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ScienceDirect

Transportation Research Procedia 72 (2023) 3625–3632

Transportation Research Procedia

www.elsevier.com/locate/procedia

Transport Research Arena (TRA) Conference

Ensuring accurate Key Performance Indicators for Battery applications by implementing consistent Reporting Methodologies

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Abstract

Batteries have been identified as a key technology enabling the transition to a low-carbon economy. To achieve the EU decarbonization target by 2050, the demand for high-performance, low-cost, and sustainable batteries is rapidly growing. Several battery technologies have been proposed for different applications, e.g., automotive, aviation, maritime, etc. In this rapidly evolving field, while key performance indicators can be readily accessed, the performance evaluation and comparison of battery technologies remain a challenging task, due to the huge variation in the quality and quantity of data reported and the lack of a common methodology. To address this challenge, Batteries Europe stakeholders have suggested reporting methodology guidelines which, if implemented, will facilitate the identification of the most promising cell technologies while highlighting areas for improvement.

Keywords: Batteries; Electrochemical cells; Key Performenace Indicators; Reporting methodologies; Technology benchmark;

1. Introduction

The electric vehicle market is one of the most dynamic areas in the clean energy world. Sales of electric vehicles (EVs) have doubled in 2021 from the previous year and nearly 10% of global car sales were electric in 2021, four times the market share in 2019 (Global EV Outlook 2022, no date).

EVs have drastically evolved within the last decade. Different battery technologies have allowed the electrified transport sector to advance, starting from lead-acid, NiCd, NiMH, and culminating in the massively adopted Li-ion chemistry. A battery for electrified vehicles is a compromise between high-power and high energy performance,

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10.1016/j.trpro.2023.11.559

ideally light, small in volume, while guaranteeing long lifetime, low cost, as well as safety, recyclability, and environmental sustainability (WG5 Batteries Europe, 2021).

Several roadmaps and strategic documents have indicated key performance indicators (KPIs) of battery technologies and projections for the near future for a successful penetration of EVs in the electrified transport market.

However, the benchmarking and performance comparison of different battery technologies are greatly hampered by the lack of a common reporting methodology. The comparative assessment of cell performance has proven to be challenging when comparing results within the same battery chemistry, between different cell chemistries, but also when trying to transfer knowledge gained from lab scale to pilot line level and eventually into large scale production. In the absence of fair comparable data globally there can be duplication of efforts and a slowing of progress in the development of the current and next generation battery technologies for implementation in the automotive sector. This is particularly poignant given battery technology is one of the key industries required to support the decarbonization of the transport sector.

To address this deficit, the working group 1 (WG1) "New and Emerging technologies" of Batteries Europe, initiated the development of common reporting methodologies guidelines (WG1 'New and Emerging technologies', 2021). The document provides the basis for the development of homogenized performance metrics and a transparent reporting methodology at cell level, necessary for the reliable benchmarking of battery chemistries. For a successful implementation, the suggested reporting methodology needs to be adopted by most scientists and implemented in all battery research projects for monitoring the progress beyond the state-of-the-art. Editors and Board members of high-level scientific journals could greatly assist in the implementation of such recommendations. This would result in setting the "gold standard" for scientific reports of battery chemistry developments in Europe and would set a trend for a worldwide implementation. Whilst this development will not have an immediate impact, it will set a best practice for results' reporting and will reduce the occurrence of "overly optimistic" claims often occurring in the field of battery research ('Thomas Edison himself said: "Just as soon as a man gets working on the secondary battery it brings out his latent capacity for lying", The Electrician (London) Feb. 17, 1883, p. 329.).

2. Context

The EU SET Plan (Strategic Energy Technology Plan) has identified batteries as one of the key technologies necessary for the energy transition and has proposed in Action 7 a classification of the current and future cell chemistries which would enable the EU to become competitive in the global battery market to serve local electromobility and stationary storage (Integrated SET-Plan Action 7, 2016). In 2019, the Batteries Europe ETIP, a technology platform covering the whole battery value chain, was established to developed an holistic Strategic Research Agenda for the European Battery R&I along with related Roadmaps and Position Papers (Batteries Europe, 2019) .

Today's optimised lithium-ion batteries (LIBs) with different cell chemistries represent the current core technologies for EVs and are expected to grow in the stationary energy storage market. LIBs and incremental improvements to them, are expected to remain the battery cells of choice for the nearest future considering the time typically required to move the technology from R&D on battery materials to large scale production (Marinaro et al., 2020). Present lithium-based battery research focuses principally on incremental improvements in the energy density of LIB cells (Armand et al., 2020). The next leap may be reached utilizing Li-metal anodes (Varzi et al., 2020) while there is plenty of room for innovation in future cell technologies or "next generation" chemistries, from which important environmental benefits are expected, but are currently at an early stage of development. Whilst energy density is one of the Key Performance Indicators (KPIs) to be considered for EV applications, where LIBs will dominate the market for the next 10-15 years (Marinaro et al., 2020), a growing variety of applications with different requirements have accelerated research towards alternative chemistries potentially able to satisfy this market diversification. The next-generation (non-lithium) chemistries also include sodium (Hasa et al., 2021), magnesium (Dominko et al., 2020), aluminium (Elia et al., 2021), zinc (Borchers et al., 2021) and calcium (Stievano et al., 2021) based systems, as well as innovative redox flow systems (Sánchez-Díez et al., 2021), where safety, cost, manufacturability, sustainability, and dependency on raw critical materials play a fundamental role.

KPIs and characteristics are generally defined at a specific level, such as cell, module, pack, or system level.

Within the frame of new and emerging technologies, continuous advances in electrode materials, electrolytes, functionalized separators, auxiliary inactive components and cell designs are reported. Today, a wide variety of electrochemical techniques and experimental conditions, cell components and cell setups are used to characterize novel battery materials and other components of interest, ultimately making accurate comparison of results from different studies extremely challenging. Furthermore, "inappropriate" selection of the cell components and/or measurement conditions, often occurring in scientific literature, can lead to results, whose interpretation is very difficult and even erroneous (Nölle et al., 2020).

All the above suggests the urgent need for the assessment of tools for benchmarking cell chemistries enabling performance comparison and facilitating a correct identification of the most promising technologies able to meet the requirements and KPIs set for the EV application.

Working group 5 (WG5) of Batteries Europe has identified KPIs at cell level for batteries to be employed in light-duty battery EVs. A summary of the most important parameters is reported in Table 1. A more comprehensive overview of battery KPIs for road, rail and air electrified transport is reported in the roadmap provided by WG5 of Batteries Europe (WG5 Batteries Europe, 2021).

Table 1. Light-duty battery electric vehicles (BEV) (WG5 Batteries Europe, 2021).

KPIs cell level	**Conditions**	**2019**	**2030**
Specific Energy (Wh/Kg)	C/3 charge and discharge, 25 °C, charge mode CCCV	250	450
Energy density (Wh/L)	C/3 charge and discharge, 25 °C, charge mode CCCV	500	1000
Specific Power (W/Kg)	180s, SOC 100%-10%, 25 °C	750	1000
Power density (W/L)	180s, SOC 100%-10%, 25 °C	1500	2200
Cycle life (80% SOH) (n° cycles)	80% DOD, 25 °C	1000	2000

In order to identify the most promising next generation battery technologies able to satisfy the KPIs and requirements of the electrified transport sector, correct benchmarking and performance assessment are crucial.

This work focuses on the identification of guidelines and methodology for reporting characteristics and performance metrics extracted from experimental investigations conducted at the cell level, where cell is defined as an electrochemical device composed of a positive (cathode) and a negative (anode) electrode, an electrolyte (liquid-separator, solid, hybrid), and passive components (e.g., current collectors, cell packaging). KPIs for module, pack and system level are not detailed in this work. The aim is to homogenize the reporting of battery results and data of mature cell chemistries and new and emerging battery technologies.

3. Challenges when comparing results: illustrative examples

Reporting methodologies are essential for accurate comparisons and reproducibility. Thus, all results should refer to consistent experimental conditions, provide a reproducible and useful data set, and ensure realistic evaluation of lab scale data for extrapolation to pilot- and industrial-scale applications. Unfortunately, a number of misleading reporting practices are commonly found in the literature (WG1 'New and Emerging technologies', 2021), which can be summarised as:

- Undefined and/or varying environmental test conditions.
- Unrealistic evaluation of cell performance in respect to feasible commercial cell design and/or operating conditions.
- Undefined implications of materials structure and/or physical-chemical reaction mechanisms affecting electrochemical response at cell level.

These inconsistencies contribute to the 3 main challenges associated with benchmarking cell chemistries as highlighted in the specific examples reported in the following subparagraphs.

3.1. Challenge 1: Comparing results within the same cell chemistry

It is well known that the cell performance strongly depends on the environmental conditions under which the cell is tested. Temperature, for instance, being the most obvious one. Detailed information about test conditions should always be given to allow a reliable comparison of cell performance. Inappropriately selected experimental conditions, as well as undefined and varying environmental test conditions, may result in confusing and/or misleading conclusions.

Fair benchmarking of the cell performance is also hindered by the adoption of unrealistic and/or widely variable cell component composition. For example, an excess of active and inactive components (electrolyte, carbon additive and binder, etc.) used in a given cell can substantially increase its performance (power, cycle life, etc.). Finally, implications of undefined materials structure and morphology make performance comparison challenging, since differences in the structure and morphology of the materials used substantially affect the cell behavior.

3.2. Challenge 2: Comparing different cell chemistry

Frequently, new emerging technologies are compared with mature commercial cell technologies. However, the same parameters cannot necessarily be easily applied or even be relevant to battery cells classified as new and emerging technologies. This makes the comparison truly challenging and leads to unrealistic conclusions. One example demonstrating this challenge is the comparison of the specific gravimetric capacity obtained for two different cell chemistries, such as LIBs and lithium-air cells. The capacity of lithium-air cells is often reported per unit mass of the carbon “electrode” (acting as substrate for deposition of discharge product), not including the weight of the discharged product lithium oxide or lithium peroxide. This is substantially different from the LIB cell case, in which the capacity is reported per mass of the discharge electrochemically active material. In addition, the carbon “electrode” used in lithium-air systems generally present a very high porosity and the discharge products have much lower density than the typical lithium-ion cathode material. So overall, the energy density of the positive electrodes for lithium-air cells is expected to be substantially lower than that of LIB cells. Nonetheless, all these aspects are rarely considered and the reported energy density values of lithium-air system are generally exceeding those reported for LIBs when investigated at a lab scale level (WG1 ‘New and Emerging technologies’, 2021).

3.3. Challenge 3: extrapolating lab scale data to industrial scale

Lab scale testing conditions are usually not directly applicable to industrial requirements. The two examples discussed demonstrate why better reporting methodologies are needed to ensure a sound evaluation of lab scale data.

Example 1: Enormous efforts have been devoted to identifying strategies to tackle the issues affecting the lithium-sulphur cell technology. Some of the proposed solutions might be useful; however, test conditions are not applicable to industry or are built on metrics that are not relevant for practical applications. For practical lithium-sulphur cells to reach an energy density >500 Wh.kg-1, the mass loading of sulphur must be at least in the range of ~7–8 mg cm-2. Such high mass loadings require thick sulphur electrodes (>300 µm). This leads to serious polarization across the electrode due to rather long electronic and ionic paths through the electrode. Additionally, the metallic lithium anode capacity should be close to stoichiometry and a limited electrolyte volume should be employed. All these parameters are rarely adopted in lab-scale research cells, in which the sulphur cathode is tested with low mass loadings, high Li excess and unclear amount of electrolyte. Regrettably, the excellent performance and cyclability of low mass loading sulphur electrodes proven at lab-scale, cannot directly be transferred to a commercially viable system.

Example 2: Hierarchically nanostructured electrodes are often reported to present promising performance. However, they generally present low tap density, making them unlikely to meet volumetric energy density demands for practical applications where high areal loading and tap density are crucial parameters to be considered. Nonetheless calendaring of the electrode to increase the density, results in destroyed hierarchical architectures affecting electrochemical performance. Therefore, a direct comparison of results obtained at lab scale and reported in literature for hierarchically nanostructured electrodes with a mature technology such as commercial LIB cells, can be misleading. This is especially true for data reported in half cells where excess electrolyte and counter electrode are frequently used.

4. Classification of cell technologies

Over the years, several cell technologies classifications have been proposed. The main difference arises from the reversibility of the conversion processes from chemical into electrical energy. Following this approach, non-rechargeable cells are defined as primary cells, while rechargeable cells are classified as secondary cells. This simple classification shows some limitations. For example, commercial Zn-air batteries are primary batteries while secondary (electrically rechargeable) zinc-air batteries are still under development. However, they can also be mechanically recharged (by adding more zinc once it is consumed) which adds extra confusion if not properly described. A plethora of classifications have been proposed, which so far are based on the electrolyte used (e.g., aqueous vs. non-aqueous), the chemistry (e.g., lithium-ion and post lithium chemistries) or the expected performance requirements (e.g., high energy vs. high power), just to mention a few examples. To maintain full neutrality with respect to the existing and new and emerging cell chemistries, we restrict the classification to the structure of the fundamental unit, i.e., the cell. A clear comparison between different cell technologies is facilitated by firstly defining the cell structure and consequently identifying the main constituents and characteristics. All rechargeable cell chemistries can be split in two large families: closed cells and open cells. Different cell structures are in turn defined by the electrode nature. Looking at the various cell architectures, it is possible to identify cells for which the maximum energy stored is fixed by, at least, one electrode. For example, even though Zn-Air cells are open to the environment on one side, their energy storage capacity is limited by the total amount of zinc that is present inside the cell, while air is in endless supply. In these types of cells, energy and power are bound because the amounts of reactants cannot be changed freely. On the other hand, in some flow cells, stored energy is in the form of dissolved ions in the catholyte and anolyte. These can be stored outside of the electrochemical cell; thus, the energy storage capability of flow cells depends on the size of the reservoirs storing the solutions. In these systems, the cell itself does not represent a limit to the energy storage capacity, but rather a limit to the power performance. This architecture enables independent power modulation upon changing the cell design and energy modulation by changing the size of the tanks. However, among the various flow-cell systems, Zn-Br batteries do not offer the above-mentioned advantage. Indeed, Zn-Br cells can store bromine/bromide species in an external reservoir, but the zinc is plated on the electrode inside the converter. Thus, in Zn-Br batteries, the energy storage capacity is determined by the maximum amount of zinc that can be deposited by the surface area of negative electrode. Similarly, metal-air cell chemistries are in general limited by the metal electrode even if oxygen is provided by air external to the cell.

Considering the different cell architectures, we divide all electrochemical cells into two main groups according to their capability to enable independent scaling of delivered power and energy. Cells in which at least one electrochemically active component is contained within the cell itself (e.g., lithium-ion or Zn-Br batteries), exhibit power and energy capabilities which are limited by the at least one of the electrodes. These types of cells are referred to as CEPc because their energy and power are coupled. On the other hand, cells where all the electrochemically active materials are stored outside of the cell (e.g., conventional redox flow cells) are referred to as DEPc.

According to such classification, the main new emerging technologies can be grouped as follows:

- **Coupled Energy and Power cells (CEPc):** Li & Li-ion, Na & Na-ion, K & K-ion, Mg & Mg-ion, Ca & Ca-ion, Al & Al-ion, Innovative Lead-acid, Zn & Zn-ion, Metal-sulphur, Metal-air, Anion Shuttle, Metal redox flow.
- **Decoupled Energy and Power cells (DEPc):** Metal-ion redox-flow, Organic redox-flow, Semi-solid redox-flow.

This classification enables a direct comparison among cell technologies within the same class, although the direct comparison between CEPs and DEPs system is not trivial.

5. Reporting requirements in Scientific journals

Several scientific publications and editorials have recently highlighted the need for a common ground for reporting research results related to batteries (Betz et al., 2019; Chen et al., 2019; Noori et al., 2019). The editorial board of Journal of Power Sources recently published a document entitled “Good practice guide for papers on batteries for the Journal of Power Sources” (Li et al., 2020). Also the editorial team at Joule (Cell Press) and Batteries & Supercaps (Wiley-VHC) recently adopted Standardized Battery Reporting Guidelines accompanied by a battery checklist (CellPress, 2020; Wiley-VCH, 2021). The initiative has been followed by many other journals inviting authors submitting battery focused manuscripts to provide the checklist at the time of submission. Additionally, within the activities of WG1 in Batteries Europe, a series of critical reports has been compiled by leading scientists evaluating the most promising new and emerging cell chemistries (Dominko et al., 2020; Li et al., 2020; Varzi et al., 2020; Borchers et al., 2021; Elia et al., 2021; Esser et al., 2021; Hasa et al., 2021; Karkera, Reddy and Fichtner, 2021; Sánchez-Díez et al., 2021; Stievano et al., 2021). All the above-mentioned documents represent a good foundation for the proper reporting aiming at reducing the occurrence of "overly optimistic" predictions and claims and promoting a more realistic and effective assessment of new and emerging cell chemistries.

6. Guidelines for the comparison of the new cell technologies

With the introduction of new cell chemistries and technologies, new reporting guidelines need to be established.

Electrochemical cell tests should provide reproducible and useful data enabling the accurate comparison within a given cell chemistry and between different cell chemistries. The information and data provided need to be at least sufficient to characterize and define the initial cell performance, but also to quantify degradation over the cell lifetime. Finally, preliminary safety testing and chemical hazard evaluations would be a valuable addition.

The new guidelines aiming at establishing comparable performance metrics and a transparent reporting methodology should include:

- Cell components characteristics.
- Details on the electrochemical measurements (electrochemical set up, testing conditions and obtained KPIs).

Among all useful information, KPIs are a set of performance metrics enabling the initial comparison of cell chemistries and technologies. However, at the materials level, the characteristic of the active materials and the final electrode's composition and properties should be given with sufficient detail for a fair analysis of the material performance to be possible. Cell components (and their constituents) are defined by characteristics and not by KPIs.

6.1. Cell components characteristics

Comparing new cell chemistries and technologies with existing ones requires the evaluation of all the cell components that can influence the performance of the final cell. The following cell components are certainly the most important: 1) Electrodes (for CEPc and DEPc); 2) Electrolytes for CEPc; 3) Separators (for CEPc and DEPc); 4) Current Collectors (for CEPc and DEPc).

In the development of new and emerging cell chemistries, a large part of the ongoing research effort is devoted to new materials discovery and the assessment of their performance. In such endeavours, accurate reporting and precise description of the synthesis procedure is important to facilitate comparison of results among different reports.

In scientific publications, all synthesis steps should be described in detail, allowing for reproducibility in other laboratories, being this the basis of any scientific report. Information associated to the scale of the synthesis (size of batch) should be provided. All the chemical precursors/solvents should be described in terms of supplier, purity, and other possible pre- and post-treatment processes (such as purification or drying) after purchasing. Synthesis conditions such as temperature, pressure, environment, concentration, amount of starting material, pH etc.., should be given. The obtained material should be described in terms of stability, and methods of further handling/storage (inert or ambient conditions) should be given. Each new material should be characterized in terms of chemical composition, physical and mechanical structure, and morphology. This should be accompanied by the detailed experimental conditions used for the analysis, including sample procedure preparation and experimental protocol for analysis and accuracy of determined values. This will ultimately enable a better data comparison, offering a clear overview of the materials properties. Regarding the electrode assembly process, details should be provided about active material and all other non-active components, the solvent (if any) used for the slurry preparation, the drying procedure, calendaring and other relevant process parameters and compounds. Overall, when going from materials to electrodes (for tests in electrochemical cells) it is important that several characteristics are given. For a full overview of the characteristics needed for electrodes, electrolyte, separator, and current collectors it is possible to consult the "Reporting methodologies" publication from Batteries Europe (WG1 'New and Emerging technologies', 2021).

6.2. Electrochemical set-up, measurements and KPIs

Transparency in reporting the selected electrochemical cell set-up and all testing conditions during electrochemical measurements is the first step for a realistic comparison between new cell technologies.

As several laboratory-scale cell setups (beaker, Swagelok-type, coin (button), and pouch cells, among others) may be employed to test novel chemistries, the electrochemical performance of a material could be affected differently by the various cell configurations. Even when a new component such as an electrode is used in conjunction with standard commercially available components, particular cell characteristics such as a large electrolyte volume (e.g., in beaker cell) or a large counter electrode could artificially increase the performance of poor electrochemical systems.

A typical example is the common performance evaluation of electrode materials for application in lithium-ion cells employing oversized metallic lithium or well-known insertion materials as counter electrodes in the so-called “half-cell configuration”. This half-cell set-up is used to determine specific thermodynamic characteristics of the investigated materials but requires the use of a counter electrode (e.g., lithium or sodium metal) which could contribute to the overall electrochemical activity. Additionally, these counter electrodes are usually oversized with respect to the investigated one, frequently hiding poor Coulombic efficiency in full cell configuration. On the other hand, these metal counter electrodes contribute, via side reactions with the electrolyte, to the formation of reactive compounds which in turn affect the electrode under investigation. Therefore, additional limitations may apply when half-cells are used for characterization of a new material. The assessment of the performance of cells requires the measurement and quantification of a series of performance metrics. Although performance metrics for individual electrodes are important (evaluated in half-cells), the evaluation of electrodes in practical cell configuration is critical for the identification of the true cell performance.

The following KPIs, referring to complete cells without casing (if casing is included it should be specified), are required for the appropriate performance comparison of different cell technologies, including the commercial ones:

Table 2. List of KPIs for complete CEPc and DEPc cells.

Necessary KPI’s
Cell type (pouch/cylindrical/prismatic, coin cells, two/three electrode T-cells) and size
Anode/Cathode balance (mass and capacity ratio)
Specific energy and energy density of the cell at two specific C rates (C/10 and 2C rate) or current densities upon (dis-)charge
Energy efficiency of the cell at C/10 and C rate (dis-)charge
Coulombic efficiency of the whole system at C/10 and C rate (of choice) (dis-) charge
Cycle life (upon SOC change per cycle of at least 80%)
Test temperature
Pressure/compression requirements during operation and cell manufacturing.
Cell volume variation % at (dis-)charge (if measurable)
Optional KPI’s (according to availability of results)
End of charge voltage / End of discharge voltage
Average (dis-)charge voltage at C/10 and a second C rate appropriate for a specific application
Overcharge behavior / Overdischarge behavior
Preliminary safety assessment

It is also important to specifically identify the testing conditions including environmental conditions such as temperature, flow rate in flow systems, pH, and the experimental set up (cell geometry, potential window for testing, etc.), which inevitably affect the above listed KPIs.

6.3. Safety testing & chemical hazards evaluation

Even if they are not paramount for a first level evaluation, preliminary safety testing and chemical hazards evaluations should be encouraged (especially for high TRL technologies) to ascertain the feasibility of developing a new cell chemistry. The following list identifies the simplest parameters that could be assessed and given along with the development of a new cell chemistry or, even more, the development of new materials for existing cell chemistry.

Table 3. List of preliminary safety, toxicity hazards characteristics for complete CEPc and DEPc cells.

Cell component level
Toxicity from MSDS (mandatory for commercial materials, if available for in lab made materials);
Thermal stability of electrolyte in combination with charged electrodes
Emissions related tests (mainly gas detection)
Flammability tests (determination of the flammability of each cell component and its emissions and decomposition products)
Cell level
Safety testing towards thermal runaway evaluation (e.g., short circuit, overcharge, overdischarge);
Self-heating properties (thermal behavior in adiabatic conditions);
Emissions related tests (mainly gas detection);

7. Summary and outlook

Consistent use of reporting methodologies are essential for accurate comparisons and reproducibility. Batteries Europe has developed clear guidelines (WG1 ‘New and Emerging technologies’, 2021) and will work further to promote implementation of these within European funded battery research projects and beyond. The reporting guidelines are recommended also as a requirement for publications in scientific journals, an implementation that is already taking place. Whilst this development will not have an immediate impact on the benchmarking of battery technologies, it will set a best practice for the reporting of results. The impact of implementing such methodologies should become apparent within 3-4 years of its adoption in research projects and journal publications. This will provide much needed clarity to the battery research community, industry stakeholders, policy makers and the integrators of battery solutions alike when accessing and choosing new battery chemistries and innovations.

Acknowledgements

The authors wish to acknowledge the input of Batteries Europe stakeholders to this work. Batteries Europe ETIP is supported by the European Commission Horizon Framework program, Contract N° ENER-2018-453-A7. SP acknowledges the basic funding of the Helmholtz Association. KE acknowledges the funding of the Swedish Strategic Research Foundation.

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