Imperial College London

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Integrated computer-aided working-fluid design and thermoeconomic ORC system optimisation

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Project aims and objectives

Key challenges in ORC system design:

- Identification of optimal working fluids
- Development of optimised systems based on thermoeconomic analyses
- Explore novel cycle architectures to enhance system performance

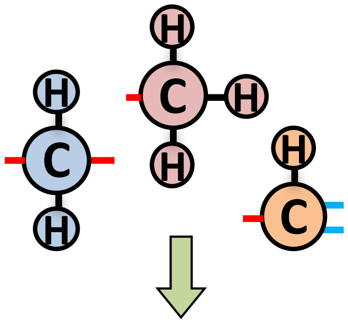
Research aim:

Develop an advanced CAMD-ORC optimisation framework based on SAFT-γ Mie capable of evaluating advanced cycle architectures, system operation parameters and fluids based on thermoeconomic performance indicators

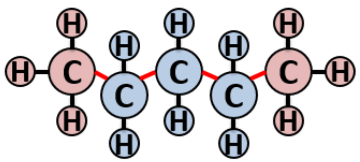
Presentation objectives:

- To introduce computed-aided molecular design (CAMD) within the context of ORC optimisation
- To apply thermoeconomic analysis within a CAMD-ORC framework

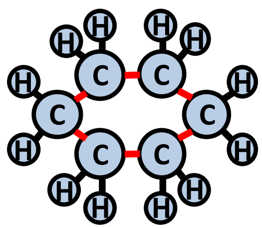
Computer-aided molecular design (CAMD)



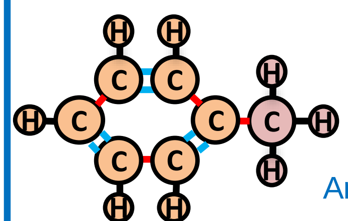
Group-contribution equation of state



Normal-alkanes

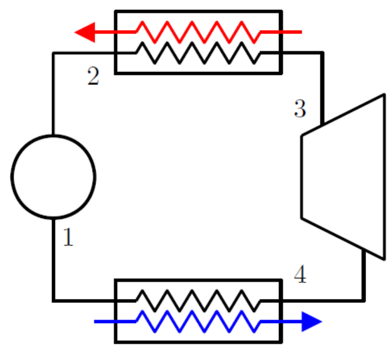


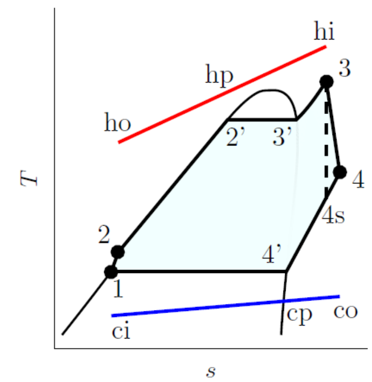
Cyclo-alkanes



Aromatics

Thermodynamic model





Mixed-integer non-linear programming (MINLP) optimisation

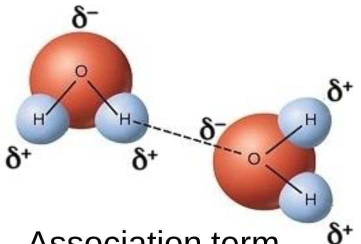
- Maximise/minimise objective function
- Integer optimisation variables: working fluid
- Continuous variables: thermodynamic cycle
- Binary variables: cycle architecture

CAMD-ORC model

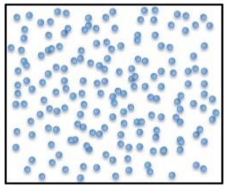
Group-contribution methods: SAFT-γ Mie

- Molecular-based, free-energy equation of state:

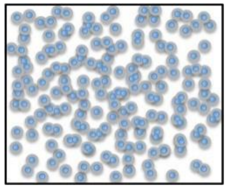
$$\frac{A(m,\sigma,\lambda,\varepsilon,u^{\text{assoc.}})}{NkT} = \frac{A^{\text{ideal}}}{NkT} + \frac{A^{\text{mono.}}}{NkT} + \frac{A^{\text{chain}}}{NkT} + \frac{A^{\text{assoc.}}}{NkT}$$



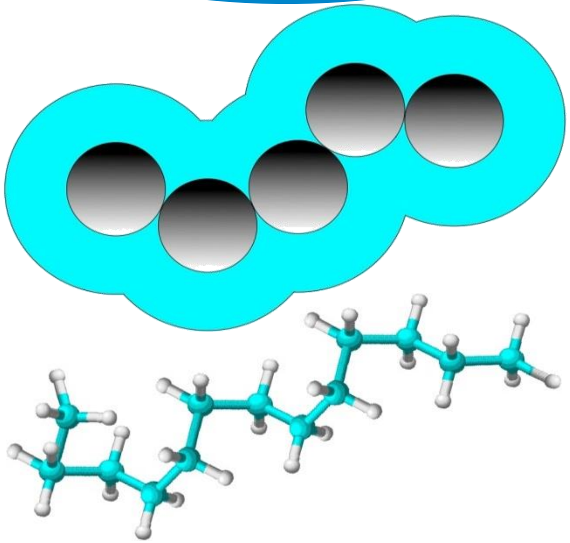
Association term



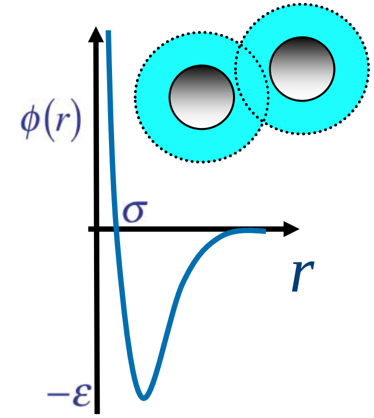
Ideal gas term



Real gas term, monomers, EoS for hard spheres



Grouping of monomers into chains
Chain term



Mie potential

[1] V. Papaioannou et al., 2014, J. Chem. Phys.
[2] S. Dufal et al., 2014, J. Chem. Eng. Data.
[3] T. Lafitte et al., 2013, J. Chem. Phys.

Group-contribution methods: Transport properties

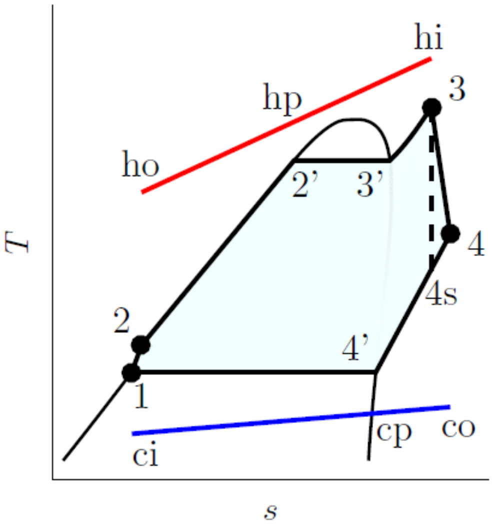
- Transport properties (k, μ, σ) are required to size heat exchangers
- Transport properties are not available from SAFT-γ Mie
- Group-contribution methods are sought that are:
  - Applicable to a large range of fluids
  - Suitable for the functional groups used within the CAMD-ORC model
  - Straightforward to implement
- Various methods have been implemented in the CAMD-ORC model (White *et al*., 2017)
- Critical properties $(T_{\mathrm{cr}}, P_{\mathrm{cr}}, V_{\mathrm{cr}})$ are estimated using Joback and Reid

	Liquid phase	Vapour phase
Dynamic viscosity	Joback and Reid (*n*-alkanes) Sastri-Rao (branched alkanes)	Reichenberg
Thermal conductivity	Sastri	Chung
Surface tension	Sastri-Rao	

White *et al*., Energy Conversion and Management, in press (2017).

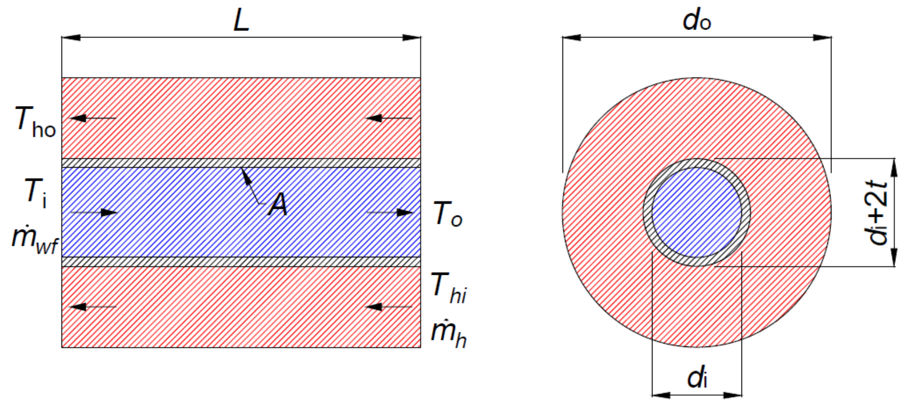
ORC thermodynamic modelling

- Simple, sub-critical, non-regenerative ORC systems
- Energy balance applied to main system components (pump, evaporator, expander, condenser)
- Defined heat source and sink (temperature, mass-flow rate and specific-heat capacity)
- Fixed pump and expander efficiencies, η_p and η_e
- ORC variables:
  - Condensation temperature, T_1
  - Reduced evaporation pressure, P_r
  - Evaporator pinch point, PP_h
  - Expander inlet condition parameter, z
- Constraints:
  - Minimum evaporator pinch point, $PP_\mathrm{h,min}$
  - Minimum condenser pinch point, $PP_\mathrm{c,min}$
  - Condensation pressure cannot be sub-atmospheric
  - Expansion cannot be into the two-phase region



Component sizing

- Evaporator and condenser units selected are of tube-in-tube construction
- Heat transfer coefficient (HTC) and heat-transfer areas (HTA) as functions of Nusselt numbers
- Evaporator is split into 3 sections:
  - Preheating section
  - Evaporating section
  - Superheating section
- Condenser is split into 2 sections:
  - Desuperheating section
  - Condensing section
- Each section is discretised spatially to account for changes in working-fluid properties over the length of the heat exchanger



Component costing

- Pump, pump motor and heat exchangers are costed using the correlations proposed by Seider *et al*. [1]:

$$C_p^0 = F \exp(Z_1 + Z_2 \ln X + Z_3 \ln(X)^2 + Z_4 \ln(X)^3 + Z_5 \ln(X)^4)$$

- Expander costed using the correlation proposed by Turton *et al*. [2]:

$$C_p^0 = F 10^{(Z_1 + Z_2 \log X + Z_3 \log(X)^2)}$$

X the sizing attribute (power, heat-transfer area etc.)

$F,\ Z_n$ correlation coefficients

- Costs converted to todays prices using the CEPCI

[1] Seider *et al*., 2009, *Product and Process Design Principles – Synthesis, Analysis and Evaluation.*

[2] Turton *et al*., 2009, *Analysis, Synthesis and Design of Chemical Processes.*

Optimisation

$$\max \left\{ \dot{W}_{\mathrm{n}}(\mathbf{x}, \mathbf{y}) \right\}$$

Subject to:

$$g(\mathbf{x}, \mathbf{y}) \leq 0 \; ;$$

$$h(\mathbf{x}, \mathbf{y}) \leq 0 \; ;$$

$$\mathbf{x}_{\mathrm{min}} \leq \mathbf{x} \leq \mathbf{x}_{\mathrm{max}} \; ;$$

$$\mathbf{y}_{\mathrm{min}} \leq \mathbf{y} \leq \mathbf{y}_{\mathrm{max}}$$

- CAMD-ORC framework developed in the gPROMS modelling environment
- MINLP optimisation solved using built-in outer approximation algorithm OAERAP

Case study

Definition

- Three heat-source temperatures considered: 150, 250 and 350 °C
- Assumptions for waste-heat recovery case study:

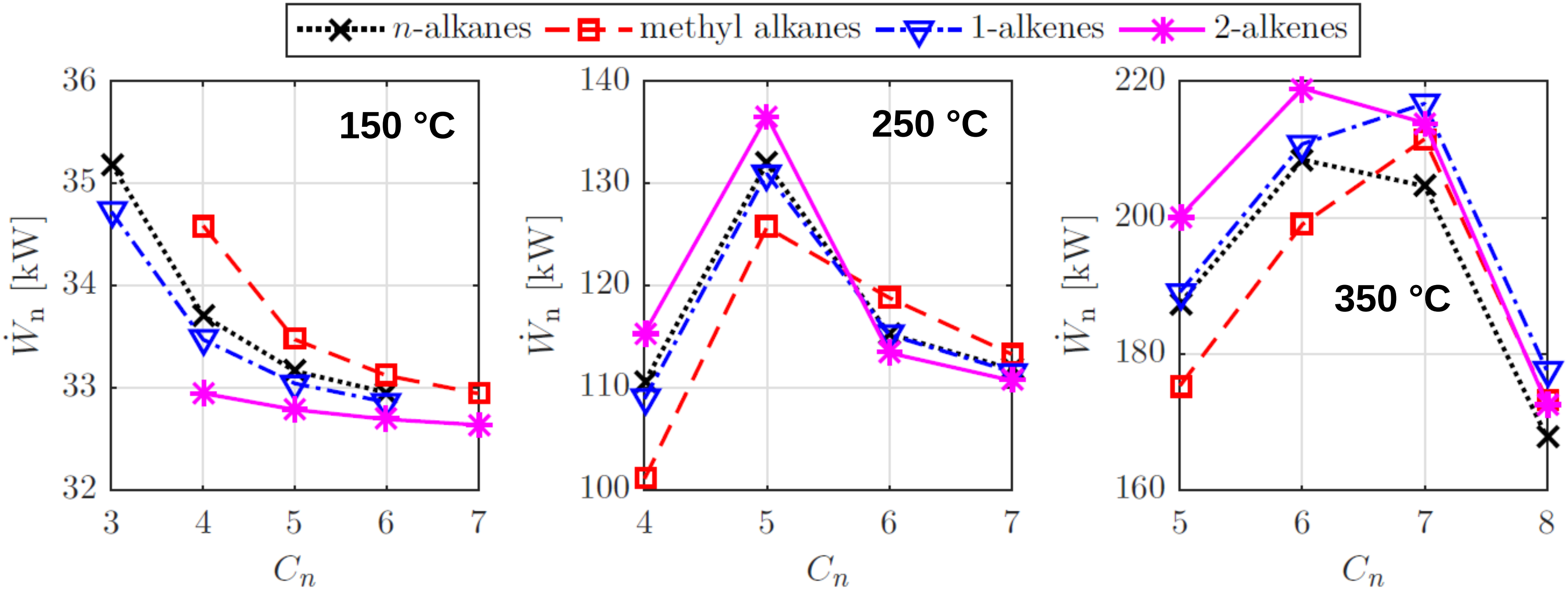
$\dot{m}_{\mathrm{h}}$ kg/s	$c_{\mathrm{p,h}}$ kJ/(kg K)	T_{ci} °C	$\dot{m}_{\mathrm{c}}$ kg/s	$c_{\mathrm{p,c}}$ kJ/(kg K)	η_{p}	η_{e}	$PP_{\mathrm{h,min}}$ °C	$PP_{\mathrm{c,min}}$ °C	$P_{\mathrm{1,min}}$ bar
1.0	4.2	15	5	4.2	0.7	0.8	10	5	0.25

- Alongside the ORC variables ($T_1, p_{\mathrm{r}}, \Delta T_{\mathrm{sh}}, PP_{\mathrm{h}}$) the effect of the number of >CH_2 groups on ORC performance is investigated for four fluid families

***n*-alkanes**	**methyl alkanes**
$CH_3 - \mathbf{(CH_2)_n} - CH_3$	$(CH_3)_2 - CH - \mathbf{(CH_2)_n} - CH_3$
1-alkenes	**2-alkenes**
$CH_2 = CH - \mathbf{(CH_2)_n} - CH_3$	$CH_3 - CH = CH - \mathbf{(CH_2)_n} - CH_3$

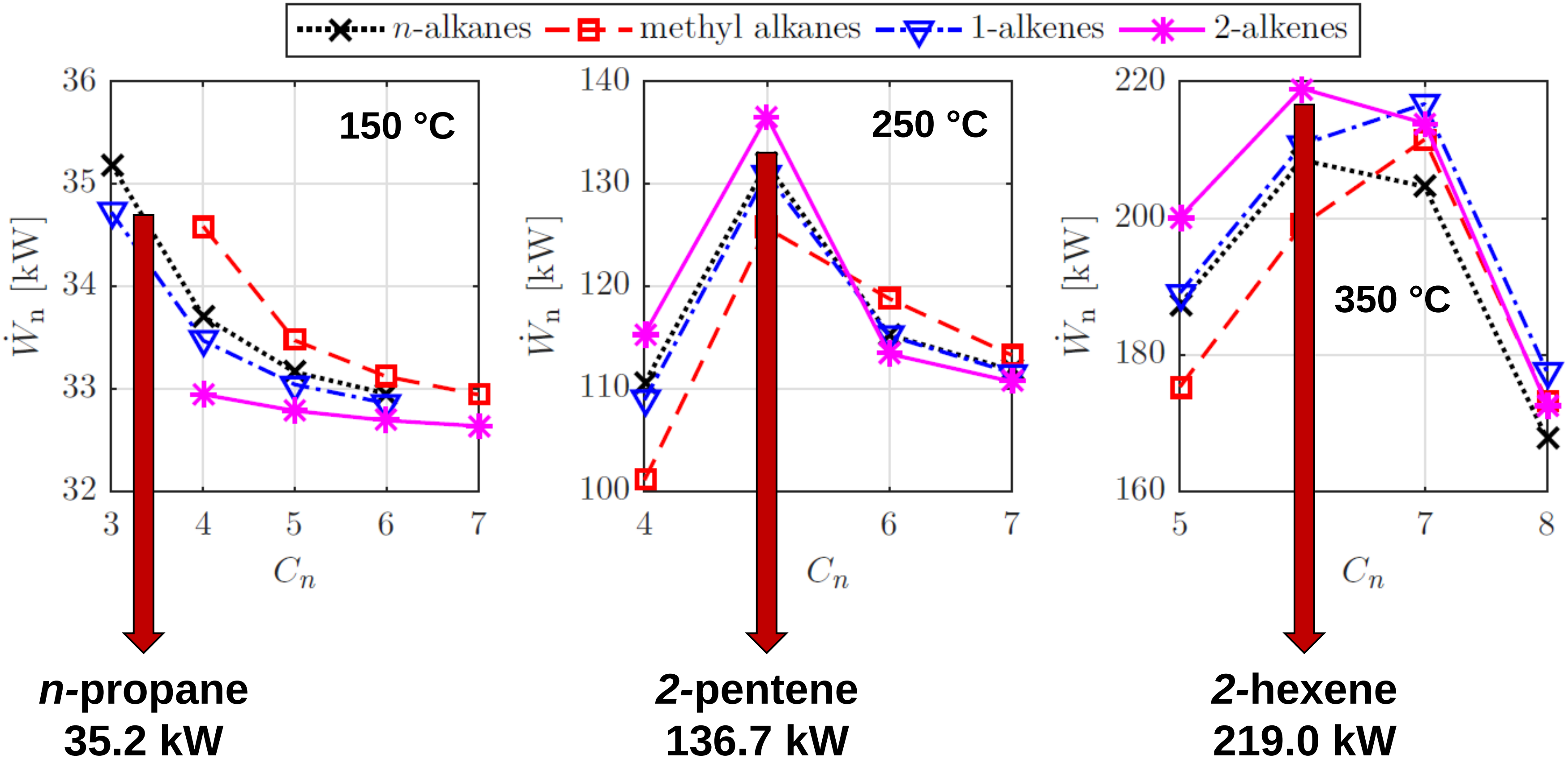
- The aim is to maximize the net power output from a basic ORC system

Thermodynamic results

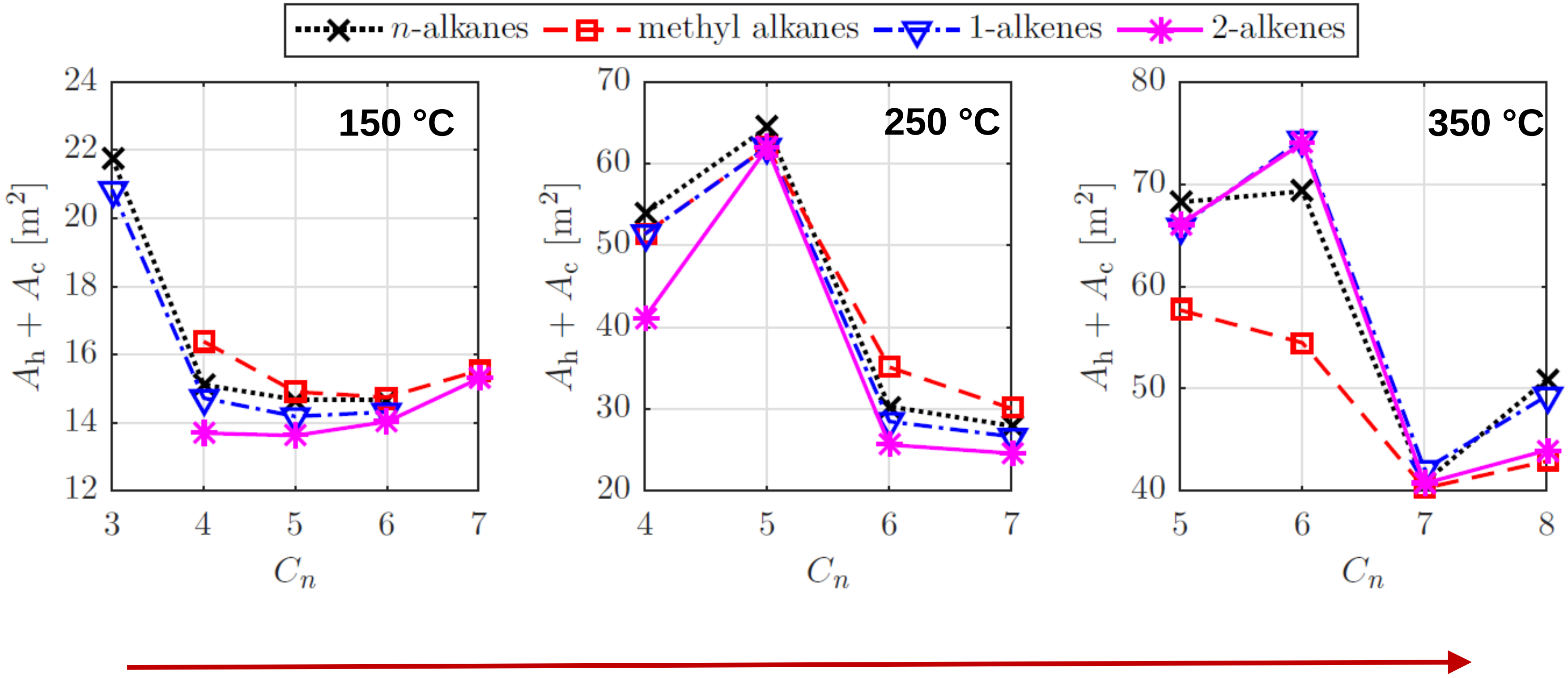


Increasing heat-source temperature → Increasing system size

Thermodynamic results

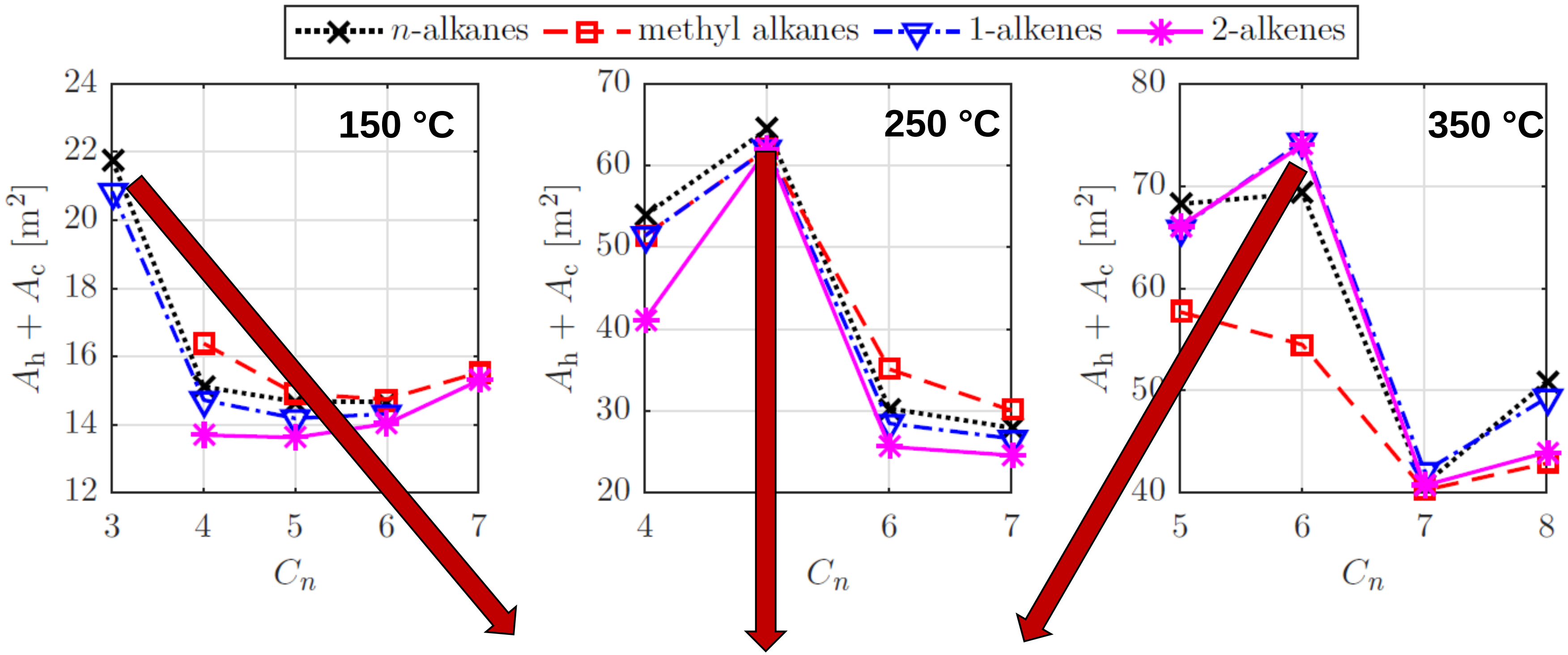


Component sizing results: Heat transfer areas



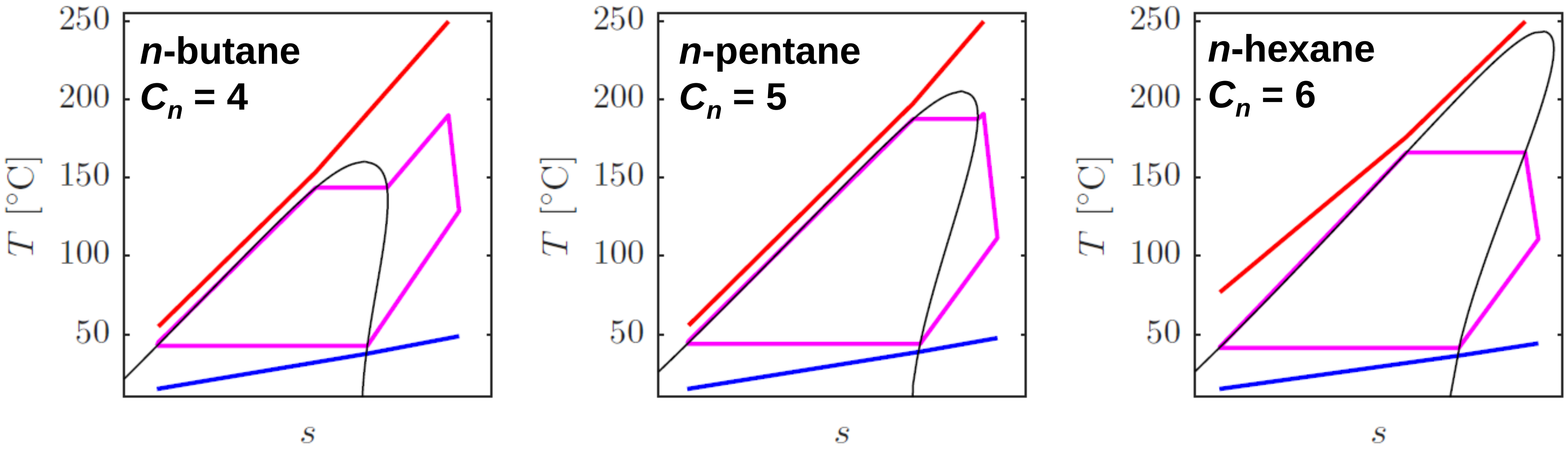
Increasing heat-source temperature → Increasing system size → Increased HTA

Component sizing results: Heat transfer areas

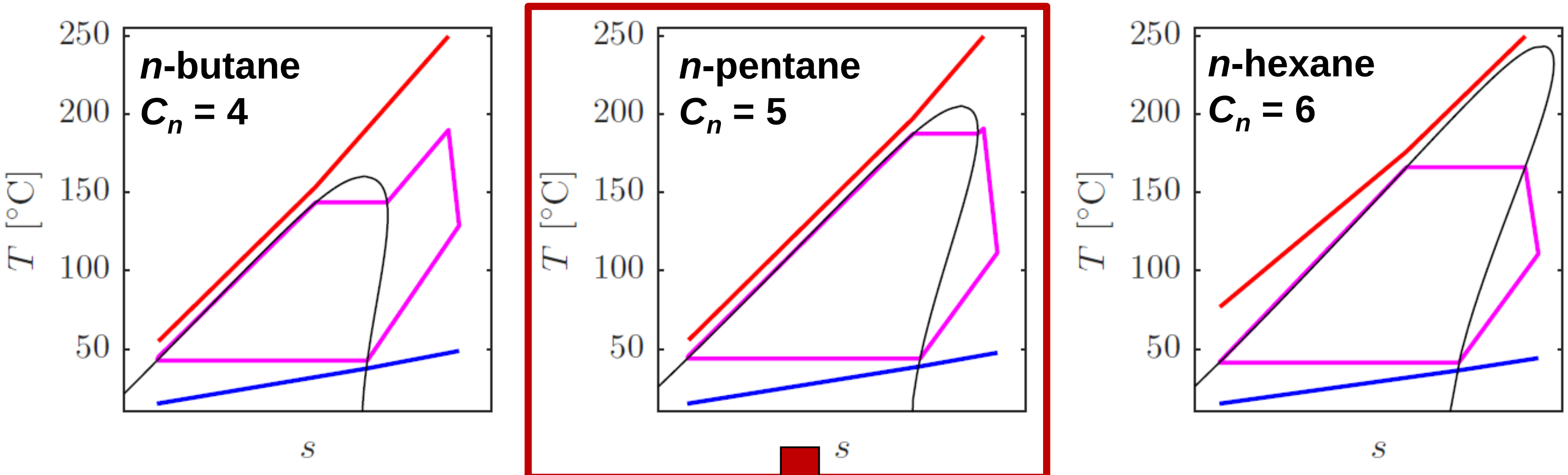


Maximum power output
Highest heat-transfer area requirements

Component sizing results: 250 °C, *n*-alkane



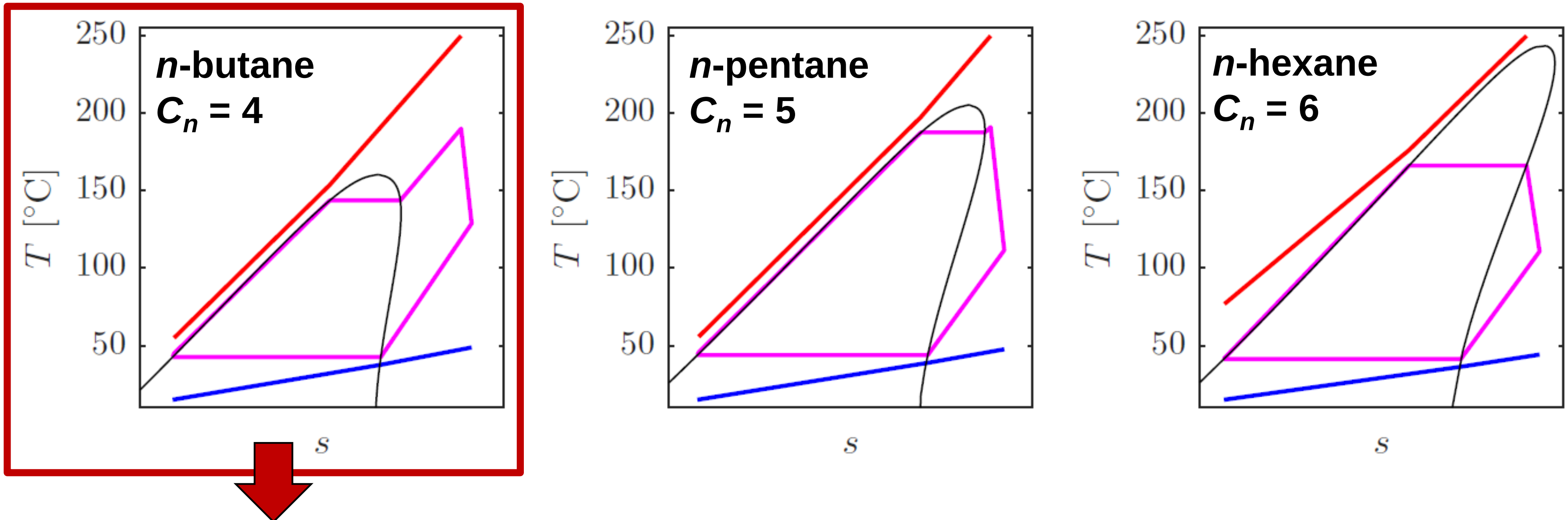
Component sizing results: 250 °C, *n*-alkane



Maximise evaporation pressure → Minimise two-phase heat transfer
Minimise superheating → Minimise vapour heat transfer
Pinch at preheater inlet → Small temperature differences

Maximise power output **Maximum heat-transfer area**

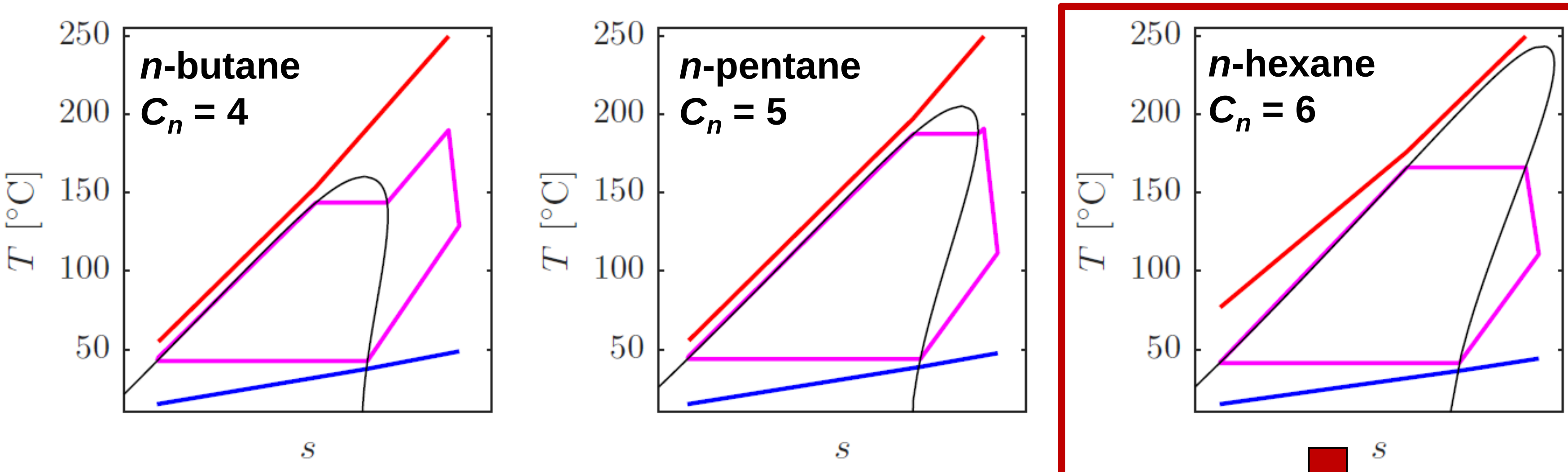
Component sizing results: 250 °C, *n*-alkane



Maximise evaporation pressure → Minimise two-phase heat transfer
More superheating required → Larger superheater but high ΔT
Pinch at preheater inlet → Small temperature differences

16% reduction in power output **16% reduction in heat-transfer area**

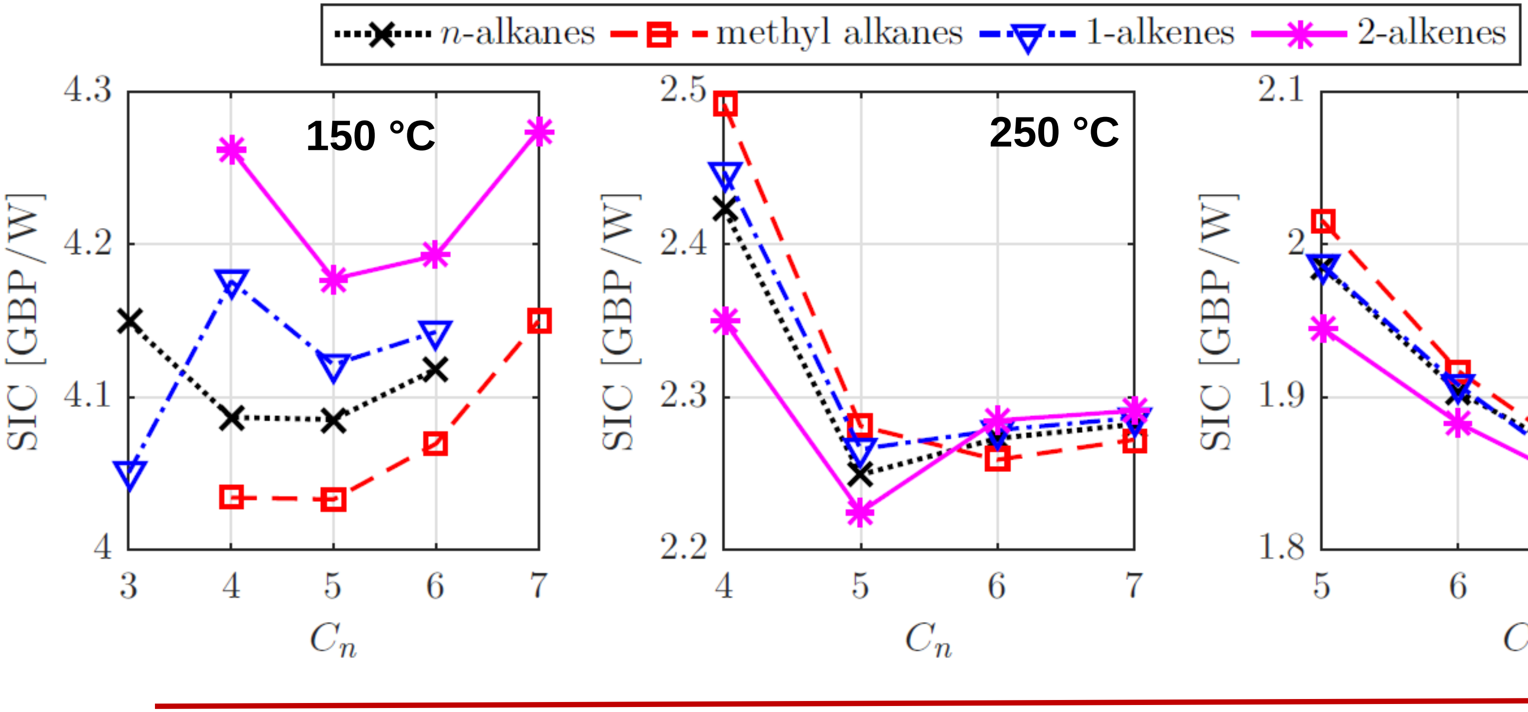
Component sizing results: 250 °C, *n*-alkane



Reduced evaporation pressure	→	More two-phase heat transfer
No superheating required	→	No superheater required
Not pinched at preheater inlet	→	Higher temperature differences

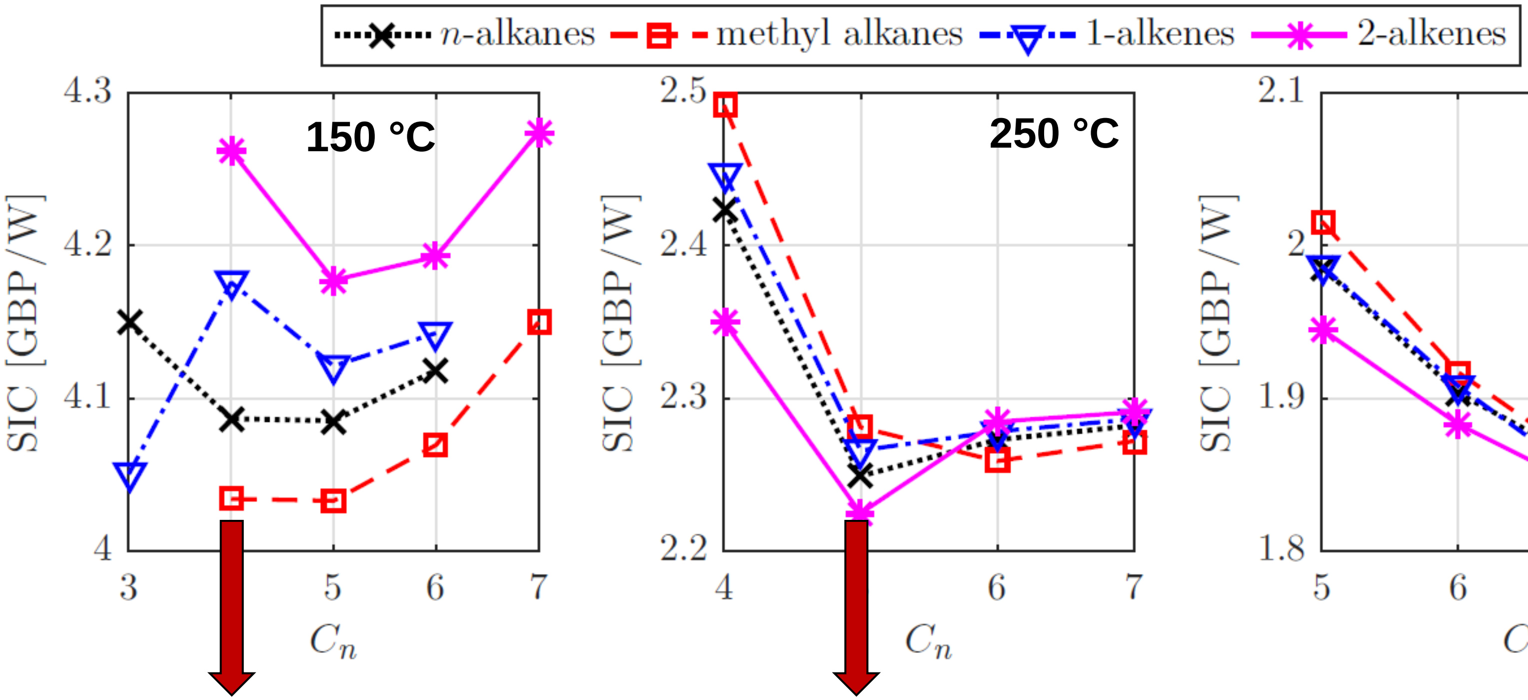
13% reduction in power output **51% reduction in heat-transfer area**

Thermoeconomic results



Increasing heat-source temperature → Increasing system size → Reduced SIC

Thermoeconomic results

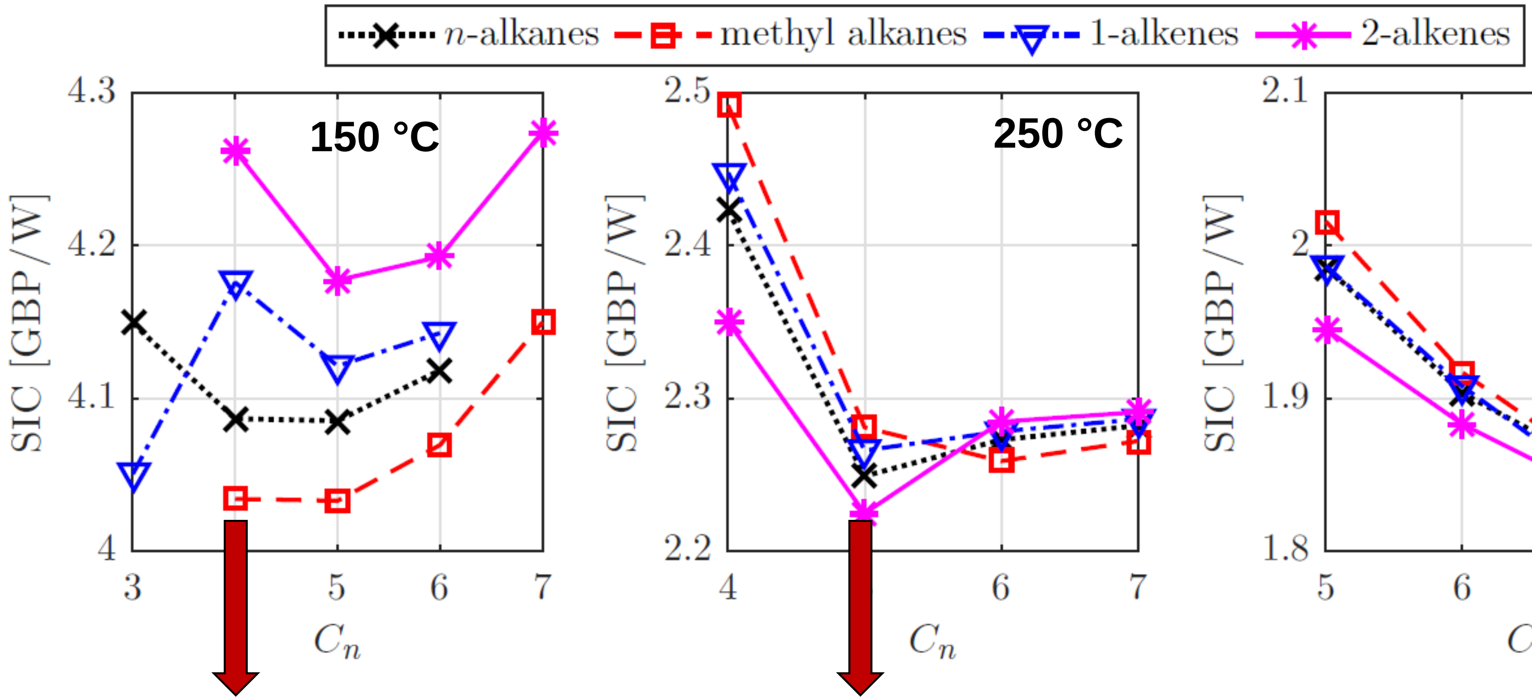


isobutane
4.03 £/W

2-pentene
2.22 £/W

2-heptene
1.84 £/W

Thermoeconomic results



isobutane
4.03 £/W
$\downarrow\dot{W}_n$ = 4.9%

2-pentene
2.22 £/W
$\downarrow\dot{W}_n$ = 0%

2-heptene
1.84 £/W
$\downarrow\dot{W}_n$ = 2.3%

Minimising SIC can identify different optimal working fluids

Conclusions

- CAMD facilitates an integrated approach to working fluid and ORC system optimisation
- SAFT-γ Mie and group-contribution transport property methods are proven to be suitable for use within a CAMD-ORC framework
- Component sizing and costing models have been implemented within the existing CAMD-ORC framework
- Optimal thermodynamic cycles have large heat-transfer area requirements
- Fluid selection based on SIC identifies different optimal working fluids:
  - 150 °C heat source → isobutane SIC = 4.03 £/W
  - 250 °C heat source → 2-pentene SIC = 2.22 £/W
  - 350 °C heat source → 2-hexene SIC = 1.84 £/W
- This highlights the importance of considering thermoeconomic performance indicators
- **Next steps:** Implement multi-objective optimisation into the CAMD-ORC model

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Thank you for listening.

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