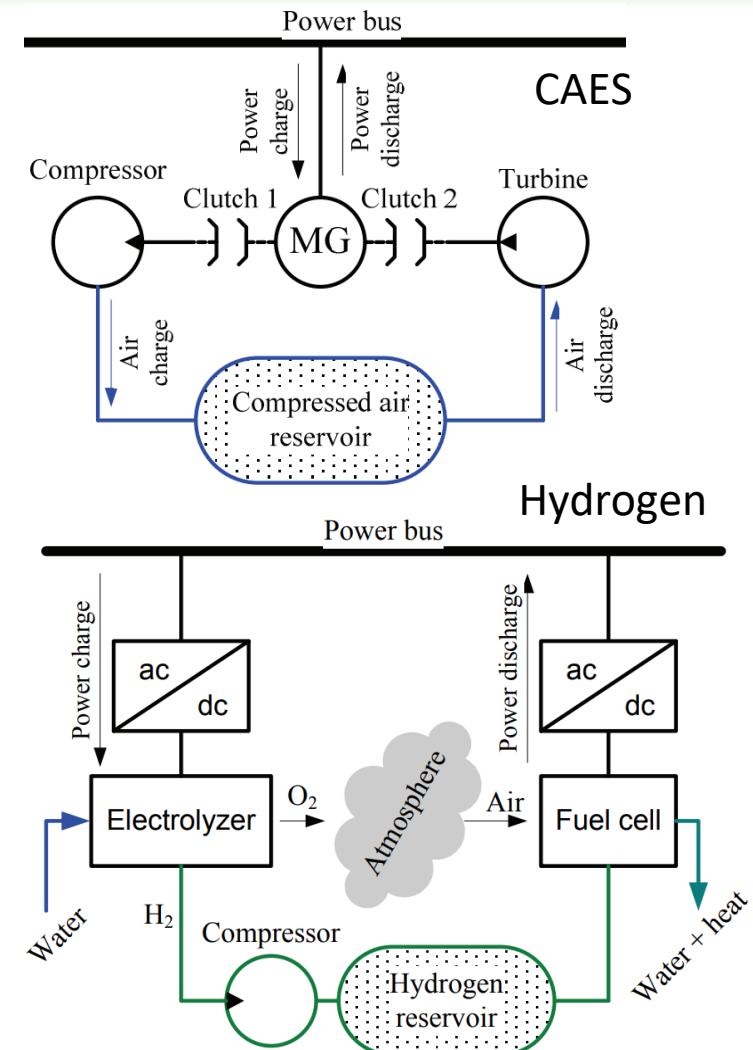
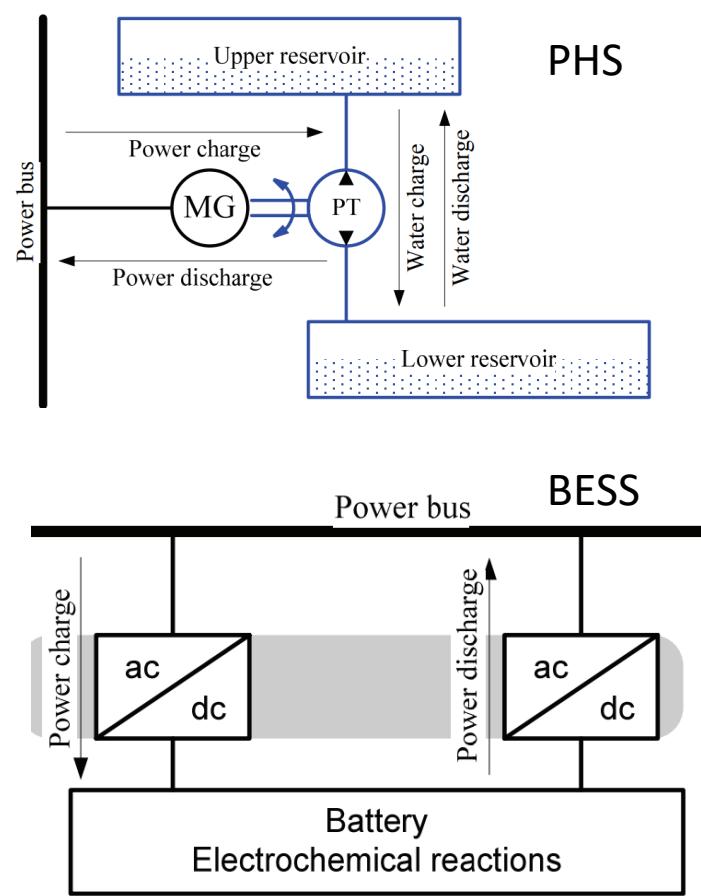
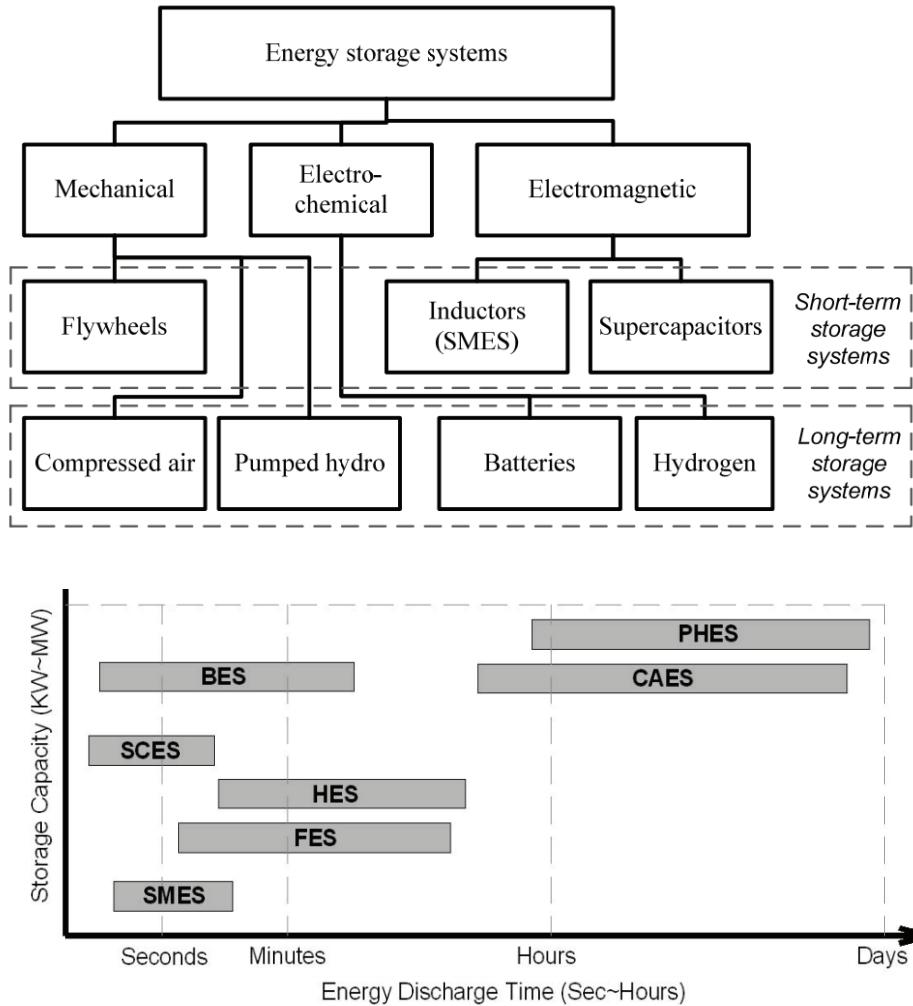


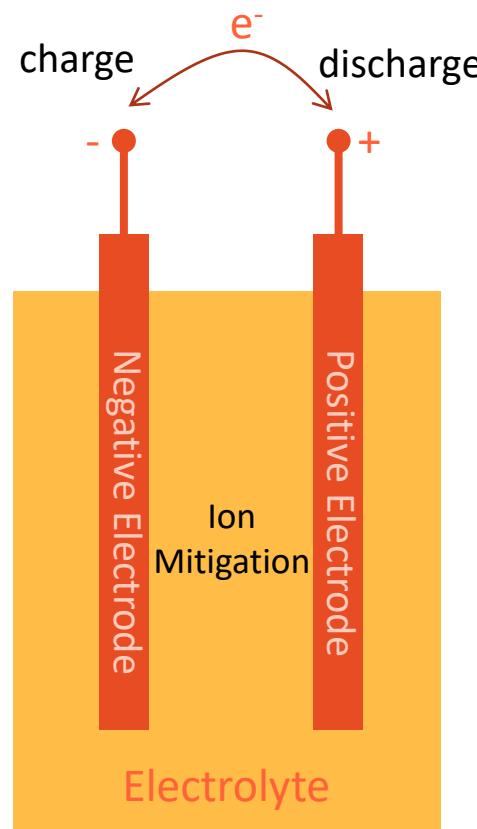
# Energy Storage Modelling & Application

Karl M.H. Lai

# Introduction – Different Types of Energy Storage

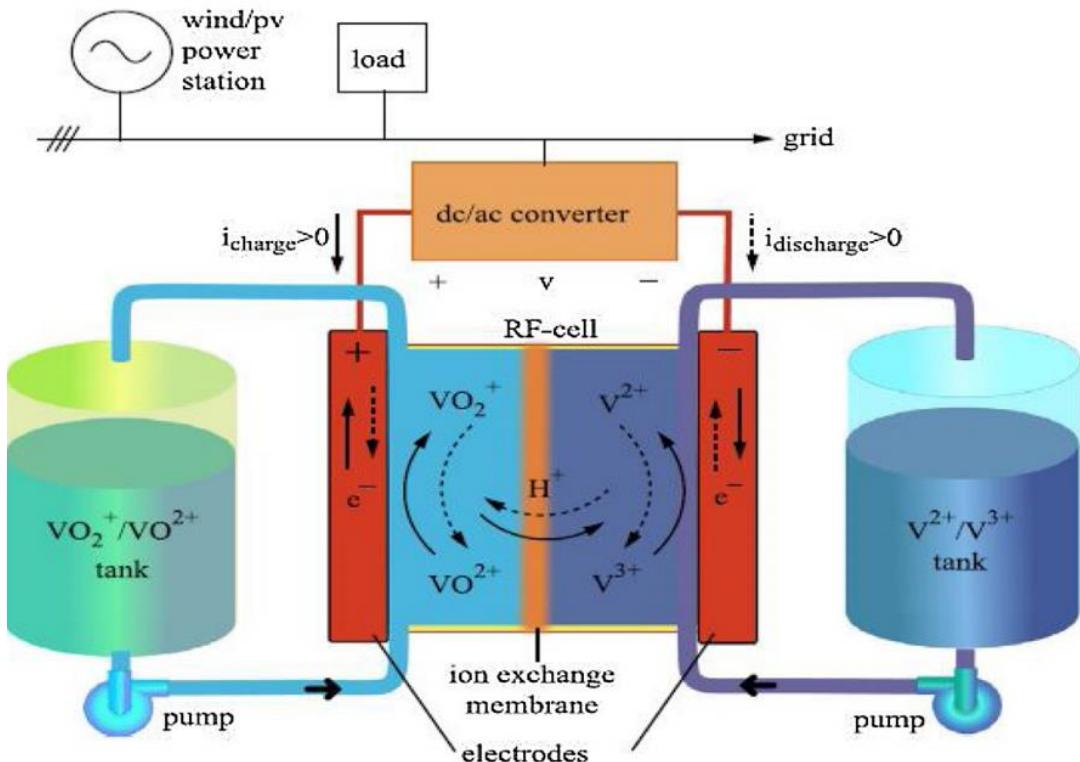


# Introduction – Electrochemistry

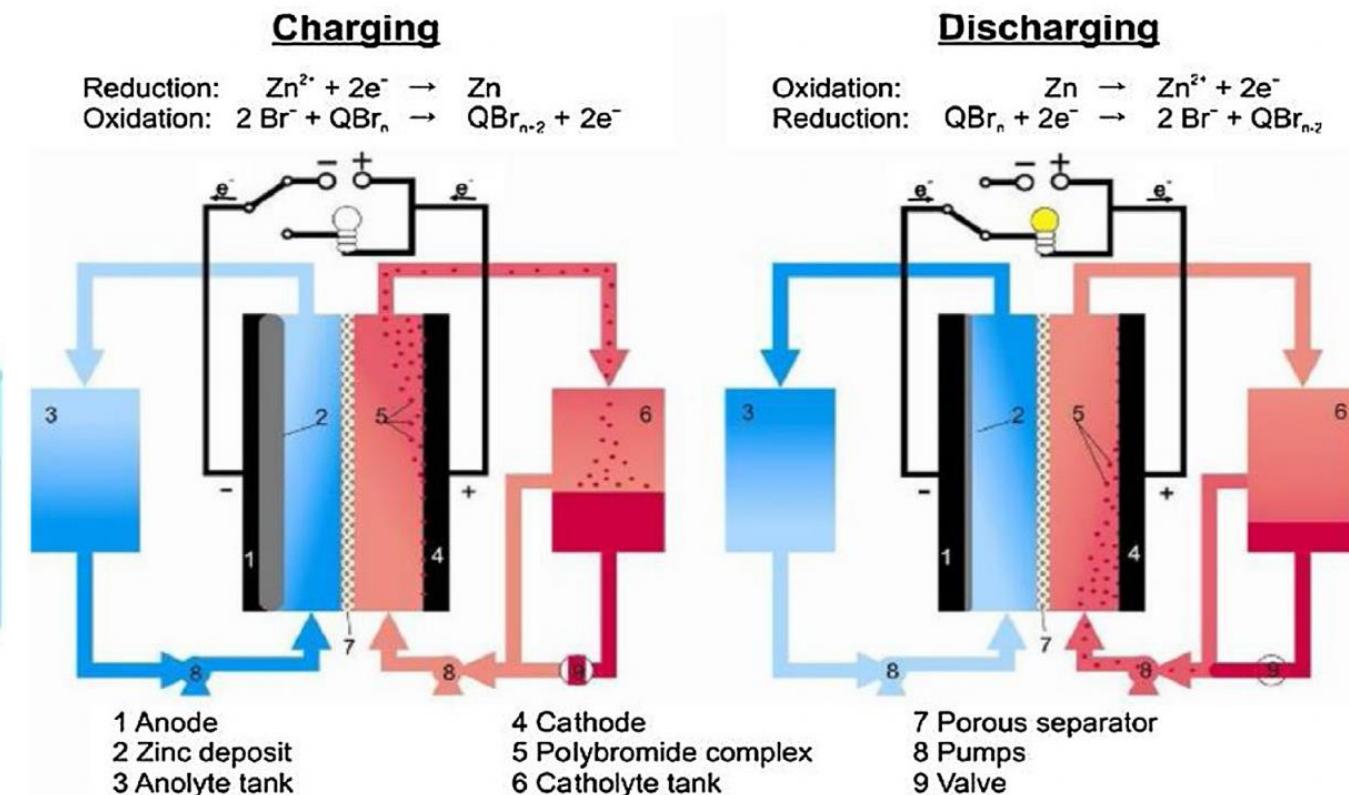


- Chemical Equations in Battery means the relative ratio the chemical needed, and subsequent dynamic equilibrium for material change
- Batteries can **charge** and **discharge**.
- Lead Acid:  $\text{Pb} + \text{PbO}_2 + 2\text{H}_2\text{SO}_4 \leftrightarrow 2\text{PbSO}_4 + 2\text{H}_2\text{O}$
- NiCd:  $\text{Cd} + 2\text{NiOOH} + 2\text{H}_2\text{O} \leftrightarrow \text{Cd}(\text{OH})_2 + 2\text{Ni}(\text{OH})_2$
- NiMH:  $\text{MH} + \text{NiOOH} \leftrightarrow \text{M} + \text{Ni}(\text{OH})_2$
- Li-ion:  $\text{Li}_x\text{C} + \text{Li}_{1-x}\text{MO}_2 \leftrightarrow \text{C} + \text{Li MO}_2$
- NaS:  $2\text{Na} + 4\text{S} \leftrightarrow \text{Na}_2\text{S}_4$

# Introduction – Electrochemistry

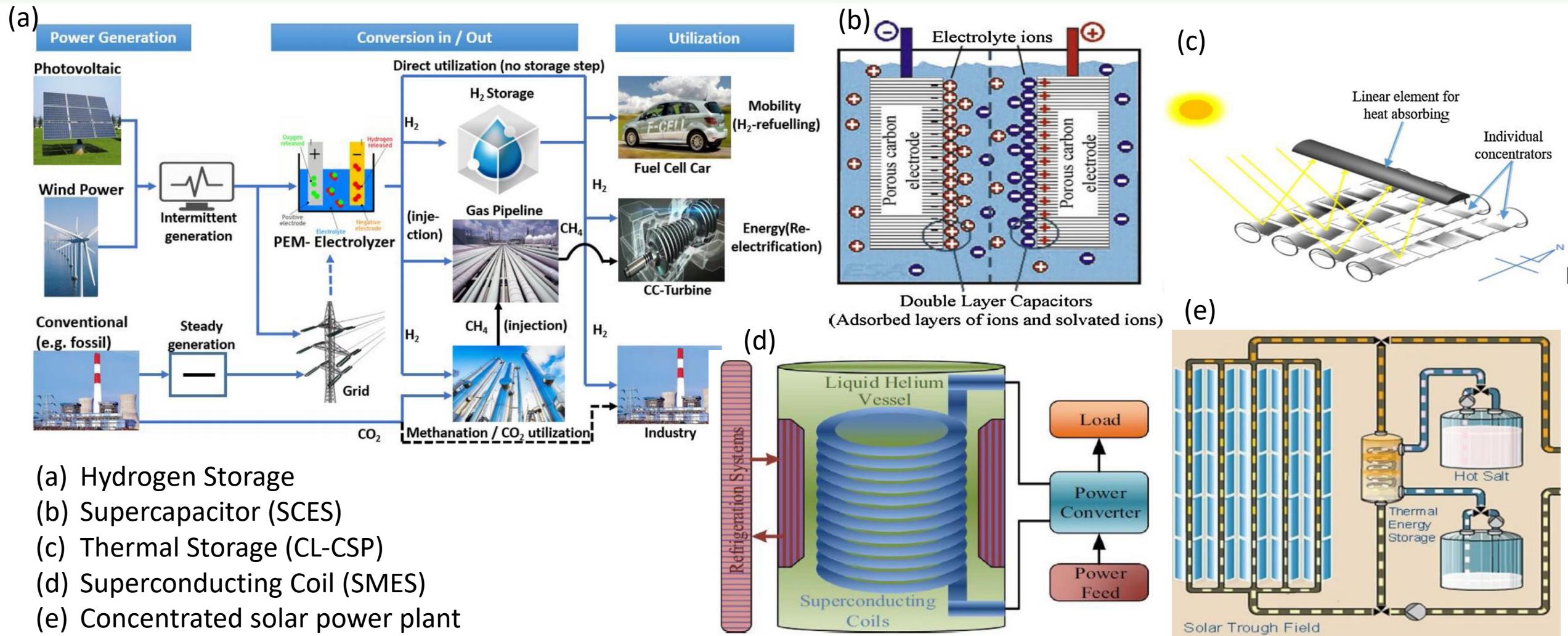


Vanadium Redox Flow Batteries



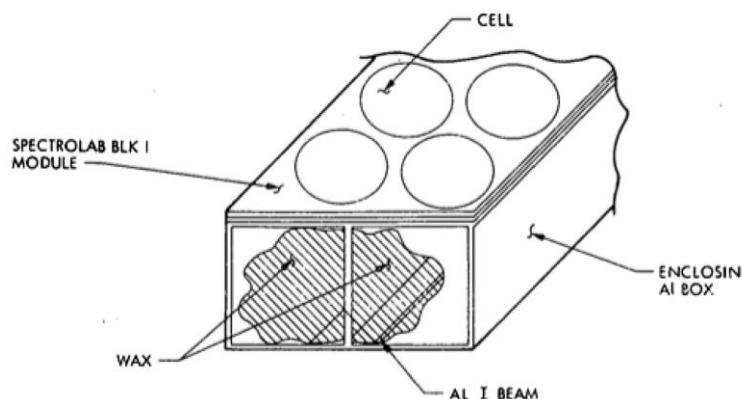
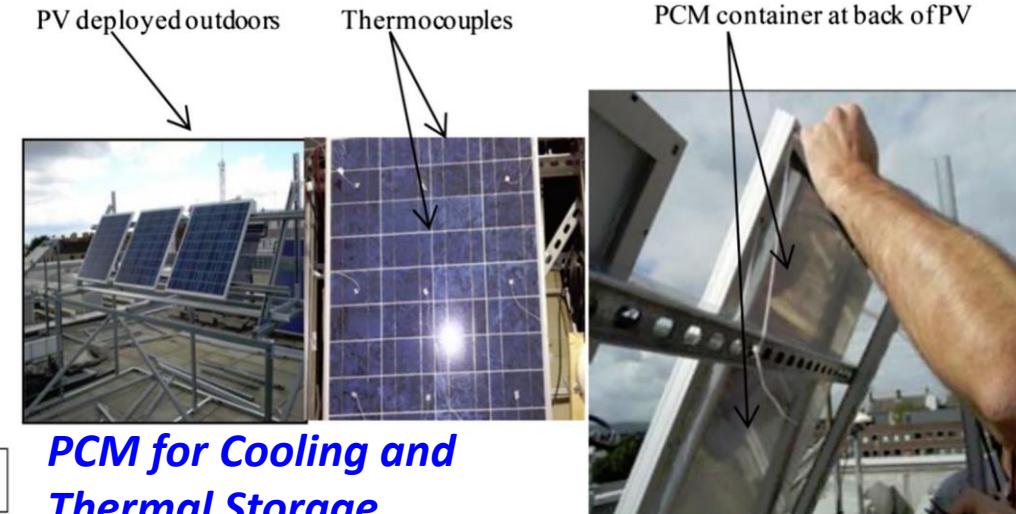
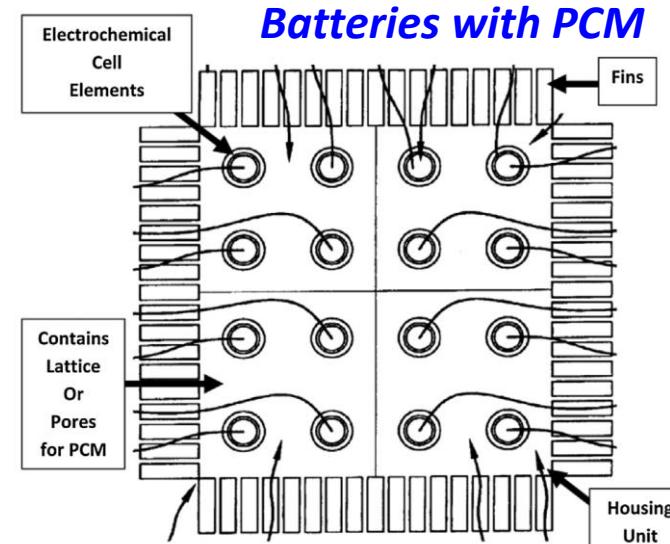
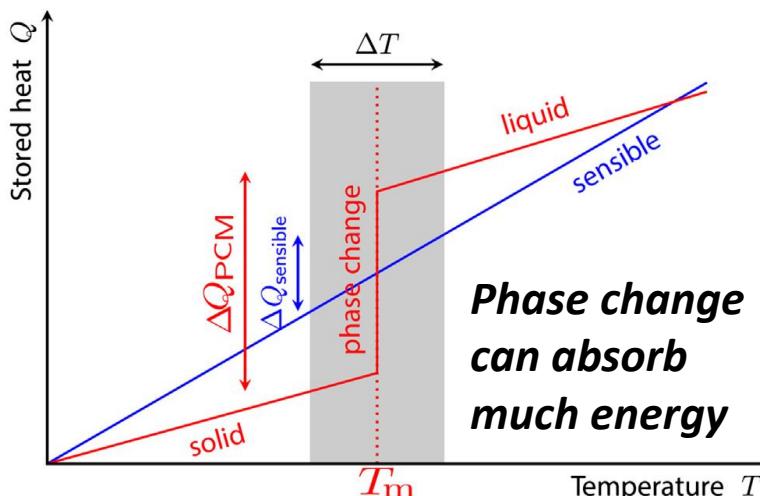
Hybrid Flow Battery (e.g. Zn-Br system)

# Introduction – Other Energy Storage



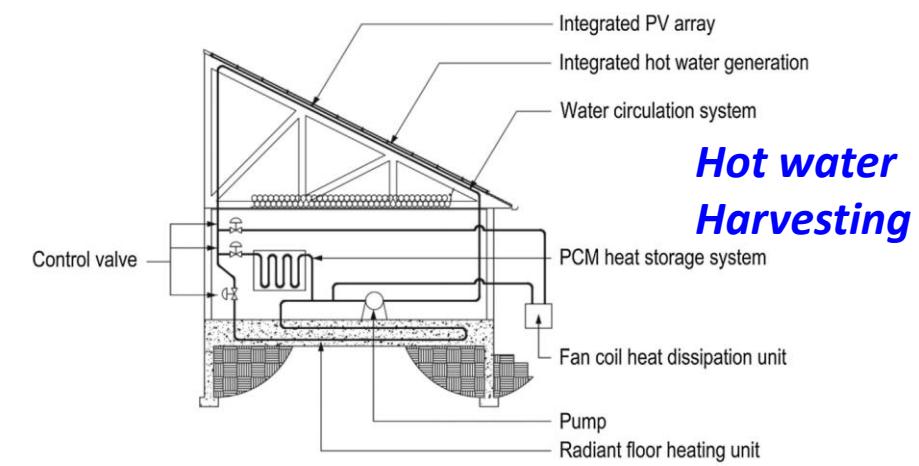
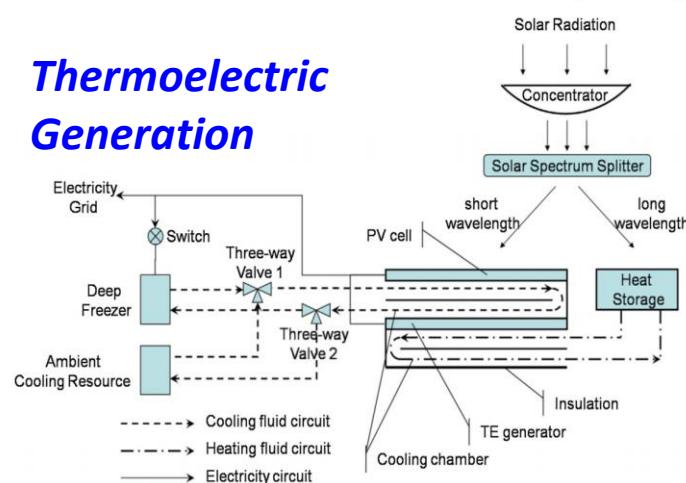
# Introduction – Thermal Storage

**PCM=Phase change material**



**PV including PCM**

## Thermoelectric Generation



# Batteries – terms, state of charge

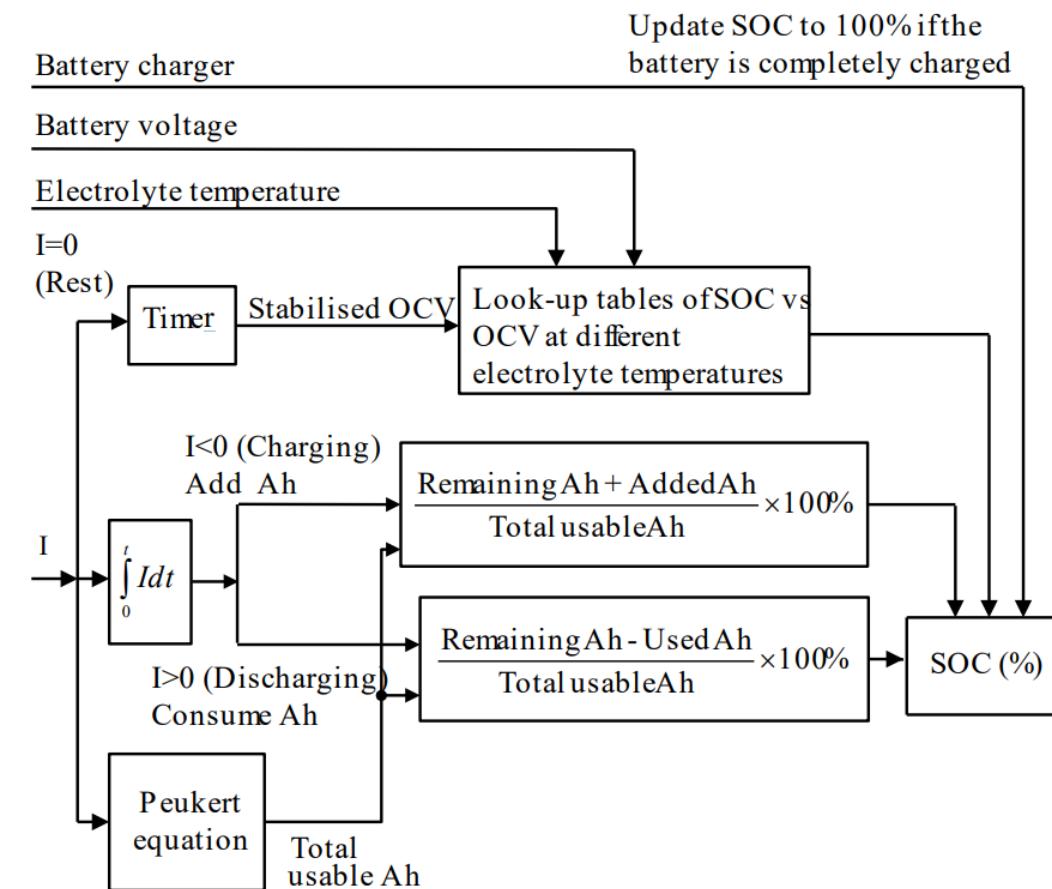
Chau, K.T. (2018), Electrochemistry, 6<sup>th</sup> Notes  
for ELEC3143 Energy Conversion

- State of Charge (SOC) is defined as  $C_r/C_t$ , where  $C_r$  and  $C_t$  are the **residual** and **total usable** coulometric capacity in Ah of the battery.
- SOC is affected by **discharging rate/current I**, **temperature T** and **aging effect**.
- Relationship between capacity and discharging current: (Peukert Equation)

$$C_{tl} = KI^{(1-n)}$$

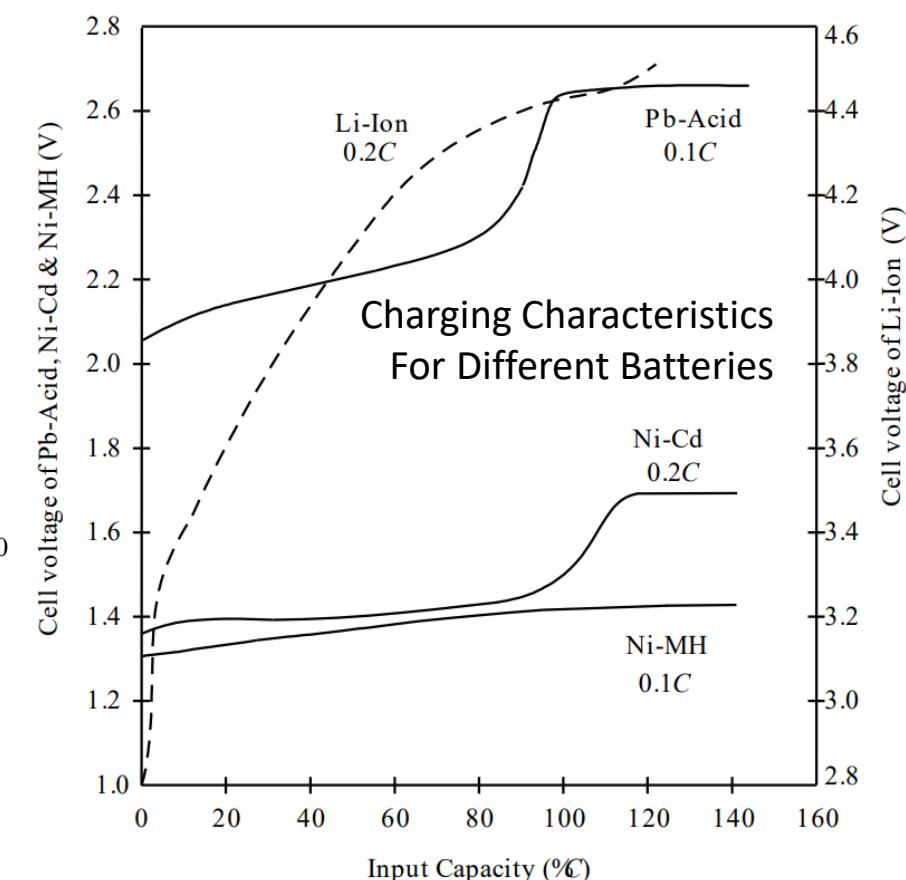
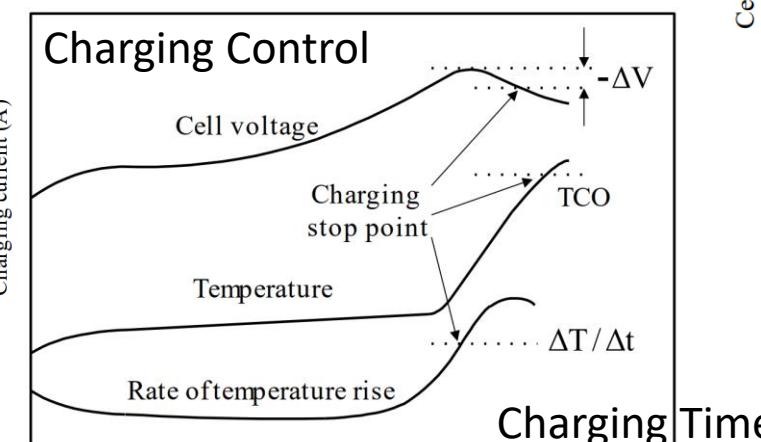
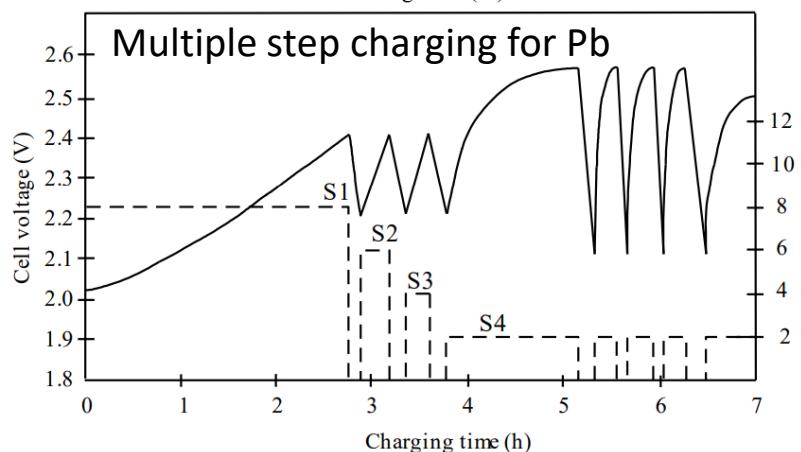
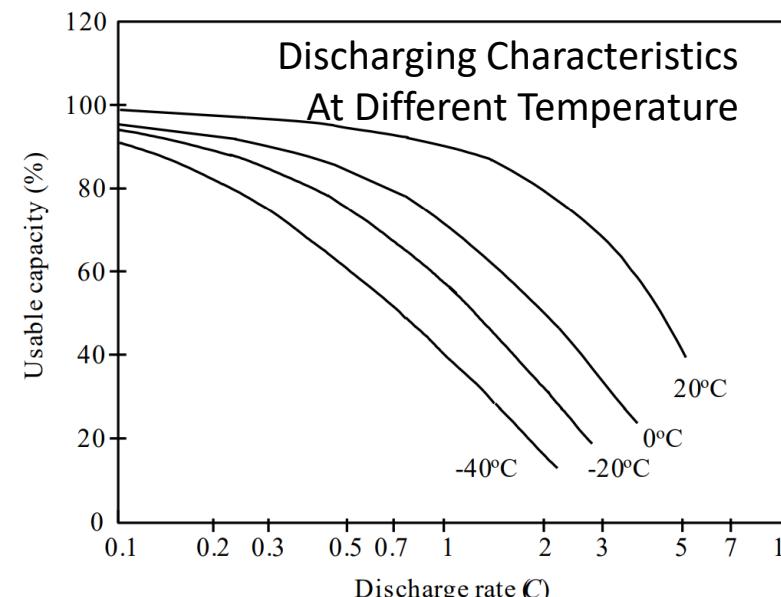
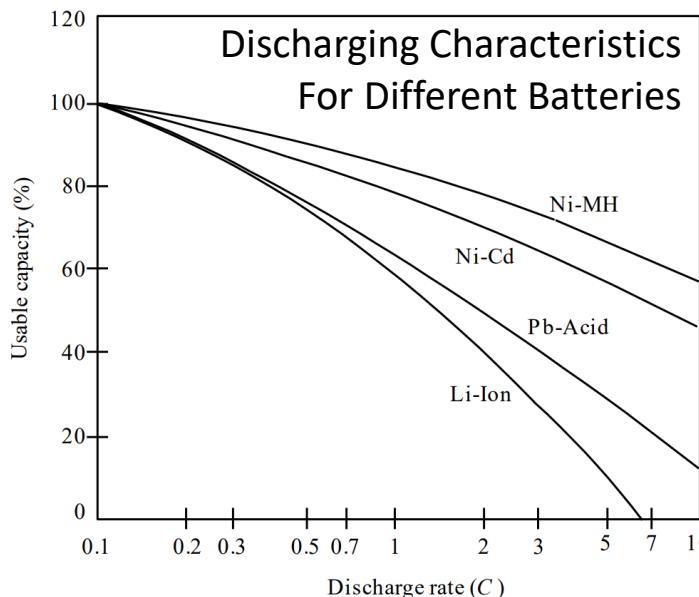
where  $C_{tl}$  is the capacity Ah under particular discharge current  $I$  in A and discharge time  $t$  in h, while  $K$  and  $n$  are constants.

- To deduce residual capacity, one can see the open circuit voltage (OCV), with Peukert Equation.



# Battery Characteristics

Chau, K.T. (2018), Electrochemistry, 6<sup>th</sup> Notes  
for ELEC3143 Energy Conversion



# Comparison between Batteries – Numbers

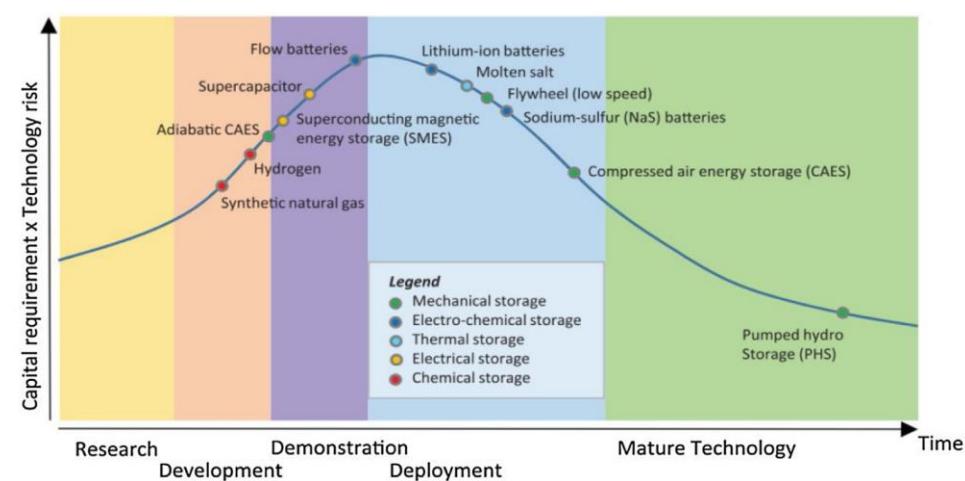
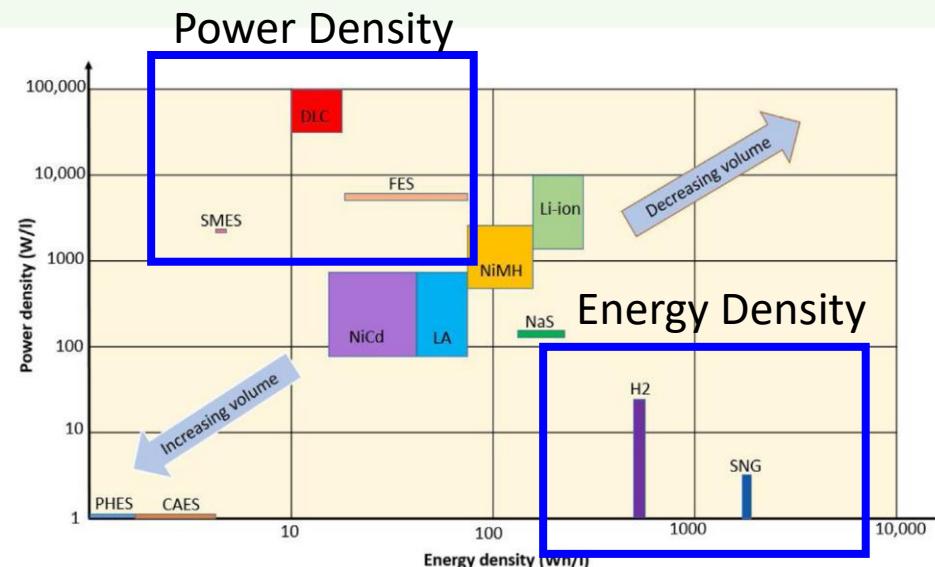
Comparison between different battery technologies.

Diouf B. &amp; Pode R. (2015), Potential of Lithium-ion Batteries in renewable energy

Specifications	Lead acid	NiCd	NiMH	Li-ion	*LiFePO <sub>4</sub>		
	3-5 years			Cobalt	Manganese	Phosphate	
Specific energy density (Wh/kg)	30–50	45–80	60–120	150–190	100–135	90–120	
Internal resistance (mΩ)	<100	100–300	200–300	150–300	25–75	25–50	
Cycle life (80% discharge)	12 V pack 200–300	6 V pack 1000	6 V pack 300–500	7.2 V 500–1000	per cell 500–1000	per cell 1000–2000	
Fast charge time	8–16 h	1 h typical	2–4 h	2–4 h	1 h or less	1 h or less	
Overcharge tolerance	High	Moderate	Low	Low. Cannot tolerate tickle charge			
Self-discharge/month (room temp.)	5%	20%	30%	<10%			
Cell voltage (nominal)	2 V	1.2 V	1.2 V	3.6 V	3.8 V	3.3 V	
Charge cutoff voltage (V/cell)	2.40 Float 2.25	Full charge detection by voltage signature			4.20	3.60	
Discharge cutoff voltage (V/cell, 1C)	1.75	1.00	2.50–3.00			2.80	
Peak load current	5C	20C	5C	>3C	>30C	>30C	
Best result	0.2C	1C	0.5C	>1C	<10C	<10C	
Charge temperature	–20 to 50 °C (–4 to 122 °F)	0 to 45 °C (32 to 113 °F)	0 to 45 °C (32 to 113 °F)			Carbon Footprint: 70kg CO <sub>2</sub> per kWh	
Discharge temperature	–20 to 50 °C (–4 to 122 °F)	–20 to 65 °C (–4 to 49 °F)	–20 to 60 °C (–4 to 140 °F)				
Maintenance requirement	3–6 months (topping charge)	30–60 days (discharge)	60–90 days (discharge)	Not required			
Safety requirements	Thermally stable	Thermally stable, fuse protection common			Protection circuit mandatory	(Explosive)	
In use since	Late 1800s	1950	1990	1991	1996	1999	
Toxicity	Very high	Very high	Low	Low	Cheaper and Cheaper !!		
Cost (ratio)	1	1 – 4			4 – 8		

5000 cycles  
For deep  
dischargeCarbon Footprint:  
70kg CO<sub>2</sub> per kWh

# Comparison between Energy Storage – Graphs



## Notes:

1. No single ES can meet all requirements.
2. Among ES, **HES** has the **highest energy density**, while for batteries **NaS and Li-ion** have **higher energy density**
3. **PHES and CAES** with long discharge duration are fit for **peak shaving and time shifting**, while **HES, TES and Flow batteries** finds **applications in medium scale**, **SMES** and supercapacitor, **flywheels and batteries** can be used for **power quality control**.
4. **PHES, CAES, HES and FB** have very little **self-discharge**
5. **CAES requires lowest capital cost** than the PHES (second) while flywheel, supercapacitors, SMES and fuel cell are expensive
6. CL-CSP and thermal storage are low cost and more efficient.
7. **Chemical deterioration** in batteries shortens their lives.
8. BES is most suitable ES to fulfil rural energy demand as it is portable and scalable
9. ES is important in large RE penetration.

# Comparison between Energy Storage – Functions

Applications Technology	Bulk Energy Application		Ancillary Services Application					End-use Energy Application		RE Integration Application	Transport Application	Off grid Application
	Energy Arbitrage	Peak Shaving	Load following	Spinning reserve	voltage support	Black start	Frequency Regulation	Power Reliability	Power quality			
<b>Mechanical Energy Storage</b>												
PHES	Y	Y	N	N	N	Y	Y	N	N	Y	N	N
CAES	Y	Y	Y	Y	N	Y	Y	Y	N	Y	N	N
FES	N	N	Y	Y	Y	N	N	Y	Y	N	N	N
<b>Electrochemical Energy Storage</b>												
Lead acid	N	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
NaS	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Li-ion	N	N	Y	N	Y	Y	Y	Y	Y	Y	Y	Y
Flow Battery	Y	Y	Y	N	Y	Y	Y	Y	Y	N	Y	Y
<b>Electrical Energy Storage</b>												
DLC	N	N	N	N	N	N	N	N	Y	N	Y	N
SMES	N	N	N	N	N	N	N	N	Y	N	Y	N
<b>Hydrogen Energy Storage</b>												
Hydrogen Fuel Cell	Y	N	N	N	N	N	N	N	N	Y	Y	Y
<b>Thermal Energy Storage</b>												
Thermal	Y	Y	Y	Y	N	N	N	N	N	N	N	N

# Comparison between Energy Storage – Functions

- **Energy Arbitrage:** Store energy when it is cheap, sell when it is expensive (\$\$)
- **Peak Shaving:** Cover the peak load, ES installed at customer side
- **Load Following:** Maintain a **balance between generation and load\***
- **Spinning Reserve:** Discharge at abnormal situation **with rated parameter values (V & f)**
- **Voltage Support:** Locally regulate the **voltage rise** problem
- **Black Start:** Restart the whole system after unexpected interrupt, balancing
- **Frequency Regulation:** Maintain **balance between generation and demand**
- **Power Quality:** Protect loads **against short-duration events**
- **Time Shifting, Capacity firming, and Energy Smoothing:** to provide energy power during a day even in worst weather without exaggerated fluctuation
- **T&D Upgrade Deferral:** Reduced loading of Tx & Cables
- **Congestion:** Take **heavy load** substations and lines to **relieve power congestion**

# Comparison between Energy Storage

## – Advantages and Disadvantages

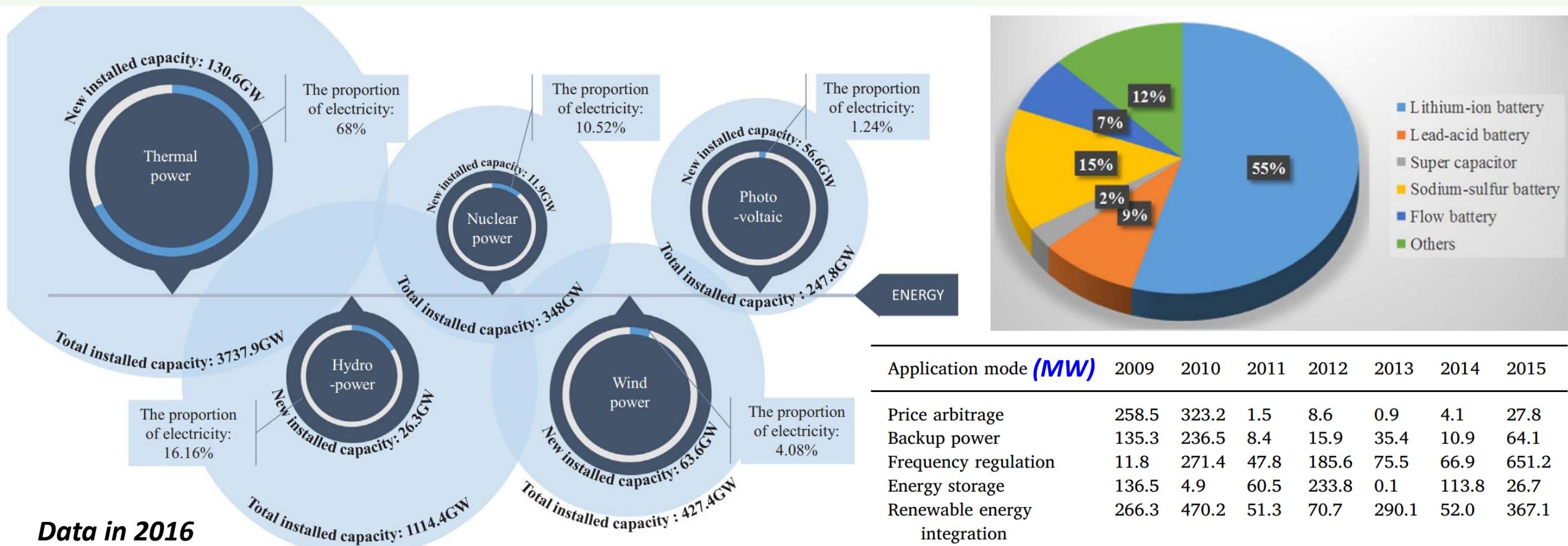
Properties	Technologies	
	BES	PSH
Cycle Efficiency (%)	60–90	70–85
Energy Density (Wh/L)	50–500	0.5–2
Response time	Milli-seconds	Seconds- Minutes
Storage Capacity* (MWh)	Up to 40 MWh	1000s of MWh
Self-discharge (%/day)	0.1–20	~ 0
Cycling times	2000–10,000	–
Period	Medium term	Long term
Status of technology	Mature	Mature
Energy Capital Cost \$/kWh	150–1000	5–100

Properties	FES	CAES
Cycle Efficiency (%)	Up to 95	40–50
Energy Density (Wh/L)	20–80	0.2–6
Response time	Milli-seconds	1–15 Minutes
Storage Capacity* (MWh)	Up to 5 MWh	1000s of MWh
Self-discharge (%/day)	20–100	~0
Cycling times	105–107	–
Period	Short term	Long term
Status of technology	Early stage	Early stage
Energy Capital Cost \$/kWh	1000–5000	2–100

EES System	Advantages	Disadvantages
Battery storage systems	Lead Acid	Fast response time Small daily self – discharge Relatively high cycle efficiencies Low capital cost
	Lithium-ion	Fast response time Compact and light weight High cycle efficiency <b>High energy densities</b>
	Sodium-Sulphur	Low self-discharges High rated capacity High recyclability
	Nickel-Cadmium	Robust Reliable Quick response High Efficiency
	Vanadium Redox flow Battery	High energy Deep discharge capability and reversibility
	Zinc-Bromine flow Battery	Higher capacity No toxic products Long life Mature and proven technology
Pumped storage hydro		No self-discharge
Flywheel energy storage		Fast response Easy maintenance Relatively high cycle efficiency
Compressed air energy storage		Low capital cost High energy density Low self-discharge
Thermal energy Storage		High operating cost Needs temperature control systems <b>High Temperature ~300°C</b>
		Environmental hazards Memory effect High operating cost Low electrolyte stability and solubility Low energy density Metal corrosion Dendrite formation Low cycle efficiency <b>Needs geographical specialties</b>
		Low energy density Long construction time
		Idling loss is present Relatively high self-discharge It cannot serve as a backup system Capital cost is high Relatively high response time Relatively low round trip efficiency Need for geographical specialties Low cycle efficiency <b>(with energy conversion)</b>

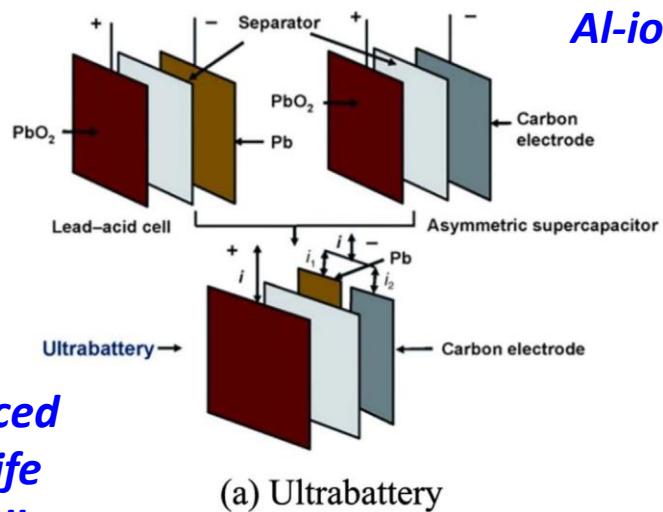
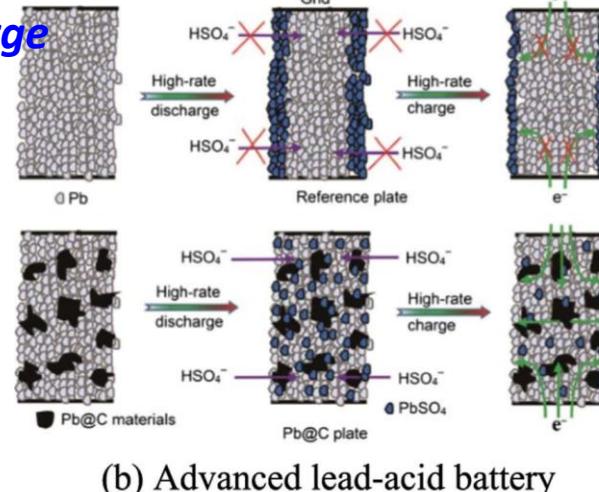
# Energy Storage: Current Situation



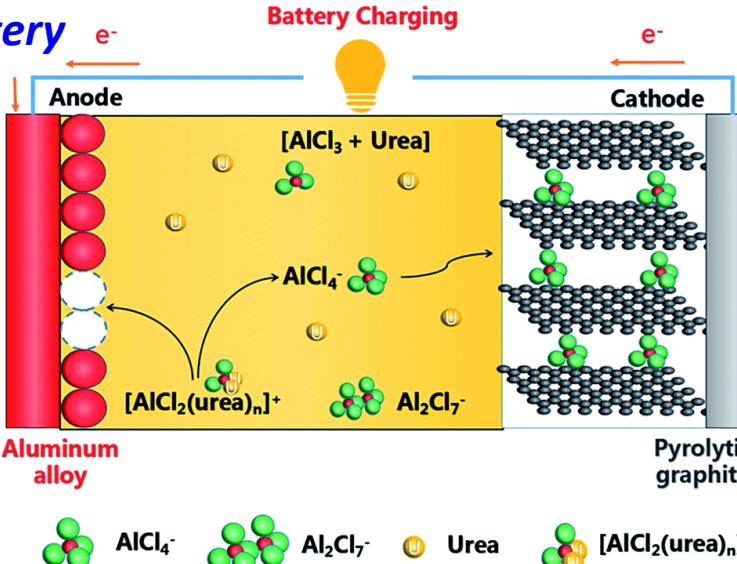
**Data in 2016**

# Energy Storage: Current Situation (Highlights)

**Enhanced Cycle life in Small Discharge**



## Al-ion Battery



- Research on Battery Power Conversion
1. Energy gap in power electronics device
  2. Good understanding but hard to compute real time in devices
  3. Multi-port converter topology
  4. Modelling of Power Electronics and Non-linear control / analysis

Battery technology	Advantages	Disadvantages	Energy storage applications
Lead-acid battery	Low capital cost	Limited life cycle, long charging time and high self-discharge rate Environmental pollution	Hot spare, frequency control and load adjustment
Lithium-ion battery	High energy densities, high efficiency, and long life cycle	High production cost, requires special charging circuit	Frequency control, load shifting and power quality
Vanadium based flow battery	High power, long life cycle, fast charge and discharge	High production cost, large area	Load shifting, emergency standby and power quality
Sodium-sulfur battery	High power and energy densities, high efficiency	Production cost and safety concerns	Load adjustment and standby power
Aluminum-ion battery (Estimated)	Low capital cost, fast charge and discharge, high efficiency	Under development Low energy densities	N/A

**Charge within 1 min**

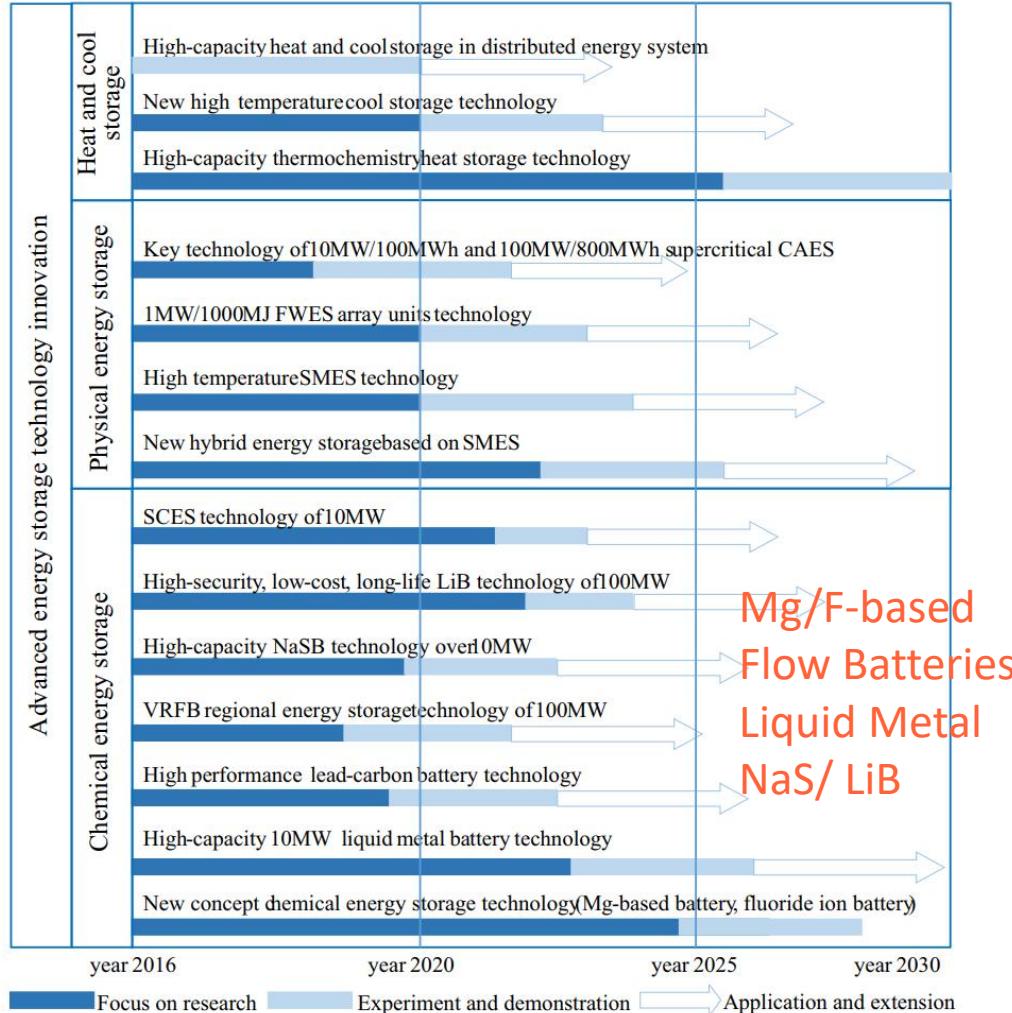
# Highlights of China's Energy Storage development (1)

- Facts:
  - **66%** of cumulative energy storage is in ***Li-ion Battery***
  - Energy Storage are installed in ***Demand Side***, and most of the ES are DG, or microgrid projects, as high capacity ES in generation is not available
  - In response to ***big peak-valley difference*** (due to high population and growing economy), energy saving, emission reduction, China government has paid attention on demand side response.
  - Need a ***clear technical route*** on development and detailed planning e.g. Germany has road map for LiB, ESEM, SES to promote progress

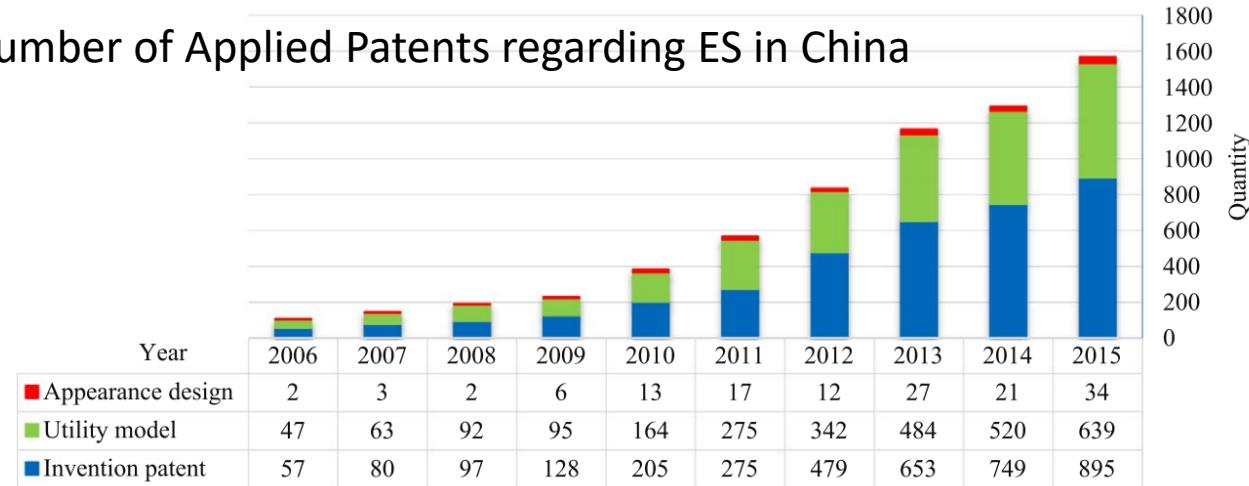
Yu, H. et al. (2017), China's Energy Storage Industry: Develop Status, Existing Problems and Countermeasures

# Highlights of China's Energy Storage development (2)

Development Roadmap for China



Number of Applied Patents regarding ES in China



China's participation in international standards

- | Year | Participation Details  |
|------|--|
| 2011 | Undertake the establishment of IEEE P2030.3TM- <i>Standard for Test Procedures for Electric Energy Storage Equipment and Systems for Electric Power Systems Applications.</i>      |
| 2012 | Undertake the work of <i>Development Roadmap of Nanotechnology (NT)</i> by IEC Market strategy bureau (MSB) Special work group 4 (SWG4)  |
| 2012 | take charge of the establishment of white book - <i>Grid integration of large-capacity renewable energy sources and use of large-capacity electrical energy storage</i> by IEC MSB |
| 2014 | Undertake the establishment of IEC 62932–2–1- <i>Flow battery systems for stationary applications-part 2–1: performance general requirements &amp; method softest</i>              |

# Highlights of China's Energy Storage development (3)

- Main Issues/ achievements in **Physical Storage**:
  - For PHS: **Pricing Policy**
  - For CAES: Compressed air into abandoned miles/ underwater tanks by high pressure → to obtain mixture of natural gas+ air  
→ Wind Power can drive compressor directly →  $\eta \uparrow$   
→ Problems in **core technology of gas turbines, lack of oil and gas reserve, or natural caves as gas storage device**
  - For FWES: → **High Self-Discharging Rate**  
→ used as UPS, regenerative braking, wind turbine storage, high-power pulse  
→ Connect to generator directly

# Highlights of China's Energy Storage development (4)

- Main Issues / achievements in **Electromagnetic Storage**:
  - **SMES**: superconducting coil to absorb EM energy
    - Good studies in **superconducting magnet separation, MHD propulsion, nuclear magnetic resonant**
    - Need **current limiter**, e.g. Gansu Province 0.5MVA SMES
  - **SCES**: similar to supercapacitor, based on electric double layer absorption, surface oxidation/reduction, insert ions
    - applied in **elevator energy saving, street lighting, robot energy storage, vehicle start-stop**
    - invented a FeOOH/graphene nanometer to lower cost of SCES

# Highlights of China's Energy Storage development (5)

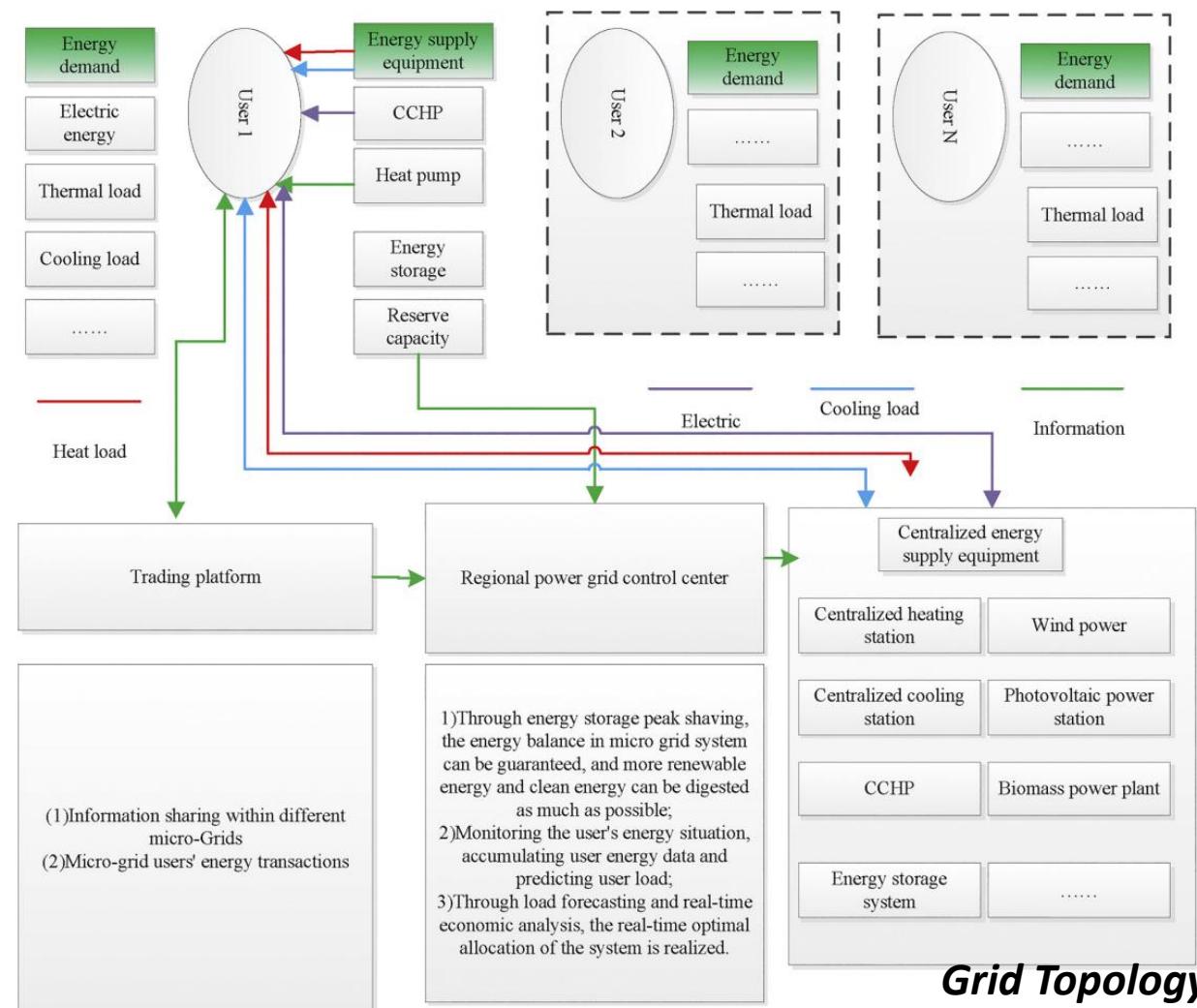
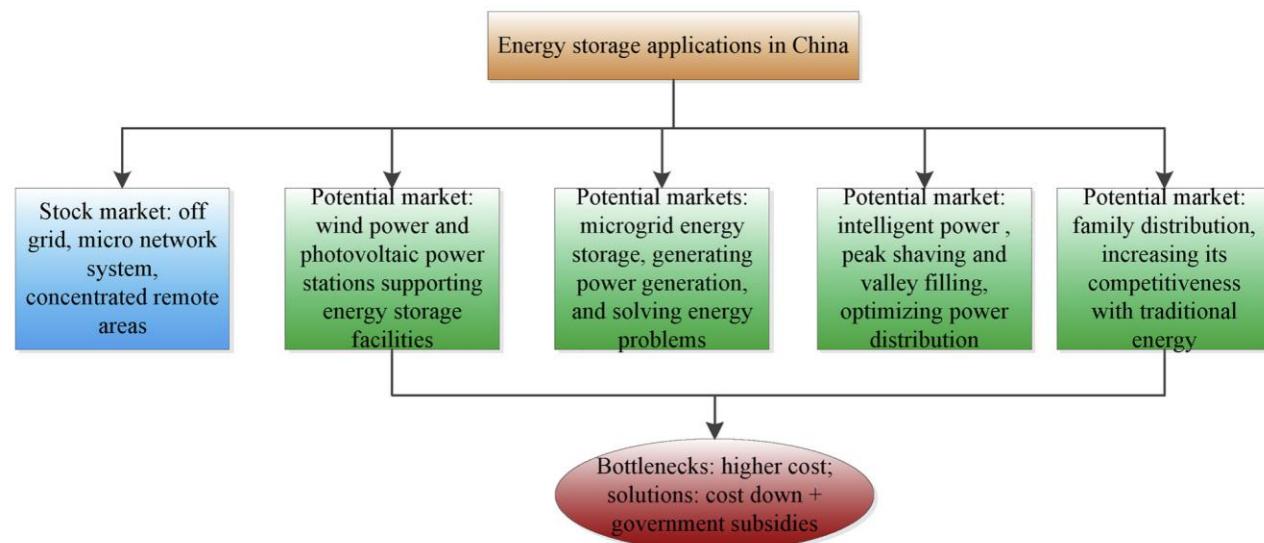
## Main Issues / achievements in **Electrochemical Storage**:

- **PbB** → Lead Fumes, dusts or waste water with Lead
- **LiB**: higher capacity, longer cycle life, no memory effect, with high energy density in weight/volume
- **NaSB**: in theory can store 4-5 times energy of LiB  
for power plant load balancing, UPS, instant power compensation, good in static environment
- **FB** (Flow Battery): VRFB/ ZnBrFB are dominating  
3MW/6MWh in Liaoning Province  
Stable output, dispatch controllability, energy saving,  
with black start, islanding, harmonic treatment

# Highlights of China's Energy Storage development (6)

Main functions of energy storage equipment in power system.

	Functions
standby powers	To help the power plant black start; to protect the independent grid and Micro-grid operation; to ensure important user power supply
peak shaving and valley filling	Delaying power generation and installation; delaying the upgrading of power transmission and distribution; saving transmission access and congestion costs
Power dispatching Power tracking	To reduce line loss Load tracking, frequency modulation, and provide spin backup
Flicker suppression	Avoid flashing effects on electrical equipment



# Highlights of China's Energy Storage development (7)

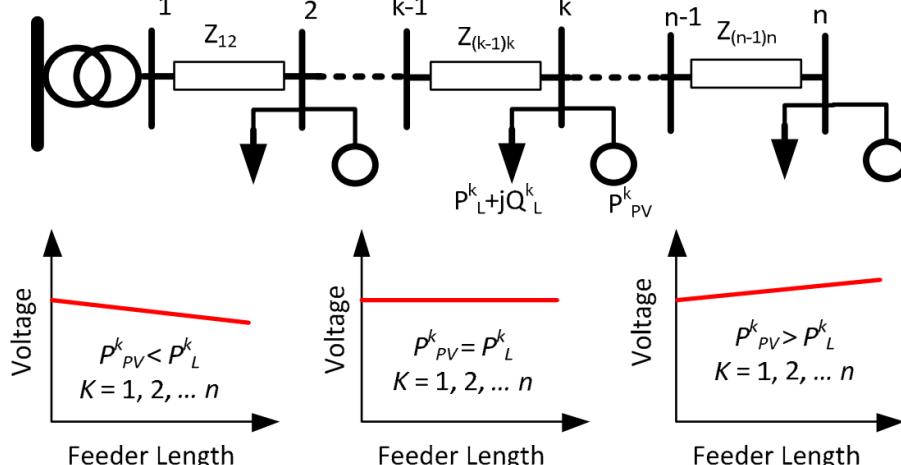
- SWOT/PEST

analysis of China's energy storage policy weakness.

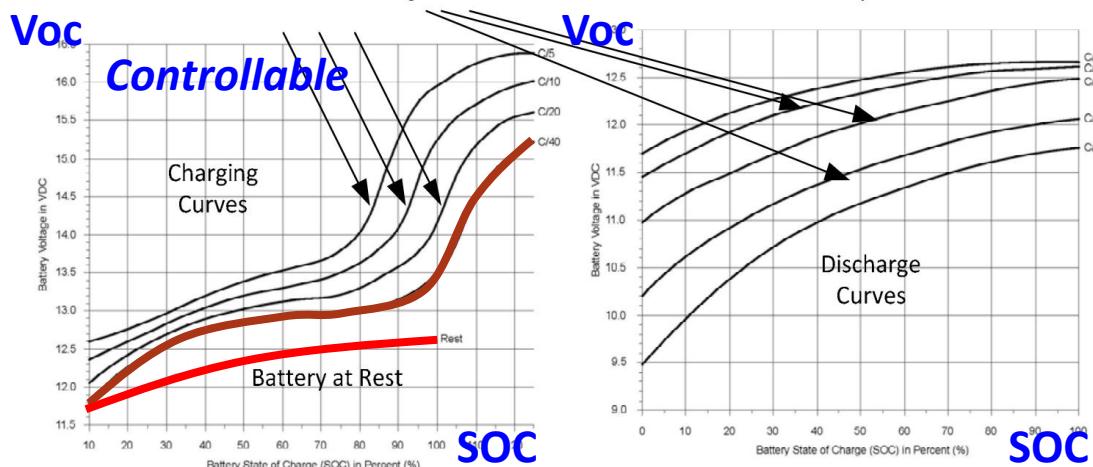
	Field			
	In demonstration project construction	Extensive policy, the lack of energy storage system program design. The experimental research of energy storage technology lacks continuity and continuity, and there is no definite electricity price and cost accounting and cost recovery plan		
	In terms of financial subsidies	Lack of energy storage financial plan, and the lack of detailed investment costs, production and operation and maintenance program.		
	In terms of investment and financing	In promoting the new energy storage industry chain industrialization, engineering application effect is not obvious		
	P Political	E Economy	S Society	T Topology
<b>Strength</b>	S the government clearly supports	Have a good industrial base	Abundant labor resources Abundant resources	The energy storage technology innovation system has been preliminarily constructed
<b>Weakness</b>	W The legal system of energy is not perfect; Energy storage policy is not matched	The energy storage industry has a low degree of intensification	In terms of energy storage, the total quantity of talents is insufficient and the quality needs to be improved	The overall technological development capability is relatively weak; Lack of core technology
<b>Opportunity</b>	O Protection of laws and regulations	Economic integration is booming; Opportunities for structural adjustment of energy	Establish various energy storage Industrial Organizations	The development of energy storage battery manufacturing technology has been widely used
<b>Threats</b>	T The state gradually reduces government support	The energy storage market is becoming more competitive; Energy storage and other high cost, cannot be industrialized	The threat of trade globalization	Energy storage technical barrier

# Voltage Rise Issue: Mitigation of Voltage Rise

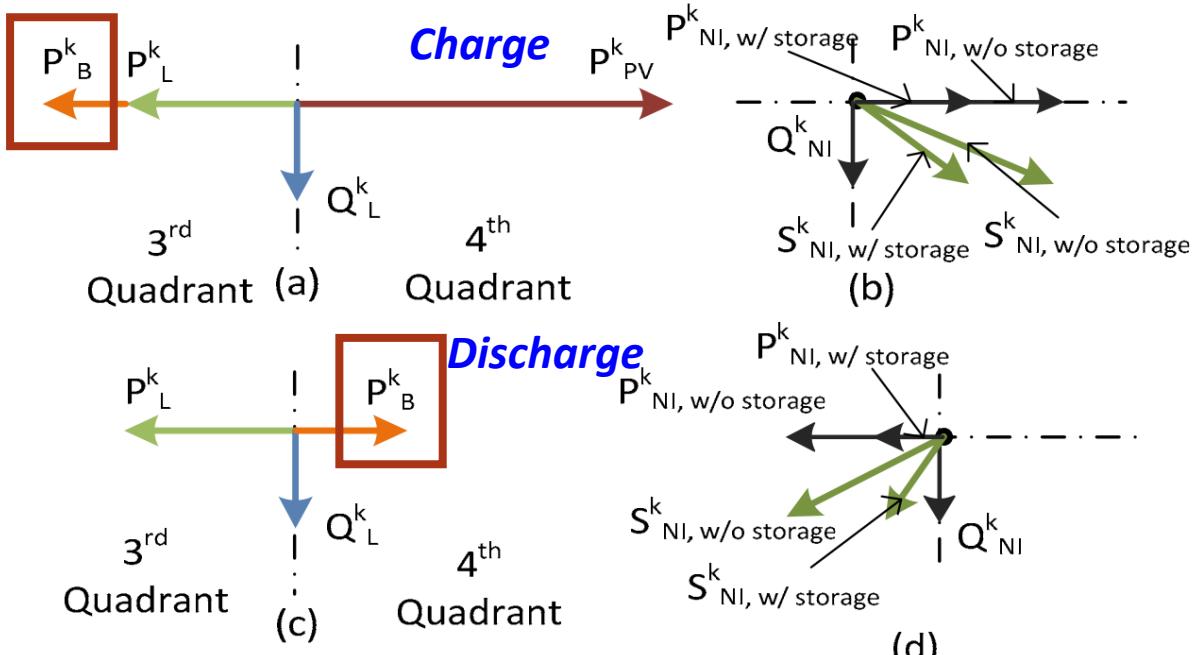
**Without ES:**



Difference in Voltage is due to Internal Resistance of the Battery



Alam, M. et al (2012), Distribution Energy Storage for Mitigation of Voltage-Rise Impact Caused by Rooftop Solar PV



$$P_{chg} = V_{chg} I_{chg}$$

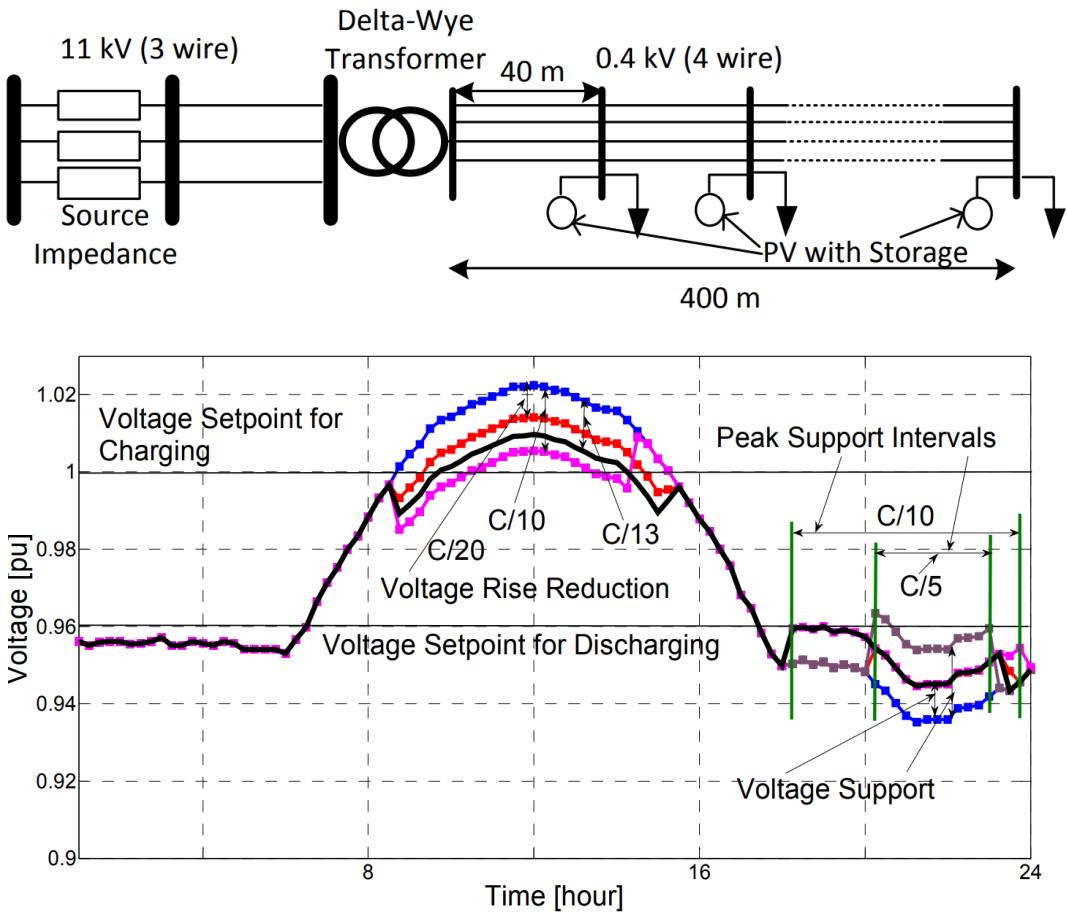
$$V_{chg} = K_1 x^4 + K_2 x^3 + K_3 x^2 + K_4 x + K_5$$

$$x = SOC(t + \Delta t) = SOC(t) + I_{chg} \Delta t$$

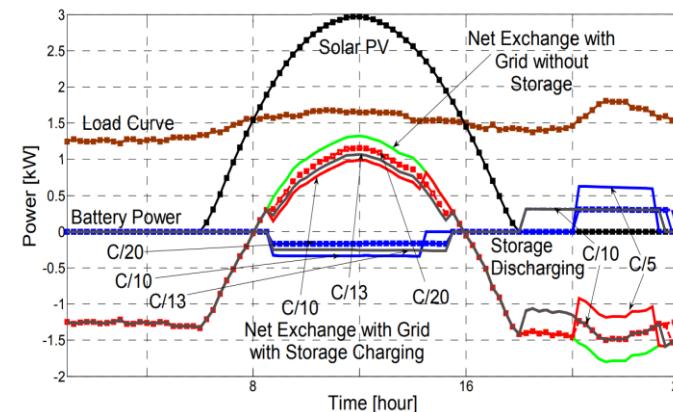
# Voltage Rise Issue: Mitigation of Voltage Rise

Alam, M. et al (2012), Distribution Energy Storage for Mitigation of Voltage-Rise Impact Caused by Rooftop Solar PV

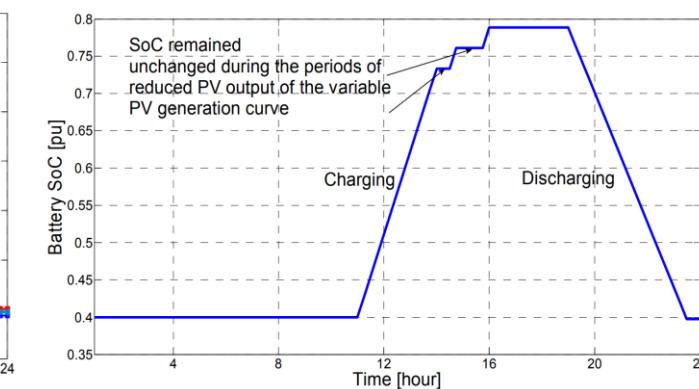
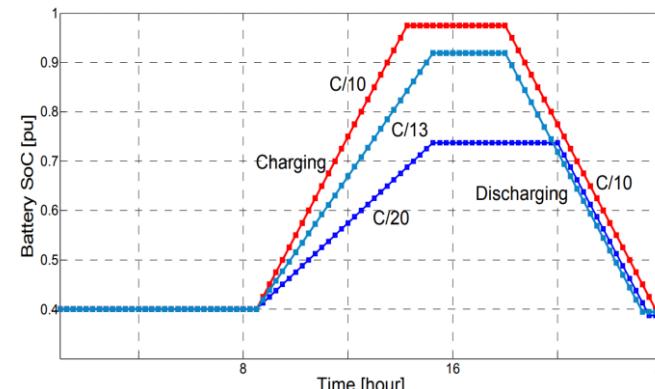
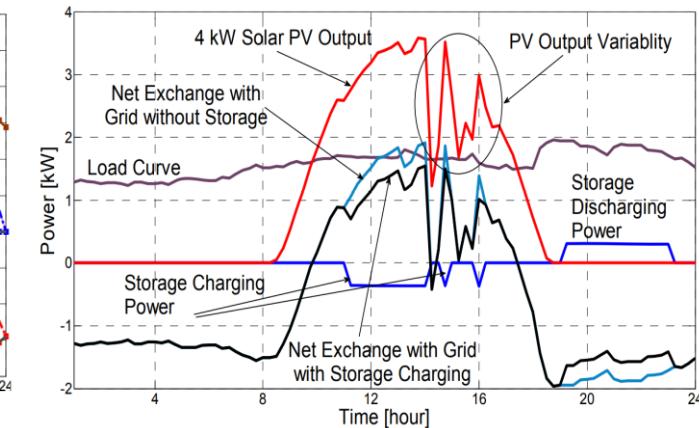
Simple LV Test Feeder



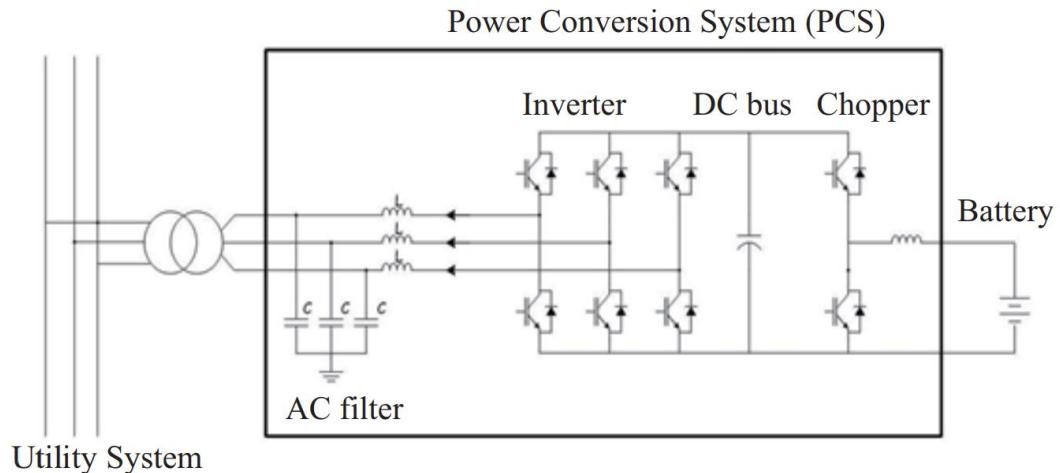
Less Fluctuation



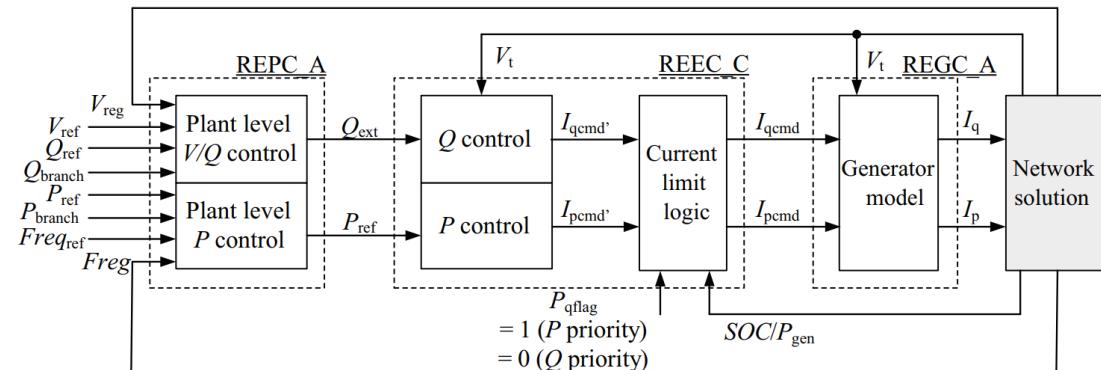
High Fluctuation



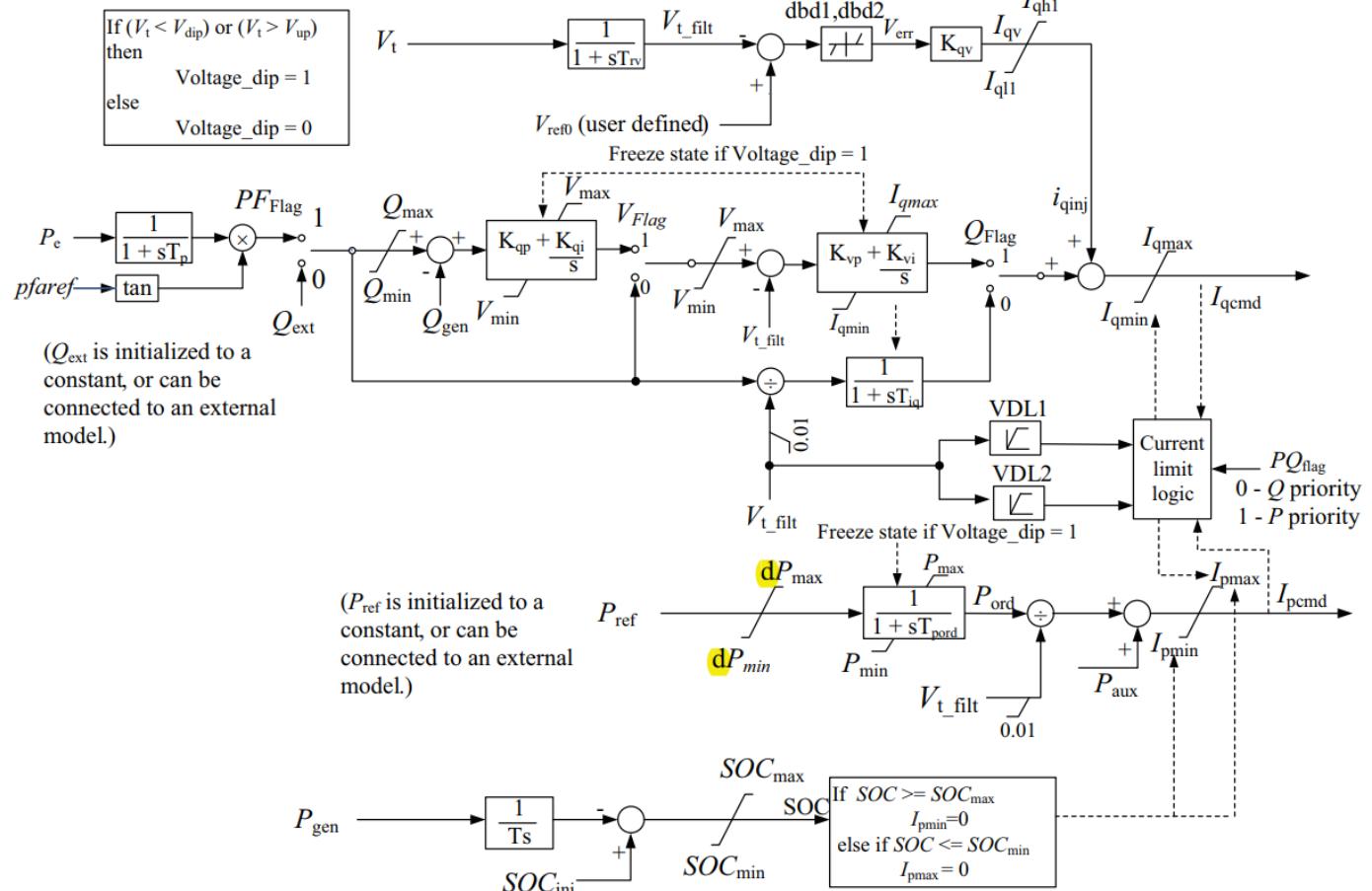
# Voltage Rise Issue: Mitigation of Voltage Rise



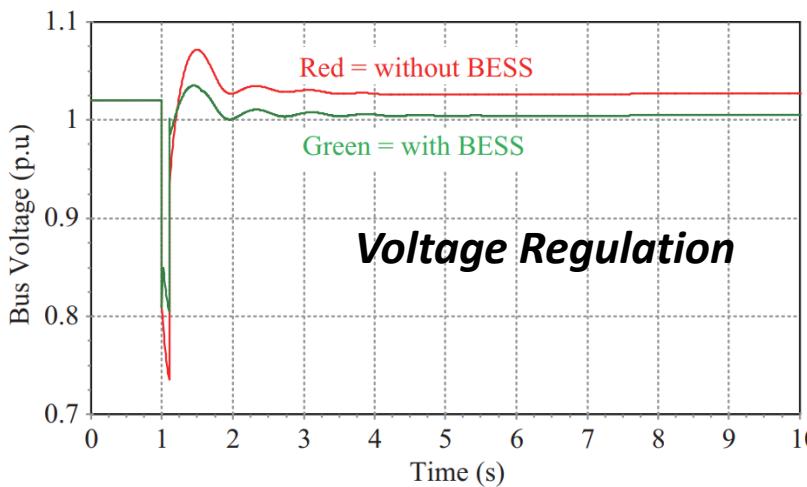
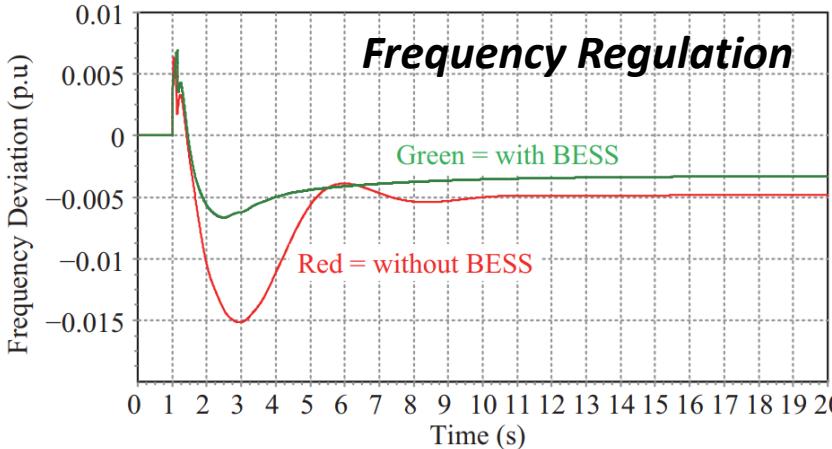
## BESS Modelling with **WECC** Generic Model



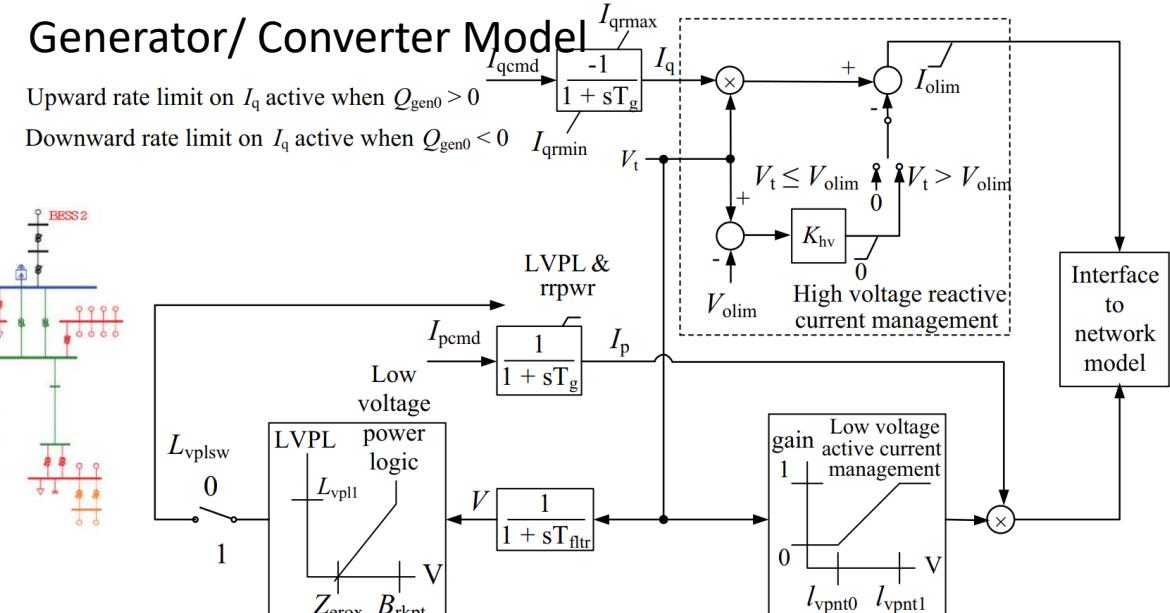
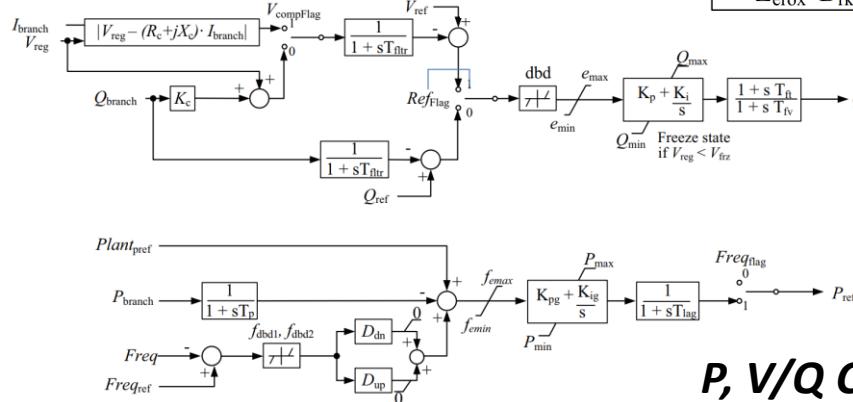
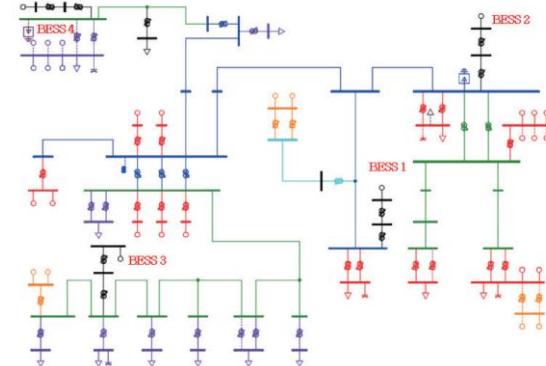
## Current Limit Logic



# Voltage Rise Issue: Mitigation of Voltage Rise



Systems:

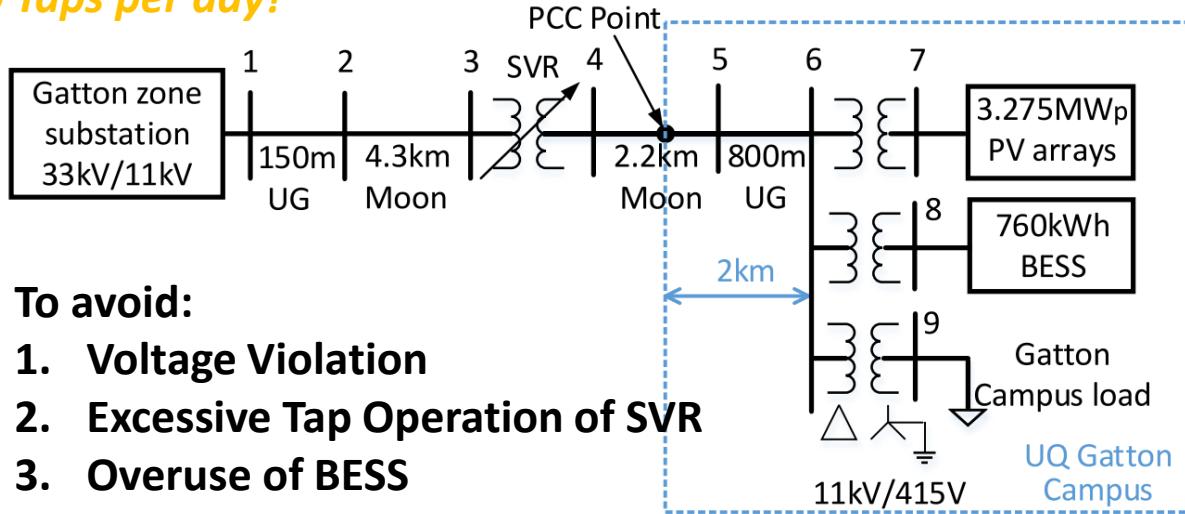


- 1) Grid frequency regulation;
- 2) economic dispatch (arbitrage);
- 3) time-shifting;
- 4) output smoothing;
- 5) output leveling.

**P, V/Q Controller**

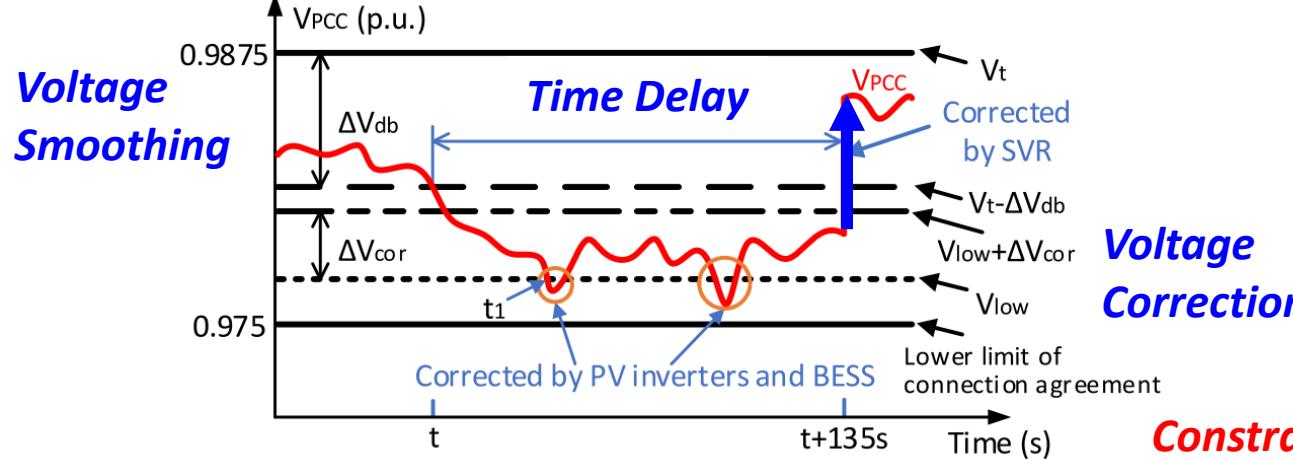
# Voltage Rise Issue: Real time voltage control

**10 Taps per day!**

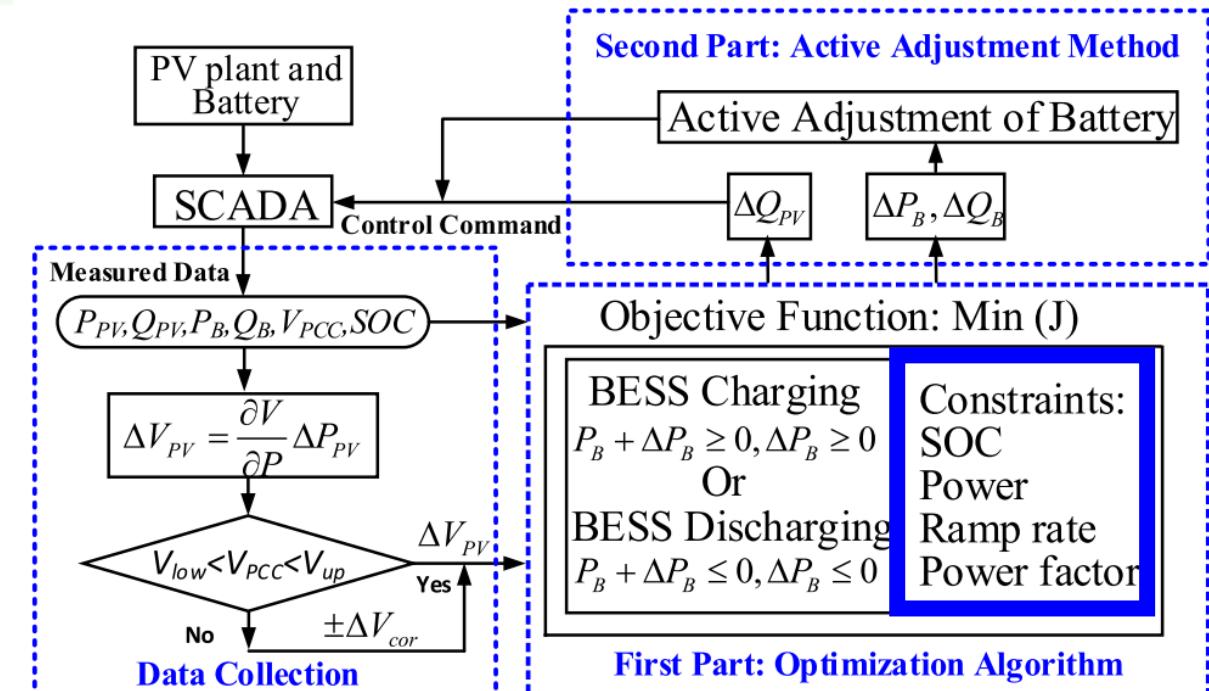


To avoid:

1. Voltage Violation
2. Excessive Tap Operation of SVR
3. Overuse of BESS



**Constraint: Ramp Rate, Power Limit, Battery Capacity, Power Factor**



Objective Function:

$$J = \left| \Delta V_{PV} + \frac{\partial V}{\partial P} \Delta P_B + \frac{\partial V}{\partial Q} (\Delta Q_B + \Delta Q_{PV}) \right| + \alpha |P_B + \Delta P_B|$$

**Voltage violation**

**Power of BESS**

# Voltage Rise Issue: Voltage Control with P-Q

Clarke Transform:  $\begin{pmatrix} i_\alpha \\ i_\beta \end{pmatrix} = \begin{pmatrix} i_L \angle \varphi \\ i_L \angle \varphi + \frac{\pi}{2} \end{pmatrix}$

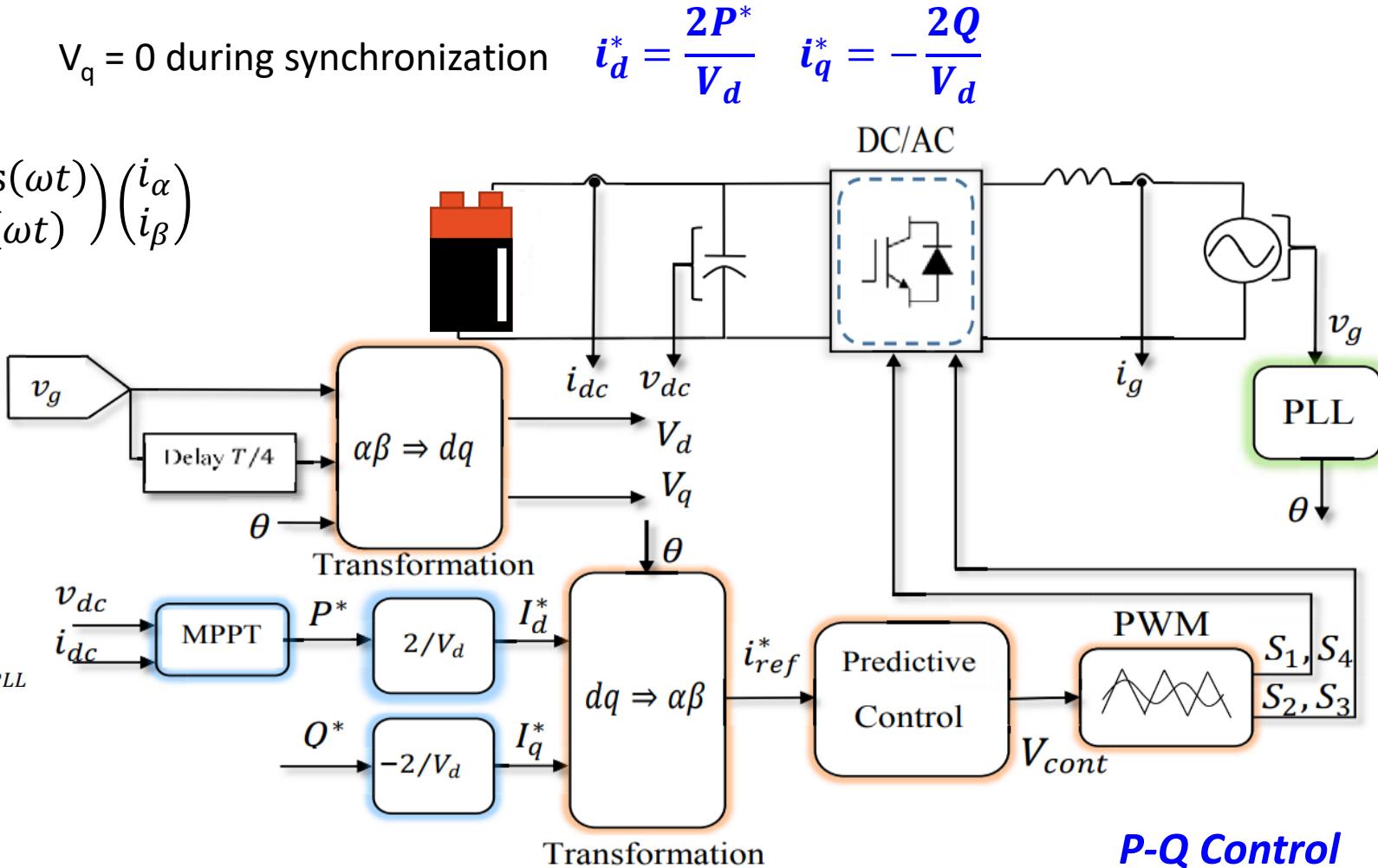
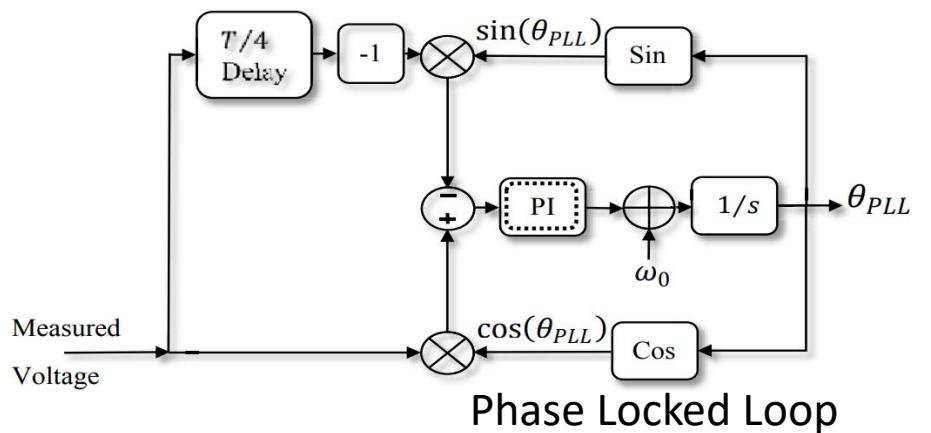
$v_q = 0$  during synchronization

$$\dot{i}_d^* = \frac{2P^*}{V_d} \quad \dot{i}_q^* = -\frac{2Q}{V_d}$$

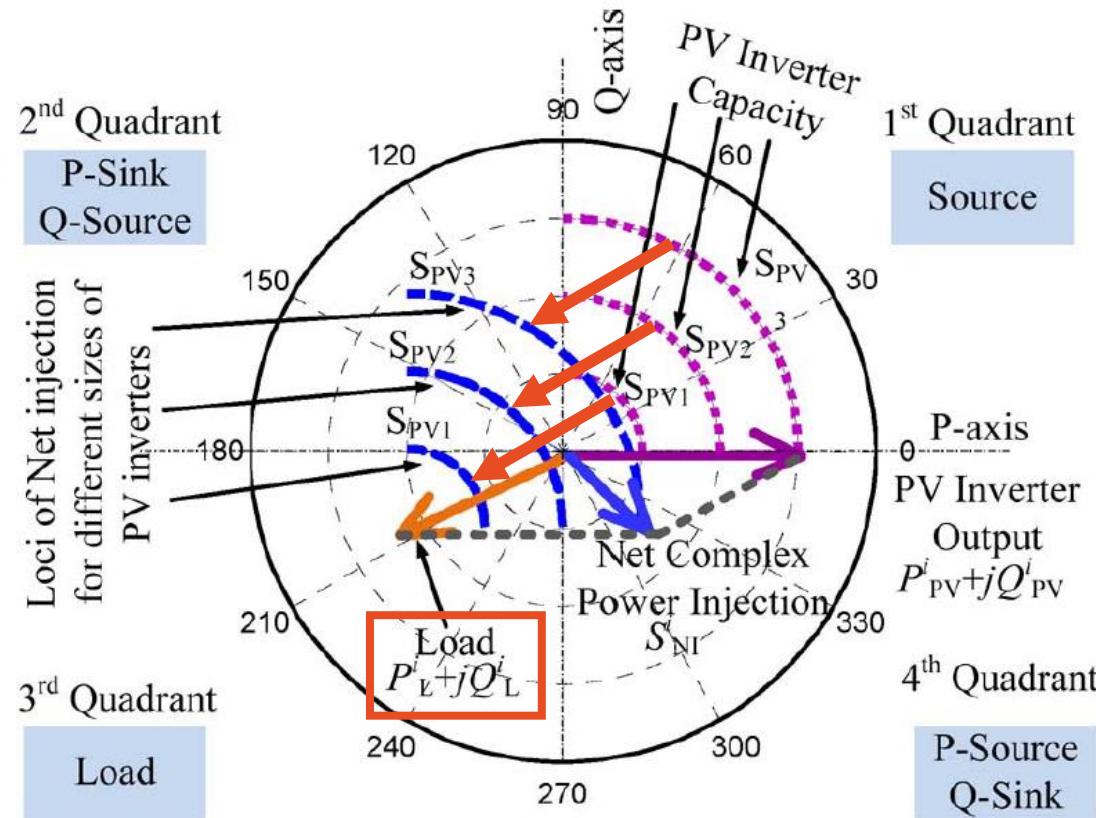
Park Transform:  $\begin{pmatrix} i_d \\ i_q \end{pmatrix} = \begin{pmatrix} \sin(\omega t) & -\cos(\omega t) \\ \cos(\omega t) & \sin(\omega t) \end{pmatrix} \begin{pmatrix} i_\alpha \\ i_\beta \end{pmatrix}$

$$P = \frac{1}{2}(v_d i_d + v_q i_q)$$

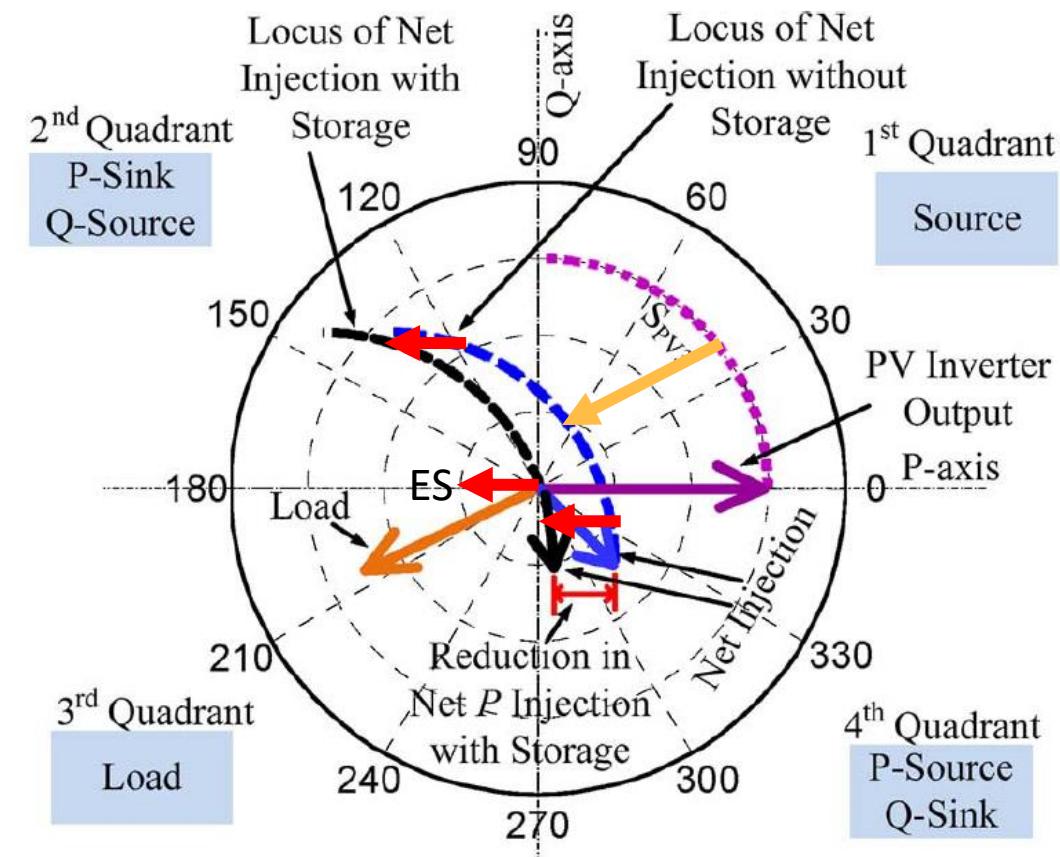
$$Q = \frac{1}{2}(-v_d i_q + v_q i_d)$$



# Voltage Rise Issue: Managing Available Capacity

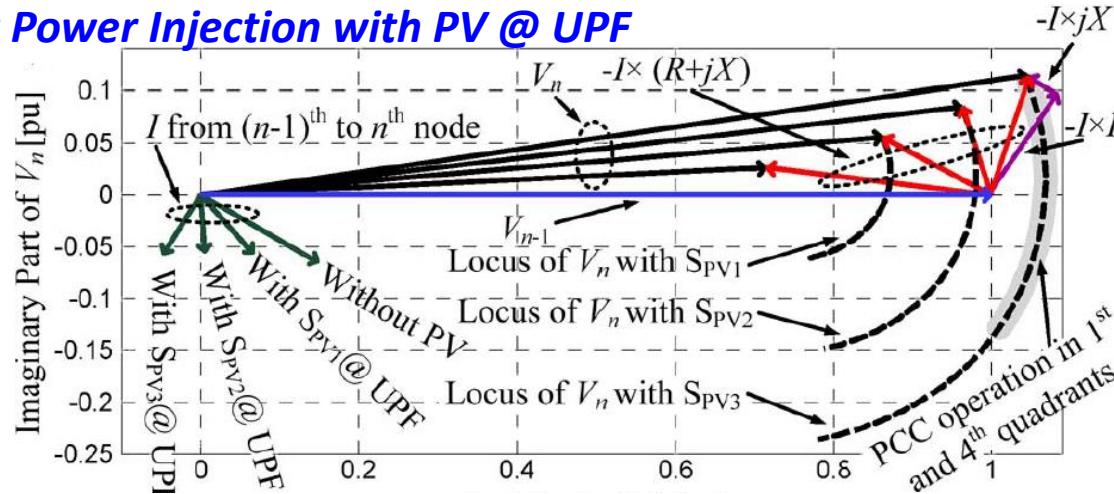
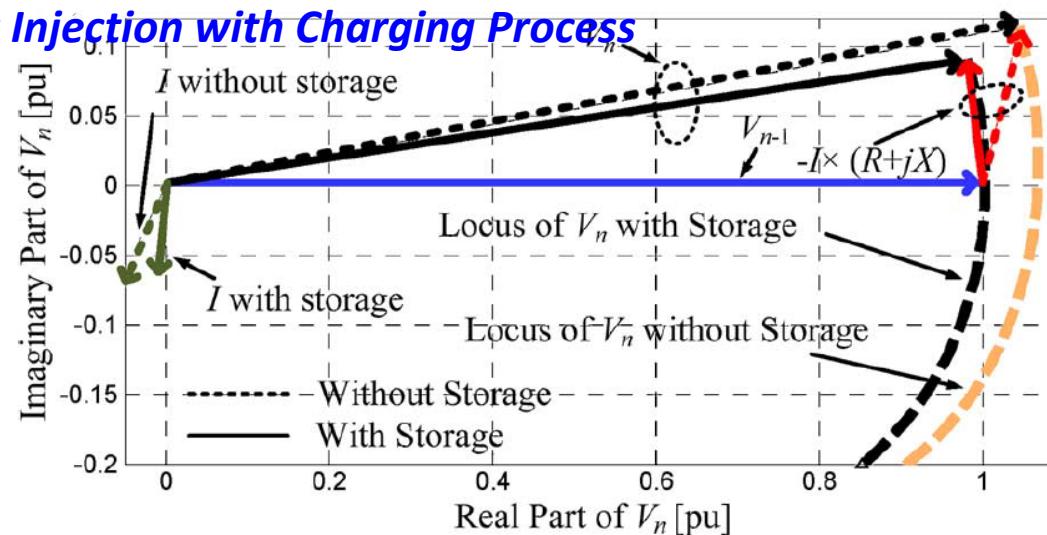
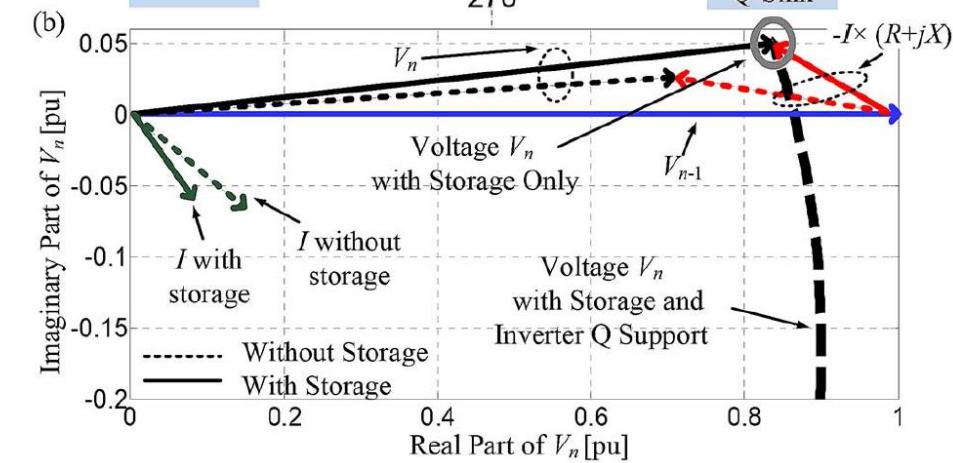
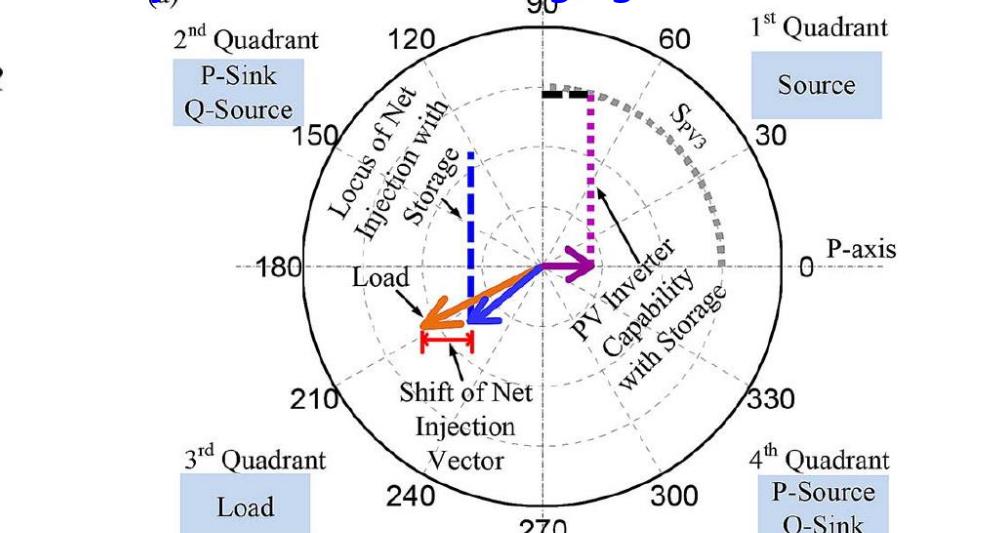


Loci of net power injection and voltage: Net power injection with different PV capacity



Four quadrant net power injection diagram with storage: Net injection in charging operation

# Voltage Rise Issue: Managing Available Capacity

**Net Power Injection with PV @ UPF****Net Injection with Charging Process****Net Injection with Discharging Process**

# Voltage Rise Issue: Managing Available Capacity

## Battery Voltage:

$$V_B = \begin{cases} V_{B0} + I_B (R_{BD} - \rho \times \text{SoC}) \\ V_{B0} - I_B (R_{BC} + \rho \times \text{SoC}) \end{cases}$$

$$(V_{oc}) V_{B0} = V_{BC} - K \times \frac{C_B}{C_B - \text{SoC}} + A e^{-B \times \text{SoC}}$$

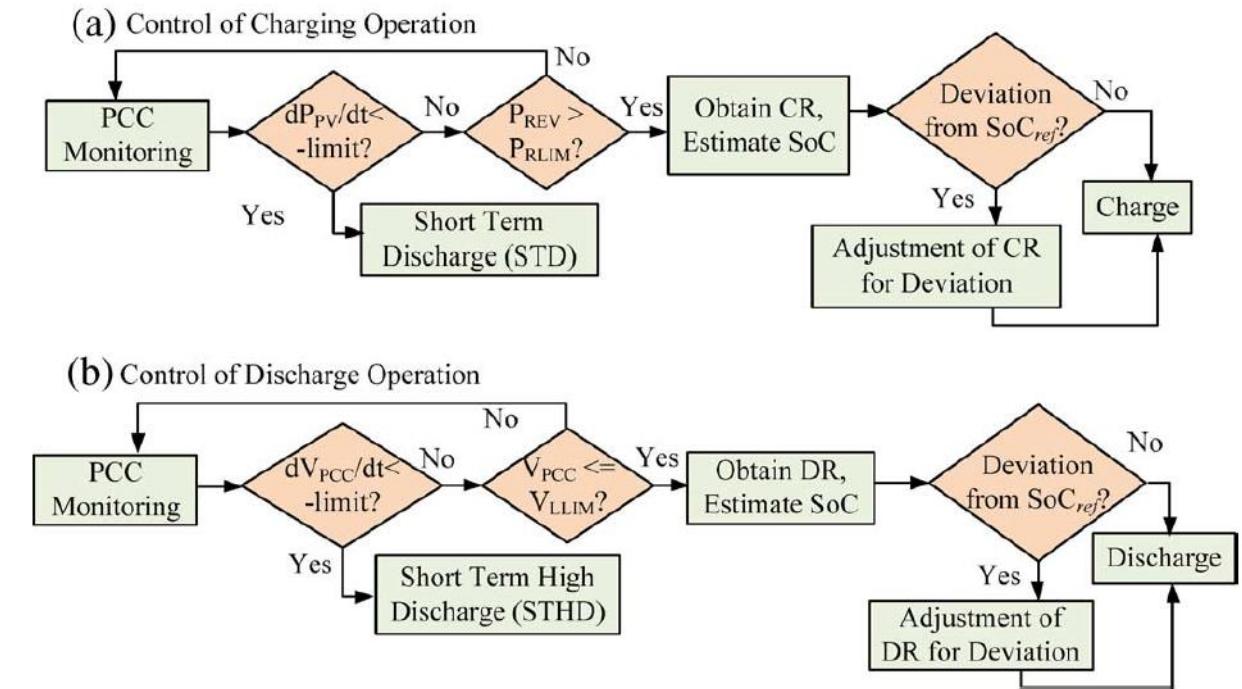
## Maximum Charging Rate:

$$\text{CR}_{\max} = \left| \frac{-(P_{L \min} - \eta_{inv} P_{PV \max})}{\eta_{inv} \times V_B^{\text{Full}}} \right|$$

where  $P_{L \min}$  = min load power,  $P_{PV \max}$  = max PV power,  
 $\eta_{inv}$  = efficiency of invertor,  $V_B^{\text{Full}}$  = Voc at 100% SOC

SCR = slope of charging rate

$$\text{Charging Rate: } \text{CR}(k) = \begin{cases} \text{CR}(k-1) + \text{SCR}, & \text{if SoC}(k-1) \leq \text{ToS}_1 \\ \text{CR}_{\text{Sat}}, & \text{if ToS}_1 < \text{SoC}(k-1) < \text{ToS}_2 \\ \text{CR}(k-1) - \text{SCR}, & \text{if SoC}(k-1) \geq \text{ToS}_2 \\ 0, & \text{if SoC}(k-1) \geq \text{SoC}_{\max}. \end{cases}$$

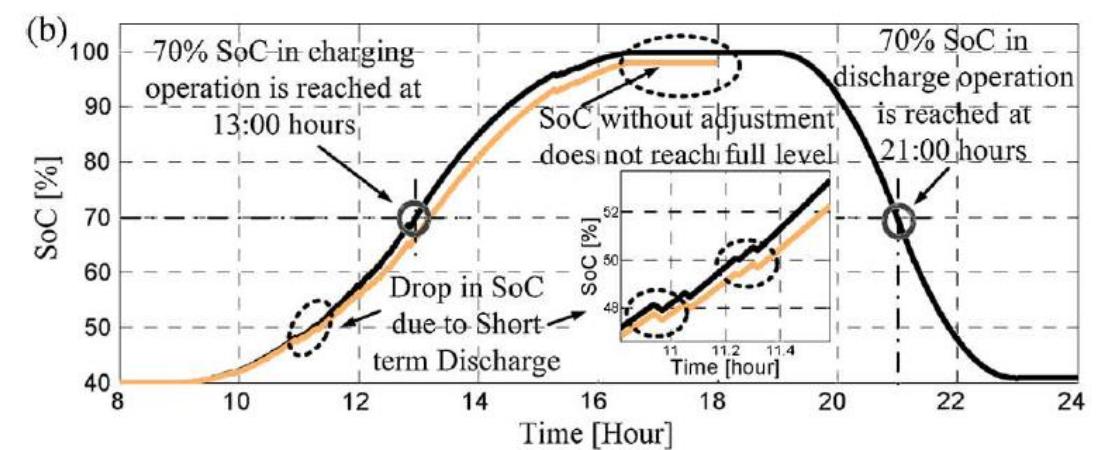
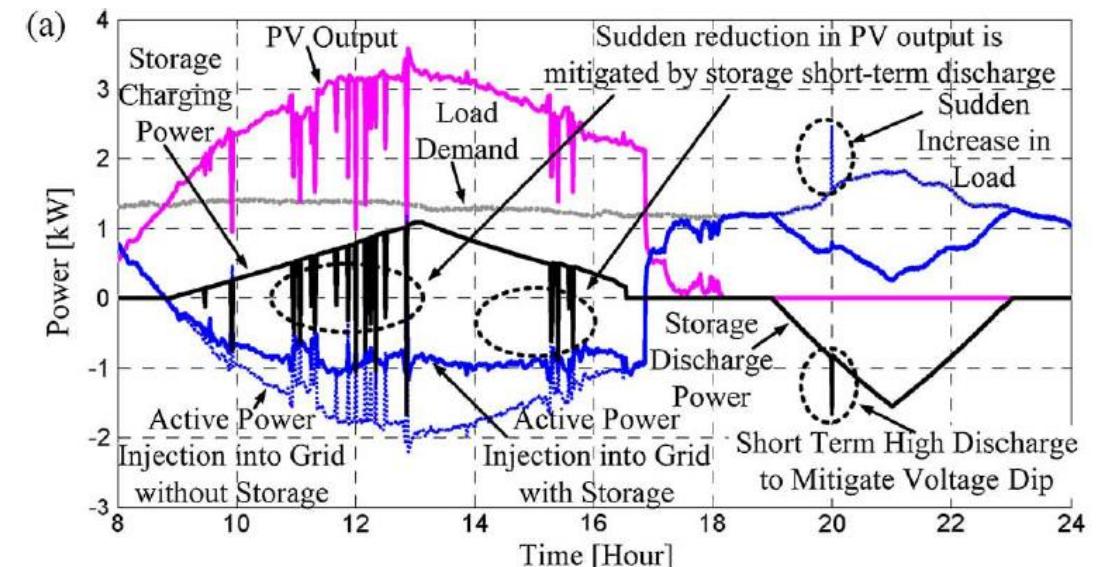
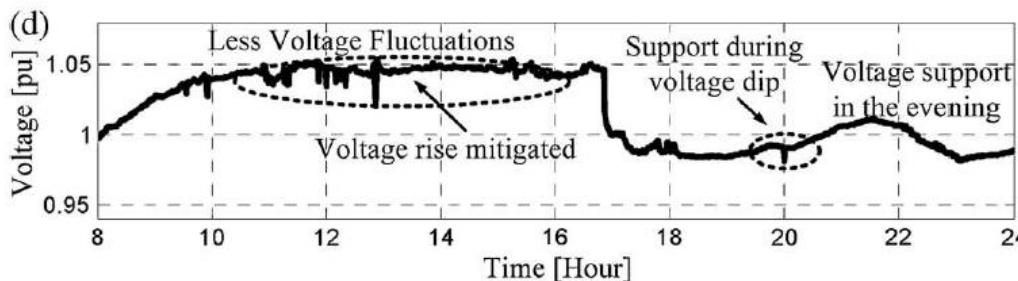
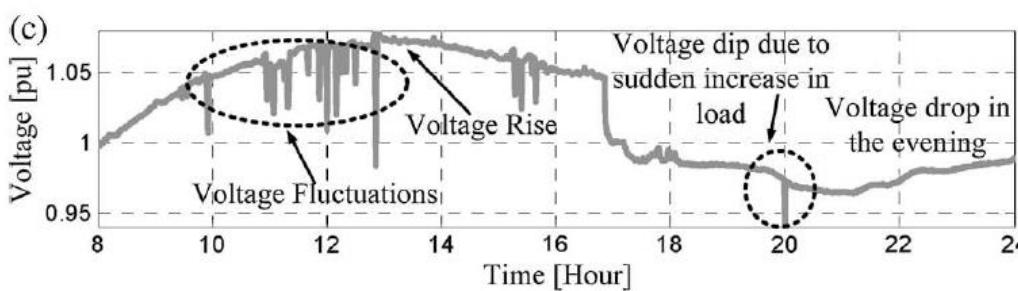
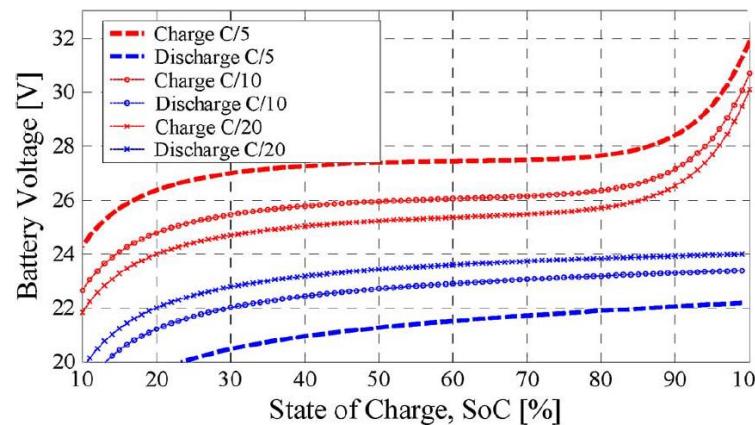
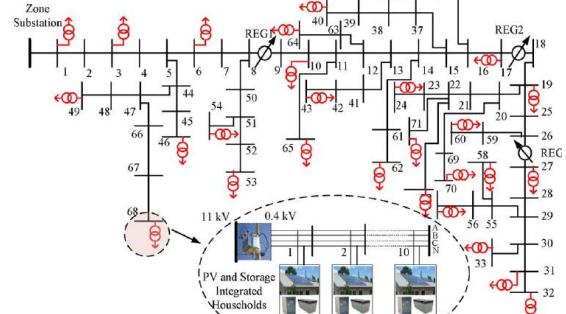


## Discharging Rate:

$$\text{DR}(k) = \begin{cases} \text{DR}(k-1) + \text{SDR}, & \text{if SoC}(k-1) \geq \text{ToS}_2 \\ \text{DR}_{\text{Sat}}, & \text{if ToS}_2 > \text{SoC}(k-1) > \text{ToS}_1 \\ \text{DR}(k-1) - \text{SDR}, & \text{if SoC}(k-1) \leq \text{ToS}_1 \\ 0, & \text{if SoC}(k-1) \leq \text{DoD}_{\max}. \end{cases}$$

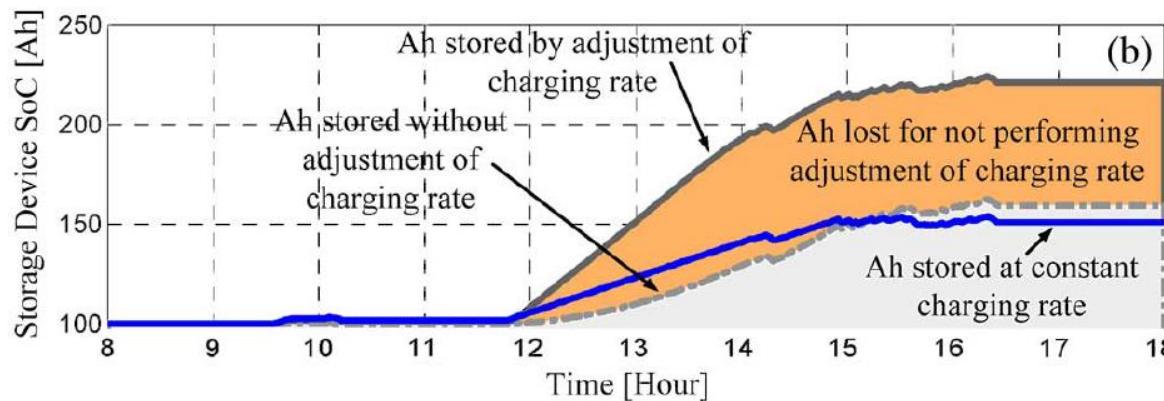
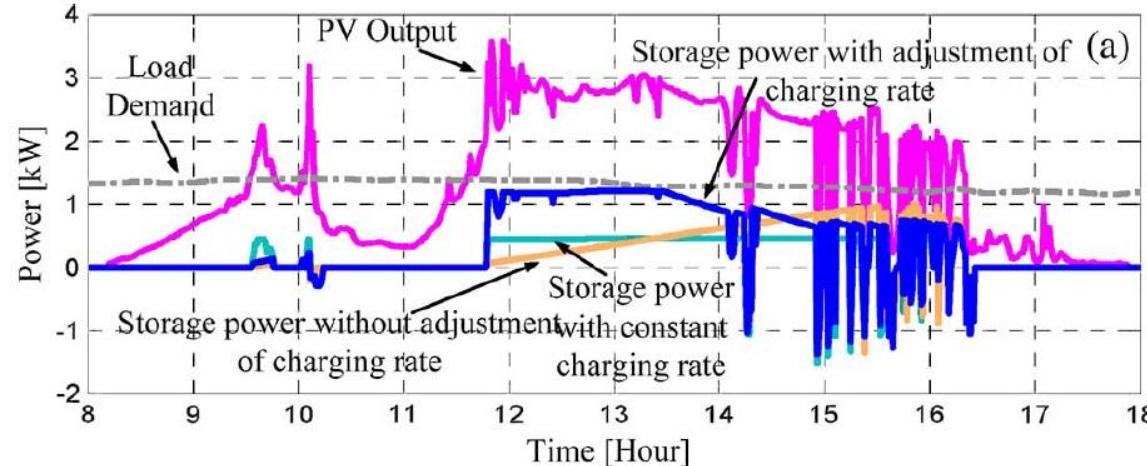
# Voltage Rise Issue: Managing Available Capacity

## Typical Feeder in Australia



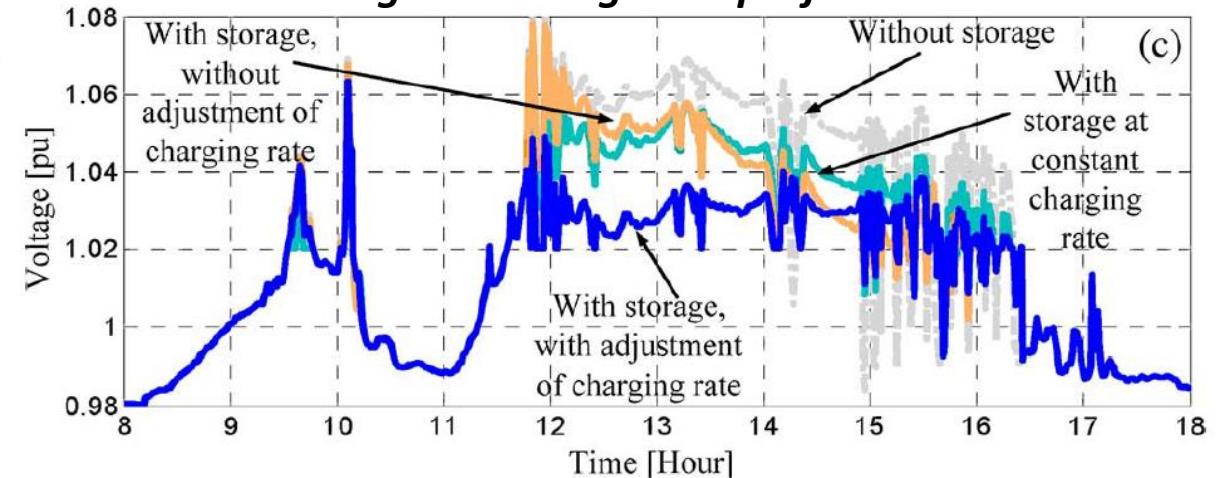
# Voltage Rise Issue: Managing Available Capacity

**Effect on power consumed by storage in charging operation**

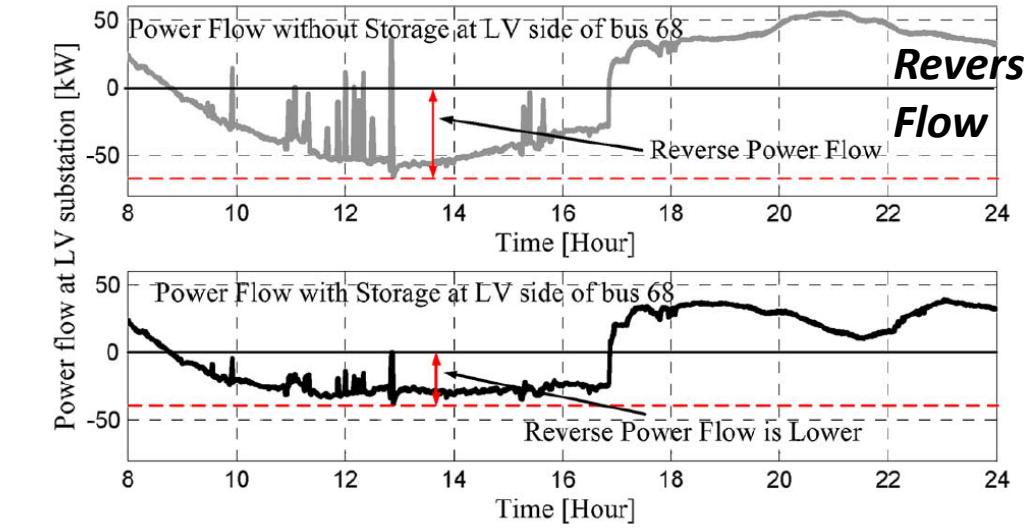


**Utilization of battery capacity.**

**Voltage rise mitigation performance**

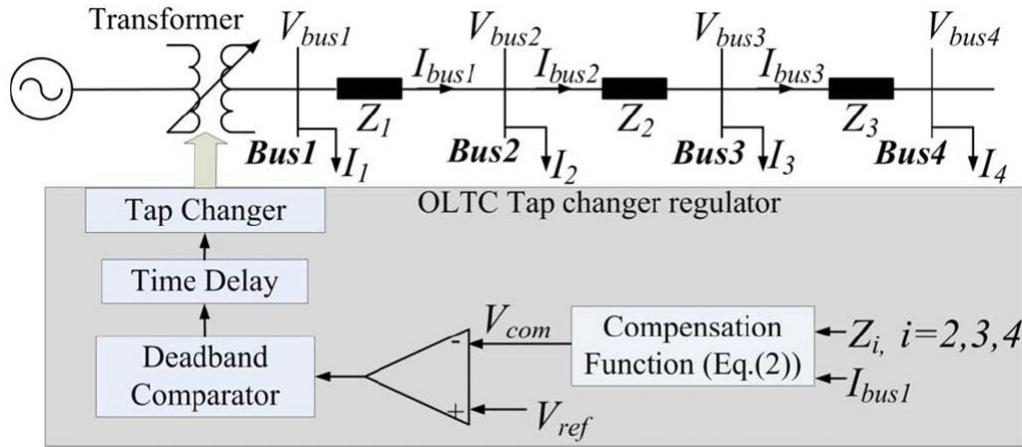


**Reverse Power Flow**



# Voltage Rise Issue: Control with OLTC

Traditional Method:



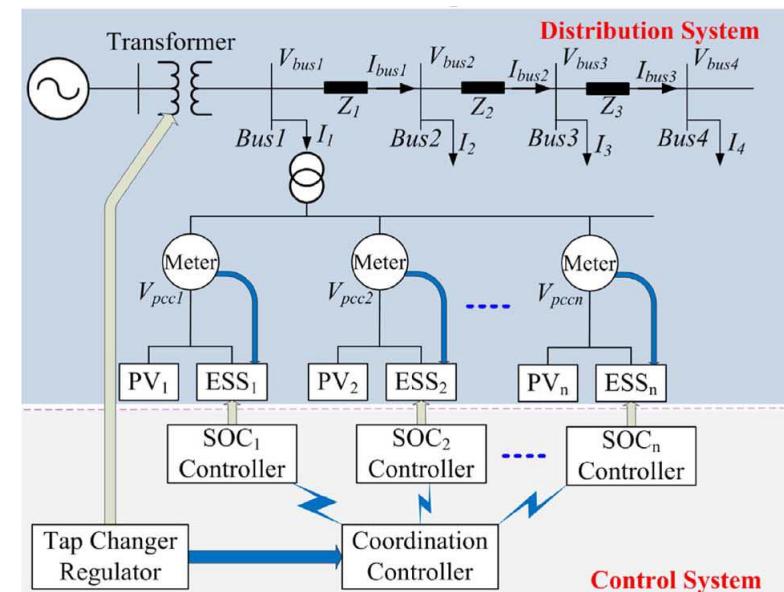
Generator Voltage:

$$V_G \approx V_2 + R(P_G - P_L) + X(Q_G - Q_L) \quad (1)$$

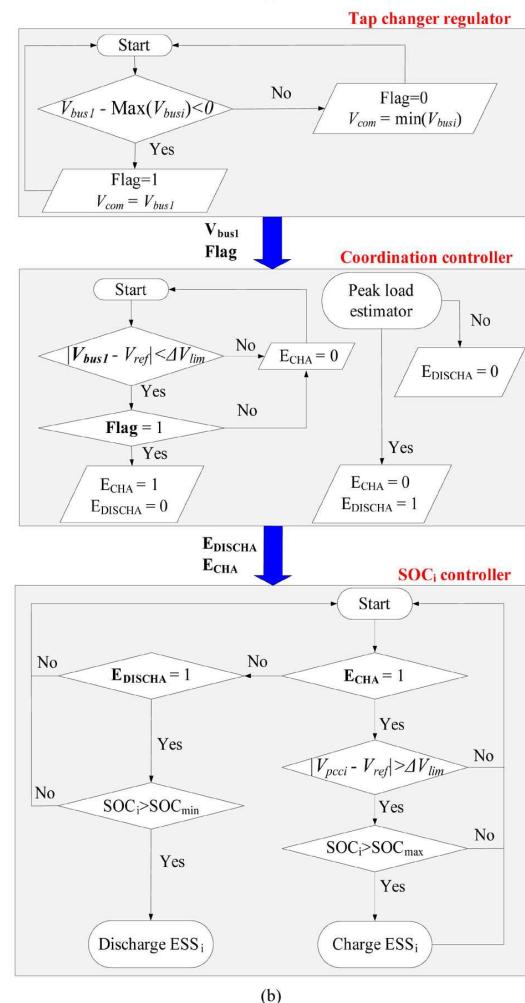
Compensation Voltage for last bus (i.e. bus 4):

$$V_{com} = V_{bus1} - Z_1 \cdot I_2 - (Z_1 + Z_2) \cdot I_3 - (Z_1 + Z_2 + Z_3) \cdot I_4. \quad (2)$$

With ESS:

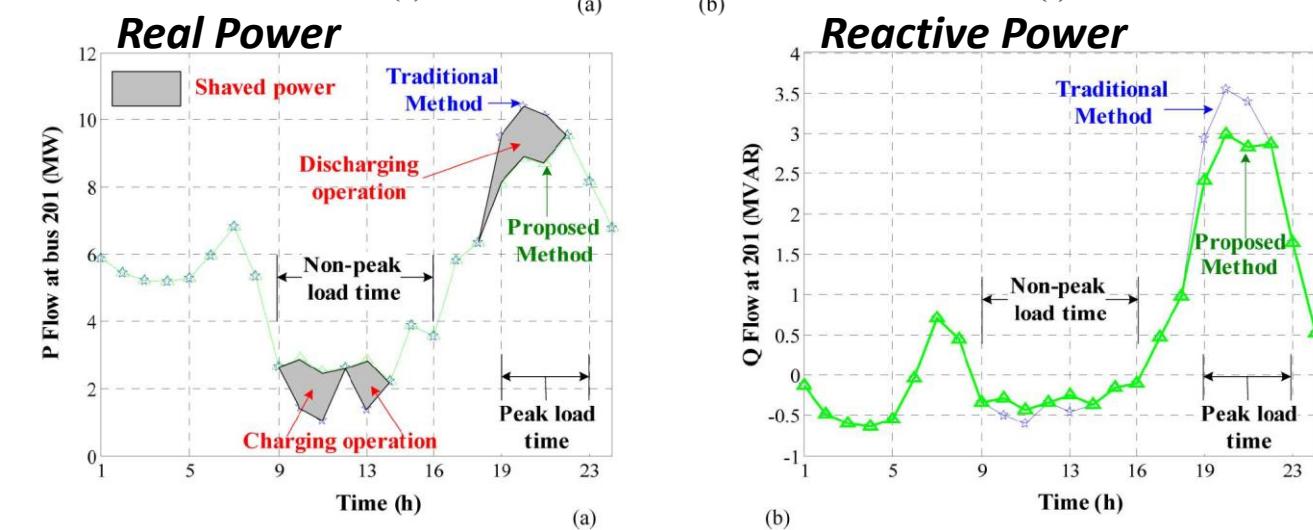
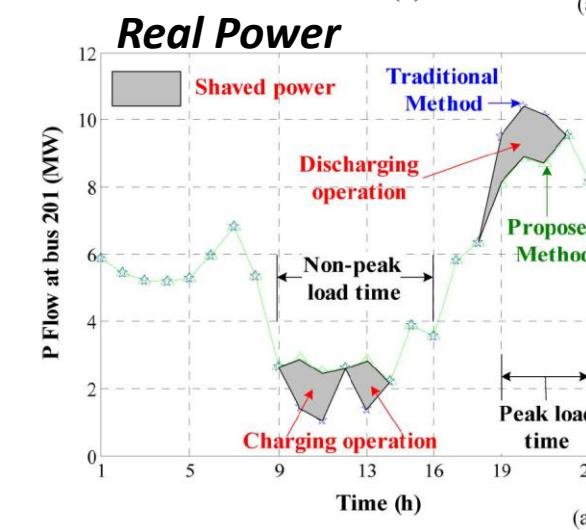
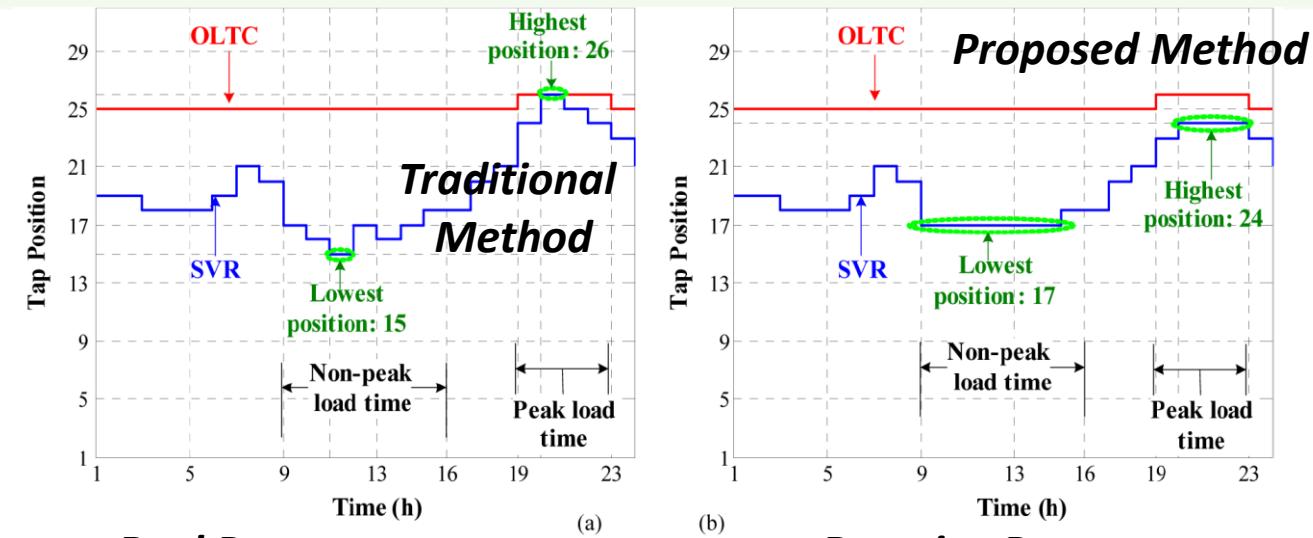
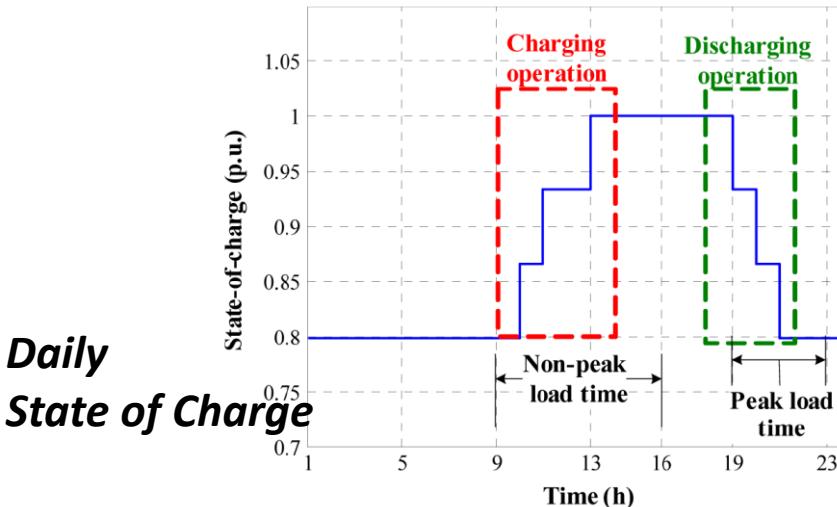
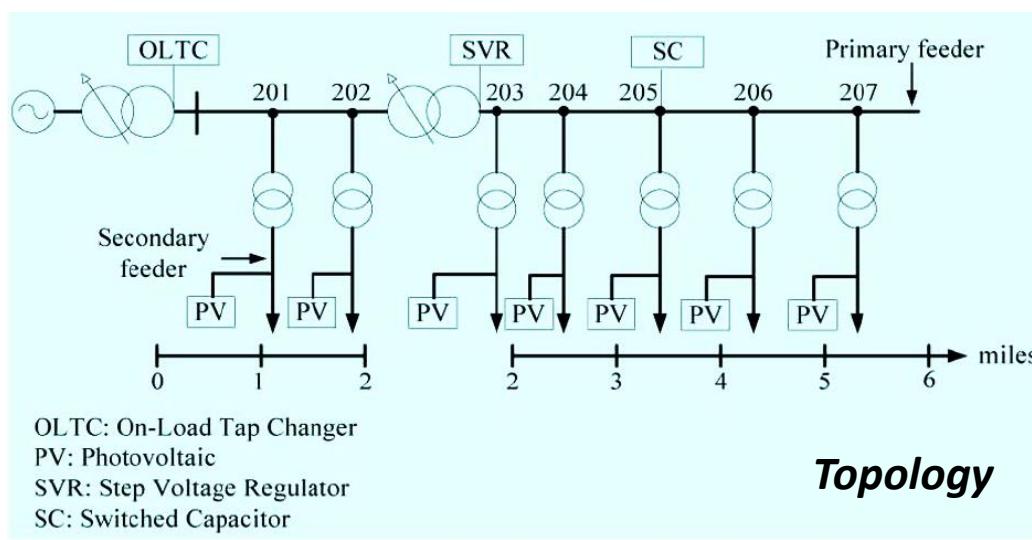


Control Strategy:



(b)

# Voltage Rise Issue: Control with OLTC



# Power Fluctuation Issue: Ramp Rate Control

## Moving Average of Ramp Rate PV output

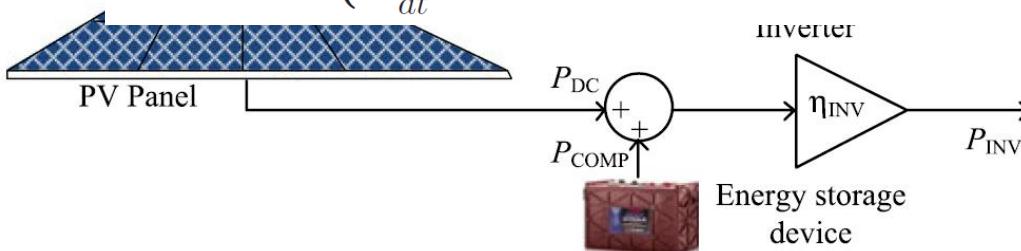
$$\begin{aligned} MoRR(k) &= \frac{1}{w} \times \frac{\sum_{i=0}^{w-1} P_{DC}(k-i) - \sum_{i=0}^{w-1} P_{DC}(k-1-i)}{t(k) - t(k-1)} \\ &= \frac{1}{w} \times \frac{P_{DC}(k) - P_{DC}(k-w)}{t(k) - t(k-1)} \end{aligned}$$

## Ramp rate of inverter output

$$\frac{dP_{INV}}{dt} = \eta_{INV} \times \left[ \frac{dP_{DC}}{dt} + \frac{dP_{COMP}}{dt} \right]$$

## Dead Band Function to force $P_{DC} = 0$ within limit

$$f\left(\frac{dP_{DC}}{dt}\right) = \begin{cases} 0, & \text{if } \eta_{INV} \times \left| \frac{dP_{DC}}{dt} \right| \leq \left| \frac{dP_{INV}}{dt} \right|_{des} \\ \frac{dP_{DC}}{dt}, & \text{otherwise.} \end{cases}$$



## Switching Function

$$S = \begin{cases} 0, & \text{if } |P_{COMP}| < \left| \frac{dP_{INV}}{dt} \right|_{des} \text{ and } f\left(\frac{dP_{DC}}{dt}\right) = 0 \\ 1, & \text{otherwise.} \end{cases}$$

## Compensated Power/ Energy Storage Output

$$\frac{dP_{COMP}}{dt} = S \times \left[ \frac{1}{\eta_{INV}} \times \left\{ \frac{dP_{INV}}{dt} \Big|_{des} - \eta_{INV} \times f\left(\frac{dP_{DC}}{dt}\right) \right\} \right]$$

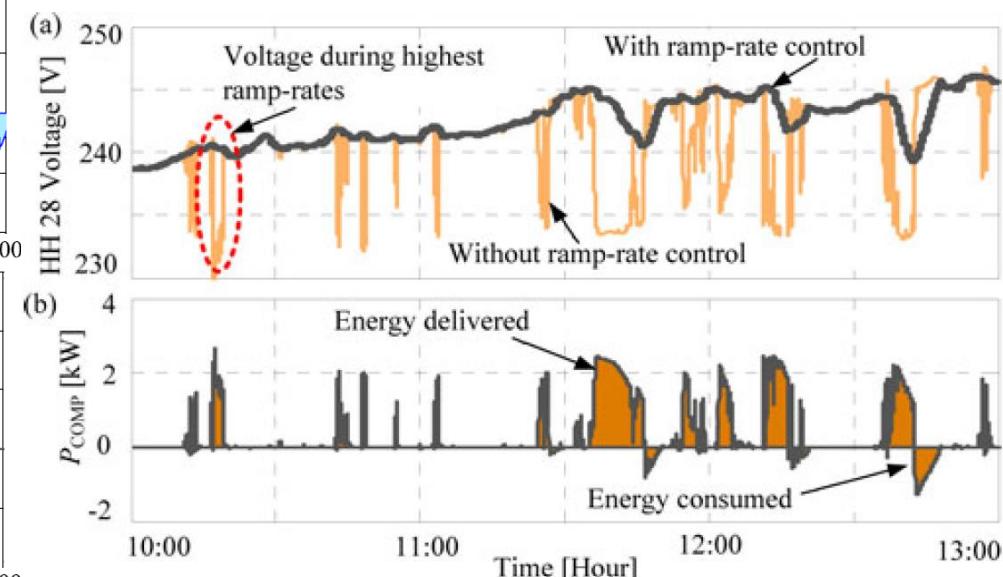
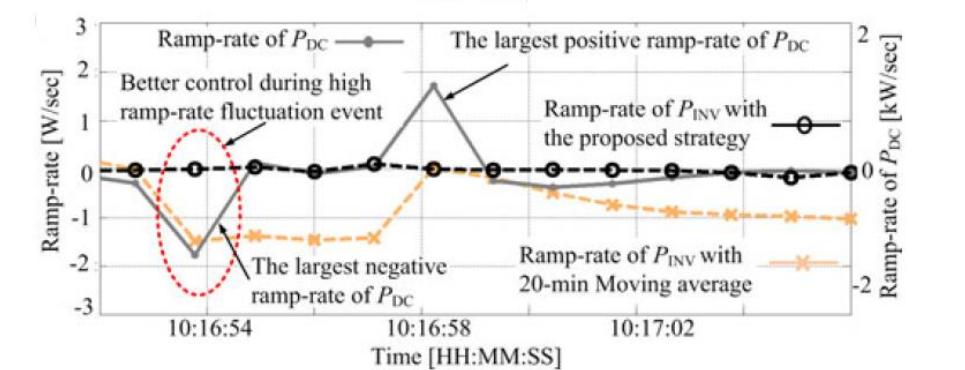
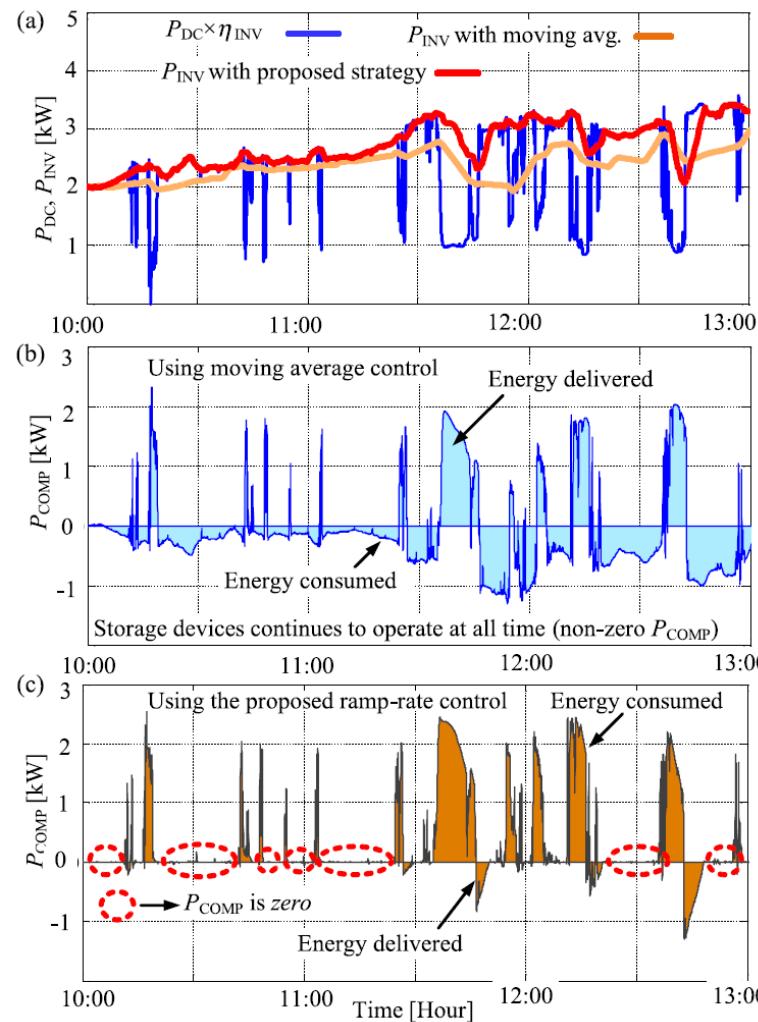
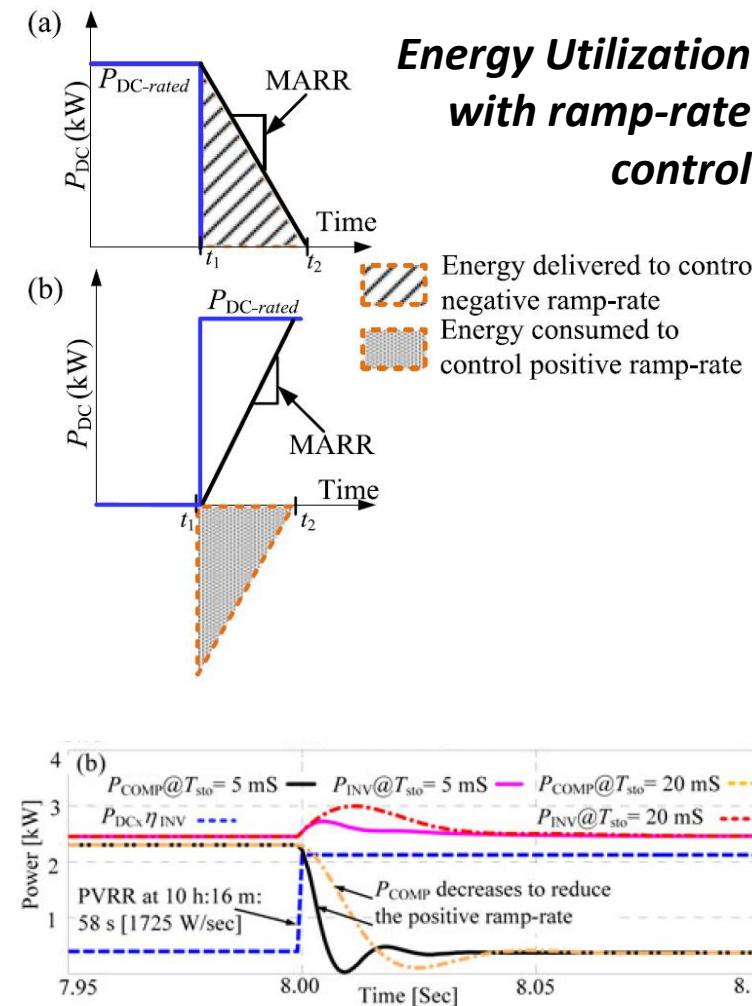
## Compensated Power Moving Average

$$P_{COMP}(k) = \frac{\sum_{i=0}^{w-1} P_{DC}(k-i)}{w} - P_{DC}(k)$$

## Maximum Allowable Ramp Rate with Moving Average and SOC droop

$$\text{MARR}_{\sigma}(k) = \begin{cases} \text{MARR}_{\min}, & \text{if } |\Delta \text{SoC}(k)| < \text{SoC}_{LB} \\ \text{MARR}_{\min} + \frac{DB_{\text{MARR}}}{DB_{\text{SoC}}} \times [|\Delta \text{SoC}(k)| - \text{SoC}_{LB}] & \text{if } \text{SoC}_{LB} \leq |\Delta \text{SoC}(k)| \leq \text{SoC}_{UB} \\ \text{MARR}_{\max}, & \text{if } |\Delta \text{SoC}(k)| > \text{SoC}_{UB}. \end{cases}$$

# Power Fluctuation Issue: Ramp Rate Control



# Energy Storage: Sizing Methods

## Sizing Techniques:

Indicator to be considered:

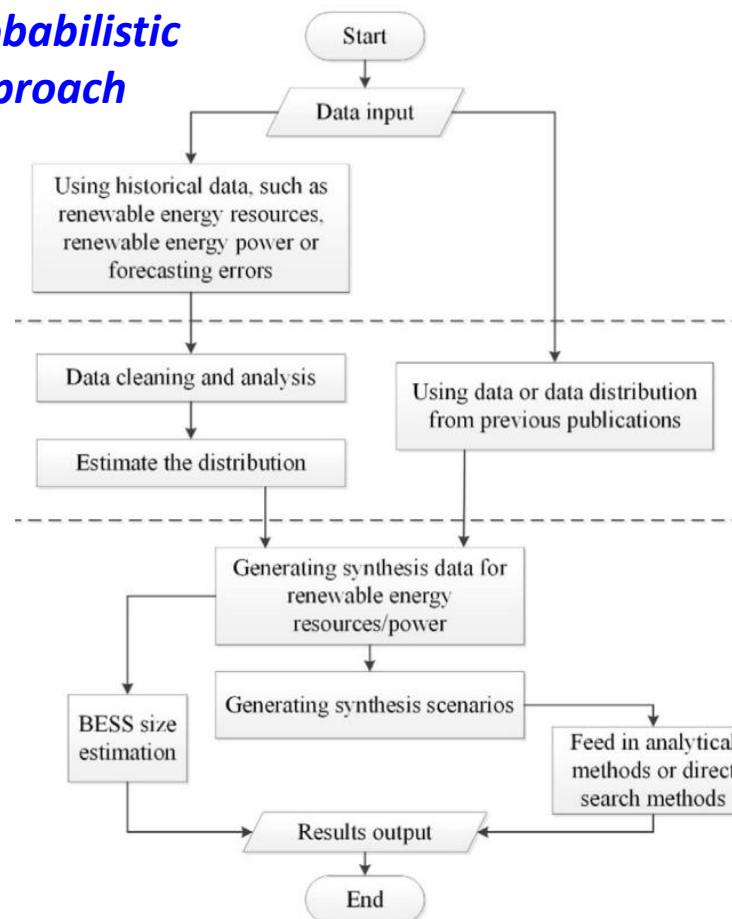
### 1. Financial Indicators

Overall cost, upfront capital cost, Operation/Maintenance cost, fuel cost, difference of op. cost w/ wo PV, disposal & recycling cost, feed in tariff

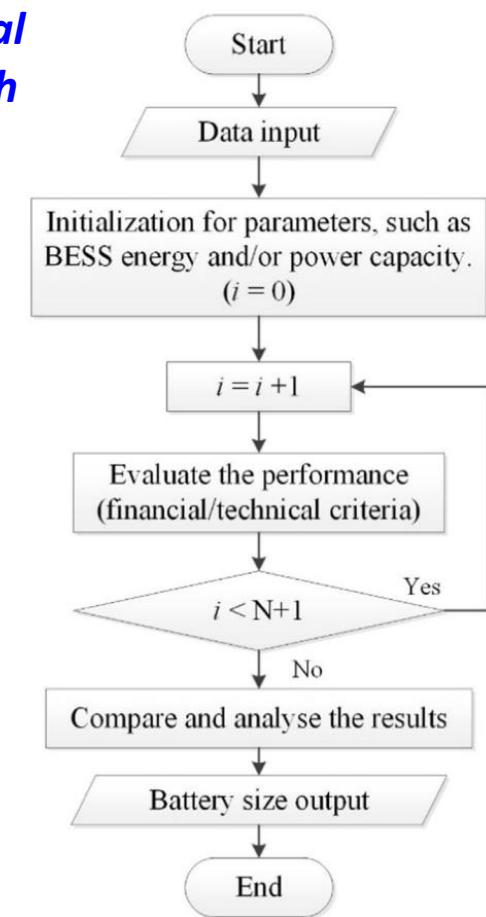
### 2. Technical Indicators

Voltage stability, frequency stability, energy curtailment, reliability, const. power output, islanded power use, depth of discharge, charge/discharge rate, state of health (SOH), round trip efficiency

### Probabilistic Approach

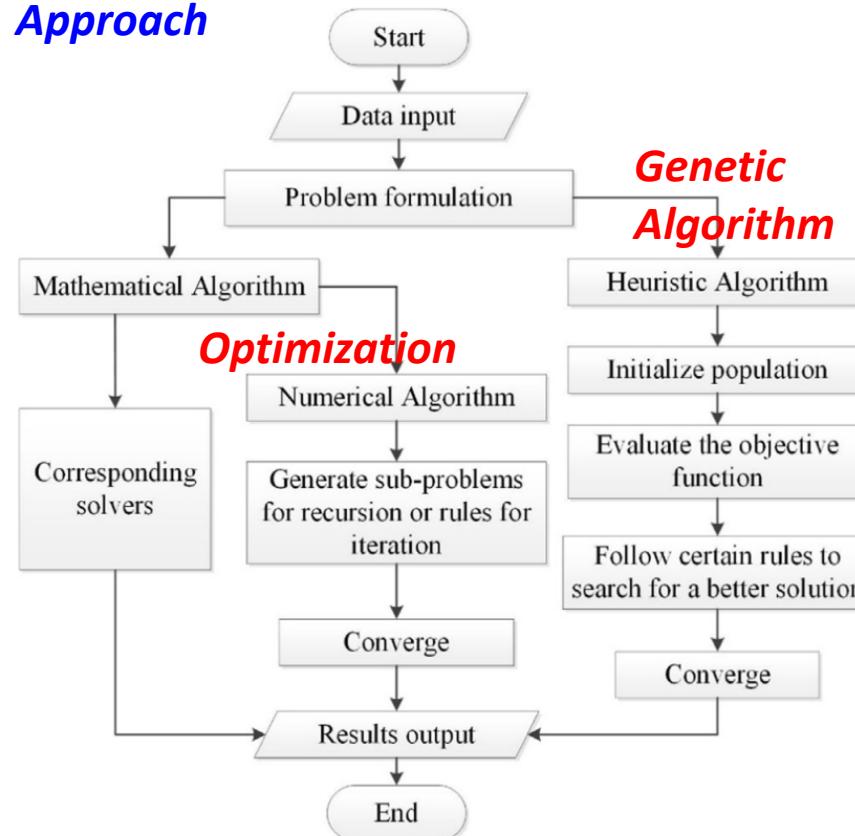


### Analytical Approach



# Energy Storage: Sizing Methods

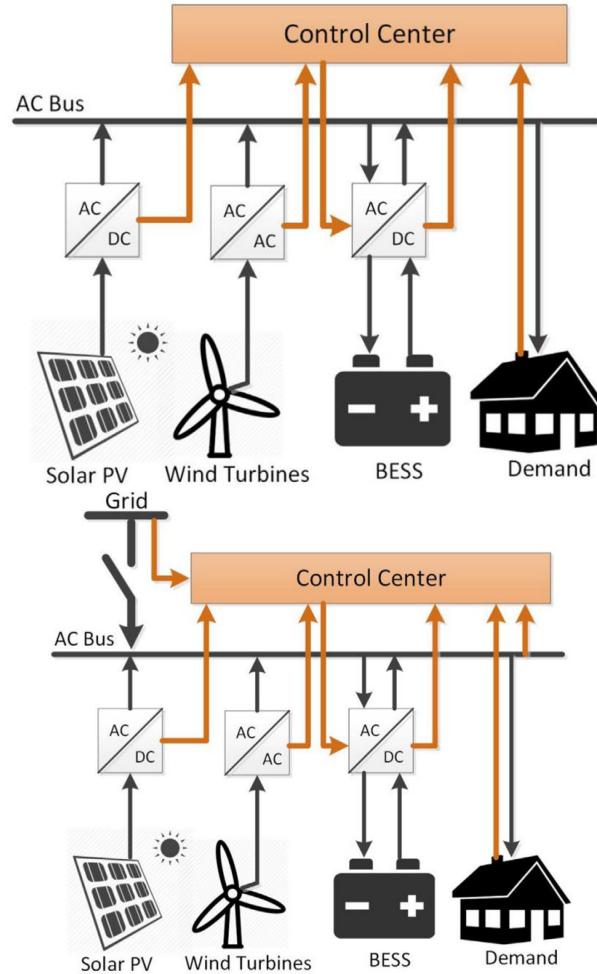
## Direct Search-Based Approach



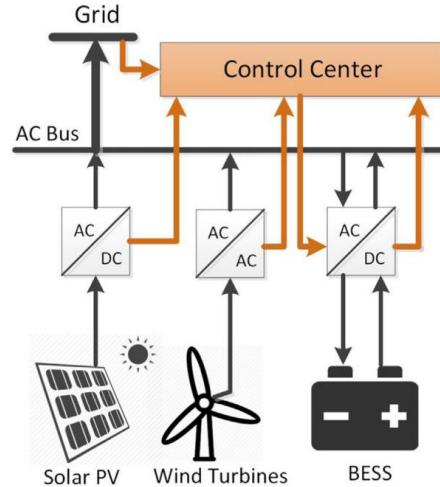
## Summary of pros and cons of BESS Sizing Techniques

Technique (Time Horizon)	Implementation	Pros	Cons
Probabilistic (depends on data resolution, more likely intra-hour, hourly data for long duration)	<ul style="list-style-type: none"> <li>Generates synthetic weather resources and PV/wind power generation data</li> <li>Generates synthetic scenarios for stochastic optimisation</li> </ul>	<ul style="list-style-type: none"> <li>Overcomes the restriction of limited data availability</li> <li>Gives results with confidence levels</li> </ul>	<ul style="list-style-type: none"> <li>Accuracy relies on the availability of historical data</li> <li>May require computational extensive resources</li> </ul>
Analytical (Applications for optimisation horizons ranging from repeated intra-hour simulations to several years assessment)	<ul style="list-style-type: none"> <li>Direct calculation based on intuitive criteria</li> <li>Repeated computation/simulation with fixed intervals</li> <li>Sensitivity analysis</li> </ul>	<ul style="list-style-type: none"> <li>Better visualization with the change of battery sizes</li> <li>Strong flexibility for all criteria and simulation environments</li> </ul>	<ul style="list-style-type: none"> <li>Computational intensive</li> <li>May miss global optimum if the data resolution is not high enough</li> </ul>
Mathematical optimisation (Applications for hourly, intra-day or daily optimisation)	<ul style="list-style-type: none"> <li>Linear, mixed-integer, quadratic programming problems</li> <li>Problems that can be linearized</li> <li>Problems that can be solved by numerical methods</li> </ul>	<ul style="list-style-type: none"> <li>Strong capability to find the global optimum</li> <li>Fast convergence and high robustness for linear problems</li> </ul>	<ul style="list-style-type: none"> <li>High efficiency limited to linear/mixed-integer/quadratic programming problems</li> <li>Linearization may require extra derivations</li> <li>Explicit mathematical formulation required</li> </ul>
Heuristic (Applications for hourly, intra-day or daily optimisation)	<ul style="list-style-type: none"> <li>Non-linear optimisation problems</li> <li>Apply nature-inspired algorithms such as GA, PSO, Tabu search and Bat Algorithms</li> </ul>	<ul style="list-style-type: none"> <li>Strong flexibility to solve all optimisation problems</li> <li>Avoid complicated derivatives</li> <li>Use less computational resources</li> <li>Simple implementation</li> <li>Large assortment of algorithms</li> <li>Combines strengths of different methods</li> </ul>	<ul style="list-style-type: none"> <li>May converge in local optimum instead of global optimum</li> <li>Less robustness and accuracy for linear problems</li> </ul>
Hybrid (Applications for hourly, intra-day or daily optimisation)	<ul style="list-style-type: none"> <li>Decoupled methods combined sequentially</li> <li>Hybridisation of different methods in a coupled way</li> </ul>	<ul style="list-style-type: none"> <li>Improves robustness and ensures global optimum found</li> </ul>	<ul style="list-style-type: none"> <li>Likely to increase the complexity</li> <li>May require high computational resources than heuristic methods</li> </ul>

# Energy Storage: Sizing Methods



**Different grid topology  
has different expectation  
on the BESS's function**



**Optimal Sizing of BESS also depends on:**

- Avoid voltage/ power/ frequency fluctuation (Microgrid)
- Absorb energy and Release Energy to reduce electricity cost
- Serve as constant voltage/frequency provider at PCC
- Reliability, Continuity and Stability of Supply (Standalone)
- Smoothing power output, load management (Power Plant)
- Avoid power curtailment, Compensate forecasting error
- Optimal Place of BESS (to avoid network congestion, upgrade, mitigate working stress of voltage regulating device)
- Application scale of Microgrid
- Auxiliary Technology (e.g. batteries, other ESS, ultracapacitors) ratio of battery to supercapacitor, expected function
- What batteries to be used? Vanadium Flow decouples energy density & power density, which has different capital cost; Zn/Br has minimized annual cost; Li-ion has less replacement;
- Selection range, Partial fulfilment, Environmental concerns, Hybrid Optimization

# Sizing of ES: Frequency Control

Rate of change of frequency:  $\bar{f} \frac{d\bar{f}}{dt} = \frac{\bar{P}_{\mu G,g} - \bar{P}_{\mu G,d}}{2 \cdot H_{\mu G}} = \frac{\Delta \bar{P}_{\mu G}}{2 \cdot H_{\mu G}}$

Equivalent Inertia:

$$H_{\mu G} = \sum_{i=1}^N \frac{H_{gen,i} \cdot S_{gen,i}}{S_{\mu G}}$$

Primary Inertia Deficiency:

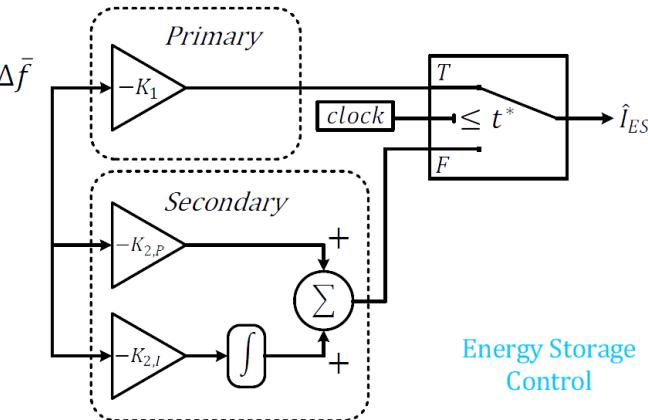
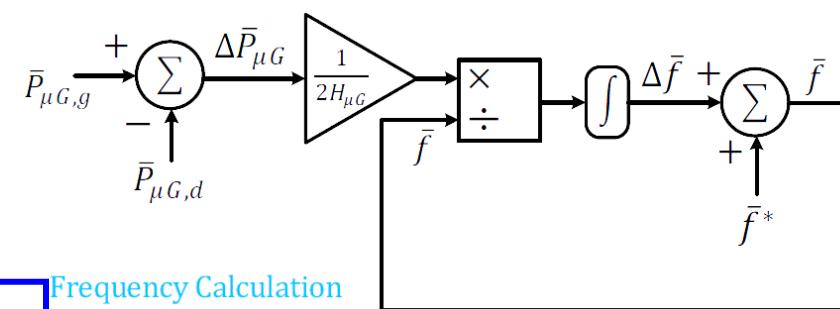
$$H_{def,1} = \frac{\Delta \bar{P}_{\mu G} \cdot \Delta t_1}{\bar{f}_2^2 - \bar{f}_1^2} - H_{\mu G}$$

$$E_{storage,1} \geq \frac{H_{def,1} \cdot P_{\mu G,g} \cdot |\Delta \bar{P}_{\mu G}| \cdot \Delta t_1}{(H_{def,1} + H_{\mu G})(3.6 \times 10^6)}$$

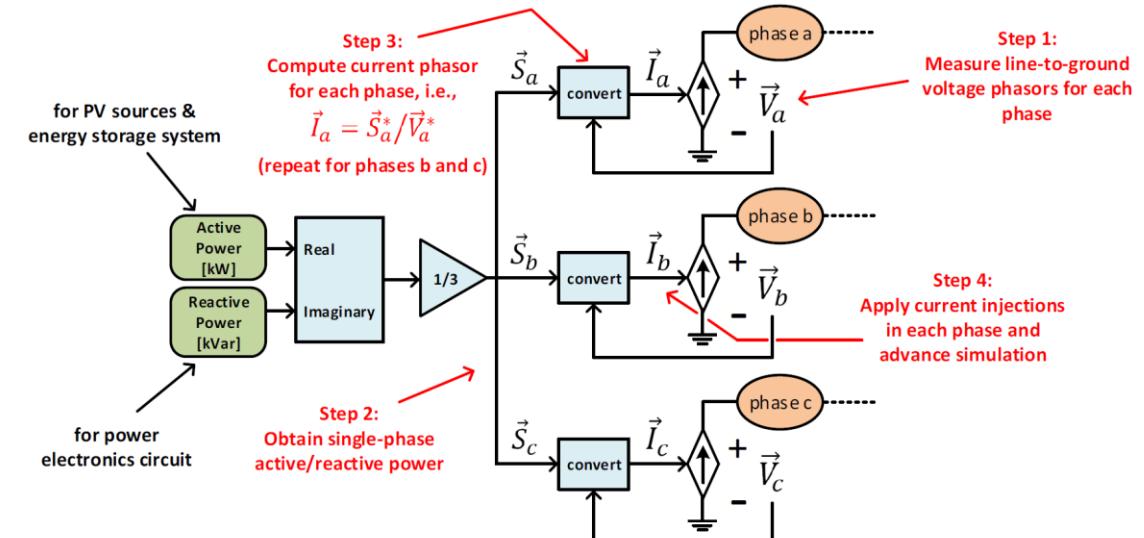
Secondary Inertia Deficiency:  $H_{def,2} = \frac{\Delta \bar{P}_{\mu G} \cdot \Delta t_2}{\bar{f}_2^2 - \bar{f}_1^2} - H_{\mu G}$

$$E_{storage,2} \geq \frac{H_{def,2} \cdot P_{\mu G,g} \cdot |\Delta \bar{P}_{\mu G}| \cdot \Delta t_2}{(H_{def,2} + H_{\mu G})(3.6 \times 10^6)}$$

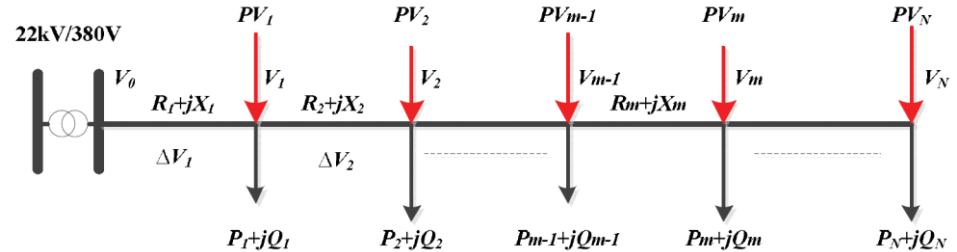
Voltage Stability:  $\Delta V_1 = V_S - V_{min} \cong \frac{P_{R,1}R + Q_{R,1}X}{V_{min}}$



Frequency Calculation



# Sizing of ES: Bee Colony Optimization



(Voltage Before PV Position)

$$V_m = V_0 - \sum_{k=1}^m \frac{((\sum_{n=k}^N P_n) - PV).rl_k + ((\sum_{n=k}^N Q_n)).xl_k}{V_{k-1}}$$

(Voltage at PV Position)

$$V_p = V_0 - \sum_{k=1}^p \frac{((\sum_{n=k}^N P_n) - PV).rl_k + ((\sum_{n=k}^N Q_n)).xl_k}{V_{k-1}}$$

(Voltage after PV Position)

$$V_m = V_0 - \sum_{k=1}^p \frac{((\sum_{n=k}^N P_n) - PV).rl_k + ((\sum_{n=k}^N Q_n)).xl_k}{V_{k-1}} - \sum_{k=p+1}^m \frac{(\sum_{n=k}^N P_n).rl_k + (\sum_{n=k}^N Q_n).xl_k}{V_{k-1}}$$

*Minimize :  $PB + dV$*

Subject to  $V_{f \min} < V_m < V_{f \max}$

$$dV = |V_{b \max} - V_{b \min}| \quad (*)$$

**Step 1:** Generate randomly the initial populations of  $n_e$  scout bees for the parameter. These initial populations must be feasible candidate solutions that satisfy the constraints. Set  $NC = 0$ .

**Step 2:** Represent the value of parameter from each population.

**Step 3:** Evaluate the fitness value of the initial populations by (\*).

**Step 4:** Select  $m$  best sites for neighborhood search. Separate the  $m$  best sites to two groups, the first group has  $e$  best sites and another group has  $m-e$  best sites.

**Step 5:** Determine the size of neighborhood search of each best size (patch size,  $ngh$ ).

**Step 6:** Recruit bees of  $n_e$  employed bees for selected sites (more bees for the best  $e$  sites).

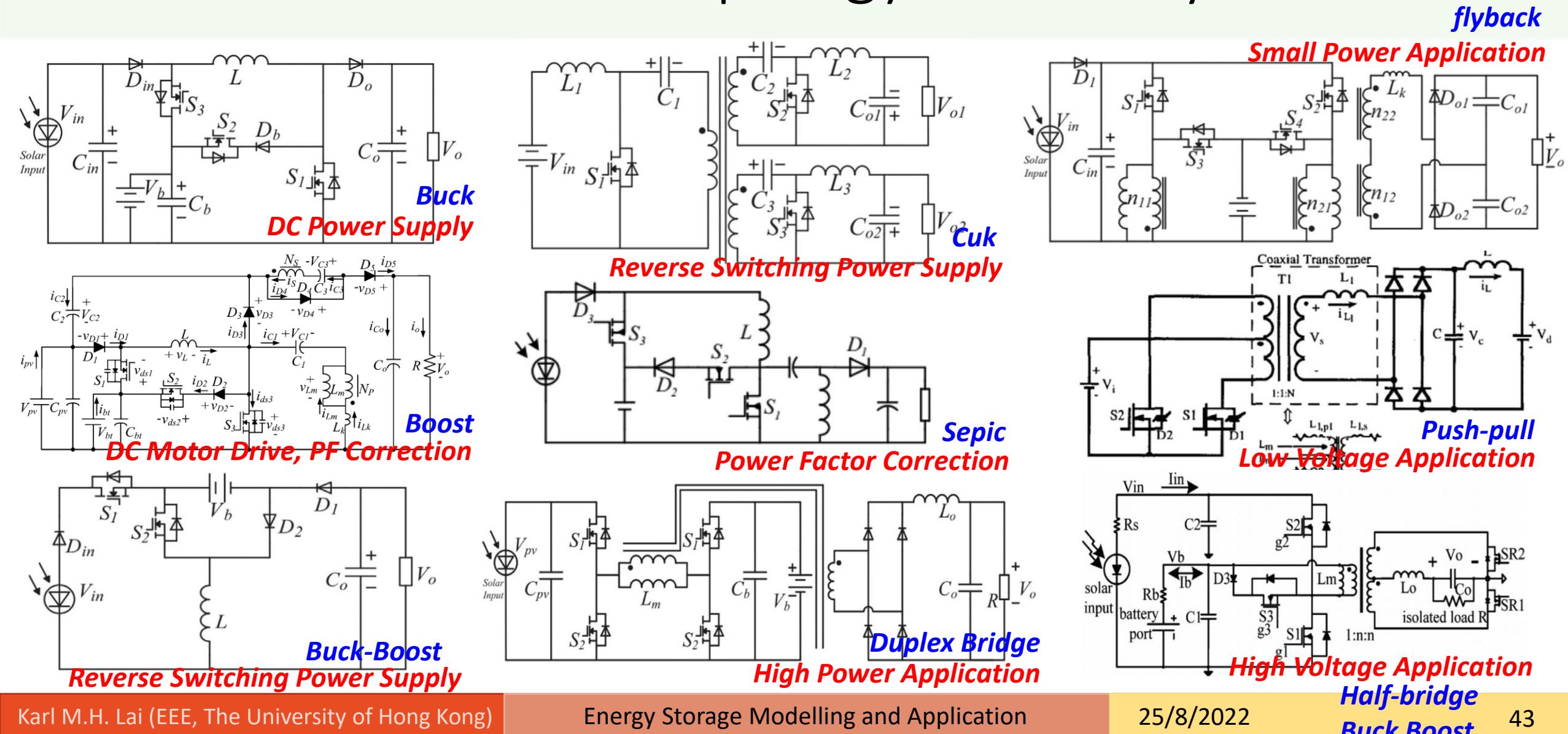
**Step 7:** Represent the value of parameter from each employed bee.

**Step 8:** Select the fittest bees from each patch.

**Step 9:** Check the stopping criterion. If satisfied, terminate the search, else  $NC=NC+1$ .

**Step 10:** Assign the  $n-m$  remaining bees to random search. Go to Step 2.

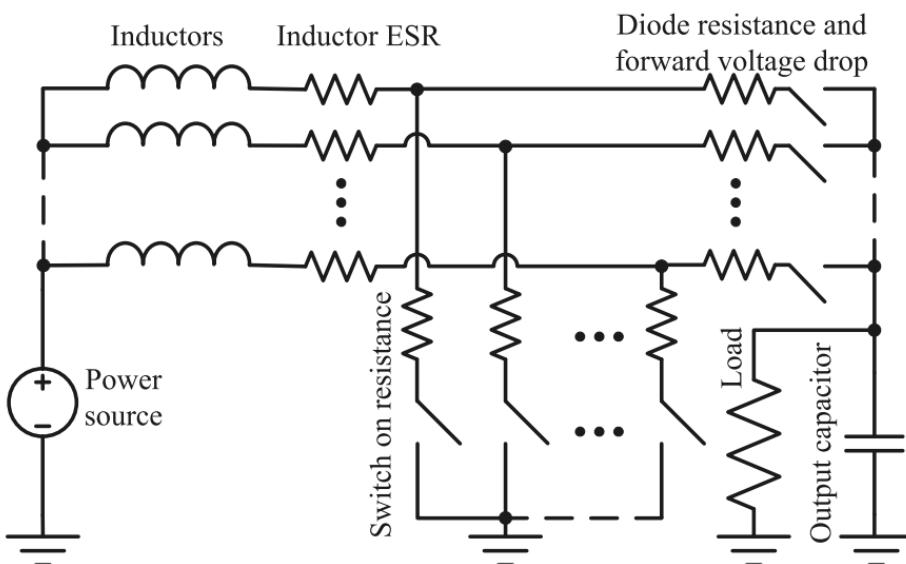
# Power Electronics Topology and Analysis



# Power Electronics Topology and Analysis

- Differential Equation Method

## Multi-phase Boost Converter



$$\begin{aligned} & \left( L_{l_{ij}} + L_{m_i} \right) \frac{di_{L_{ij}}(t)}{dt} - L_{m_i} \sum_{k=1, k \neq j}^N \frac{di_{L_{ik}}(t)}{dt} \\ & = v_g(t) - [1 - s_{ij}(t)]v_c(t) - [1 - s_{ij}(t)]v_D \\ & \quad - \{ R_{L_{ij}} + s_{ij}(t)R_{ONij} + [1 - s_{ij}(t)]R_{Dij} \} i_{L_{ij}}(t) \end{aligned}$$

$$C_f \frac{dv_c(t)}{dt} = \sum_{i=1}^M \sum_{j=1}^N [1 - s_{ij}(t)] i_{L_{ij}}(t) - \frac{v_c(t)}{R} - i_o(t)$$

while  $s_{ij}(t) = \begin{cases} 0 & \text{switch ON} \\ 1 & \text{switch OFF} \end{cases}$

Disturbance input:  $w = [v_g(t), i_o(t), v_D]$

Inductor current & cap. voltage:  $x = [i_{L_{11}}(t), \dots, i_{L_{MN}}(t), v_c(t)]$

State Equation:  $K\dot{x} = A[S(t)]x + B[S(t)]w$

# Power Electronics Topology and Analysis

- Differential Equation Method (cont')

Switch Period Averaging:  $\sum_{\alpha=1}^n t_{\alpha} = T \quad \sum_{\alpha=1}^n \frac{t_{\alpha}}{T} s_{ij}{}_{\alpha} = d_{ij}(t)$

Denote  $\sum_{\alpha=1}^n \frac{t_{\alpha}}{T} = \Gamma$

The averaged switching period model:

$$K\dot{x} = \left[ \frac{1}{T} \sum_{\alpha=1}^n t_{\alpha} A(S_{\alpha}) \right] x + \left[ \frac{1}{T} \sum_{\alpha=1}^n t_{\alpha} B(S_{\alpha}) \right] w$$

Define Duty Cycle Vector:

$$D(t) = [d_{11}(t), \dots, d_{1N}(t), d_{21}(t), \dots, d_{MN}(t)]^T$$

With linearity of circuit differential equations,

$$\Gamma A(S_{\alpha}) = A[D(t)] \quad \Gamma B(S_{\alpha}) = B[D(t)]$$

Average State Equation:  $K\dot{x} = A[D(t)]x + B[D(t)]w$

$L_{l_{ij}}$	leakage inductance of phase $j$ , group $i$ ;
$L_{m_i}$	mutual inductance of group $i$ ;
$i_{L_{ij}}(t)$	inductor current of phase $j$ , group $i$ ;
$v_g(t)$	power source voltage;
$v_D$	diode forward voltage drop;
$v_c(t)$	voltage of output capacitor;
$R_{D_{ij}}$	diode resistance of phase $j$ , group $i$ ;
$R_{ON_{ij}}$	switch conduct resistance of phase $j$ , group $i$ ;
$R_{L_{ij}}$	inductor ESR of phase $j$ , group $i$ ;
$R$	load resistance;
$C_f$	output capacitance;
$i_o$	output current;
$s_{ij}(t)$	switching state of phase $j$ , group $i$ ; and

$$s_{ij}(t) = \begin{cases} 0 & \text{switch turned OFF} \\ 1 & \text{switch turned ON.} \end{cases}$$

# Power Electronics Topology and Analysis

- Differential Equation Method (cont')

For steady state analysis,  $D(t) \rightarrow D$  and  $\dot{x} = 0$

$$\dot{x} = -A(D)^{-1}Bw$$

With elementary row transformation we can obtain the inverse of  $A(D)$ .

$$I_{Lij} = \frac{W-P(1-d_{ij})}{WR_{ij}(d_{ij})}v_g + \frac{1-d_{ij}}{WR_{ij}(d_{ij})}i_0 - \frac{1-d_{ij}}{WRR_{ij}(d_{ij})}v_D$$

$$V_c = \frac{P}{W}v_g - \frac{1}{W}i_o - \left(1 - \frac{1}{RW}\right)v_D$$

where W and P are defined as

$$W = \frac{1}{R} + \sum_{i=1}^M \sum_{j=1}^N \frac{(1-d_{ij})^2}{R_{ij}(d_{ij})}$$

$$P = \sum_{i=1}^M \sum_{j=1}^N \frac{1-d_{ij}}{R_{ij}(d_{ij})}$$

For Dynamic Analysis,

$$D(t) = \bar{D} + \tilde{D}(t)$$

$$w(t) = w + \tilde{w}(t)$$

Similarly,

$$K \frac{d\tilde{x}}{dt} = \tilde{A}(t)\bar{x}(t) + \bar{A}(t)\tilde{x}(t) + \tilde{B}(t)\bar{w}(t) + \bar{B}(t)\tilde{w}(t)$$

$$\tilde{A}(t)\bar{x}(t) + \tilde{B}(t)\bar{w}(t) = \bar{H}\bar{D}(t)$$

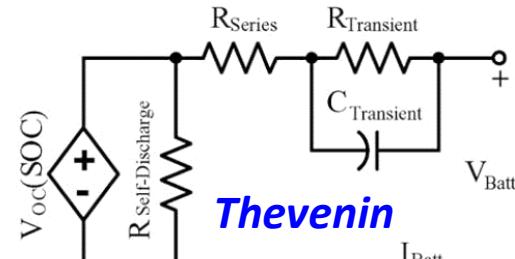
$$H = \begin{pmatrix} \delta(V_{ij}) \\ [-I_{Lij}]^T \end{pmatrix} \text{ and } V_c - \left( R_{ONij} - R_{Di,j} \right) I_{Lij} + v_D$$

$$K \frac{d\tilde{x}}{dt} = \bar{A}(t)\tilde{x}(t) + \bar{H}\bar{D}(t) + \bar{B}(t)\tilde{w}(t)$$

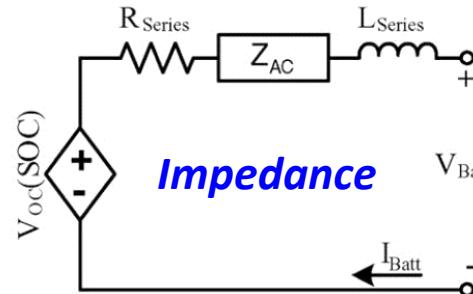
If  $x(0)=0$ ,  $Ks\tilde{x}(s) = \bar{A}(s)\tilde{x}(s) + \bar{H}\bar{D}(s) + \bar{B}(s)\tilde{w}(s)$

$$\tilde{x}(s) = (Ks - \bar{A})^{-1} \bar{H}\bar{D}(s) + (Ks - \bar{A})^{-1} \bar{B}\tilde{w}(s)$$

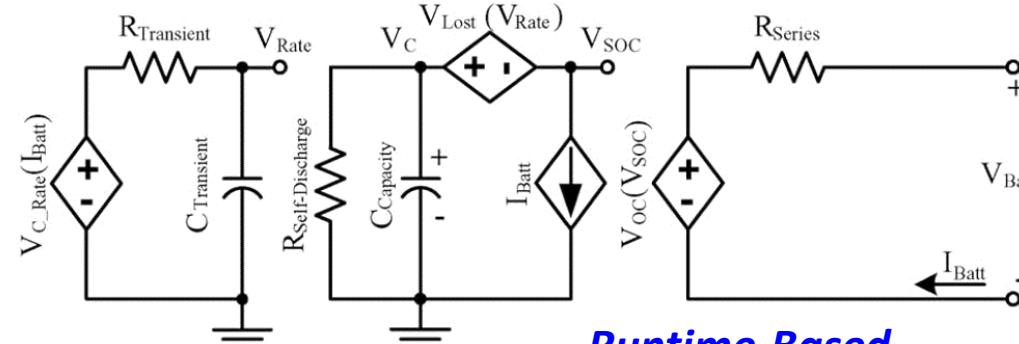
# Battery Models: (Integer) Equivalent Circuit



(a)

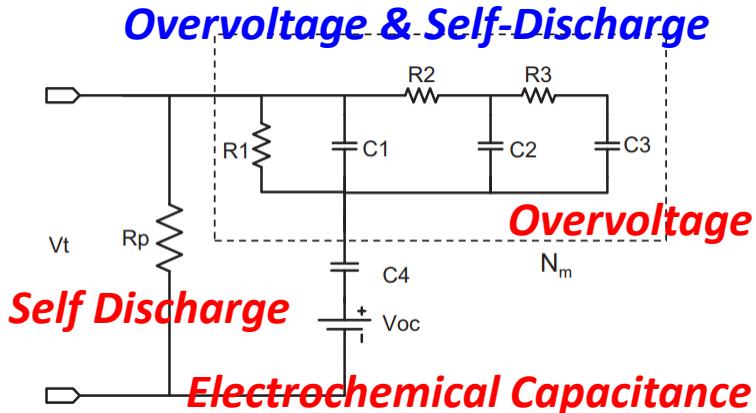


(b)



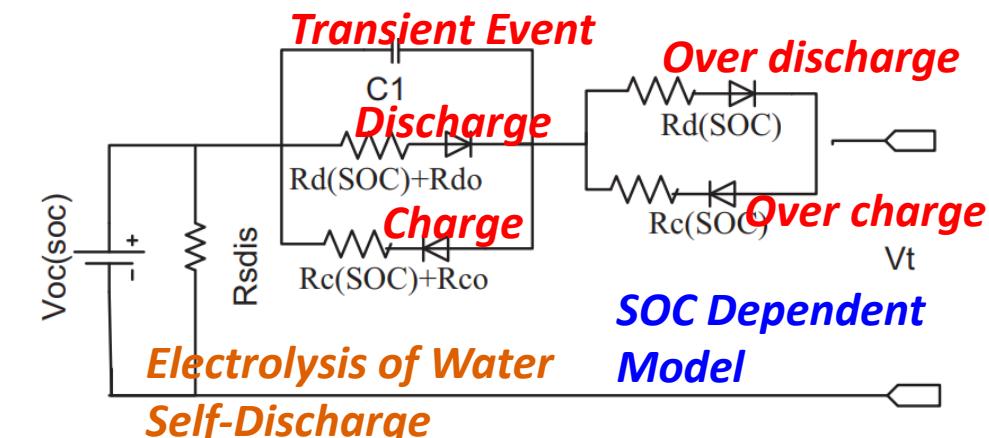
Runtime-Based

(c)



Self Discharge

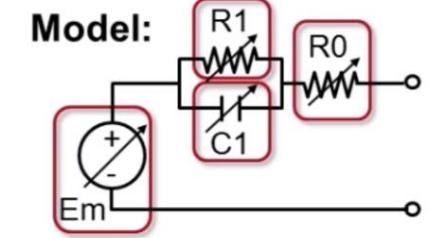
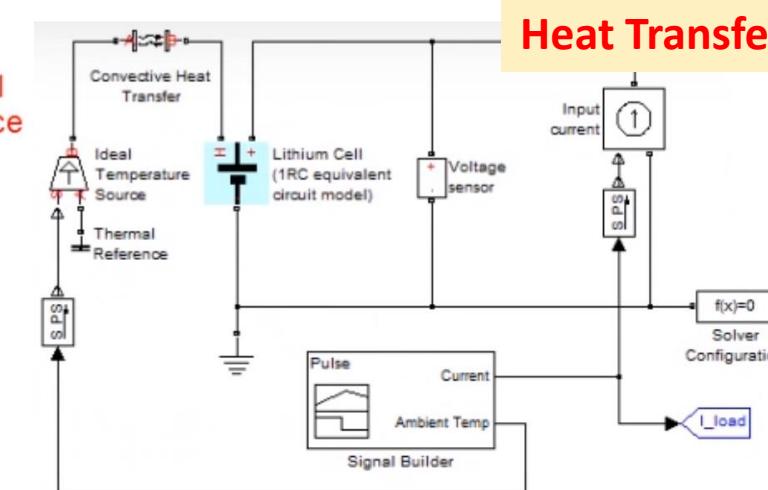
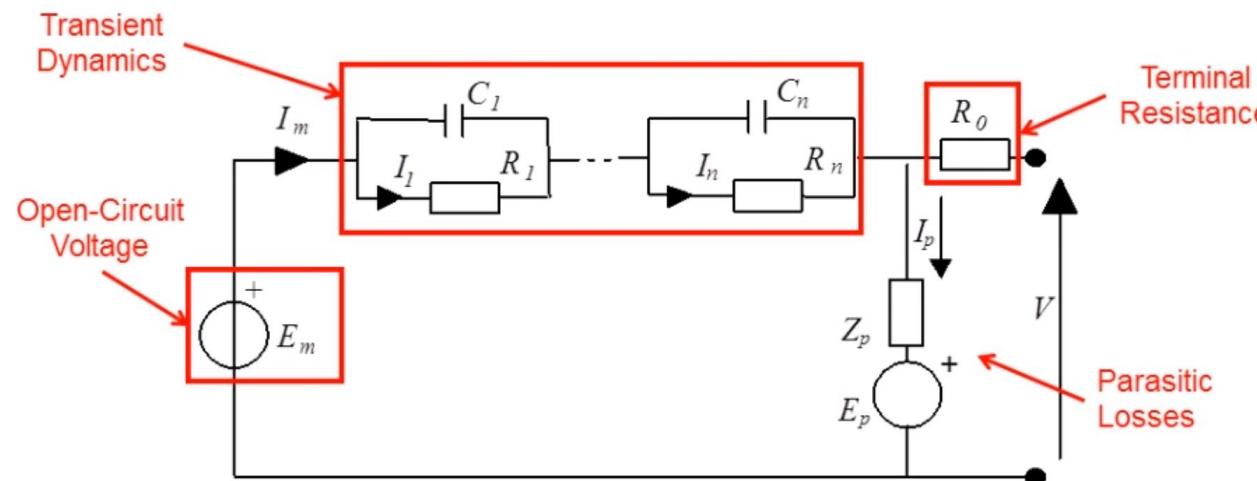
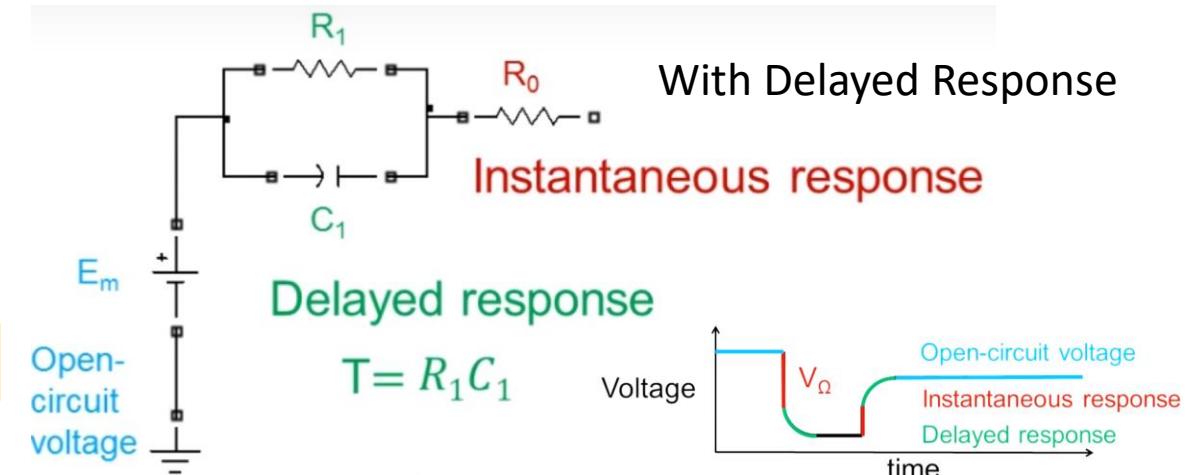
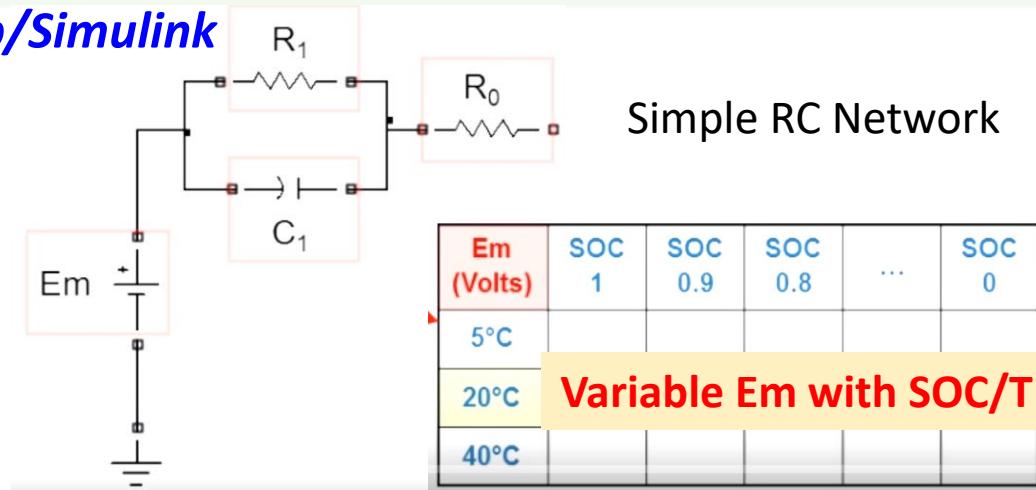
Electrochemical Capacitance

Electrolysis of Water  
Self-DischargeSOC Dependent  
Model

Mousavi S.M. & Nikdel M. (2014), Various Battery Models for Various Simulation Studies and Applications

# Battery Models: (Integer) Equivalent Circuit

**Matlab/Simulink**

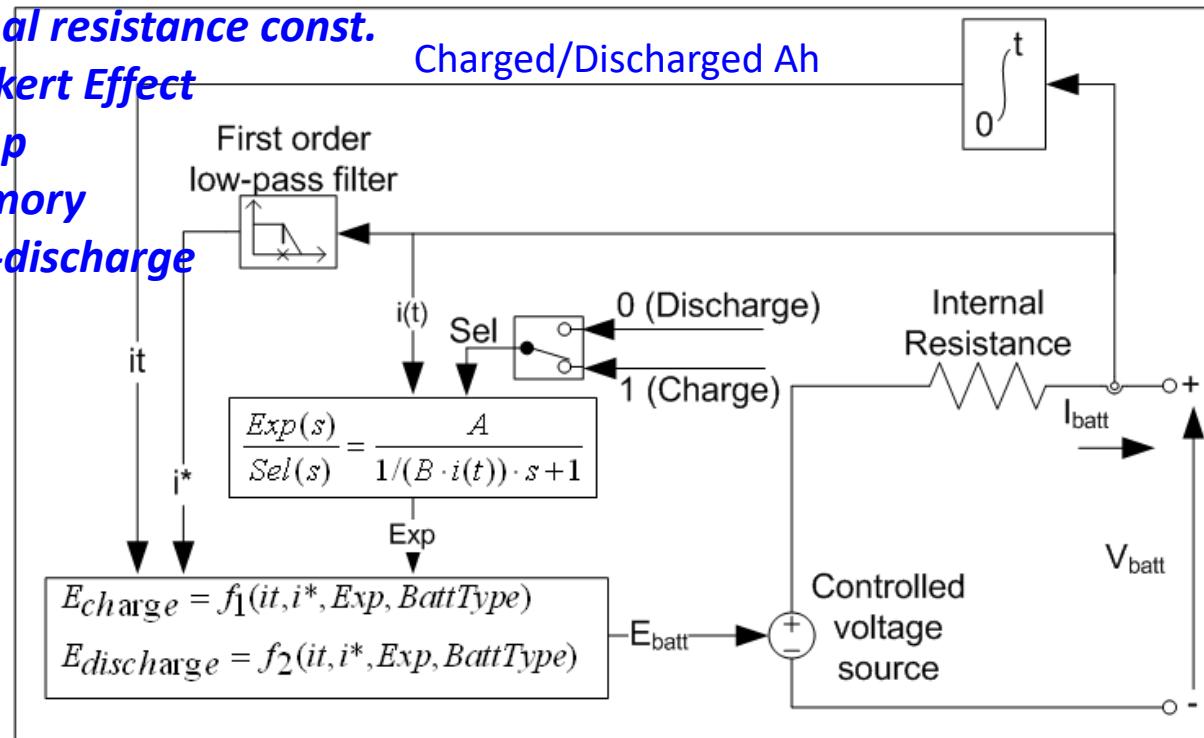


Behavior varies with  
SOC, temperature, etc.

# Battery Models: (Integer) Equivalent Circuit

**Assumption:**

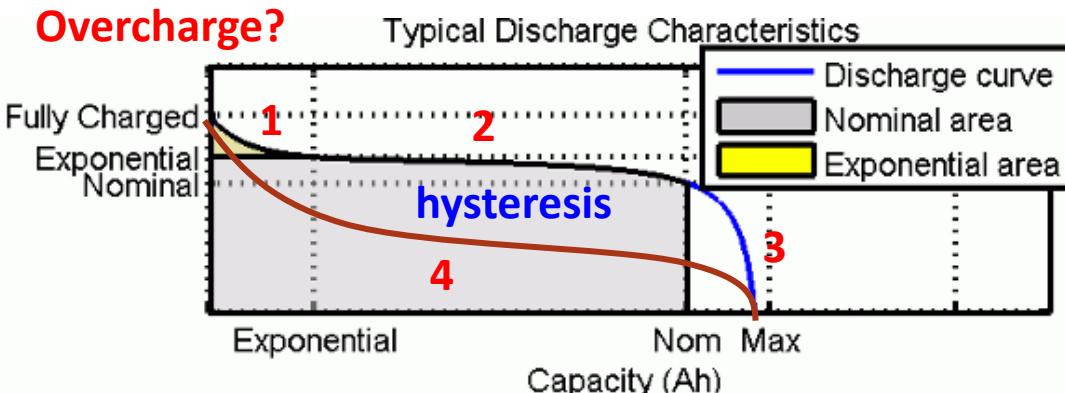
- Internal resistance const.
- X Peukert Effect
- X Temp
- X memory
- X self-discharge



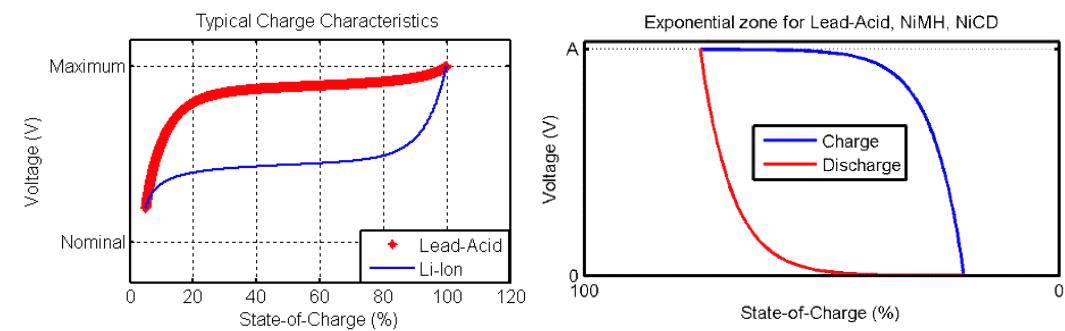
For Li-ion Cell:

$$\text{Discharge Model } (i^* > 0): f_1 = E_0 - k \frac{Q}{Q-it} i^* - K \frac{Q}{Q-it} it + Ae^{-B it}$$

$$\text{Charge Model } (i^* < 0): f_2 = E_0 - K \frac{Q}{it+0.1Q} i^* - K \frac{Q}{Q-it} it + Ae^{-B it}$$



1. Exponential Voltage Drop when the battery is charged
2. Charge can be extracted from the battery until voltage drop below nominal voltage
3. Total discharge of battery, when voltage drops rapidly
4. Battery current negative, battery recharges.



# Battery Models: (Integer) Equivalent Circuit

For Li-ion Battery: (With Temperature Effect)

Discharge Model ( $i^* > 0$ )

$$f_1 = E_0(T) - K(T) \frac{Q(T_a)}{Q(T_a) - it} (i^* + it) + Ae^{-B it} - C it$$

$$V_{batt}(T) = f_1 - R(T)i$$

Charge Model ( $i^* < 0$ )

$$f_2 = E_0(T) - K(T) \frac{Q(T_a)}{it + 0.1Q(T_a)} i^* - K(T) \frac{Q(T_a)}{Q(T_a) - it} it + Ae^{-B it} - C it$$

$$V_{batt}(T) = f_2 - R(T)i$$

with

$$E_0(T) = E_0|_{T_{ref}} + \frac{\partial E}{\partial T} (T - T_{ref})$$

$$K(T) = K|_{T_{ref}} e^{\alpha \left( \frac{1}{T} - \frac{1}{T_{ref}} \right)}$$

$$Q(T_a) = Q|_{T_a} + \frac{\partial Q}{\partial T} (T_a - T_{ref})$$

$$R(T) = R|_{T_{ref}} e^{\beta \left( \frac{1}{T} - \frac{1}{T_{ref}} \right)}$$

under cell temperature,  $T$ , at time,  $t$

$$T(t) = L^{-1} \left\{ \frac{P_{loss} R_{th} + T_a}{1 + st_c} \right\}$$

$$P_{loss} = (E_0(T) - V_{batt}(T))i + \frac{\partial E}{\partial T} iT$$

Obtained in: <https://www.mathworks.com/help/physmod/sps/powersys/ref/battery.html>

where

$T_{ref}$  = nominal ambient temperature

$T$  = cell temperature

$T_a$  = ambient temperature

$E/T$  = reversible voltage temperature coefficient

$\alpha$  = Arrhenius rate constant for polarization resistance

$\beta$  = Arrhenius rate constant for internal resistance

$\partial Q / \partial T$  = maximum capacity temp coefficient

$C$  = nominal discharge curve slope in V/Ah

$t_c$  = thermal time constant

# Battery Models: (Integer) Equivalent Circuit

Cyclic Ageing Effect for Li-ion Cell: with  $n = kT_h$

$$\text{Capacity: } Q(n) = \begin{cases} Q_{BOL} - \varepsilon(n)(Q_{BOL} - Q_{EOL}) & \text{if } k/2 \neq 0 \\ Q(n-1) & \text{otherwise} \end{cases}$$

$$\text{Internal Resistance: } R(n) = \begin{cases} R_{BOL} - \varepsilon(n)(R_{EOL} - R_{BOL}) & \text{if } k/2 \neq 0 \\ R(n-1) & \text{otherwise} \end{cases}$$

where

$T_h$  = half-cycle duration in s

$Q_{BOL}$  = battery max capacity in Ah, at beginning

$Q_{EOL}$  = battery max capacity in Ah, at end of life

$R_{BOL}$  = Internal resistance at BOL, nominal T

$R_{EOL}$  = Internal resistance at EOL, nominal T

$\varepsilon$  = battery aging factor ( $=0$  at BOL,  $=1$  at EOL)

$$\text{Battery Aging Factor: } \varepsilon(n) = \begin{cases} \varepsilon(n-1) + \frac{0.5}{N(n-1)} \left( 2 - \frac{DOD(n-2) + DOD(n)}{DOD(n-1)} \right) & \text{if } \frac{k}{2} \neq 0 \\ \varepsilon(n-1) & \text{otherwise} \end{cases}$$

where

DOD = depth of discharge (%) after half-cycle

$$N(n) = H \left( \frac{DOD(n)}{100} \right)^{-\xi} \exp \left( -\Psi \left( \frac{1}{T_{ref}} - \frac{1}{T_a(n)} \right) \right) \left( I_{dis\_ave}(n) \right)^{-\gamma_1} \left( I_{ch\_ave}(n) \right)^{-\gamma_2}$$

where: H is cycle number constant,  $\xi$  = exponential factor for DOD,  $\Psi$  = Arrhenius rate constant for cycle number,

$I_{dis\_ave}$  = average discharge current (A) during half-cycle,  $I_{ch\_ave}$  = average charge current (A) during half-cycle

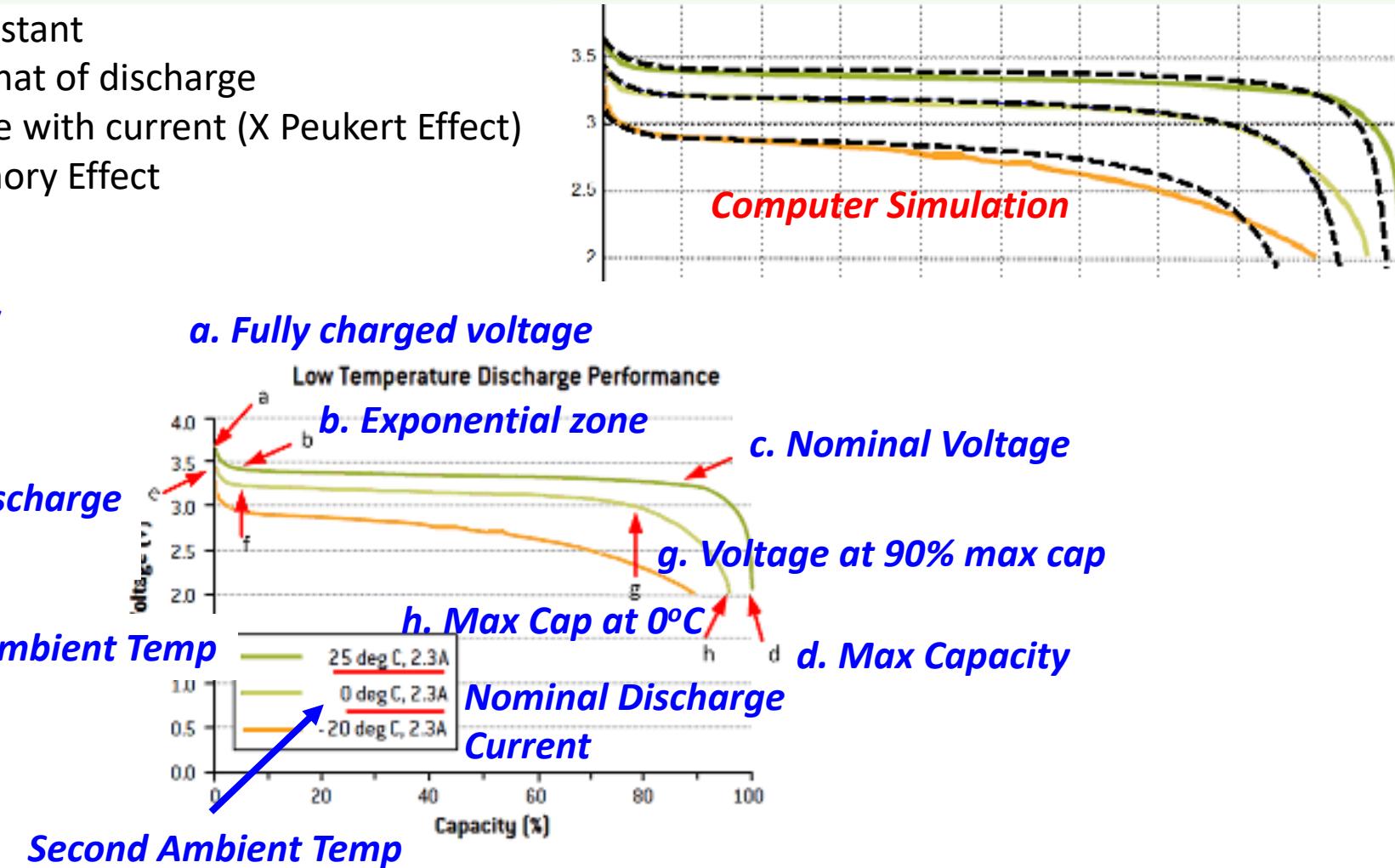
$\gamma_1$  = exponent factor for the discharge current and  $\gamma_2$  = exponent factor for the charge current.

# Battery Models: (Integer) Equivalent Circuit

- Assumption:
- Internal Resistance = constant
  - Parameter for charge = that of discharge
  - Capacity does not change with current (X Peukert Effect)
  - No Self-Discharge / Memory Effect

Extracting Information from Data Sheet:

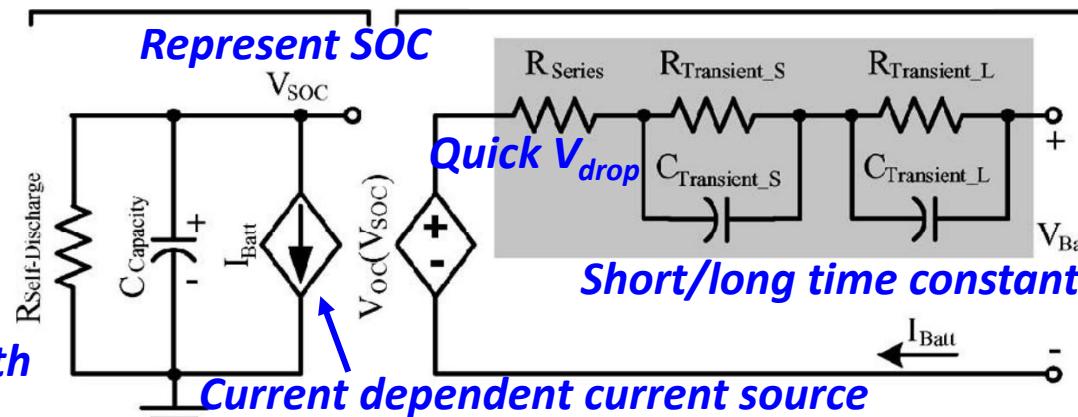
Specifications	Rated Capacity
Nominal capacity and voltage	2.3 Ah, 3.3 V
Internal impedance (1kHz AC)	8 mΩ typical
Internal resistance (10A, 15°C)	10 mΩ typical
Recommended standard charge method	
Recommended fast charge current	
Maximum continuous discharge	
Pulse discharge at 10 sec	
Cycle life at 10C discharge, 100% DOD	
Recommended pulse charge/discharge cutoff	
Operating temperature range	-30°C to +60°C
Storage temperature range	-50°C to +60°C
Core cell weight	70 grams



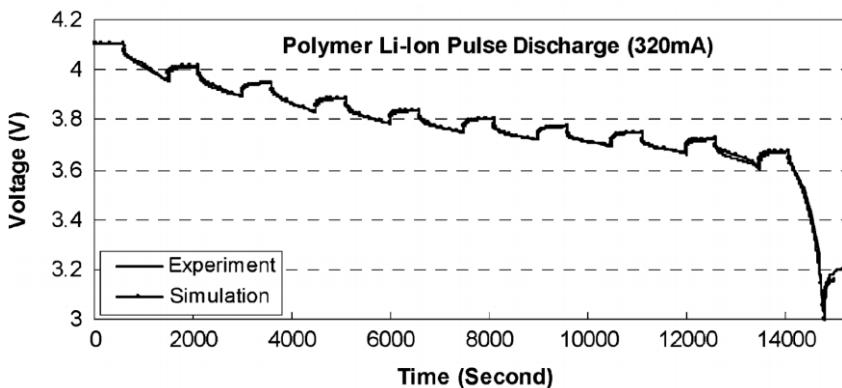
# Battery Models: (Integer) Equivalent Circuit

## MapleSim Equivalent Circuit Model

### Capacity Circuit      Time Response Circuit



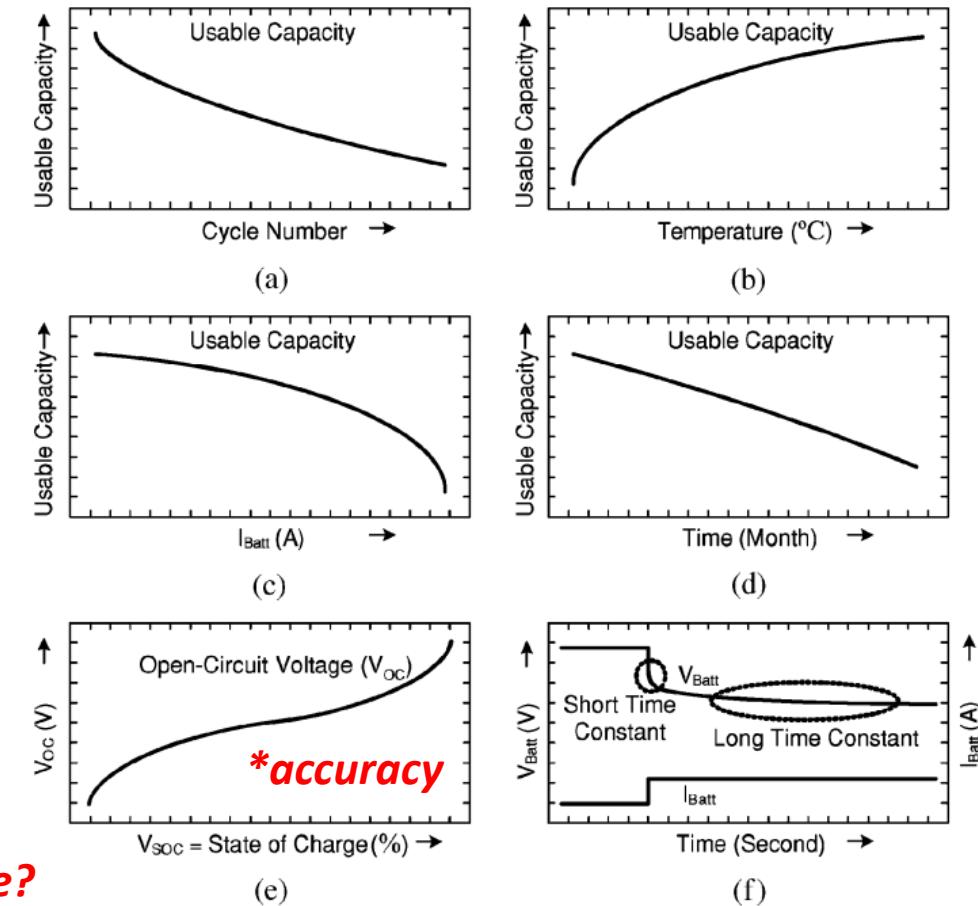
Parameters are temp, SOC, current and cycle dependent!



Max Error Voltage (mV)	Runtime Error * (%)
15	0.039%
17	0.118%
18	0.020%
21	0.029%

What will be the runtime?

Usable Cap  $\downarrow$  when cycle number, discharge current, storage time  $\uparrow$  and temperature  $\downarrow$



# Battery Models: (Fractional) Equivalent Circuit

- **Fractional Calculus** suits for infinite dynamic processes, such as movement of charge carriers through electrolytes, charge-transfer reactions, solid-phase diffusion, to stray storage and cyclic operation and ageing process. It takes into account the entire past trajectory, with a long memory property.

Impedance of Capacitance:  $Z_{CPE} = \frac{1}{C_\alpha(j\omega)^\alpha}$  for  $\alpha \in (0,1)$  CPE = constant phase element,  $C_\alpha$  = pseudo cap

Fractional Order Derivative of the CPE is given as:

$${}_0D_t^\alpha = \frac{d^\alpha(.)}{d(.)^\alpha} = \lim_{T \rightarrow 0} \frac{1}{T^\alpha} \sum_{k=0}^{t/T} (-1)^k \langle \alpha, k \rangle f(t - kT)$$

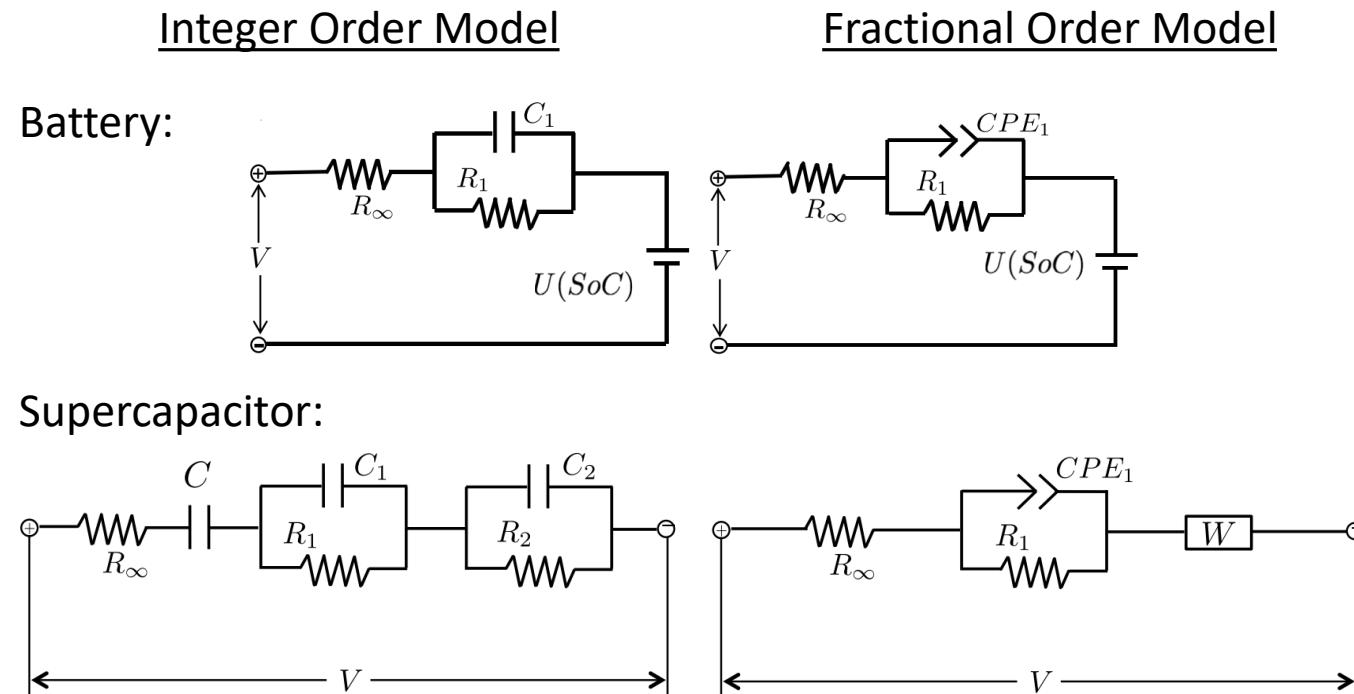
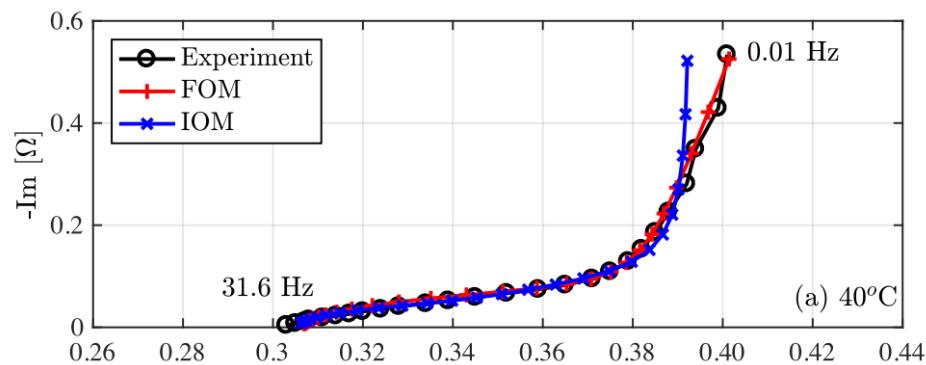
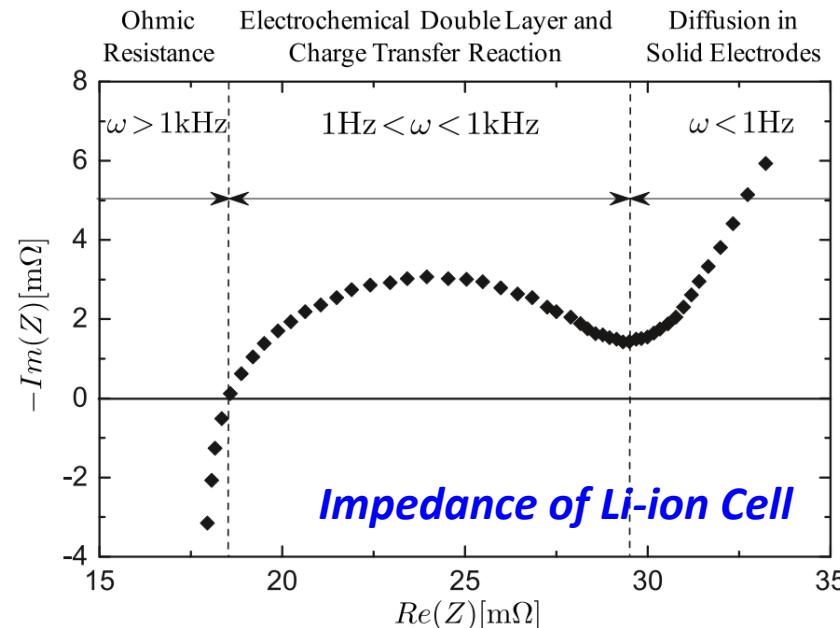
for Newton-Binomial coefficient:

$$\langle \alpha, k \rangle = \frac{\Gamma(\alpha + 1)}{\Gamma(k + 1)\Gamma(\alpha - k + 1)}$$

and Gamma Function:

$$\Gamma(\alpha) = \int_0^\infty \xi^{\alpha-1} e^{-\xi} d\xi$$

# Battery Models: (Fractional) Equivalent Circuit



# Battery Model: Electrochemical Modelling

## Porous Electrode Theory

Governing Equations

**Diffusive Flow in Liquid Phase**

$$\varepsilon_i \frac{\partial c}{\partial t} = \nabla \cdot D_{eff,i} \nabla c + a_p (1 - t_+) j_i \quad \text{KCL + Ohm's Law}$$

$$-\nabla \cdot [\sigma_{eff} \nabla \Phi_1] - \nabla \cdot [\kappa_{eff} \nabla \Phi_2] + \nabla \cdot \left[ \frac{2\kappa_{eff} RT}{F} (1 - t_+) \nabla \ln c \right] = 0$$

$$\sigma_{eff,i} \nabla^2 \Phi_1 = a_i F j_i \quad \text{Charge Conservation}$$

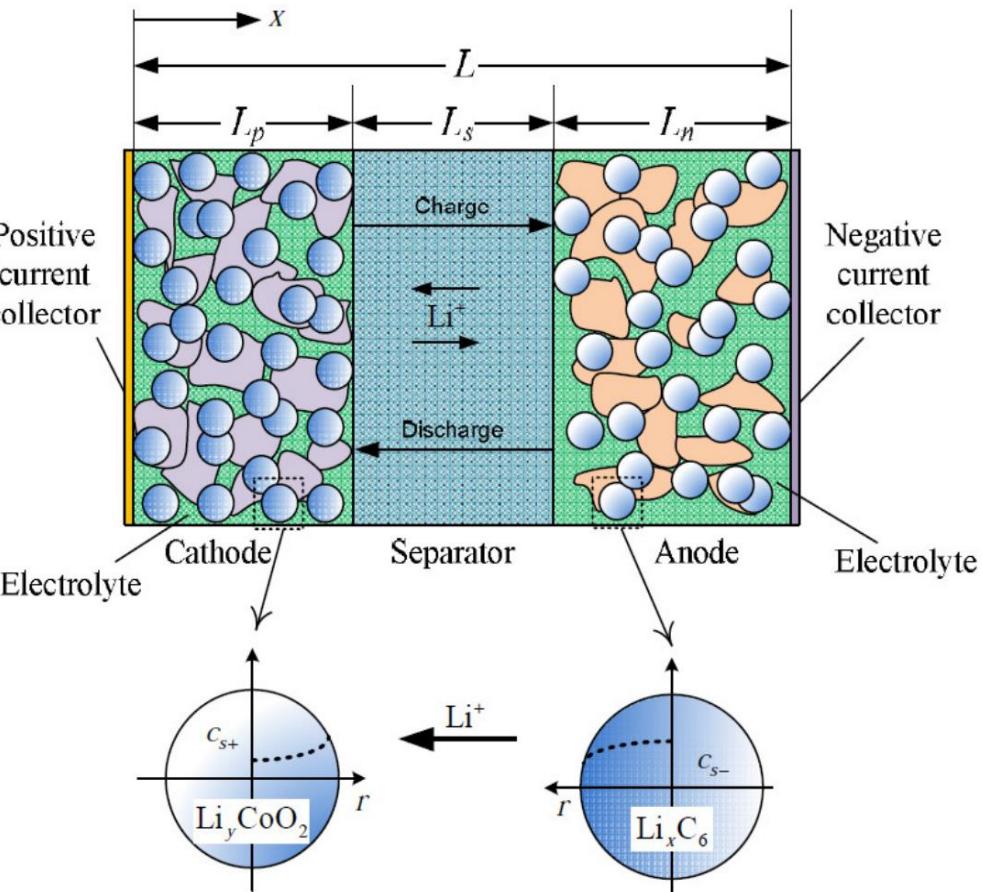
$$\frac{\partial c_p^s}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 D_p^s \frac{\partial c_p^s}{\partial r} \right] \quad \text{Diffusive Flow in Solid State}$$

$$\rho_i C_{p,i} \frac{dT_p}{dt} = \nabla \cdot \lambda_i \nabla T + Q \quad \text{Heat Transfer}$$

$\frac{\partial T}{\partial y} = 0$	$\frac{\partial C}{\partial y} = 0$	$\frac{\partial \Phi_1}{\partial y} = 0$	$\frac{\partial \Phi_2}{\partial y} = 0$
Cathode	Separator	Anode	
$\frac{\partial T}{\partial x} = 0$	$\frac{\partial C}{\partial x} = 0$	$\frac{\partial \Phi_1}{\partial x} = 0$	$\frac{\partial \Phi_2}{\partial x} = 0$
$\sigma_p \frac{\partial \Phi_1}{\partial x} = -I_{app}$		$\sigma_n \frac{\partial \Phi_1}{\partial x} = -I_{app}$	
$\frac{\partial \Phi_2}{\partial x} = 0$		$\frac{\partial \Phi_2}{\partial x} = 0$	

**Boundary Condition**

$\frac{\partial \Phi_1}{\partial y} = 0$		
Cathode	Separator	Anode
$\int_0^L \sigma_p \frac{\partial \Phi_1}{\partial x} dy = -I_{app}$		$\int_0^L \sigma_n \frac{\partial \Phi_1}{\partial x} dy = -I_{app}$
$\Phi_1(x=0, y, t) = f(t)$		$\Phi_1(x=L, y, t) = f(t)$



**Anatomy of a lithium ion cell**

# Battery Model: Electrochemical Modelling

- Single Particle Model (Current density, conc., over-potential)

$$\text{Butler-Volmer Equation: } j = k(c_{s,max} - c_{s,surf})^{0.5} (c_{s,surf})^{0.5} c_e^{0.5} \sinh\left(\frac{0.5F\mu}{RT}\right)$$

$$V(t) = (U_p(t) - U_n(t)) - (\phi_e(L_c, t) - \phi_e(0, t)) - (\eta_p(t) - \eta_n(t)) \\ - (R_r(t) + R_c)I(t) - V_h(t) \quad (\text{Electrical})$$

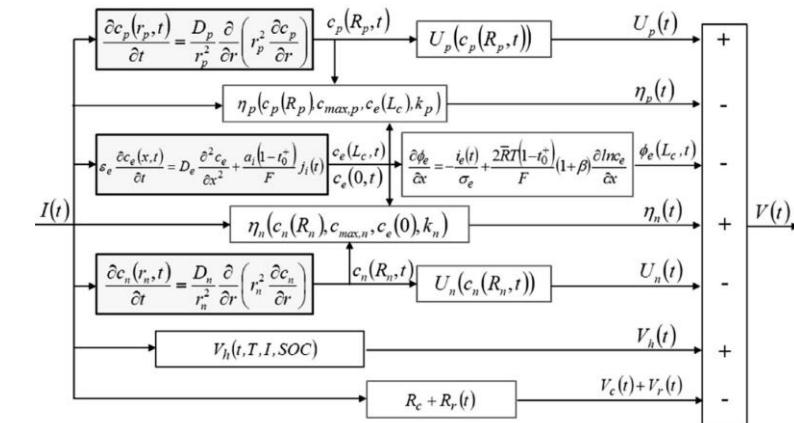
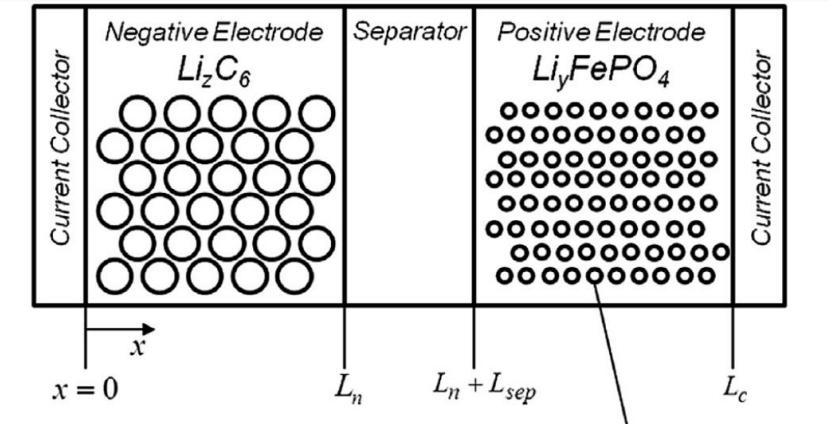
$$\frac{dV_h}{dt} = |I|\tau_h(T)(H(T, SOC) - V_h) \quad (\text{Hysteresis})$$

$$R_r(t) = \frac{R_p L_{\text{cond}}(t)}{3L_b A \varepsilon_b} \frac{1}{\sigma_b} \quad (\text{Increasing } R \text{ with depth of discharge}) \quad \frac{dL_{\text{cond}}}{dt} = \frac{\pi R_p |I|}{Fc_{\max,p} L_p A \varepsilon_p}$$

$$\frac{\partial c_i}{\partial t} = \frac{D_i}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_i}{\partial r} \right) \quad \text{Mass diffusion equation (overpotential)}$$

$$\frac{\partial c_e}{\partial t} = D_e \frac{\partial^2 c_e}{\partial x^2} + \frac{a_i(1-t_0^+)}{F} j_i(t) \quad (\text{Ohmic Transport in Liquid state})$$

$$\frac{\partial \phi_e}{\partial x} = -\frac{i_e(t)}{\sigma_e} + \frac{2\bar{R}T(1-t_0^+)}{F} (1+\beta) \frac{\partial \ln(c_e)}{\partial x} \quad (\text{potential-concentration relation})$$



Marcicki, J. et al. (2013) Design and parametrization analysis of a reduced-order electrochemical model of graphite/LiFePO4 cells for SOC/SOH estimation

# Battery Model: Electrochemical Modelling

- Observer Design

Let  $x$  be a vector of concentration and  $u$  be a vector of current  $I$ .

$$\begin{aligned} \frac{dc_n}{dt} &= \frac{S_{n-1}}{r_n - r_{n-1}} \frac{D_s}{V_n} c_{n-1} \\ &\quad - \left( \frac{S_{n-1}}{r_n - r_{n-1}} + \frac{S_n}{r_{n+1} - r_n} \right) \frac{D_s}{V_n} c_n \\ &\quad + \frac{S_n}{r_{n+1} - r_n} \frac{D_s}{V_n} c_{n+1}, \end{aligned}$$

$$\frac{dc_{N_s}}{dt} = \frac{S_{N_s-1}}{r_{N_s} - r_{N_s-1}} \frac{D_s}{V_{N_s}} (c_{N_s-1} - c_{N_s}) + K_I^s I.$$

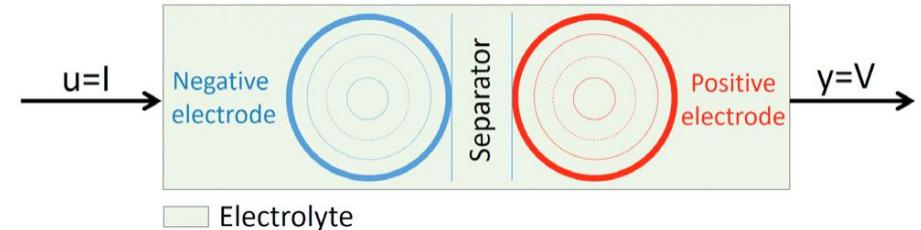
$$c_1^{neg} = K + \sum_{i=2}^{N_{neg}} \beta_i^{neg} c_i^{N_{neg}} + \sum_{i=1}^{N_{pos}} \beta_i^{pos} c_i^{N_{pos}}$$

$$K := \frac{Q}{\alpha_{neg} V_1^{neg}}$$

$$\beta_i^{neg} := -\frac{V_i^{neg}}{\alpha_{neg} V_1^{neg}} \quad \beta_i^{pos} := -\frac{\alpha_{pos} V_i^{pos}}{\alpha_{neg} V_1^{neg}}.$$

$$(Voc) \quad y := OCV_{pos}(c_{pos}^{surf}) - OCV_{neg}(c_{neg}^{surf}) + g(u)$$

$g(u)$  is current dependent

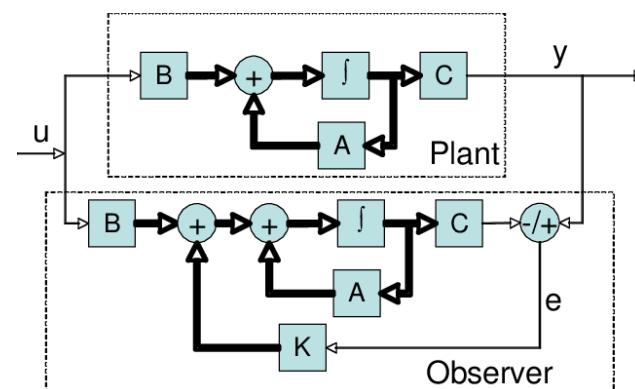


State Equation:  $\begin{cases} \dot{x} = Ax + Bu + K + Ew \\ y = h(x) + g(u) + Dz, \end{cases}$

$Ew$  is perturbation  
 $Dz$  is measurement noise

State Observer:  $\begin{cases} \dot{\hat{x}} = A\hat{x} + Bu + K + L(y - \hat{y}) \\ \hat{y} = h(\hat{x}) + g(u), \end{cases}$

Estimation error:  $\dot{e} = Ae + Ew - L(h(x) - h(\hat{x})) - LDz.$



State space analysis and state observer

# Battery Model: Electrochemical Modelling

- Kalman Filter

State-Space Eqt:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{z}, u) & \mathbf{x} &= [\mathbf{c}_s, \mathbf{c}_e, T]^T \\ 0 &= \mathbf{g}(\mathbf{x}, \mathbf{z}, u) & \mathbf{z} &= [\mathbf{j}^{Li}, \phi_{s,c}^0, \phi_{s,a}^0]^T \\ \mathbf{y} &= [H_x \quad H_z] \begin{bmatrix} \mathbf{x} \\ \mathbf{z} \end{bmatrix} + H_u u\end{aligned}$$

$\mathbf{y} = [\mathbf{V} \quad \mathbf{T}]$   
V = voltage

T = temp

$H_x, H_z, H_u$  is derived from electrochemical eqts

For a linear State-Space:  $\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + Bu(t) + \mathbf{w}(t)$

$$\mathbf{y}_k = C\mathbf{x}_k + \mathbf{v}_k$$

$$\widehat{\mathbf{x}}_{k+1}^- = \Phi \widehat{\mathbf{x}}_k + \int_{t_k}^{t_{k+1}} \Phi B \mathbf{u}(\tau) d\tau$$

Time Update:

$c_s$  = solid-phase conc

$c_e$  = electrolyte conc

T = bulk temperature

$j$  = volumetric reaction rate

$\phi_{s,c}^0$  = potential at cathode

$\phi_{s,a}^0$  = potential at anode

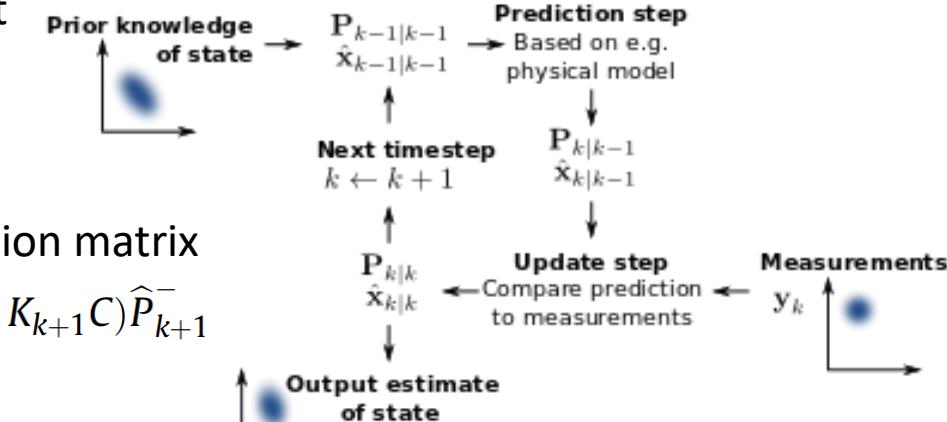
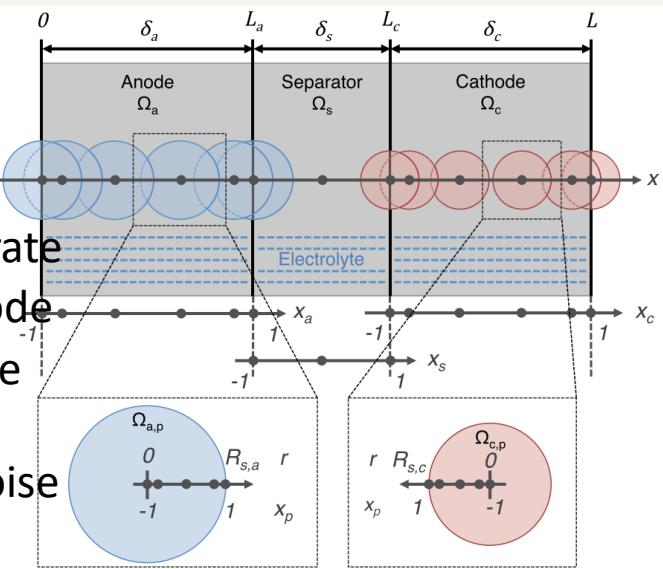
$\mathbf{w}(t)$  = white Gaussian Noise  
with covariance Q

$\mathbf{v}_k$  = measurement  
noise with  
covariance R

Measurement Update:  $\widehat{P}_{k+1}^- = \Phi \widehat{P}_k \Phi^T + Q$   $\Phi$  = state transition matrix

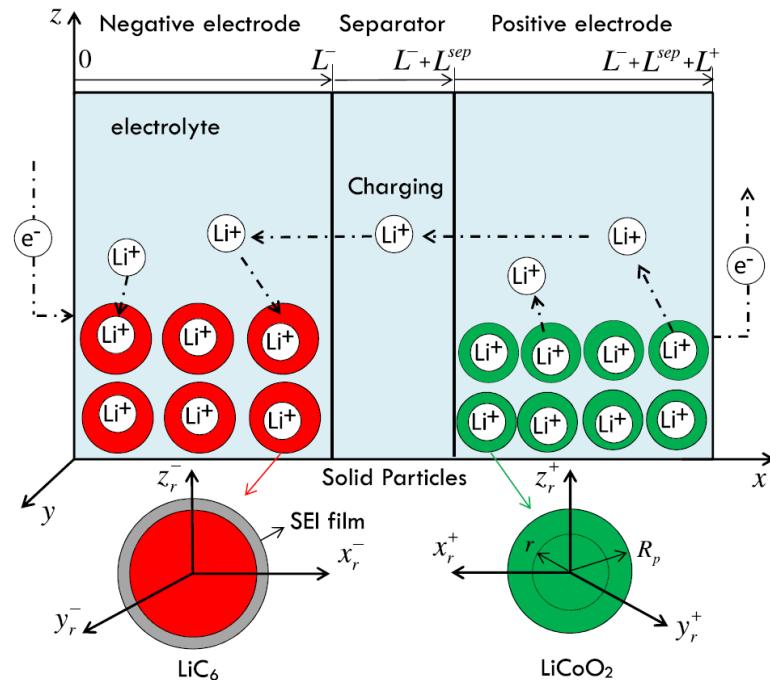
$$\begin{aligned}K_{k+1} &= \widehat{P}_{k+1}^- C^T \left( C \widehat{P}_{k+1}^- C^T + R \right)^{-1} & \widehat{P}_{k+1} &= (I - K_{k+1} C) \widehat{P}_{k+1}^- \\ \widehat{\mathbf{x}}_{k+1} &= \widehat{\mathbf{x}}_{k+1}^- + K_{k+1} (\mathbf{y}_{k+1} - \widehat{\mathbf{y}}_{k+1}^-)\end{aligned}$$

State time update -> linearization -> error time update -> linearization -> measurement update

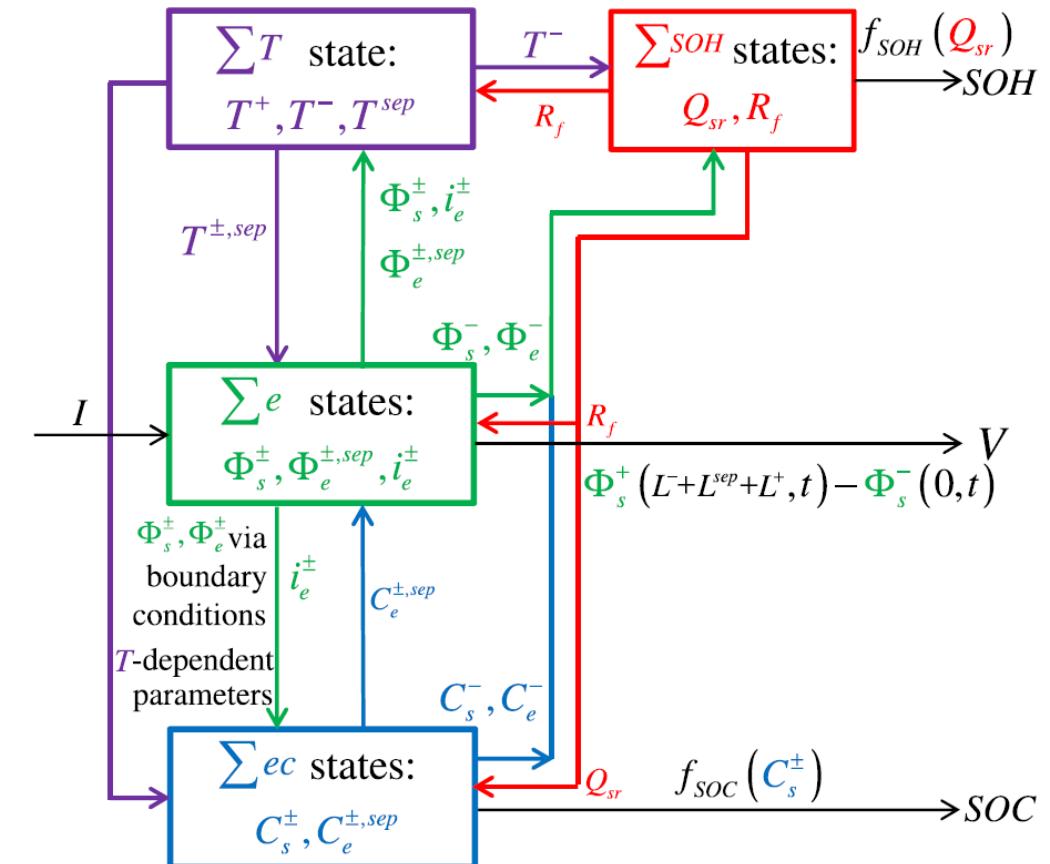


# Battery Model: Electrochemical Modelling

- 3D Model



Transformation to Hilbert to obtain infinite D and easier separate solution for short time and long time.



State estimation is needed for charging strategy evaluation, residual capacity, lifetime estimation, fast charging control...

# Battery Model: Electrochemical Modelling

## Latest Development:

- Extended Single Particle Model (ESPM)
- Multiple Particle Model (MP)
- Pade Approximation Method
- Orthogonal Decomposition

## Detailed model is needed for:

- Cycling
- Capacity Fade
- Hysteresis
- Memory Effect
- Recovery Effect
- Endothermic Effect

\* Stochastic Model can only tackle a specific characteristics

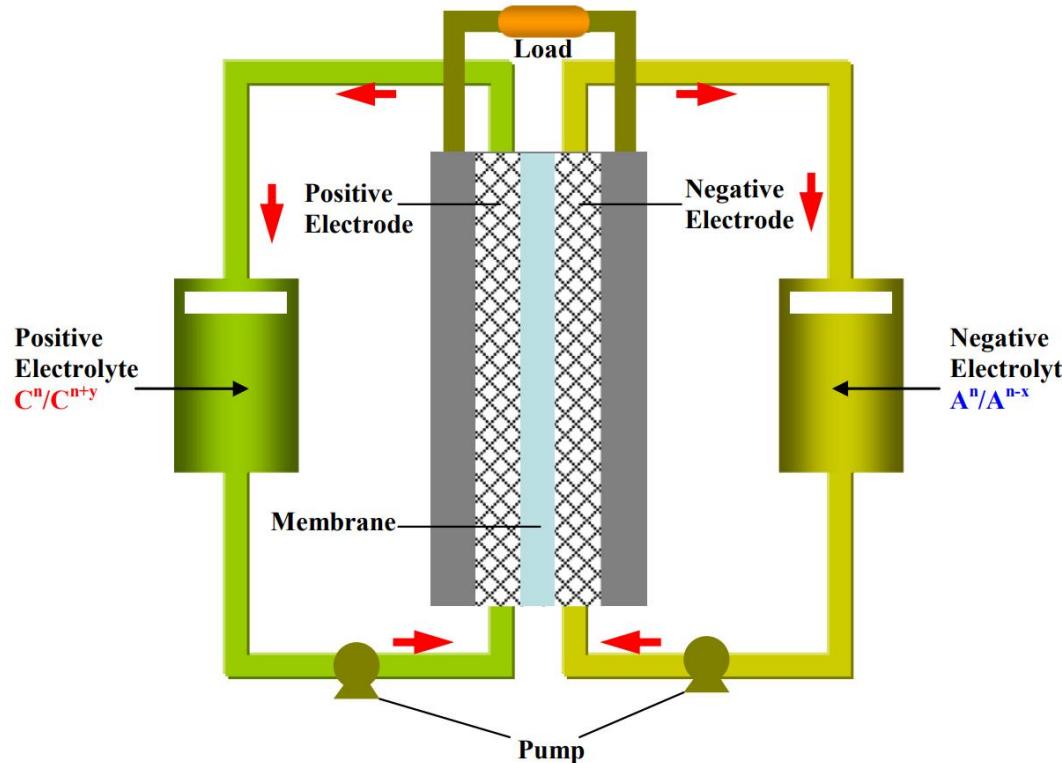
## Further studies:

1. Rank the **most influential parameters** in Li-ion cell
2. Higher-order polynomial / non-polynomial **profile**
3. **Coupled Electrochemical and Thermal** Equations for real-time
4. Develop simplified P2D model with **aging** phenomena
5. Real time model for internal properties Li-ion cell based on **inverse heat transfer methods**
6. Simplified model compatible with **LiFePO<sub>4</sub>** cathode materials (different batteries, different structures, different equations)
7. **Multiple Cells** with series and parallel connection studies
8. **Bifurcation studies** and **fractional calculus method** for memory effect with **simplification** in solving are needed
9. Real time transient model with fluctuating load is lacked

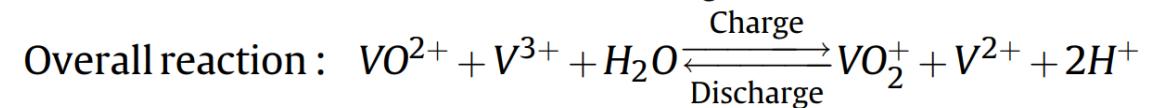
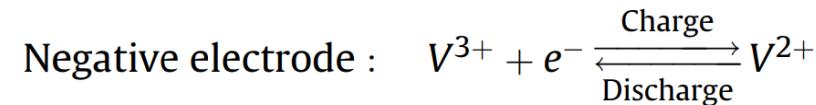
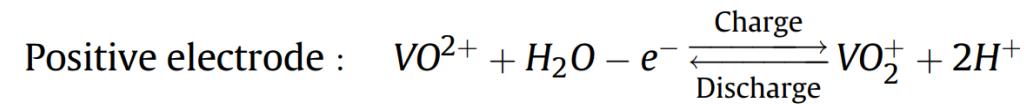
Mohammed YS et al. (2014), Hybrid renewable energy systems for off-grid electric power: Review of substantial issues  
 Suresh, R. et al. (2016), Modeling of Rechargeable Batteries  
 Jokar A. et al. (2016), Review of simplified P2D models of lithium ion batteries

# Battery Model: Electrochemical Modelling

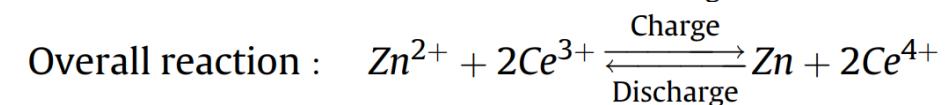
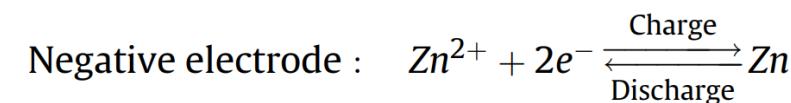
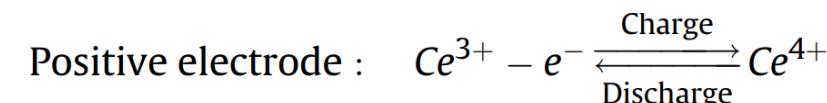
- Flow Battery



## Vanadium Redox Flow Battery (VRFB):



## Zinc/Cerium Redox Flow Cell (Zn/Ce FB)



# Battery Model: Electrochemical Modelling

$$\frac{\mu}{K} \vec{u} = -\nabla p \quad (\text{Darcy's Law})$$

$$\nabla \cdot \vec{u} = 0 \quad (\text{Mass Balance})$$

$$p_c = p_g - p_l = \sigma \cos \theta_c (\varepsilon/K)^{0.5} J(s) \quad (\text{Capillary Pressure})$$

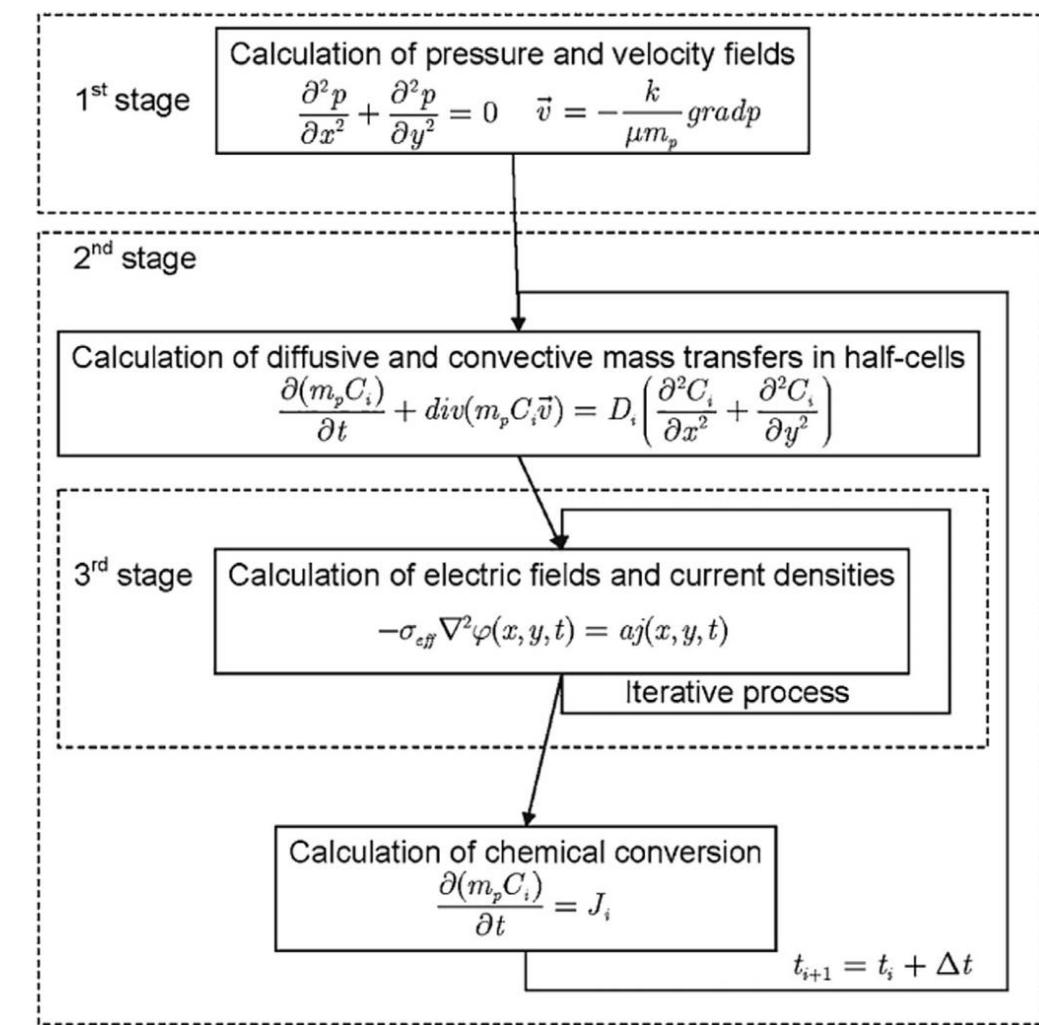
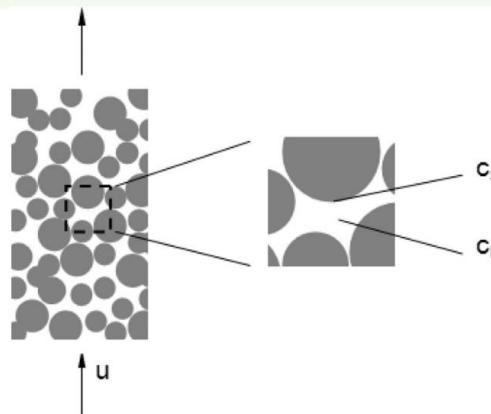
$$\vec{u}_{\text{slip}} = \frac{d_b^2}{18\mu_l} \nabla p \quad (\text{Slip Velocity})$$

$$(\text{Mass Transport}) \quad \frac{\partial c_i}{\partial t} = \nabla \cdot (D_i^{\text{eff}} \nabla c_i) + \frac{F Z_i}{R T} \nabla \cdot (D_i^{\text{eff}} c_i \nabla \phi_s) - \nabla \cdot (\vec{u} c_i) + S_i$$

$$(\text{Energy Transport}) \quad \frac{\partial}{\partial t} (\overline{\rho C_p} T) + \nabla \cdot (\vec{u} \overline{\rho C_p} T) = \bar{\lambda} \nabla^2 T + \sum_k Q_k$$

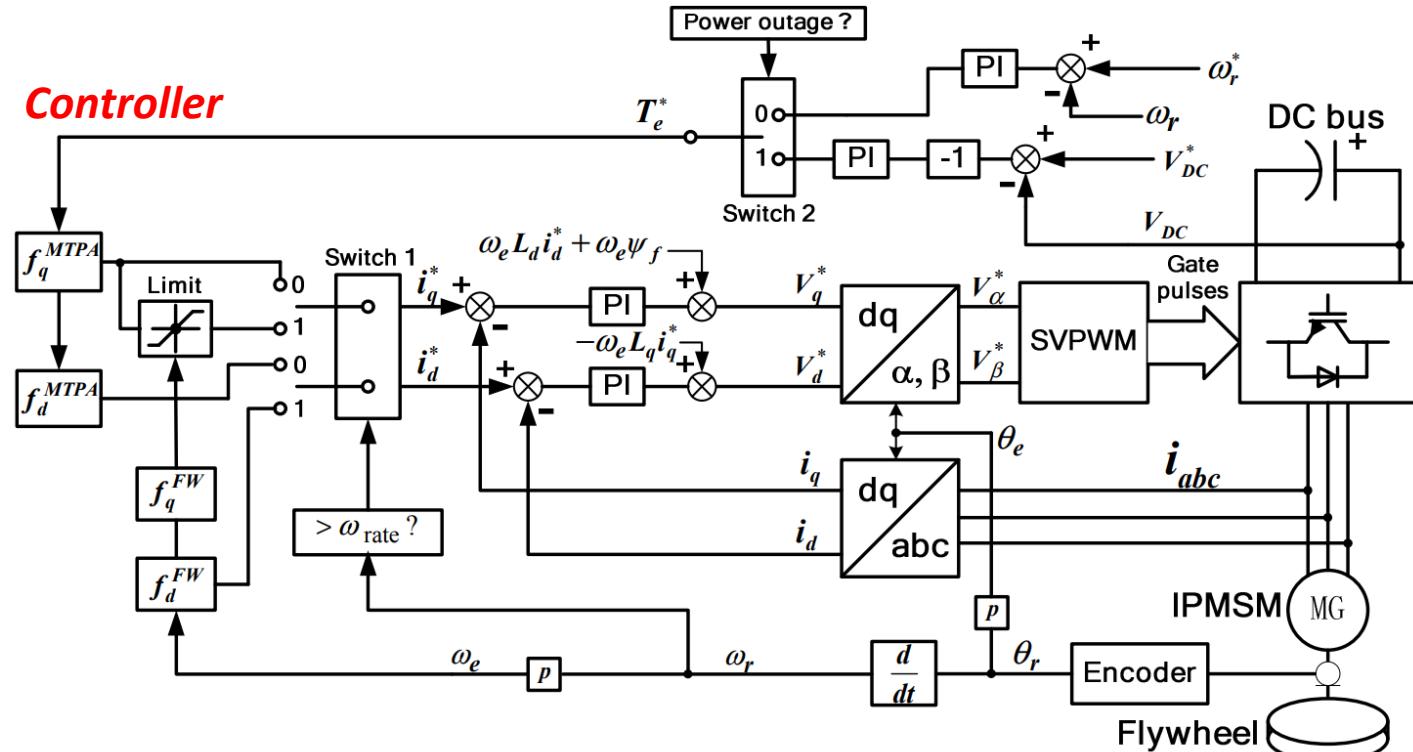
$$j_1 = \varepsilon A_v F k_1 \left( c_{V(III)}^s \right)^{\alpha_{-,1}} \left( c_{V(II)}^s \right)^{\alpha_{+,1}} \left\{ \exp \left( \frac{\alpha_{+,1} F \eta_1}{RT} \right) \right.$$

$$(\text{Butler-Volmer Eqt}) \quad \left. - \exp \left( - \frac{\alpha_{-,1} F \eta_1}{RT} \right) \right\}$$



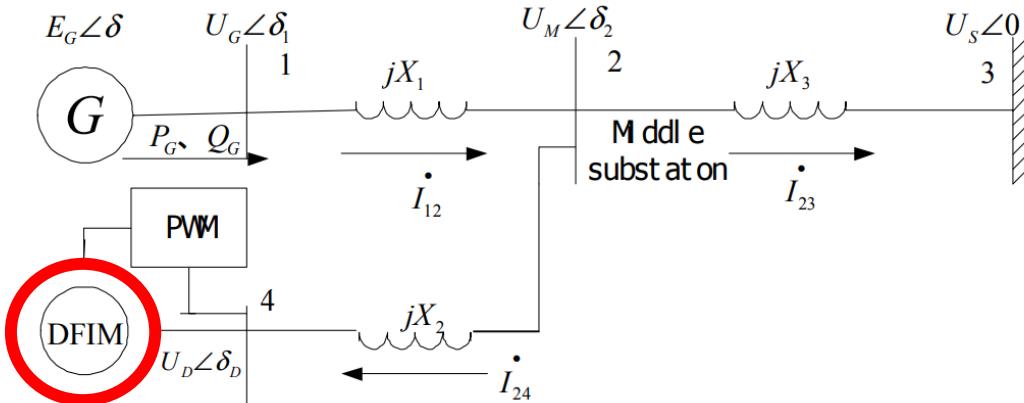
# Flywheel Model

**Controller**



$$E'_d = -\frac{x_m}{X_{rr}} \Psi_{qr} \quad X_{rr} = x_r + x_m; x_{ss} = x_s + x_m; X' = x_{ss} - \frac{x_m^2}{X_{rr}}$$

$$E'_q = \frac{x_m}{X_{rr}} \Psi_{dr} \quad T'_{d0} = \frac{X_{rr}}{\omega_0 r_r}; T_e = \Psi_{qr} I_{dr} - \Psi_{dr} I_{qr} = E'_d I_{ds} + E'_q I_{qs}$$



**Flywheel = Doubly-Fed Induction Motor**

$$U_{ds} = E'_d - X' I_{qs}$$

$$U_{qs} = E'_q + X' I_{ds}$$

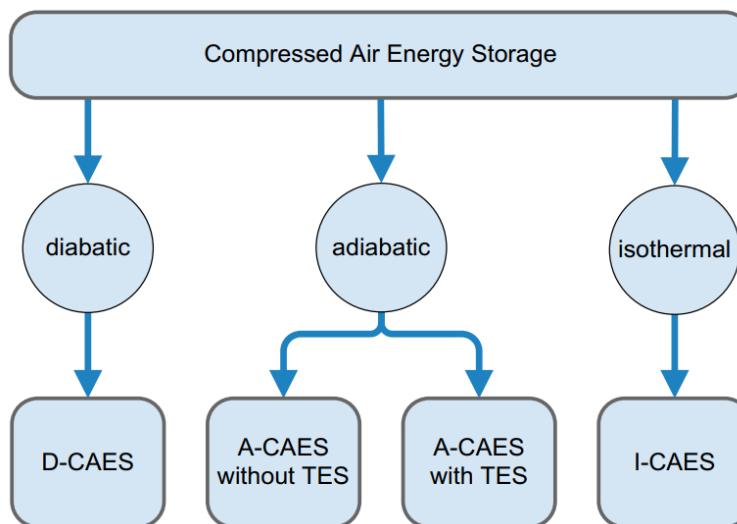
$$\frac{dE'_d}{dt} = -\frac{\omega_0 x_m}{X_{rr}} U_{qr} - \frac{1}{T'_{d0}} E'_d + s\omega_0 E'_q - \frac{x_{ss}-X'}{T'_{d0}} I_{qs}$$

$$\frac{dE'_q}{dt} = \frac{\omega_0 x_m}{X_{rr}} U_{dr} - \frac{1}{T'_{d0}} E'_q - s\omega_0 E'_d + \frac{x_{ss}-X'}{T'_{d0}} I_{ds}$$

$$\frac{ds}{dt} = \frac{1}{T_j} (-T_e) \quad s = \frac{\omega_0 - \omega_r}{\omega_0}$$

# Compressible Air Energy Storage Model

	Diabatic		Adiabatic		Isothermal	
Cycle efficiency (AC to AC)	Today 0.54	Goal 0.6	Today –	Goal 0.7	Today 0.38	Goal 0.8
Energy density (per m <sup>3</sup> of CAS)	2–15 kW h/m <sup>3</sup>		0.5–20 kW h/m <sup>3</sup>		1–25 kW h/m <sup>3</sup>	
Start-up time	10–15 min		5–15 min		<1 min	
Power range	5 MW–1 GW		1 MW–1 GW		5 kW–1 GW	
Development status	Application/Demonstration		Research/Demonstration		Research/Demonstration	



D-CAES: heat resulting from air compression is wasted to ambient, external heat source is needed to prevent condensation during expansion process

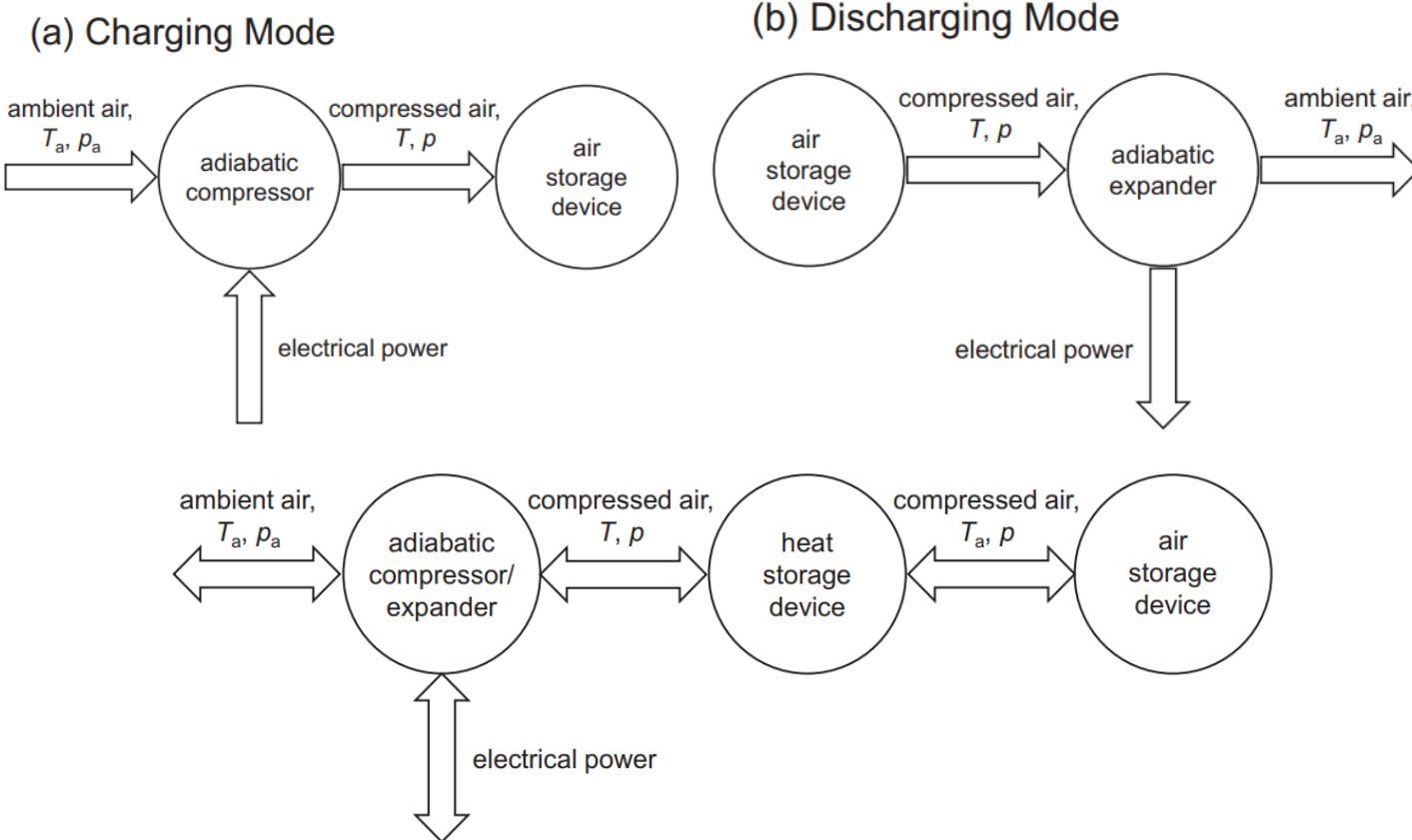
A-CAES: heat of compression is captured in additional TES devices and is utilized for expansion

I-CAES: heat of compression is minimized and prevented in I-CAES

**How heat is handled during compression and prior to expansion of the air?**

# Compressible Air Energy Storage Model

For A-CAES:



$$\text{First Law: } P_{el} = \dot{m}(h(T, p) - h(T_a, p_a))$$

Assuming adiabatic and relatively const.  $c_p$

$$h^0(T, p) - h^0(T_a, p_a) = c_p^0(T - T_a)$$

$$s^0(T, p) - s^0(T_a, p_a) = c_p^0 \ln\left(\frac{T}{T_a}\right) - R_L \ln\left(\frac{P}{P_a}\right)$$

Exergy:  $P_{el}$

$$= \dot{m} \left[ T_a c_p^0 \left( \frac{T}{T_a} - 1 - \ln\left(\frac{T}{T_a}\right) \right) + T_a R_L \ln\left(\frac{p}{p_a}\right) \right]$$

For adiabatic compressor:

$$\frac{T}{T_a} = \left( \frac{p}{p_a} \right)^{\frac{k-1}{k}}$$

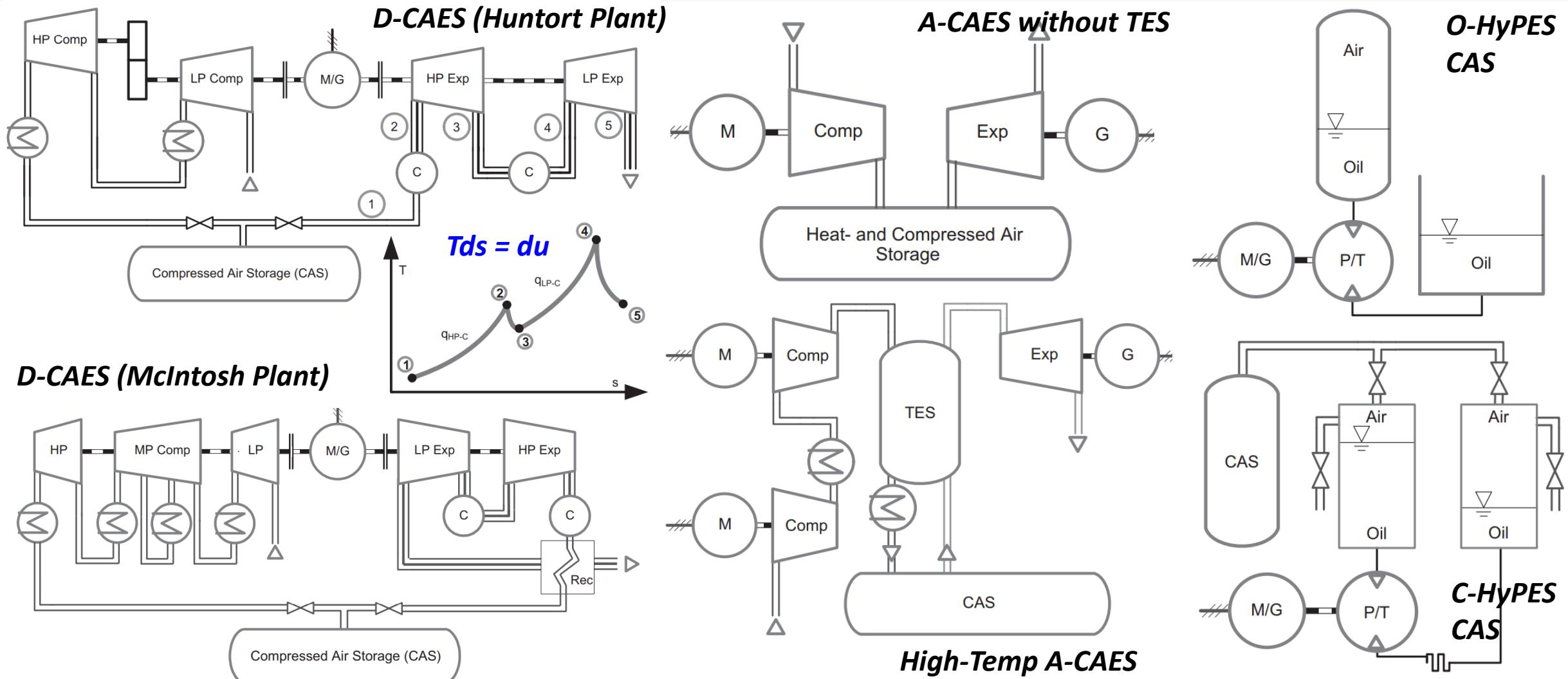
Heat flow  $Q_{storage}$  becomes power supplied to compressor.

$$Q_{storage} = P_{el} = \dot{m} c_p^0 (T - T_a)$$

Efficiency:

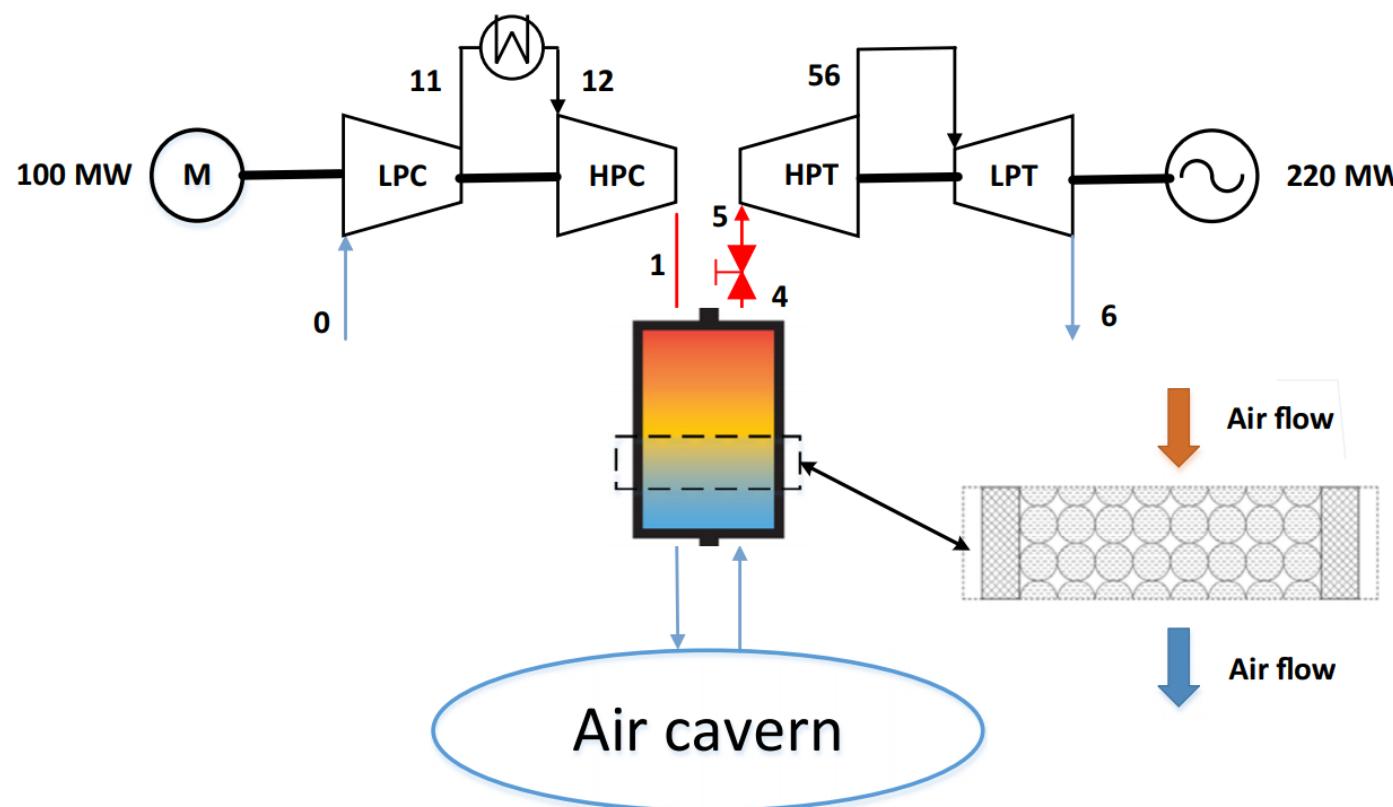
$$\eta_{cyc} = \frac{E_{out}}{E_{in}}$$

# Compressible Air Energy Storage Model



# Compressible Air Energy Storage Model

## Typical A-CAES Cycle and Typical Data



Quantity	Value
Ambient temperature	293.15 K
Ambient pressure	1.01325 bar
Expansion train rated power	220 MW
HP turbine design inlet temperature	905.15 K
HP turbine design inlet pressure	46 bar
HP turbine design expansion ratio	4.18
LP turbine design inlet temperature	655.15 K
LP turbine design inlet pressure	11 bar
LP turbine design expansion ratio	11
Turbines design efficiency	88%
Compression train rated power	100 MW
HP compressor design inlet temperature	480.15 K
HP compressor design compression ratio	8.4
LP compressor design compression ratio	8.4
Cavern volume	230,000 m <sup>3</sup>
Cavern min/max pressure	46/72 bar
Cavern wall heat transfer coefficient	$0.02356 + 0.0149 \dot{m}_{in} - \dot{m}_{out} ^{0.8}$

A-CAES performance for full load charging/discharging.

Quantity	Value
Number of cycles (-)	30
Round trip efficiency $\eta_{cycle}$ (-)	74%
Total output energy (MW h <sub>e</sub> )	22,100
Charge time (h)	9.1
Discharge time (h)	3.3
Thermal energy stored (MW h <sub>th</sub> )	940
Thermal energy storage efficiency $\eta_{th}$ (-)	93%

<sup>a</sup> Averaged value over 30 cycles.

# Compressible Air Energy Storage Model

Compressor:

$$T_{c,out}^{isen} = T_{c,in} \beta^{\frac{k-1}{k}}$$

$$\eta_c = \frac{T_{c,out}^{isen} - T_{c,in}}{T_{c,out} - T_{c,in}}$$

where  $\beta$  is compression ratio.

Power of Compressor:

$$W_c = \dot{m}_c (h_{c,out} - h_{c,in})$$

Heat Exchanger:

(Energy Balance and  $\varepsilon$ -NTU Method)

$$\varepsilon = \frac{1 - \exp(-NTU(1 - \chi))}{1 - \chi \exp(-NTU(1 - \chi))}$$

$$NTU = \frac{UA}{c_{min}} \text{ and } \chi = \frac{c_{min}}{c_{max}}$$

Charge process effectiveness:

$$\Phi = \varepsilon c_{min} (T_{in,h} - T_{in,c})$$

Turbine:

$$T_{t,out}^{isen} = T_{t,in} / (\pi_i)^{\frac{k-1}{k}}$$

$$\eta_t = \frac{T_{t,in} - T_{t,out}}{T_{t,out} - T_{t,in}^{isen}}$$

where  $\pi_i = p_{in}/p_{out}$

Power output:

$$W_t = \dot{m}_t (h_{t,out} - h_{t,in})$$

Flugel Formula: (off-design)

$$\frac{\dot{m}_t}{\dot{m}_{t0}} = \alpha \sqrt{\frac{T_{t0,in}}{T_{t,in}}} \sqrt{\frac{\pi_t^2 - 1}{\pi_{t0}^2 - 1}}$$

$$\frac{\eta_t}{\eta_{t0}} = (1 - t(1 - \dot{n}_t)^2) \left(\frac{\dot{n}_t}{\dot{G}_t}\right) \left(2 - \frac{\dot{n}_t}{\dot{G}_t}\right)$$

Compressed Air Reservoir:

$$\begin{aligned} \frac{dT_r}{dt} &= \frac{1}{m_r} \left[ \left(1 - \frac{1}{k}\right) (m_{in} T_{in} - m_o T_r) \right. \\ &\quad \left. + \frac{h_w A_w (T_w - T_r)}{c_{p,a}} \right] \end{aligned}$$

$$\frac{dm_r}{dt} = m_{in} - m_o$$

Thermal Energy Storage Packed Bed:

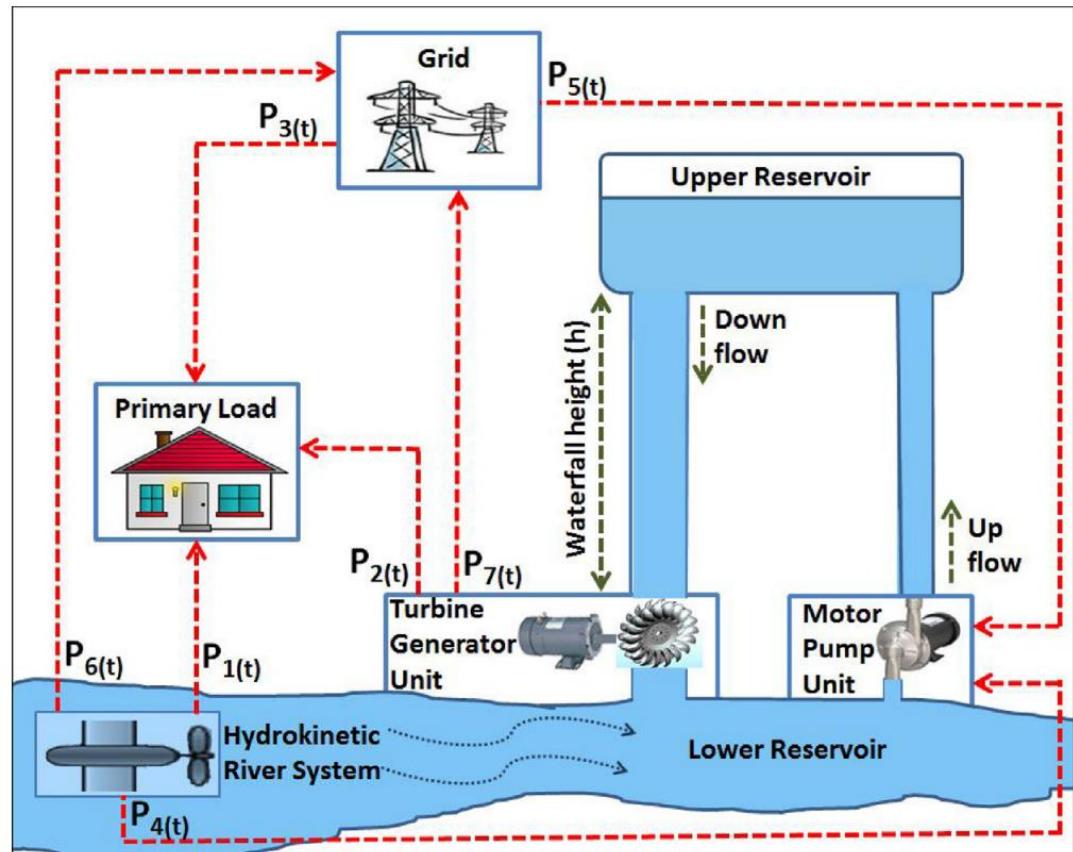
$$\begin{aligned} \varepsilon \rho_a c_{p,a} \frac{\partial T_a}{\partial t} + \varepsilon \rho_a c_{p,a} u_a \frac{\partial T_a}{\partial x} \\ = k_a \frac{\partial^2 T_a}{\partial x^2} - h_v (T_a - T_s) - U_w (T_a - T_0) \\ (1 - \varepsilon) \rho_s c_{p,s} \frac{\partial T_s}{\partial t} = k_s \frac{\partial^2 T_s}{\partial x^2} + h_v (T_s - T_a) \end{aligned}$$

# Compressible Air Energy Storage Model

## ***Concerns***

- CAES shows lower cycle efficiency than PHES or batteries
- No off-the-shelf machinery available that is suitable for efficient CAES plants, especially for high temperature adiabatic ones
- Low flexibility in short start-up times and fast ramping
- Site independence and low cost air reservoir are needed.
- Heat storage devices with high power and energy densities are needed for A-CAES
- (Turbo)machinery capable of being used as compressor or turbine to increase efficiency
- Tools for detailed simulations including humidity, part-load and dynamic operation of machinery needs to be developed.

# Pumped Hydro Storage Model



Energy Pumped up to certain height (H):

$$P_{M:P} = \frac{\rho_W \times g \times H \times Q_{M:P}}{\eta_{M:P}}$$

Power Generated in Turbine Generator:

$$P_{T:G} = \rho_W \times g \times H \times Q_{T:G} \times \eta_{T:G}$$

Cost Function:

$$F = \sum_{j=1}^N C_j \cdot (P_{3(j)} + P_{5(j)}) \cdot \Delta t - C_j \cdot R_a \sum_{j=1}^N (P_{6(j)} + P_{7(j)}) \cdot \Delta t$$

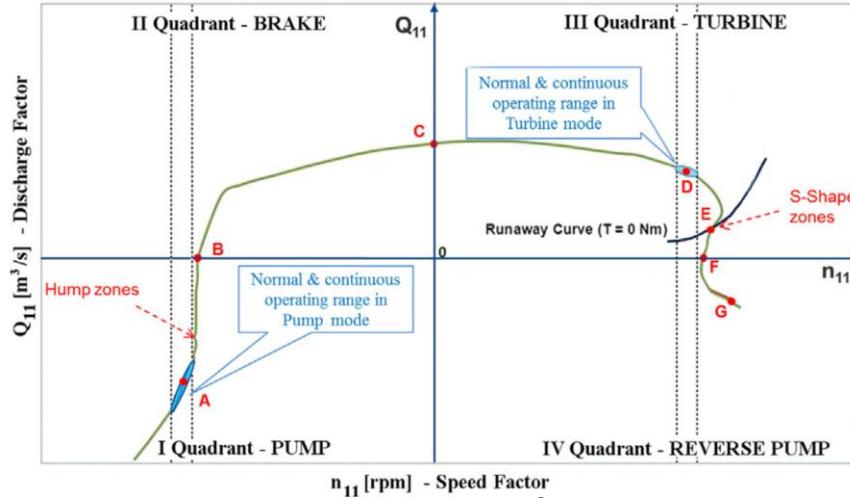
Power Constraint:  $P_{Load(j)} = P_{1(j)} + P_{2(j)} + P_{3(j)} \quad (1 \leq j \leq N)$

Storage Constraint:  $Cap^{\min} \leq Cap_{(j)} \leq Cap^{\max}$

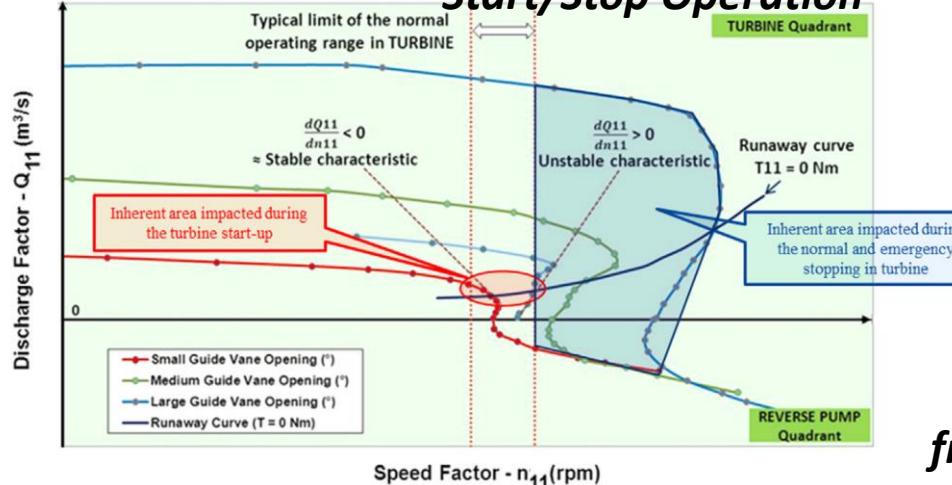
Final State Constraint:  $\sum_{j=1}^N (P_{4(j)} + P_{5(j)}) - \sum_{j=1}^N (P_{2(j)} + P_{7(j)}) = 0$

# Pumped Hydro Storage Model

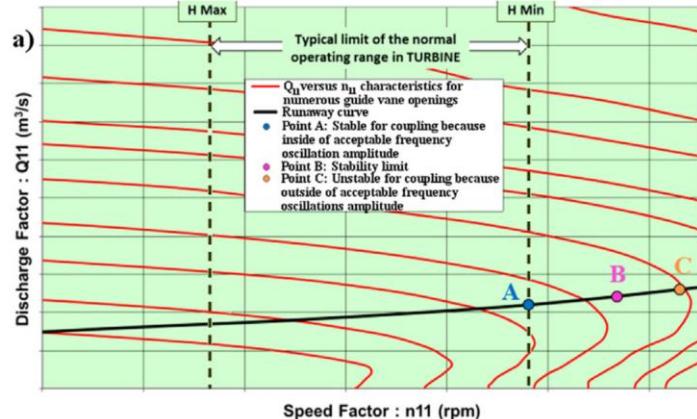
## Four Quadrants of Operation



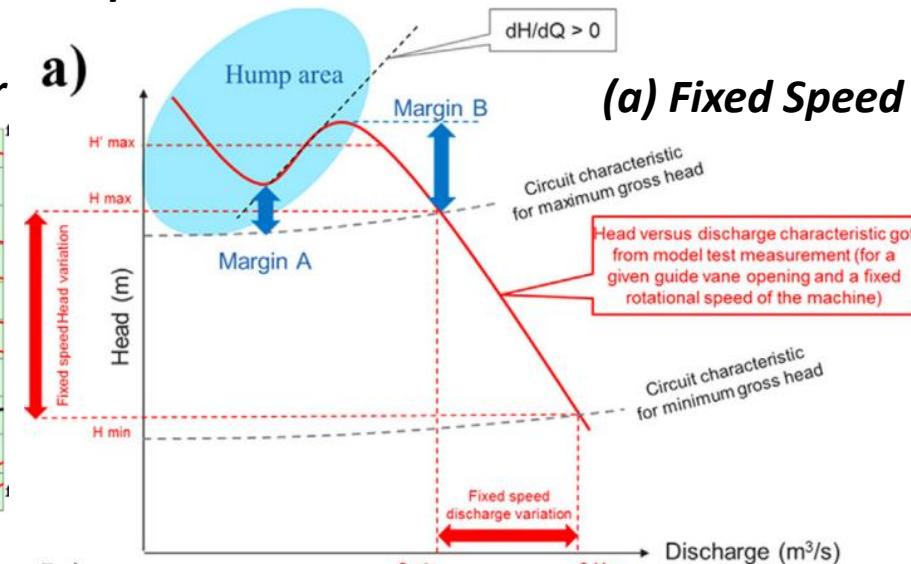
## Start/Stop Operation



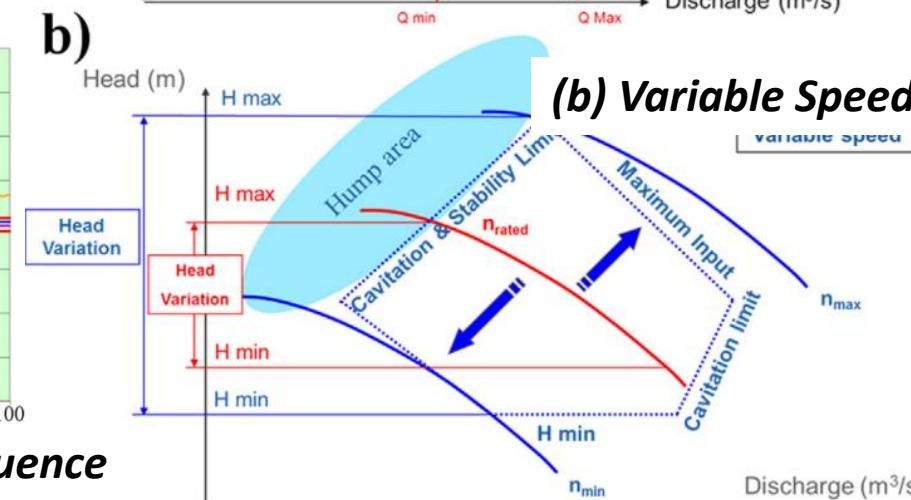
## Discharge factor Vs speed factor



## Operation Domain



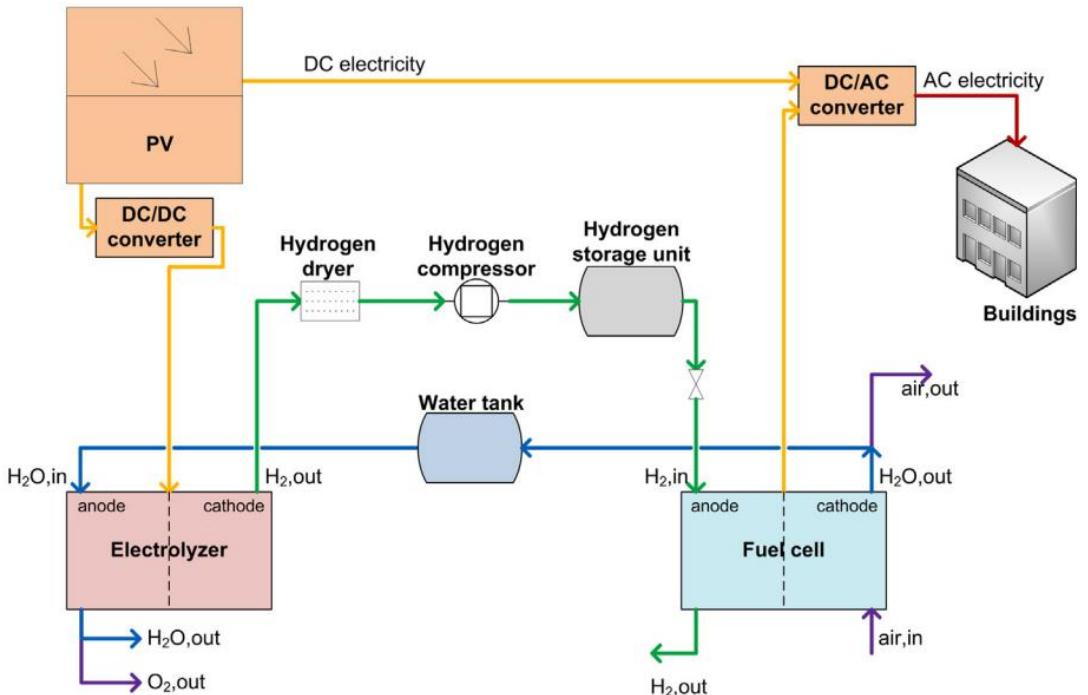
## (a) Fixed Speed



## (b) Variable Speed

## frequency Vs time at start-up sequence

# Hydrogen Storage Model



Suggested book: Nand, K. & Jesus F.A. (2017)

Modeling and Dynamic Behaviour of Hydropower Plants  
Electrolyzer – hydrogen storage – fuel cell subsystem

Anode, Cathode and Ohmic Overpotential:

$$\eta_a = \left( \frac{R \cdot T_{fc}}{\alpha \cdot F} \right) \cdot \operatorname{arcsinh} \left( \frac{i}{2 \cdot k_{eh} \cdot \theta_{H_2}} \right)$$

$$\eta_c = \left( \frac{R \cdot T_{fc}}{\alpha \cdot F} \right) \cdot \ln \left( \frac{i}{i_{oc}} \right)$$

$$\eta_{ohmic} = i \cdot R_{ohmic}$$

Electrolyzer voltage:

$$V_{cell,ec} = V_0 + (\eta_a + \eta_c + \eta_{ohmic})$$

Surface Coverage Differential for oxidation part:

$$\frac{d\theta_{H_2}}{dt} = \frac{k_{fh} \cdot y_{H_2} \cdot p_{ec} \cdot (1 - \theta_{H_2} - \theta_{CO} - \theta_{O_2})^2 - b_{fh} \cdot k_{fh} \cdot \theta_{H_2}^2 - i - k_{oh} \cdot \theta_{H_2}^2 \cdot \theta_{O_2}}{\rho} = 0$$

Hydrogen (initial) mass flow rate:

$$\dot{m}_{H_2,s} = \dot{m}_{H_2,s0} + \dot{m}_{H_2,ecs} - \dot{m}_{H_2,fcs}$$

Fuel Cell Efficiency:

$$\eta_{fc} = \frac{\dot{P}_{fc}}{\dot{m}_{H_2,cons} \cdot HHV_{H_2}}$$

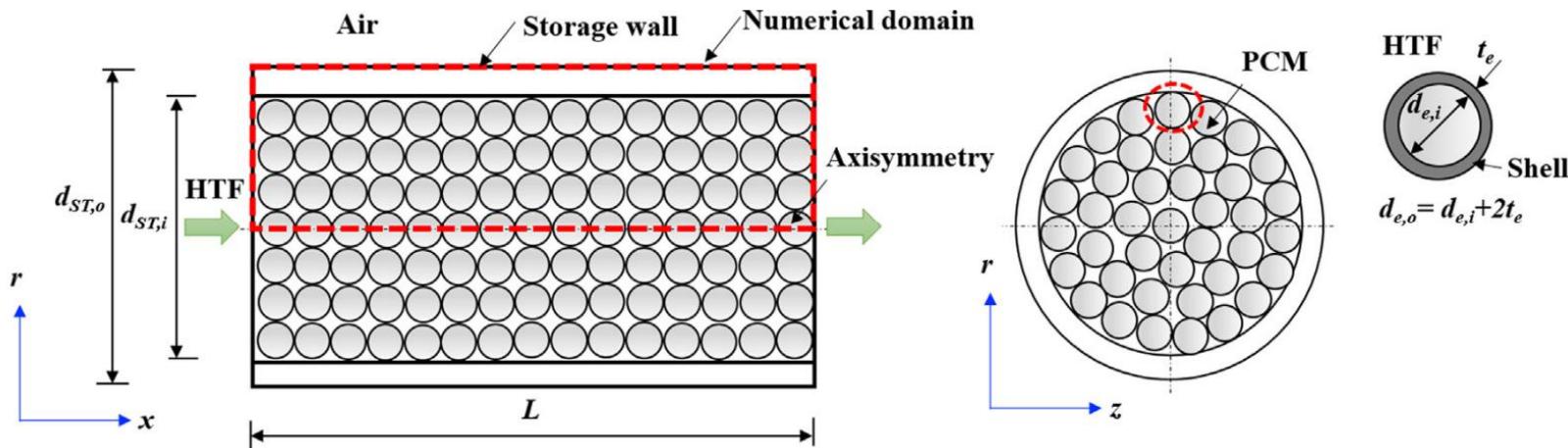
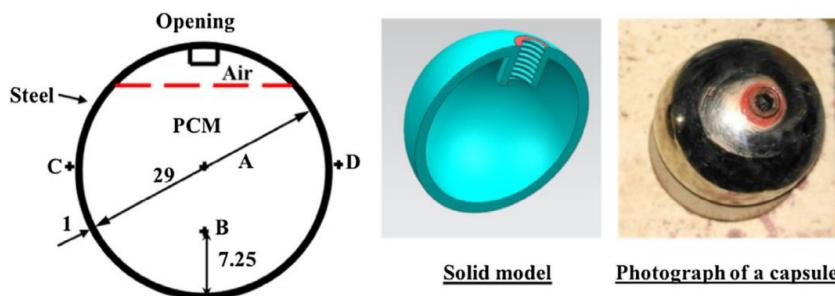
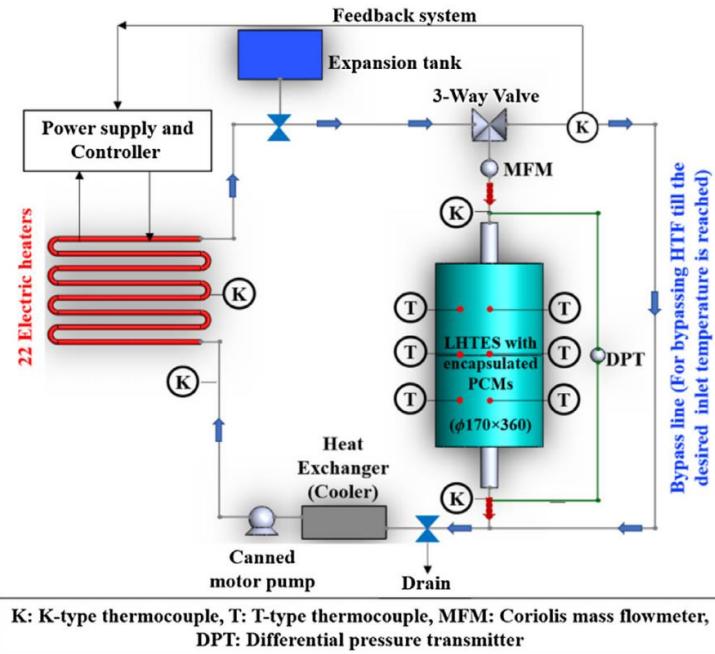
Electrolyzer Efficiency:

$$\eta_{ec} = \frac{\dot{m}_{H_2,gen} \cdot HHV_{H_2}}{\dot{P}_{ec}}$$

HHV:  
Higher  
heating value

# Thermal Storage Modelling

**For a PCM Thermal Storage:**



Heat Transfer Fluid:

$$\varphi \rho_F c_{p,F} \frac{\partial T_F}{\partial t} + \frac{\partial (\rho_F c_{p,F} T_F u)}{\partial x} = \frac{\partial^2 (\varphi k_F T_F)}{\partial x^2} + h_{conv,F} \mathcal{A}_e (T_S - T_F) + h_{conv,F-ST} \mathcal{A}_{ST,i} (T_{ST} - T_F)$$

Phase Change Material:

$$(1-\varphi) \rho_S c_{p,S} \frac{\partial T_S}{\partial t} = \frac{\partial^2 [(1-\varphi) k_S T_S]}{\partial x^2} + h_{conv,F} \mathcal{A}_e (T_F - T_S) + S_2$$

(Latent Heat Content):  $S_2 = -(1-\varphi) \rho_S \frac{d \Delta E}{dt}$

# Thermal Storage Modelling

Latent Heat change:

$$[\Delta E_P]_{n+1} = [\Delta E_P]_n + \lambda c_{p,S} \frac{a_p}{a_p^0} ([T_{PCM}]_n - T_m)$$

$$[\Delta E_P]_n = 0 \quad \text{If } [\Delta E_P]_{n+1} < 0$$

$$[\Delta E_P]_n = L_{lat} \quad \text{If } [\Delta E_P]_{n+1} > L_{lat}$$

Energy Storage for wall:

$$\rho_{ST} c_{p,ST} \nabla \frac{\partial T_{ST}}{\partial t} = h_{conv,F-ST} \mathcal{A}_{ST,i} (T_F - T_{ST}) - h_{conv,amb} \mathcal{A}_{ST,o} (T_{ST} - T_{amb})$$

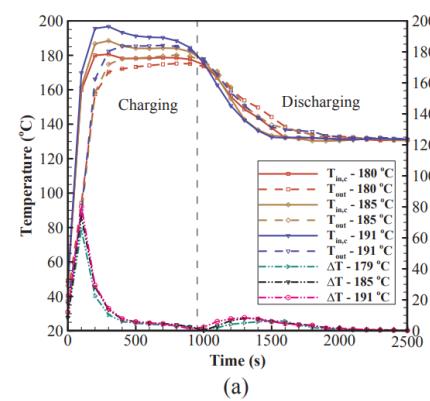
$$\text{Storage wall volume: } \forall = \left\lceil \frac{V_{ST,o} - V_{ST,i}}{V_{ST,i}} = \left( \frac{d_{ST,o}}{d_{ST,i}} \right)^2 - 1 \right\rceil$$

$$\text{Packed void fraction: } \varphi = 0.4272 - 4.516 \times 10^{-3} \left( \frac{d_{ST,i}}{d_{e,o}} \right) + 7.881 \times 10^{-5} \left( \frac{d_{ST,i}}{d_{e,o}} \right)^2$$

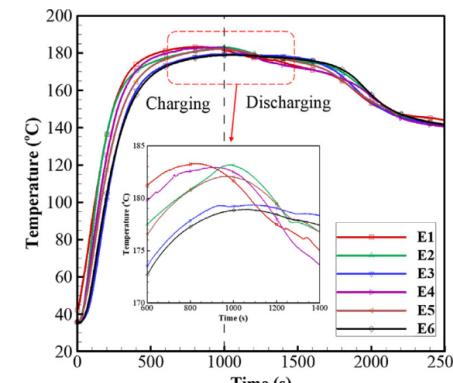
$$\text{Convection coeff: } h_{conv,Fo} = \frac{6(1-\varphi)(2.2Re^{0.6} Pr^{1/3})k_F}{d_{e,o}^2}$$

$$\text{Pressure Change: } \frac{\Delta P}{L} = 0.061 \left( \frac{1-\varphi}{\varphi^3} \right) \left( \frac{d_{ST,i}}{d_{e,o}} \right)^{0.2} (1000Re^{-1} + 60Re^{-0.5} + 12) \left( \frac{\rho_F}{d_{e,o}} \right) U^2$$

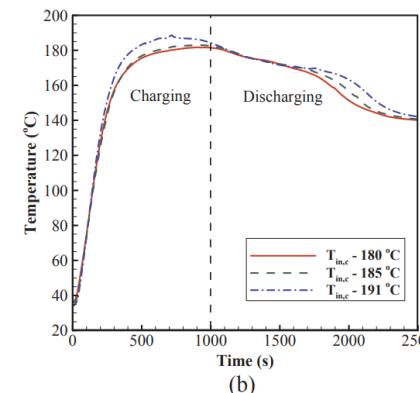
## Temperature Profile



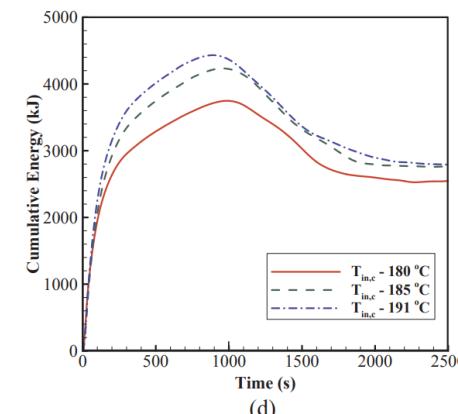
(a)



(c)

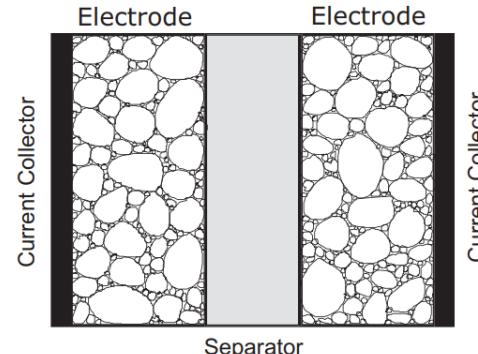


(b)



(d)

# Supercapacitor Modelling – Physical Model



- Charge conservation across the double layer

$$aC \frac{\partial(\phi_1 - \phi_2)}{\partial t} = \sigma \frac{\partial^2 \phi_1}{\partial \chi^2}$$

- Electrolyte diffusion

$$\epsilon \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial \chi^2} - \frac{aC}{F} \left( t_- \frac{dq_+}{dq} + t_+ \frac{dq_-}{dq} \right) \frac{\partial(\phi_1 - \phi_2)}{\partial t},$$

- Ohm's law

$$\begin{aligned} & \kappa \left( \frac{RT(t_+ - t_-)}{F} \right) \frac{\partial}{\partial \chi} \ln(c) + \sigma \frac{\partial(\phi_1 - \phi_2)}{\partial \chi} \\ & + \left( \kappa \frac{\partial}{\partial \chi} + \sigma \frac{\partial}{\partial \chi} \right) \phi_2 + i = 0 \end{aligned}$$

State-Space Form:

$$\begin{bmatrix} \epsilon & \frac{aC}{F} (t_- \frac{dq_+}{dq} + t_+ \frac{dq_-}{dq}) & 0 \\ 0 & aC & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{c} \\ \dot{\phi}_1 - \phi_2 \\ \dot{\phi}_2 \end{bmatrix} = \begin{bmatrix} D \frac{\partial^2}{\partial \chi^2} & 0 & 0 \\ 0 & \sigma \frac{\partial^2}{\partial \chi^2} & \sigma \frac{\partial^2}{\partial \chi^2} \\ 0 & \sigma \frac{\partial}{\partial \chi} & \kappa \frac{\partial}{\partial \chi} + \sigma \frac{\partial}{\partial \chi} \end{bmatrix} \begin{bmatrix} c \\ \phi_1 - \phi_2 \\ \phi_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{\kappa RT(t_+ - t_-)}{F} \frac{\partial}{\partial \chi} \\ 0 \end{bmatrix} \ln(c) + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} i$$

$$\begin{bmatrix} \epsilon & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{c} \\ \dot{\phi}_2 \end{bmatrix} = \begin{bmatrix} D \frac{\partial^2}{\partial \chi^2} & 0 \\ 0 & \kappa \frac{\partial}{\partial \chi} \end{bmatrix} \begin{bmatrix} c \\ \phi_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \kappa \left( \frac{t_+ - t_-}{f} \right) \frac{\partial}{\partial \chi} \end{bmatrix} \ln(c) + \begin{bmatrix} 0 \\ 1 \end{bmatrix} i. \quad y = V = \phi_1|_{x=0} - \phi_1|_{x=L}.$$

Convert DAE into ODE for  $\phi_2$ :

$$\begin{aligned} & \sigma \hat{\mathbf{D}}_{\phi_1} (\phi_1 - \phi_2) + (\kappa \hat{\mathbf{D}}_{\phi_2} + \sigma \hat{\mathbf{D}}_{\phi_1}) \phi_2 \\ & \kappa \left( \frac{t_+ - t_-}{f} \right) \hat{\mathbf{D}}_{\ln c} \ln(c) + i = 0 \end{aligned} \longrightarrow \begin{aligned} \Phi_2 &= -(\kappa \hat{\mathbf{D}}_{\phi_2} + \sigma \hat{\mathbf{D}}_{\phi_1})^{-1} [\sigma \hat{\mathbf{D}}_{\phi_1} (\phi_1 - \phi_2) \\ & \kappa \left( \frac{t_+ - t_-}{f} \right) \hat{\mathbf{D}}_{\ln c} \ln(c) + i]. \end{aligned}$$

State-Space Representation:

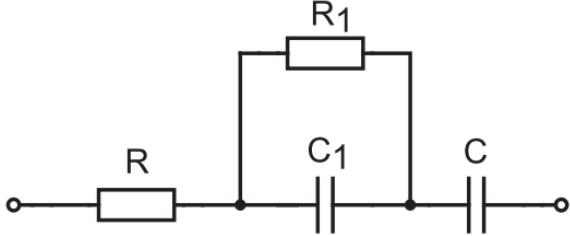
$$M \dot{x} = Ax + \tilde{B}_1 \ln(c) + \tilde{B}_2 i$$

$$y = Cx + \tilde{D}_1 \ln(c) + \tilde{D}_2 i$$

$$x := [c^T, \Phi_1^T - \Phi_2^T]^T$$

# Supercapacitor Modelling – Equivalent Circuit

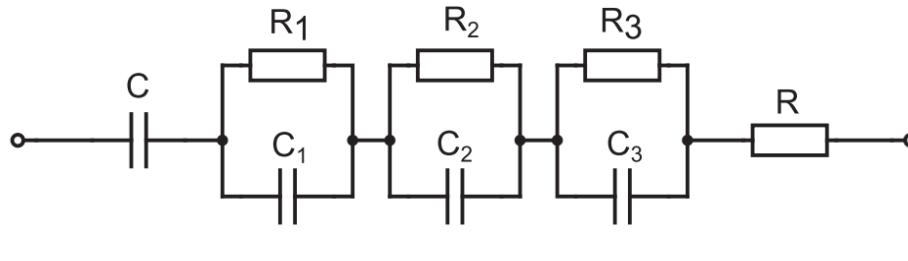
Classic Topology



$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & -\frac{1}{R_1 C_1} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{C} \\ \frac{1}{C_1} \end{bmatrix} i$$

$$V = x_1 + x_2 + Ri.$$

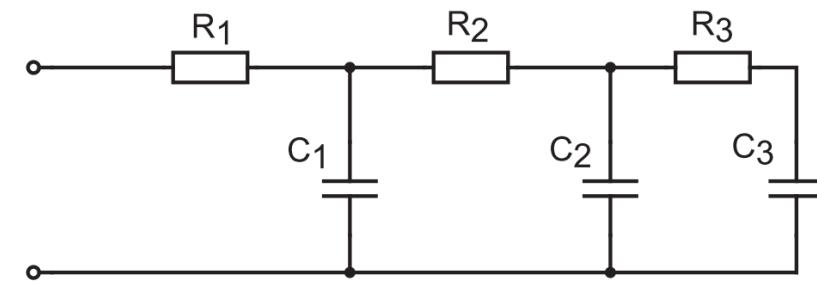
Dynamic Topology



$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{R_1 C_1} & 0 & 0 \\ 0 & 0 & -\frac{1}{R_2 C_2} & 0 \\ 0 & 0 & 0 & -\frac{1}{R_3 C_3} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} + \begin{bmatrix} \frac{1}{C} \\ \frac{1}{C_1} \\ \frac{1}{C_2} \\ \frac{1}{C_3} \end{bmatrix} i$$

$$V = x_1 + x_2 + x_3 + x_4 + R_s i.$$

Ladder Topology

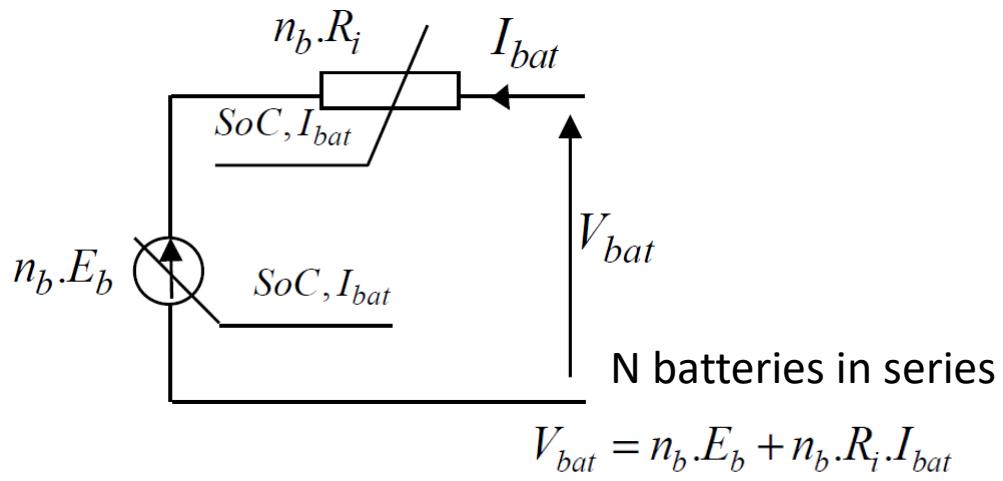
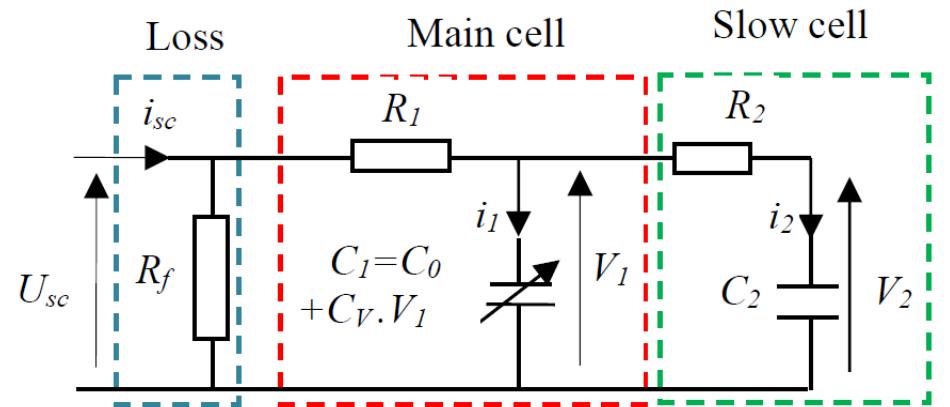


$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -\frac{1}{R_2 C_1} & \frac{1}{R_2 C_1} & 0 \\ \frac{1}{R_2 C_2} & -\frac{1}{R_3 R_2 C_2} & \frac{1}{R_3 C_2} \\ 0 & \frac{1}{R_3 C_3} & -\frac{1}{R_3 C_3} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} \frac{1}{C_1} \\ 0 \\ 0 \end{bmatrix} i$$

$$V = x_1 + R_1 i.$$

# Supercapacitor Modelling – Equivalent Circuit

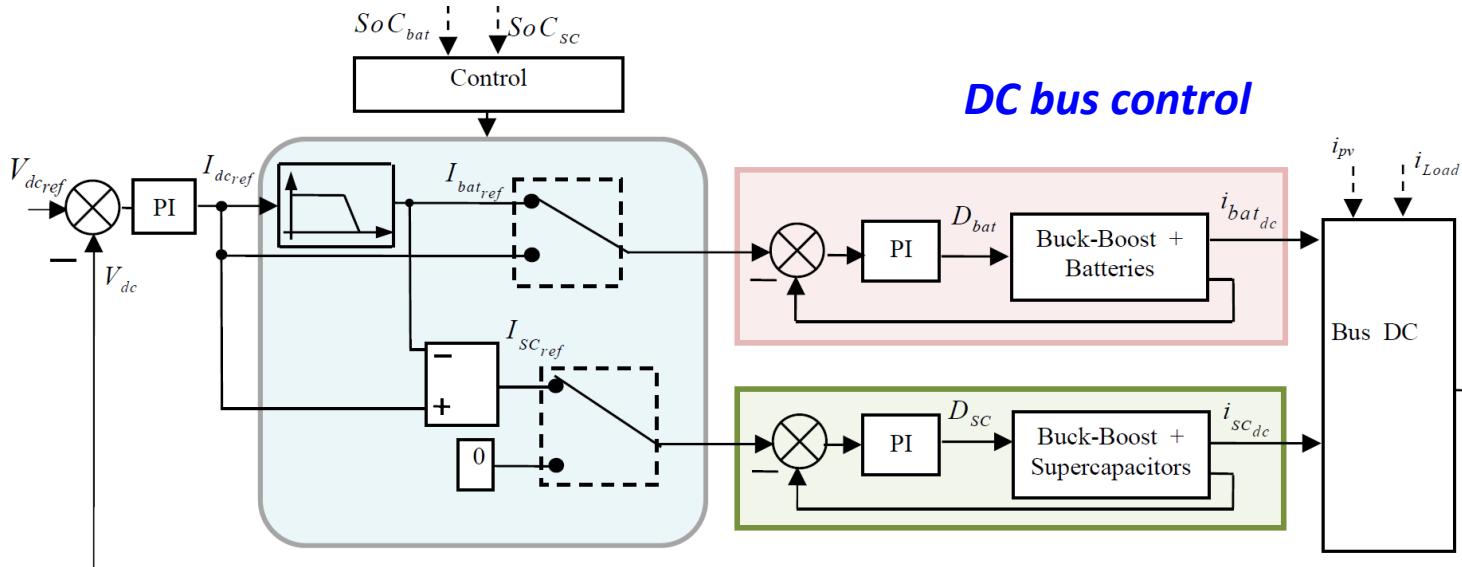
## Zubieta and Bonert model



$$U_{SC} = N_{SSc} v_{sc} = N_{SSc} \left( v_1 + R_1 \frac{I_{SC}}{N_{Psc}} \right)$$

$$v_2 = \frac{1}{C_2} \int i_2 d t = \frac{1}{C_2} \int \frac{1}{R_2} (v_1 - v_2) d t.$$

$$i_1 = C_1 \frac{dv_1}{dt} = \frac{dQ_1}{dt} = (C_0 + C_v y_1) \frac{dv_1}{dt}$$



# Energy Storage – Testing and Commissioning

No.	Test items	Type tests	Production tests	Commissioning tests	Periodic tests
1	Temperature stability	✓			
2	State of charge (SOC)	✓			✓
3	Conversion efficiency	✓			
4	Response time	✓			✓
5	Ramp-rate	✓			✓
6	Synchronization	✓	✓	✓	
7	Reconnection after abnormal condition	✓	✓		
8	Harmonics	✓			✓
9	Flicker	✓			
10	Voltage unbalance	✓			
11	Open phase	✓			
12	Overcurrent	✓	✓		
13	DC injection	✓			
14	Response to abnormal voltage condition	✓	✓		✓
15	Response to abnormal frequency condition	✓	✓		✓
16	Unintentional islanding	✓	✓	✓	
17	Low-voltage ride through (LVRT)	✓	✓		
18	Interconnection integrity	✓			
19	Continuous operation	✓	✓		
20	Stop charging/discharging	✓		✓	

Note:

This standard allows **simulated Electrical Power System (EPS)** with Energy Storage Systems (ESS)

However, the following should be satisfied.

Requirement	Allowance
THD	50% as in EPS
Steady State	1% $U_n$ fluctuation
Voltage Deviation	$\pm 3\%$ of $U_n$
Frequency Deviation	$\pm 0.01\text{Hz}$
Unbalance of 3 phases	$\pm 3\%$ of $U_n$ $\pm 3^\circ$ of phase angle

# SimulationX – Consideration in designing ES

## System Level:

- How much **energy** must the energy storage be able to store and release **over a certain period of time**?
- How much **storage** may be needed **in average** and how much for peak loads?
- How **long** must energy be stored in the storage?
- Which storage solution (electro-chemical, mechanical, thermal etc.) keeps **losses** between the generating and the consuming devices at a minimum?
- **What losses** are to be expected during transmission and conversion?

## Reliability:

- How does a **failing component** impact the entire system?
- How can I **prevent a component or system breakdown**?
- How does an alternative system layout impact the system's **reliability and safety**?

## CAES

- Determine and optimize **energy efficiency**
- Specify system components to meet the given requirements
- Develop and test the **optimum control strategy** for your compressed air energy storage
- Master **thermal effects** and increase the efficiency by making use of occurring heat

## Flywheel

- Simulate the **interactions** between all assemblies including flywheel mass, **magnetic bearing**, generator, vacuum pump and **cooling system**
- Dimension your components precisely already during the conceptual phase through conceptual simulations
- Identify **undesired vibrations** and examine **eigenfrequencies** with torsional vibration analyses

# SimulationX – Consideration in designing ES

Batteries:

- Master the **thermal behavior** of batteries through simulation with respect to material and the **geometrical, mechanical and electrical** properties of the cells and their interactions with each other
- Develop **optimized battery management systems** (BMS) in regard to the battery's **state of charge** (SOC) and **state of health** (SOH)
- Ensure a **sustained usage** of the battery system
- Make **reliable predictions** about a battery's **range** and **aging effects**
- Make profound estimations about a battery's lifespan by simulating calendric and **cyclical aging**
- Channel **waste heat** of batteries effectively by dimensioning the cooling system optimally through simulation

Power to Gas/ Gas to Power:

- Analyze the behavior of valves for inlet and outlet under **high pressure**
- Simulate the **fluid's properties** for variable boundary conditions. Which fluid phase occurs when and where?
- Design a **cooling system** fast and reliably
- Prove the safety of the pressure system **with automated fault tree analyses** (FTA) and **failure mode and effect analyses** (FMEA)

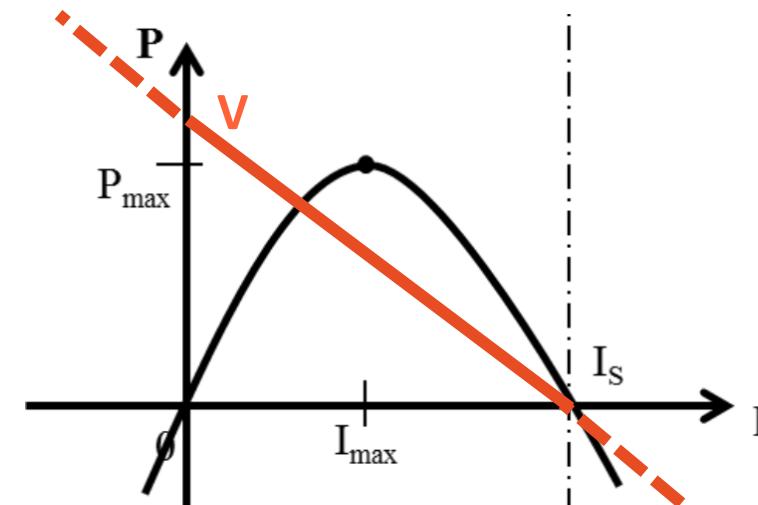
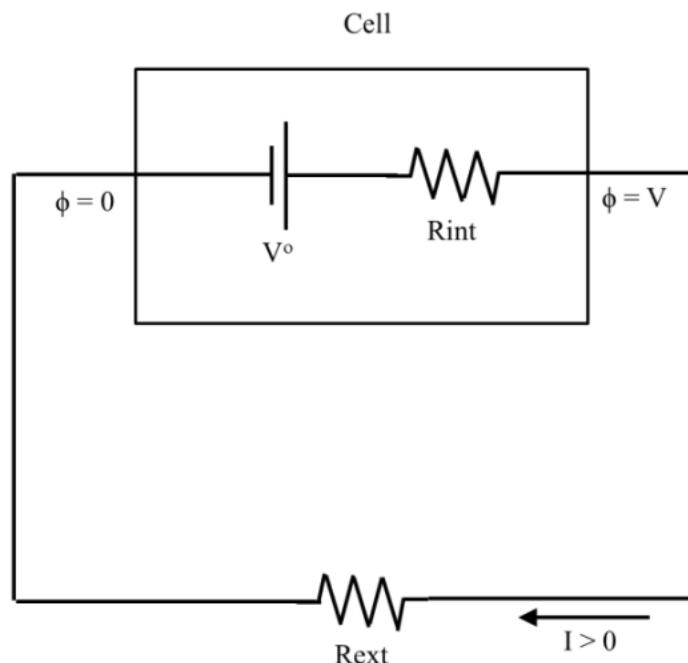
Thermal Storage:

- Design heat and cold storage systems through detailed simulation:
- Investigate **temperature distribution and heat transfer**
- Analyze the behavior of fluids for **phase changes** (e.g. in latent heat storage systems)
- Specify **compressors**, condensers, pipes, heat exchangers etc. for efficient functionality throughout the entire system
- Select the appropriate cold or heat storage on the basis of the simulation results for the whole system including **heat sources, heat sinks, storages and pipes**

# Appendix: Basic Physics of Cells

- Cell Voltage  $V(I, Q, \dots) = \Delta G/ne$   
 $= [\text{Free energy difference of net reaction}] / [\text{charge transferred}]$

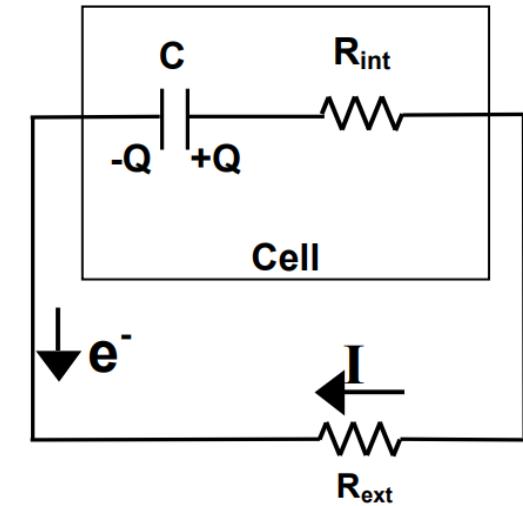
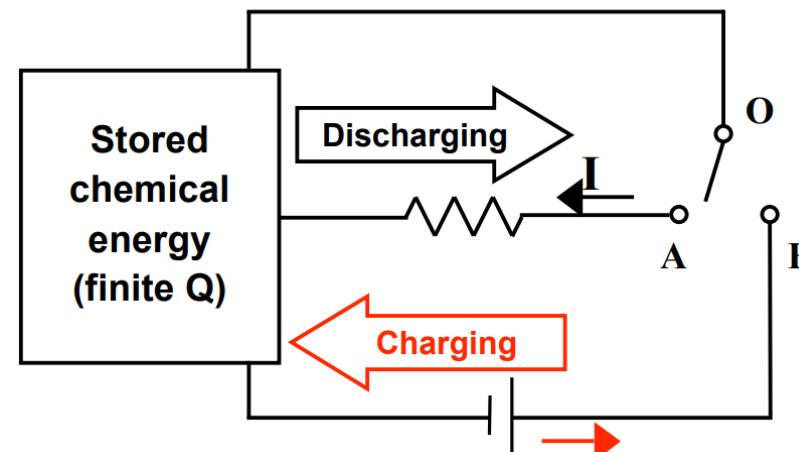
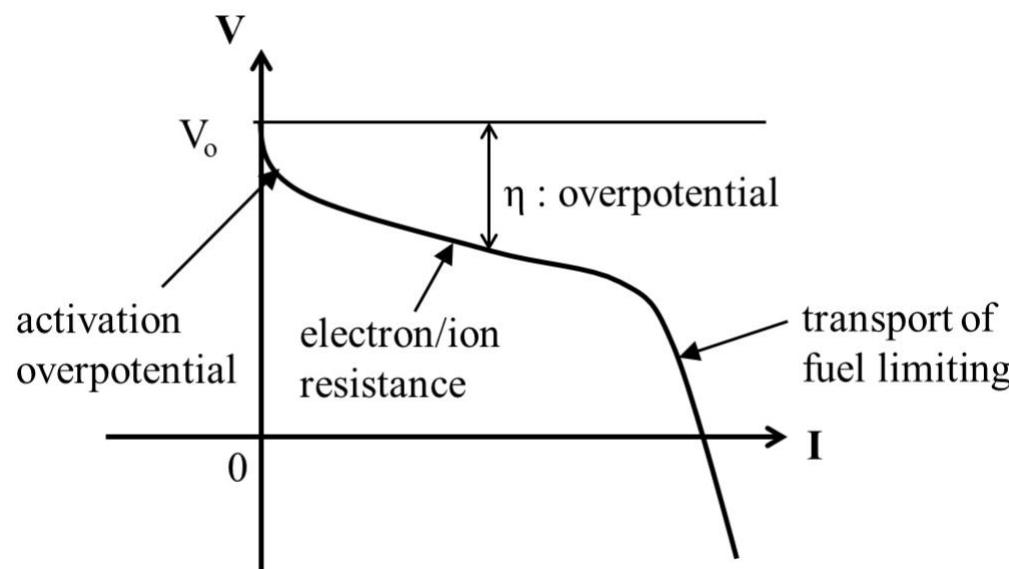
- Consider the equivalent circuit.



Electrolytic Regime	Galvanic Regime	Super Galvanic Regime
$P < 0$ $I < 0$ $V > V_o$	$P > 0$ $I > 0$ $0 < V < V_o$	$P < 0$ $I > I_S$ $V < 0$
Electrical Energy → Chemical Energy Storage e.g. charging a Li-ion battery by applying a reverse voltage	Chemical Energy → Electrical Energy + Heat Loss e.g. discharging a battery through an external load	Chemical + Electrical Energy → Heat Loss e.g. forcing the battery to discharge faster than $I_S$ by applying a voltage externally

# Appendix: Basic Physics of Cells

Resistance are normally current dependent and there are limiting factors in charge / ion transport.



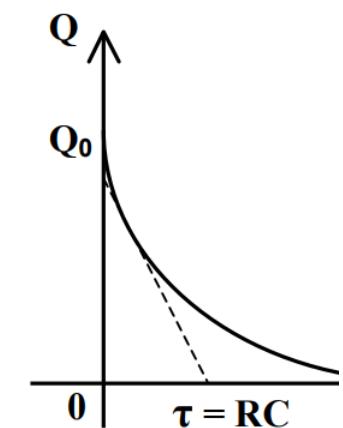
$$I = -\frac{dQ}{dt} = -C \frac{dV_C}{dt}$$

$$V = \frac{Q}{V_C} - IR_{int} = IR_{ext}$$

$$Q = -RC \frac{dQ}{dt}$$

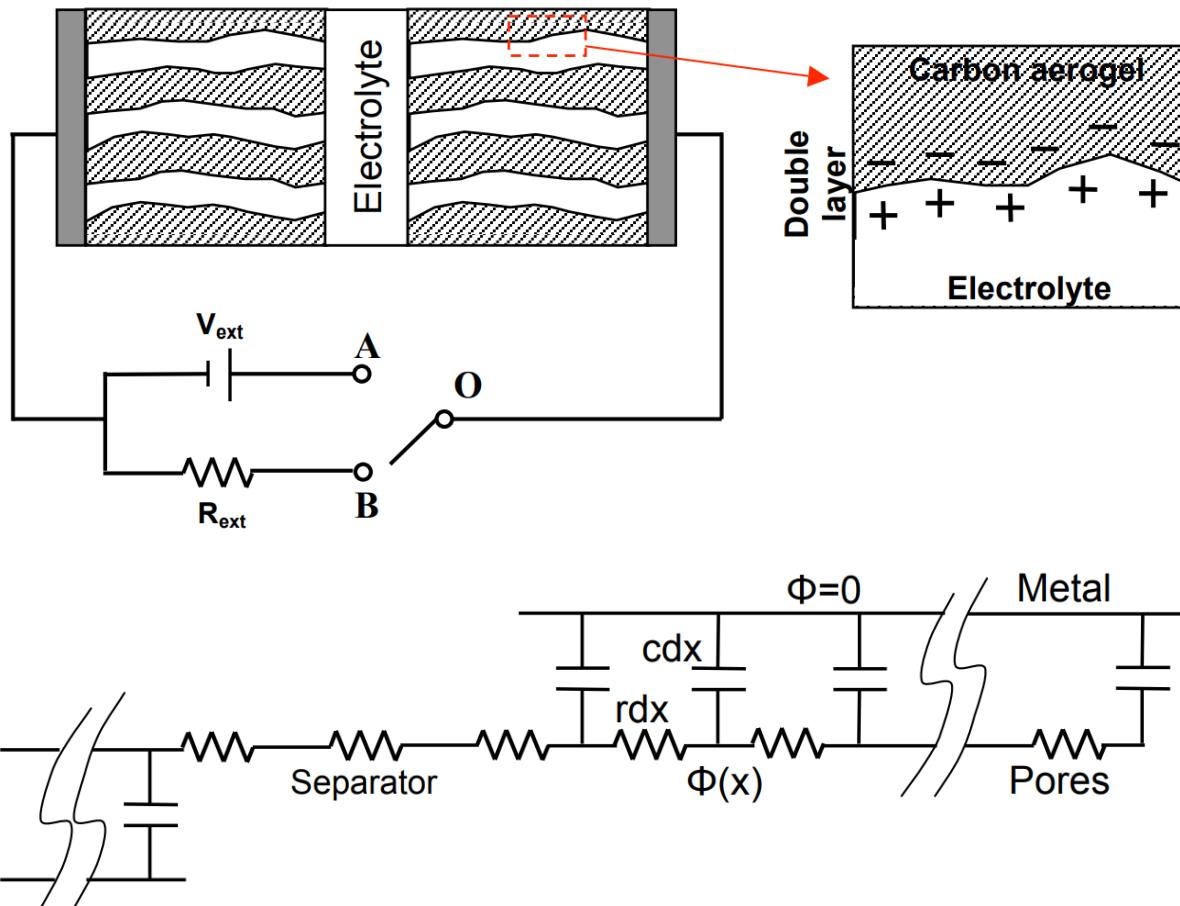
$$Q = Q_0 e^{-\frac{t}{RC}}$$

***t = RC as time constant***



# Appendix: Basic Physics of Cells

## **Supercapacitor**



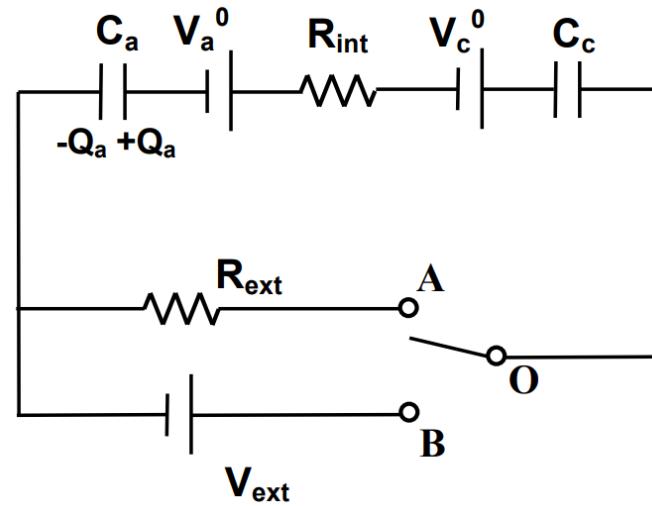
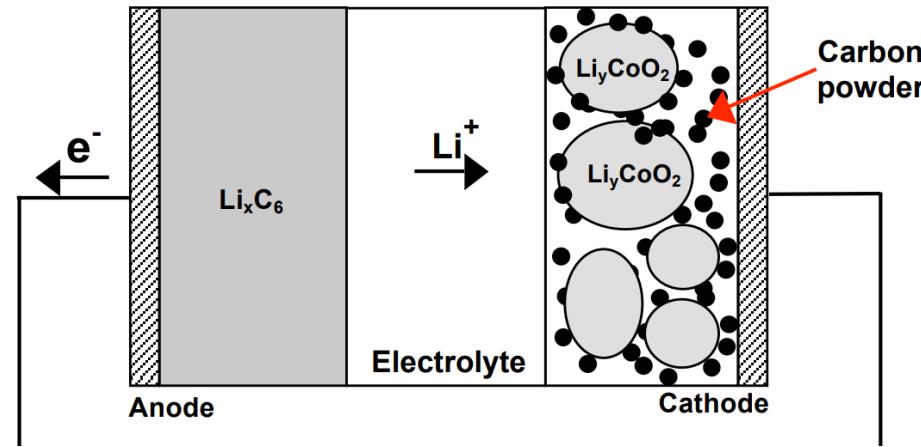
Consider two identical porous electrodes with thickness  $L$ , and electrolyte-filled pore space has constant volume-average resistance per length  $r$  and cap per length  $c$ . The mean potential satisfies diffusion eqt:

$$rc \frac{\partial \varphi}{\partial t} = \frac{\partial^2 \varphi}{\partial x^2}$$

For a sudden change of voltage at  $x = 0$ ,

$$I \sim \begin{cases} V \sqrt{\frac{c}{rt}} & , t \ll rcl^2 \\ \frac{V}{rl} e^{-\frac{t}{rcl^2}} & , t \gg rcl^2 \end{cases}$$

# Appendix: Basic Physics of Cells

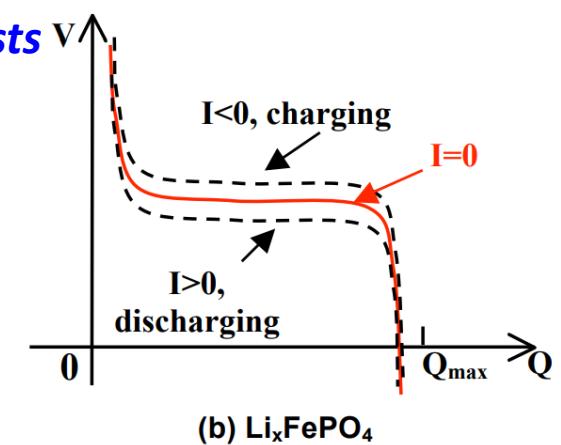
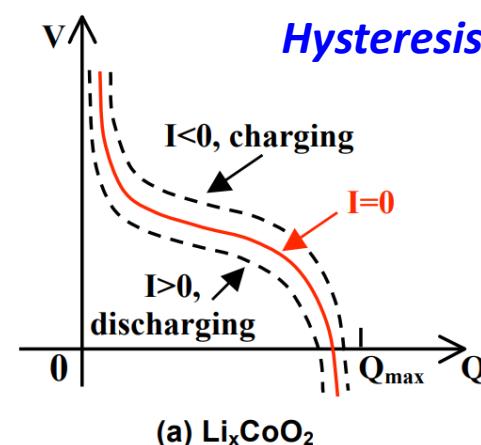


1) Discharging (connect OA in Figure ):

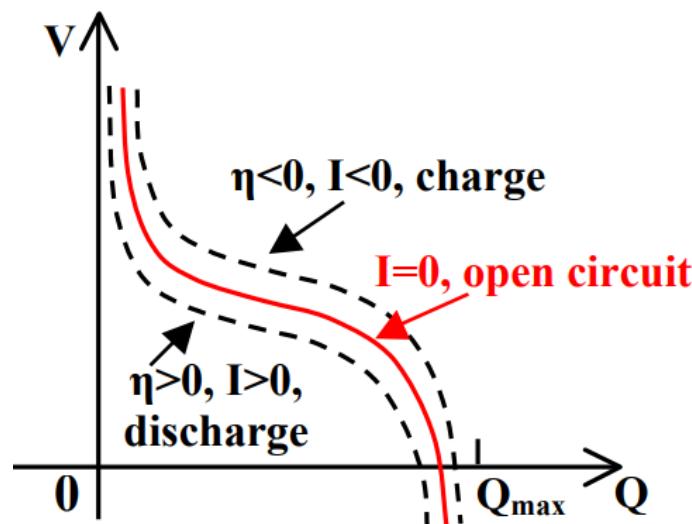
$$\left\{ \begin{array}{l} I = -\frac{dQ_a}{dt} = \frac{dQ_c}{dt} = \frac{V_a^0(Q_a) + V_c^0(Q_c)}{R} \\ Q_a(t=0) = Q_a^0 \\ Q_c(t=0) = 0 \end{array} \right.$$

2) Charging (connect OB in Figure ):

$$I = \frac{V_a^0(Q_a) + V_c^0(Q_c) - V_{\text{ext}}}{R} < 0$$



# Appendix: Basic Physics of Cells



$$V = V_o(Q) - \eta(I, Q) = I R_{\text{ext}}$$

Linear Response: Assume  $V = V(Q, I)$

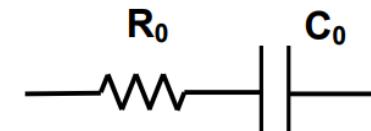
$$\Delta V = \left. \frac{\partial V}{\partial Q} \right|_{Q_0, I_0} \Delta Q + \left. \frac{\partial V}{\partial I} \right|_{Q_0, I_0} \Delta I$$

Define differential internal resistance:  $R_0 = \left. \frac{\partial V}{\partial I} \right|_{Q_0, I_0}$  and differential cell cap:

$$\frac{1}{C_0} = \left. \frac{\partial V}{\partial Q} \right|_{Q_0, I_0} = \left( \frac{dV_o}{dQ} - \frac{\partial \eta}{\partial Q} \right)_{Q_0, I_0}$$

$$\Delta V = \frac{1}{C_0} \Delta Q + R_0 \frac{d\Delta Q}{dt}$$

Equivalent Circuit:



# Appendix: Basic Physics of Cells

Constant Load:

$$V(t) = V_o(Q) - \eta \left( \frac{dQ}{dt} \right), Q = \frac{dQ}{dt} R_{ext}$$

$$V = V_o(Q) - \frac{dQ}{dt} R_{int}(Q) = \frac{dQ}{dt} R_{ext}$$

$$\frac{dQ}{dt} = \frac{V_o(Q)}{R_{ext} + R_{int}(Q)}$$

Assume the overpotential is linearly dependent on current

$$\int_{Q_0}^Q \frac{(R_{ext} + R_{int}(Q))dQ}{V_o(Q)} = - \int_0^t dt = -t$$

Constant Current:

$$Q = Q_0 + It$$

$$V(t) = V_o(Q_0 + It) - \eta(I, Q_0 + It) = IR_{ext}(t)$$

$R_{ext}(t)$  should be continuously varying to suit for constant current.

# Appendix: Basic Physics of Cells

Constant Power:

$$P = IV = \text{constant}$$

$$P = \left[ V_0(Q) - \eta \left( \frac{dQ}{dt}, Q \right) \right] \left( \frac{dQ}{dt} \right)$$

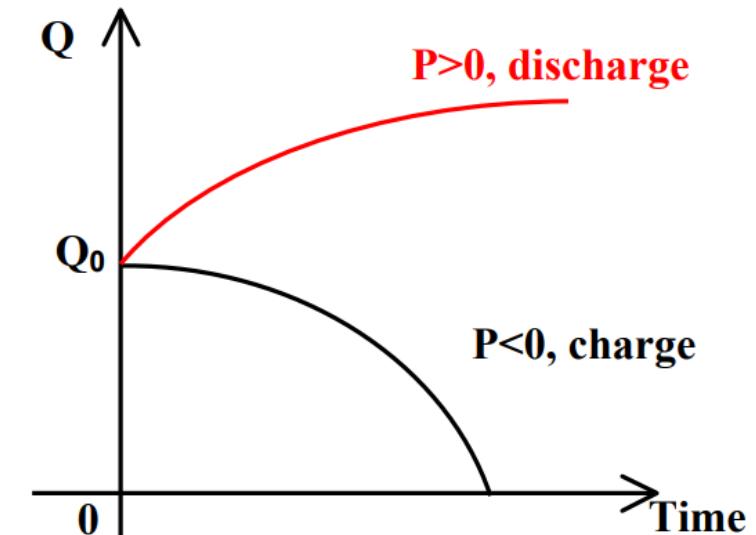
C rate:

$$\text{C rate} = \frac{\text{total capacity}}{n \text{ hours}} = \frac{C}{n}$$

$C/60$  = batteries discharge total capacity (Ah) in 60 hours.  
 $60C$  = batteries discharge total capacity (Ah) in 1 minutes.

Frequency Response:

$$V \approx \frac{Q}{C_{\text{ref}}} + R_{\text{ref}}i\omega Q = \frac{I}{i\omega C_0} + R_0 I$$



Complex Impedance:  $Z = \frac{V}{I} = \frac{V}{|I|} e^{-i\phi}$

Complex Capacitance:  $C = \frac{Q}{V}$

# Appendix: Basic Physics of Cells



$$Z = R_{\text{ref}} + \frac{1}{i\omega C_{\text{ref}}}$$

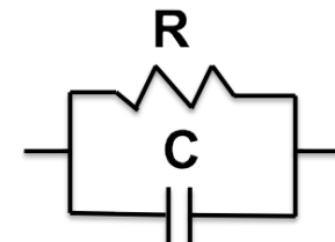
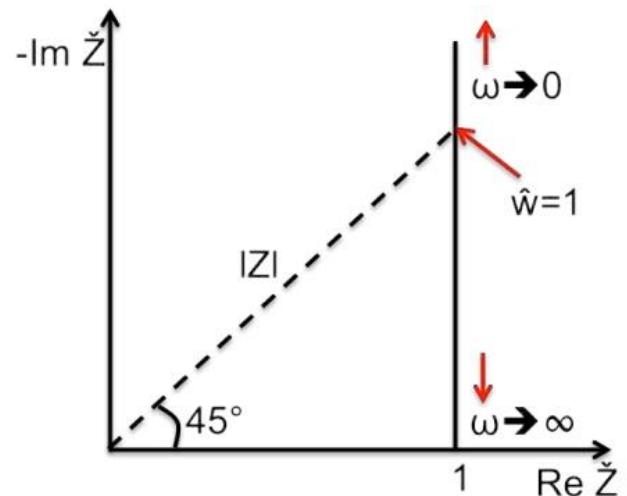
$$Y = \frac{i\omega C_{\text{ref}}}{1+i\omega R_{\text{ref}} C_{\text{ref}}}$$

$$C = \frac{C_{\text{ref}}}{1+i\omega R_{\text{ref}} C_{\text{ref}}}$$

$$\tilde{Z} = 1 + \frac{1}{i\tilde{\omega}}$$

$$\tilde{Y} = \frac{i\tilde{\omega}}{1+i\tilde{\omega}}$$

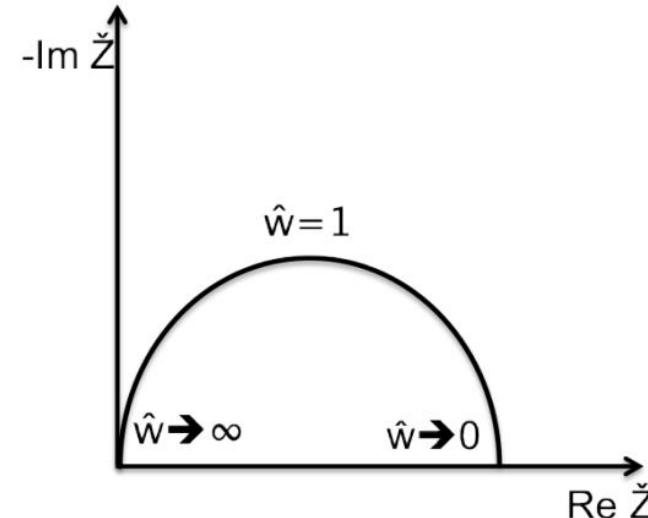
$$\tilde{C} = \frac{1}{1+i\tilde{\omega}}$$



$$\tilde{Z} = \frac{1}{1+i\tilde{\omega}}$$

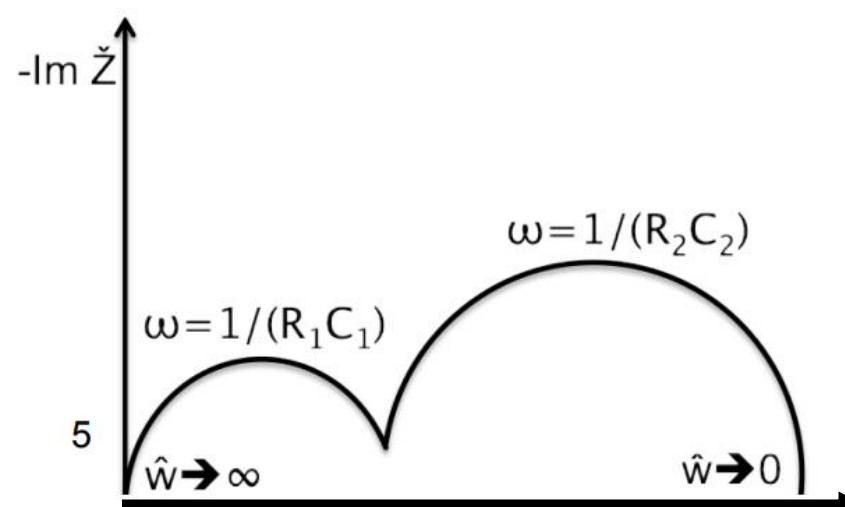
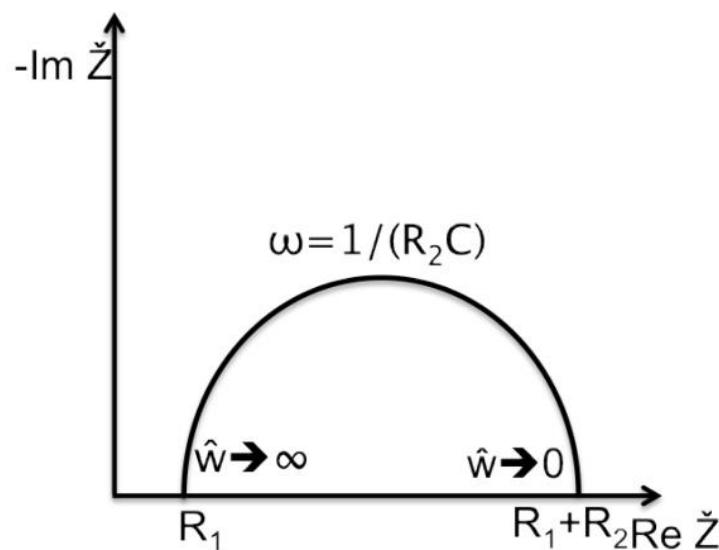
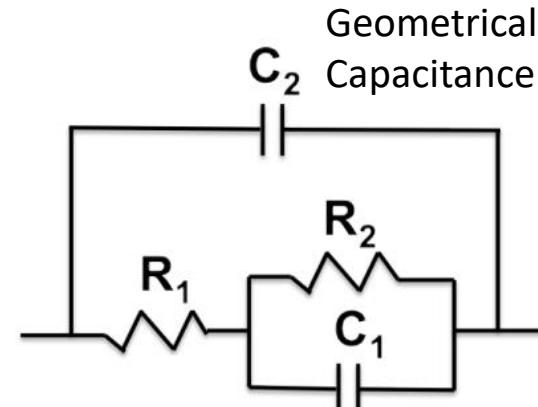
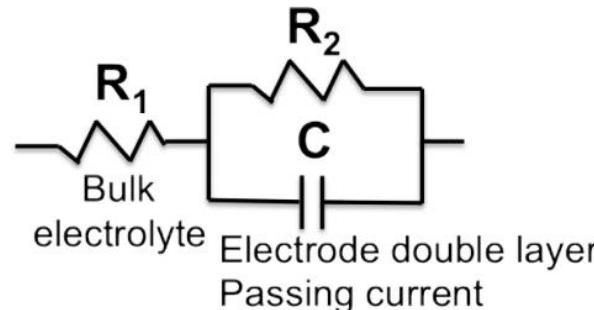
$$\tilde{Y} = 1 + i\tilde{\omega}$$

$$\tilde{C} = 1 + \frac{i}{\tilde{\omega}}$$



Dimensionless form:  $\tilde{\omega} = \omega R_{\text{ref}} C_{\text{ref}}$ ,  $\tilde{Z} = \frac{Z}{R_{\text{ref}}}$ ,  $\tilde{Y} = Y R_{\text{ref}}$ ,  $\tilde{C} = \frac{C}{C_{\text{ref}}}$

# Appendix: Basic Physics of Cells



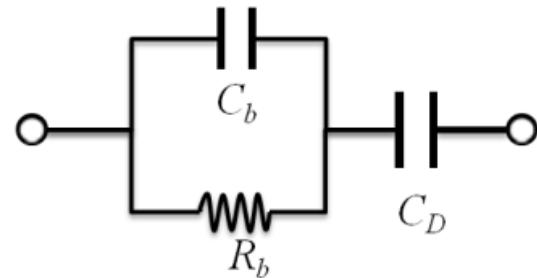
For an R-C parallel network, one can obtain a linear transformation for further analysis:

$$\tilde{Z} = \frac{1}{1 + i\tilde{\omega}}$$

$$\bar{Z} = 2\tilde{Z} - 1 = \frac{1 - i\tilde{\omega}}{1 + i\tilde{\omega}}$$

# Appendix: Basic Physics of Cells

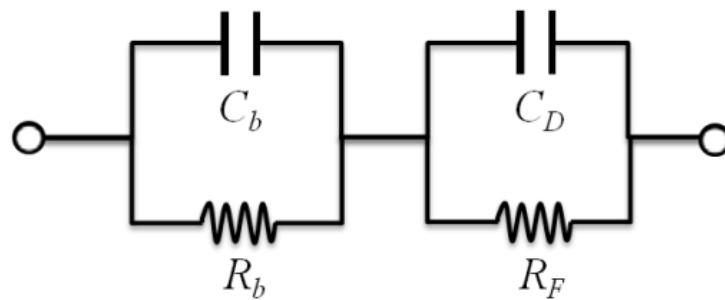
Ideal Blocking Electrode:



$$Z = \frac{1}{i\omega C_D} + \frac{1}{i\omega C_b + \frac{1}{R_b}}$$

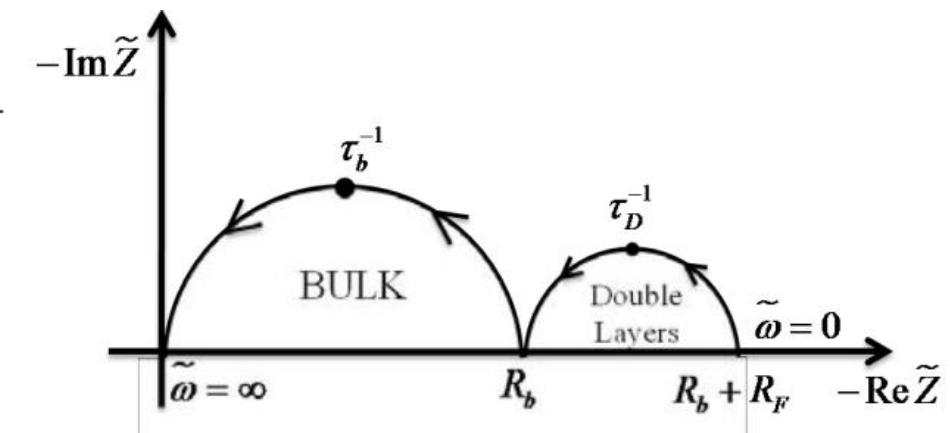
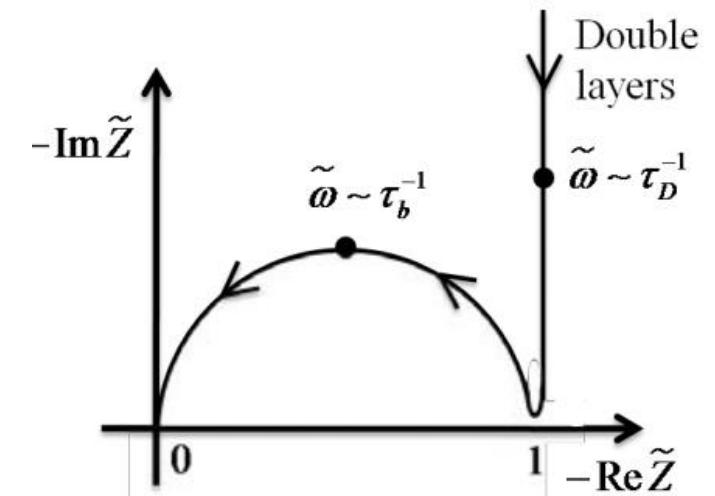
$$\tilde{Z} = \frac{1}{i\omega\tau_D} + \frac{1}{1 + i\omega\tau_b}$$

Partially Polarizing Electrode:



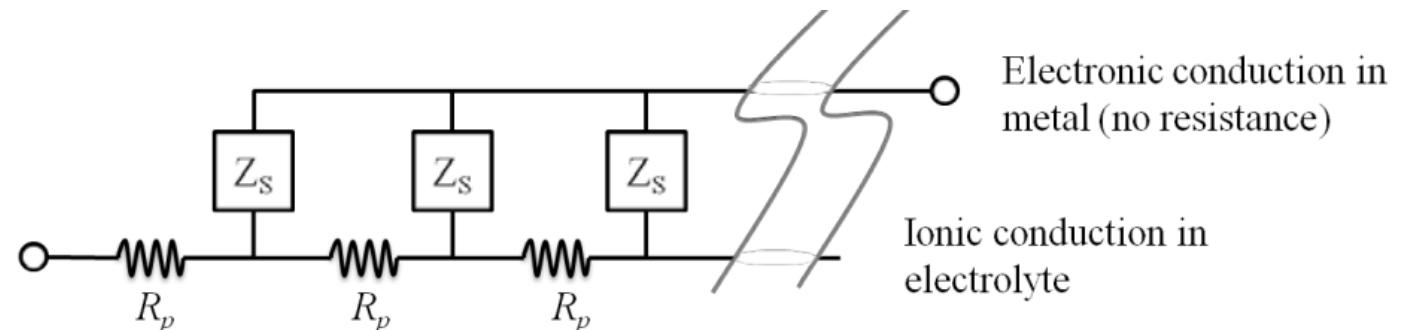
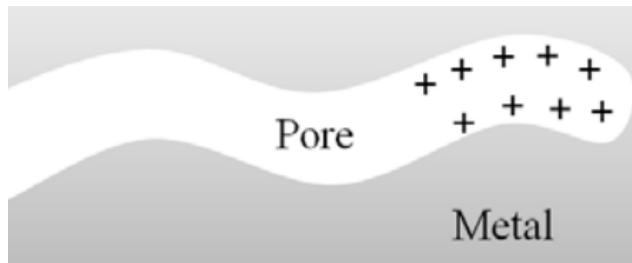
$$Z = \frac{1}{i\omega C_D + \frac{1}{R_F}} + \frac{1}{i\omega C_b + \frac{1}{R_b}}$$

$$\tilde{Z} = \frac{1}{i\omega\tau_D + \frac{R_b}{R_F}} + \frac{1}{1 + i\omega\tau_b}$$

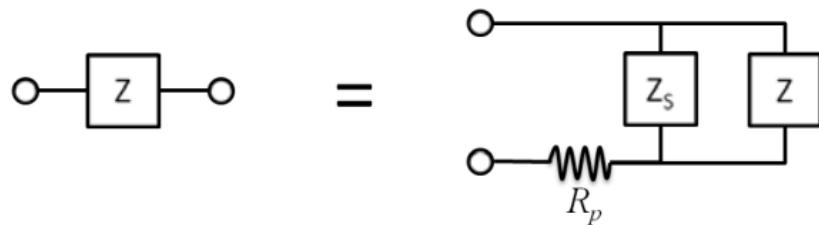


# Appendix: Basic Physics of Cells

Homogeneous Microstructures:



Solving the equivalent impedance equation:  
(Assuming infinite long with pattern)

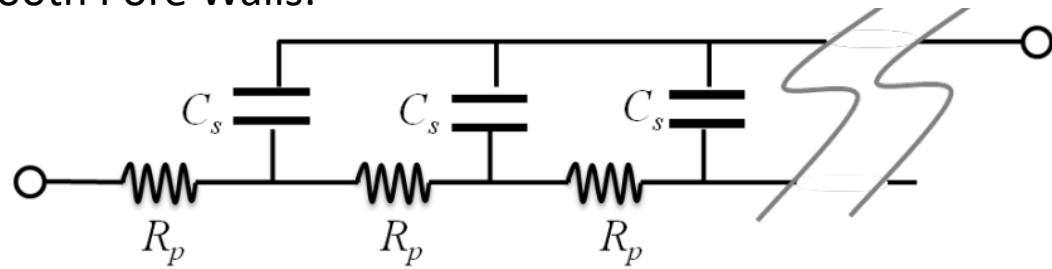


$$\tilde{Z} = \frac{1 + \sqrt{1 + 4\tilde{Z}_s}}{2} \sim \begin{cases} 1 & \text{for } \tilde{Z}_s \ll 1 \\ \sqrt{\tilde{Z}_s} & \text{for } \tilde{Z}_s \gg 1 \end{cases}$$

Where,  $\tilde{Z}_s = Z_s/R$  and  $\tilde{Z} = Z/R$

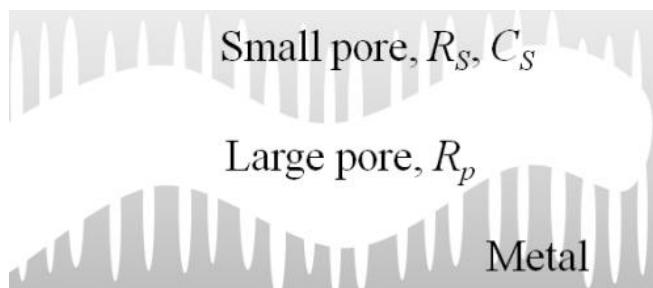
# Appendix: Basic Physics of Cells

Smooth Pore Walls:

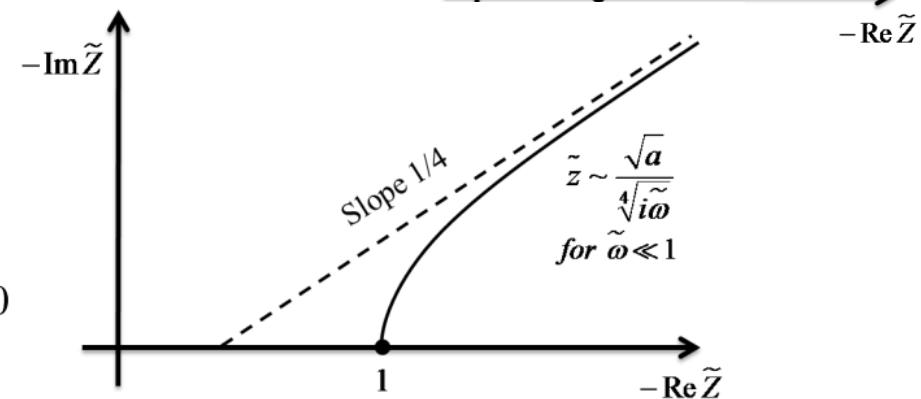
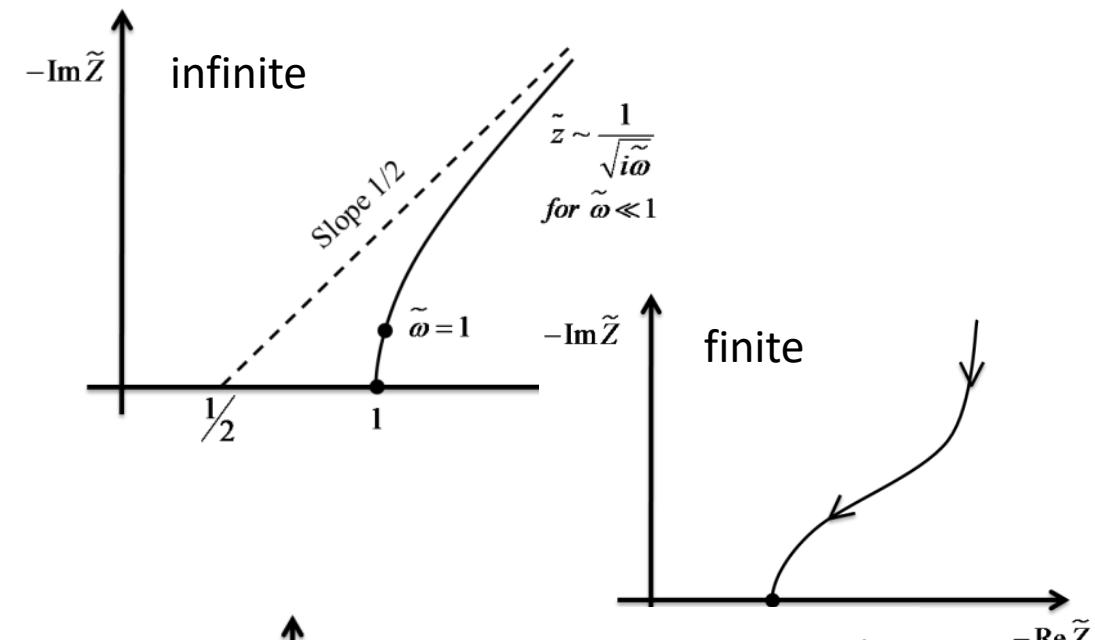


$$\tilde{Z}_s = \frac{1}{i\tilde{\omega} R C_s} = \frac{1}{i\tilde{\omega}} \quad \tilde{Z} = \frac{1 + \sqrt{1 + \frac{4}{i\tilde{\omega}}}}{2} \sim \begin{cases} \frac{1}{\sqrt{i\tilde{\omega}}} & \text{for } \tilde{\omega} \ll 4 \\ 1 & \text{for } \tilde{\omega} \gg 4 \end{cases}$$

Porous Pore Wall:



$$\tilde{Z}_s = \frac{1 + \sqrt{1 + \frac{4}{i\tilde{\omega}}}}{2} \quad \tilde{Z} = \sqrt{\frac{1 + \sqrt{1 + \frac{4}{i\tilde{\omega}}}}{2}} \sim \frac{1}{(i\tilde{\omega})^{1/4}} \text{ for } \tilde{\omega} \rightarrow 0$$



# Appendix: Warburg Element

Suppose  $\Delta V \sim \frac{k_B T}{ne} \ln\left(\frac{C_0 + \Delta C}{C_0}\right) \sim \frac{k_B T}{ne} \frac{\Delta C}{C_0}$  for linear response (e.g. Nernst equation,  $\Delta C \ll C_0$ ) and  $\Delta I \sim -neAD \frac{\partial C}{\partial x}(x=0)$

Also, assume quasi-equilibrium reactions at  $x=0$  and linear diffusion.

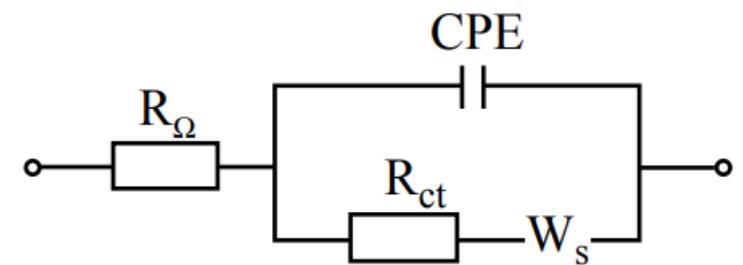
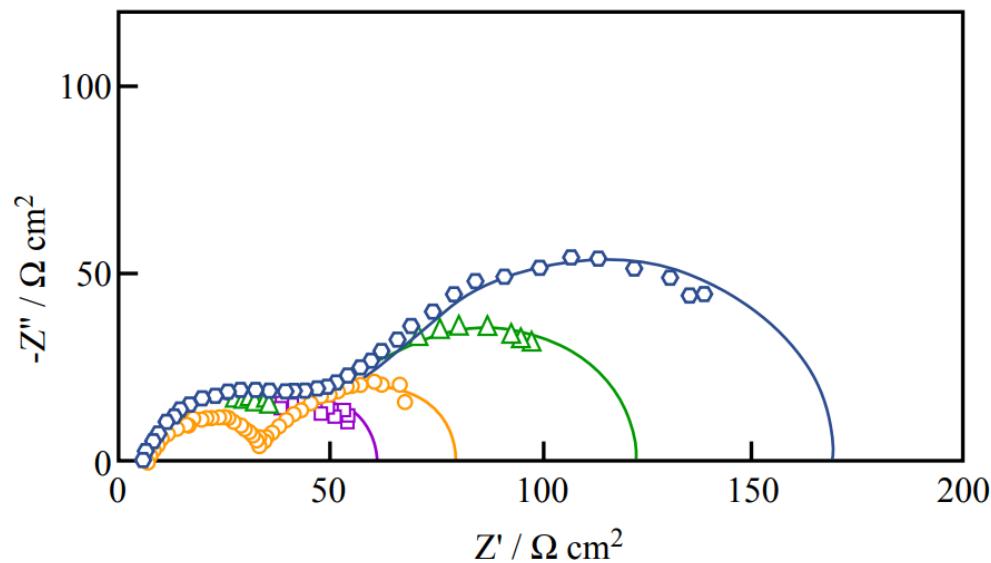
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Alternating current:  $\Delta V = \text{Re}[Ve^{j\omega t}]^{\text{Real } V} = V \cos(\omega t)$   
 $\Delta I = \text{Re}[Ie^{j\omega t}] = |I| \cos(\omega t + \varphi)$     $I = |I|e^{j\varphi}$   
 $\Delta C = C(x, t) - C_0 = \text{Re}[Ce^{j\omega t}]$

Therefore,  $iwC = DC''$

Hence,  $C = C(x=0)e^{-\sqrt{\frac{iw}{D}}x}$  ( $C \rightarrow 0$  as  $x \rightarrow \infty$ )

$$\frac{C(x=0)}{-C'(x=0)} = \sqrt{\frac{D}{iw}}$$

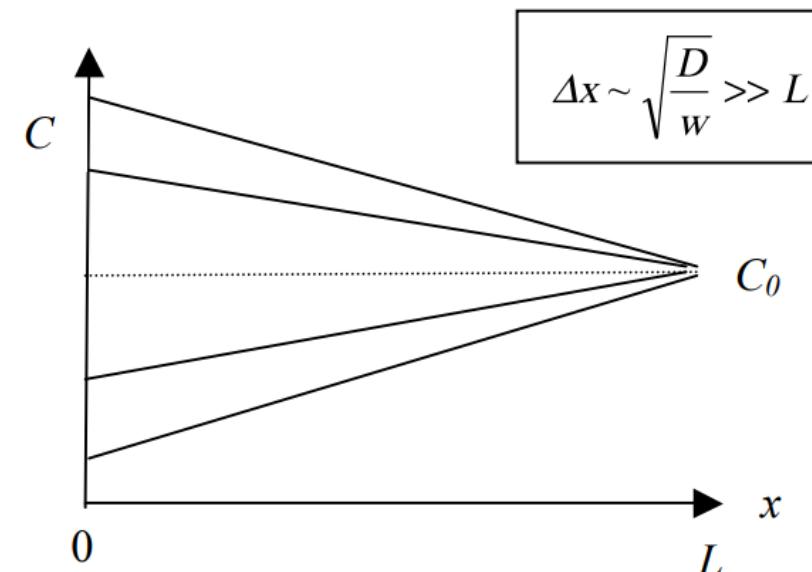
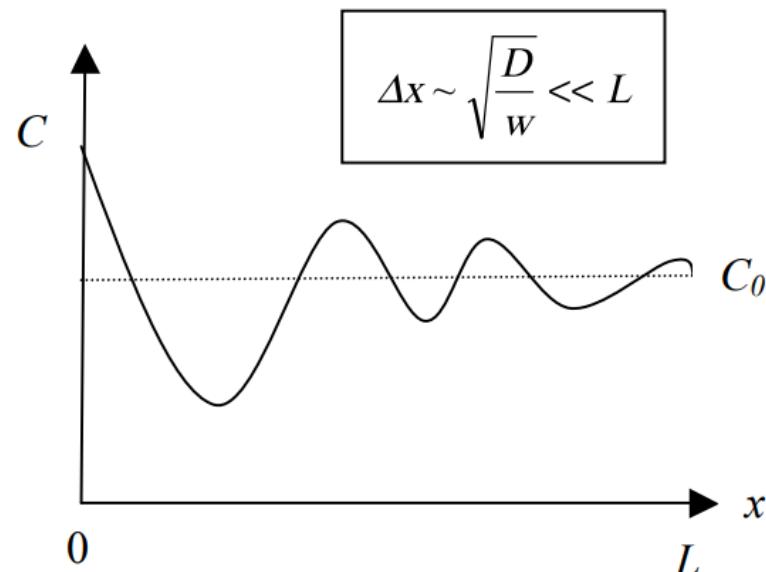


# Appendix: Warburg Element

Thus, impedance is

$$Z = \frac{\Delta V}{\Delta I} = \frac{k_B T}{(ne)^2 A D C_0} \frac{C(x=0)}{C'(x=0)} = \frac{A}{\sqrt{iw}}, \quad A = \frac{k_B T}{(ne)^2 A C_0 \sqrt{D}}$$

For oscillating diffusion layer, the characteristic length is  $\Delta x \sim \sqrt{Dt} = \sqrt{\frac{D}{w}}.$  **(Fuel Cell)**



# Appendix: Warburg Element

Now,  $C=C_0$  is imposed on  $x=L$ , not at the infinity. At low frequency ( $w \rightarrow 0$ ), FLW acts like a resistor. This situation is depicted in above figure.

Solve  $iwC = DC''$  with  $C=0$  at  $x=L$ .

The general solution is  $C = A\sinh\left[\sqrt{\frac{iw}{D}}(L-x)\right] + B\cosh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$ .

$B=0$  due to  $C(x=L) = 0$ . Thus,

$$C = A\sinh\left[\sqrt{\frac{iw}{D}}(L-x)\right], \quad C' = -\sqrt{\frac{iw}{D}}A\cosh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$$

$$\frac{C(x=0)}{-C'(x=0)} = \sqrt{\frac{D}{iw}} \tanh\left(\sqrt{\frac{iw}{D}}L\right)$$

Hence, the impedance is,

$$Z = \frac{\Delta V}{\Delta I} = \frac{k_B T}{(ne)^2 A D C_0} \frac{C(x=0)}{-C'(x=0)} = Z_0 \frac{1}{L} \sqrt{\frac{D}{iw}} \tanh\left(\sqrt{\frac{iw}{D}}L\right), \quad Z_0 = \frac{k_B T L}{(ne)^2 A D C_0}$$

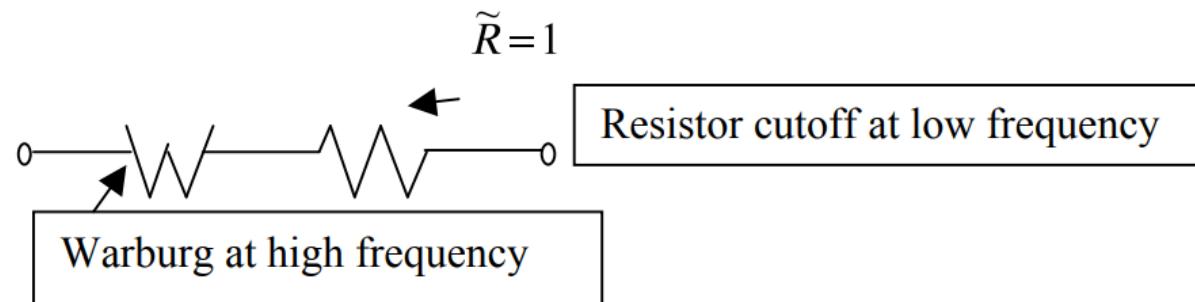
# Appendix: Warburg Element

$$\tilde{Z} = \frac{Z}{Z_0} \text{ and } \tilde{w} = \frac{wL^2}{D}$$

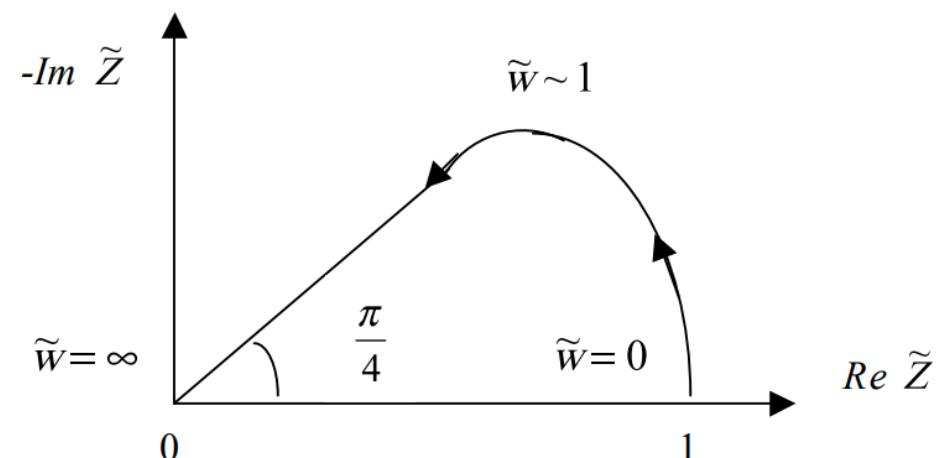
Then, dimensionless impedance is

$$\tilde{Z} = \frac{1}{\sqrt{i\tilde{w}}} \tanh(\sqrt{i\tilde{w}}) \sim \begin{cases} \frac{1}{\sqrt{i\tilde{w}}} (\tilde{w} \gg 1) \\ 1 - \frac{i\tilde{w}}{3} + \dots (\tilde{w} \ll 1) \end{cases}$$

Hence, this is similar to the following circuit, except in the transition region:

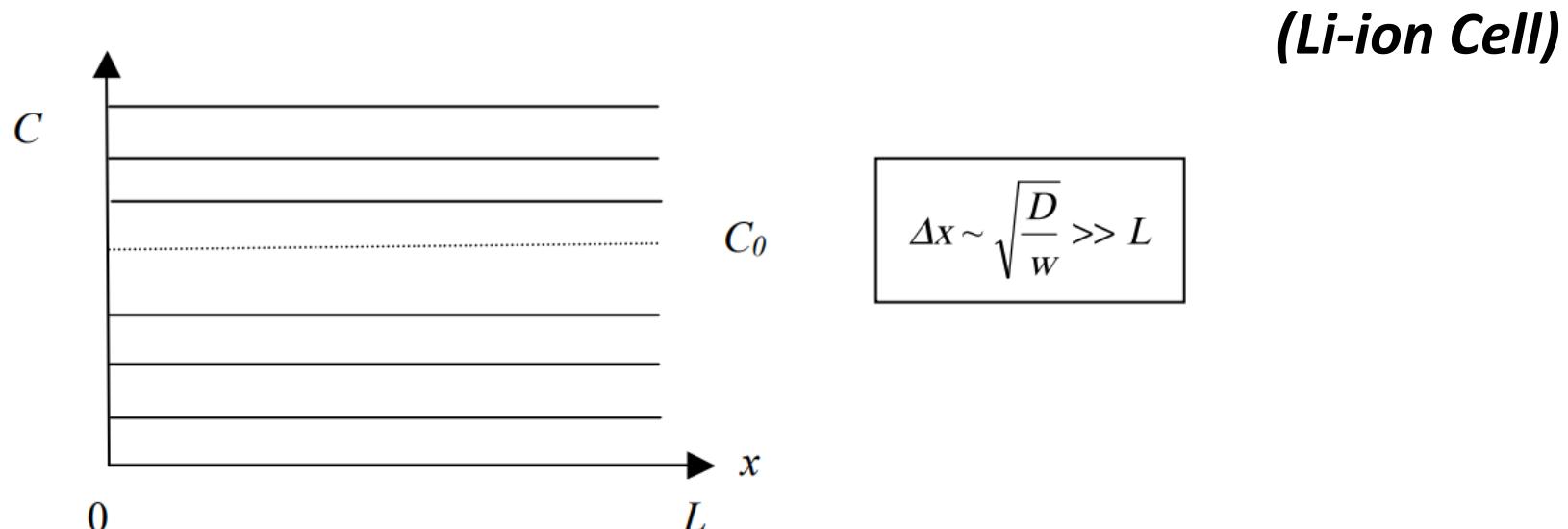


The Nyquist plot is,



# Appendix: Warburg Element

Now apply a zero flux Neuman BC at  $x=L$  instead of Dirichlet BC, to represent the finite end of intercalation particle. At higher frequency, this system has the same Warburg impedance as before. However, this system acts as a capacitor at low frequency at this time. Schematic figure is as follows.



Still, general solution is  $C = A\sinh\left[\sqrt{\frac{iw}{D}}(L-x)\right] + B\cosh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$ .

# Appendix: Warburg Element

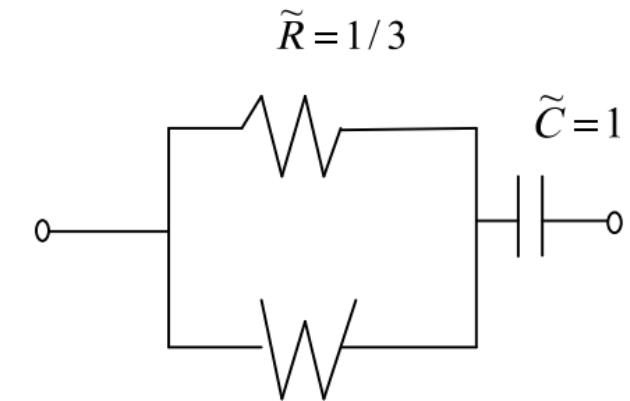
Still, general solution is  $C = A \sinh\left[\sqrt{\frac{iw}{D}}(L-x)\right] + B \cosh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$ .

With  $C(x=L) = 0$ ,  $A=0$ .  $C = B \cosh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$ ,  $C' = -\sqrt{\frac{iw}{D}} B \sinh\left[\sqrt{\frac{iw}{D}}(L-x)\right]$

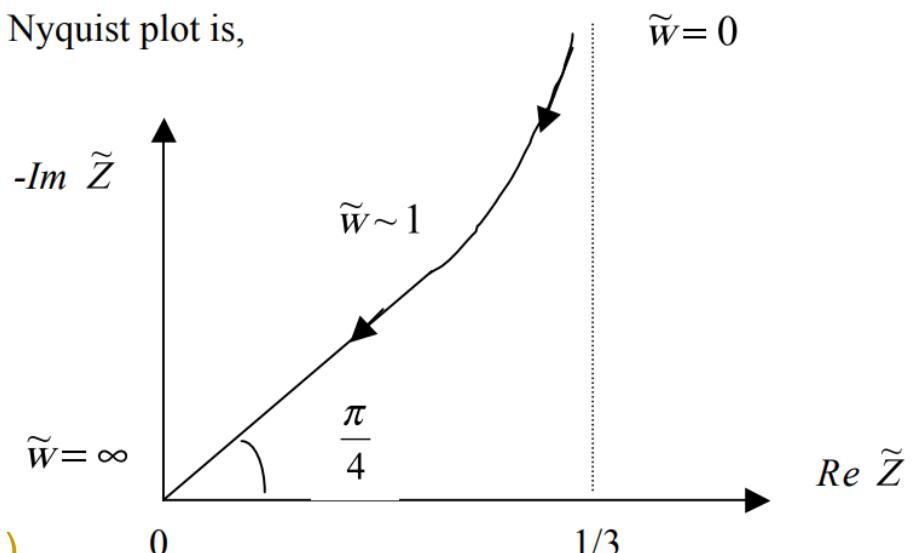
$$\frac{C(x=0)}{-C'(x=0)} = \sqrt{\frac{D}{iw}} \coth\left(\sqrt{\frac{iw}{D}}L\right)$$

Use the same notation as before. Then, dimensionless impedance is

$$\tilde{Z} = \frac{1}{\sqrt{iw}} \coth\left(\sqrt{iw}\right) \sim \begin{cases} \frac{1}{\sqrt{iw}} (\tilde{w} \gg 1) \\ \frac{iw}{1} + \frac{1}{3} \dots (\tilde{w} \ll 1) \end{cases}$$



The Nyquist plot is,



Materials taken from [10.626 Electrochemical Energy Systems \(Spring 2011\)](#)