Techno-economic optimization of high-temperature heat pumps using pure fluids and binary mixtures

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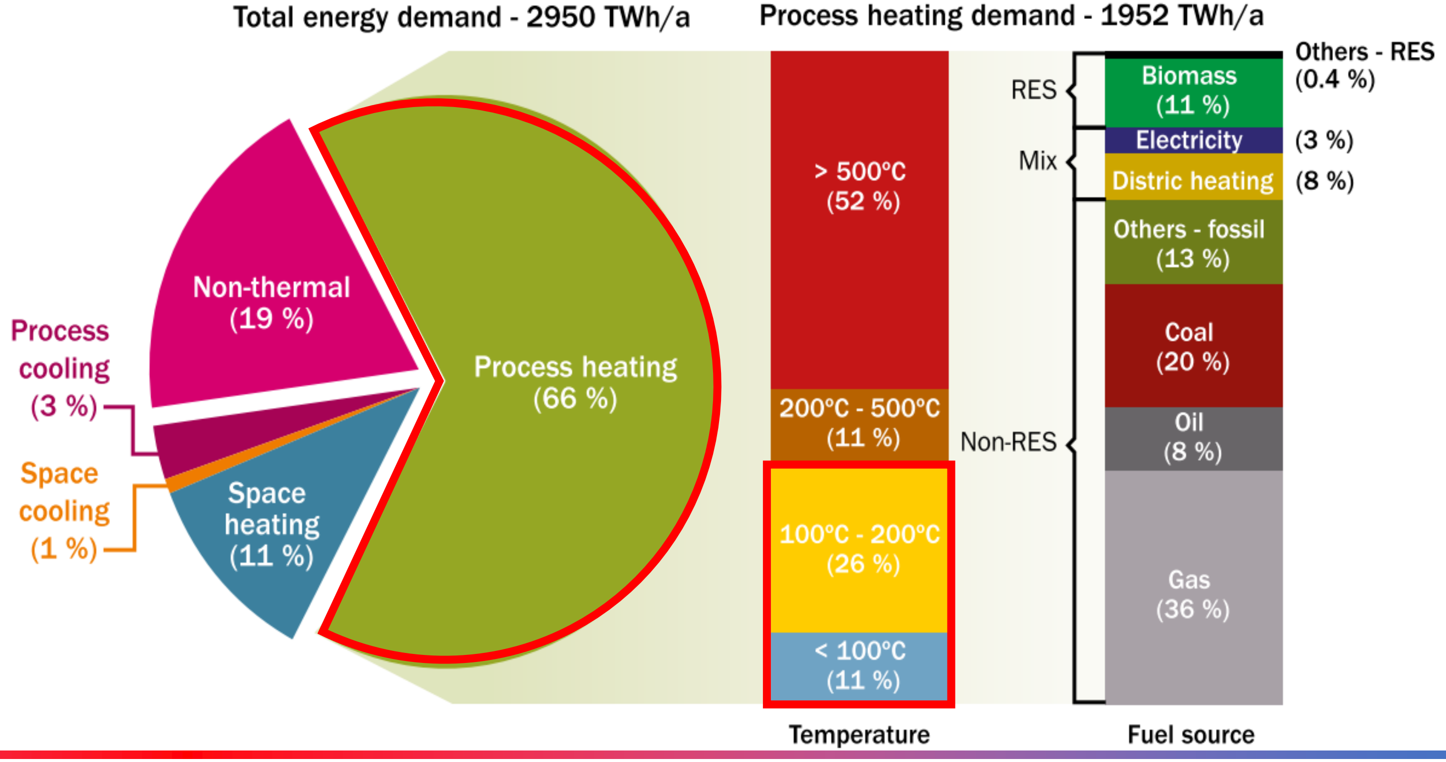
Why high-temperature heat pumps?

- The energy use in industry (2019): 40 % of the global CO_2 emission's
  - ➢ Mainly attributed to the demand in heat.

Total energy demand European industry [2]:



Research gap in high-temperature heat pumps

Research: maximizing COP

- Refrigerant selection
- Heat pump configurations
- Component development/optimization
- …

→ Is the increase in investment cost worth it?

Some research, but:

This research

- Supply temperatures < 120-150 °C → 160-200 °C
- Few working fluids → All fluids within REFPROP 10.0, including binary mixtures
- Specific case studies → Large set of generalized cases
- Simple cycles →

Single stage	Double stage
Internal heat exchange	No internal heat exchange

The starting point: Thermodynamic model

General assumptions:
- No pressure drops
- No heat losses

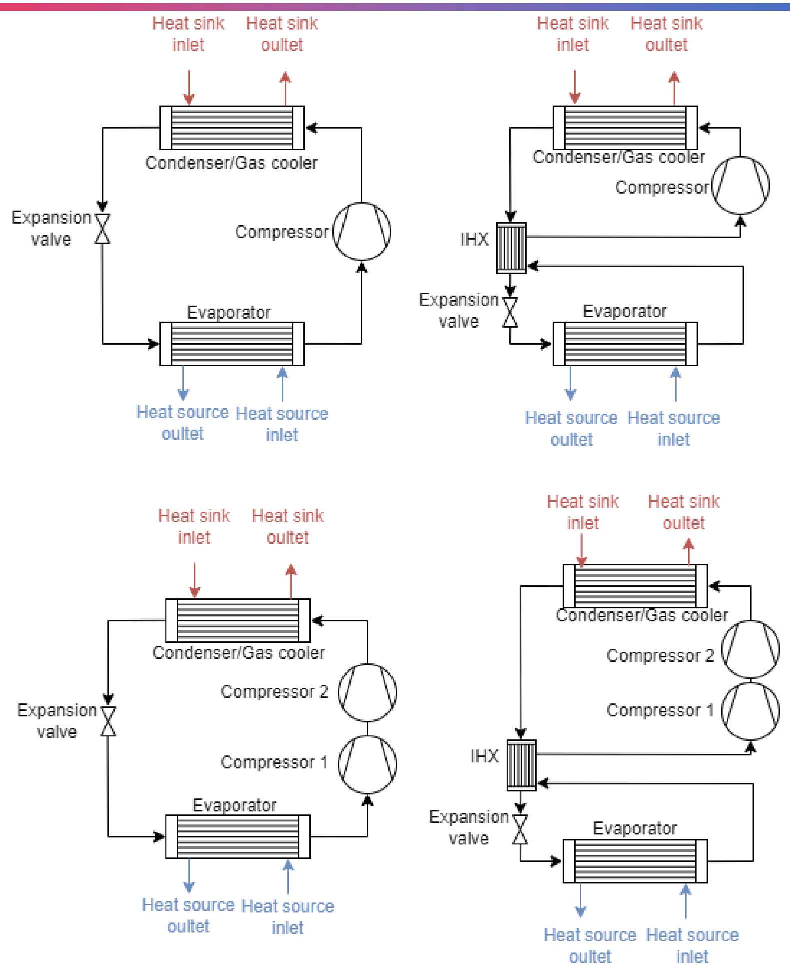
Compressor:
- $\eta_v = 90\ \%$
- $\eta_{is} = 75\ \%$
- $\eta_{drive} = 95\ \%$
- Maximum pressure ratio per stage: 6

Expansion valve:
- Isenthalpic

Evaporator/ condenser/ gas cooler / gas heater:
- Minimum temperature approach

Internal heat exchanger:
- ε: 0.75

Generic model



Extension: Financial aspects

$$LCOH(\text{€/kWhth}) = \frac{C_{CAPEX}+\sum_{t=1}^{n}\frac{C_{OPEX,t}}{(1+i)^t}}{\sum_{t=1}^{n}\frac{Q_t}{(1+i)^t}}$$

Capital expenditure

$C_{CAPEX} = \ C_{TM}$ (Turton et al. [3])

- $C_{comp} = f(\dot{v}_{comp,in})$
- $C_{drive} = f(\dot{W}_{comp})$
- $C_{hex} = f(A)$
- $C_{valve} = f(\dot{m}_{ref})$

Parameter	Value
Heat pump lifetime (n)	15 year
Interest rate (i)	5 %
Maintenance fraction (f_{maint})	0.06
Annual operating hours (h_a)	7000 h
Specific electricity cost (c_e)	0.0806 €/kWh_{el}
Heating capacity ($\dot{Q}_{process}$)	500 kW_{th}

Operational expenditure

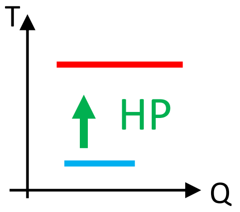
$$C_{OPEX} = C_e + C_{maint} \ = \ c_e \cdot \left(\frac{\dot{Q}_{process}}{\boxed{COP}}\right) \cdot h_a + f_{maint} \cdot C_{CAPEX}$$

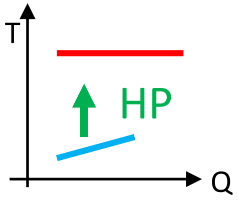
Case studies

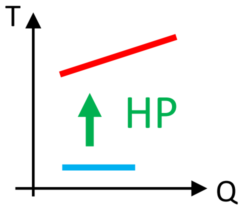
Heat source	Heat sink	Example application
Latent	**Latent**	Distillation
Sensible	**Latent**	Direct steam production from hot water
Latent	**Sensible**	Superheated steam drying
Sensible	**Sensible**	Hot air drying

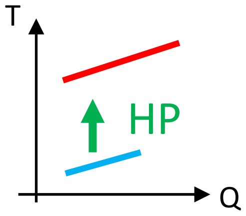
Heat sink outlet temperature: 160 - 200 °C

Heat source inlet temperature: 80 - 120 °C





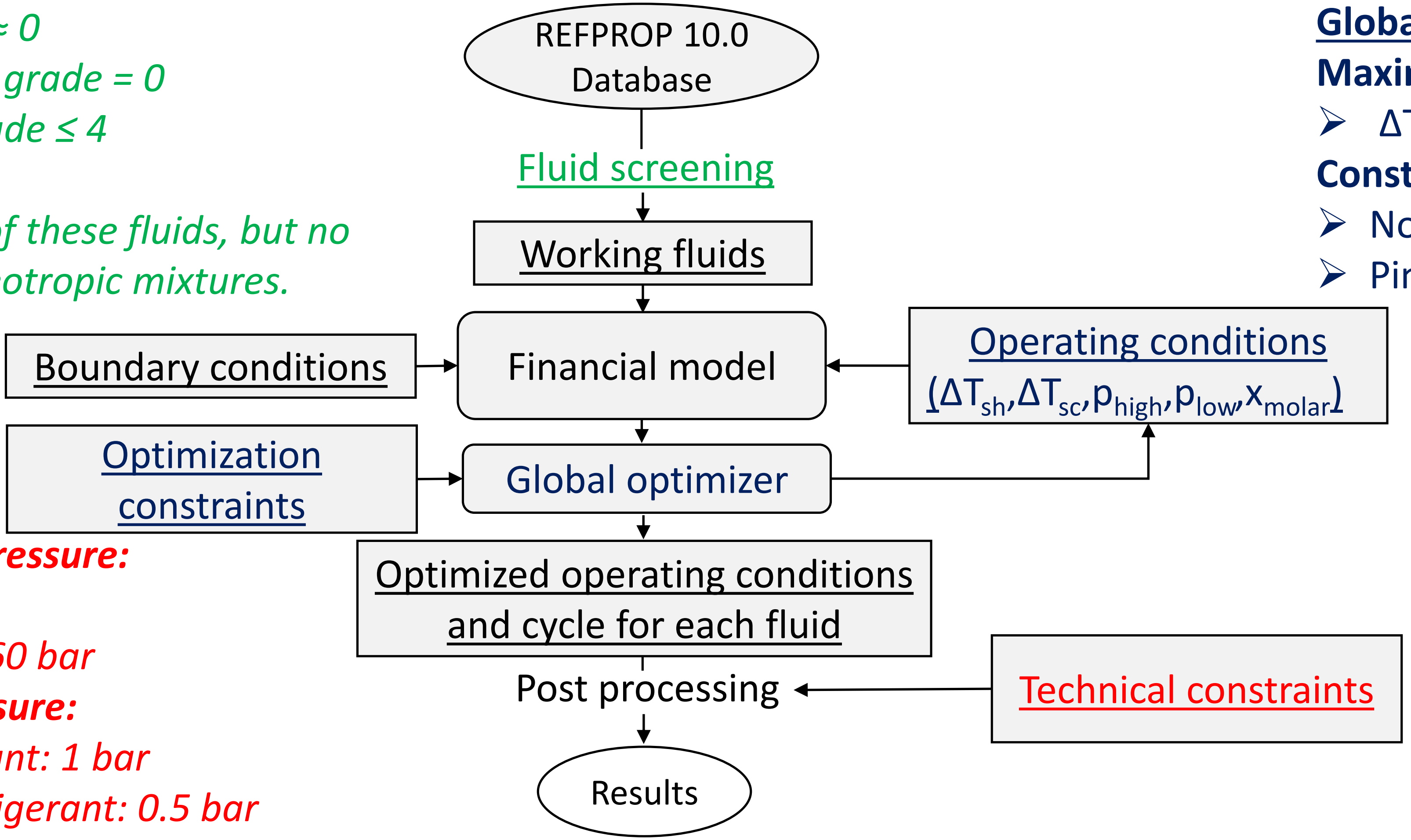




Financial optimization model

- *GWP ≤ 150 & ODP ≈ 0*
- *NFPA 704 instability grade = 0*
- *NFPA 704 health grade ≤ 4*
- *Thermally stable*

→ All binary mixtures of these fluids, but no focus on transcritical zeotropic mixtures.



Global optimizer in SciPy

Maximize LCOH:

- ΔT_{sh}, ΔT_{sc}, p_{high}, p_{low}, x_{molar}

Constraint:

- No wet compression
- Pinch point HEX: 5 K

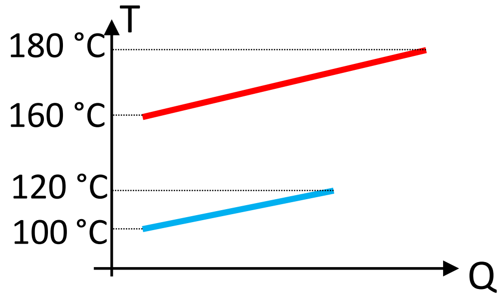
Maximum discharge pressure:

- *CO_2: 150 bar*
- *Other refrigerants: 60 bar*

Minimum suction pressure:

- *Flammable refrigerant: 1 bar*
- *Non-flammable refrigerant: 0.5 bar*

A ‘sensible sensible’ case study: Results



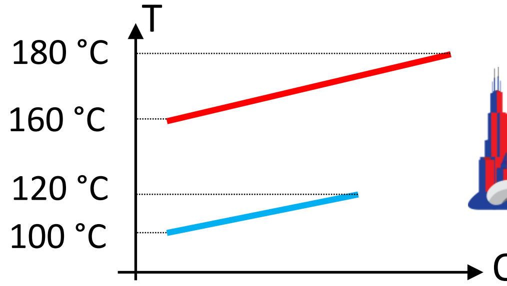
The five best performing working fluids:

Working fluid	Molar fraction first component	Stages	IHX	COP	LCOH [€/kWh$_{th}$]	c_{inv} [€/kW$_{th}$]
Methanol/ammonia	0.685	1	No	3.84	0.0290	372
Cis-2-butene/methanol	0.585	1	Yes	3.56	0.0305	363
Benzene/methanol	0.684	1	Yes	4.10	0.0307	512
Cyclobutene/toluene	0.955	1	Yes	3.45	0.0309	351
Cyclobutene/heptane	0.963	1	Yes	3.46	0.0310	357

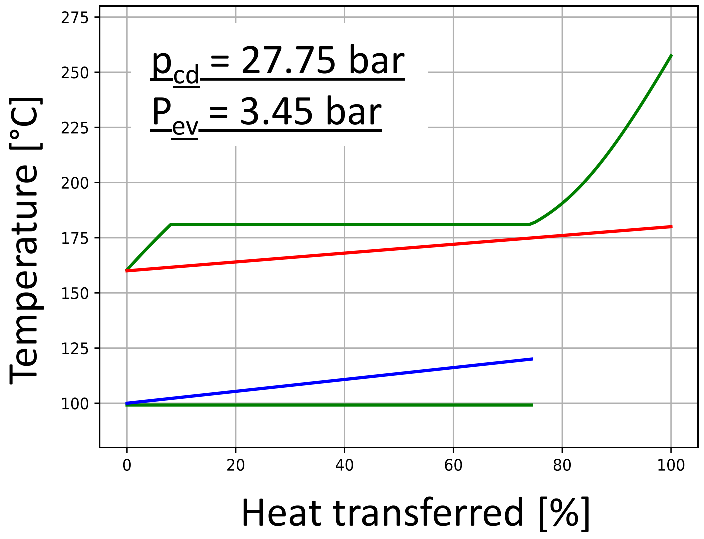
The respective pure working fluids:

Working fluid	Molar fraction first component	Stages	IHX	COP	LCOH [€/kWh$_{th}$]	c_{inv} [€/kW$_{th}$]
Cyclobutene	-	1	Yes	3.37	0.0317	357
Methanol	-	2	No	3.71	0.0331	528
Cis-2-butene	-	1	Yes	3.18	0.0339	396
Benzene	-	2	Yes	3.82	0.0400	871

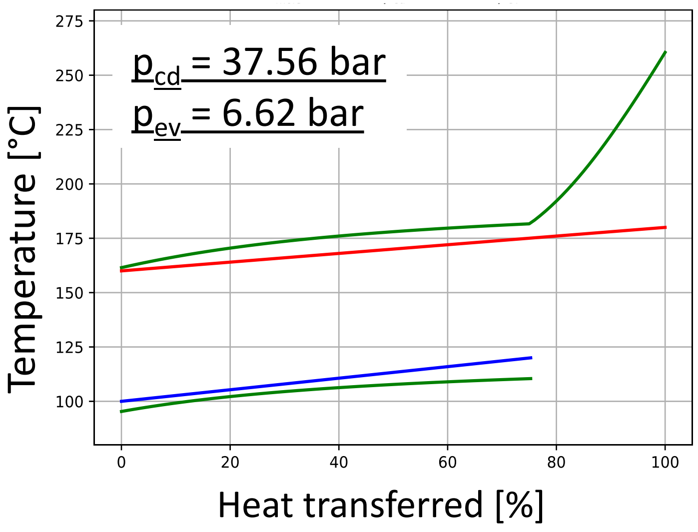
A ‘sensible sensible’ case study: Potential of binary mixtures



Methanol



Methanol&ammonia



Binary mixtures:

(1) Increase the COP

- ➢ Improved temperature matching.
- ➢ More favorable thermophysical properties?

(2) Reduce the investment cost

- ➢ Less compression stages
- ➢ Lower volume flow rate compressor inlet

$$\pi = \frac{p_{cd}}{p_{ev}} = 8.04$$

$$\pi = \frac{p_{cd}}{p_{ev}} = 5.67$$

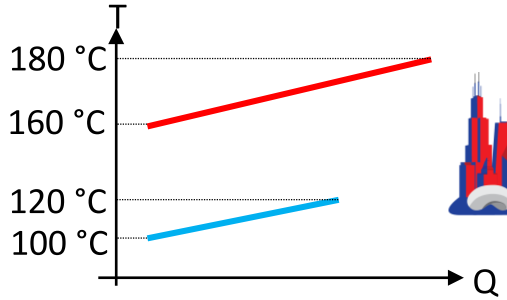
→ 42 % higher for pure methanol

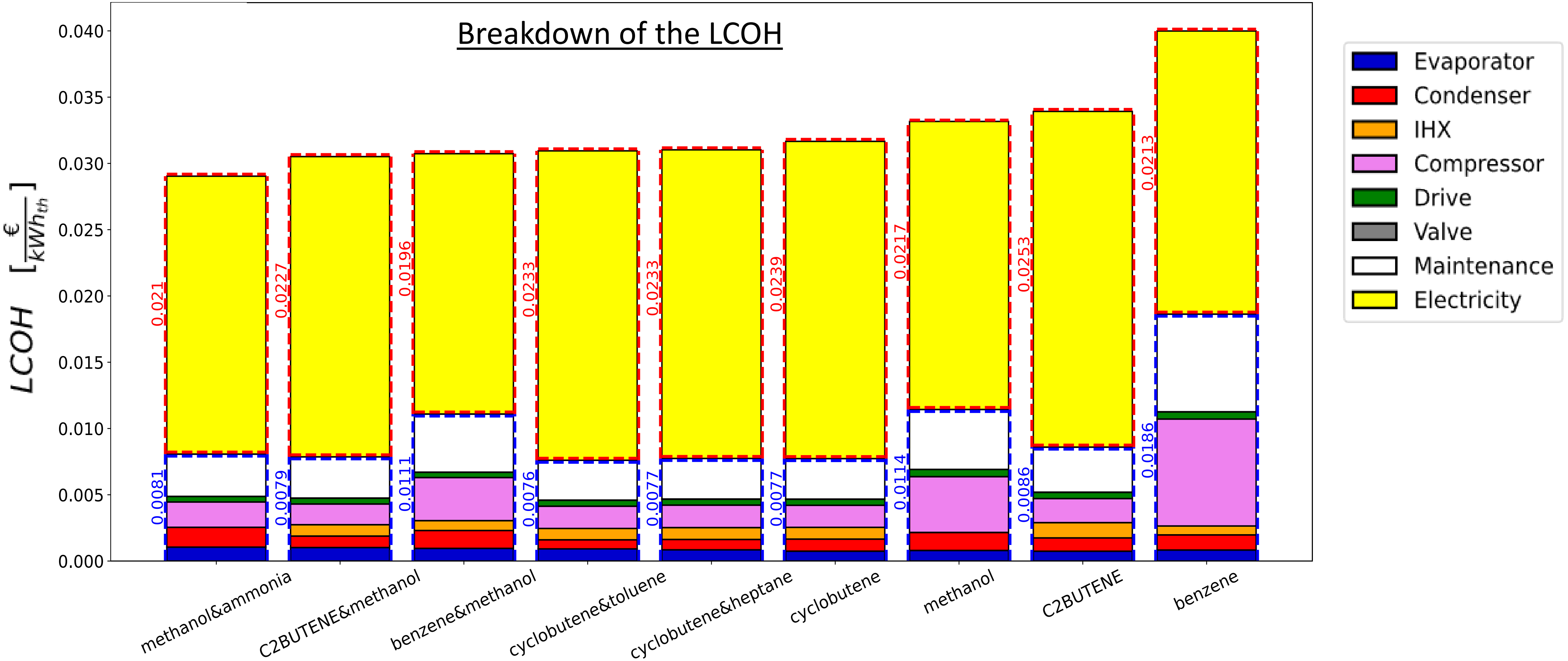
$$\dot{v}_{comp,in} = 0.130 \, \frac{m^3}{s}$$

$$\dot{v}_{comp,in} = 0.083 \, \frac{m^3}{s}$$

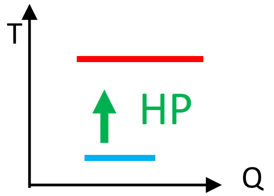
→ 57 % higher for pure methanol

A ‘sensible sensible’ case study: LCOH breakdown





Generalized selection matrix:



Heat sink: Latent

Heat source: Latent

(Near-) azeotropic mixtures

Flammable:
- Mixtures of hydrocarbons (always)
- Mixtures of water and hydrocarbons (medium T_{source})

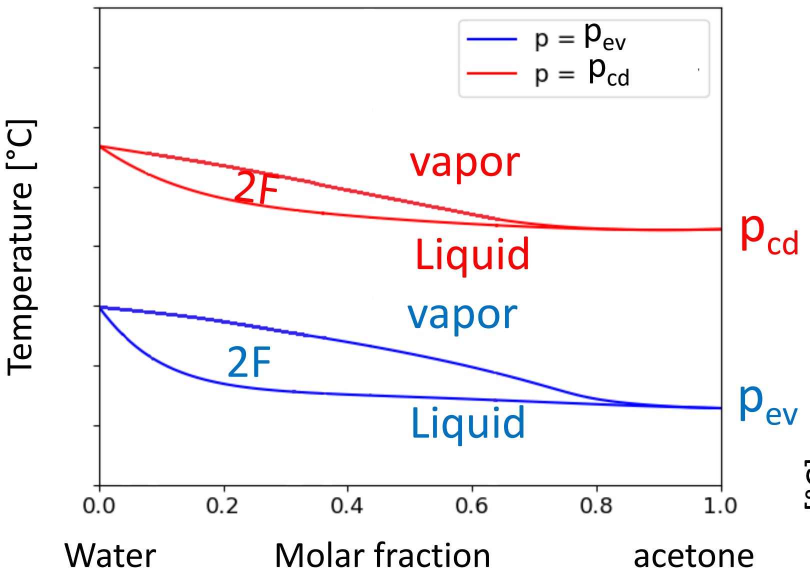
Non/mildly flammable:
- None

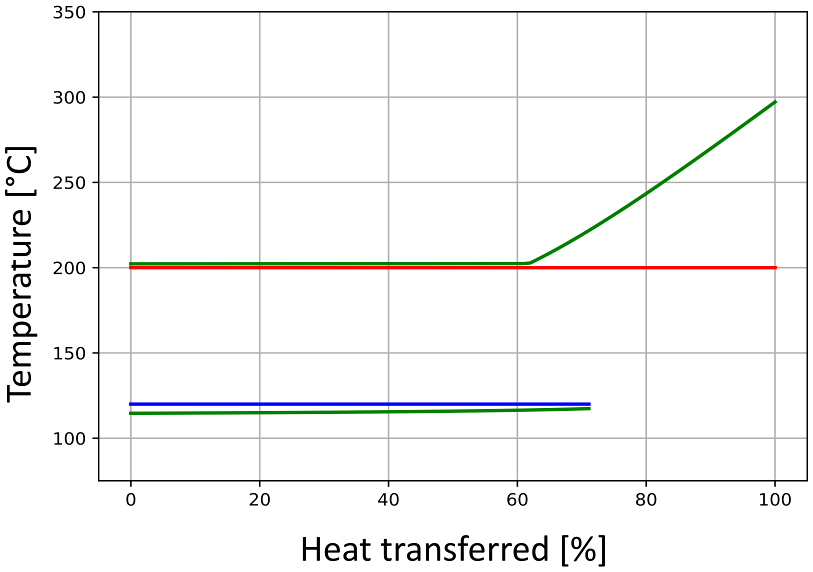
Pure fluids

Flammable:
- Acetone, methanol, ethanol (always)
- Cyclobutene (low T_{source} and T_{sink})

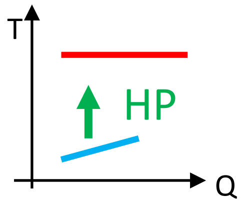
Non/mildly-flammable:
- Water (high T_{source})
- HFOs and HCFOs (low T_{source} and T_{sink})

Acetone&water





Generalized selection matrix



Heat source: Sensible

Heat sink: Latent

Zeotropic mixtures

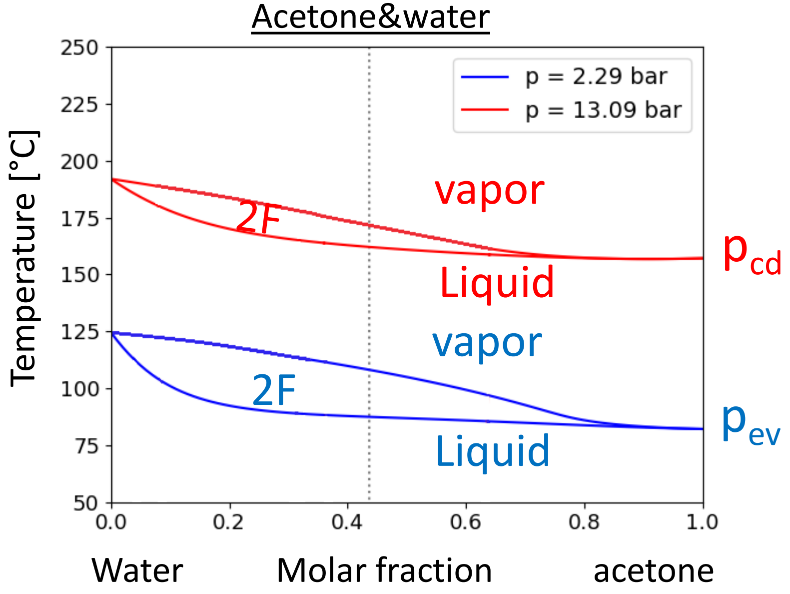
Flammable:
- Mixtures of hydrocarbons and mixtures of hydrocarbons and ammonia (always)
- Mixtures of water and hydrocarbons (medium T_{source})

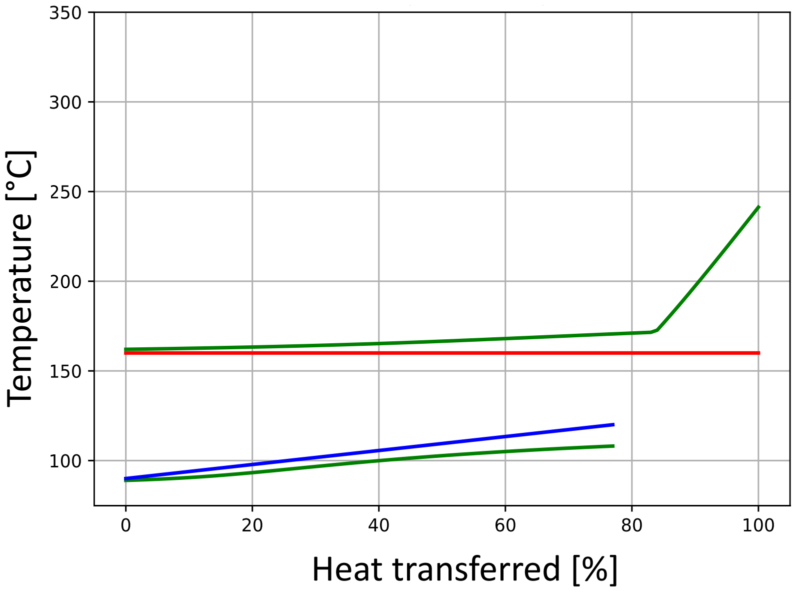
Non/mildly-flammable:
- Water/ammonia (high T_{source})

Pure fluids

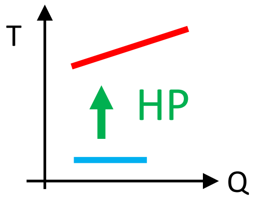
Flammable:
- Cyclobutene, Cyclopentane, Cis-2-Butene (low T_{sink})
- Acetone, Methanol, Ethanol (high T_{sink})

Non/mildly-flammable:
- Water (high T_{sink} and T_{source})
- HFOs and HCFOs (low T_{sink} and T_{source})





Generalized selection matrix



Heat source: Latent

Heat sink: Sensible

(near-) azeotropic mixtures

Flammable:

- Mixtures of hydrocarbons (high T_{sink})
- Mixtures of hydrocarbons and water or ammonia (high T_{source} and high T_{sink})

Non/mildly-flammable:

- None

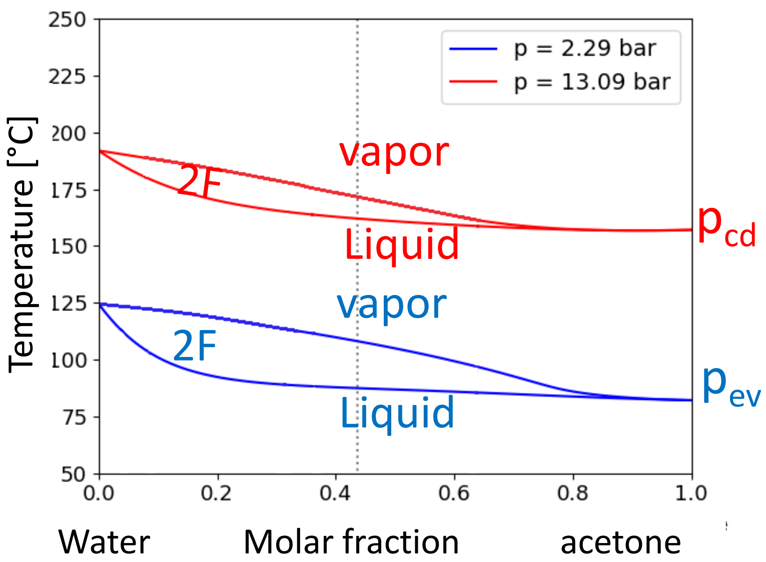
Pure fluids

Flammable:

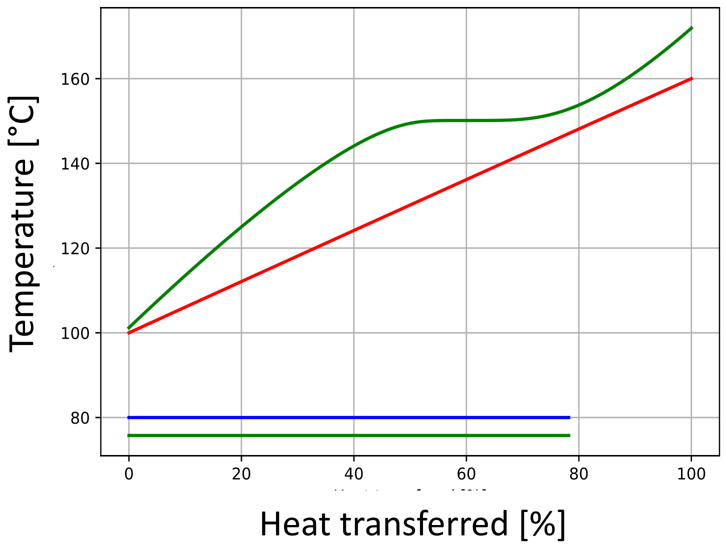
- Cyclobutene and Cis-2-Butene (low/medim T_{sink})

Non/mildly-flammable:

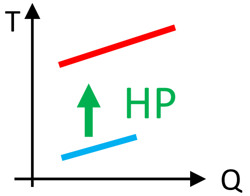
- HFOs and HCFOs (low/medium T_{sink})
- Water (high T_{source} and T_{sink})



Transcritical pure working fluid



Generalized selection matrix



Heat source: Sensible

Heat sink: Sensible

Zeotropic mixtures

Flammable:

- Mixtures of hydrocarbons and mixtures of hydrocarbons and ammonia (always)
- Mixtures of water and hydrocarbons (medium T_{source})

Non/mildly-flammable:

Water/ammonia (medium T_{source})

Discussion: Limitations to the model

The model: preliminary screening.

Best performing working fluids, (re)consider:

- Non-fixed heat transfer coefficients.
- Cost of the refrigerant.
- Influence of material compatibility or pressure.
- Off-design behaviour.
- Non-fixed isentropic efficiency.
- Influence of costs related to ATEX compliance.

Conclusions

- Investment cost of heat pump cannot be neglected.
- Discrepancy between optimum LCOH and optimum COP.
- Best performing working fluid: case study dependent
  - ➢Often binary mixtures (natural refrigerants):
    - ❖Favorable temperature matching: COP ⬈
    - ❖Favorable operational conditions: Investment cost ⬊
  - ➢Heat sink (large ΔT), heat source (small ΔT):
    - →Transcritical cycles

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References

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