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An Assessment of Working-Fluid Mixtures in ORCs for Waste Heat Recovery using SAFT-VR

Aly Taleb, Oyeniyi Oyewunmi, Andrew Haslam, Christos N. Markides

NB: Some information from the original presentation has been omitted for confidentiality reasons.

Aims & Objectives

To evaluate the advantages of different working fluid mixtures for optimal organic Rankine cycles by:

1. Calculating relevant fluid properties of a wide range of working fluid mixtures with SAFT-VR
2. Linking SAFT-VR with a thermodynamic model of an ORC and calculating performance parameters (efficiency, power output, costs)

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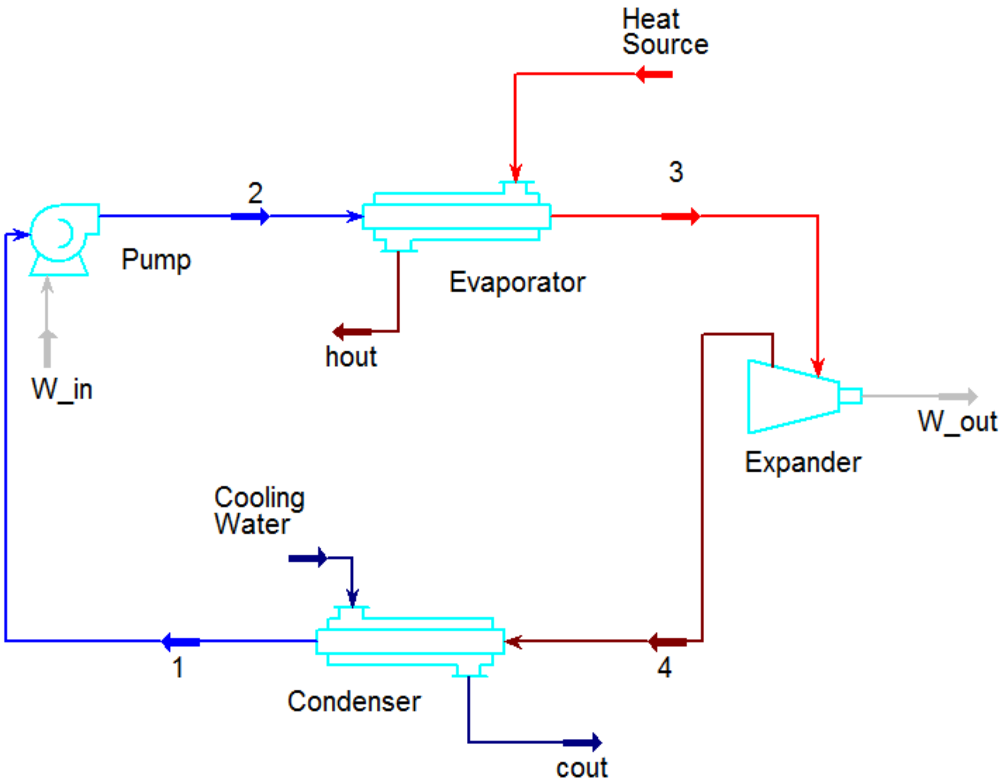
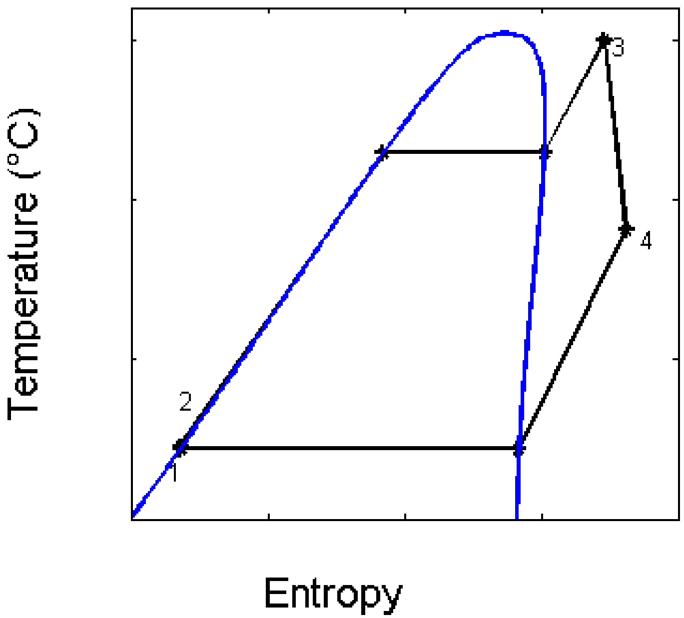
The Organic Rankine Cycle (ORC)



ORC schematic



ORC with butane on a *T*-*s* plot

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ORC Model

Cycle definition:

Pump (1 → 2)

- $\dot{W}_{\text{pump}} = \dot{m}_{\text{wf}}(h_2 - h_1)$

Evaporator (2 → 3)

- $Q_{\text{in}} = \dot{m}_{\text{hs}} c_{\text{p,hs}} (T_{\text{hs,in}} - T_{\text{hs,out}})$
- $Q_{\text{in}} = \dot{m}_{\text{wf}}(h_3 - h_2)$

Expander (3 → 4)

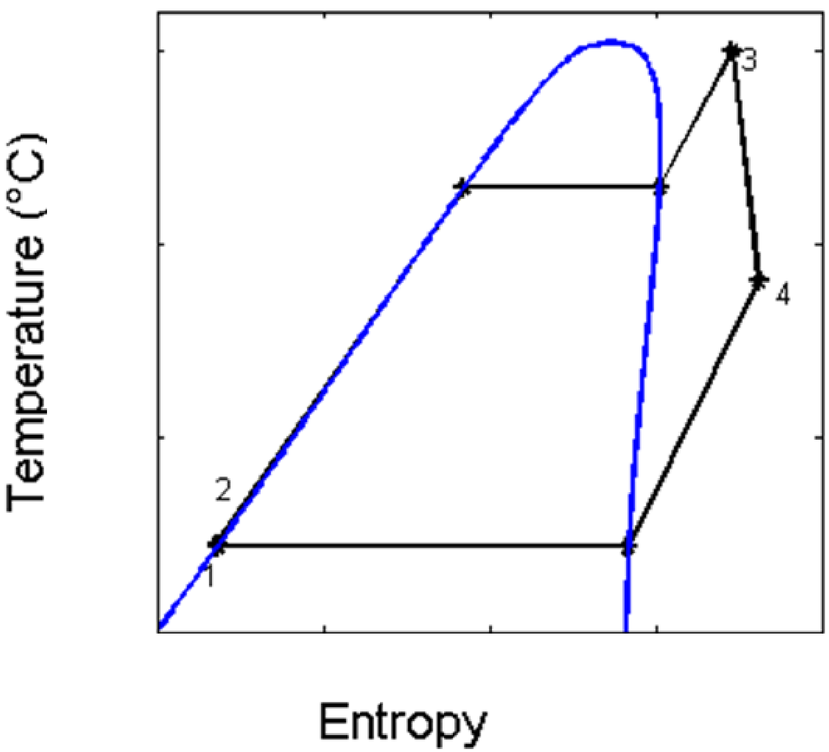
- $\dot{W}_{\text{exp}} = \dot{m}_{\text{wf}}(h_3 - h_4)$

Condenser (4 → 1)

- $Q_{\text{out}} = \dot{m}_{\text{cs}} c_{\text{p,cs}} (-T_{\text{cs,in}} + T_{\text{cs,out}})$
- $Q_{\text{out}} = \dot{m}_{\text{wf}}(h_4 - h_1)$

$$\eta_{\text{th}} = \frac{\dot{W}_{\text{exp}} - \dot{W}_{\text{pump}}}{Q_{\text{in}}}$$

Case considered: Heat source – Flue gas from a refinery preheater (200 °C, 560 kg/s)



Component Cost Calculation

Heat exchangers – **C-value method**

- $\text{Cost} = \text{C}\frac{Q}{\Delta T_{Lm}} = \text{C} \times (\text{UA})$

Pumps and Expanders – **Market survey**

Component costs ≈ 0.45 - 0.7 x overall costs for typical ORCs for waste heat recovery (Koehler 2005, Lukawski 2009, Bejan et al. 1996)

NB: Costs shown in this work are not TOTAL system costs; but the added costs of the basic ORC system components (i.e. heat exchangers, pumps and expanders)

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Model Parameters and Variables

Inputs:

- Variable
  - Expander inlet temperature T_3
  - Evaporation pressure P_{23}
  - Mass flow rate $\dot{m}$
  - Working fluid mixing ratio
- Fixed parameters
  - Pinch temperature 10 °C
  - Heat source T = 200 °C
- Fluid properties
  - Pure properties from NIST database
  - Mixture properties from SAFT-VR EoS

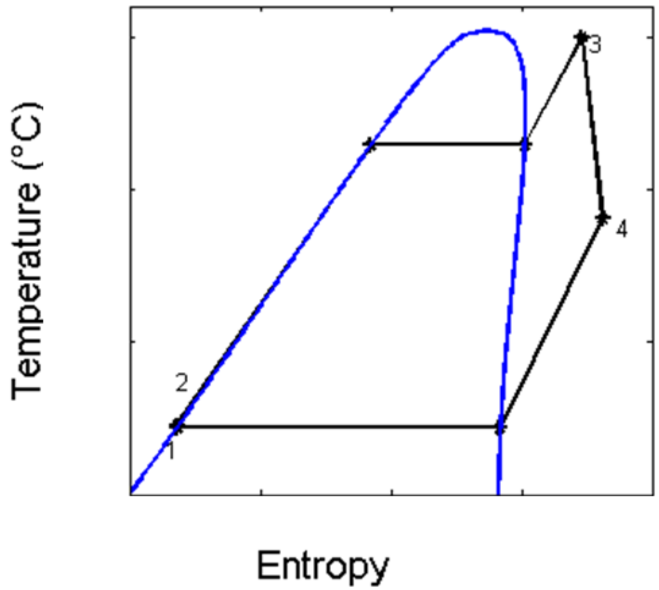
Outputs:

Power output ($\dot{W}_{\text{exp}}$)

Thermal efficiency (η_{th})

Capital cost (£)

Cost per unit power (£/kW)



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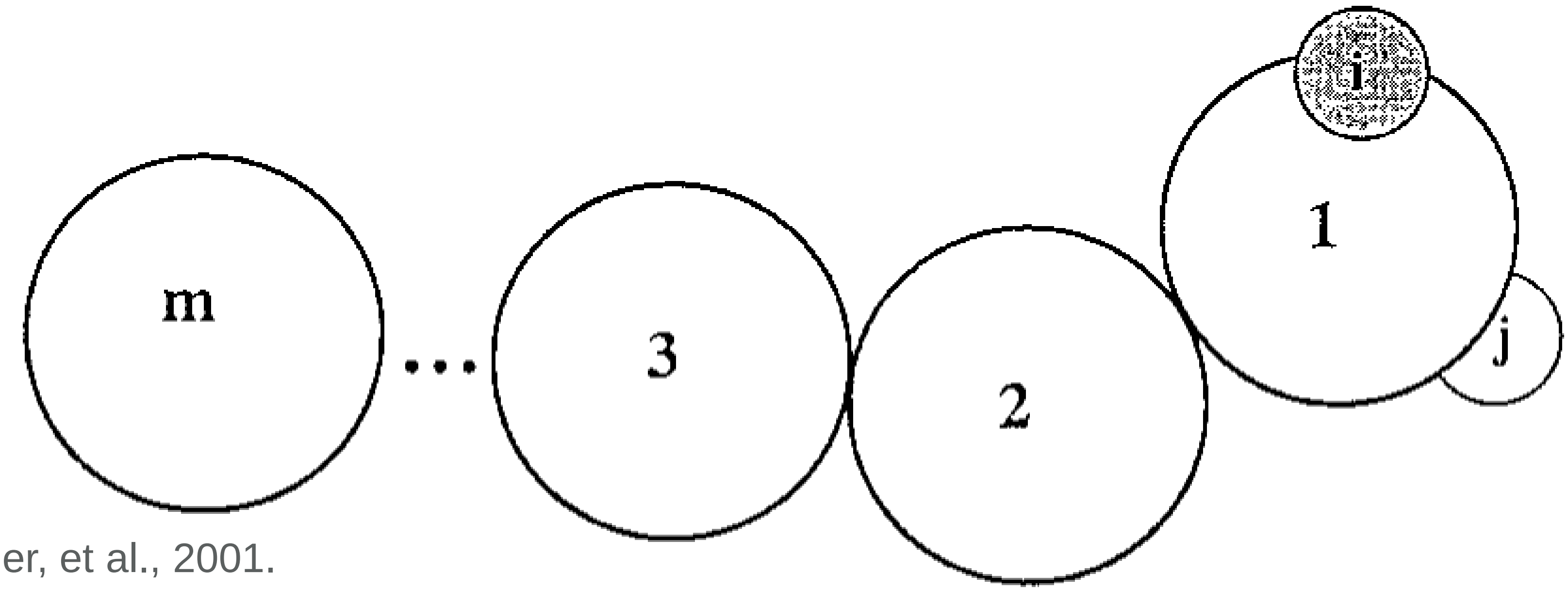
SAFT-VR for Mixture Fluid Properties

- SAFT-VR divides molecules into building blocks or spheres
- Each sphere can have four different effects:

$$A = A^{\text{ideal}} + A^{\text{mono}} + A^{\text{chain}} + A^{\text{assoc.}}$$



Müller, et al., 2001.

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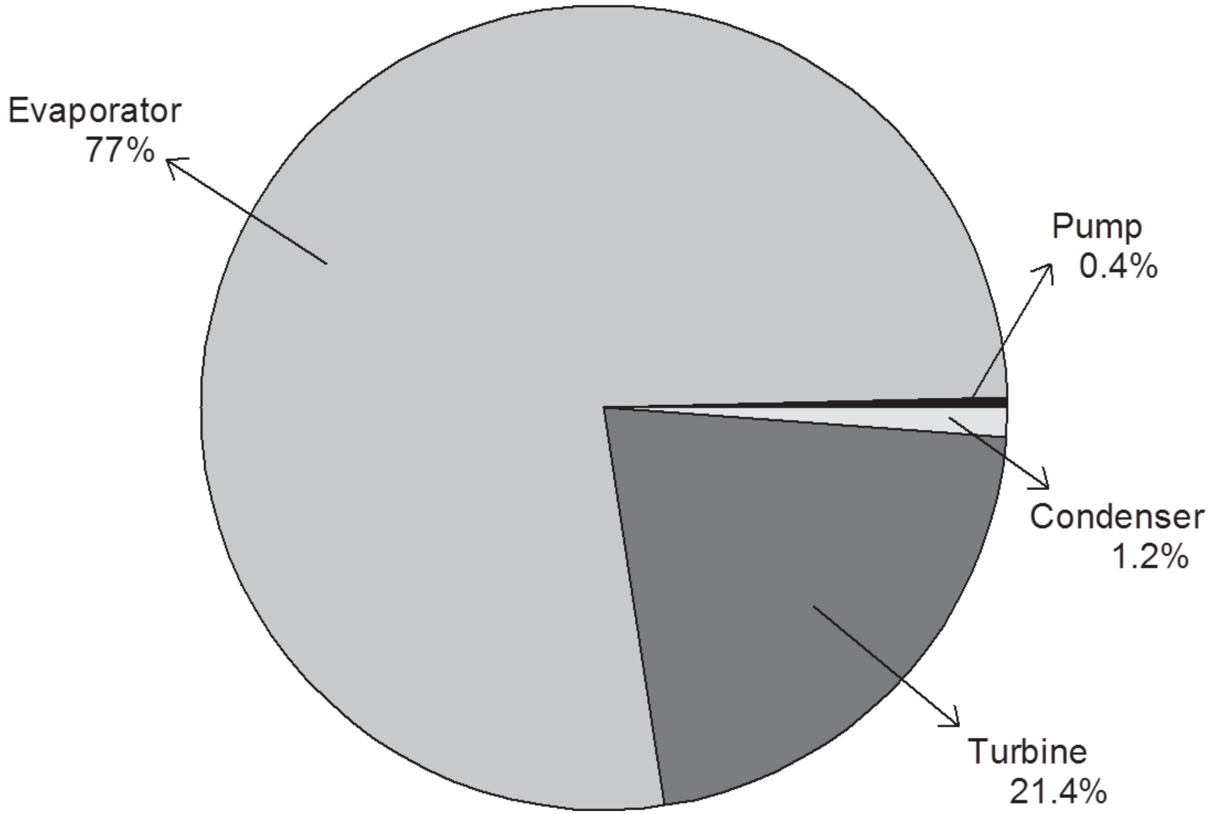
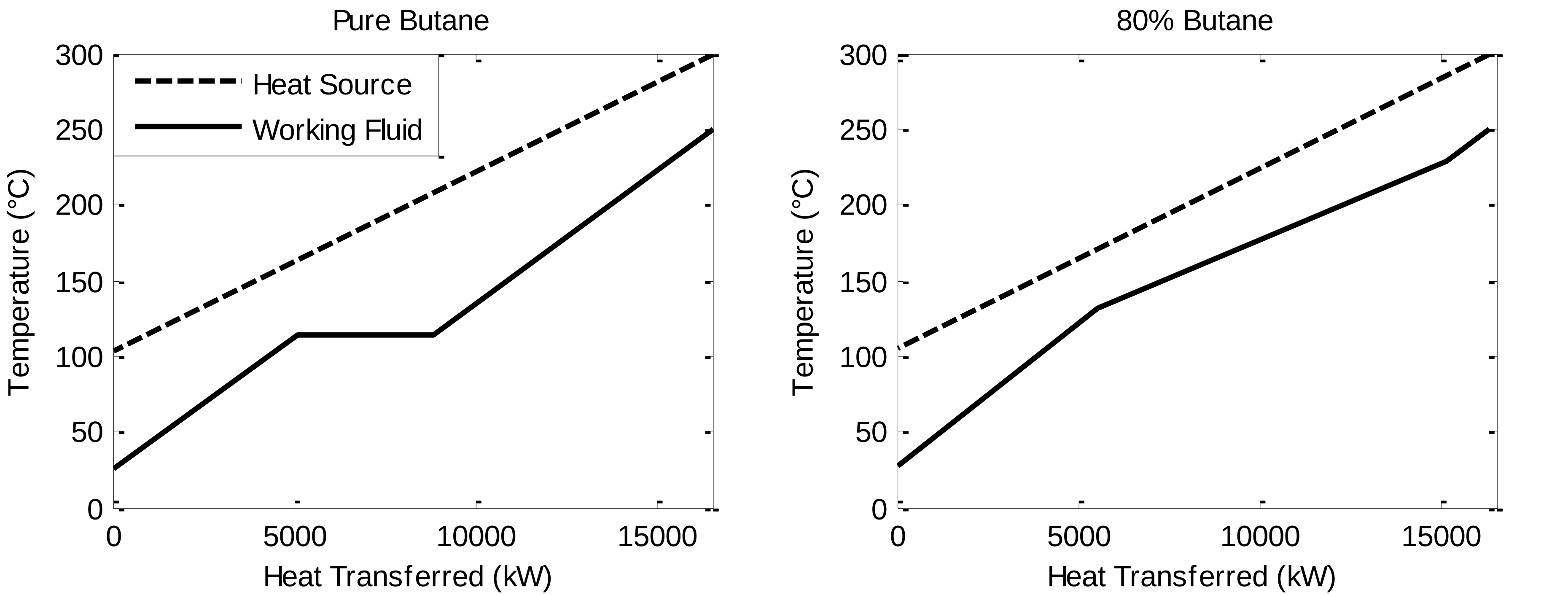
Why Working Fluid Mixtures - Exergy Loss in a typical ORC



- Main source of **exergy destruction** in ORC is the heat exchanger of the **evaporator**
- Exergetic losses in evaporator must be reduced

Pure Working Fluids vs. Working Fluid Mixtures



- By increasing **average temperature** of heat addition

→ **Efficiency and power output** increased

- Caution: average temperature of heat rejection may also be increased which leads to efficiency losses

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Perfluoroalkane (C_4F_{10} + C_5F_{12}) Mixtures

Working fluid conditions:

- 8 bar $\leq P_{23} \leq$ 20 bar
- 100 °C $\leq T_3 \leq$ 190 °C
- 1 kg/s $\leq \dot{m}_{wf} \leq$ 600 kg/s
- $0 \leq C_4F_{10} \leq 1; 1 \geq C_5F_{12} \geq 0$

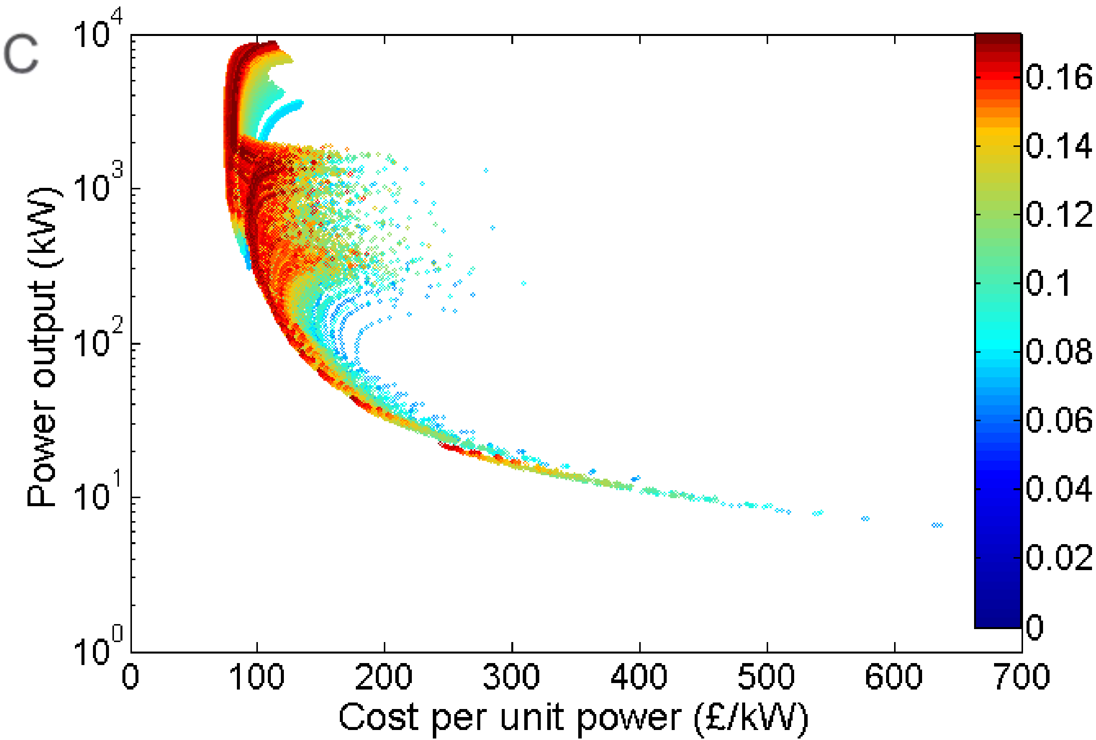
Heat Source: Flue gas at 200 °C

Power Output: 0.1 – 10 MW

Efficiency: 16 –17%

Costs: down to 100 £/kW

(**NB: component costs only**)



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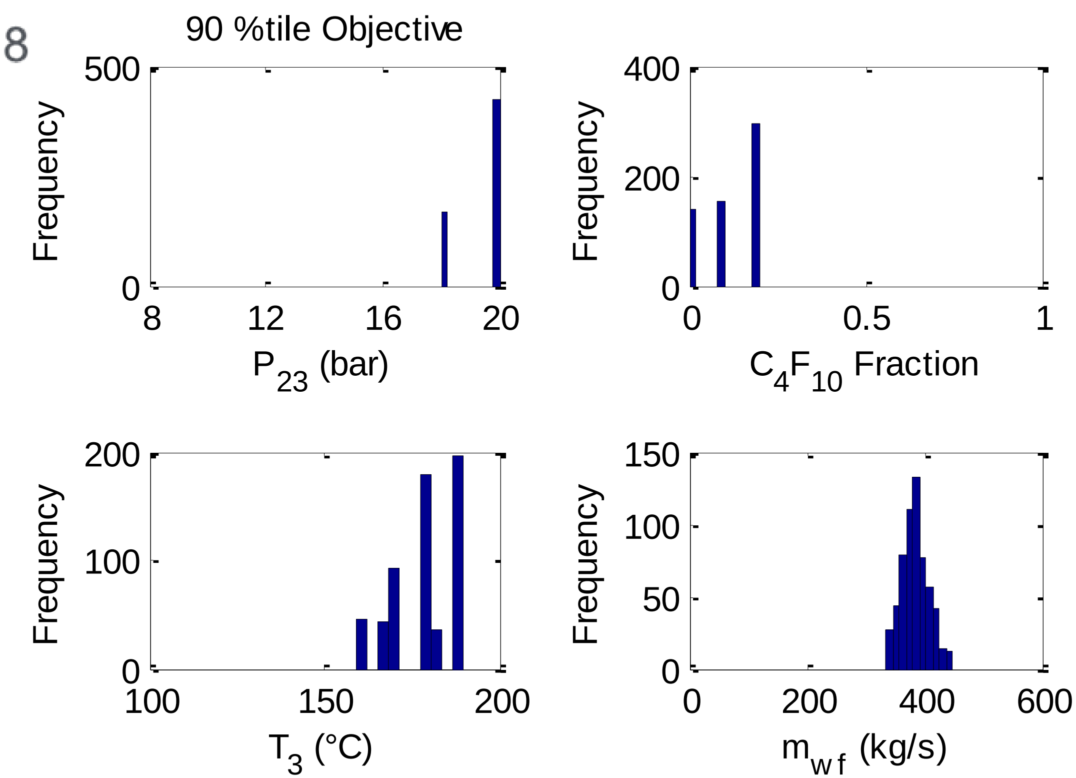
Optimal Operation Conditions for Perfluoroalkane Mixtures

Satisfactory working fluid conditions:

- $18 \text{ bar} \leq P_{23} \leq 20 \text{ bar}$
- $160\ °\text{C} \leq T_3 \leq 190\ °\text{C}$
- $300 \text{ kg/s} \leq \dot{m}_{\text{wf}} \leq 450 \text{ kg/s}$
- $0 \leq C_4F_{10} \leq 0.2;\ 1 \geq C_5F_{12} \geq 0.8$

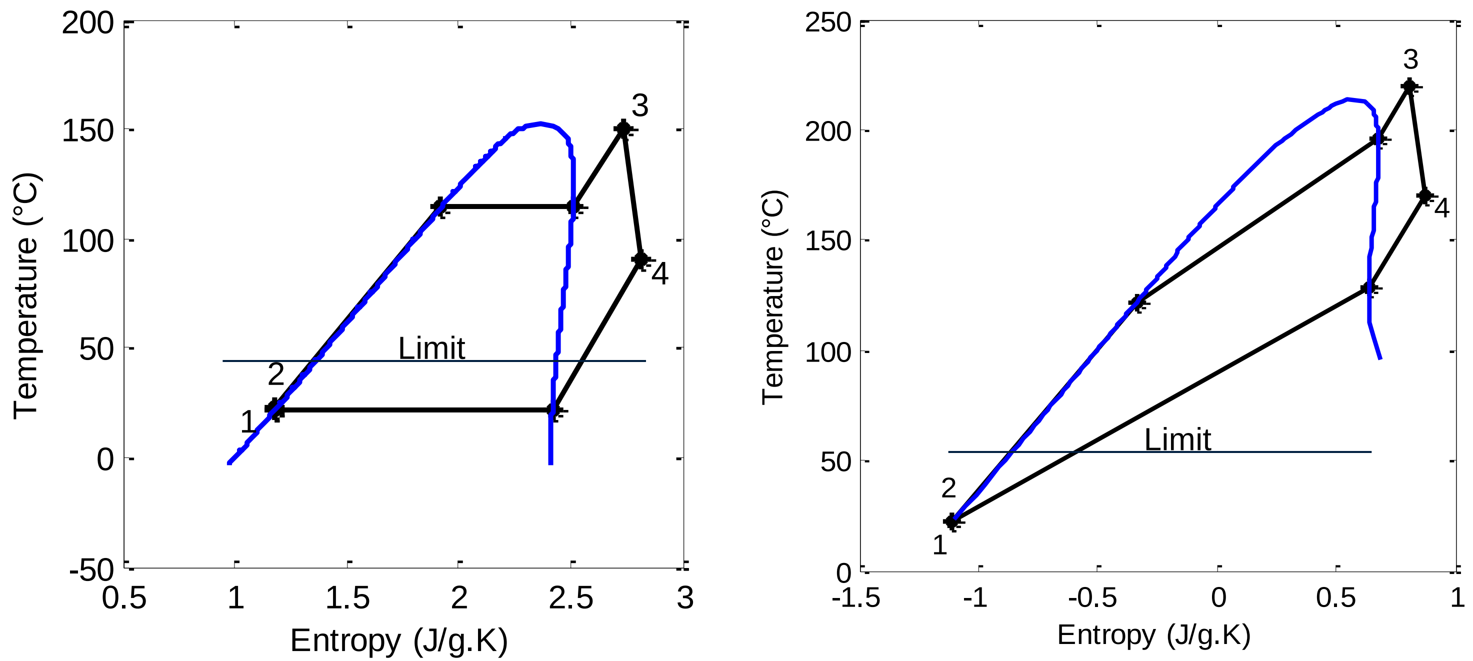


Decane + Butane Working Fluid with Regenerators

Why use regenerators?

Increased efficiencies but additional costs

Increased mass flowrates → Increased power output



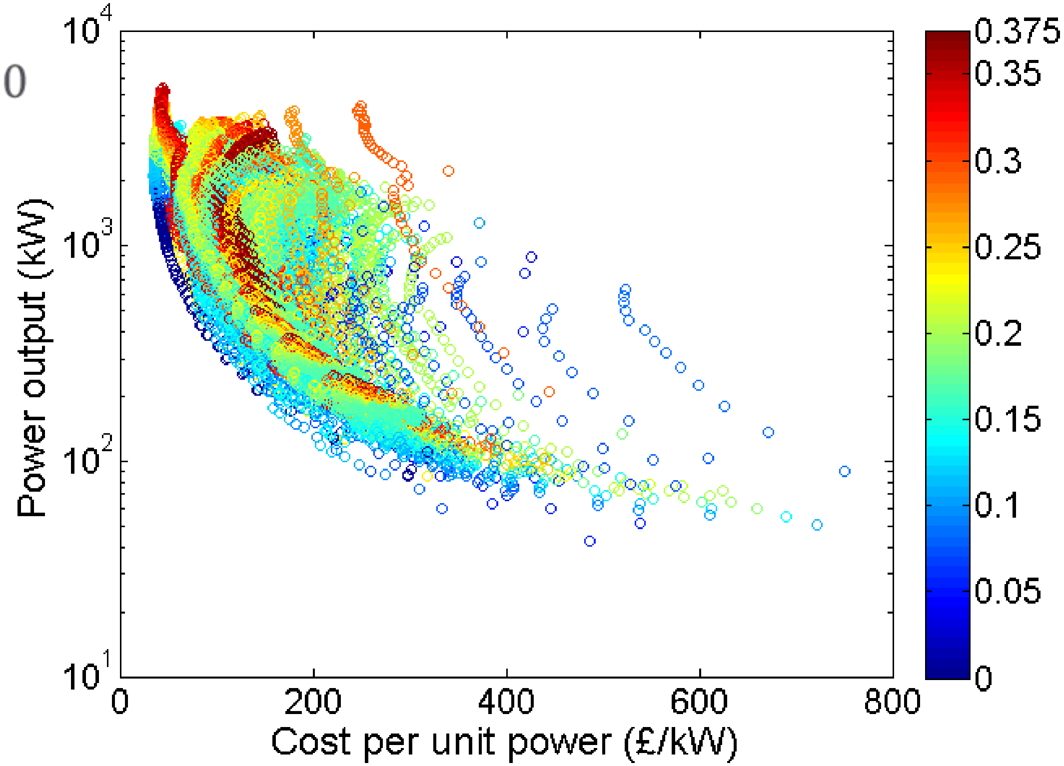
T-*s* plot for: (a) Pure working fluid (b) Mixture working fluid

Decane + Butane Working Fluid with Regenerators

Flue gas at 330 °C

Working fluid conditions:

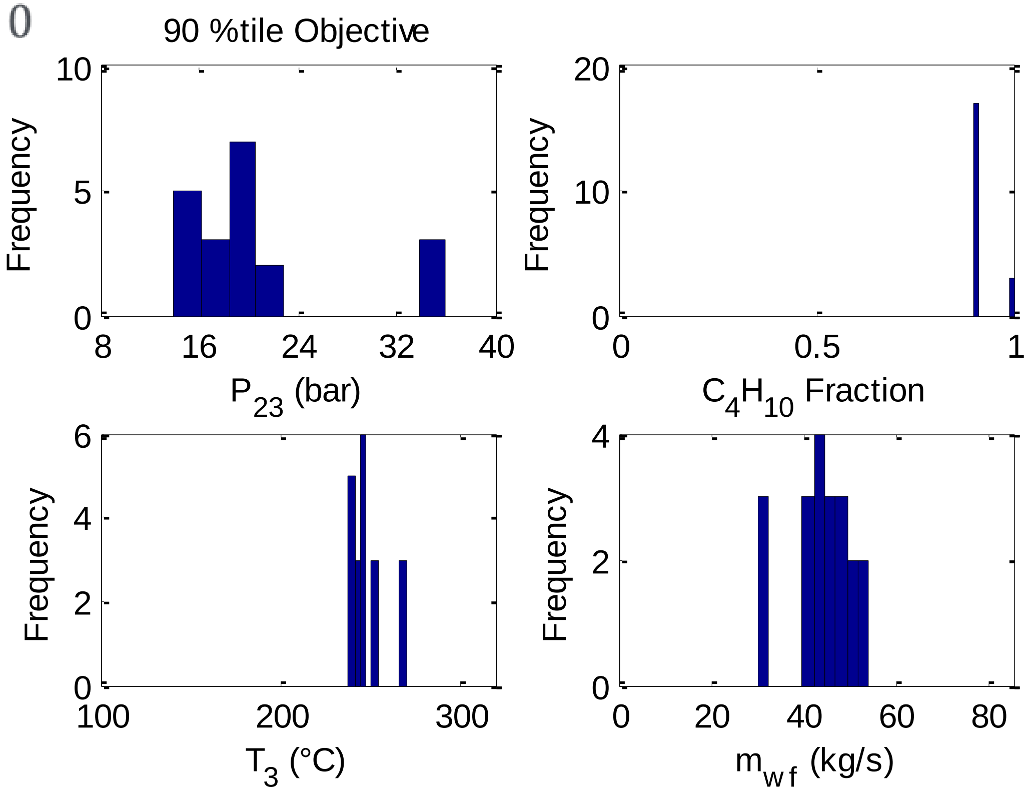
- 6 bar $\leq P_{23} \leq$ 40 bar
- 100 °C $\leq T_3 \leq$ 320 °C
- 1 kg/s $\leq \dot{m}_{wf} \leq$ 80 kg/s
- $0 \leq C_4H_{10} \leq 1;\ 1 \geq C_{10}H_{22} \geq 0$



Maximize Power Output, Efficiency and Minimize Costs per Unit Power

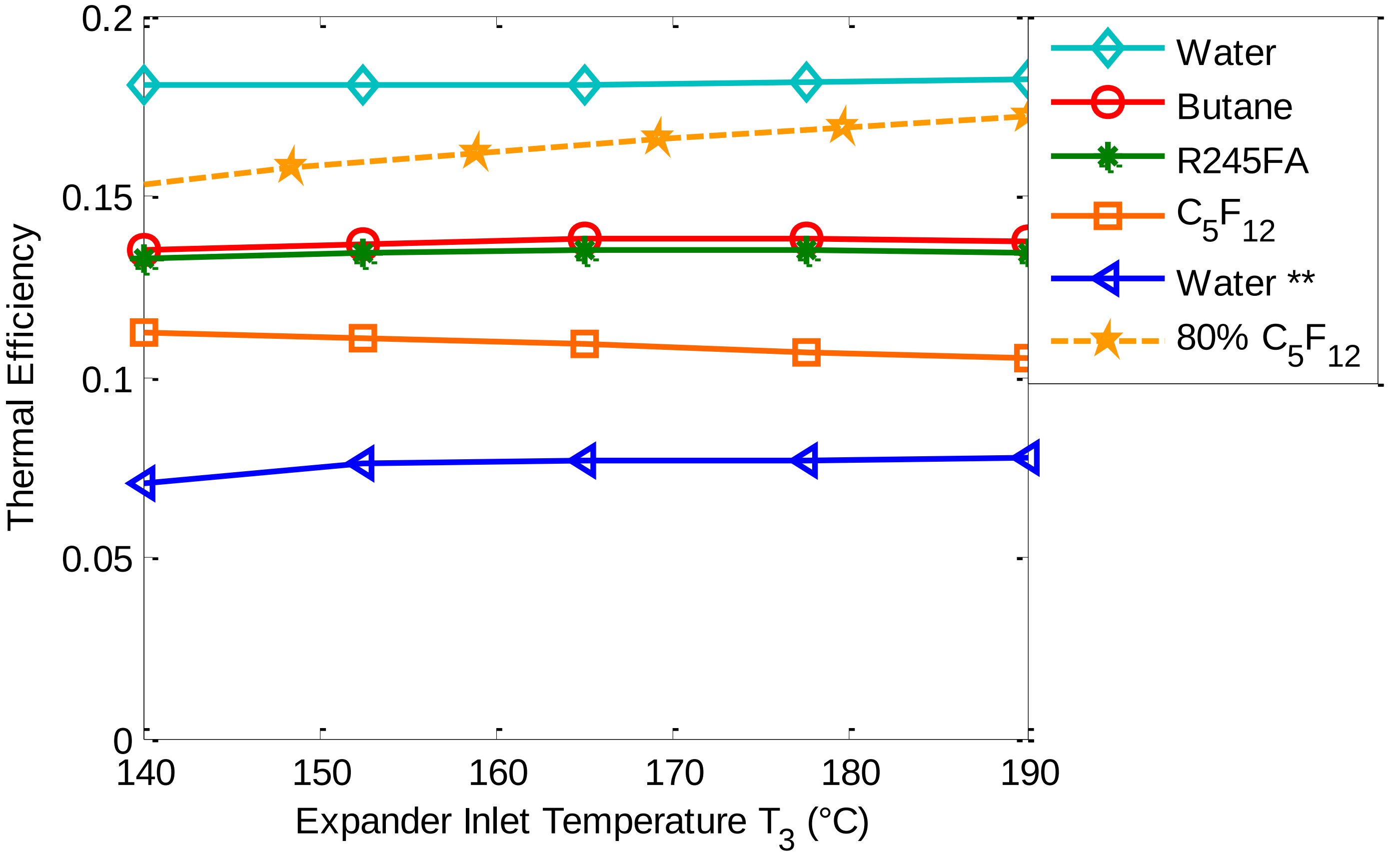
Satisfactory working fluid conditions:

- 14 bar $\leq P_{23} \leq$ 32 bar
- 250 °C $\leq T_3 \leq$ 280 °C
- 30 kg/s $\leq \dot{m}_{wf} \leq$ 55 kg/s
- $0.9 \leq C_4H_{10} \leq 1; 0.1 \geq C_{10}H_{22} \geq 0$

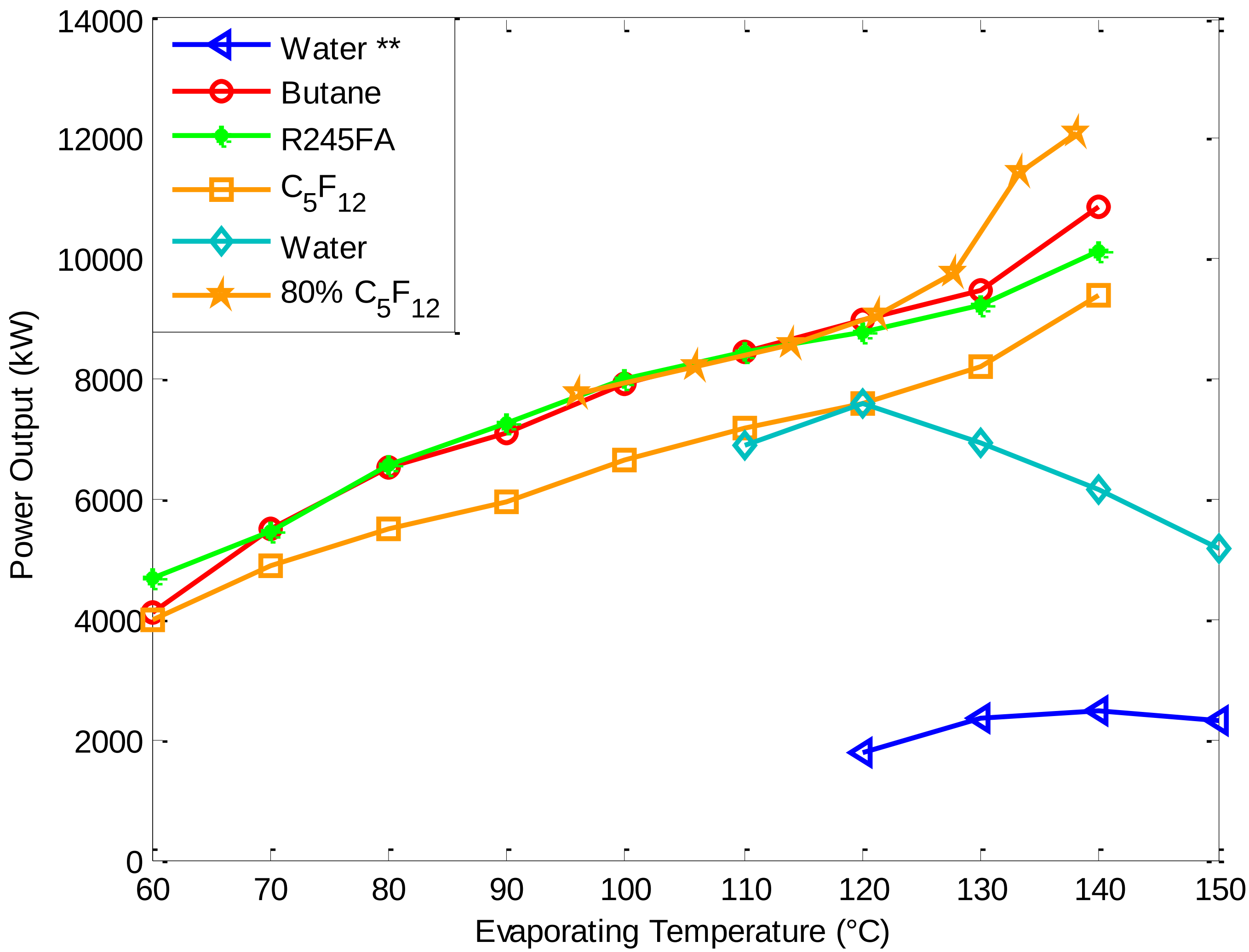


Thermal Efficiencies – Pure Working Fluids

- Organic fluids and water condensing at 30°C
- ** Water condensing at 1 bar (100°C)
- Evaporating at 140°C
- Heat source at 200°C



Maximum Power Output – Pure Working Fluids

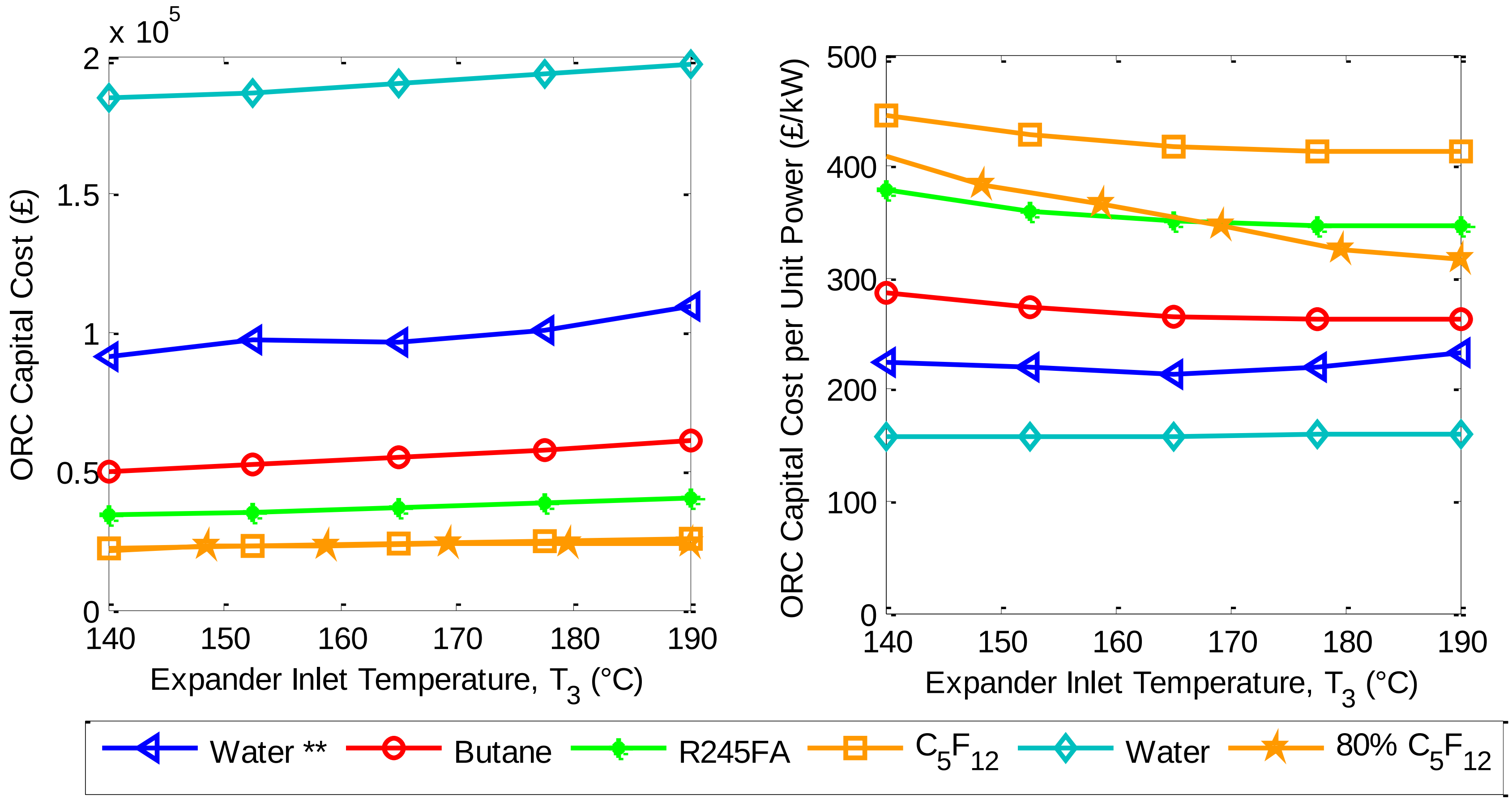


Component Cost Comparisons

$\dot{m} = 2.5 \text{ kg/s}$

Condensing at 30°C, 100°C for water

Evaporating at 140 °C and superheating to 190 °C



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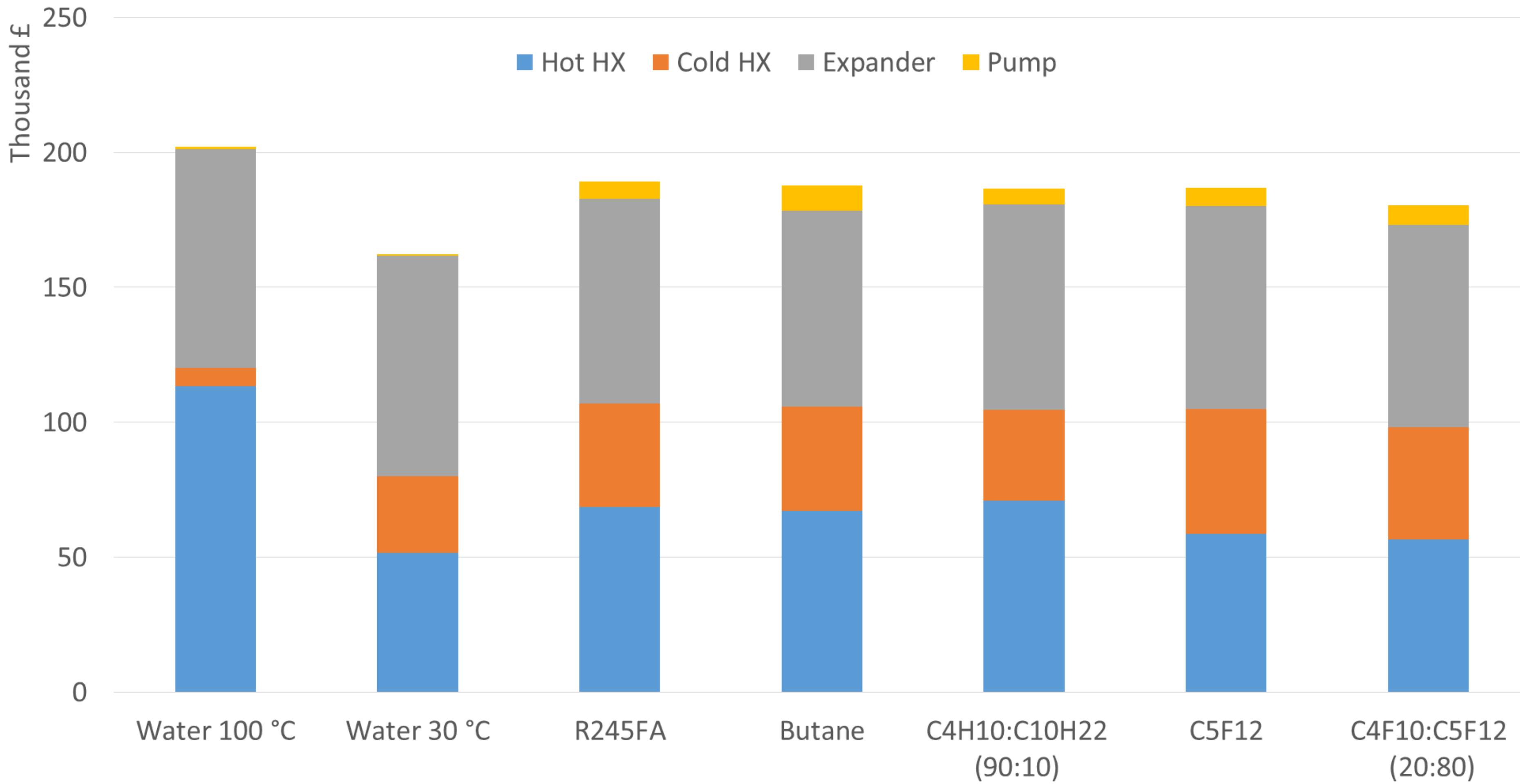
Component Cost Breakdown Comparison at 1 MW Output



Summary

- Heat source: 200 °C, 560 kg/s (modelled refinery flue gas)

Results with perfluoroalkane mixture:

- Efficiency: 16 – 17%
- Power output: 0.1 – 10 MW
- Component cost: <100 £/kW

Comparison perfluoroalkane mixtures, water, pure organic fluids:

- Highest efficiency: perfluroalkane mixture and water (however, condensation at 0.04 bar!)
- Highest maximum power output: perfluoroalkane mixture

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Summary and Conclusions

SAFT-VR calculates working fluid mixtures very accurately

There is no “perfect” working fluid mixture (cycle parameters + application)

Carefully selected working fluid mixtures can improve cycle performance

Future Work

- Water mixtures (e.g. water-ethanol, etc.)
- Different homologous series (e.g. alkane + refrigerant)
- Azeotropic mixtures
- SAFT-VR for "reverse" engineering / design:
  - Define properties first and derive from that molecular structure

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