Level 3 Industrial Case Study

Battery Designer and Materials for Transportation

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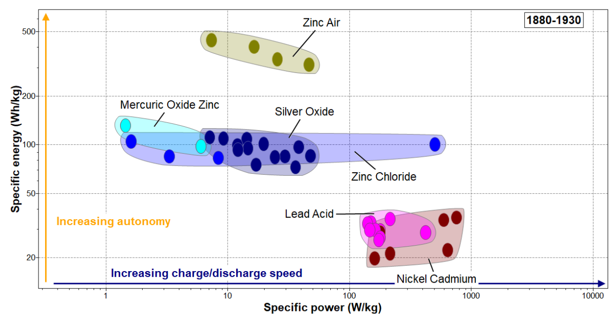
The benefits of Electrification

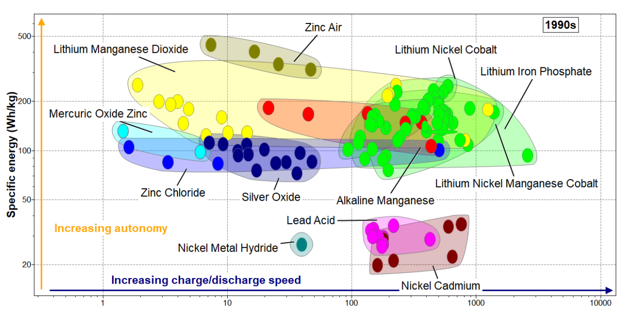
Nobody could have missed the shift towards electrification in society, with increasing number of electric cars and electric bicycles on the streets around us. This development is partly driven by a realization that fossil fuels need to be phased out and environmental concerns. It is also boosted by technological developments of battery performance, enabling more energy to be stored electrochemically using new improved materials. This has led to reduced local pollution where electric vehicles have replaced combustion engine-based mobility in city traffic.

Moreover, there are new types of recreational modes of transport, such as electric skateboards, hoverboards and even monowheels. If the batteries are charged using renewable energy, it has never been so fun to be environmentally aware, at least in terms of direct emissions from your transportation.

Historically, many of the first electrochemical batteries, more than 200 years ago, were based on zinc as the anode. Zinc-Carbon and Alkaline batteries with zinc powder are still popular today but have limited lifespan. In contrast to the single use primary batteries, rechargeable batteries are called secondary batteries. The first truly rechargeable batteries (by reverse current) were lead-acid type cells developed in the mid-1800's.



These are now considered heavy and bulky in relation to the amount of energy they can hold. However, they can produce remarkably large currents in bursts, which make them suitable for starting combustion engines etc. Therefore, they are still the dominant battery type in traditional cars and heavy vehicles.



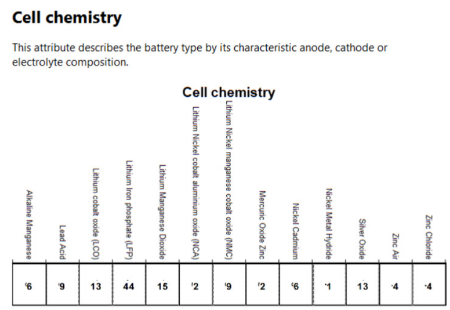
Nickel Cadmium alkaline batteries have been around for more than a hundred years and hold significantly better energy density than previous types. They are still used in handheld applications despite being considered quite expensive. The next significant step for portable energy storage was also nickel based, but with metal hydrides instead of cadmium. Nickel Metal Hydride batteries have long lifespan and are now popular in power tools.

Lead and Cadmium are heavy metals with significant environmental and health risks associated. The current battery type that is dominating electric mobility and household appliances is instead Lithium based, with the first Lithium-ion battery prototype developed as late as in the 1980's. Since then, designs with various metal oxide cathodes (Ni, Mg, Co, Fe…) on the market have exploded. These have superior performance, as we shall see in this case study. John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino were awarded the Nobel Prize in Chemistry 2019 for their development of lithium-ion batteries.

In an electric bicycle, the purpose of the motor is to assist the transport, to enable enhanced speed and range. Weight and volume might not be the primary target for minimization but in most cases (if not all), the goal is to reduce the cost while maximizing range. For electric skateboards and eScooters, in addition to the amount of energy stored, there are limitations to the volume of the battery pack. It must fit under the deck where you stand without interfering with the wheels and touch the ground. This scenario constitutes the main example of this case study. For a drone, which is our second example below, the energy storage to weight ratio is the crucial properties to optimize. For racing purposes, like electric motorbikes, the power to weight ratio is more important, as well as the charge and discharge rate properties and safety considerations.

What can Granta EduPack do?

The battery designer tool in Ansys Granta EduPack contains new battery materials and performance data alongside a synthesizer model that enables you to create a complete battery pack design from concept to selection of electrochemistry. The purpose is to introduce key concepts to non-experts rather than being encyclopedic. In this case study, we show how to introduce students to general design concepts and explore batteries for the electrification of transportation. We apply visual selection to the initial design of an e-Scooter battery pack. This is an example where you want to maximize energy content onboard while space under the footboard is limited.

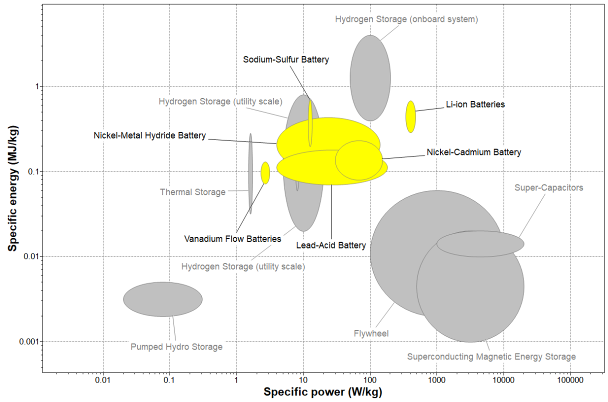


Add Record Tool	Favorites
Comparison Table	Find Similar
Engineering Solver	Synthesizer
Enhanced Eco Audit	Reference

Advanced databases of Granta EduPack have the Battery Designer Synthesizer tool module and a Battery Cell data-table. In this case study, we will make use of the Sustainability Level 3 database which is used in teaching relating to Engineering or Design for project or classroom work. It enables a wider range of learning outcomes linked to materials. Of course, it also contains a comprehensive set of mechanical, thermal, optical, electrical and environmental properties for over 4,000 engineering materials as well as energy storage data.

In traditional materials selection using EduPack, a free design parameter is needed in combination with a performance index to rank the material options and choose the best one for the application, in stiffness or strength limited design. A database of specific products, such as batteries, will evolve with time and in the existing energy storage solutions, the geometries are already given. Thus, the best performance is guided directly by an index without a free parameter. This means that for the total amount of energy stored (the range), we have two possible performance indices. We can choose energy density [J/m^3] if we have a limited volume to work with. Alternatively, the specific energy [J/kg] can be used if we want to keep the weight down. The energy density can be calculated from the specific energy by multiplying with the effective battery density [kg/m^3].

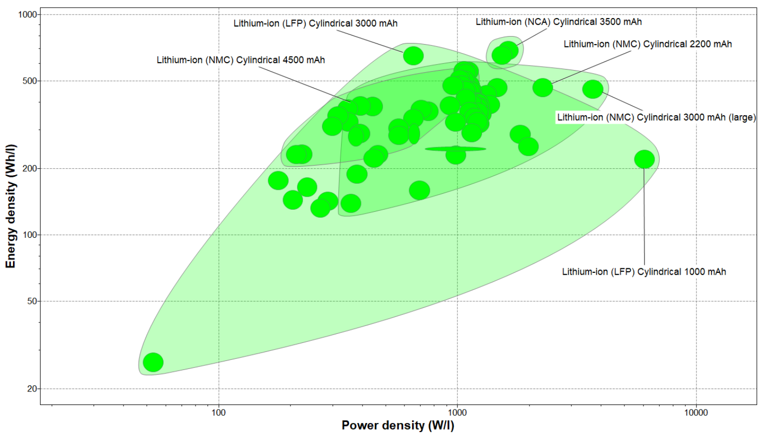
If, on the other hand, we need access to that energy as fast as possible [J/s], we can choose the power density [W/m^3] for minimum volume or specific power [W/kg] for lightweight performance. These parameters are available in the Battery Cells data-table and in the Energy storage data-table within the sustainability database. There is also information on specific energy and power for other energy storage systems than batteries, as shown here. A plot of specific energy vs specific power is called a Ragone plot and is very useful for comparisons.



Maximum energy density (limited volume) – the eScooter

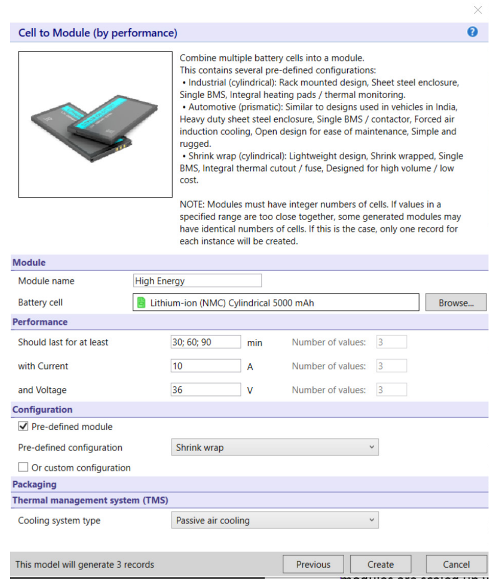
We will work on an e-scooter design with a set of constraints for initial screening on battery cells. As mentioned above, we assume a limited volume for the battery pack, meaning that the energy density [MJ/m^3] is used as performance index. Furthermore we will consider only rechargeable cells with at least a 1000 charge-discharge cycles of life expectancy to meet the typical 3-years warranty of such products (every day charge). In a first step we identify eligible cells using these constraints. Zinc technology and Lithium Manganese Dioxide are quickly eliminated, while the cycle constraint takes out some of the remaining cells. Top candidates are: Lithium Cobalt Oxide (LCO), Lithium Iron Phosphate (LFP) and Lithium Nickel Manganese Cobalt Oxide (NMC) chemistry.

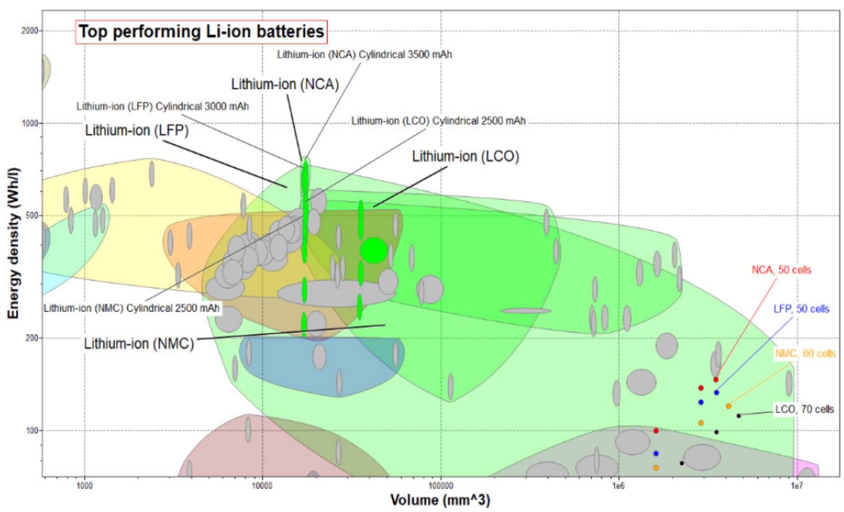
The available space under the e-scooter decking varies depending on size and model but is always limited by the board length and safe distance to the ground. The width is naturally greater than the length of a standard cylindrical battery, typically 65 mm long and 18 mm in diameter (18650), due to the need for foot space on the board. The nominal voltage of Li-ion cells is inherently 3.6-3.7 V.



As can be seen in the Lithium cell plot to the left, the cylindrical batteries are at the top performing corner of the diagram. Next, we use the synthesizer tool, and employ the Cell to module (by performance) model to estimate properties of different cell configurations. We will not consider geometry and packaging of the cells, since cylindrical geometry can be adapted to fit many types of spaces. We will use a cell module, not a pack.

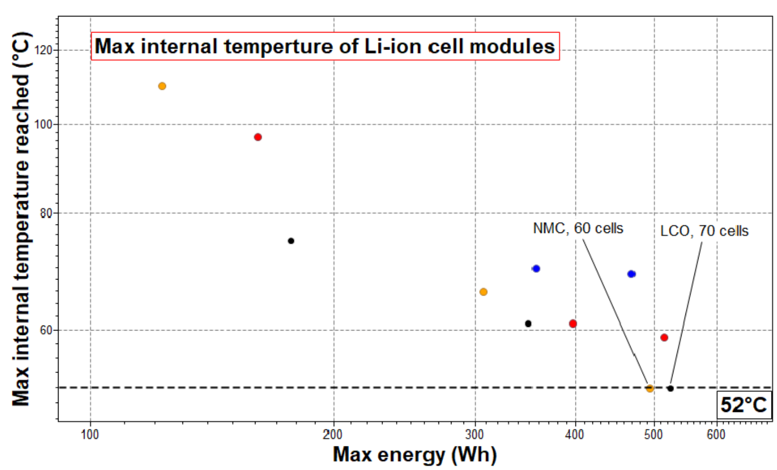
The top performing batteries from each Li-ion family that fulfill the constraints mentioned above are elaborated further; the cylindrical 3500mAh NCA cell, 3000 mAh LFP cell, 2500 mAh LCO cell and 2500 mAh NMC cell. The eScooter typically operates on 36 V with a maximum current of around 10 A, resulting in around 3-400 W of power for a module. In order to obtain 36 V, the number of cells in series will be automatically assigned to stacks of 10 and by requesting the charging time to be 30, 60 or 90 min the synthesizer will sweep different configurations of parallel stacks to fullfill these requirements. The pre-defined shrink wrapped configuration (not the industrial or automotive) is the one most suitable for our application. This is designed for high volume / low cost, as described in the specification sheet of this module. Passive air cooling is assumed here. Click the help icon (?) for further general information.

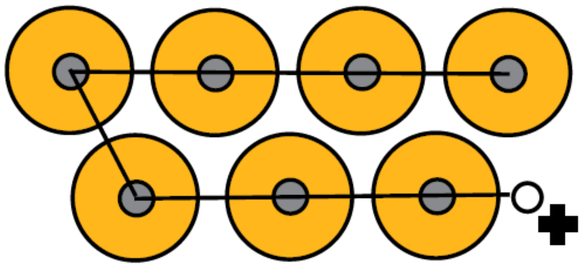




Four series of configurations were generated in the synthesizer tool by completing the boxes in the form and naming them after their respective cell chemistry. As expected, the performance of the battery modules are scaled up with the stack sizes, but not in a linear fashion. In the generated records, some of the estimated properties are also summarized in yellow at the bottom of each datasheet.

For example, the charging temperature of some modules with fewer parallel stacks is very high, around or even over 100°C. Only two alternatives have realistic values for safe design, the 70 cell LCO module and the 60 cell NMC module. Both have parallel stacks of 10 cells in series to generate 36-37 V and achieve their moderate temperatures by operating around 30%, as can be read in records generated by the synthesizer tool.





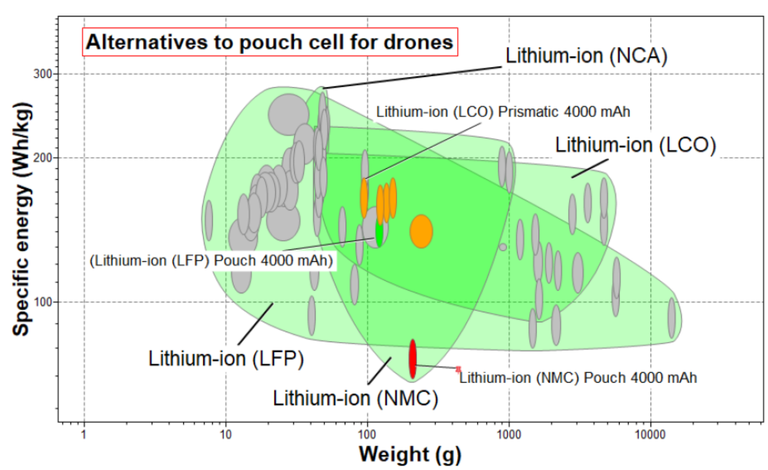
The volume calculated for the modules shown in the Ashby plot above is based on a very simplistic model, resulting in a total volume of over 4 l for the 70 cell LCO solution of 18650 batteries. A 7 x 10-stack configuration as shown to the left (end view) would fit within 653 x 100 x 30 mm which would be feasible. The 60 cell NMC solution would be somewhat smaller.

Maximum specific energy (lightweighting) – the drone

We now consider the battery requirements for drones. While speed and power is important, consumer drones, such as those for photography/filming or delivery, in most cases prioritize flight time. This means that low weight is more important than small dimensions so battery size is not a major issue, as can be seen in the example to the right with a large pouch-type battery. It is therefore natural to use the specific energy of the battery pack as the performance index in drone-type applications.

A typical drone battery can be up to 4000 mAh in capacity and may be of Li-ion or Lithium polymer (Li-Po) type. Since Li-ion is less costly and can store more energy, we will investigate this type and compare pouch batteries available in our database, with possible alternatives of the prism type. A couple of examples of these types are shown in the pictures to the left. A search in the Ansys Granta EduPack 2021 Battery Cells data-table for ‘pouch’ shows two candidates for drones available; the 4000 mAh LFP cell and the 4000 mAh NMC cell. The LFP option is not suitable, since it has a nominal voltage of only 3.2 V. Hence, the 4000 mAh NMC cell is set as reference and made red, using right-click.

The specific energy can now be plotted, for the custom subset of Lithium cell chemistry prismatic type cells, against the cell weight, in order to scrutinize alternatives. Prismatic alternatives to this pouch cell can be identified utilizing a limit stage with a minimum of 4000 mAh of capacity and a maximum weight of 206 g, which is the mass of the reference cell. There are several prismatic cells that pass these requirements, the lightest one being the 4000 mAh LCO type cell, to consider.



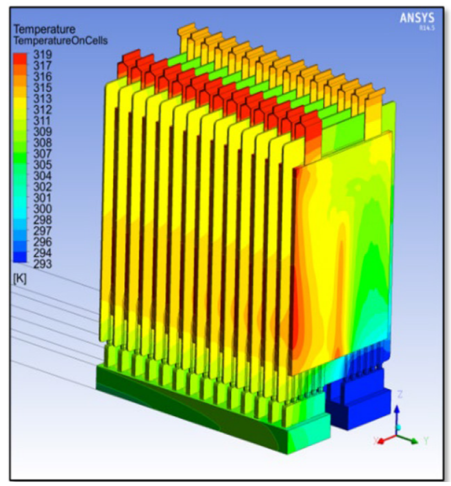
Comparison - Battery Cells

All Data | Project Data | Ranges | Averages | # Values | % Change | Highlight % Change

	Lithium-ion (NMC) Pouch 4000 mAh	Lithium-ion (LCO) Prismatic 4000 mAh
General		
Cell chemistry	Lithium Nickel manganese cobalt oxide (NMC)	Lithium cobalt oxide (LCO)
Rechargeable	✓	✓
Cycle life (cycles)	500 - 1000	1000
Specific energy (Wh/kg)	69.3 - 83.8	150 - 182 ↑
Energy density (Wh/l)	127 - 153	278 - 337 ↑
Specific power (W/kg)	177 - 214	277 - 335 ↑
Power density (W/l)	324 - 392	514 - 622 ↑
Size		
Cell geometry	Pouch	Prismatic
Weight (g)	206	90 - 97 ↓
Length (mm)	251	64.8 - 71 ↓
Width (mm)	136	37.1 - 46 ↓
Thickness (mm)	3.3	18.5 - 18.9 ↑
Volume (mm^3)	113000	44500 - 57000 ↓
Nominal ratings		
Nominal capacity (mAh)	4300	4000 - 4400
Nominal voltage (V)	3.65	3.65 - 3.7

The data can now easily be compared, side-by-side, using a comparison table that is created using the reference battery cell and right clicking on the cells that should be included in the comparison, here the 4000 mAh LCO type cell. As can be seen, this prismatic alternative performs as good or better in most categories, where significant differences are highlighted in orange. The All data option includes more attributes than is shown here, and there is also an option to only include project data, which presents a more concise table. In the full comparison table, it can be seen, e.g., that the Max discharge C-rate is lower for the LCO cell, 1.8C vs 3C compared to the NMC cell.

Reality check



Recent studies of performance in the operation of Li-ion batteries show that elevated temperatures contributes to the permanent loss of capacity, even from as low as 40°C. Additional considerations in battery design would therefore be to optimize the geometry of the battery pack, or change casing materials, to reduce the maximum internal temperature reached. It is uncertain that the assumption for the eScooter that passive air cooling is accurate for battery compartments, ventilated or not. Optimizing temperature is something that can also be looked into during other phases of product development. Complementary multi-physics simulation software, such as Ansys Fluent, allows detailed thermal-electrical-fluidic simulations of battery packs in operation to be carried out but, realistically, only for high value products (automotive, aerospace), not for consumer drones/eScooters.

There are also environmental and safety concerns to consider when working with electrification of transport systems. It matters greatly for the total emissions how the electricity is generated. Some countries, like Norway, have a near fossil-free energy mix, whereas some of the largest consumer markets are still dominated by fossil sources in their energy mix. Finally, there are also many problems to address when it comes to extraction and recycling of the critical elements involved in batteries and magnets for electric motors. Lithium, Cobalt and rare earth elements, such as Neodymium and Dysprosium are examples of these.

The Sustainability Level 3 database contains a data-table covering the periodic table with useful geo-economic property data on all the elements included in the battery cells, which informs students about potential risks. It can help discussions about major problems around scarcity, mining conditions and harmfulness of metals such as Li, CO or Ni. Recent studies also question the electrification gains in terms of CO2-emissions per passenger-km in transportation systems. Until the energy mix of countries where batteries are produced becomes decarbonized, improvements with regard to mitigating climate change from public mobility are limited. Important R&D initiatives are being carried out to address urban mining and recycling of critical elements, but also to achieve technology breakthroughs that would exclude critical elements with conserved performance.

Conclusions

The Battery Designer is an early-stage battery pack design tool for initial comparisons across different module and pack configurations. It uses simplified models and selection data from commercially available cell types to estimate key performance metrics, taking choice of cell, configuration, casing and insulation materials, and thermal management system into account.

In this advanced industrial case study, we have demonstrated how the battery cell data-table can be used for performance overviews and screening of design options for two major design scenarios; max energy storage at limited space or for minimum weight.

A database of products, such as the battery cell one, will evolve with time and results will depend on which systems are available. It is also fundamentally different in selection than selection of materials based on material properties. Ashby charts and a performance index technique can still be used, as discussed in these cases.

Special thanks to Dr Billy Wu, Dr Samuel Cooper and Nathasha Gjerløv Fiig of Imperial College London for their contributions to the tool and data table schema.

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