ElectroChemical Application for advance energy System

Korea-EU horizon Europe researchers networking forum

Mechanical engineering, Chung-Ang university

Associate professor

Dongkyu Kim

#0 Self-Introduction

- **Dong Kyu Kim**
  - Ph.D. in mechanical engineering
  (thesis: Studies on the performance of hybrid system which is consisted of a polymer electrolyte membrane fuel cell coupled with organic Rankine cycle)
- **Education & position**
  - B.S., & Ph. D., Department of Mechanical and Aerospace Engineering, Seoul National University.
  - Visiting researcher, Microfluidics group/ Energy research, KIST-Europe, Germany
  - Guest scientist, Transfer center Sustainable Electrochemistry, Germany
  - Associate professor, Chung-Ang university, Korea
  - Guest researcher, National Institute of Science and Technology, USA
- **Research experience**
  - Research on organic Rankine cycle(ORC) for low-grade heat with temperature below 100^{o}C.
  - Research on PEM fuel cell system for automotive.
  - Research on oil cooing for motor-reducer assembly.
  - Research on hydrogen infrastructure.
  - Research on electrochemical devices.
  - Research on thermal runaway of battery.
  - Extensive background in refrigeration cycle.

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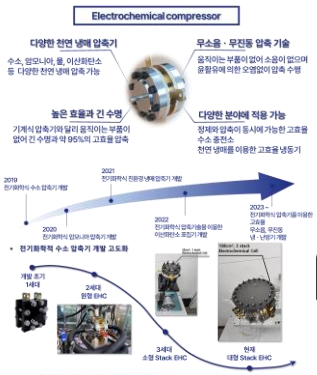
Research introduction

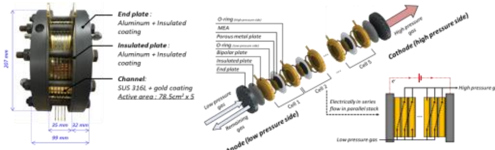
중앙대학교
CHUNG-ANG UNIVERSITY

1. Research areas

#1 Research areas

Electrochemical compressor & heat pump





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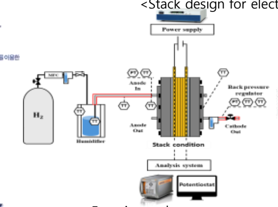

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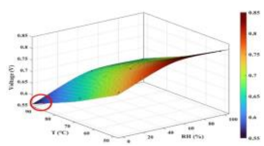

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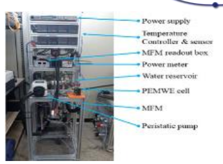
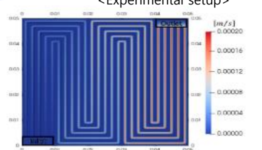
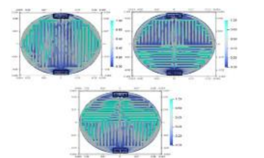
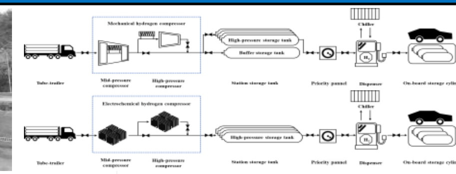




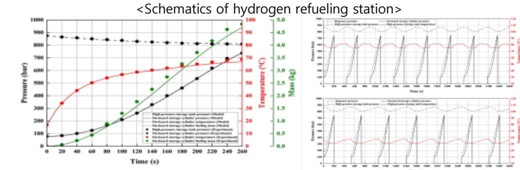


<CFD analysis on channel>

Fault detection on hydrogen refueling station



<Schematics of hydrogen refueling station>



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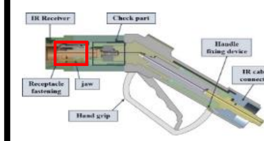

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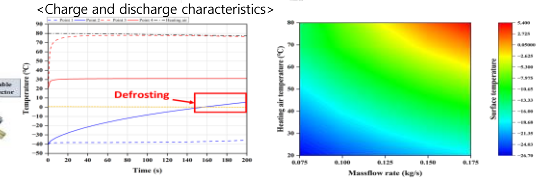

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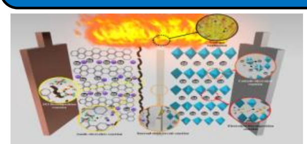
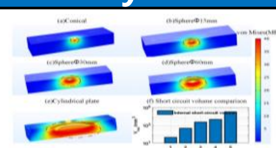
Thermal runaway of batteries





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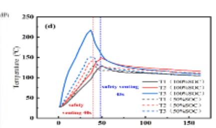

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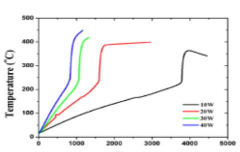
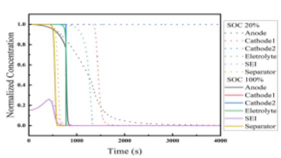


<characteristics of thermal runaway>



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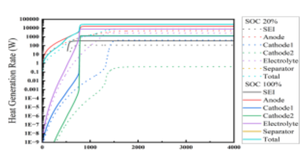
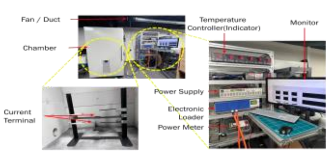


<Heat release rate>



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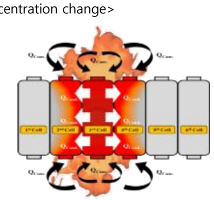
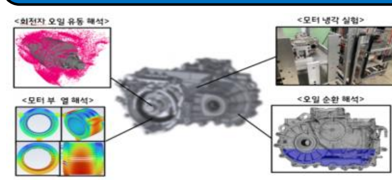


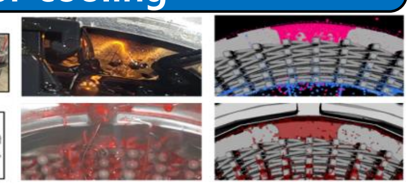
<Heat propagation>

<battery module fire>

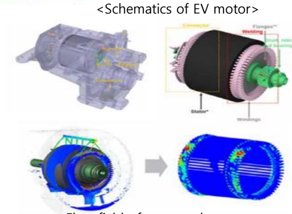
EV motor cooling



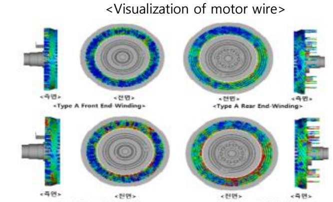
<Schematics of EV motor>



<Visualization of motor wire>



<Flow field of rotor and stator>



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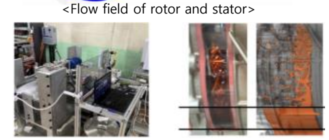

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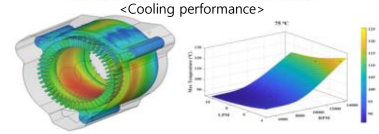
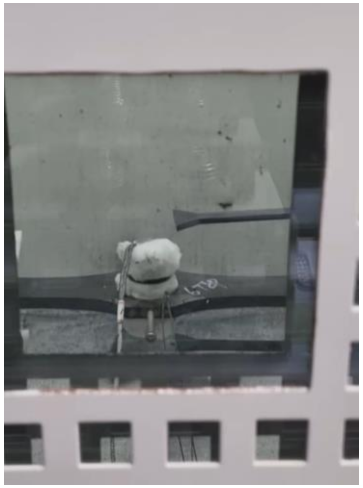


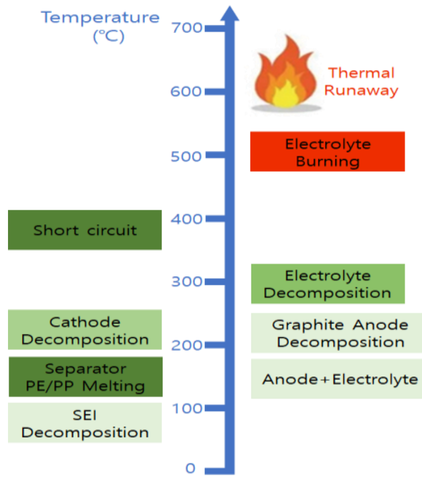
<Local temperature distribution>

2. Related topics

#2-1 Thermal runaway of Li-ion batteries



<Experiments of TR>



<Mechanism of TR>

$$\frac{dc_{sei}}{dt} = -A_{sei} \exp\left[-\frac{E_{sei}}{RT}\right] c_{sei}^{m_{sei}} \longrightarrow \dot{q}_{sei} = H_{sei} W_{sei} \left|\frac{dc_{sei}}{dt}\right|$$

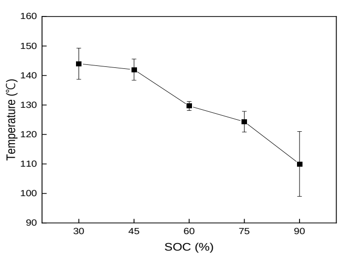
$$\frac{dc_{ne}}{dt} = -A_{ne} \exp\left(-\frac{t_{sei}}{t_{sei,ref}}\right) \exp\left[\frac{E_{ne}}{RT}\right] c_{ne}^{m_{ne}} \longrightarrow \dot{q}_{ne} = H_{ne} W_{ne} \left|\frac{dc_{ne}}{dt}\right|$$

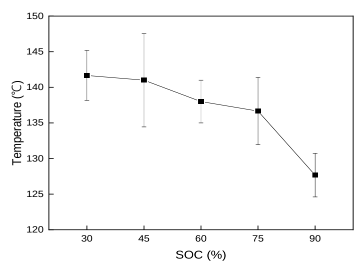
$$\frac{d\alpha}{dt} = A_{pe} \exp\left[-\frac{E_{pe}}{RT}\right] \alpha^{m_{pe,1}} (1-\alpha)^{m_{pe,2}} \longrightarrow \dot{q}_{pe} = H_{pe} W_{pe} \left|\frac{d\alpha}{dt}\right|$$

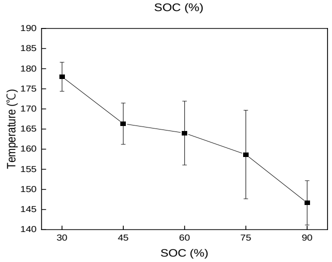
$$\frac{dc_e}{dt} = -A_e \exp\left[-\frac{E_e}{RT}\right] c_e^{m_e} \longrightarrow \dot{q}_e = H_e W_e \left|\frac{dc_e}{dt}\right|$$

$$\frac{dSOC}{dt} = -ISC_{cond} \cdot SOC \cdot A_{ec} \cdot \exp\left(-\frac{E_{ec}}{RT}\right) \longrightarrow \dot{q}_{ISC} = H_{ec} \left|\frac{dSOC}{dt}\right|$$

<Governing equations of TR>







<Changes in starting temperature of TR depending on SOC>

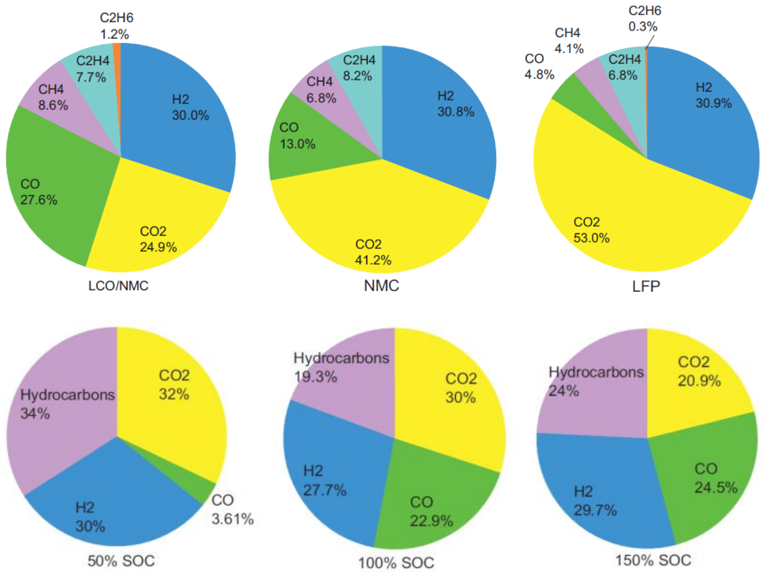
배터리 NO.	방전 C-rate	방전완료 전압[V]	실험시작 전 전압[V]	충전 C-rate	대기 온도	충전 SOC	단열 유무	가열 시작	벤팅 시각	열폭주 유/무	비고
1	1C	2.5V	2.81	1C	20	100	X	3608	3838	Y	벤팅과 동시에 열폭주
2	1C	2.5V	2.57	1C	20	100	X	3610	3956	Y	큰 폭발, 뚜껑파손
3	1C	2.5V	2.82	1C	20	100	X	3610	3912	Y	벤팅과 동시에 열폭주
4	1C	2.5V	2.71	1C	21	100	O	3610	3825	Y	벤팅과 동시에 열폭주, 뚜껑파손
5	1C	2.5V	2.72	1C	21	100	O	3610	3802	Y	벤팅과 동시에 열폭주, 뚜껑파손
6	1C	2.5V	2.72	1C	24	100	O	3610	3816	Y	벤팅과 동시에 열폭주, 뚜껑파손
7	1C	2.5V	2.9	1C	25	80	X	2888	3321	Y	뚜껑파손
8	1C	2.5V	2.84	1C	23	80	X	2889	3380	Y	
9	1C	2.5V	2.9	1C	24	80	X	2889	3211	Y	큰 폭발
10	1C	2.5V	2.6	1C	24	80	O	2888	3250	Y	뚜껑파손
11	1C	2.5V	2.83	1C	24	80	O	2888	3200	Y	뚜껑파손
12	1C	2.5V	2.5	1C	24	80	O	2890	3203	Y	뚜껑파손
13	1C	2.5V	2.8	1C	23	60	X	2169	2517	Y	
14	1C	2.5V	2.8	1C	24	60	X	2179	2699	Y	
15	1C	2.5V	2.83	1C	23	60	X	2168	2795	Y	
16	1C	2.5V	2.8	1C	23	60	O	2160	2536	Y	
17	1C	2.5V	2.5	1C	23	60	O	2167	2509	Y	
18	1C	2.5V	2.8	1C	23	60	O	2169	2530	Y	
19	1C	2.5V	2.89	1C	20	40	X	1450	1856	Y	
20	1C	2.5V	2.85	1C	20	40	X	1445	1801	Y	벤팅과 동시에 열폭주
21	1C	2.5V	2.8	1C	20	40	X	1450	1913	Y	
22	1C	2.5V	2.89	1C	24	40	O	1440	2098	Y	
23	1C	2.5V	2.63	1C	19	40	O	1450	1728	Y	벤팅과 동시에 열폭주
24	1C	2.5V	2.5	1C	11	40	O	1448	1909	Y	
25	1C	2.5V	2.89	1C	20	20	X	726	2018	N	
26	1C	2.5V	2.58	1C	20	20	X	727	1182	Y	
27	1C	2.5V	2.8	1C	21	20	X	728	1368	Y	뚜껑파손
28	1C	2.5V	2.59	1C	20	20	O	730	1394	Y	
29	1C	2.5V	2.6	1C	11	20	O	720	—	N	
30	1C	2.5V	2.5	1C	11	20	O	720	1394	Y	벤팅과 동시에 열폭주

<Reproducibility test>

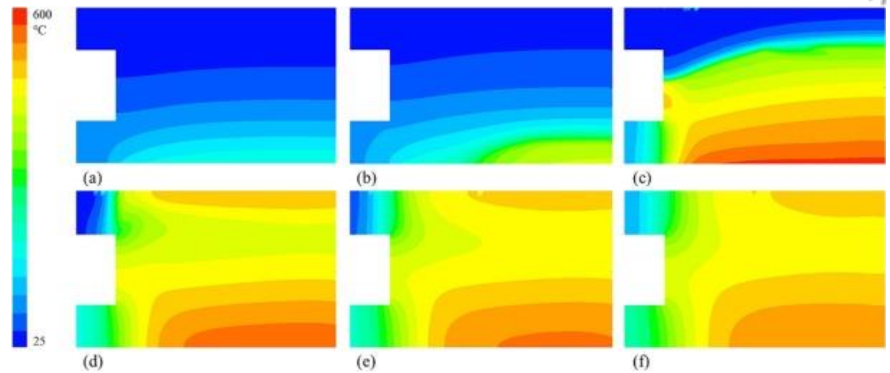
- **We analyzed thermal runaway mechanism of Li-ion batteries by conducting experimental and numerical analysis.**

#2-1 Thermal runaway of Li-ion batteries

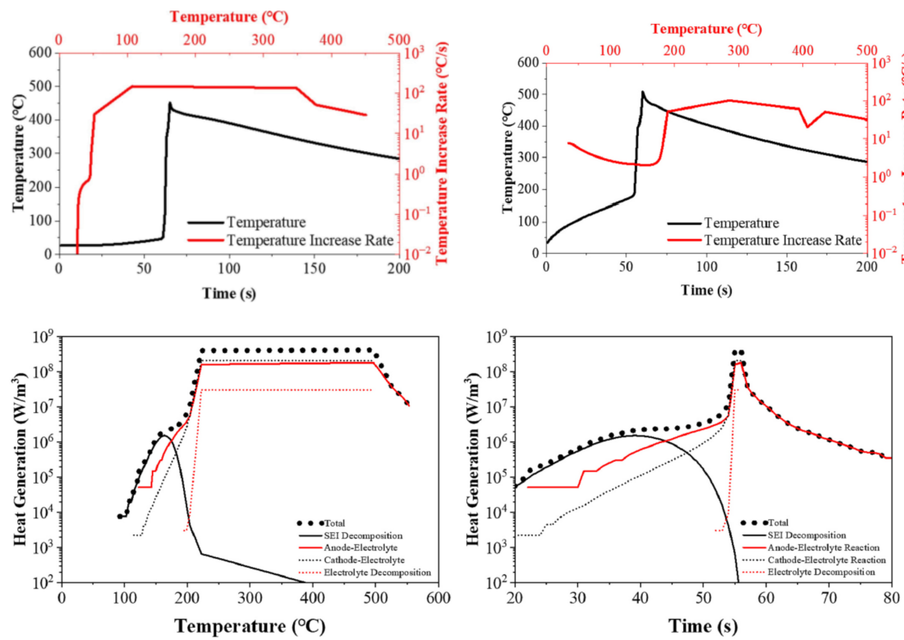
Electrolyte /Cathode	274.2-300 ℃: Oxygen release $LCO-NCA-NCM-LMO-LFP$ $LCO: Li_xCoO_2 \rightarrow xLiCoO_2 + \frac{1}{3}(1-x)Co_3O_4 + \boxed{\frac{1}{3}(1-x)O_2}$ $Co_3O_4 \rightarrow 3CoO + 0.5O_2 \quad CoO \rightarrow \boxed{CO + 0.5O_2}$	[150-153]
Electrolyte decomposition	200 ℃ $C_2H_5OCOOPF_4 \rightarrow \boxed{PF_3O + CO_2 + C_2H_4 + HF}$ $DMC: 3O_2 + C_3H_6O_3 \rightarrow \boxed{3CO_2} + 3H_2O$ $EC: 2Li + 2EC \rightarrow LiO(CH_2)_4OLi + \boxed{2CO_2} \xrightarrow[2STEP]{} \boxed{POF3}$ $PC: -$	
Separator	135-166 ℃ (PE, PP)	
Electrolyte /Anode	100 ℃ $2Li + C_3H_4O_3(EC) \rightarrow Li_2CO_3 + \boxed{C_2H_4}$ 에틸렌 1400kJ/mol $2Li + C_4H_6O_3(PC) \rightarrow Li_2CO_3 + \boxed{C_3H_6}$ 프로판 2058kJ/mol $2Li + C_3H_6O_3(DMC) \rightarrow Li_2CO_3 + \boxed{C_2H_6}$ 에탄 1560kJ/mol	[21,151,160]
SEI decomposition	90-120 ℃ : $(CH_2OCO_2LI)_2 \rightarrow LI_2CO_3 + \boxed{C_2H_4 + CO_2 + \frac{1}{2}O_2}$ 51-69 ℃ : carbon exothermic reaction	[150-153] [154]



<Various vent gases>



<Temperature distribution>

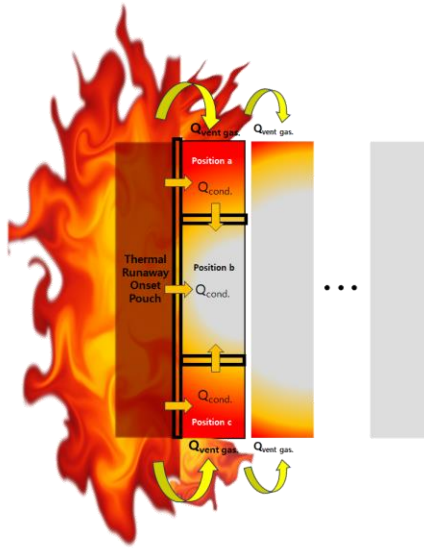


<Changes in temperature during TR>

- We analyzed heat release rate and temperature change during thermal runaway.
- We considered combustion by vent gases.

#2-1 Thermal runaway of Li-ion batteries

<Experiment>



<Heat propagation>

$$\Delta Q = mC_P \frac{dT_{cell}}{dt} = Q_{abuse} + Q_{vent\ \mathrm{gas}} - Q_{ht}$$

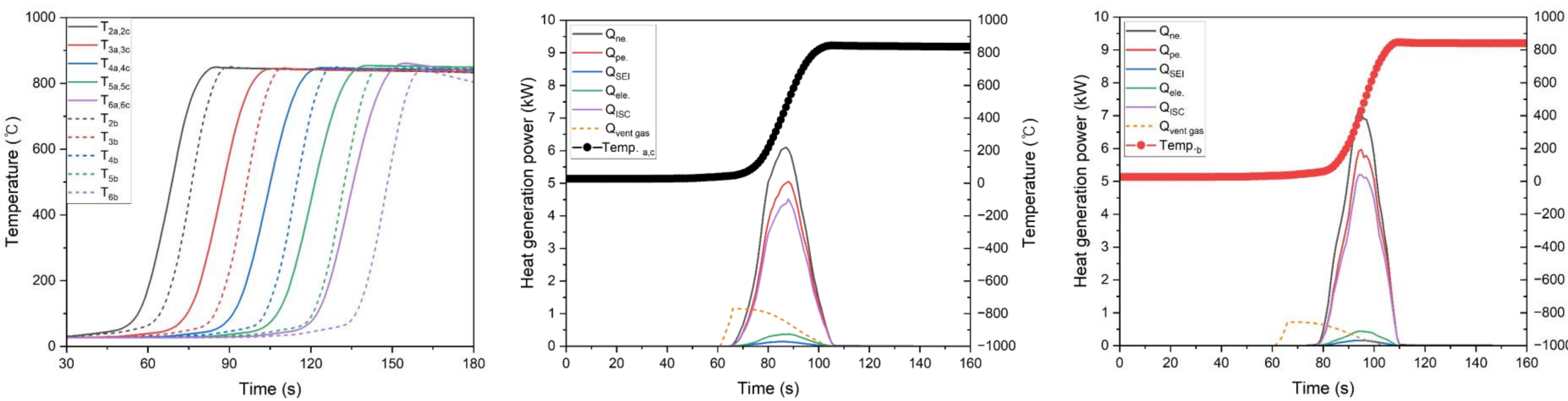
$$Q_{ht} = \iiint_V \nabla(\lambda \nabla T) - hA(T - T_{amb.})$$

$$Q_{vent\ gas} = \begin{cases} 0 \\ a_0 \exp(b_0 t) + c_0 \exp(d_0 t) \\ a_1 \sin(b_1 t + c_1) + a_2 \sin(b_2 t + c_2) + a_3 \sin(b_3 t + c_3) \end{cases}$$

$$V = \frac{Q_{cond.}}{A\rho c_p (T_H - T_L)} \qquad Q_{cond.} = -Ak_j \Gamma$$

$$V = \frac{-k_j \Gamma}{\rho c_p (T_H - T_L)} \quad (j = x, y, z)$$

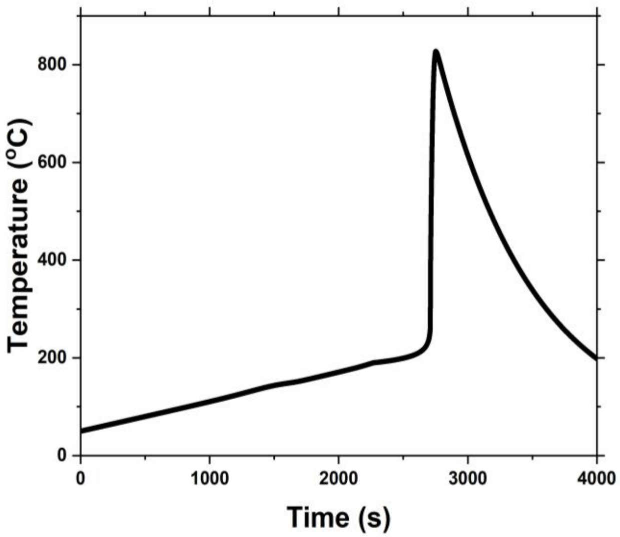
<Governing equations related to combustion>



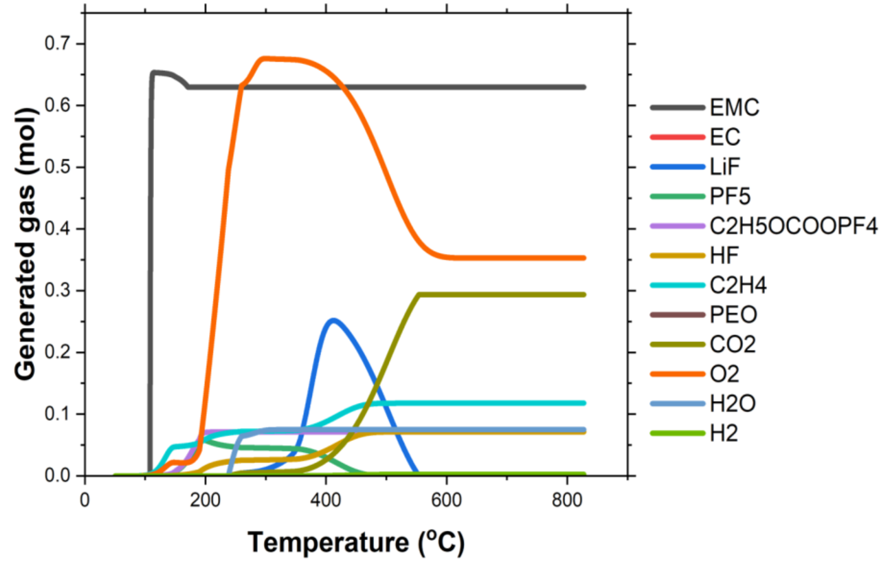
<Changes in the batteries during TR>

- **We analyzed heat propagation of 6 pouch cells during thermal runaway. Heat transfer by convection is the most important factor.**

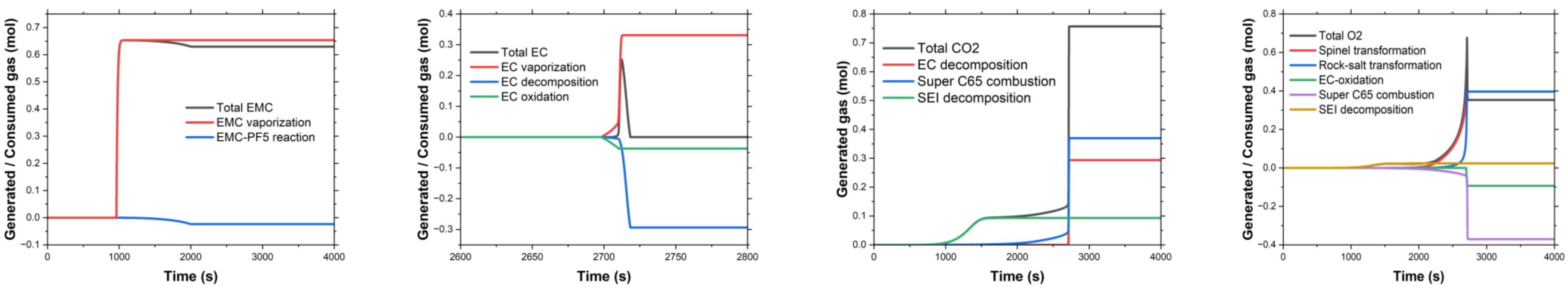
#2-1 Thermal runaway of Li-ion batteries



<Temperature change during TR>



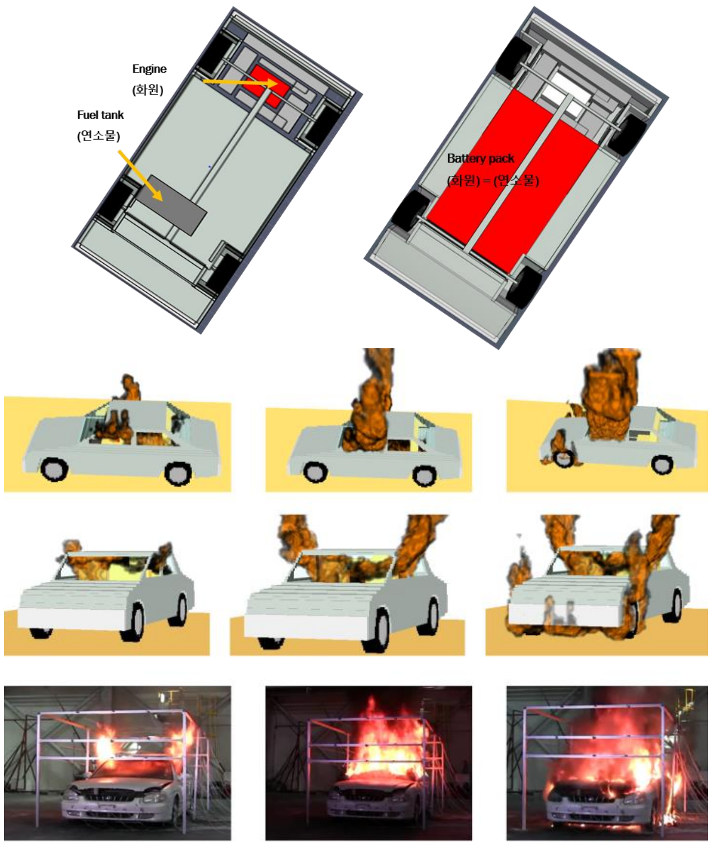
<Variations in vent gases>



<Specific sub-reactions related to gas generation>

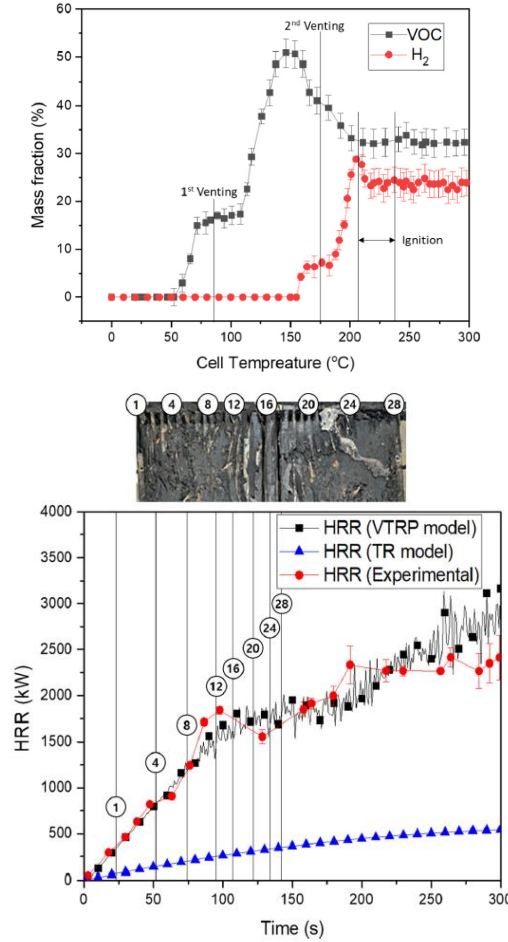
- Various redox reactions occurs sequentially depending on the temperature.
- At early stage, electrolytes are mainly evaporated, and SEI is decomposed.
- Damage of separator results in oxygen generation reaction.
- SEI decomposition generates carbon dioxide.

#2-1 Thermal runaway of Li-ion batteries



250 s 800 s 1200 s

<EV fire>



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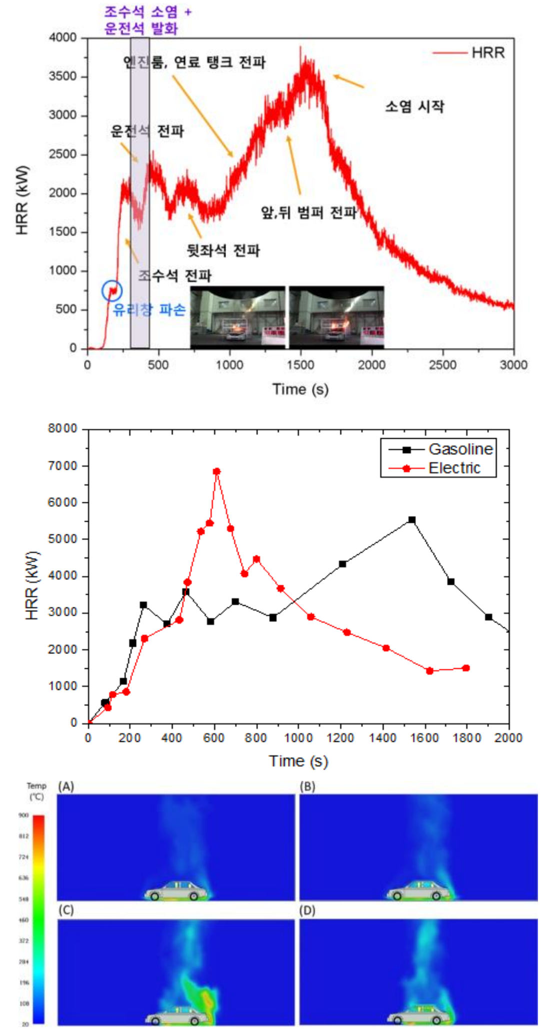
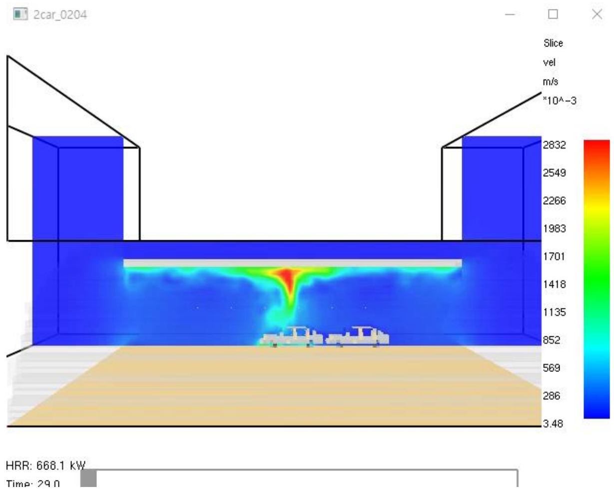
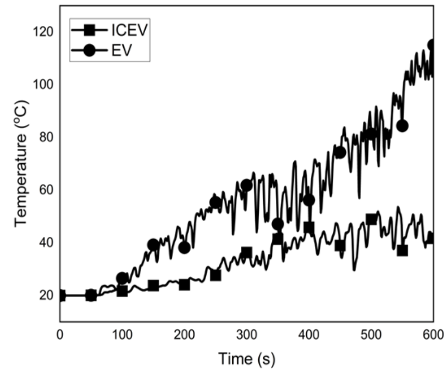


<Temperature change>

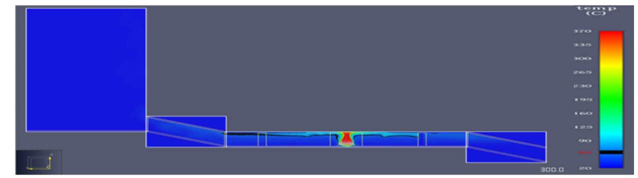
- **We analyzed EV car fire and compared to ICE fire. The EV car fire is dramatic.**

#2-1 Thermal runaway of Li-ion batteries

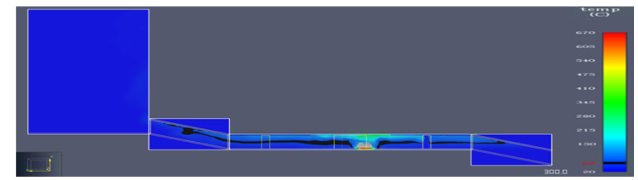




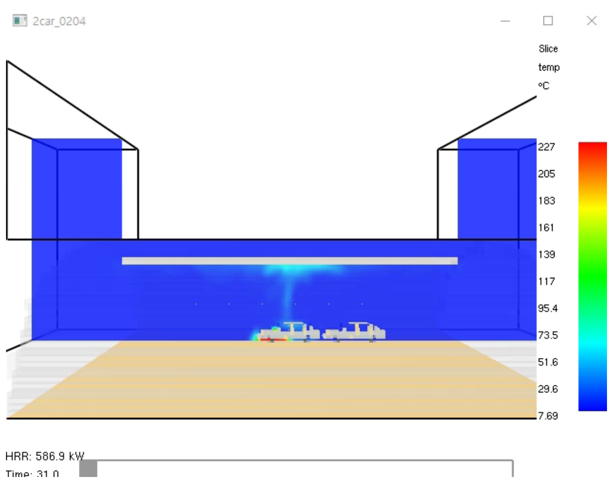
화재 발생시 온도 변화 비교

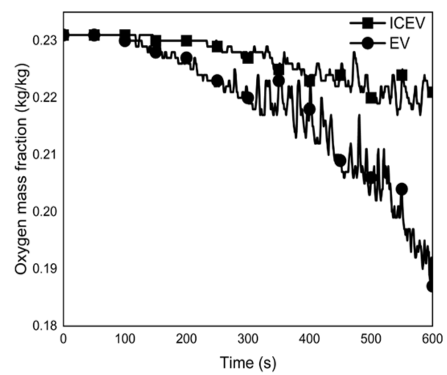


ICEV

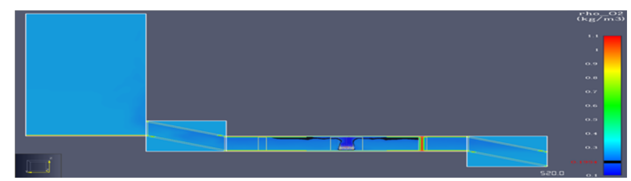


EV

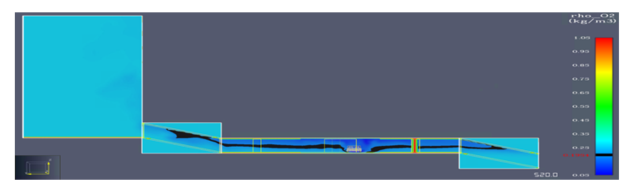




화재 발생시 산소농도 변화 비교



ICEV



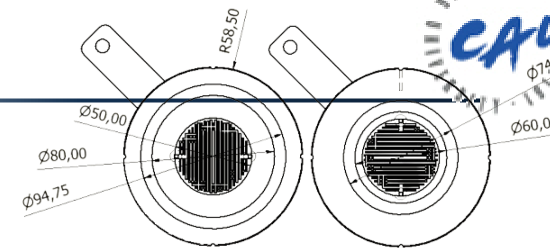
EV

<Comparison of fire propagation>

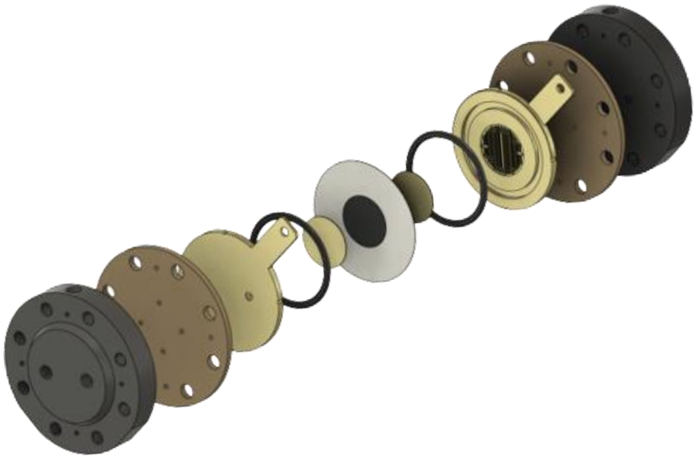
<Fire of EV car in the basement>

- We analyzed danger of EV car fire by comparing ICE car fire. EV is more dangerous.

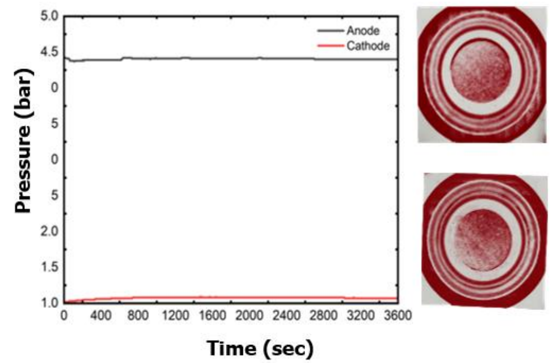
#2-2 Electrochemical compressor



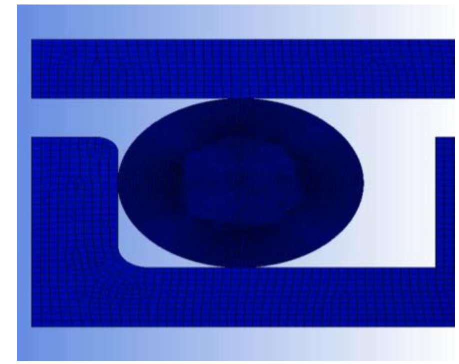
❖ Electrochemical hydrogen compressor



<Electrochemical hydrogen compressor>



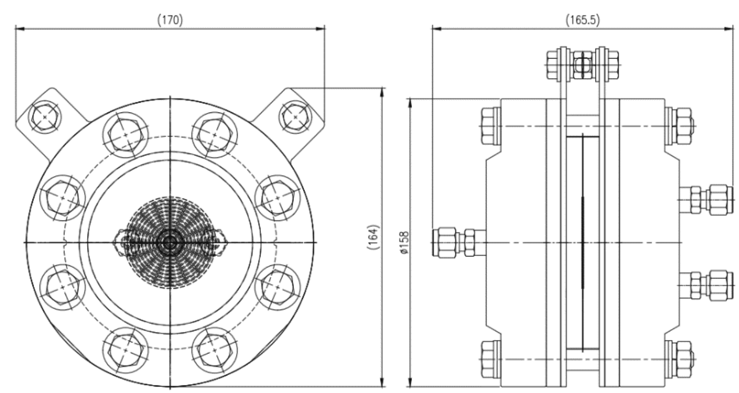
<Sealing test>



<Gasket design>

Nafion™ XL	Nafion™ 212	Nafion™ 115	Nafion™ 117
진행 X	1단계 실험결과 차압 6 bar	40 bar 이상 버팀	40 bar 이상 버팀
효율 89% 달성	효율 86% 1단계 실험결과 차압 6 bar	효율 85%	시작전압 0.4V 이상 막손상 우려로 중단
 체결 시 막 찢어짐	.	효율 85% 이하 설계 변경 후 다시 실험예정	.
 체결 시 막 찢어짐	 체결 시 막 찢어짐	효율 85% 이하 설계 변경 후 다시 실험예정	.

<Membrane selection>

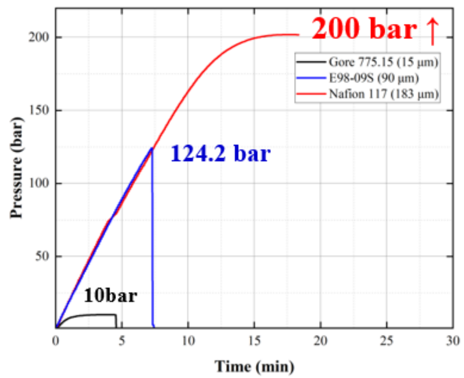


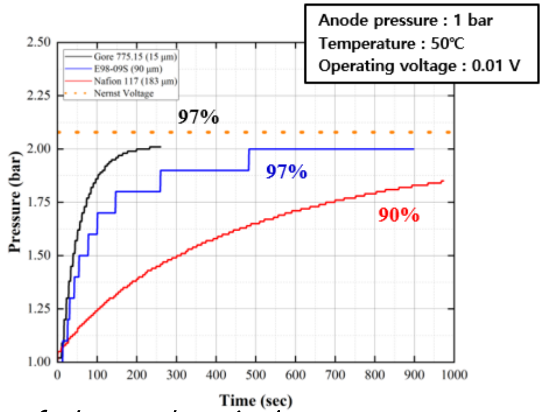
<Design electrochemical compressor>

- **Electrochemical compressor is similar to electrolysis cell that can compress target gas to over hundreds bars.**

#2-2 Electrochemical compressor

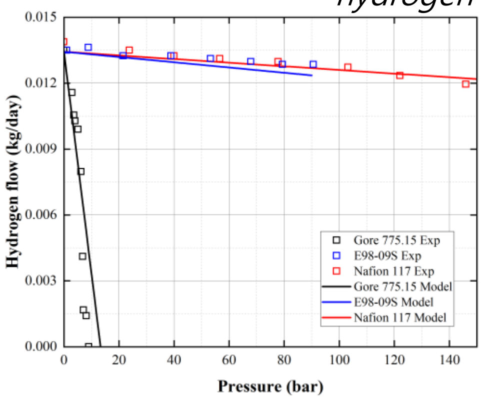
❖ Electrochemical hydrogen compressor

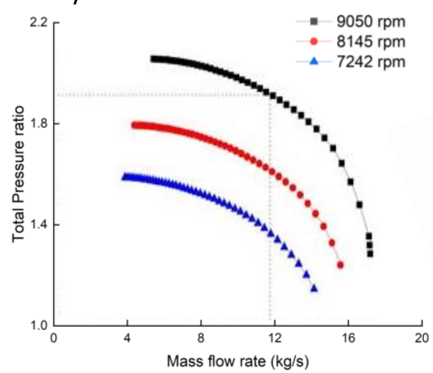




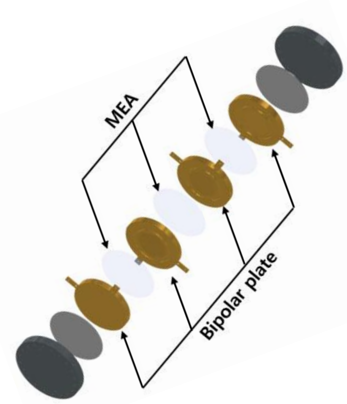
<performance of electrochemical hydrogen compressor>

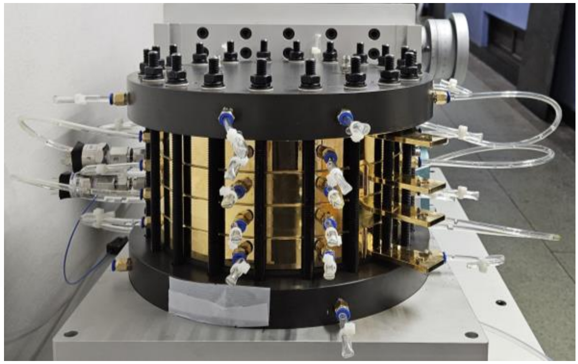
<10 bar EHC>





<Characteristic of EHC>



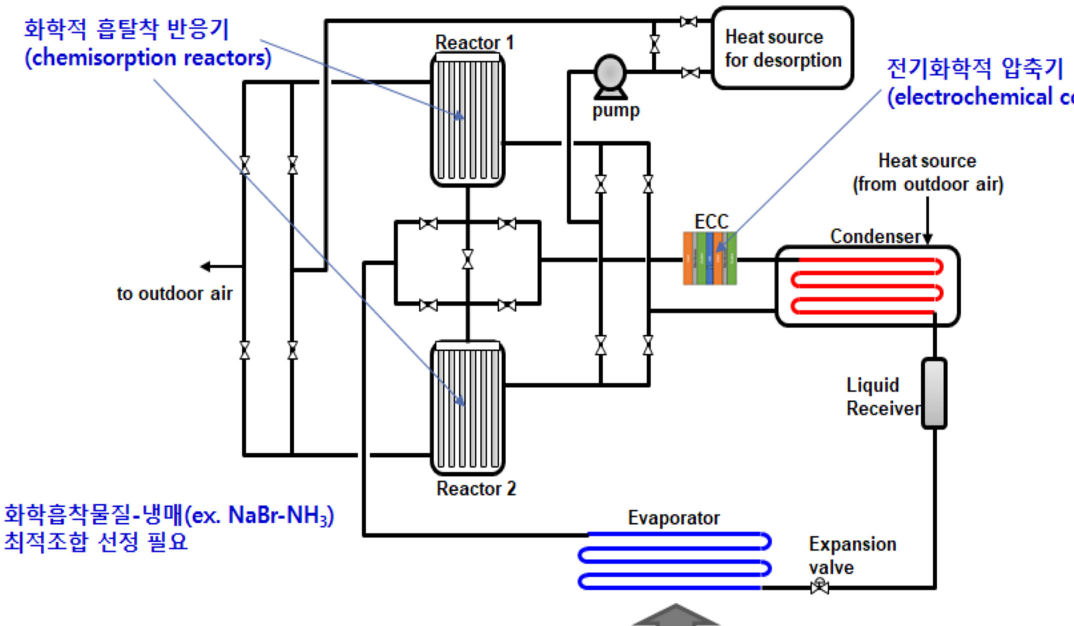


<large capacity compressor>

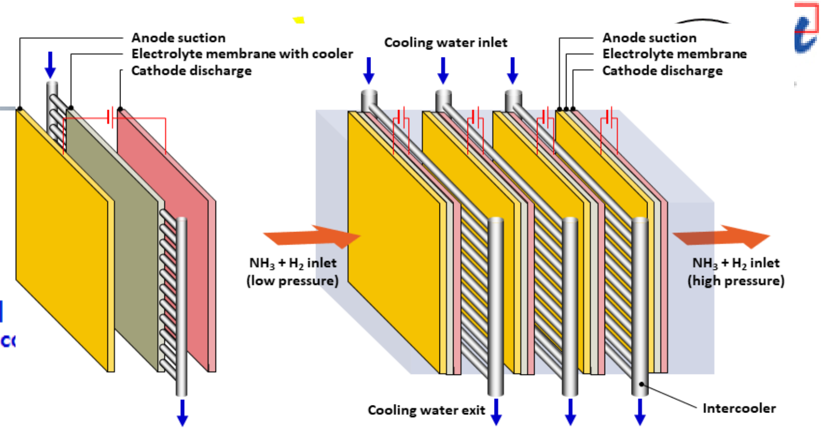
- The EHC shows almost constant mass flow rate according to pressure difference.
- The efficiency of EHC is much higher than that of mechanical compressor.

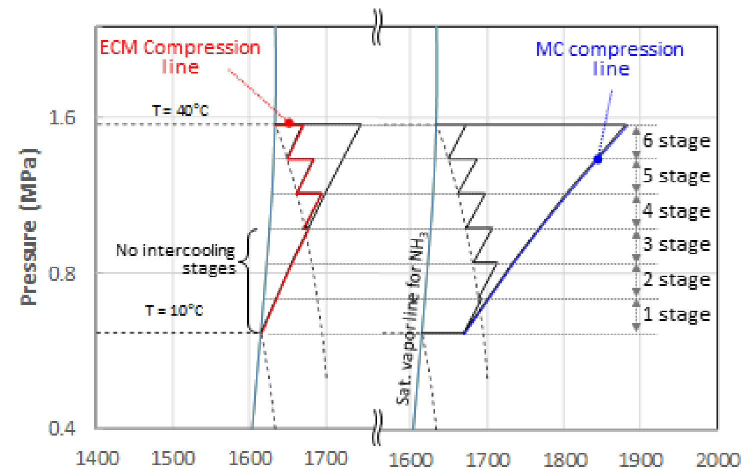
#2-2 Electrochemical compressor

❖ Alchemist project (2019~2025)



<Schematics of chemisorption heat pump>





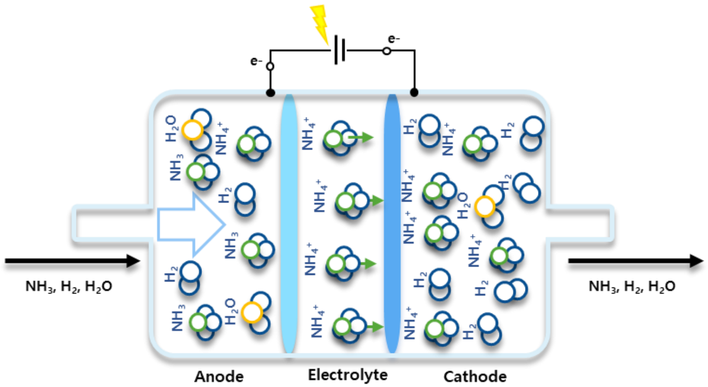
<HP with ECC>

- **Chemisorption heat pump :**

- Through the electrochemical compressor, we can decrease the pressure of chemisorption reactor and manage the pressure and temperature simultaneously. Therefore, COP of the cycle can be further increased.
- The electrochemical compressor can compress refrigerant in isothermal process, because intercooling channel is located between the membrane.

#2-2 Electrochemical compressor

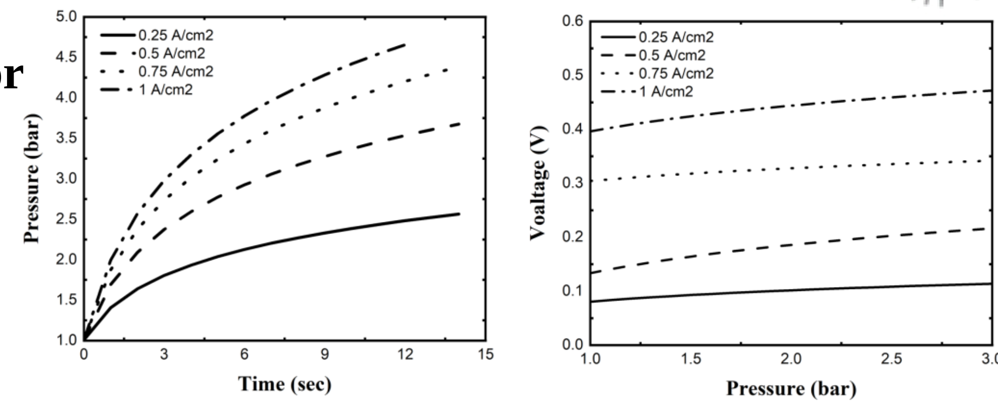
❖ Electrochemical Ammonia compressor



Anode $: 2NH_3 + H_2 \rightarrow 2NH_4^+ + 2e^-$

Cathode $: 2NH_4^+ + 2e^- \rightarrow 2NH_3 + H_2$

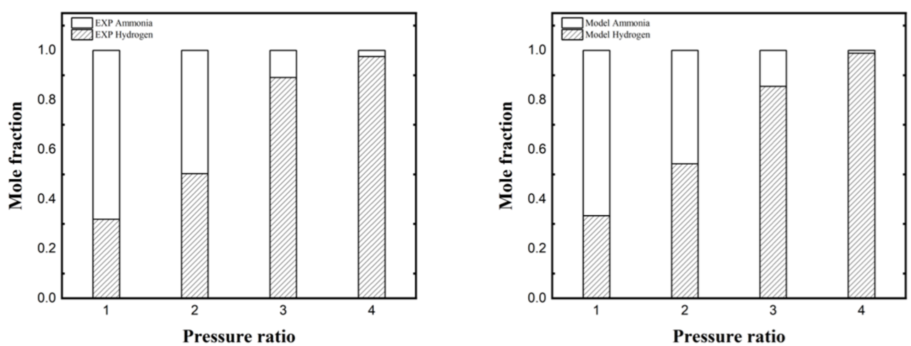
<Electrochemical ammonia compressor>



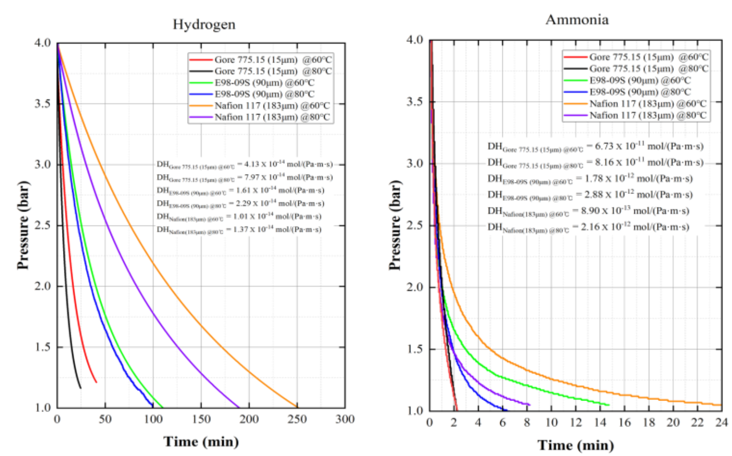
<changes in outlet pressure>

Area [mV.s]	Height [mV]	Area [%]	Compound Name
2144.552	803.655	31.2	Hydrogen
2055.837	394.018	65.9	Ammonia
279.146	24.069	2.9	Water
4479.535	1221.741	100.0	

<Constituent of gas at compressor outlet>



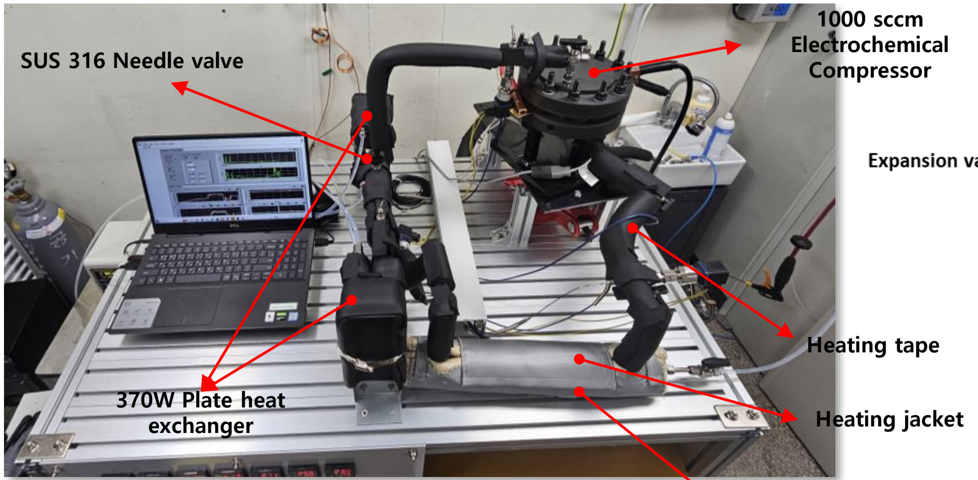
<NH3/H2 mole fraction depending on pressure ratio>



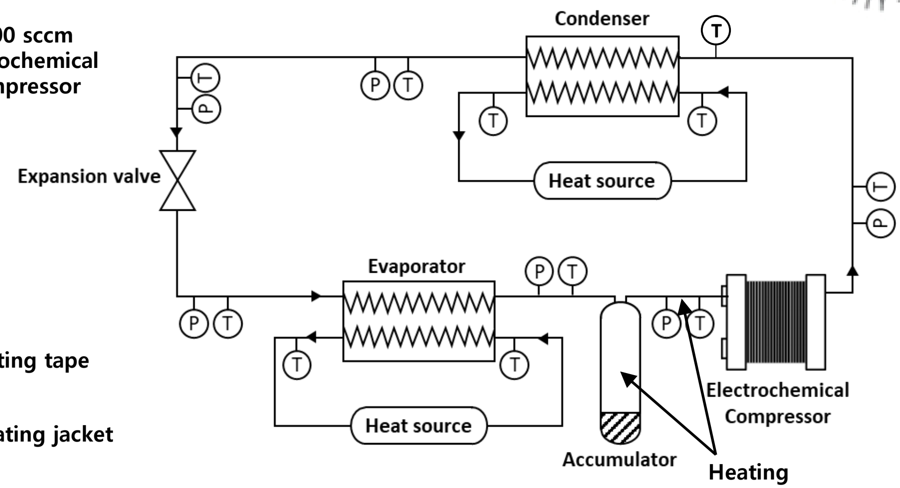
<Effect of back diffusion>

- **The EAC uses $H_2/NH_3/H_2O$, so it needs special management.**

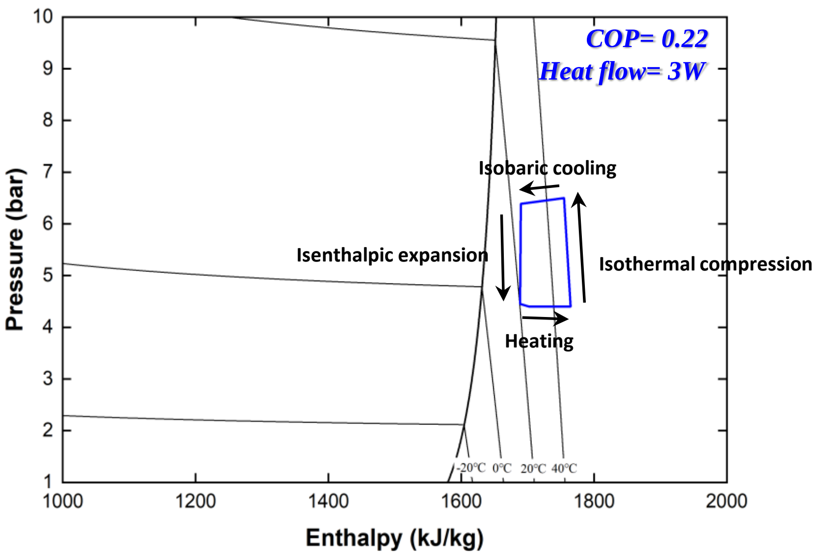
#2-2 Electrochemical compressor



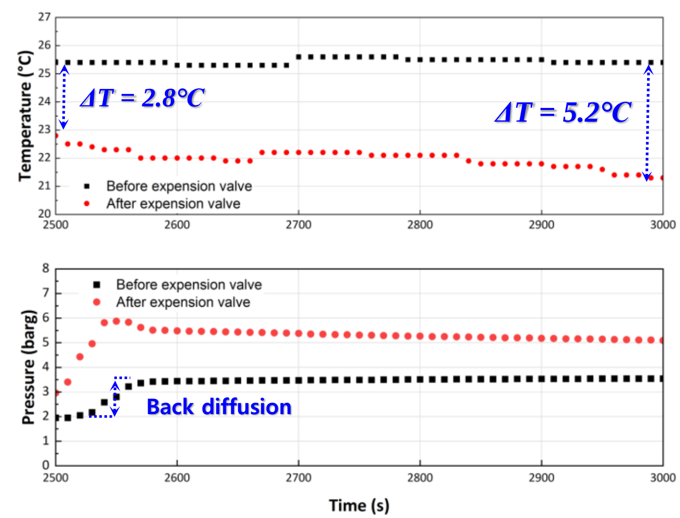
<Picture of HP with ECC>



<Schematic diagram of HP-ECC>



<P-h diagram of HP-ECC>



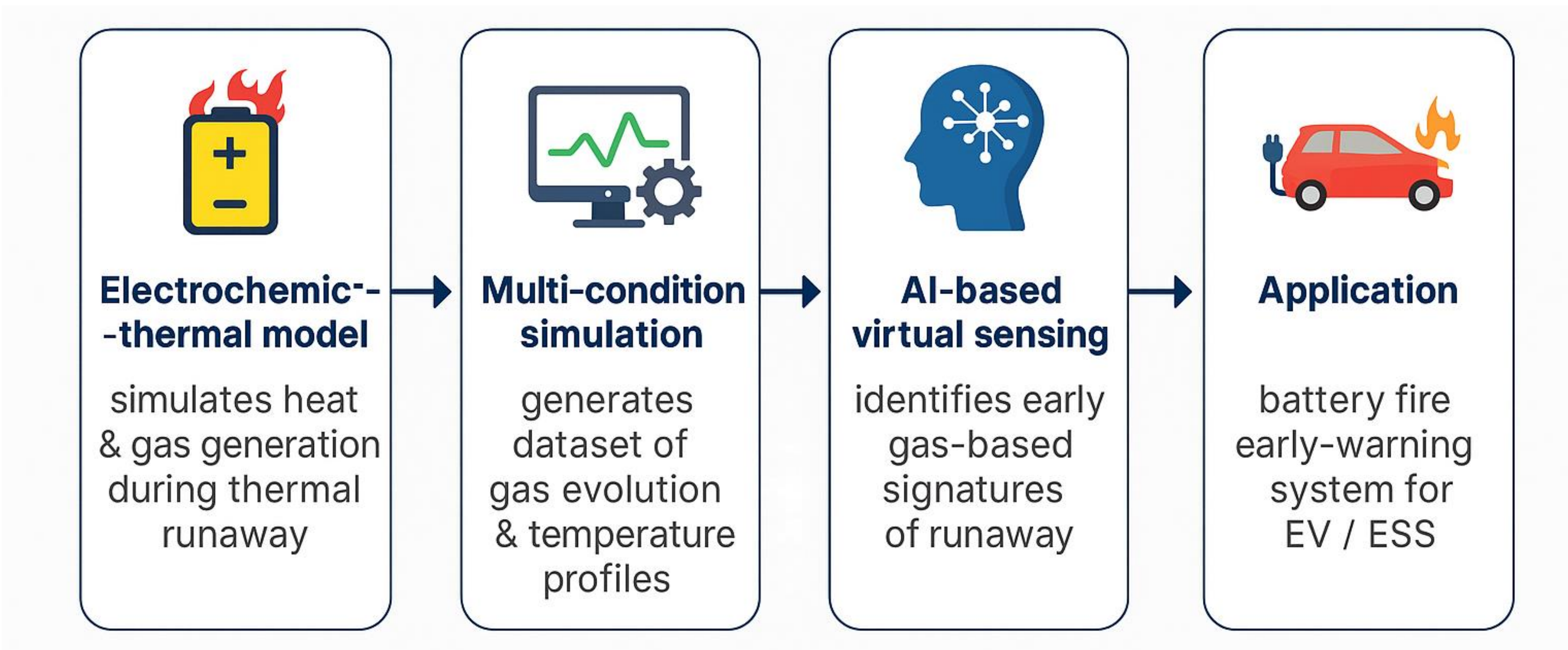
<(Up)Temperature change, (down) Pressure change>

- Manu improvements are needed in the electrochemical compressor for use in the thermodynamic cycle.

3. Research proposal

#3-1 Research proposal

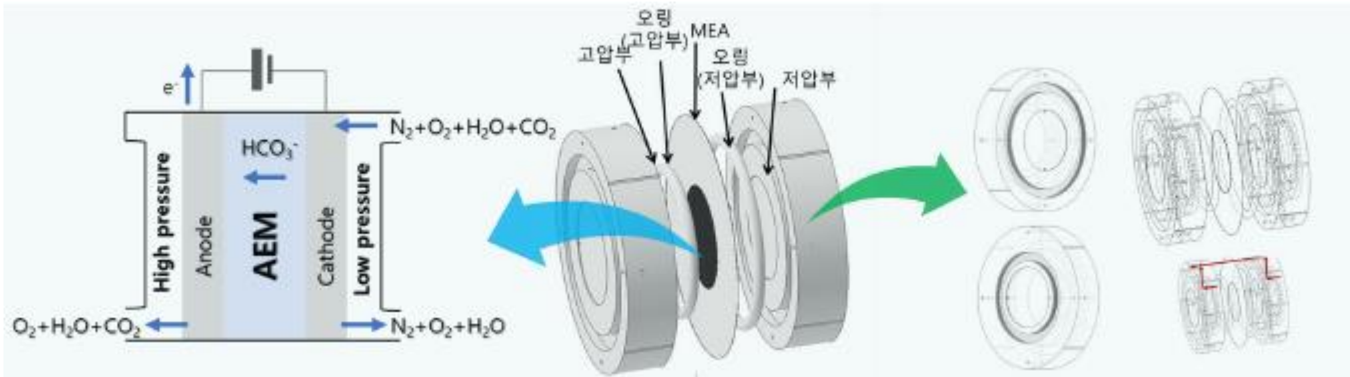
❖ **Targeted call: HORIZON-CL5-2027-03-D5-06: Fire prevention and mitigation for EVs in confined areas (2ZERO Partnership)**
>> Main objectives: Virtual sensor for on-board fire detection



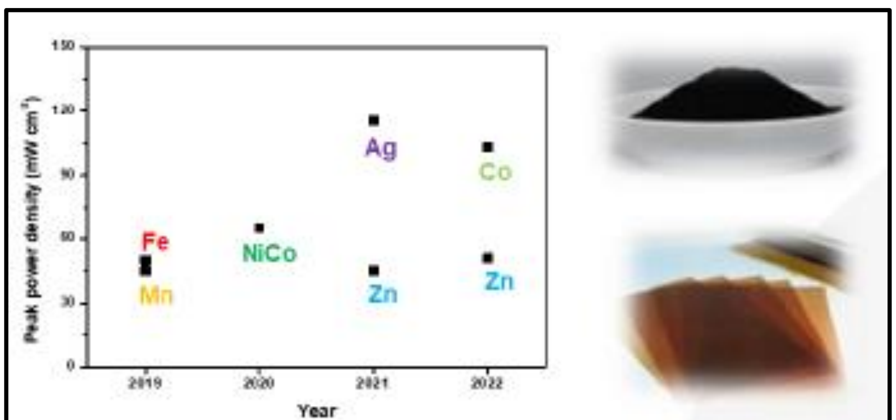
- **Early detection of battery thermal runaway through model-based sensing.**
- **Reduction in dependency on expensive physical gas sensors.**
- **Improved safety for EVs, ESS battery systems.**

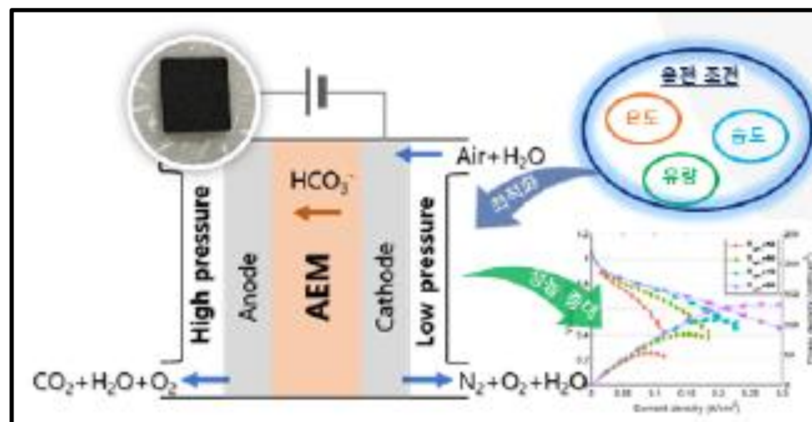
#3-2 Research proposal

❖ **Targeted call: HORIZON-CL5-2027-02-D3-31: Advancements in Direct Air Capture**
>> Main objectives: Electrochemical CO2 separation cell for direct air capture



▪ Electrochemical CO2 separation using anion exchange membrane cell





▪ Performance analysis depending on membrane, catalyst, GDL, and channel.

▪ Design stack to prevent leakage problem under high pressure condition.

Thank you

ElectroChemical Application for advanced energy System Laboratory