Chapter 3: Modeling and Simulation (alsc)

24. What is the interpretation of the Arrhenius term in the reaction kinetics?

$$r_1 = k_1 c_R e^{-\frac{E_{A1}}{RT}}$$

r is reaction rate, c is concentration, E_A is activation energy, T is temperature.

25. What contribution has the temperature in the Arrhenius term?

As the temperature increases, the exponential term increases, leading to a higher reaction rate. In the context of batteries, by incorporating the Arrhenius term into battery models, it is possible to predict the behavior of the battery under different temperature conditions and optimize the battery performance.

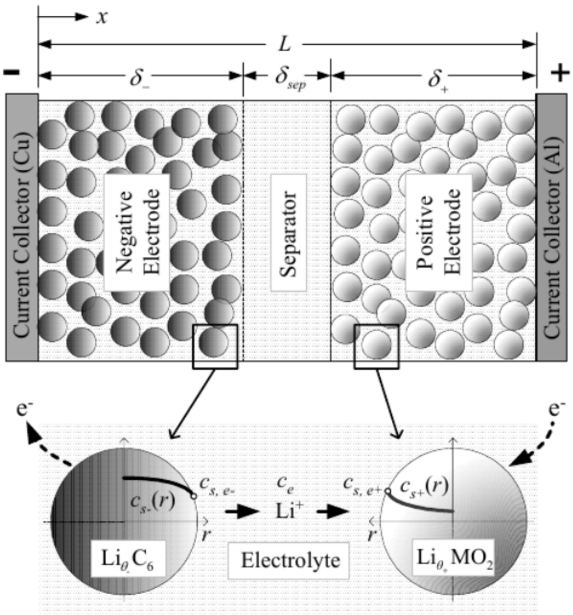
26. What is the interpretation of activation energy for a battery when charging?

In lithium-ion batteries, the activation energy for the charging reaction is generally higher than that for the discharging reaction. This is because the crystal structure of the positive electrode material is more open and can more easily accommodate the intercalation of lithium ions during discharging compared to the extraction of lithium ions during charging, which requires more energy to overcome the higher activation energy barrier. Batteries with high activation energy will have higher voltages.

19. Explain the basic idea of the single particle model.

1:00:03

- Normally all the particles inside the electrodes are not homogenous in terms of size, distribution and so on. So in order to reduce the complexity, we assume that the battery is flat and thin, which reduces the model from 3D to 2D;
- And we just consider the sphere as a single particle on a large scale (because we are just interested in the overall behavior).
- So now we only have 2 single particles to model the electrodes (negative and positive respectively), and the diffusion within the particles are homogenous radially (only take into account radial directions), same to the kinetics of the electrochemical reactions that occur at the electrode-electrolyte interfaces. As for the diffusion within the electrolyte, it will be only modeled in x-direction. As a result r- and x-directions are kind of decoupled.



20. Why is the single particle model nonlinear?

Due to the couplings and the nonlinearities in each PDE equation.

21. Is the ion diffusion process in an electrode described by a linear or nonlinear equation?

46:52

Nonlinear, because in the diffusion equation, the diffusion coefficient D is dependent on x or c.

$$\frac{\partial c}{\partial t}(x,t) = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}(x,t)\right)$$

More importantly, the concentration changes with time not only because of the diffusion, but also of the electrochemical reactions at the electrode surface. This coupling also introduces nonlinearity.

22. How are the equations for the different components coupled?

1:07:06

The 3 diffusion PDEs are coupled by Butler-Volmer equation, which describes the reaction kinetics, since the concentrations change with time due to the electrochemical reaction; And the B-V equation itself implies the coupling between electrode potential and the ion concentration.

23. What is the relation between reaction kinetics and electrical current in a battery model?

51:00 Butler-Volmer equation

Based on Faraday's law, the current is proportional to the rate of electron transfer (i.e., the flow of electrons) at the electrode, which is related to the rate of the electrochemical reaction occurring at the electrode surface.

27. What influences the thermal behavior of a battery?

55:00

The thermal energy produced by electrical power dissipation (Q=k*U*I*t), the heat conduction inside the battery, the heat transport with the environment, and the heat radiation (related to its surface area).

28. What methods do you know for solving the related partial differential equations?

- ODEs involve derivatives with respect to a single independent variable, usually time; while PDEs, which are used to describe the behavior of systems that vary continuously in space and time, involve derivatives with respect to multiple independent variables.
- The 1st method introduced is the Finite Differences Method (FDM). It uses values of the function (with boundary conditions) at nearby points to approximate the (partial) derivatives, based on its Taylor series expansion.

$$\frac{\partial c}{\partial x}(x) = \begin{cases} \frac{c(x+\Delta x)-c(x)}{\Delta x} + \mathcal{O}(\Delta x), & \text{forward difference} \\ \frac{c(x)-c(x-\Delta x)}{\Delta x} + \mathcal{O}(\Delta x), & \text{backward difference} \\ \frac{c(x+\Delta x)-c(x-\Delta x)}{2\Delta x} + \mathcal{O}^2(\Delta x), & \text{central difference} \end{cases}$$

$$\frac{\partial^2 c}{\partial x^2}(x) = \frac{c(x+\Delta x) - 2c(x) + c(x-\Delta x)}{(\Delta x)^2} + \mathcal{O}^2(\Delta x)$$

In our diffusion model, FDM is applied to approximate the 2nd spatial derivative (w.r.t x) of the concentration, which is proportional to its temporal derivative. At the end, we can write the equality to a classical state-space form in terms of the linear system. And then the temporal evolution of the concentration c can be easily integrated by any numerical ODE method.

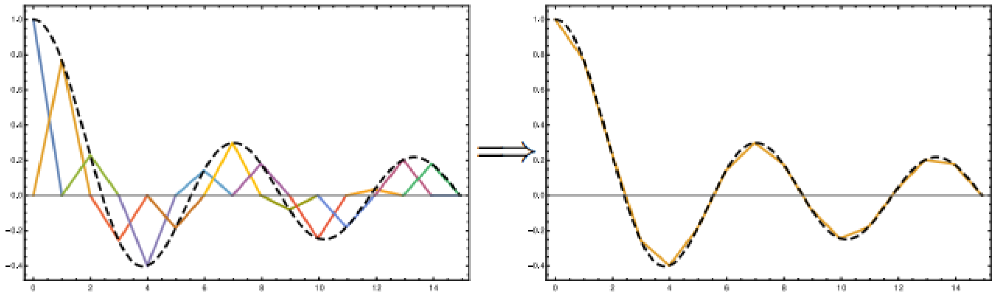
Setting $c_i(t) = c(x_i, t)$ this yields

$$\frac{dc_i}{dt}(t) = \frac{a}{(\Delta x)^2}(c_{i+1}(t) - 2c_i(t) + c_{i-1}(t)),$$

C_dot = A*C + b*v, where C=[c_0,c_1,...,c_N-1] ’

- The 2nd method is the Finite-Element Method (FEM). The basic idea behind is to divide the geometric domain into smaller, simpler parts namely finite elements, where the unknown function is approximated by a piecewise polynomial function V_k. The basis chosen was named as linear tent functions.

Approximation of the Bessel function J_0



However, due to the approximation the strong form cannot be satisfied anymore. So we have to transform it to a so-called weak formulation. The weak form is derived by multiplying the strong form of the PDE by a test function \lambda and integrating over the domain of interest.

$$\int_0^L \lambda \frac{\partial c}{\partial t} dx = \int_0^L \lambda \frac{\partial^2 c}{\partial x^2} dx$$

After constructing the test function in terms of V_k, the weak form will reach an ODE problem again. So within each element, the temporal evolution of the coefficients c_k of the polynomial function can be solved by any discrete integrator.

Chapter 4: Battery Control and Management (alsc)

1. What is the task of the battery management system?

- Battery management systems are required for system monitoring, e.g., state of charge (SOC), state of health (SOH) and control (optimization of charging time and operation).
- In particular this is achieved by state estimation and control, including Optimal charging/discharging; Reference (value) governing; Cell balancing.

2. What information is essential for the battery management system to work adequately?

Voltages, currents, temperatures.

3. How are battery packs conformed?

Battery packs are typically made up of multiple individual battery cells connected together in a series or parallel configuration, depending on the desired voltage and capacity of the overall pack.

4. What estimation tasks do you know for battery systems?

SOC, SOH (related to R0).

5. What is the underlying system-theoretic property that ensures that these estimation tasks can be carried out adequately?

Observability (related to state estimation) and identifiability (related to parameter identification).

6. What is key information that cannot be measured directly but must be estimated?

SOC.

7. Is it possible to directly measure the state of charge or state of health?

- A possible way to find the SoC is to measure the open circuit voltage Voc of the battery since it only depends on the SoC. But the problem is that the Voc can be measured directly only if the battery has been resting for a certain time.
- The simplest and more intuitive way is to use the number of charge/discharge cycles or time to get SOH. However, it may be useful only as a rough indicator.
- So practically speaking, it's not possible for EV applications.

8. What specific control tasks do you know and can explain for battery systems?

Optimal charging/ discharging; thermal management (charging/ discharging rate); cell balancing.

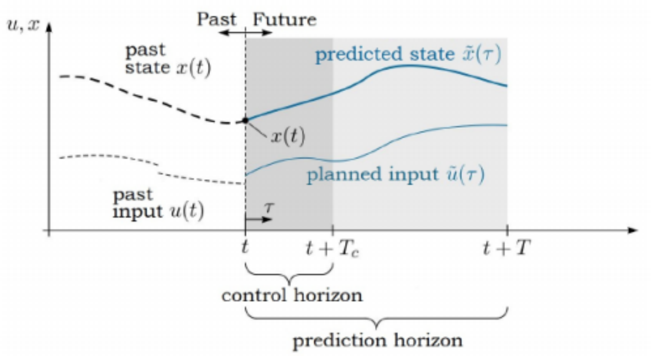
9. Is it possible to design controllers directly for a single particle model?

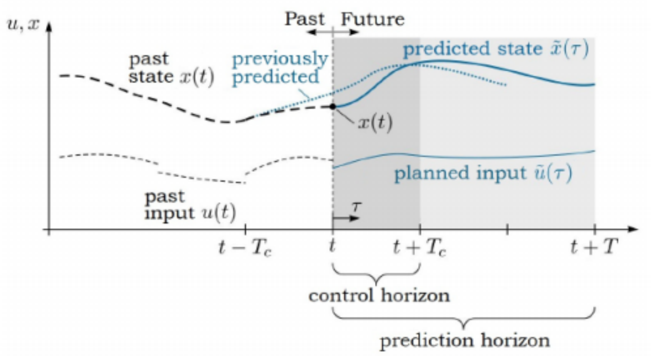
While single particle models can be useful for understanding basic battery behavior and developing more complex models, they are not typically used directly for designing battery controllers due to their limited accuracy and practicality.

10. What is the main idea of optimal control?

The goal of optimal control is to design controllers that are not only effective but also efficient and cost-effective, taking into account the specific objectives and constraints of the system being controlled.

11. What is the main idea in model-predictive control?





12. What information does a controller need to do its job?

The state and/or the model of the system, the reference of the output, the constraints of the input, and sometimes the past information.

13. Can essential battery states be estimated without using the single particle model?
    Equivalent circuit models.
14. What is the main requirement for building up a purely data-driven model?
    Complete opportunity of recording the states and generating auto-diagnostic function during complete life time.
15. How is the battery dynamics represented in an equivalent circuit model?
    High order pairs of resistor and capacitor.

Chapter 5: Power Electronics (hab)

1. What are the differences between on-board chargers and off-board chargers?

Page 12

- If AC power (level 1 or 2) is used, from the AC charging station, the current passes through the charging cable to the on-board charger, which converts the AC to DC and sends it to the battery via the Battery Management System (BMS).
- If the car is charged with DC (level 3), then the current is sent via the BMS directly to the battery. Therefore, the on-board charger is bypassed during DC charging, but this charging style has higher demands on the BMS.

Level 1	AC (slow)	standard household 120-volt AC outlet (1-phase)	2 kW
Level 2	AC	240-volt AC outlet (1-phase) or sometimes 400 V (3-phase)	20 kW
Level 3	DC (fastest)	3-phase power is used, which provides voltage of 200~800 V	100 kW

2. What are the functions of a battery-based energy storage for the grid?

To do peak shaving, load management and so on.

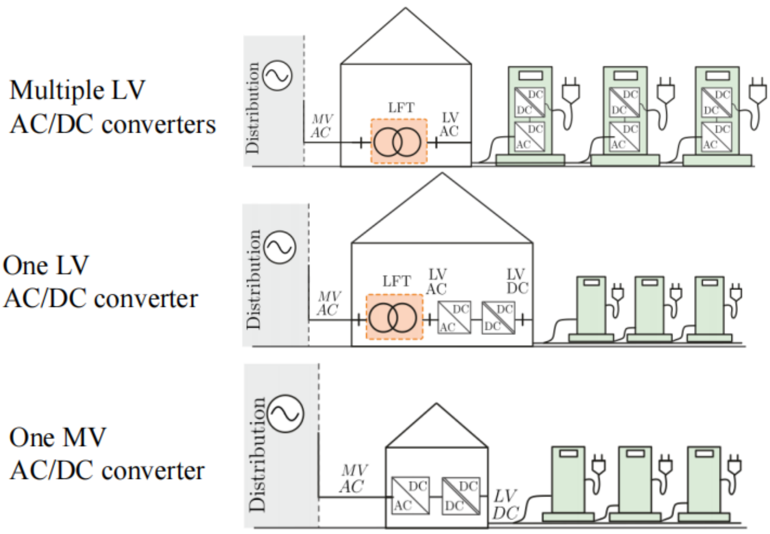
3. What is the power range for an on-board EV charger?

Generally, on-board EV chargers have a power range between 3 kW and 20 kW. The power range for an on-board EV charger can vary depending on the model of the EV, as well as the charging capacity of the charging station being used.

4. Explain the fast charging station architectures based on the MV converter and transformer stages.

Page 13

- In general, the industrial available fast-charging stations need a low-voltage (LV) grid connection for feeding the system. Therefore, normally the voltage adaption from the MV to the fast-charging station is provided by a 50/60-Hz low frequency transformer (LFT), but it increases weight/volume and losses.
- By constructing the MTB dc-dc converter properly (see smart MTB dc-dc transformers), we can establish direct medium-voltage (MV) connection, see the 3rd topology. So it only has 2 stages, stage 1: convert MV AC to MV DC by a ac-dc rectifier; stage 2: convert MV DC to LV DC by a smart multi-winding-based dc-dc converter. From stage 2 we can see that it should be used for large-scale charging stations, i.e. multiple charging piles.



5. Why is galvanic isolation important for EV charging stations?

- Galvanic isolation between AC and DC is mandatory in electric vehicle (EV) charging stations according to the IEC 61851-23 Standard.
- On the one hand, galvanic isolation provides a barrier between the high-voltage charging circuit and the low-voltage vehicle electronics, preventing electrical faults or surges in the gird from damaging the vehicle's sensitive electronic components; on the other hand, galvanic isolation helps protect the charging station and the grid from electrical faults caused by the EV.
- Normally galvanic isolation is achieved by the multi winding transformer on the AC side, however we can also do it on the DC side by using MTB dc-dc converters.

6. Name two popular DC-DC converter topologies for fast charging stations.

The classical topology is based on multiple two-winding transformers (2WTs). During the lecture MTB topology was introduced. Moreover, multiple-active-bridge (MAB) is the most common MTB topology, such as DAB TAB QAB.

7. What is the benefit of partial power processing converters?

Page 53

Improve efficiency and power density; reduce power losses and cost.

8. Explain the principle of soft switching in resonant converters?

Soft switching is a technique used in resonant converters to reduce power loss and improve efficiency by switching at a time when the voltage and current are both low. By using a resonant circuit tuned to a specific frequency, the converter can switch more smoothly and gradually, reducing energy loss and improving performance.

9. What is the impact of increasing the frequency on the transformers?

Page 35 and 36

High efficiency and smaller size.

10. What are the advantages of Smart Transformer for battery integration?

Page 49 and 53

Limit the number of power stages; with high efficiency and safety; participate in condition monitoring and battery management.

Chapter 6: Battery Economics (alsc)

1. What types of costs are important for battery systems?

Page 8 9

The costs of energy storage system, power conversion system, and overheads; the former one is related to energy capacity([€/kWh]), while the latter two are related to power capacity ([€/kW]).

$$C_{cap}\left[\frac{€}{kWh}\right] = \frac{C_{PCS}}{h} + \frac{C_{OH}}{h} + C_{sto}$$

2. What do you understand about life cycle costs?

Page 10

It refers to the total cost of the ESS over its entire life cycle, including (fixed and variable) operation & maintenance, replacement, and disposal and recycling.

3. What examples do you know for variable operating costs?

Variable operating costs: Electricity costs, raw material costs, maintenance and repair costs;

Fixed operating costs: Rent or lease payments, property taxes, salaries and wages.

4. What is the influence of a battery storage system's efficiency on the costs?

- Higher efficiency ESSs can be more cost-effective over their lifetime because they are able to store and release more energy per unit of input energy, reducing the overall cost of operation.
- Higher efficiency ESSs tend to have a lower degradation rate, which means that they can maintain their ability to store and release energy for longer periods of time before needing to be replaced.

5. What is the idea of energy arbitrage?

- Energy arbitrage is the practice of buying and storing energy during periods when the price is low, and then selling it back to the grid or using it during periods when the price is high. This can be done using ESSs.
- Energy arbitrage can be particularly useful for renewable energy sources, which may produce excess energy during periods of low demand or when weather conditions are favorable. By storing this excess energy and selling it back to the grid when demand is higher, renewable energy producers can increase their revenue and improve the economics of their operations.

6. Sketch the qualitative behavior of levelized costs of discharged electricity over the full load hours and explain its meaning.

The qualitative behavior of the levelized cost of discharged electricity (LCDE) over full load hours can be described as a U-shaped curve. At low full load hours, the LCDE is higher due to the higher fixed costs associated with the energy storage system. As the full load hours increase, the LCDE decreases as the fixed costs are spread out over more hours of operation. However, at some point, variable costs (such as electricity, maintenance) begin to outweigh the benefits of spreading out fixed costs, causing the LCDE to increase again.

7. What points are important to consider for the offer for ancillary services, in particular of primary reserve control (PRC)?

Page 19

- Capacity: PCR plants need to have sufficient capacity to provide the required amount of power.
- Response Time: PCR plants need to have a fast response time to be able to provide power quickly when requested by the grid operator. The response time is typically a few seconds.
- Cost: The PCR plant should be cost-effective, and the cost of providing the service should be competitive with other PCR plants in the market.

8. What are typical costs to be considered for primary reserve control (PRC)?

Basically the same as ESSs, plus the cost of transmission and distribution.

Some taxes and costs for generation and marketing.

9. What degrees of freedom should be considered for ensuring that the SOC is about its nominal value for offering PRC services?

Page 22

The power demand can be increased, the frequency range can be deviated, the response time can be within 30s, and the SoC can be changed by trading electricity.

10. How does aging play a role in the considerations of costs and offers in PRC services?

- Reduced revenue: As the BESS ages and experiences capacity degradation, its ability to provide PCR services may become limited. This reduction in revenue can affect the overall profitability of providing PCR services and may require the provider to adjust the PCR offer to maintain profitability.
- Increased maintenance costs: As the BESS ages and experiences capacity degradation, it may require more frequent maintenance and repairs to keep it operating efficiently. These additional maintenance costs can increase the overall cost of providing PCR services.

Chapter-1

1. Explain the structure of a lithium ion battery: (electrodes, separator, electrolyte)

Li-ion batteries consist of largely four main components: cathode, anode, electrolyte, and separator.
"Cathode" determines the capacity and voltage of a Li-ion battery
"Anode" sends electrons through a wire
"Electrolyte" allows the movement of ions only
"Separator", the absolute barrier between cathode and anode

2. What are the differences between primary and secondary batteries?

Primary cells are non rechargeable. They have a solid electrolyte hence the internal resistance is too high and chemical reaction can't be reversed. They have low self discharge
Secondary cells are rechargeable. They have liquid electrolyte and the internal resistance is low. The chemical reaction is reversible. they have high self discharge rates

3. Name some of the existing secondary batteries. (NiCd, NiMh, Li-ion, Li-S, …)

Lithium-ion (Li-ion) batteries,Nickel-metal hydride (NiMH) batteries,Lead-acid batteries,Nickel-cadmium (NiCad) batteries,Lithium-polymer (LiPo) batteries,Sodium-ion batteries etc

4. Name the lithium ion battery chemistry with the highest theoretical capacity.

Li-air batteries could achieve a specific energy of up to 10,000 Wh/kg, which is several orders of magnitude higher than current lithium-ion batteries.

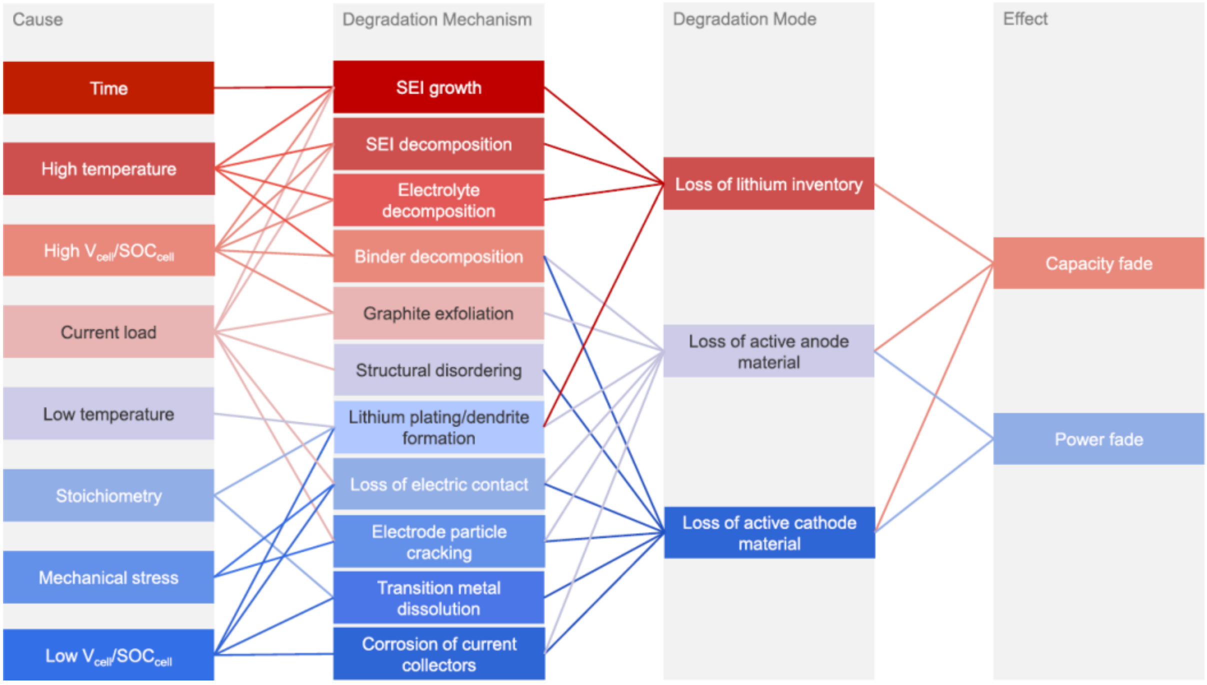
5. What kind of materials have been used in Li-ion batteries (Intercalation materials: Graphite, Conversion materials: sulfur, alloying materials: Silicon)

Anode: The anode is typically made from carbon-based materials such as graphite or lithium titanate ($Li_4Ti_5O_{12}$).
Cathode: The cathode can be made from a variety of materials, including lithium cobalt oxide ($LiCoO_2$), lithium iron phosphate ($LiFePO_4$), lithium manganese oxide ($LiMn_2O_4$), and lithium nickel manganese cobalt oxide ($LiNiMnCoO_2$ or NMC).
Separator: The separator is typically made from a porous polymer material that allows lithium ions to pass through while preventing the anode and cathode from coming into contact.

Electrolyte: The electrolyte is the substance that allows the flow of ions between the anode and cathode. It is typically made from a lithium salt (such as lithium hexafluorophosphate or lithium trifluoromethanesulfonate) dissolved in an organic solvent (such as ethylene carbonate or propylene carbonate).

6. What are the aging mechanisms of Li-ion batteries?

Lithium plating is one aging mechanism which ends the life of a battery more rapidly due to the formation and growth of lithium dendrites.
Lithium Plating, Electrolyte Breakdown,Separator Degradation,Cathode Degradation,Capacity Fade etc.



7. What is lithium plating? How does it happen?

Lithium plating is one aging mechanism which ends the life of a battery more rapidly due to the formation and growth of lithium dendrites. The decomposition of the electrolyte and subsequent formation of the film surface layer on the anode, cause an increase in the impedance and the consumption of recyclable lithium ions. These degradation mechanisms rarely affect the crystal structure of the anode electrode.

8. What is the SEI layer?

The solid electrolyte interface (SEI) is a passivation layer formed on the surface of lithium-ion battery (LIB) anode materials produced by electrolyte decomposition.
or
SEI stands for Solid Electrolyte Interface, which is a thin layer of solid electrolyte that forms on the surface of the anode in a lithium-ion battery during the initial charging cycle. The SEI layer is formed as a result of the reaction between the electrolyte and the anode material.

9. Why SEI layer is important?

The SEI (Solid Electrolyte Interface) layer is important in a lithium-ion battery because it serves as a protective layer that stabilizes the battery's performance and prevents further reactions between the electrolyte and the electrode materials. It forms during the initial charging of the battery. It can also contribute to the aging and degradation of the battery over time.

10. Explain the irreversible losses?

Irreversible losses in a battery refer to the loss of capacity, life span and performance that cannot be recovered through the normal charging and discharging cycles
SEI Layer Formation,Electrolyte Breakdown,Active Material Loss,Mechanical Stress,Internal Resistance are few major irreversible losses.

11. Do you think in a li-ion battery, anode is aged faster or cathode?

Yes, in general, the anode of a lithium-ion battery tends to age faster than the cathode. This is because the anode undergoes more complex electrochemical reactions during the battery's charging and discharging cycles, which can cause more damage to its surface and reduce its performance over time.

12. What is the big challenge of silicon to be used as the anode material?

Silicon has attracted huge attention in the last decade because it has a theoretical capacity ~10 times that of graphite. However, the practical application of Si is hindered by three major challenges: large volume expansion during cycling (~300%), low electrical conductivity, and instability of the SEI layer caused by repeated volume changes of the Si material.

13. Explain the intercalation mechanism. Why it is called intercalation?

Intercalation is the process by which a mobile ion or molecule is reversibly incorporated into vacant sites in a crystal lattice. It occurs in batteries during the process of charging and discharging. It refers to the insertion of ions or molecules into the layered structure of a solid electrode material, such as graphite, which is commonly used as the anode material in lithium-ion batteries.

14. What is dendrite growth and why it is harmful for the battery?

Dendrites are tiny needle-like structures that can form on the surface of the electrode, typically the anode, and can grow and penetrate the electrolyte, causing a short circuit between the anode and cathode. They can also cause capacity loss and further creates overheat issues leading to safety concerns.

15. What is thermal runaway?

Thermal runaway begins when the heat generated within a battery exceeds the amount of heat that is dissipated to its surroundings.If the cause of excessive heat creation is not remedied, the condition will worsen. We use BMS to maintain the right thermal conditions.

Chapter 2

1. Can you name some of the most popular battery cell formats?

Coin/button, cylinder, prismatic and pouch

2-4. What are the advantages and disadvantages of cylindrical cell, prismatic and pouch cells?

Cylindrical cells

Advantages - high energy density, robust, low-self discharge, high current output and cost effective.

Disadvantages - limited shape options, heating

Major disadvantages in terms of safety and flexibility at cell level (Answer in PPT)

- Due to current cell design larger formats are difficult to realize and for many applications (automotive / ESS) extremely high number of cells would be required in the pack
- Nature of the winding process leads to uneven distribution of pressing forces inside to outside the cells
- With increasing energy density, increased pressure build-up inside the cell and safety risk
- The high number of units results in challenges for the BMS fault detection and the assembly and connection technology (AVT)

Prismatic cells

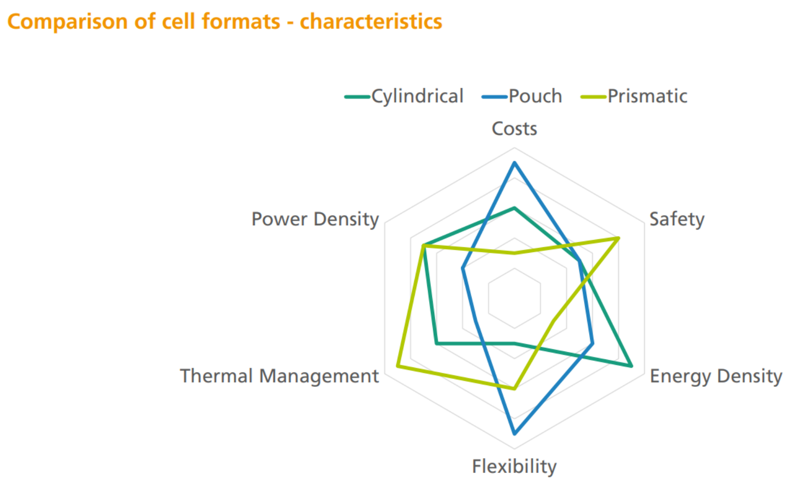
Advantages - Customizable shapes, stable temperature,high capacity

Disadvantages- More fragile, limited options, low output current, high cost, low energy density

Pouch cells

Advantages - Customizable shape, light and thin, high energy density, stable temperature ,Homogeneity (internal pressure distribution) and heat removal from the cel

Disadvantages- More fragile, limited options, low output current, vulnerable to puncher.



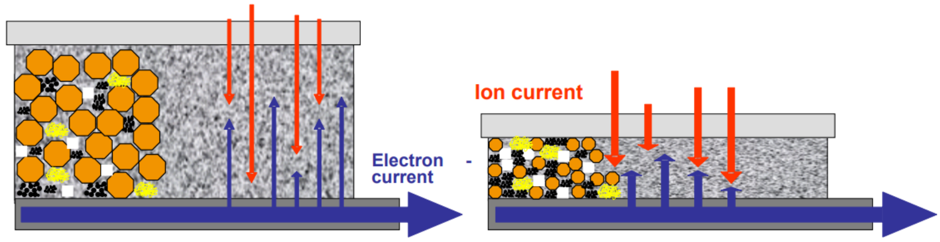
5. Which cell format has the best thermal performance?

Prismatic cells have best thermal performance due to their flat design that allows better heat dissipation compared to the other.

6.Explain the exiting trade-off between specific power and specific energy when designing a battery.

The trade-off between specific power and specific energy arises because the two characteristics are inversely proportional.This is because increasing the specific power usually involves increasing the rate at which the battery discharges, which can reduce the amount of energy that it can store.

Recipe development and trade-offs



High specific energy density: [Wh/kg]

- High levels of large active material (AM) granules
- High layer thickness (capacity occupancy)
- Lower polymer binder content
- Low content of conductive additives
- Low porosity
- Processing sophisticated, ionic and electrical conductivity and long diffusion paths
- = **Low specific power**

High specific power density: [W/kg]

- small "nano" - particle AM
- low layer thickness (low capacity)
- high conductive additive share
- high porosity
- High binder content required for cohesion, lower AT content, much electrolyte
- = **Low specific energy**

7. Explain the coating process in battery production line.

Battery production lines often involve a coating process to apply a layer of active material onto a substrate to create a positive or negative electrode.

- Mixing: The active material, along with other components such as binders and conductive additives, is mixed in a solvent to create a slurry.
- Coating: The slurry is then applied onto a substrate using a coating technique such as doctor blade or slot die coating. The thickness and uniformity of the coating are critical to the performance of the battery.
- Drying: The coated substrate is then dried to evaporate the solvent and create a solid film of the active material on the substrate.
- Calendering: The dried film may be calendered, which involves pressing the film between rollers to improve its density and reduce its thickness.
- Cutting: The coated substrate is then cut into the desired size and shape to form the electrode.
- Assembly: The electrodes are then assembled with other components such as a separator and electrolyte to create a complete battery cell.

8. What are the objectives of electrode calendaring?
to increase the conductivity of electrode and improve the quality of electrode as well
Aim of the process: Homogenous electrodes, Defined porosity.

9. What is the Galvanostatic Cycling with Potential Limitation (GCPL)?
Galvanostatic Cycling with Potential Limitation (GCPL) is a testing technique used to evaluate the performance of batteries and electrochemical cells. It is a type of electrochemical cycling test that combines a constant current (galvanostatic) mode with a voltage limitation (potential limitation) mode.

10. What is the drawback of GCPL and how to solve it?
Time consuming, limited information, limited acceptability, reliance in predetermined voltage limits, artificial degradation.soluation to use pules test method and EIS method

11. What is a pulse test?
The pulse test is an electrochemical testing technique used to evaluate the performance of batteries. under differents loads during time