

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

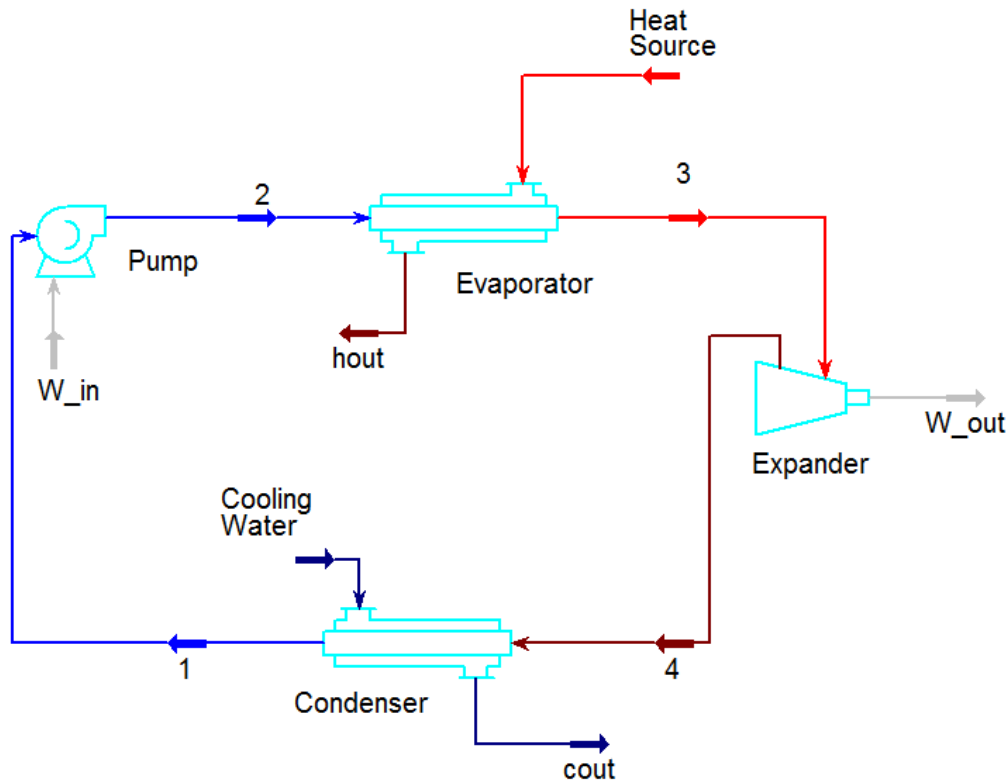
Aly Taleb, Oyeniyi Oyewunmi, Andrew Haslam, Christos N. Markides

Aims & Objectives

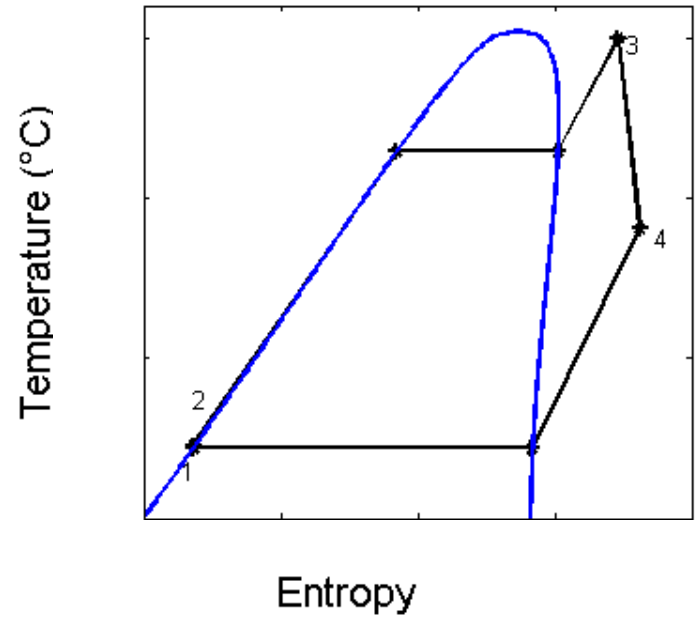
To evaluate the advantages of different working fluid mixtures for optimal organic Rankine cycles by:

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**)

The Organic Rankine Cycle (ORC)



ORC schematic



ORC with butane on a T - s plot

ORC Model

Cycle definition:

Pump (1 → 2)

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

Evaporator (2 → 3)

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

Expander (3 → 4)

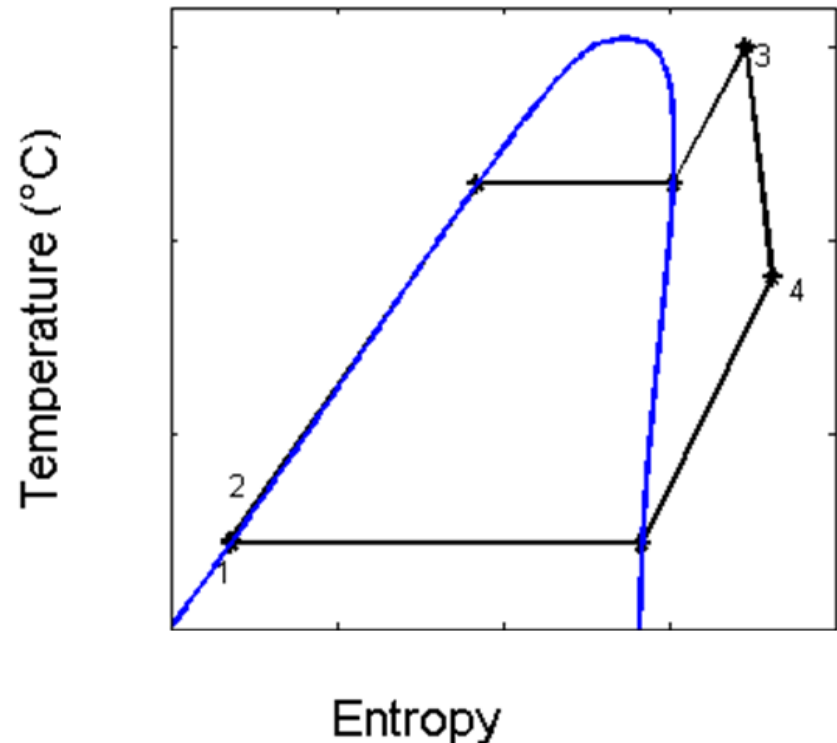
- $\dot{W}_{\text{exp}} = \dot{m}_{\text{wf}}(h_3 - h_4)$

Condenser (4 → 1)

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

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

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



Component Cost Calculation

Heat exchangers – **C-value method**

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

Pumps and Expanders – **Market survey**

Component costs $\approx 0.45 - 0.7$ 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**)

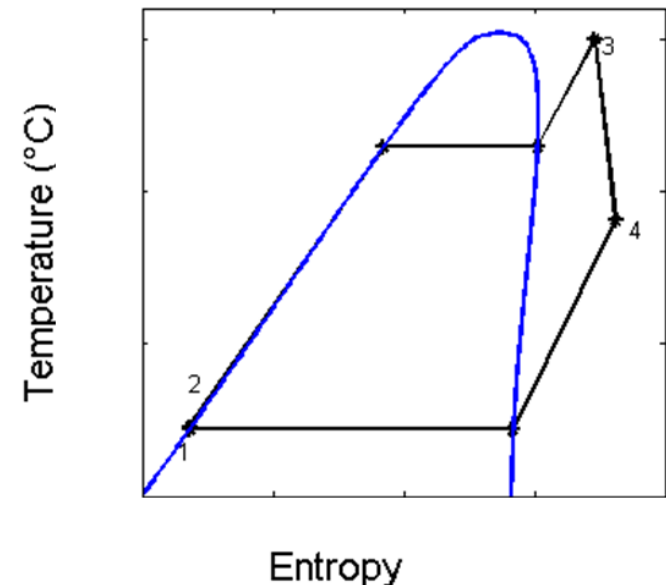
Model Parameters and Variables

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:

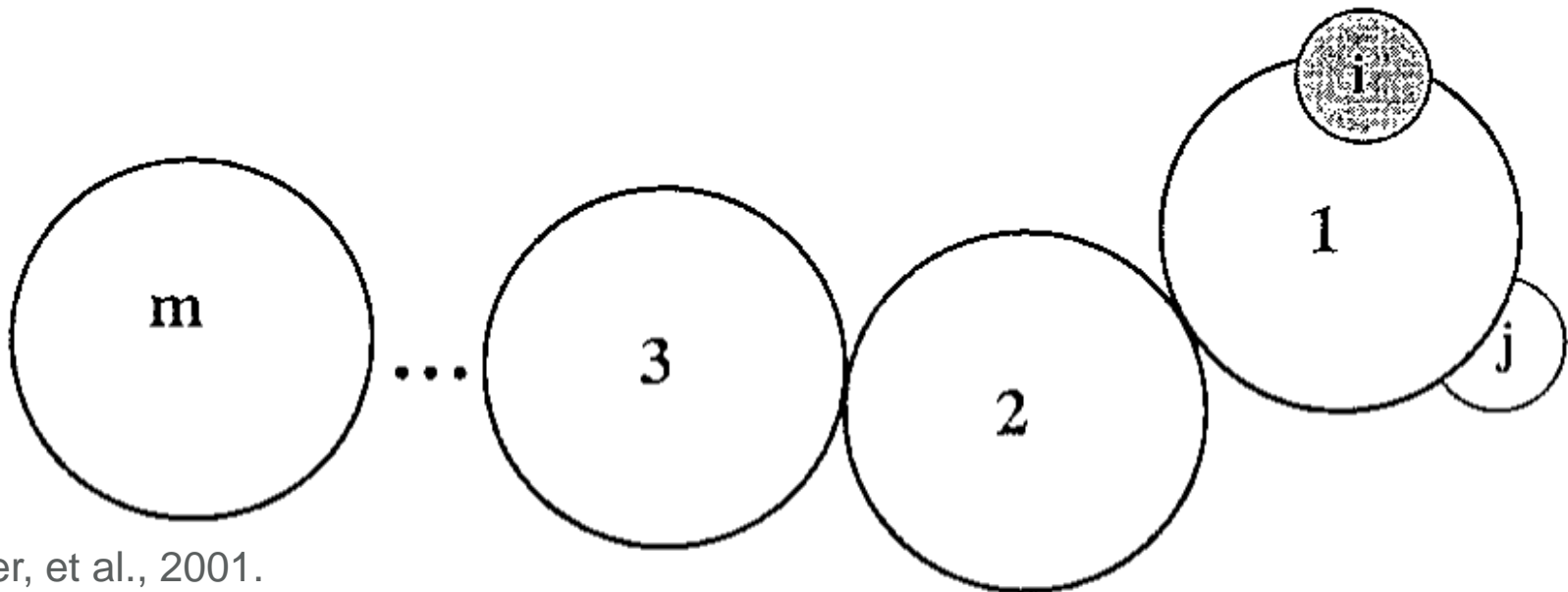
- Power output (\dot{W}_{exp})
- Thermal efficiency (η_{th})
- Capital cost (£)
- Cost per unit power (£/kW)



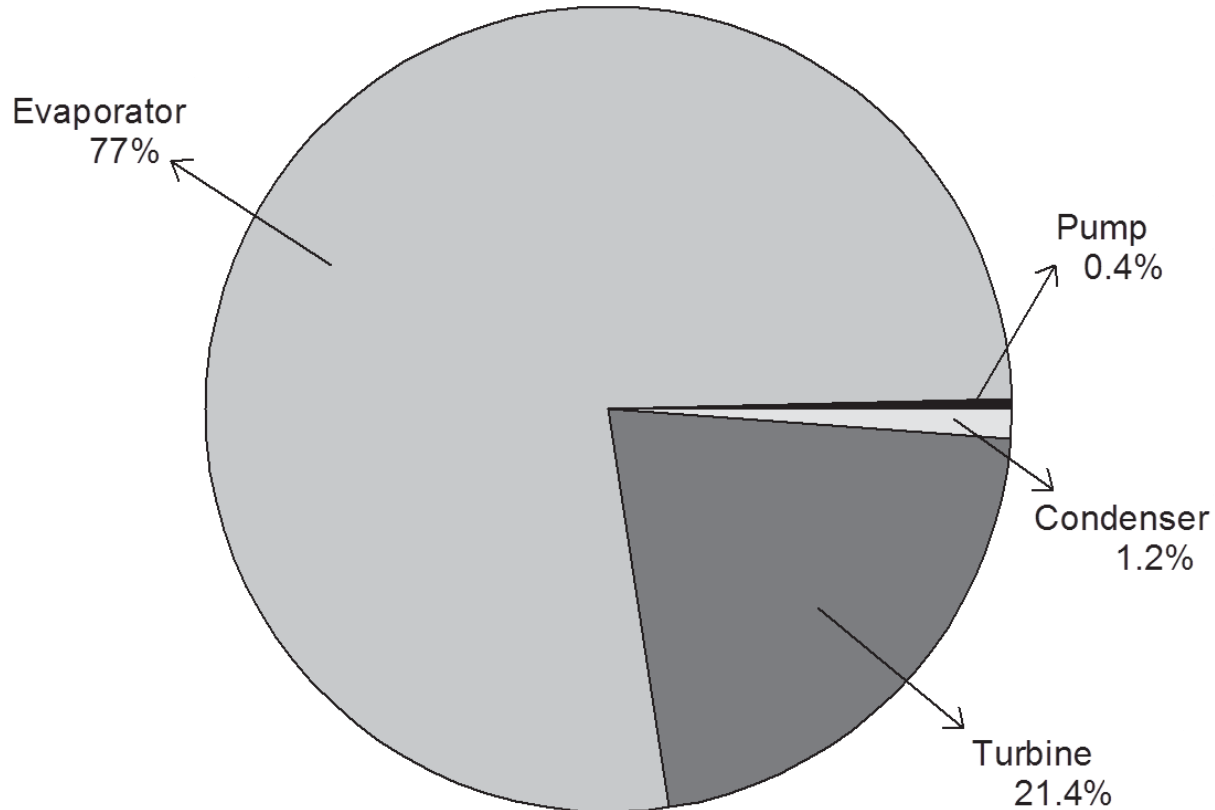
SAFT-VR for Mixture Fluid Properties

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

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

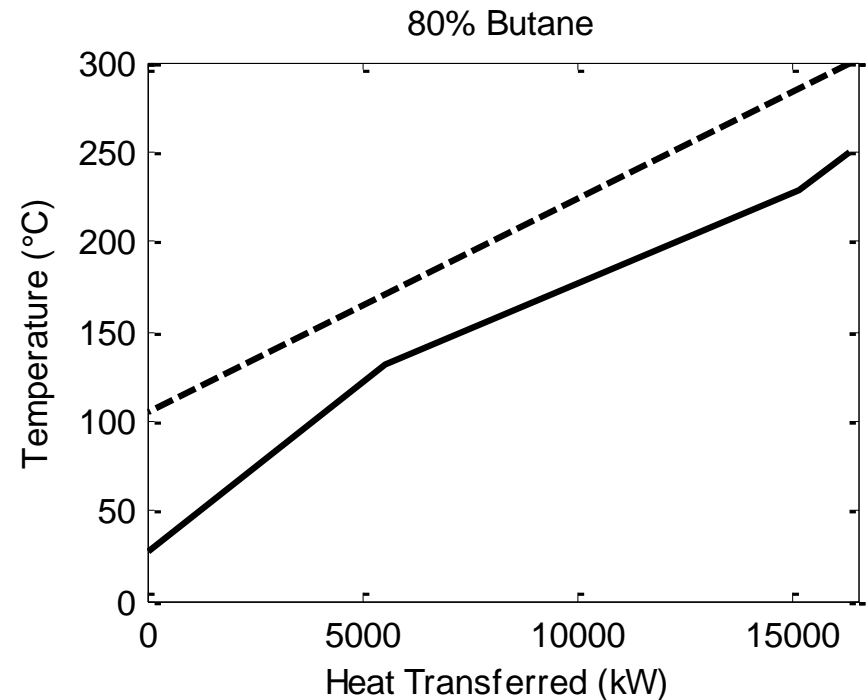
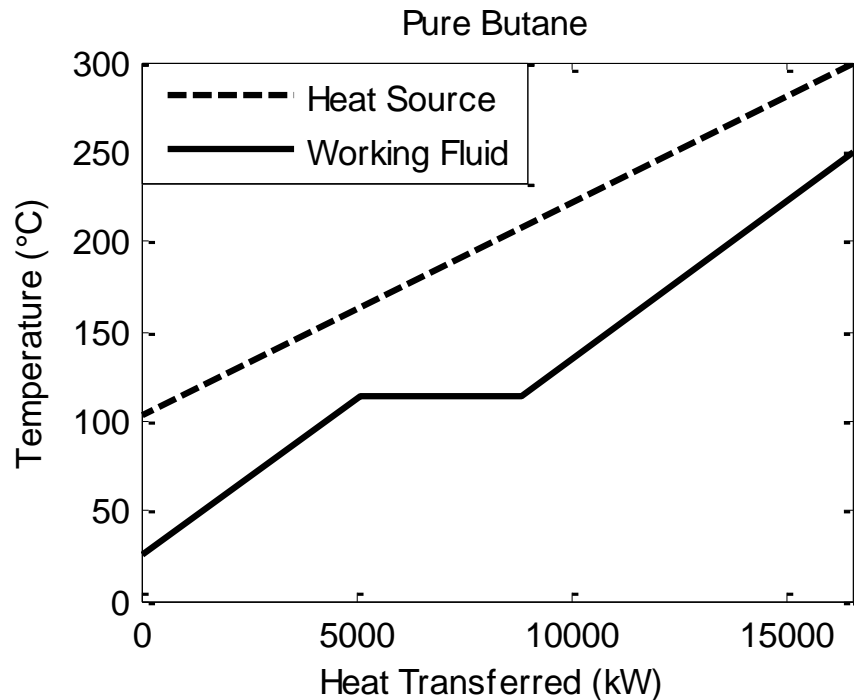


Why Working Fluid Mixtures - Exergy Loss in a typical ORC



- 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

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

Working fluid conditions:

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

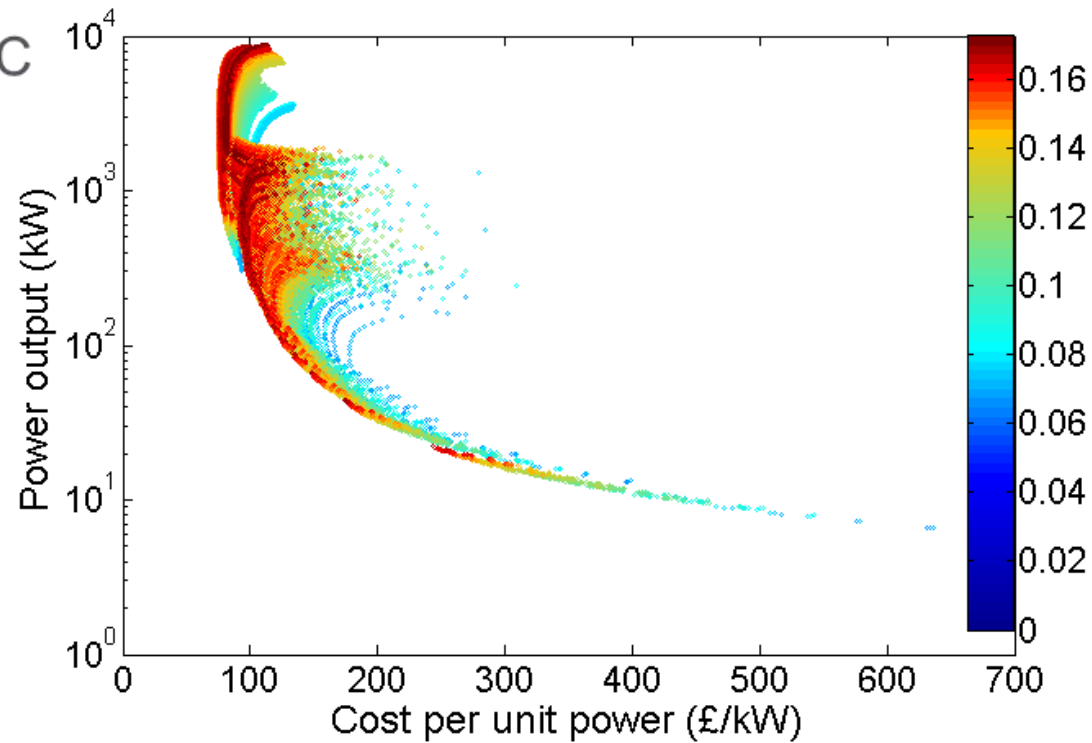
Heat Source: Flue gas at $200 \text{ }^\circ\text{C}$

Power Output: 0.1 – 10 MW

Efficiency: 16 – 17%

Costs: down to 100 £/kW

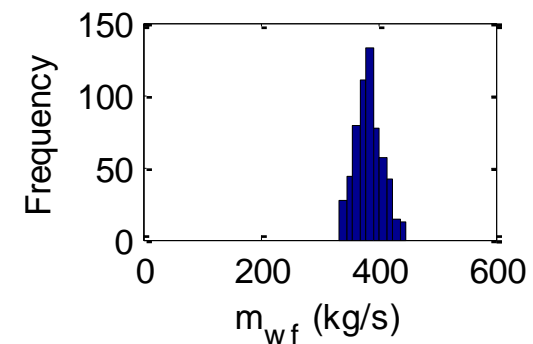
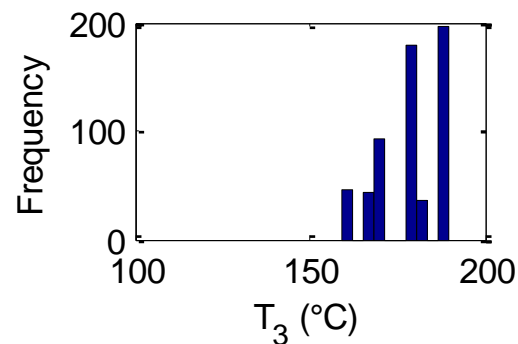
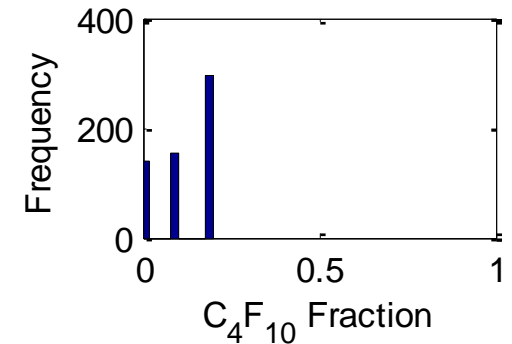
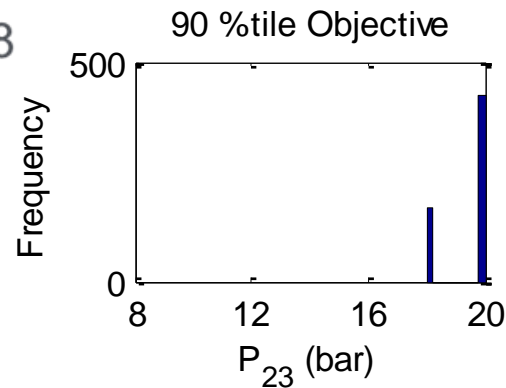
(NB: component costs only)



Optimal Operation Conditions for Perfluoroalkane Mixtures

Satisfactory working fluid conditions:

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

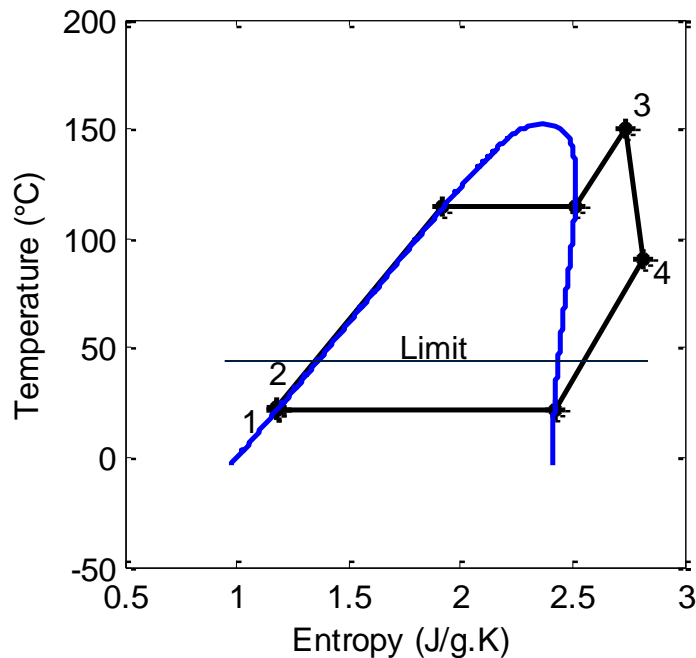


Decane + Butane Working Fluid with Regenerators

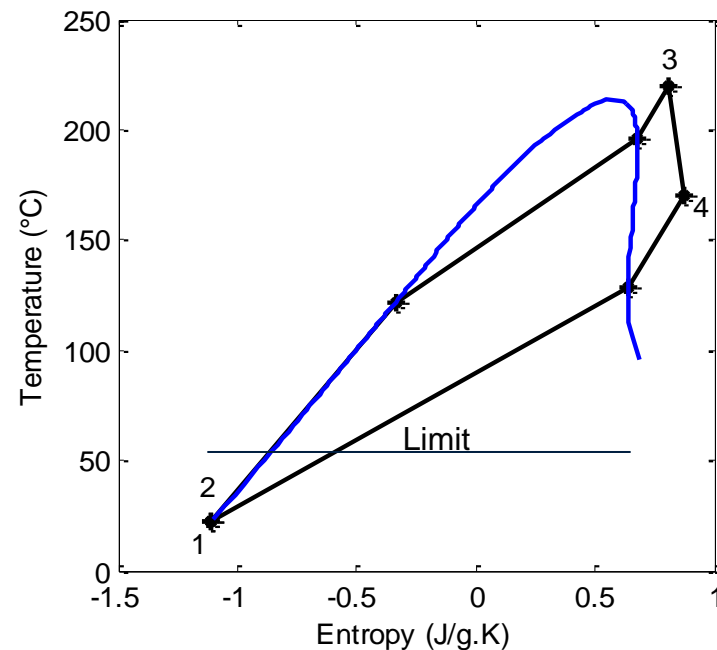
Why use regenerators?

Increased efficiencies but additional costs

Increased mass flowrates → Increased power output



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



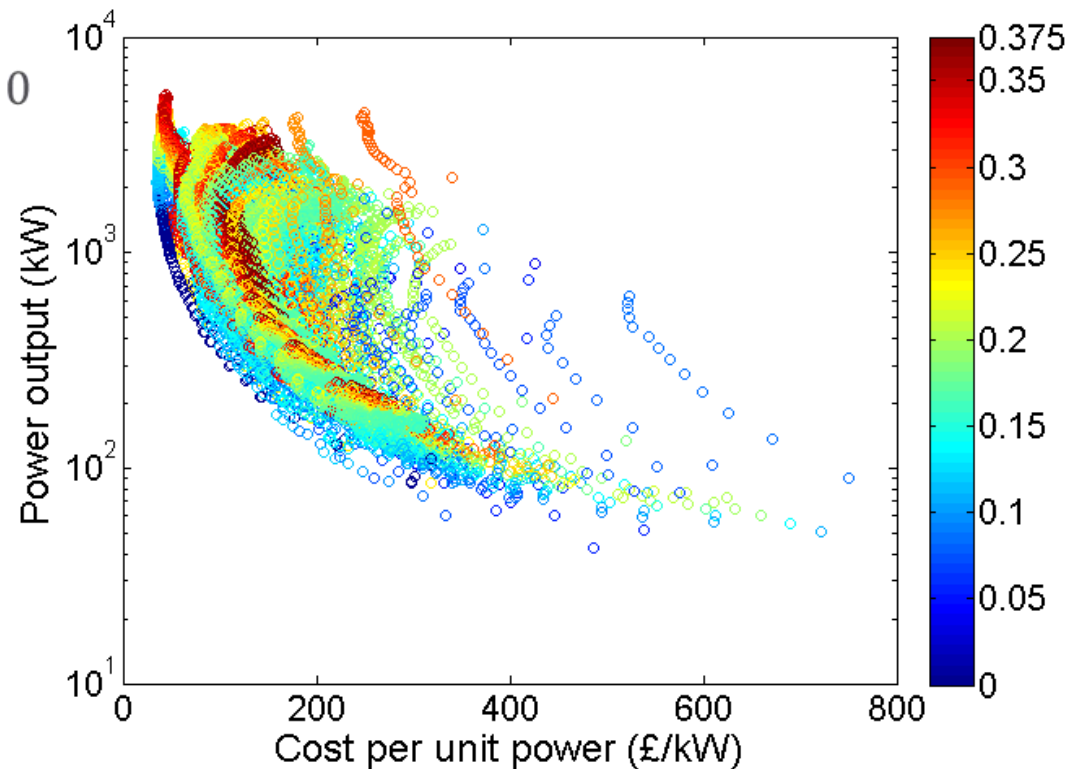
(b) Mixture working fluid

Decane + Butane Working Fluid with Regenerators

Flue gas at 330 °C

Working fluid conditions:

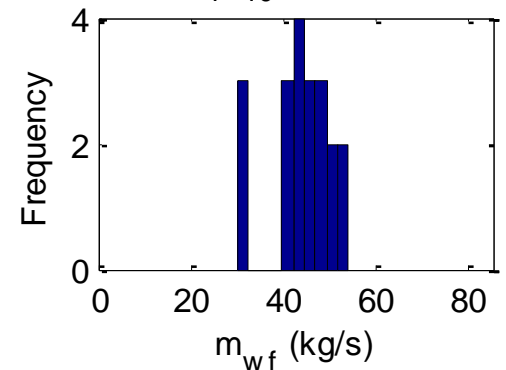
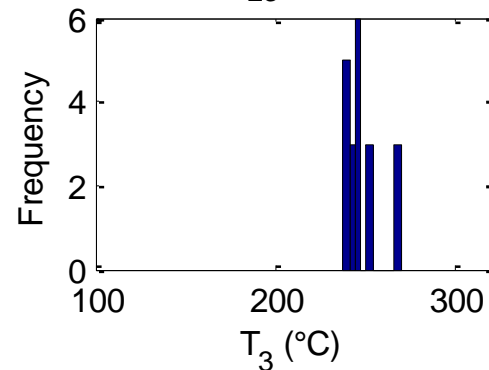
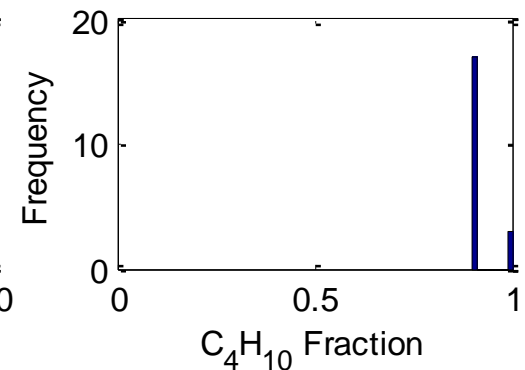
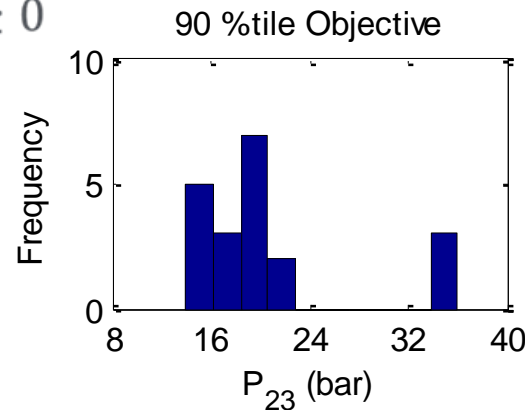
- $6 \text{ bar} \leq P_{23} \leq 40 \text{ bar}$
- $100 \text{ °C} \leq T_3 \leq 320 \text{ °C}$
- $1 \text{ kg/s} \leq \dot{m}_{\text{wf}} \leq 80 \text{ kg/s}$
- $0 \leq C_4H_{10} \leq 1; 1 \geq C_{10}H_{22} \geq 0$



Maximize Power Output, Efficiency and Minimize Costs per Unit Power

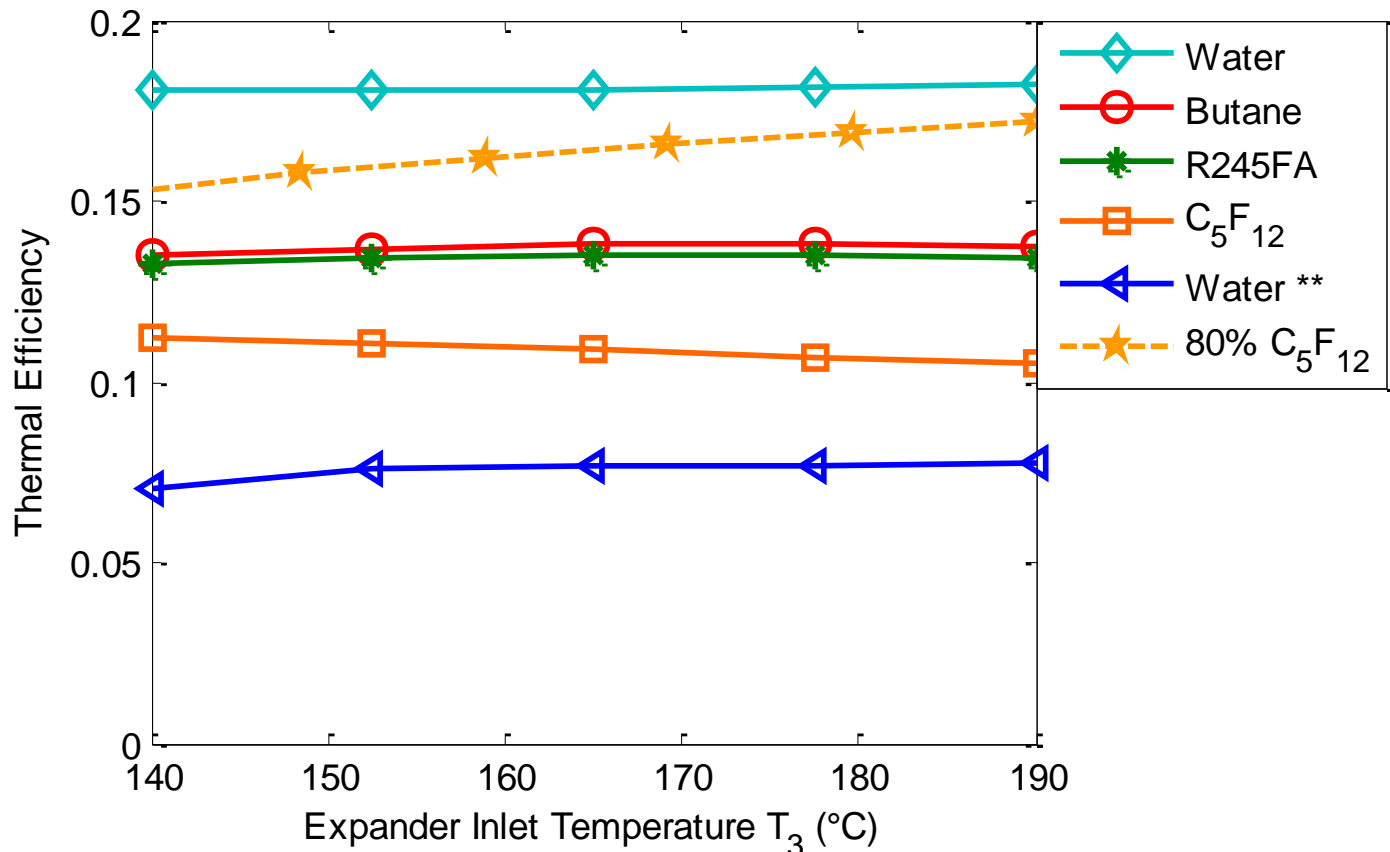
Satisfactory working fluid conditions:

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

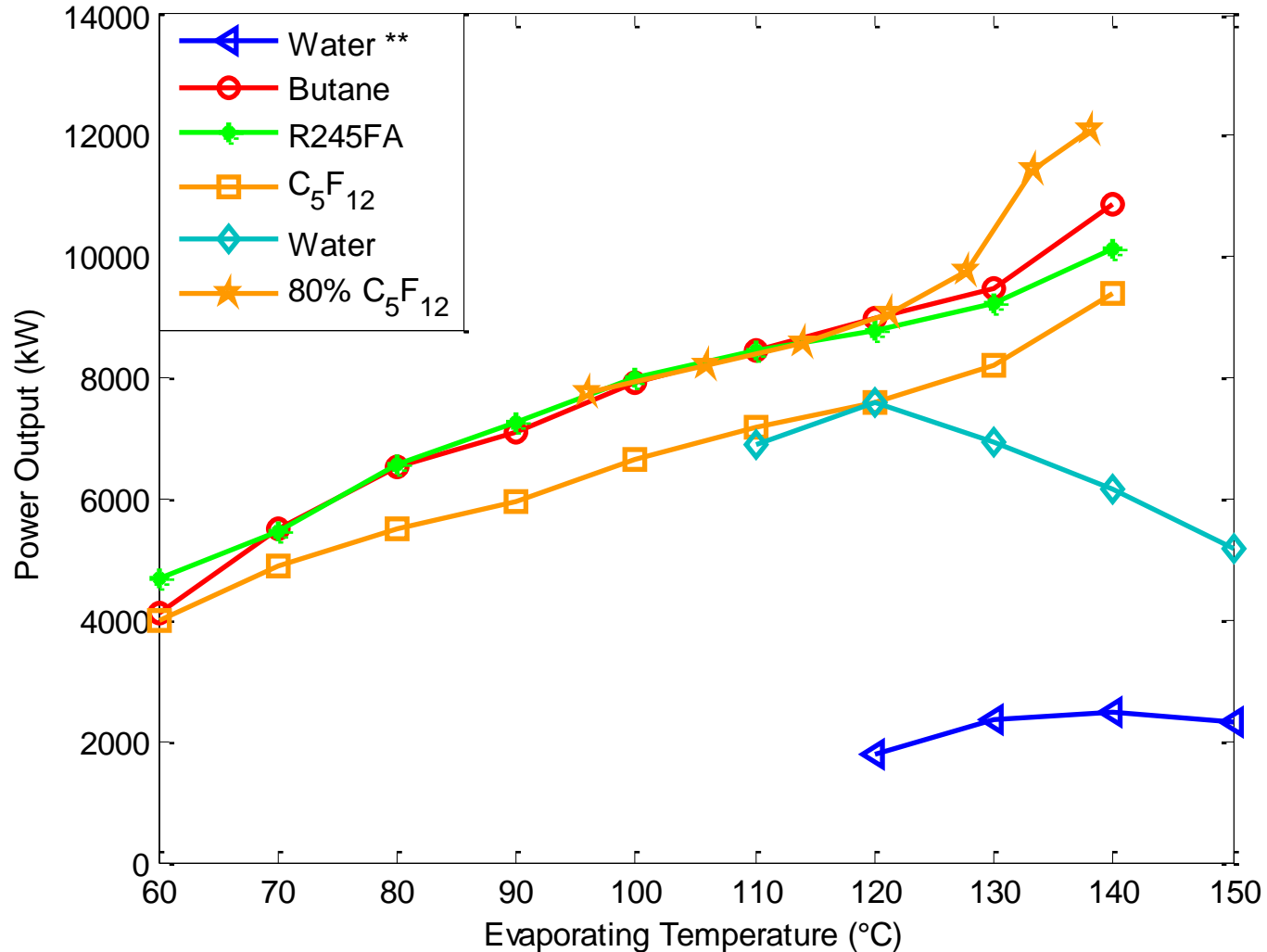


Thermal Efficiencies – Pure Working Fluids

- 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

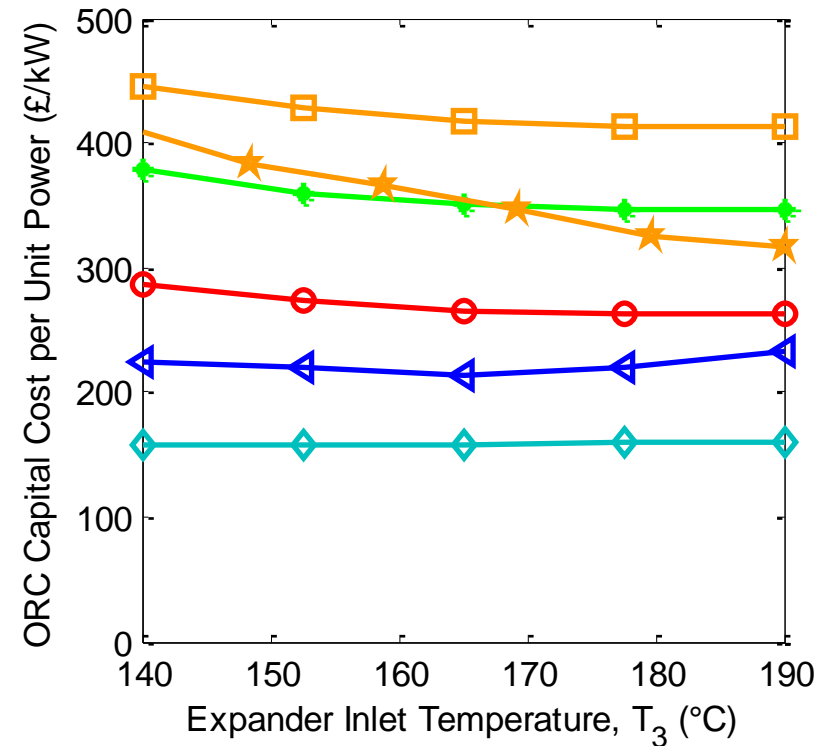
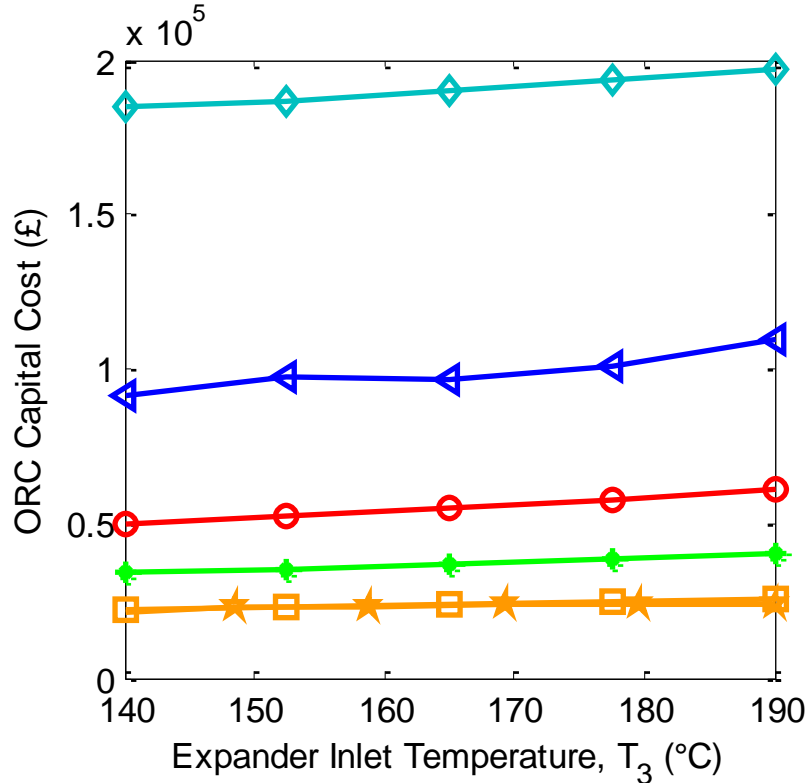


Component Cost Comparisons

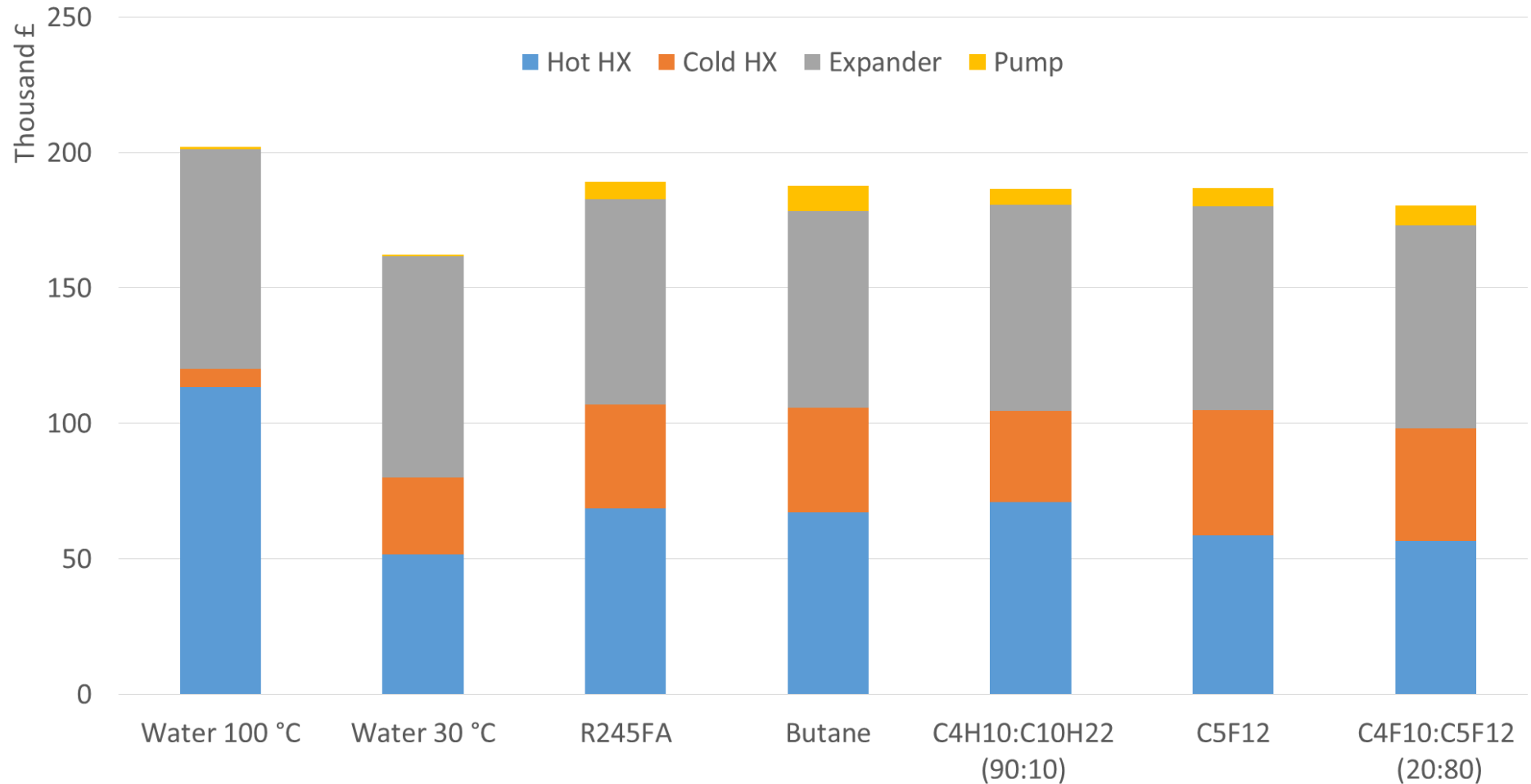
$\dot{m} = 2.5 \text{ kg/s}$

Condensing at 30°C , 100°C for water

Evaporating at 140°C and superheating to 190°C



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

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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