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Designing tomorrow's Li-ion battery

Providing an integrated engineering approach for electric vehicle batteries

Executive summary

Together with environmental concerns, the introduction of Li-ion chemistries in automotive batteries has driven the beginning of a vehicle electrification wave over the past 10 years. During the coming decade, battery electric vehicles (BEVs) will have to become commonplace and start yielding profit for original equipment manufacturers (OEMs). To achieve this, battery and vehicle manufacturers will have to further mitigate the current gaps compared to internal combustion engine (ICE) driven cars. These include cost, range, charging speed, reliability and safety. In this white paper we discuss the implications of powertrain electrification on the vehicle development process, which aspects drive lithium-ion (Li-ion) battery pack design, which physics are involved and which types of analysis are required in this context.

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Abstract

The battery is so intertwined with the BEV that both the battery and BEV development processes need to happen simultaneously and require continuous collaboration between the various discipline experts. This should be facilitated by deploying a common engineering environment that helps to remove silos between stakeholders. At the same time, such a platform should include the best-in-class solution for all steps in the process. In Simcenter™ software and hardware simulation and testing solutions, everyone involved will find the right tool to address his/her engineering challenges, from initial sizing and architecture definition, electrochemistry analysis and cell, module and pack design, to integration in the vehicle and final validation. Using Simcenter enables engineers to connect all these process steps, study the impact of their choices on all battery and BEV performance aspects, and allows them to use optimization and design exploration to effectively discover innovative solutions.

The unstoppable rise of BEVs

BEVs have been around throughout automotive industry history. But major roadblocks such as limited range and an inadequate charging infrastructure have always impeded attempts to broad commercialization.[1] Today, however, we are in disruptive times. BEVs, and by extension all gradations of hybrid electric vehicles (HEVs), are on the rise again, and this time they will be unstoppable. Converging technological innovation and evolving circumstances is leading to radical change. Three major drivers have created an unprecedented momentum for electrified traction, which has made batteries the center of attention, where they are likely to stay.

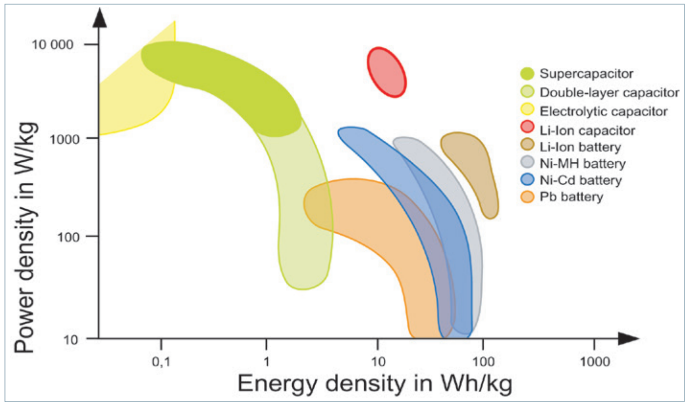

Figure 1. Ragone plot, showing the power capacity and energy capacity potential of current commercial capacitor and battery cell type technologies.[7]

The availability of suitable battery technology

First, there is the spectacular evolution that has taken place during the last decades of the 20th century in the field of battery cell technology, mainly driven by the needs of the consumer electronics industry. The market introduction of Li-ion battery cell chemistries in the 1990s has been a gamechanger.[2]

Compared to predecessor candidate traction technologies such as Nickel-Cadmium (Ni-Cd) and Nickel-Metal Hydride (Ni-MH), Li-ion batteries (in all their chemistry variants) provide a high energy density and open circuit voltage, faster charge and low self-discharge.[3,4] Despite the fact all Li-ion technologies still suffer from notable disadvantages, such as vulnerability for over-charge and deep-charge (requiring a protection circuit), temperature sensitivity, as well as disputable sustainability and recyclability,[5] it's definitely fair to state they have contributed tremendously to the vehicle electrification wave we're witnessing. And they will probably continue being dominant during the coming decade, or at least until new groundbreaking technologies will be ready for the market.[6]

Just to illustrate how fast things are changing, since 2010 mass production has decreased Li-ion battery cost by 87 percent while energy density has tripled. Automakers now offer BEVs with more than a 200-mile range compared to over 100 miles just 10 years ago while maintaining the same price point.[8,9]

Digitalization as both additional load and technology catalyst

Secondly, the thorough digitalization that is taking place in the automotive industry is on the one hand slowly but certainly raising the bar for battery cell technologies, but at the same time paving the pathway for full electric driving.

The number of electric systems in cars has increased dramatically over the past 20 years. Some of today's vehicles easily include more than 150 electronic control units (ECUs) with accompanying software.[10] In this field, consumers have eagerly adopted one innovation after the other, often for their safety and comfort. Advanced driver-assistance systems (ADAS) such as pedestrian detection, adaptive cruise control (ACC), collision avoidance, lane correction and automated parking are gradually become commonplace, while fully autonomous cars are already being tested on public roads. It is predicted that by 2030 these systems will represent a significant proportion of the market (up to 15 percent according to McKinsey), even in the most prudential scenarios.[11]

ADAS systems are, just like starting, lighting, ignition (SLI) and auxiliary, part of the low-voltage circuits where classic lead-based batteries are currently still the preferred technology.[12] They are fail-safe and robust to support safety-critical functions under all environmental circumstances. However, as the amount of equipment grows to enable connected and autonomous driving functions, classic 12-volt (V) power architectures are pushed to the limit and consume an amount of power that can considerably affect an EV's driving range.[13] The latter even leads to interesting discussions on whether both autonomous and full electric driving can be achieved simultaneously in the near future.[14] It's clear these challenges dramatically raise the pressure for better battery technologies than are available today.

Despite all the concerns and caution of some, most industry leaders are convinced that autonomous and connected driving only makes sense if it is fully electric. An important element here is they also envision that digitization will yield new forms of mobility and associated business models, such as shared mobility, the internet of vehicles and more.[15,16] ICEs that regularly need to be refueled at defined locations do not fit that story. They will still have a role to play in HEVs to temporarily compensate for BEV shortcomings, such as driving range. But eventually the future will be fully electric, and the ICE will disappear. Several prominent OEMs are already moving in that direction.

Global warming as the ultimate driver of radical change

Finally, global warming urges us toward greener mobility, including BEVs. What's unique about climate change compared to earlier environmental concerns is it affects all of us. There is a worldwide scientific consensus that man-made carbon dioxide (CO_2) emissions, primarily caused by fossil fuel consumption, is a major driver and the international community has taken clear action by consolidating ambitious long-term targets into a legally binding treaty.

The Paris Agreement, an initiative of the Intergovernmental Panel on Climate Change (IPCC), is a historical landmark for multilateral collaboration and will probably be remembered as the ultimate tipping point to automotive electrification. Having a binding commitment from all industries and (almost) all governments around the world to drive green initiatives is unprecedented and is providing carmakers with a unique and durable opportunity to by-pass two main hurdles to wider adoption of electric driving: price and infrastructure.

Whereas before the success of BEVs depended on the goodwill of consumers to pay more for less driving range and limited charging comfort for merely ecological motives, now they are encouraged by incentive schemes and tax waivers. While in the past deploying charging infrastructure at scale seemed impossible, now there is dynamism and creativity in that field. Societies used to look at aspects such as mobility, energy and housing in a fragmented manner. Thanks to the goals that were set in the Paris Agreement, there is a lot of activity, both private and public, on different levels, to look at these holistically. That is leading to innovative initiatives, new business models and an enormous momentum for green mobility, including the tailpipe CO_2-neutral BEVs.

The Li-ion battery in charge during the 2020s

The transition is already happening. During the previous decade, the total number of electric passenger cars on the world's roads grew from just about 17,000 in 2010 to about 7.2 million in 2019, of which 67 percent were fully electric. This decade will become extremely important as it should become the time when EVs become commonplace and achieve a significant market share by 2030. Whereas the 2010s were just the beginning, the 2020s will bring the final breakthrough.

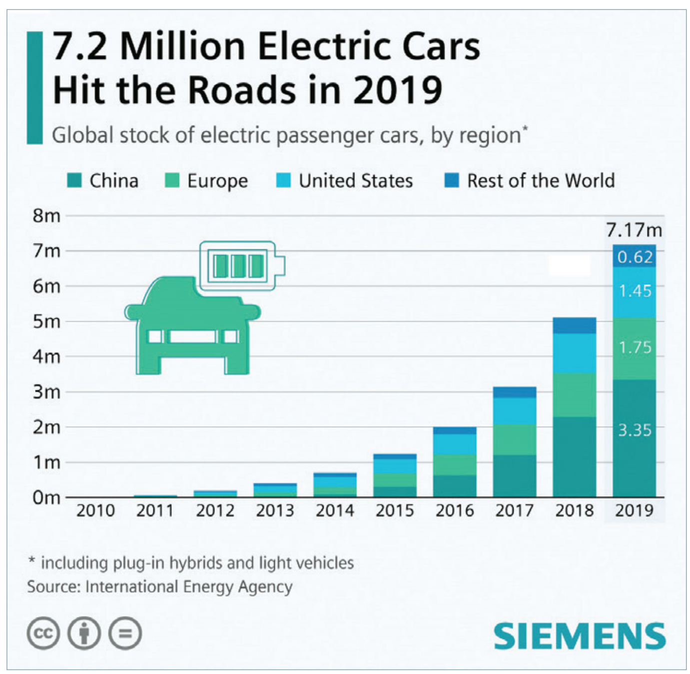

Figure 2. Global stock of electric passenger cars by region between 2010 and 2019.[17]

This is obviously good news for Li-ion battery cell-type manufacturers, who have enormous potential to upscale their activities.[18] Success will partly depend on the speed and extent by which improvements can be made. Current BEVs are just starting to approach the overall performance of ICE-driven cars. Driving range and lifespan are still major concerns but are gradually reaching acceptable levels. However, charging speed is also an important factor for range anxiety. And that is currently perceived to be the biggest gap that's left. Today's premium batteries can handle an 80 percent charge in around 30 minutes, but ultra-fast charging would be highly desirable. This is a challenging engineering problem, as higher charging speed requires decreasing the thickness of the electrodes, which tends to increase cost and lower the energy density. And a good design of the pack, including the thermal management system, will be necessary to mitigate the impact of faster charging on the battery's lifetime and safety.[19]

For all elements, anode, cathode and electrolyte, there is still a significant margin for including better performing chemistries. It is expected they will be implemented during the coming five to 10 years. By then, the theoretical limit of Li-ion will probably be reached However, further improvements can possibly be found in cell design and on the system level, particularly the battery pack and its integration into the wider vehicle system. Later in this document we discuss how OEMs and pack suppliers can make a difference. We discuss the implications of powertrain electrification on the vehicle development process; which aspects drive Li-ion battery pack design, which physics are involved and which types of analysis are required in this context. The more conceptual choices that are to be made are beyond the scope of this white paper, such as exact chemistry, which is mainly driven by application, market readiness and cost; and in-vehicle positioning, which is more related to vehicle structural development and driving dynamics.

Transforming the vehicle development process

Despite this utterly prosperous outlook, the reality today is OEMs still struggle to achieve profitability with BEVs. A battery is so different from an ICE and so omnipresent and dominant in the overall vehicle system that all established processes, in terms of design, manufacturing and lifecycle management, must be reconsidered. Strong industry players cannot simply fall back on the knowledge and infrastructure they have been building up over the decades so they must invest heavily. That poses great risks, as new players are eager to take their place. Manufacturers that show the most flexibility to make the switch quickly will have the best chance to survive. Below we summarize some of the most impactful measures that need to be taken in the vehicle development process. In fact, these recommendations will help any manufacturer of products with inherent complexity.

Move away from working in silos

Successfully developing a new vehicle requires the combined knowledge of various application experts, who often have conflicting targets. In order to effectively find the right balance, it is important that all aspects are considered simultaneously as early as possible, otherwise the development process can get stuck in endless iterations. The more complex products become, and the more multi-physics systems are involved, the more important this becomes.

Such a highly collaborative approach seems more obvious than it really is. Traditionally, OEMs have various departments for different disciplines, sometimes even spread over several sites. This easily ends up in a siloed development approach with difficult exchange of information and data. To be competitive today, OEMs must remove these silos by using in an integrated environment where engineers can collaborate on comprehensive models from the very beginning of the design cycle.

This will significantly shorten the total development time and will in the case of BEVs be essential to achieve profitability.

Increase the focus on simulation

Such an integrated approach that aims to front load design decisions naturally leads to an increased focus on simulation. But more needs to be done than that, especially for BEV development. A classic verification-centric methodology that ultimately relies on prototype testing and where simulation is merely used for analysis and troubleshooting is no longer practicable. A battery behaves in a nonlinear way with respect to ambient temperature and its state of charge (SOC).

So, when integrated in the vehicle system, this leads to an enormous number of operating regions. It is just impossible to cover all these using physical testing only. Instead, OEMs must deploy a comprehensive digital twin, a set of models and data that can predict the real behavior of the vehicle with the highest possible accuracy. The digital twin gets initiated during the concept phase, when the vehicle architecture is defined and then gradually includes more detail as development advances. Ultimately the comprehensive digital twin mirrors the final product and can be used for virtual verification and validation.

Rethink the role of physical testing

This focus shift doesn't mean physical testing is about to disappear. Crucial development phases, such as certification or final verification and validation, will never be fully simulation-based. But as creating a prototype and doing measurements is relatively slow and expensive compared to performing calculations on a digital twin, testing cycles will need to shorten to keep the overall development time and cost under control.

On the other hand, test departments will see an increase of new activities during earlier development stages, as real measured data becomes more important than ever to endorse modeling accuracy, especially when exploring uncharted design areas. Realistic simulation, the comprehensive digital twin cornerstone, implies continuous testing on components, new materials, boundary conditions and more, often involving multiple physics, including some that are new to automotive testing departments. To be successful as a team, test and simulation engineers need to exchange knowledge, align their workflows and exploit synergies they create by combining their tools.

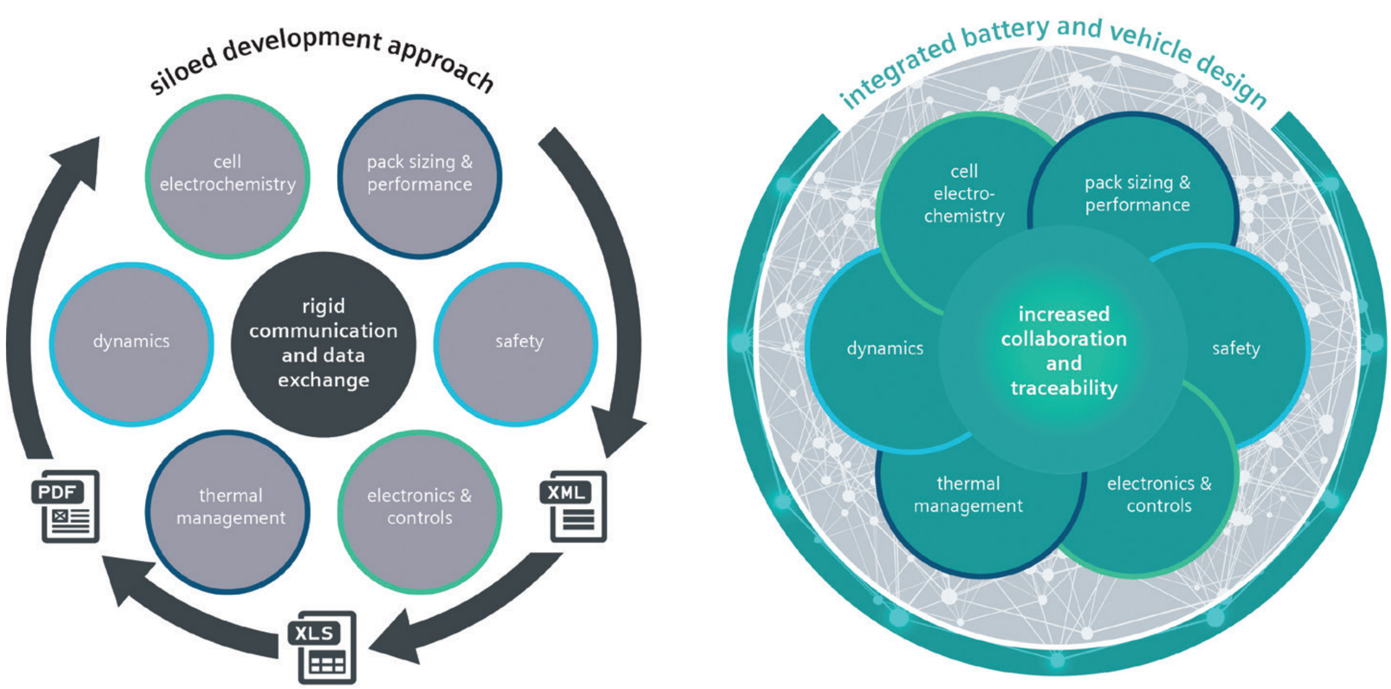

Figure 3. A siloed approach impedes collaboration between battery design stakeholders, whereas an integrated approach facilitates communication, collaboration and traceability.

Intensify the collaboration between OEMs and suppliers

The presence of the battery in a BEV is in all respects more pronounced than of the ICE in a conventional vehicle. Its range of action goes far beyond mere propulsion. The battery is connected to all systems in the vehicle, touches all engineering disciplines and even determines to a large extent what the structure of the vehicle looks like. To put it simply: An ICE is an important component of a conventional vehicle, but a BEV is a battery on wheels. Studies indicate at certain production volumes it could even benefit OEMs to take part or all of the battery development activities in-house, even if it would require a huge investment and a lot of knowledge gathering outside their core business.[20] That demonstrates how important the battery is as a component.

Whoever is or should be involved, it's clear the various phases in the battery engineering process, namely cell development, pack sizing and design and vehicle integration, cannot be simply separated from each other. If these are done by different stakeholders, it is important those are connected in a streamlined process that enables communication, teamwork and data exchange. Such an intense collaboration should, for example, facilitate OEMs to effectively communicate design requirements to suppliers who then provide a digital twin that can be used in further development stages. This is in the end also a form of removing silos.

Battery development process and stakeholders

As mentioned in the previous section, the battery engineering process touches diverse engineering disciplines and requires the combined expertise of a large amount of people. All these stakeholders must collaborate, keeping the most important battery design criteria in mind: range, charging speed, reliability safety and lifetime. Often, these criteria can conflict with other vehicle performance requirements they are aiming for. In this section, we will elaborate on who does what during the different parts of the battery engineering process. We describe them as individuals, but obviously sometimes they can be multiple people, or even an entire team.

Battery cell design

The battery cell type is usually chosen from what is commercially available. Chemistry is obviously an important factor, but also configuration plays a major role. The different types that are actively used in BEVs are cylindrical, prismatic and pouch. All three of them score differently on various characteristics, such as capacity, weight, safety aspects, flexibility, manufacturability, cost and more. But as technology and market are in full evolution, it's hard to say which one is best, and a listing of all the advantages and disadvantages would be beyond the scope of this white paper. Besides, what is true today may not be tomorrow. Cylindrical cells are currently by far the most common type, mainly due to costs because they are easy to manufacture, but also because they have a good mechanical stability.

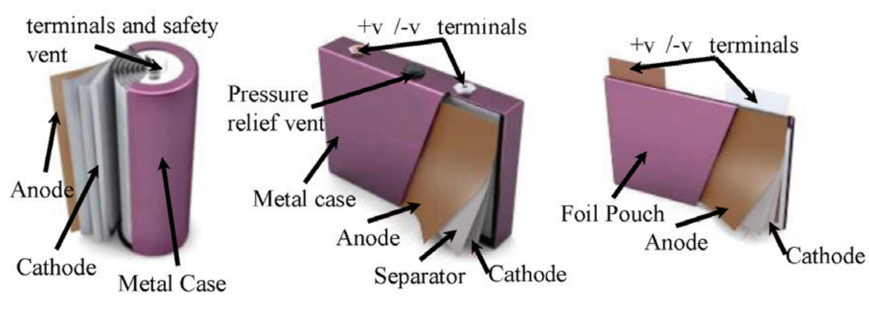

Figure 4. Commonly used Li-ion cell types in automotive batteries.[21]

The electrochemical and materials engineer
The battery cell choice has a huge influence on the further process, as the entire pack design is affected by the shape as well as the chemical, electrical and electrothermal characteristics of the cells. The task of the cell designer consists of properly drawing up these properties in simulation models. This can range from molecular chemistry and microstructure electrochemistry aspects to a detailed geometric representation of the complete cell. Part of the necessary information to create these models can come from the cell manufacturer and another part might require reverse engineering, involving measurements. The cell designer can then play with chemical and geometric parameters to optimize cell performance and make suggestions for improvement; for example, to lower voltage drops and heat generation while increasing energy density. The precision of his/her models are crucial for the relevance of further simulations that happen during battery pack design.

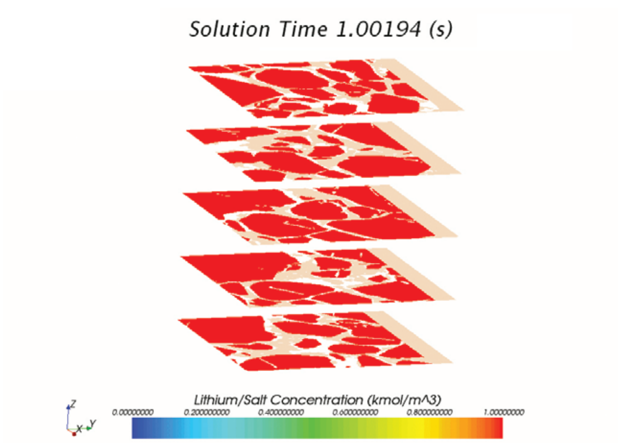

Figure 5. 3D simulation of salt concentration in the battery microstructure in different sections.

Battery pack sizing and design

In parallel with the research that is being done on the chosen cell, the design of the battery pack can start, for which endless possibilities exist. As mentioned before, this is preceded by lots of conceptual choices with major impact on the overall vehicle behavior, such as the position in the car, which affects the structural and spatial layout and drivability. We make abstractions of these and focus on the functional aspects of the battery pack design. This includes how many cells are needed, how are they bundled and packed, how are they protected and cooled and how the system is integrated into the overall vehicle in order to achieve the best possible performance for multiple design requirements.

The powertrain architect
The first question that needs to be answered is about the sizing and internal wiring. The powertrain architect studies the battery on a system level and determines the necessary amount of battery cells and the preferred series-parallel wiring topology to meet the battery's technical targets for power, voltage and energy. To achieve serviceable units, cells are grouped in modules. The powertrain architect will sketch the layout of these in an electrical scheme, looking for the most robust and manageable configuration. He/she will also integrate this component model in a full vehicle system model and do early simulations on various battery in-vehicle performance aspects, such as energy consumption and thermal behavior, and study the interaction between the battery and other vehicle systems, such as the electric drive and the battery thermal management system.

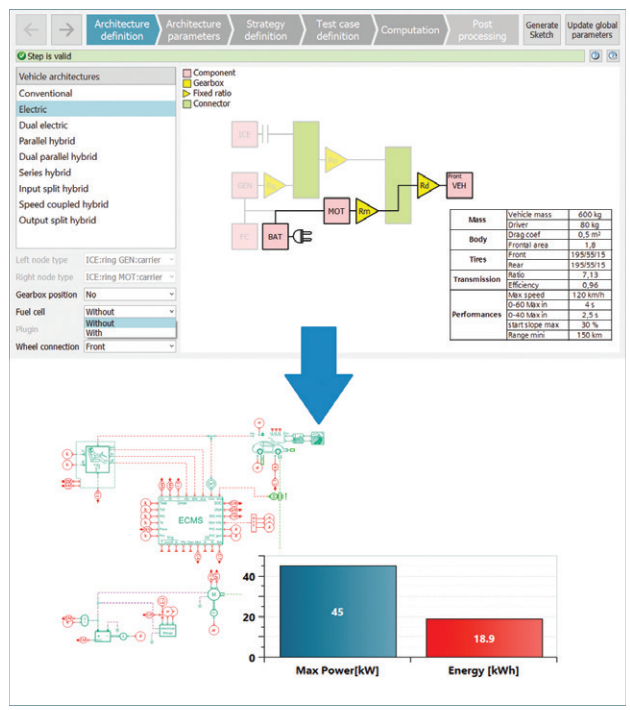

Figure 6. The powertrain architect sizes the battery (capacity, power, voltage) to reach the desired vehicle performance.

The multi-physics CAE/CFD expert
Once cell geometry, configuration and modularity have been fixed, the geometry of the pack can be elaborated. This is mainly driven by both mechanical and thermal requirements. Mechanical damage or deformation of the cells are among the biggest threats to battery safety. In other words, the cells must structurally be optimally protected. At the same time, thermal

management, such as air or liquid cooling, but also mutual thermal insulation between modules, is crucial for the overall battery performance, its safety and life-time. These two aspects together fully determine what the battery pack looks like and cannot be separated from each other. The objective of this thermal and structural analysis is to obtain a design that is strong, lightweight and facilitates a homogeneous temperature distribution during simulated drive cycles.

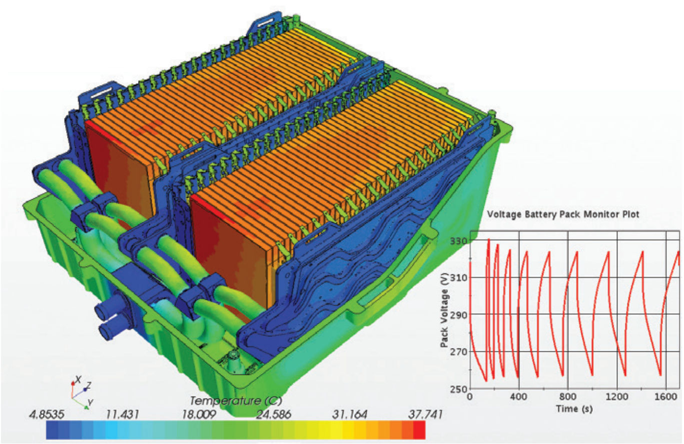

Figure 7. The 3D thermal simulation of the battery pack including cooling system – courtesy of Automotive Solution Center for Simulation (ASCS), Stuttgart and Behr.

The multi-physics computer-aided engineering (CAE)/ computational fluid dynamics (CFD) expert starts off from the model created by the electrochemical engineer who designed the cell. This one can be either physics-based or a 3D equivalent circuit model (RCR-type model) that replicates the cell voltage behavior in an empirical manner for computational efficiency. He/she then builds the entire battery system in a dedicated computer-aided design (CAD) or CAE/CFD software, and completes it with all other components, such as bus bars, electrical insulation pad, cooling channels and battery casing. After meshing and specifying the material and coolant properties, the expert runs large-scale electrothermal simulations, including conjugate heat transfer (CHT), to the coolant flow of the entire battery pack over transient scenarios using a dedicated multi-physics solver. He/she then optimizes the performance of the new design by making tweaks to the geometry, materials and boundaries to balance strength and weight, minimize temperature differences, increase cooling capacity and reduce pressure drop in the coolant flow, which should decrease the amount of energy the coolant pump needs from the battery.

The multi-physics CAE/CFD engineer also pays special attention to thermal runaway, a phenomenon to which Li-Ion batteries are particularly sensitive. This problem can be initiated by an abusive load, such as extreme overcharge or discharge, a cell that is exposed to heat for a long time (cells can become thermally unstable after 60 degrees Celsius), or an internal short circuit; for example, because of cell deformation or damage by impact. This can provoke exothermic chemical chain reactions in the cell, leading to even more heat generation at a rapid pace and the formation of flammable gases, which accumulate and eventually lead to spontaneous combustion or explosion. A good battery pack design should control the problem and/or mitigate the consequences, as any such incident can obviously have enormous consequences and harm the reputation of the OEM or even the entire industry. The multi-physics CAE/CFD engineer will study the propagation of the thermal runaway in comprehensive models that couple electrochemistry, combustion, flow and heat transfer. He/she will then look for pack designs that can, for example, slow down the mutual heat transfer between cells and modules or drain stacked reactant gasses in a more controlled manner.

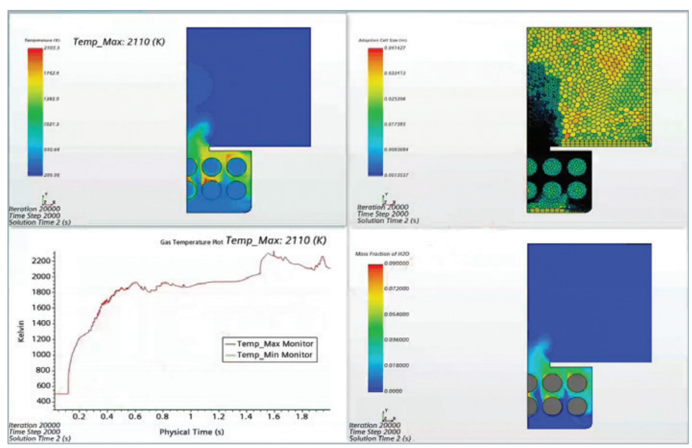

Figure 8. Studying thermal runaway propagation and safety using 3D simulation.[22]

The software and controls engineer

In parallel, the software and controls engineer develops the battery management system (BMS): The assembly of electronic control circuits that optimizes use of remaining energy equally balances the stored charge between different cells and prevents the battery from operating outside the safety boundaries, such as deep-charge and over-charge. For this purpose, the battery is equipped with the necessary sensors to measure pack voltage, current, cell voltages and temperature and more. These values are then employed in software algorithms that calculate data such as SOC, state of health (SOH) and state of function (SOF) and then communicate them to the vehicle user interface and autonomously initiate smart, corrective measures to improve the performance, lifetime and functional safety of the battery.

The task of the software and controls engineer is to develop robust software algorithms and set up a scalable model-based design (MBD) framework that enables virtual verification and validation during the different stages of the development cycle. The expert uses model-based system simulation techniques to generate battery models that are both fast and accurate in terms of dynamics, and couples those with control models, control codes and real controls in model-in-the-loop (MiL), software-in-the-loop (SiL) and hardware-in-the-loop (HiL) test configurations. This allows a multitude of test scenarios to happen before the battery prototype is available, a virtual assessment of the response of the battery as it ages and effective optimization of the control strategy for performance and lifespan. The software and controls engineer and the CAE/CFD expert often also share their models, one as input for the other, or in co-simulation scenarios.

Integration in the vehicle

As the battery is progressing to its final shape, the vehicle also grows further in the development cycle. With details becoming available on other components, further refinements must be made based on performance simulations that take this evolving information into consideration. Model-based system simulation is an effective way to do so. This technique is highly scalable in several ways. It lets engineers efficiently model a complete vehicle concept based on predefined components, and then gradually refine them. It also allows you to study both the overall vehicle as well as to zoom in on individual subsystems or applications that have closer interaction with the battery. This technology is inherently multi-physics and embraces data from any source. In this way, engineers can be sure they are working with the most realistic information available at the instant of simulation. Below are listed some vehicle engineering stakeholders whose applications closely interact with battery design.

The vehicle thermal systems engineer

Unlike an ICE-driven car, a BEV cannot recover waste heat from the powertrain to warm the cabin. Instead, cabin comfort must be achieved with other mechanisms, such as a resistive heater, which drains the battery. This can dramatically reduce the driving range in cold environments. Additionally, high ambient temperatures can be problematic as an air conditioning system consumes a lot of battery energy. The vehicle thermal systems engineer is focused on finding the optimal balance between driving range and cabin comfort while keeping the battery (and also other electric components) in optimal thermal operating conditions. To achieve this, he/she will include the battery in a comprehensive vehicle thermal model, including all the relevant components, such as the cooling pump, heat exchangers, valves, chillers and more, and optimize the entire system by making tweaks to all of them. Today, there is also an increasing trend to include heat pumps in vehicles. They could increase overall energy efficiency, but at the same time add even more complexity to this application.[23]

The power electronics engineer

The main purpose of the battery is to provide the electric motor with adequate traction energy over a sufficiently long driving range. But also all other electrical systems in the vehicle are powered by the battery in one way or another. Optimizing the entire electrical system and implementing it in an electric board is carried out by the power electronics engineer. He/she chooses an electric circuit topology and designs a power flow chart in which the battery is a central and crucial component. Particularly for a BEV, this is especially complex as it also contains elements such as inverters, converters and on-board chargers. The design space of all these components, including the battery, is therefore partly constrained by the outcome of this engineering process.

The vehicle integrator

As mentioned, the battery is connected to all systems and touches all vehicle engineering disciplines. As a BEV is practically a battery on wheels, the development of both happens nearly simultaneously. The vehicle integrator must orchestrate the various parallel subsystem development tracks. During the early design stages, he/she translates vehicle performance requirements into targets for all the individual subsystems or components. Along the duration of the vehicle project, the vehicle integrator populates his/her multi-level models with increasing detail and evolving data, while continuously safeguarding that with choices made on subsystem level, the targeted balance between major vehicle performance attributes is being maintained. Those include energy consumption, range, thermal comfort, drivability, ride and handling, noise, vibration and harshness (NVH) and more.

The vehicle integrator uses all possible methodologies to make his/her models as realistic and complete as possible throughout the process. In addition to model-based system simulation, this involves testing, even for target setting. It is common to put a competitor or predecessor vehicle on a test bench. A dedicated vehicle energy management (VEM) setup in a climate-controlled room can yield energy flows in the vehicle under imposed driving conditions. This data can be converted in different simulation models for various attributes. By doing what-if scenarios on them, the vehicle integrator can study the performance of the vehicle in specific conditions and see what are the pros and cons of the vehicle architecture, where there is room for improvement, so that he/she can give directions to colleagues who work on components, like the battery. Ultimately, when the end of the development cycle approaches, there will be a phase of refinement and possibly troubleshooting on the physical prototype. Testing is crucial at that moment. Via a similar VEM test setup, the performance of all components, including the battery, can be validated in their operating environment.

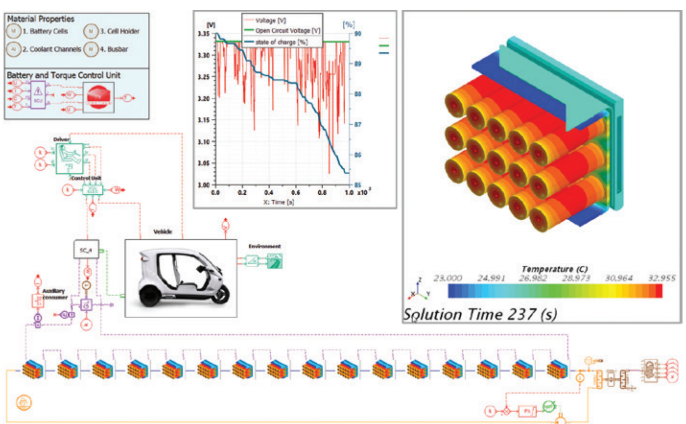

Figure 9. Vehicle level simulation using reduced order models.

Battery design within the wider vehicle engineering process

In the above sections, we've depicted the main stakeholders in the BEV engineering process that have, in varying degrees, direct influence on the battery and pack design. But there are many other engineering disciplines that are massively affected by the presence of the battery. Numerous specialists, who are mainly on the vehicle side of the story, must take specific new challenges into consideration when studying their domain. For them as well, it is mandatory to dispose of accurate battery models and data, to be in close contact with the stakeholders in the battery design process, and, if possible, to work on a common platform that facilitates collaboration. Without going into the full detail, we selected some examples.

An electromagnetics engineer must study the cables around the battery that transport high current at low frequency. This produces a large magnetic field that can negatively affect other electronics in the vehicle and requires high-shielding attenuation. At the same time, the battery and its circuits must be protected from any incoming electromagnetic interference.[24]

The battery is continuously subject to vertical low-frequency, road-induced vibrations and shocks. This could ultimately lead to problems, such as loss of electrical continuity or fatigue failure of the casing. When designing the vehicle structure, the NVH engineer must understand the dynamics behavior of the battery and make sure critical frequencies are absorbed and modules are prevented from moving.[25]

Finally, as mentioned, damage by impact is one of the most common causes, leading to the hazardous thermal runaway phenomenon. Moreover, when a battery catches fire, it's impossible to extinguish because when the cathodes degrade they continuously release oxygen. The vehicle crash engineer must investigate all possible impact scenarios and make sure that in all of them the structural integrity of the battery can be maintained.

Simcenter solutions for battery design

As illustrated, successful battery design requires many different discipline experts to continuously collaborate; on cell design, pack development and integration into the vehicle, with a lot of overlap and interdependencies between their working areas. It is impossible to be effective if these domain specialists are trapped in their silos. Given the number of parameters, the broad operating range, and the inherent multi-physics complexity of the battery engineering problem, it is also mandatory to follow a systematic predictive simulation-based approach. This one should be underpinned by highly specialized testing technologies to validate all these complex models, physics and materials. Ideally, all the necessary tools are available in a common environment for OEMs and suppliers in which it is easy to share data and knowledge, where co-simulations can be set up without the need for extensive scripting and where requirements, targets and design decisions are captured as traceable artifacts.

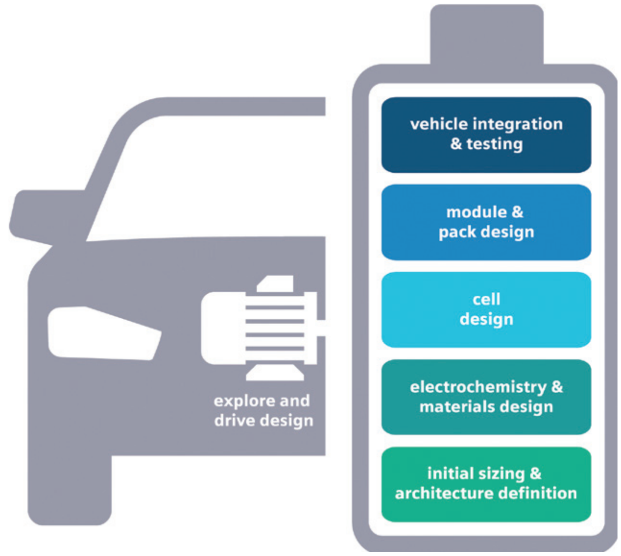

Figure 10. Simcenter for battery design workflow.

Introducing the Simcenter solutions portfolio

This is exactly what the Simcenter portfolio is all about. Simcenter, which is a part of the Xcelerator™ portfolio, the comprehensive and integrated portfolio of software and services from Siemens Digital Industries Software, uniquely integrates multi-physics system simulation, 3D CAE, CFD, electromagnetics and physical testing, and combines this with design exploration and data analytics, all in one environment. This open, scalable and flexible engineering platform helps OEMs and suppliers accurately predict battery and BEV performance aspects, optimize designs and deliver innovations faster and with greater confidence. Simcenter simulation and testing solutions allow engineers to generate a set of validated ultrarealistic, multi-physics models and data that can predict battery and BEV behavior. These are essential to implement the comprehensive digital twin, the industry paradigm that helps OEMs and suppliers design robust and safe batteries that combine high power, long range, fast charge and continued reliability through their structure, systems, software, controls and innovative materials.

Simcenter has a long, proven track record in complex product design. As a global industry leader with a clear focus on innovation, Siemens strives to deliver solutions that will allow businesses in the entire transportation sector to take the next steps in digitalization. Siemens has achieved this by making substantial investments in research and development (R&D) as well as by strategic partnering and acquiring technology pioneers that can provide decades of engineering proficiency in the sector. The ones that focus on product design and development have been unified as Simcenter. All the solutions are backed by a global team of engineering specialists that are dedicated to helping OEMs and suppliers meet the challenges of their industry and exceed the expectations of their market. In the following paragraphs we highlight the Simcenter products that specifically fit the battery design process.

Simcenter Battery Design Studio

Simcenter Battery Design Studio helps electrochemical engineers build and validate a 3D Li-ion cell model starting from standardized, yet customizable specifications for cell shapes and components such as electrodes, tabs and current collectors. The software also includes predefined standard mixture formulations as well as cell characterization tools so the mixture formulation can be reverse engineered from experimental input.

Simcenter Battery Design Studio can be used to calculate cell responses to pulses or duty cycles based on several levels of performance models: a physics-based macro-homogeneous model to get insight into the cell's electrochemical mechanisms; and an RCR model, which is an empirical approach to simulating cell behavior in a computationally effective way. The software also comes with an aging model to study the effect of calendar and cycle aging by resolving the mechanism of solid electrolyte interface (SEI) growth, as well as capabilities to simulate thermal abuse tests, such as the oven test and accelerating rate calorimeter (ARC) test. The model can then be configured to predict the point at which the cell enters the thermal runaway.

Simcenter Battery Design Studio models and data can be exported in a dedicated file format that can be opened in both Simcenter STAR-CCM+™ software and Simcenter Amesim™ software.

Simcenter Culgi

Simcenter Culgi™ software includes an extensive set of tools for multiscale computational chemistry, ranging from quantum mechanics to fluid dynamics and from molecular dynamics to statistical modeling. The software has proprietary mappers, wrappers and scripting environments that allow engineers to deal with industrially relevant formulations.

Simcenter Culgi is particularly well suited to study battery material performance at the molecular level, such as the transport of ions through membranes at ambient and nonambient conditions. At the same time, degradation effects caused by the charging cycles and possible other environmental factors can be studied. After model validation has been completed, engineers can virtually screen for new materials to improve battery performance.

Simcenter STAR-CCM+

Simcenter STAR-CCM+ is a dedicated 3D software that allows the multi-physics CAE/CFD expert to accurately predict battery performance, including all physics of influence, including the ones that cross the boundaries of traditional engineering disciplines.

Using Simcenter STAR-CCM+ enables the user to take multi-physics literally. The software even has tools to predict the spatial distribution of ions and potential within an arbitrary, multi-phase microstructure region, such as the electric potential and salt concentration in electrolytes, and concentration of Lithium in active electrode parts. These functionalities are helpful for electrode design.

However, the core value of Simcenter STAR-CCM+ for the battery design process is in its capabilities to simulate the electrothermal behavior of modules and pack including coolant flow, all coupled for optimal accuracy. The software includes the Simcenter Battery Simulation module to easily build a module or pack based on Simcenter Battery Design Studio input as well as high-performance automated meshing capabilities and includes dedicated modeling tools and methodologies. Simulations in Simcenter STAR-CCM+ allow multi-physics CAE/CFD experts to study the electrochemical behavior of cells in their thermal environment, to predict 3D heat maps and to evaluate cooling strategies in real drive cycle conditions.

Additionally, Simcenter STAR-CCM+ includes highly specialized capabilities that are necessary to study thermal runaway progress and related safety aspects.

Finally, Simcenter STAR-CCM+ can be coupled with Simcenter Amesim in co-simulation scenarios.

Simcenter Amesim

Simcenter Amesim is an open, integrated and scalable multi-physics system simulation platform, allowing engineers to virtually assess and optimize the performance of all types of mechatronic systems. The software drives the balancing of multiple design requirements from start to finish, from concept design to final validation and controls calibration.

Simcenter Amesim combines ready-to-use and validated multi-physics libraries with application-oriented solutions and powerful platform capabilities to let simulation engineers rapidly create models and perform accurate analysis. The tool is particularly fit for battery design stakeholders who need to consider the battery pack as part of a bigger system, such as powertrain architects, software and controls engineers, vehicle systems engineers, power electronics engineers, vehicle integrators and more.

At the start of the pack design, engineers can use Simcenter Amesim for battery pre-sizing based on a database of pre-calibrated cells or by importing characteristics from a Simcenter Battery Design Studio RCR model and technical targets that have been determined by cascading vehicle requirements down to the component level.

As both battery and EV development evolve, Simcenter Amesim improves collaboration between the teams on both tracks by enabling them to predict in-vehicle battery performance and assess future interactions between the battery and surrounding systems. This enables engineers on both sides to front load design decisions and avoid endless iterations. As such, the software can help to significantly shorten the overall design cycle.

Simcenter Amesim can easily include 3D simulation or tested data for increased accuracy or can be engaged in co-simulation scenarios with Simcenter STAR-CCM+, for example, for designing the battery management system.

As Simcenter Amesim models are capable of running in real time, the tool is particularly suitable for validation of control strategies in SiL, MiL and HiL scenarios.

Simcenter HEEDS

All steps in the battery design process that spans Simcenter Battery Design Studio, Simcenter STAR-CCM+ and Simcenter Amesim can be automated. As a result, choices that must be made at different levels can be subjected to design exploration studies. This can be done in Simcenter HEEDS™ software.

Simcenter HEEDS multi-disciplinary design exploration and optimization capabilities enable engineers to fully exploit their simulation models by enabling extensive parameter studies in an environment that embraces input from various origins. All this can happen with optimal use of the available computational resources and supported by efficient search algorithms. In this way, engineers can discover new designs, optimize performance and improve robustness in a fraction of time it would take otherwise.

For example, engineers can use Simcenter HEEDS to study the battery at the cell level, to maximize its capacity considering a fixed pack design but only working on cell chemistry, or at the battery module level, working on its geometry and characteristics.

Simcenter HEEDS allows semiautomatic, efficient and safe exploration of hundreds of design variations aiming to balance the performance of multiple aspects while respecting system constraints.

Simcenter Engineering services and VEM test facilities

During all battery and BEV design process steps, OEMs and suppliers can get in touch with Simcenter Engineering and Consulting services experts. They have a broad engineering proficiency across industries and applications and can provide help with scalable projects tailored to the customer's needs, from troubleshooting problems, to larger parts of the product development, to methodology deployment, all in a collaborative atmosphere and with the possibility of technology transfer.

Simcenter Engineering and Consulting services can include all simulation applications as depicted above or can also provide complementary development efforts such as implementing testing methodologies for benchmarking and target setting, the experimental determination of parameters related to new materials and technologies, or final prototype validation. The experts use Simcenter testing solutions and leading-edge 3D and 1D simulation to significantly speed up the development time of a new battery and its vehicle integration.

Simcenter Engineering and Consulting services has proprietary VEM testing facilities, where predecessor or competitor vehicles have been studied in the context of target setting, or where the final battery prototype can be tested for various drive cycles inside the vehicle and in climate-controlled conditions.

Figure 11. the vehicle energy management testing facilities in Lyon, France.

Conclusion

In this white paper we have discussed the specific challenges that come with designing Li-ion automotive batteries and their integration into BEVs.

Making a Li-ion battery that performs well, can be rapidly charged and is reliable and safe requires the combined knowledge of many engineering discipline experts. As the battery is connected to all its subsystems, the battery design process cannot be entirely decoupled from the BEV engineering process. We depict the importance of following a simulation-driven approach, complemented by physical testing on a platform that encourages collaboration and diminishes the danger of stakeholders working in silos.

With Simcenter, we offer OEMs and battery suppliers a complete, open and scalable engineering environment that includes all the components they need to be successful. This includes Simcenter Culgi for materials engineering, Simcenter Battery Design for cell definition, Simcenter STAR-CCM+ for pack and cooling design, Simcenter Amesim for the design of, and integration with all the surrounding systems and Simcenter testing for target setting and final prototype validation. And, if necessary, supported by Simcenter Engineering and Consulting services experts.

Simcenter solutions include all the necessary physics that drive Li-ion battery development, such as advanced electrochemistry, structural, thermal and flow analysis, as well as tools for numerous applications, such as the development of software and controls, battery management systems, power electronics and vehicle thermal systems.

By deploying Simcenter solutions in their battery and BEV engineering processes, OEMs and suppliers can profitably make the switch to an electrified fleet.

References

1. E.H. Wakefield (1994). "History of the electric automobile, society of automotive engineers," pp. 2–3, ISBN 1-56091-299-5.
2. M.V. Reddy, A. Mauger, C.M. Julien, A. Paolella and K. Zaghib. "Brief history of early lithium-battery development. Materials," 2020, 13, 1884.
3. Y. Miao, P. Hynan, A. von Jouanne and A. Yokochi. "Current Li-Ion battery technologies in electric vehicles and opportunities for advancements." Energies 2019, 12, 1074.
4. Yuan-Li Ding, Zachary Cano, Aiping Yu, Jun Lu, Zhongwei Chen. (2019). "Automotive Li-Ion batteries: current status and future perspectives. Electrochemical energy reviews." 2. 1-28. 10.1007/s41918-018-0022-z.
5. https://ingenuity.siemens.com/2020/06/sourcing-resources-how-efficient-battery-recycling-helps-reduce-costs-and-emissions/
6. International Energy Agency (IEA), Clean Energy Ministerial, and Electric Vehicles Initiative (EVI) (June 2020), Global EV Outlook 2020: Entering the decade of electric drive?
7. https://commons.wikimedia.org/wiki/File:Energiespeicher3.svg
8. BloombergNEF, battery pack prices Fall as market ramps up with market average at $156/kWh in 2019, December 3, 2019.
9. BloombergNEF: Lithium-Ion battery cell densities have almost tripled since 2010, February 19, 2020.
10. Embitel: "'ECU' is a three letter answer for all the innovative features in your car: know how the story unfolded." https://www.embitel.com/blog/embedded-blog/automotive-control-units-development-innovations-mechanical-to-electronics
11. Paul Gao, Hans-Werner Kaas, Detlev Mohr, Dominik Wee. McKinsey: "Automotive revolution – perspective towards 2030," January 1, 2016. https://www.mckinsey.com/industries/automotive-and-assembly/our-insights/disruptive-trends-that-will-transform-the-auto-industry/de-de
12. C. Allen, C. Telford: Automotive Battery Technology Trends Review (June 2020), European Automobile Manufacturers' Association (ACEA) https://www.acea.be/uploads/publications/ES-TECH-TRENDS-V10.pdf
13. A. Mohan, S. Sripad, P. Vaishnav et al. "Trade-offs between automation and light vehicle electrification." Nature Energy 5, 543–549 (2020). https://doi.org/10.1038/s41560-020-0644-3
14. https://www.autonews.com/article/20171211/OEM06/171219941/hybrids-are-better-for-autonomy-ford-says
15. Santhanakrishnan Narayanan, Manos Chaniotakis and Constantinos Antoniou. (2020). "Shared autonomous vehicle services: A comprehensive review. Transportation Research Part C Emerging Technologies." 111. 255-293. 10.1016/j.trc.2019.12.008.
16. Eun-Kyu Lee, Mario Gerla, Giovanni Paul, Uichin Lee and Jae-Han Lim. (2016). "Internet of vehicles: from intelligent grid to autonomous cars and vehicular fogs." International Journal of Distributed Sensor Networks. 12. 10.1177/1550147716665500.
17. F. Richter, Statista: "7.2 million electric cars hit the roads in 2019," June 15, 2020. https://www.statista.com/chart/17178/global-electric-car-ownership/
18. World Economic Forum, 2019. "A vision for a sustainable battery value chain in 2030 unlocking the full potential to power sustainable development and climate change mitigation." http://www3.weforum.org/docs/WEF_A_Vision_for_a_Sustainable_Battery_Value_Chain_in_2030_Report.pdf.
19. Anna Tomaszewska, Zhengyu Chu, Xuning Feng, Simon O'Kane, Xinhua Liu, Jingyi Chen, Chenzhen Ji, Elizabeth Endler, Ruihe Li, Lishuo Liu, Yalun Li, Siqi Zheng, Sebastian Vetterlein, Ming Gao, Jiuyu Du, Michael Parkes, Minggao Ouyang, Monica Marinescu, Gregory Offer and Billy Wu, "Lithium-ion battery fast charging: a review," eTransportation, Volume 1, 2019, 100011, ISSN 2590-1168, https://doi.org/10.1016/j.etran.2019.100011.
20. Andreas Breither, Paul Hackert, Will Han, Russel Hensley and Dennis Schwedhelm. McKinsey: "improving battery-electric-vehicle profitability through reduced structural costs," September 3, 2020. https://www.mckinsey.com/industries/automotive-and-assembly/our-insights/improving-battery-electric-vehicle-profitability-through-reduced-structural-costs
21. https://www.engineering.com/story/battery-recycling-technologies-part-1-introduction-and-recycling-preparation
22. A.R. Baird, E.J. Archibald, K.C. Marr and O.A. Ezekoye. "Explosion hazards from lithium-ion battery vent gas," J. Power Sources, 446 (2020), p. 227257
23. Wang Peng, Haijun Xu, Xiaojun Xu and Cunyun Pan. (2017). "Design and simulation of liquid cooled system for power battery of PHEV." IOP Conference Series: Materials Science and Engineering. 231. 012025. 10.1088/1757-899X/231/1/012025.
24. Orazio Aiello, Paolo Crovetti and Franco Fiori. (2015). "Susceptibility to EMI of a battery management system IC for electric vehicles." 10.1109/ISEMC.2015.7256257.
25. Shashank Arora, Ajay Kapoor. (2018). "Mechanical design and packaging of battery packs for electric vehicles." 10.1007/978-3-319-69950-9_8.

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