current and forthcoming EU R&I actions. Those KPIs were developed based on the hazards identified for LIB but were chosen to be able to cover several technologies with minimal adaptations concerning specific hazards or adaptation of scale.

To organise the work and follow the Batteries Europe structure, the LIB value chain was divided into 3 levels: material (WG3), cell (WG4) and system level (regrouping automotive (WG5) and stationary storage applications (WG6)). Each related Batteries Europe working group was invited to give their input. Those KPIs aim to evaluate safety levels from the end-user point of view and is not intended to be used as an engineering tool (e.g., for selection of cells by OEM). They should concern the operation of the battery; other initiatives should be taken or are ongoing to evaluate safety of LIB during other life cycle phases (i.e., safety of dismantling or safety during transport[4]). All the KPIs are not yet in the form of absolute values and the experimental methods to assess them are only indicated in this document since this need to be dealt with in standardisation groups. Examples of methods are nonetheless proposed to ensure the possibility of measurement of each indicator proposed. To avoid the multiplication of indicators that would complexify their practical use, a maximum of four KPIs per level – identified as being the more relevant – are presented.

[1]https://ec.europa.eu/energy/sites/ener/files/documents/batteries_europe_strategic_research_agenda_december_2020__1.pdf
[2] *https://energy.ec.europa.eu/safety-task-force-position-paper-0_en*
[3]https://eucar.be/wp-content/uploads/2019/08/20190710-EG-BEV-FCEV-Battery-requirements-FINAL.pdf
[4] https://unece.org/sites/default/files/2022-06/UN-SCETDG-60-INF11e_0.pdf

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To facilitate comprehension and ensure homogeneity of the document, each KPI is presented according to the following structure:

- Definition of the KPI, explaining what it measures and why it is important for safety evaluation.
- Usable SI units for quantification.
- When possible, reference values based on present commercial Li-ion batteries and/or technical literature.
- Example of a possible measurement methodology to ensure that it can be practically assessed. No detailed protocol is given since this document is not a normative one.

At material level, an original concept to consider both the hazard of material itself and hazard caused by the interaction between materials in the cell is proposed. KPIs focus on reactions that can occur inside a cell, leading to thermal runaway and other hazards. To evaluate those indicators, test on small “concept cells”, which are not entering the thermal runaway during the testing, are preconised, event if not yet precisely defined.

At cell level, addtionally the combustion of materials and consequences of the thermal runaway as well as the architecture of the cell will be considered.

At pack level, interaction between cells and possible propagation of the incident outside of the pack itself is evaluated.

In overall the focus of this document is on research and the aim is to give an indication of the most relevant hazard to consider from the user point of view in a general application.

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2 KPIs at material level

As a preliminary information, we state that KPIs at this level are intended as related to the materials testing in “concept” cells, e.g.: semi-cells or small full cells (button/coin or pouch with low capacity, which doesn’t lead to initiation of combustion processes during the corresponding test procedure). Battery materials present hazards both per se and because of manipulation/integration in reference cells. Concerning the first point, aspects such as toxicity/carcinogenicity and ecotoxicity, corrosiveness and flammability (chiefly of the electrolyte solution) are properly reported and described in corresponding Safety Data Sheets. Therefore, corresponding safety countermeasures for their storage and processing are expected to be governed by specific EU and international regulations and will not be discussed here. The same considerations can be made for the treatment of nanoscale materials (nanosolids), both for simple manipulation and for assembling concept cells. Additional hazards may arise from the integration of materials in the cell, building electrochemical interfaces and resulting in unexpected chemical/electrochemical interactions. The basic hazards coming from a particular electrochemistry defined by specific material combinations are potentially induced by:

- liquids, gas, and particles leakage into environment
- venting of toxic gases
- heat release caused by self-heating and potentially leading to thermal runaway (TR).

Even if the countermeasures against critical events are mostly undertaken on cell and system levels, the energy and power evolved during short-circuit (i.e., by dendrite formation), external overheating and overcharging (BMS malfunction) is strongly dependent on the materials utilised in the cell. Therefore, it seems useful to define KPIs also at the material level, albeit with the limitations reported above about the type of cells that are considered.

For systematic consideration and avoidance of hazards, the distinction of energy released due to electrochemical processes (i.e., short-circuiting discharge, decomposition of cathode with oxygen release, etc.) and due to combustion is important, as the electrochemical energy release rate defines the increase of the temperature inside the cell and battery pack. If this temperature increase can be maintained below the ignition temperature (leading to combustion and pressure increase inside the cell/cell enclosure), the hazard for the environment and humans can be minimised. For this reason, the **specific characteristics related to material combinations** resulting in different electrochemistries and their behaviour regarding heat release, toxic gas release, oxygen release, and pressure increase coming from total gas release **due to electrochemical reactions excluding combustion processes** are in the focus of material safety KPI definition.

The evaluation of corresponding KPI values is performed by comparison to reference electrochemistries for a corresponding cell concept (i.e., liquid electrolyte, solid-organic electrolyte, and inorganic electrolyte-based cells) that remain to be defined in normative framework. This approach enables a pathway for classification of safety characteristics of different electrochemical cells inside the corresponding cell type, as well as comparison of different types of cells. In this way, even the novel material combinations and cell concepts can be evaluated in terms of their safety potential, in addition to well-established evaluation regarding energy and power density, specific capacity, etc.

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2.1 Heat release

The heat release during internal short-circuiting is the fundamental risk for electrochemical cell related to its safety. The short-circuiting can be caused by dendrite formation as result of normal cycling, fast charge cycling and multiple deep discharge cycles. The properties of corresponding materials combination, building the cell electrochemistry, can be measured on small cells (i.e., coin cells or similar) and include only contributions coming from electrochemical processes during the short-circuiting event. Unfortunately, limited data is available in the literature and no standardised, or even at least harmonised, procedure for measurement of related characteristics yet exists. Nevertheless, the methodology of such measurements is already discussed in the literature[5] and can be used for development of suitable normative documents for corresponding testing.

For heat release, two characteristics should be evaluated:

- total heat release (in kJ g^{-1} (heat normalised to the weight of the cell under test including current collectors) and kJ Wh^{-1} (heat normalised to the electrochemical energy stored in the cell))
- heat release rate (in kW g^{-1} and kW Wh^{-1})

Both characteristics can be obtained from calorimetric (e.g., isothermal microcalorimetry, or accelerated rate calorimetry) measurements on small cells as illustrated in figure 1. The heat release rate is particularly crucial for temperature increase inside the cell and battery pack and must be minimised to avoid ignition, combustion and thermal runaway. A protocol for heat release measurements from cathode materials during cycles has been recently proposed in the literature[6]. Typical values of the order of 0.1-1 kJ g^{-1} are expected for common cathode materials. Decomposition heats of cathode materials with different solvents and electrolytes up to 2 kJ g^{-1} are expected from thermodynamics[7]. Contribution from anode materials is also less than 2 kJ g^{-1} [8].

For commercialised cells, the heat release rates are not yet specified up to date, and systematic effort should be undertaken in the near future to quantify the proposed characteristics and create the safety matrix for existing and coming electrochemistries.

[5] C. Ziebert et al. "Electrochemical-thermal characterization and thermal modelling for batteries" in ISBN 97803232977

[6] F. Friedrich et al 2022 J. Electrochem. Soc. 169 040547, DOI: 10.1149/1945-7111/ac6541

[7] Randy C. Shurtz 2020 J. Electrochem. Soc. 167 140544, DOI: 10.1149/1945-7111/abc7b4

[8] J. He, Ionics, Ionics (2020) 26:3343–3350, https://doi.org/10.1007/s11581-020-03509-5

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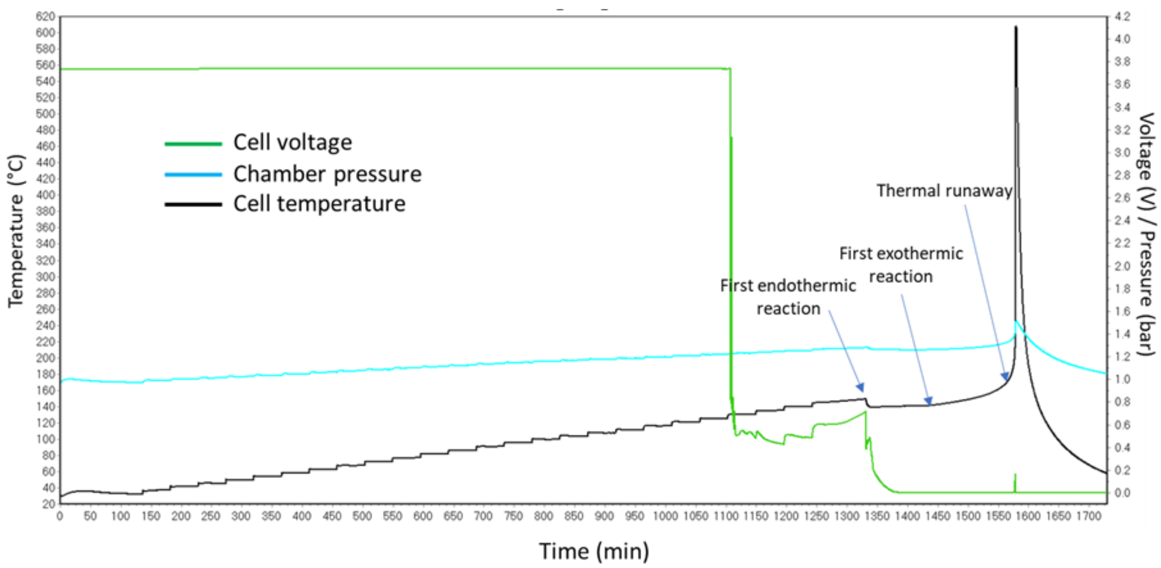

Figure 1: typical ARC test on pristine cell at SOC 50%[9]

2.2 Pressure

The pressure increase is caused by gas evolution during the cell operation often combined with cell temperature increase. Even when venting occurs, the sudden pressure increase can cause strong cell and battery pack damage and should be avoided. The gas evolution comes often from material combinations used and electrochemical processes going in the cell. The example for experimental setup and measurement of such pressure increases in 18650 cylindrical Li-ion cell, using pressure sensors is provided in the work of Lei *et al.*[10] However, this work is dealing with practical, i.e. not concept, cells. Other possible sensors are currently under research and example are given in the Lu *et al*. review[11]. No standards or harmonised testing protocols for testing of small cells (<1 Ah) are yet available. Here, the development of normative documents, round robin tests and systematic investigation on commercialised electrochemistries and promising material combinations are necessary to quantify the corresponding characteristics. It is proposed to use the maximum absolute pressure (Pa) and pressure increase rate (Pa s^{-1}) as well as released gas volume (L g^{-1} (gas volume per gram of cell including current collectors) and L Wh^{-1} (gas volume per electrochemical energy stored)) and gas evolution rate (L $g^{-1}s^{-1}$) recalculated from pressure measurements as characteristics for KPI quantification. As a general indication of the order of magnitude, it should be considered that $\Delta P \sim$ 100-1000 Pa (1-10 mBar) for 1 mL cell volume are expected to correspond to a gas evolution of 2.24-22.4 mL g^{-1} (0.1-1 mmol g^{-1}) of active material[12].

[9] Thi Thu Dieu Nguyen. Understanding and modelling the thermal runaway of Li-ion batteries. Material chemistry. Université de Picardie Jules Verne, 2021.
[10] Lei, B. et al. Experimental analysis of thermal runaway in 18650 cylindrical Li-ion cells using an accelerating rate calorimeter. Batteries 3, 14 (2017).
[11] Lu, X.; Tarascon, J.-M.; Huang, J., Perspective on commercializing smart sensing for batteries. Elsevier: 2022.
[12] Breitung et al., Batteries & Supercaps, 2020, 3, 361, https://doi.org/10.1002/batt.202000010

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2.3 Hazardous gas emission

In case of venting event, especially, the hazardous gas emissions (i.e., toxic gas amount) are crucial for humans and environment and should be strictly limited. During combustion, the gaseous products contain multiple hazardous components (potentially toxic and explosive), but even during the electrochemical operation some toxic molecules can appear. The target of investigation on material level is to identify the formation of hazardous gas components in the small cell during electrochemical cell operation without entering combustion phase. In this area, only marginal knowledge exists. However, similar setups used for measurement of pressure increase can be utilised for gas sampling and its analysis (ie. gas chromatography, ion-chromatography, FTIR, etc.). The released gas volume at normal conditions of pressure and temperature (L g^{-1} (gas volume per gram of cell including current collectors) and L Wh^{-1} (gas volume per electrochemical energy stored)) and gas evolution rate (L $g^{-1}s^{-1}$)) of every hazardous gas component (e.g CO, HF, organic carbonates vapours…) are proposed as characteristics for quantification. The development of normative documents, round robin tests and systematic investigation on commercialised electrochemistries and promising material combinations are necessary to quantify this KPI and create incentive-based, materials development strategies.

2.4 Oxygen release

The high energy cathode materials used in many commercial cells tend to exothermal decomposition and oxygen release under charged conditions upon increased temperature. The decomposition reaction strongly depends on state of charge and operating temperature of the cell and it is a part of thermal runaway process caused by external heat, increasing the overall cell temperature. Thus, the onset temperature at which the decomposition and oxygen release starts, often defines the critical point where thermal runaway takes place. The measurement of onset temperature using calorimetry or thermogravimetry is widely reported in the literature, but without a harmonisation of measurement procedures. Often only the "onset temperature" is reported as a critical parameter. In contrast, however, the amount of heat released (J g^{-1} (heat per gram of cathode electrode – including graphite, binder etc. and excluding current collector – or J Wh^{-1} (heat per electrochemical energy stored in the cathode)) and heat release rate (W g^{-1} and W Wh^{-1}) resulting from exothermal cathode material decomposition are rarely - reported. It is proposed to use at least these three measures as characteristics for safety quantification. Additionally, the released oxygen amount (L g^{-1}) and oxygen release rate (L $g^{-1}s^{-1}$) can be considered as further safety-related characteristics. Here, the development of normative documents, round robin tests and systematic investigation on commercialised electrochemistries and promising material combinations are necessary to obtain the values, which can be used for KPI quantification. As a preliminary information, gas volumes of the order of few millilitres per cell (mL) during NMC-based coin cells operation were reported[13]. Finally, the "onset temperature" is an easily measurable and important indication of the materials' thermal and electrical stability when combined in an electrochemical system, which can also be used to determine chemistry robustness

[13] D. J. Xiong et al 2017 J. Electrochem. Soc. 164 A3025, DOI: 10.1149/2.0291713jes

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3 KPIs at cell level

Evaluation of safety at cell level is crucial because it is the lowest level at which safety behaviour can be directly assessed and managed, as it is the smallest constitutive element of an electrochemical energy storage system. Contrary to characteristics obtained on material level, the characteristics resulting from testing on cell level include heat release connected with combustion of materials used in the cell. The results obtained on material level allow to make a distinction between combustion related and non-combustion related phenomena.

Three majors KPIs have been identified at this level, reflecting the hazards identified as the most concerning ones. Other hazards, like electrolyte leakage or pressure increase, are pertinent in some scenarios but are not considered here, to keep reasonable the number of KPIs and make them usable. Some properties were not considered like electrical hazard because of the low voltage or mechanical strength because this parameter is affected by choices made at pack and system level). Additionally, internal short-circuit is not directly addressed but its consequences (heat release and gas emission are present in this work. Some of these KPIs are in line with the ones identified on the material level and provide more integral values typical for real cell size and specific designs.

3.1 Heat release

The first KPI considered is the quantity of heat released by the cell when submitted to an abnormal situation, either due to an external or internal defect. This parameter is paramount because it affects the propagation of thermal runaway to the neighbouring cells within the module or battery pack.

To quantify this parameter, two options are possible:

- the total thermal energy released by the cell in kJ
- the Heat Release Rate (HRR) peak in kW, representing the maximal instantaneous energy released by the cell, and somehow the power of the reaction.

To be able to fairly compare various size of cells, those values should be taken relatively to the cell energy or weight in units homogeneous to kJ Wh^{-1}, kJ kg^{-1}, kW Wh^{-1} or kW kg^{-1}.

Based on commercial Li-Ion cell abuse test feedback, examples of values that can be found in the literature are comprised between 2 kJ Wh^{-1} up to 50 kJ Wh^{-1} in terms of the total energy released and 0.2 to 1.1 kW Wh^{-1} in terms of HRR. This wide range of values is explained by the variety of cell size and chemistry as well as the variety of contributions that can be considered or not. For example in figure 2, contributions are separated between combustion heat (blue), non-burnt gas that could contribute to heat released in some scenarios, depicted in orange, and other contributions (Joule effect, chemical reactions …), depicted in grey.

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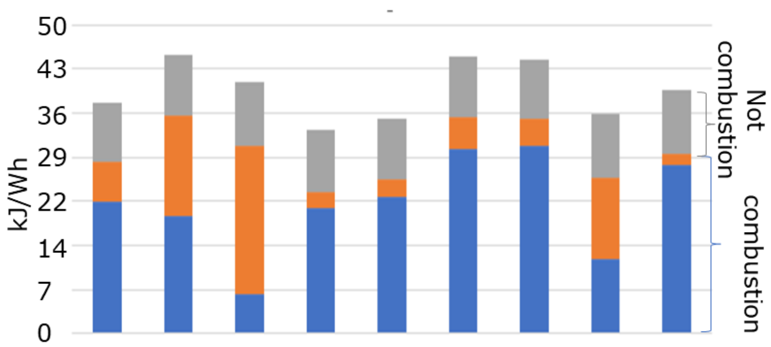

Figure 2: typical values of total energy released and HRR of Li-ion cells. Contributions are separated between combustion heat (blue), non-burnt gas that could contribute to heat released in some scenarios (orange) and other contributions (Joule effect, chemical reactions…) (grey)

The heat release can be measured experimentally by using different methods and equipment. To trigger a thermal runaway, the cell can be placed in a thermal chamber under air where a thermal ramp is applied to the cell through an external heater. The total heat of combustion can be calculated based on the measurement of O_2 consumption or CDG (CO/CO_2) generation. Also, to measure the radiation heat, flux sensors can be placed on the cell surroundings.

However, these techniques do not allow to measure the heat generation due to Joule effect (electric process) nor the heat generation due to the chemical process (e.g. inorganic component decomposition), that can count for a non-negligible part of the total heat release depending on the test procedure.

To assess these components, the test can be performed using calorimetry. One option is to use ARC and applying the so-called Heat-Wait-Search, an incremental heating of the cell to a set point where the cell starts self-heating or temperature ramp method. Another option is to use inhouse calorimeters developed for such measurements.

3.2 Hazardous fumes emission

The second key indicator identified is the quantity of hazardous gas emitted by the cell when submitted to an abnormal situation, either due to an external or internal defect. This parameter is also paramount, because it can affect human health due to the toxicity and temperature of the gases and because of the explosive nature of some released gases.

The toxic and flammability hazards are dependent on external parameters (e.g., volume of the space in which the reaction occurs, ventilation, …) that could not be considered in the definition of a KPI. That is why, to measure this parameter, the total volume of gases emitted at normal conditions of pressure and temperature by the cell relatively to the energy of the cell ($L\ Wh^{-1}$) or to its weight ($L\ kg^{-1}$) has been chosen.

In the literature, usual values are comprised between 0.5 to 6 $L\ Wh^{-1}$ for the current LIB technology [14] [15]. Of course, the nature of gas emitted plays a crucial role and, if technically

[14] D. Sturk et al. Analysis of Li-Ion Battery Gases Vented in an Inert Atmosphere Thermal Test Chamber, Batteries, MDPI, 2019

[15] FAA report DOT/FAA/TC-15/59 on vent gas analysis, https://www.fire.tc.faa.gov/pdf/TC-15-59.pdf

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possible, the volume of gas can be reconsidered by considering only known toxic (e.g. CO, HF…) and flammable (e.g. CO, H_2…) gas contents[16].

The total volume of emitted gas can be measured experimentally by different means. First, by inducing a thermal runaway, through thermal, mechanical, or electrical abuse, to a cell placed in a close container and in an inert atmosphere. Using a pressure sensor in the container will allow to measure the level of pressure due to the gas release and to estimate the volume of emitted gas.

Another option is based on analysis through FT-IR, μGC and other adapted gas analysers that enable the assessment of the nature of the gas emitted as well as their concentration. In controlled conditions, this allows to approximate the total volume of emitted gas. This method is more laborious than the first one, but gives important information about the composition of the gases and the possible associated risks.

In addition to the quantity of gases emitted, it would be of interest to consider the fume toxicity, as well as the particles emission to fully assess the toxicity of the species released by the cell under thermal runaway. At present, the knowledge in this field is not mature enough to be considered in an indicator but systematic effort should be undertaken in the near future to realize holistic quantification of fume emission toxicity.

3.3 Entering in thermal runaway (TR)

Contrary to material level, some hazards at cell level can be mitigated or even avoided by passive protection systems. The last identified KPI is linked to the thermal and electrical reactivity of the cell and its ability to avoid or delay TR. This KPI seemed more difficult to define and is currently at a lower level of readiness.

The first dimension is to evaluate thermal stability and, more specifically, determine when a thermal runaway is triggered and cannot be stopped while the root cause of the defect has been removed (for example stopping the overcharge or reducing the environmental temperature of the cell). When a thermal runaway is triggered, cascading adverse events can indeed occur, such as fire, flying parts of the cell, explosion, etc.

This is determined by measuring the temperature at which the cell enters in TR. Several approaches can be used to define this temperature, for example by using a self-heating rate threshold or by examining the apparitions of outside effects (e.g., degassing…)

It can be measured experimentally by performing an abuse thermal test on the cell placed in a calorimeter (ARC for example) and by applying the Heat-Wait-Search or temperature ramp method. Cell failure can also be induced by simply applying a thermal ramp on the cell using a thermal resistance surrounding the cell placed in a thermal chamber. The temperature at which commercial cells begin to enter in thermal runaway is on average comprised between 150 to 200°C for LIB.

[16] A. Bordes et al., New insight on the risk profile pertaining to lithium-ion batteries under thermal runaway as affected by system modularity and subsequent oxidation regime, Journal of Energy Storage, 2022

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The second dimension is to evaluate electrical stability, which can be determined by imposing an electrical abuse (overcharge seems adapted) on the cell until reaction, or eventually triggering a passive safety device. For each dimension, the produced effects can be evaluated according to the EUCAR level scale.

Eventually, fore some application (e.g. automotive), testing the cell using mechanical abuse would be an option but it seems more adapted to evaluate this at higher levels (module/pack/system).

The resulting KPI is then a correlation between thermal stability, effect of the thermal runaway (according to EUCAR) in case of thermal abuse, electrical abuse (eg. overcharge, overdischarge, external short circuit) and eventually mechanical abuse.

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4 KPIs at pack level

A battery pack consists of several cells. Therefore, the hazardous effects of damage at pack level may be many times that of a single cell. While a spill from one cell does not necessarily cause other cells to leak, a thermal event can spread to the pack level. Electrical dangers also can be identified directly by the battery specifications. Therefore, only the hazards from a thermal runaway event are considered for the safety KPIs at pack level. Concerning the particle emission also, the scenario needs to be considered (e.g. sight of a driver, human lungs…). Corrosiveness is not so much a topic (rather a long term effect.

At the same time the pack level offers different options for safety measures in addition to the characteristics of the cells. Other safety measures could be taken into consideration (eg time to escape from a car in case of TR, management of fumes in aerospace application…), however those parameters belong to system level which is excluded from this work because they are specifical to the application.

The following three most severe hazards can be identified: cell-to-cell propagation of the thermal runaway (hazards: flames, projectiles, liquid metal), hazardous (explosive, toxic, particles) fume gas emission and high temperatures inside and outside the system.

4.1 Cell-to-cell propagation

While the effect of a single cell undergoing the thermal runaway in most cases does not cause a major threat to the environment, it will do so if the cell ignites the neighbouring cells and thereby forces the full pack (or parts of it) into the thermal runaway. This ability of cell-to-cell propagation resulting in a thermal event of the whole pack is, therefore, the main cause of severe hazardous situations for the environment (humans or neighbouring goods) [17]. While a short-term flame / thermal reaction of an isolated cell may not cause a critical situation, the long-lasting high temperatures and flames may ignite nearby objects and materials and the large amounts of toxic and flammable gases from the pack may lead to hazardous atmospheres.

Apart from the ability to react at all on cell level, the cell-to-cell propagation, therefore, is considered as the most significant KPI at pack level. The ability of cell-to-cell propagation can be tested by a propagation test, e.g. as described by the UN IWG lithium batteries[18]. However, in order to verify the ability of cell-to-cell propagation for the pack, module or battery level, a suitable sample unit size needs to be identified to represent the full pack. Heat sinks in the battery case, isolation and air/ separation (e.g., constructural separation as in battery stationary applications) may be addressed in this respect, testing will require ignition of an inner cell. Suitable initiation methods are e.g., heating (heater, flame), mechanical (nailing) or electric (overcharging). The pass criterion can be a yes/no decision or a time-dependent evaluation.

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[17] Ruiz Ruiz, V. and Pfrang, A., JRC exploratory research: Safer Li-ion batteries by preventing thermal propagation, EUR 29384 EN, Publications Office of the European Union, Luxembourg, 2018, ISBN 978-92-79-96399-5, doi:10.2760/096975, JRC113320

[18] Work of the informal working group on hazard-based classification of lithium batteries and cells, expert from France on behalf of the informal working group, UNECE SCTDG 2022, https://unece.org/sites/default/files/2022-06/UN-SCETDG-60-INF11e_0.pdf

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Following this approach, a two component KPI can be defined.

The first component, evaluating the number of elements involved in the pack thermal runaway. In the best case, only the abused element reacts, whereas in the worst case, the TR propagates to all the elements composing the pack in a chain reaction. In intermediate cases, the TR propagates only to a limited number of elements or sub-systems (module, rack…).

The second component aims to reflect the propagation speed, which may vary depending on the cell type used and system geometry, as shown in figure 3. The speed of the reaction is linked to the effect severity, and consists in the evaluation of the quantity of energy (Wh) reacting simultaneously. The proposed unit would be Wh (of battery reacting)/min. The mass loss per minute can be used to estimate this parameter or by calculating the number of cells reacted per time unit through measurement of temperature distribution in the pack or by numerical simulation. Other possibilities are to directly assess the "severity" parameters by measuring maximal HRR (as done at cell level) or the amount of gas emitted/min in absence of gas combustion. To reflect the worst-case event, the maximal instantaneous value of this indicator should be reported.

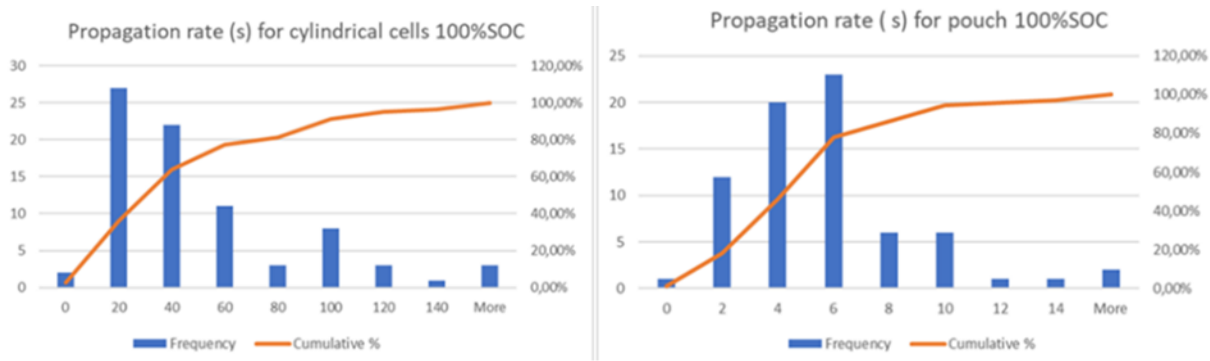

Figure 3: example of propagation rate measured for cylindrical and pouch cell. Source: recharge and UN IWG on transport of dangerous goods

In order to get fair and representative results, the existing thermal runaway mitigation means should be considered and taken into account in the testing protocol. However, for each application they should be clearly defined and listed depending on the usage environment of the system.

4.2 Hazardous fume emission

The fume emission of a lithium battery pack in a closed room will in most cases be a hazardous event. With today's commonly used cell chemistries the fuel gases are toxic for humans (e.g., CO, HF, …) and/or may lead to explosive atmospheres (e.g., CO, H_2, …). Even for

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small cylindrical cells (eg : 18650 format) a gas volume of example up to 10 L may be expected[19].

The gas emission volume and the concentration of the contained species will be measured in a thermal runaway experiment. In cases where there will be significant mitigation effects / contributions of the housing material of the battery, a pack / module / battery test may be required. In other cases, cell testing may be sufficient. Depending on the gas measured (HF, CO, …) different test methods are possible (e,g, FT-IR, laser diode, washing bottle…).

KPIs for hazardous fume emission would allow to evaluate, if the emission is problematic or not, in an accidental scenario. Concerning toxic hazards, we propose to assess the concentration of each toxic gas component that is found and compare it to the AEGL2 limit. Concentration should be assessed considering the environment in which the battery is used (large room, outside, ventilation, sprinklers…) Concerning explosive hazard, the concentration of explosive gas should be assessed and compared with their Lower Explosive Limit.

Again, concentration should be assessed considering the environment in which the battery is used (large room, outside, ventilation, sprinklers…).

4.3 Effects of the temperature increase from the system to its environment

The maximal temperatures reached by both single cell or pack forced into thermal runaway are in the range of ca. 600-1000°C)[20]. However, it is also the duration time of the peak temperature that will affect the surrounding flammable materials and goods. The maximum temperature can be detected with thermocouples and the time / temperature curve will be recorded. In this respect, flames are also considered as a temperature increasing element and the effect will be captured by a temperature measurement. For this reason, the flammability and explosibility are not considered as independent KPIs.

Temperatures need to be measured on the pack / system / application levels, because there may be mitigation tools or there may be additional fire load.

For the Dangerous Goods Transport regulations, a maximum outside surface temperature of 100°C has been established a pass criterion (UN recommendations[21]). In order not to be a danger for the environment (goods, humans) the pack level needs to have prevention or mitigation measures in place. This can be isolation, shut-off mechanisms or sprinklers as examples. Looking into the future there will be artificial intelligence solutions or programmed routines for determining the temperature.

The related KPI will depend on the end application and integration and compares maximal temperature reached on the surface of the system with the critical temperature of the surrounding elements. Various thresholds can be proposed (Bursting including projectiles, flames, temperature value e.g., 238°C for cardboard).

[19] Meta-analysis of heat release and smoke gas emission during thermal runaway of lithium-ion batteries, Tim Rappsilber, Nawar Yusfi, Simone Krüger, Sarah-Katharina Hahn, Tim-Patrick Fellinger, Jonas Krug von Nidda, Rico Tschirschwitz, Journal of Energy Storage, 2023

[20] Experimental study on thermal runaway and vented gases oflithium-ion cellsLiming Yuan⁎, Tom Dubaniewicz, Isaac Zlochower, Rick Thomas, Naseem RayyanPittsburgh, Process, safety and environmental protection, 2020

[21] https://unece.org/sites/default/files/2022-06/UN-SCETDG-60-INF11e_0.pdf

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Tests 4.2 (hazardous gas emissions) and 4.3 (surface temperature) only need to be performed in case the cells / packs show cell-to-cell propagation (Tests 4.1). In this case, the values obtained on cell level could be used.

Maximum temperatures and fume composition will vary depending on

- Chemical composition
- State of charge
- Energy density (e.g., density of cells inside [4])

Those and possibly further parameters should be selected to reflect foreseeable worst-case scenario.

The initiation temperature which leads to a thermal runaway event also differs for the different cell types. However, this parameter will be covered by the investigations on cell level.

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5 Overview and conclusion

The Batteries Europe Safety Task Force, composed of experts form the academic, research organisations and industry sector, has defined an overview of Safety KPIs. The objective of the present document is to kick off the definition of the Safety KPIs that can be used as a reference and guidance for current and forthcoming EU R&I actions. To fulfil this aim, the defined overview is structured as follows: 3-4 KPIs per level (material, cell, pack) are identified and the definition of each KPI, unit, reference values and examples for measurement of each of the KPIs are provided as well. These KPIs were developed based on the hazards identified for LIB but were chosen to be able to cover several technologies with minimal adaptations concerning specific hazards or adaptation of scale. Following those guidelines, in the previous chapters a detailed overview of the most critical KPIs has been defined which is summarised in Table 1.

Level/ Hazard	Heat	Pressure	Hazardous Gas emission	Onset Temperature O_2 evolution	Propagation (cell to cell)	Temperature (outside the system)	Entering in TR
Material (Trigger)	X	X	X	X			
Cell	X		X				X
Pack			X		X	X	

Table 1: Summary of the selection of KPIs per level

The present classification can be treated as a starting point, guideline, or reference, however the provided KPIs are not yet quantified in the form of absolute values. In addition, although the provided methods proposed to ensure the possibility of measurement of each indicator proposed, they are not precisely described in this document since this is an issue to be reported and resolved at the level of standardisation committees (IEC or CENELEC). A possible successful transfer and follow up on this regard would be the integration of the KPIs into the one already existing in normative and regulatory framework. Several European research projects are ongoing focusing on developing different sensors and self-healing that would lead to the development of long lasting and safer batteries. A good overview of this activities can be found in the roadmap of Batteries 2030+[22]. In addition, the present overview focuses on the integration and understanding of the battery ecosystem in overall by integrating the different levels. For example, the hazard "Hazardous Gas Emission" was highlighted by the different treated levels independently. This KPI shows the importance of the hazard at different levels and could be a successful transfer to novel approaches such as the Battery Passport[23].

Although there are many other aspects which should be covered and discussed at safety level, such as storage, recycling, manufacturing, as well as specified for specific applications (mobility, storage), the present work focuses on the hazards connected with battery operation. This work can be extended and expanded on other applications and use cases in which a different KPI list can come into place. In the same way, future and emerging technologies could benefit from this reference work with the aim to transfer the lessons

[22] https://battery2030.eu/research/roadmap/
[23]https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A52020PC0798&qid=1608192505371

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learned and accelerate the market time by providing safety limits that should be detected per level. The study of other applications, critical aspects and the transfer to novel technologies has been listed as the next step in the Safety Task group which is currently in place.

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