Numerical evaluation of simultaneous cooling and heating absorption system using H_2O/ionic liquid and R32/ionic liquid as working fluids

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Contents

1. Research purpose

1-1 Background [Climate Change conferences]

- ✓ International movement to counter climate abnormalities
- ✓ Various agreements such as the 1992 UNFCCC, 1997 Kyoto Protocol, and the 2015 Paris Agreement
- ✓ Influencing the direction of various industries

Fig. 1 UNFCCC.

Fig. 2 Kyoto protocol.

Fig. 3 Paris Climate Change Accord.

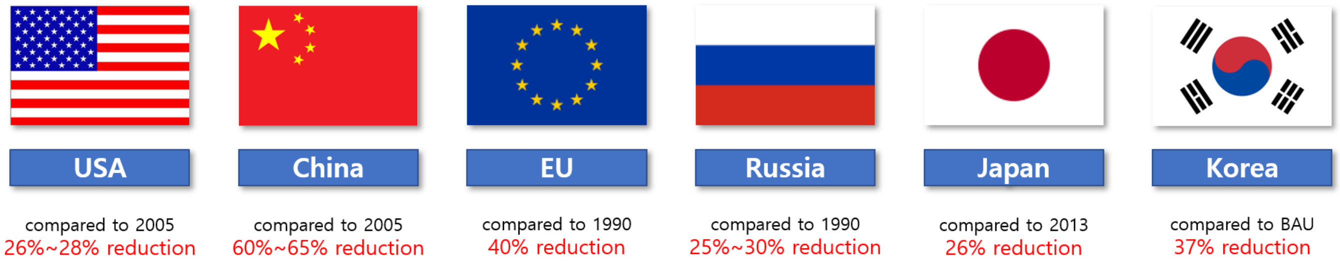

Fig. 4 Greenhouse gas reduction targets of six major countries.

1-1 Background [Necessity for waste heat utilization]

- ✓ About 68% of energy is wasted across industries
- ✓ In the case of waste heat among the energy wasted, low-temperature waste heat below 200°C possesses 66% of the total waste heat
- ✓ Absorption systems that can utilize low-temperature waste heat are starting to attract attention

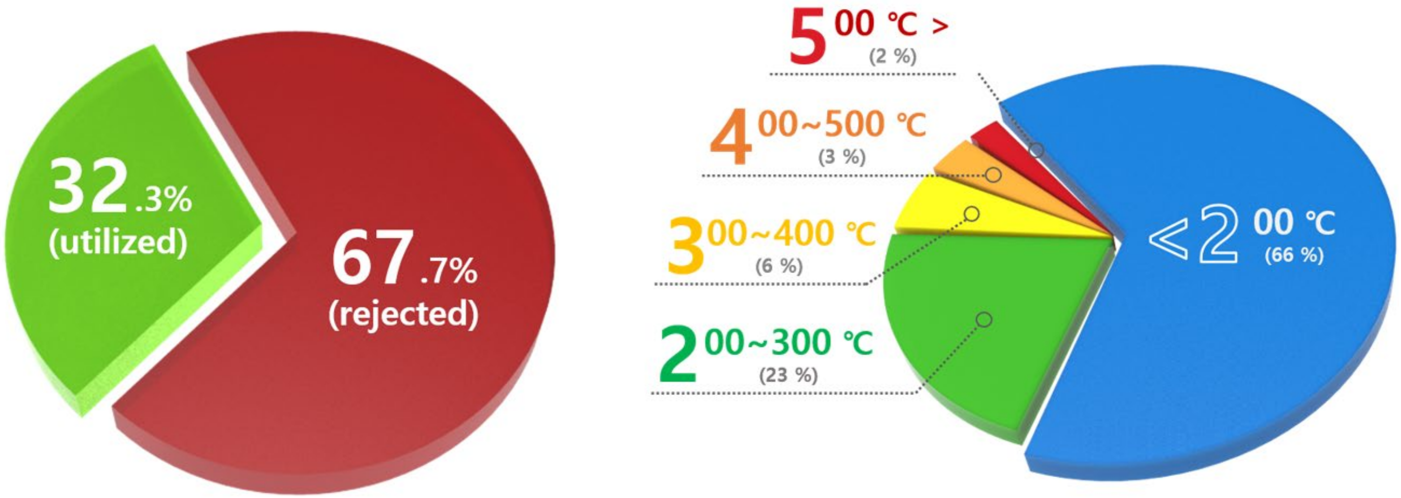

Fig. 5 (Left) electricity conversion efficiency of average energy technology and (right) temperature distribution of waste heat.

1-1 Background [Absorption system]

- ✓ A system that can achieve cooling and heating effects through generation, condensation, evaporation, and absorption processes
- ✓ Depending on the working fluid (refrigerant/absorbent), it can be operated at a relatively low temperature (90°C~)
- ✓ Most commercial working fluids are H_2O/LiBr, NH_3/H_2O

Fig. 6 Absorption heat pump *2

1-2 Necessity [Problems and Solutions of Existing Absorption Systems]

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- ✓ The working fluid of the existing commercial absorption system has clear problems.
- ✓ Developing new working fluids and solving problems using Imidazolium-based ionic liquids

Table 1. Advantages and disadvantages of working fluid.

Existing working fluid	Disadvantages
H_2O/LiBr	**Poor circulation due to absorbent crystallization**
	High corrosivity
	High production cost due to relatively large heat transfer area
	Vacuum design
NH_3/H_2O	**High toxicity**
	High flammability and explosivity
	High pressure design

Strengths of ionic fluid
Exists as a liquid over a wide temperature range (-150°C to 400°C)
Low corrosivity
Low toxicity
Low flammability
High thermostability even at a temperature of 400K
High thermal conductivity and low specific heat

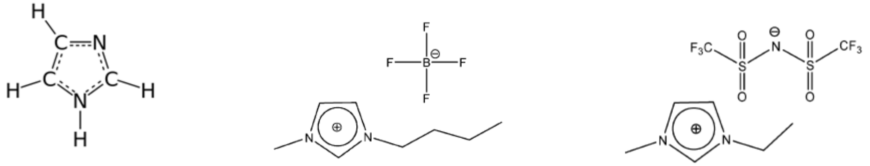
1-2 Necessity [Ionic liquid]

✓ What is an ionic liquid?

It refers to a salt in a liquid state. The constituent molecules are not neutral molecules, but cation and anion molecules, and have a low melting point, high evaporation point, vapor-free pressure, and high thermal stability.

✓ What is Imidazolium ionic liquid?

1. The most stable substance among ionic liquids
2. Since it is an ionic liquid that is being studied most actively, it is relatively easy to secure physical properties.
3. Exists as a liquid at 15°C to 400°C
4. Aromatic heterocyclic compound of formula $C_3H_4N_2$



(a) (b) (c)

Fig. 7 Imidazolium ILs
(a) Imidazol, (b) [BMIM][BF_4], (c) [EMIM][Tf_2N].

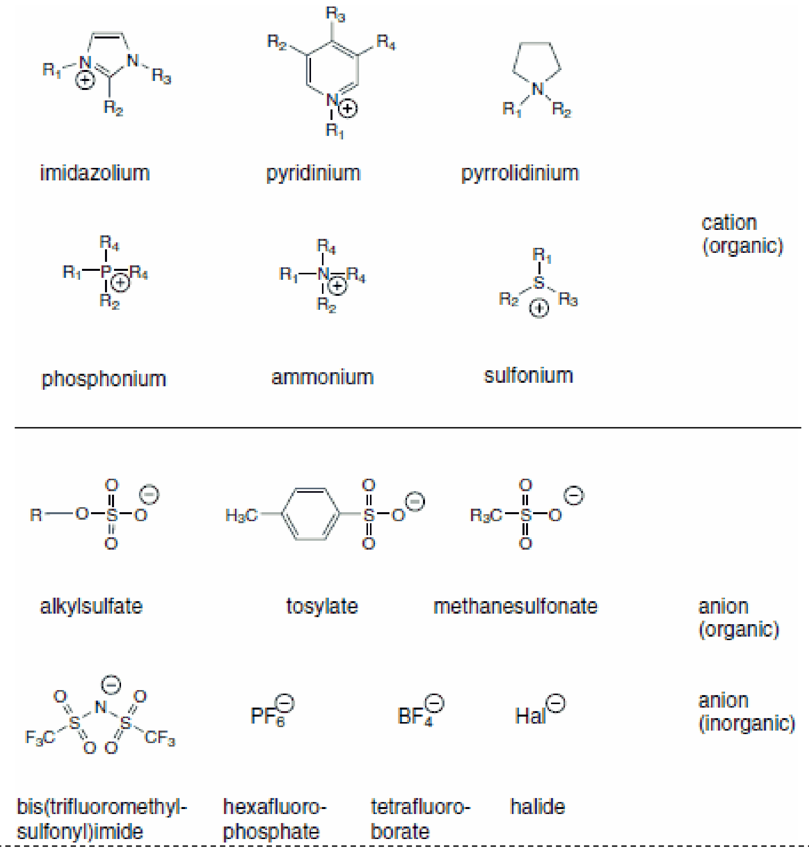


Fig. 8 Types of ionic liquid.

1-3 Previous researches

- ✓ Refrigerant/ionic liquid combination investigation
- ✓ Most of the Type I absorption simulation studies

Table 2. List of references.

[1] Wu et al, 2019	[13] PreiZinger et al, 2013
[2] Kim et al, 2012	[14] Liu et al, 2019
[3] Kühn et al, 2020	[15] Shiflett and Yokozeki, 2006
[4] Kim and Kohl, 2014	[16] Zheng et al, 2014, Review
[5]Wu Wei, 2018	[17] Takalkar et al, 2019
[6] Zhang and Hu, 2011	[18] Khamooshi et al, 2013, overview
[7] Dong et al, 2012	[19] Moreno et al, 2018
[8] Yokozeki and Shiflett, 2010	[20] He et al, 2018
[9] Zuo et al, 2010	[21] Wu et al, 2018
[10] Wang et al, 2007	[22] Liu et al, 2016
[11] Sujatha and Venkatarathnam, 2018	[23] Sun et al, 2020
[12] Zhang and Hu, 2012	

Table 3. Refrigerants, cations and anions of ionic fluid.

Refrigerant
H_2O
R32
R152a
R1234ze(E)
R1234yf
R1233zd

Ionic liquid cation
DMIM
EMIM
EEIM
BMIM
HMIM
OMIM

Ionic liquid anion
Ac
BF_4
Cl
$C_2H_5SO_4$
$(CH_3)_2PO_4$
$(C_2H_5)_2PO_4$
DMP
DEP
$EtCO_2$
$EtSO_4$
PF_6
Tf_2N
TfO

1-4 Research purpose

1. Development of simulation model configuration for simultaneous cooling and heating absorption system

2. Performance evaluation according to working fluid selection and generation temperature

3. Performance comparison analysis for each working fluid

2. Research method

2-1 Simulation modeling

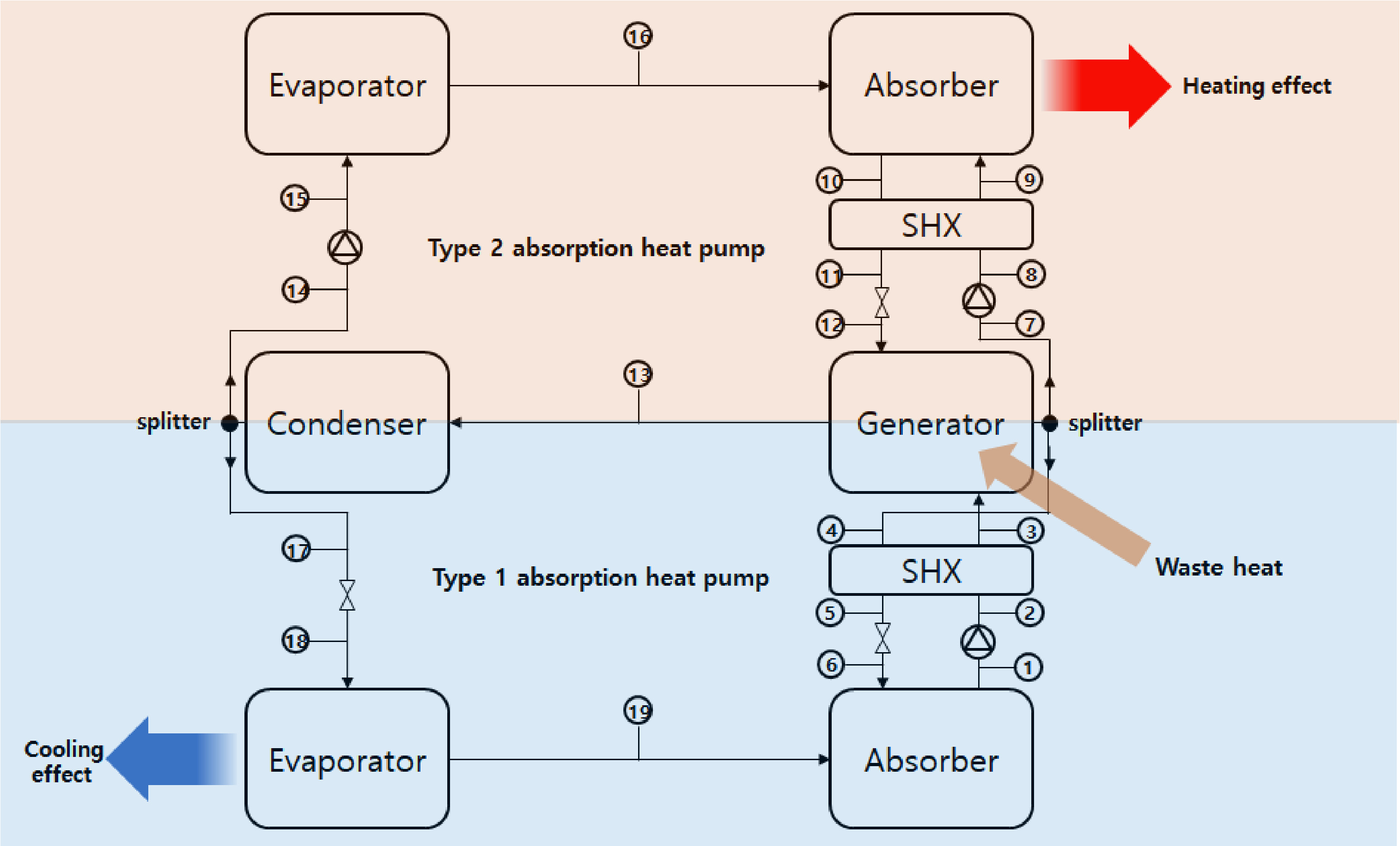


Fig. 9 Schematic diagram of simultaneous cooling and heating absorption system.

2-1 Simulation modeling

- ✓ Model composition : generator / condenser / evaporator / absorber / solution heat exchanger

- ✓ Cycle modeling :
  - Mass balance equation
  - Energy balance equation
  - VLE equilibrium
  - NRTL model (Non-Random Two-Liquid model)

- ✓ Assumptions

① Evaporator outlet : refrigerant saturated vapor,
low pressure 5°C/ high pressure 50°C

② Absorber outlet : solution saturated liquid, vapor-liquid equilibrium,
low pressure 30°C / high pressure 77°C

③ Generator outlet : vapor-liquid equilibrium

④ Ignoring changes in mixing enthalpy for solutions that are not in equilibrium

⑤ Ignoring pressure drop

2-1 Simulation modeling

✓ Calculation of cycle operation characteristics according to generator outlet temperature

⇒ (1) $COP_{cooling} = \frac{\dot{Q}_{evap1}}{\dot{Q}_{gen}}$ (2) $COP_{heating} = \frac{\dot{Q}_{abs2}}{\dot{Q}_{gen}}$ (3) $COP_{total} = COP_{cooling} + COP_{heating}$

✓ Key parameters

(1) $r_g(Split\ ratio\ of\ generator) = \frac{m_7}{m_4 + m_7}$

(2) $r_c(Split\ ratio\ of\ condenser) = \frac{m_{14}}{m_{14} + m_{17}}$

(3) $T_{gen} = T_4$

2-1 Simulation modeling

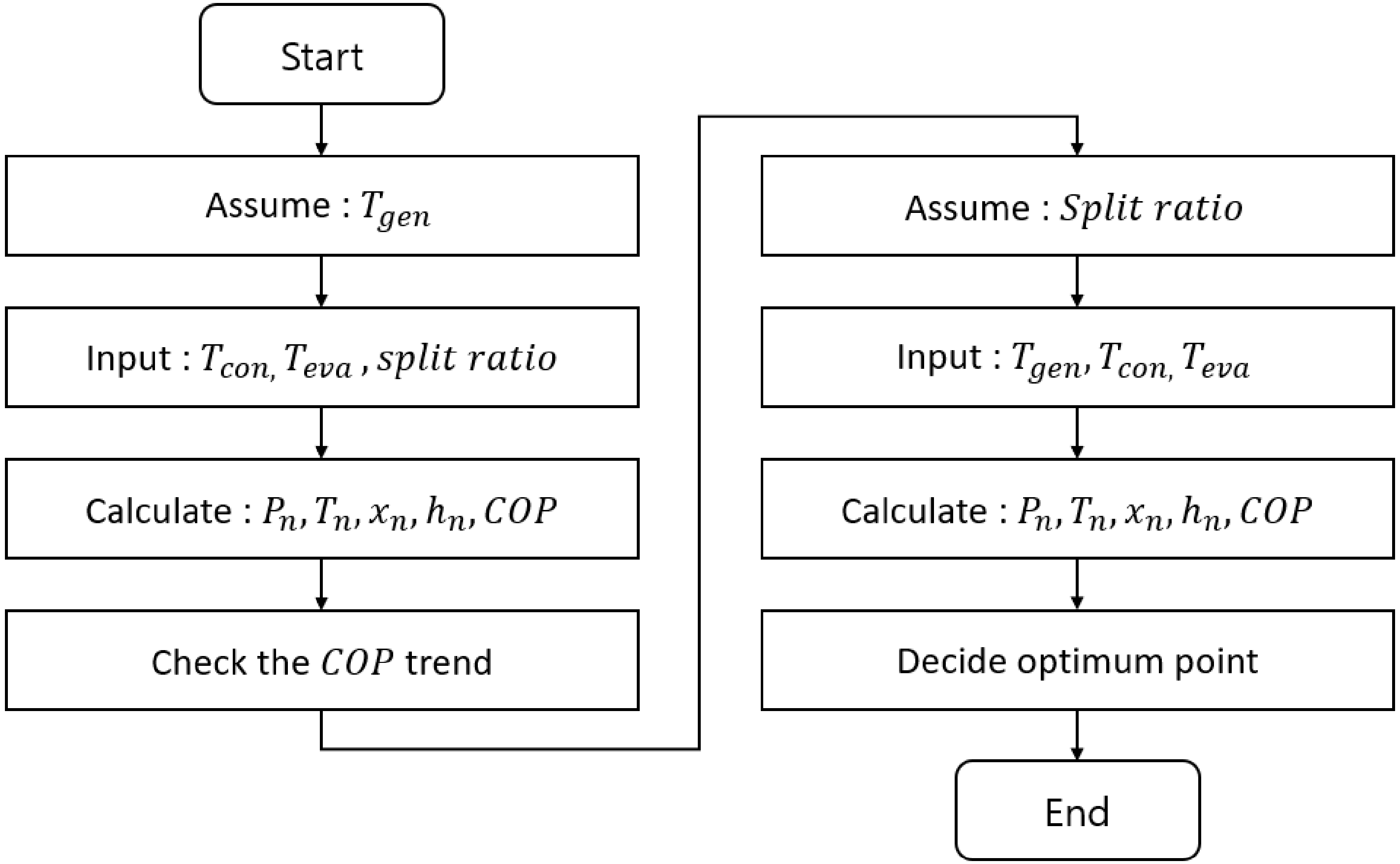


Fig. 10 Simulation flow chart

2-2 Selecting working fluid

✓ Why H_2O, R32 refrigerant?

H_2O :
1. Most commercial refrigerants for absorption system
2. Solving the biggest problems with considering the direction of keeping refrigerant

R32 :
1. Refrigerant exhibiting the highest COP excluding water
2. Availability of sub-zero cooling
3. advantageous for miniaturization of device, because of smaller specific volume than water

Table 4. Basis for selection of working fluid.

Working fluid	Reason for selection	Ref.
H_2O/[DMIM][(a)][DMP][(d)]	• Easy to collect material properties and data as there are the most research papers • While producing a COP close to that of H_2O/LiBr, the operable temperature range is extended	• [7]
H_2O/[EMIM][(b)][DMP][(d)]	• Lower temperature operation possible than H_2O/LiBr • Higher COP than H_2O/[DMIM][DMP]	• [6] • [13]
H_2O/[EMIM][(b)][BF_4][(e)]	• Highest COP among combinations with H_2O	• [2]
R32/[HMIM][(c)][Tf_2N][(f)]	• Relatively high COP • Ionic liquids with relatively high refrigerant solubility due to their long chemical structure • Analyzed as the most suitable ionic liquid for R32	• [2] • [11] • [11]

(a) : 1,3-Dimethylimidazolium , (b) : 1-Ethyl-3-methylimidazolium, (c) : 1-Hexyl-3-methylimidazolium, (d) : Dimethyl phosphate, (e) : Tetrafluoroborate, (f): bis(trifluoromethylsulfonyl)imide

2-3 Simulation condition

Table 5. Simulation condition of H_2O/[DMIM][DMP], [EMIM][DMP], [EMIM][BF_4].

	Low-temperature absorber outlet	High-temperature absorber outlet	Condenser outlet	High-temperature evaporator outlet	Low-temperature evaporator outlet
Location	1	10	14, 17	16	19
Temperature	30 °C	77 °C	30 °C	50 °C	5 °C
pressure	0.8725 kPa	12.35 kPa	4.247 kPa	12.35 kPa	0.8725 kPa
State	solution liquid	solution liquid	refrigerant liquid	refrigerant vapor	refrigerant vapor

Split ratio generator : 0.9 / condenser : 0.9

Table 6. Simulation condition of R32/[HMIM][Tf_2N].

	Low-temperature absorber outlet	High-temperature absorber outlet	Condenser outlet	High-temperature evaporator outlet	Low-temperature evaporator outlet
Location	1	10	14, 17	16	19
Temperature	30 °C	77 °C	30 °C	50 °C	5 °C
Pressure	951.5 kPa	3141 kPa	1928 kPa	3141 kPa	951.5 kPa
State	solution liquid	solution liquid	refrigerant liquid	refrigerant vapor	refrigerant vapor

Split ratio generator : 0.9 / condenser : 0.9

- ✓ **Software : EES (Engineering Equation Solver)**
- ✓ **Thermodynamic properties :** EES(Pure substances and gas mixtures), NRTL model(Property prediction chemistry model)

3. Results

3-1 Result [variable : split ratio]

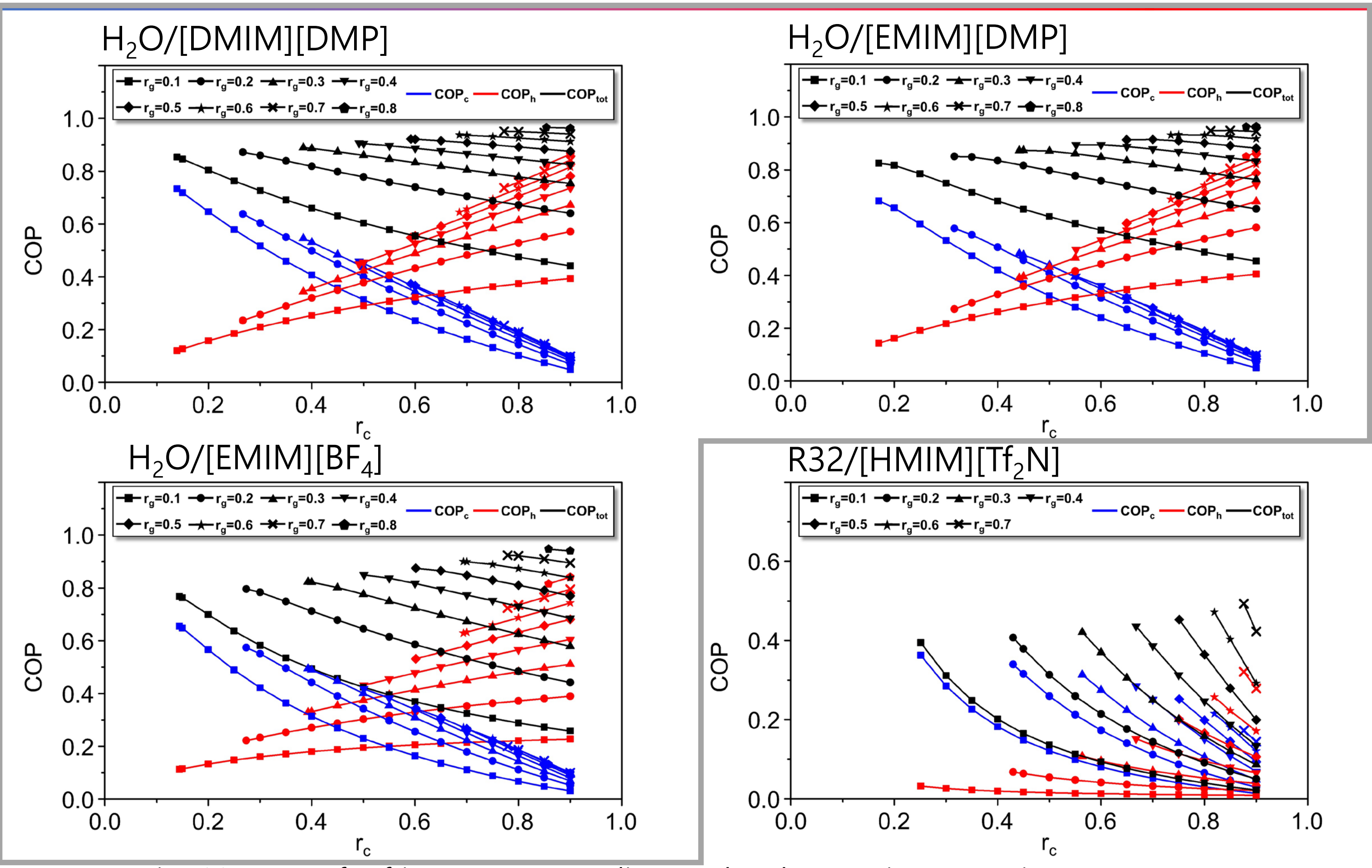


Fig. 11 COPs of refrigerant/IL according to the changes in generation temperature

✓ The r_g, r_c needs to be controlled according to the required cooling and heating load.

3-2 Result [variable : generator outlet solution temperature]

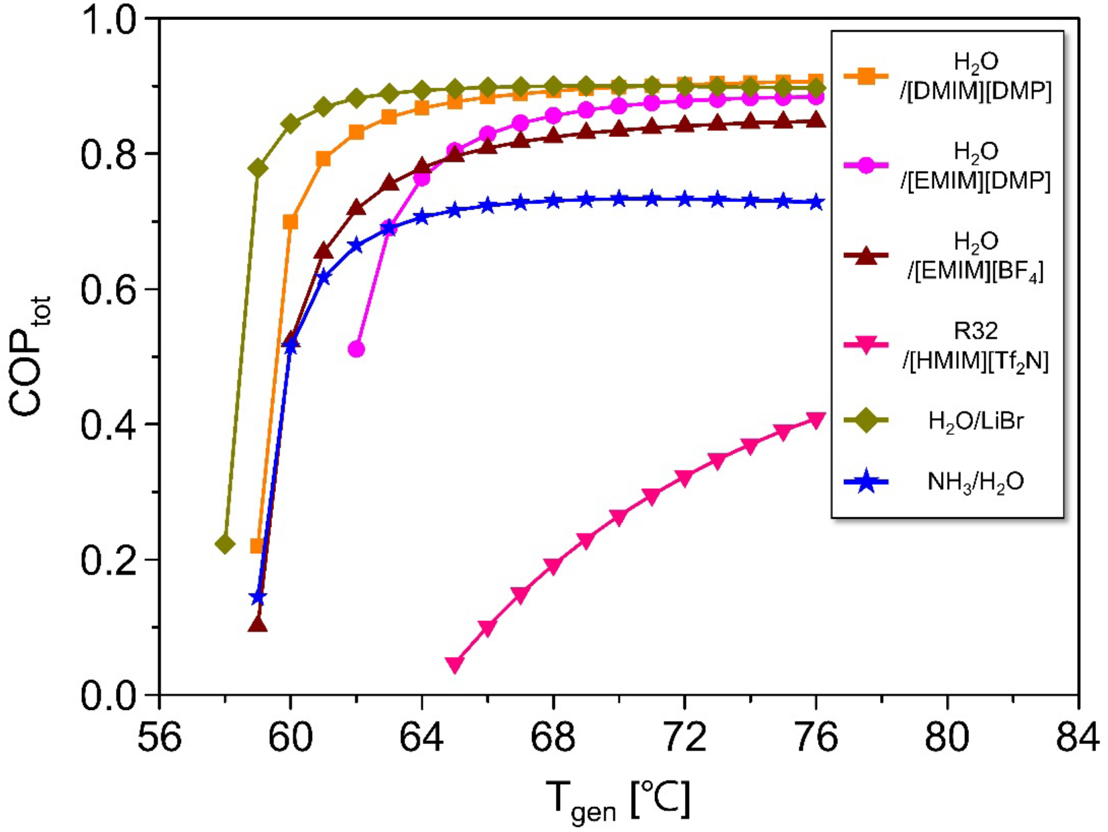


Figure. 12 Simulation results when generator temperature is a variable.

- ✓ Efficiency similar to H_2O/LiBr even when H_2O/ionic liquid is applied to the simultaneous cooling/heating absorption cycle.
- ✓ R32/IL shows about 50% efficiency compared to H_2O/IL.

4. Conclusion

4. Conclusion

(A) Simultaneous cooling and heating absorption system model

- ✓ **Confirmation of COP** and steady state operation characteristics of simultaneous cooling/heating absorption system applied with refrigerant/ionic liquid

(B) Simulation analysis

- ✓ Effect of split ratio
  - As split ratio of the generator ↑, cooling and heating COP of H_2O/IL↑, cooling COP of R32/IL ↓, heating COP of R32/IL ↓
  - **Split ratio of the condenser needs to be controlled** according cooling and heating load
- ✓ Effect of generation temperature
  - COP changes rapidly from the minimum operating temperature
  - Tend to maintain a constant COP above a certain temperature

(C) COP calculation and discussion

- ✓ H_2O based working fluid : cooling COP=0.1, heating COP=0.88, total COP=0.98

  (H_2O/LiBr cooling COP=0.1, heating COP=0.88, total COP=0.98)
- ✓ The selected H_2O/ionic liquid is suitable for simultaneous cooling and heating absorption system
- ✓ R32/ionic liquid needs further research to increase COP

Thank you