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-\(\gamma\) Mie**

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

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

Group-contribution methods: Transport properties

- Transport properties \((k, \mu, \sigma)\) are required to size heat exchangers
- Transport properties are not available from SAFT-\(\gamma\) 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 \((T_{cr}, P_{cr}, V_{cr})\) are estimated using Joback and Reid

<table>
<thead>
<tr>
<th></th>
<th>Liquid phase</th>
<th>Vapour phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic viscosity</td>
<td>Joback and Reid ((n\text{-alkanes}))</td>
<td>Reichenberg</td>
</tr>
<tr>
<td></td>
<td>Sastri-Rao ((\text{branched alkanes}))</td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>Sastri</td>
<td>Chung</td>
</tr>
<tr>
<td>Surface tension</td>
<td>Sastri-Rao</td>
<td></td>
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</tbody>
</table>
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, $\eta_p$ and $\eta_e$

- 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, $PP_{h,\text{min}}$
  - Minimum condenser pinch point, $PP_{c,\text{min}}$
  - 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]:

\[ C_p^0 = F10^{(Z_1+Z_2 \log X+Z_3 \log(X)^2)} \]

\[ X \quad \text{the sizing attribute (power, heat-transfer area etc.)} \]
\[ F, Z_n \quad \text{correlation coefficients} \]

• Costs converted to todays prices using the CEPCI

Optimisation

\[
\text{max } \{ \dot{W}_n(x, y) \}
\]

Subject to:

\[
g(x, y) \leq 0 ;
\]

\[
h(x, y) \leq 0 ;
\]

\[
x_{\text{min}} \leq x \leq x_{\text{max}} ;
\]

\[
y_{\text{min}} \leq y \leq y_{\text{max}}
\]

- 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:

<table>
<thead>
<tr>
<th>$\dot{m}_h$ kg/s</th>
<th>$c_{p,h}$ kJ/(kg K)</th>
<th>$T_{ci}$ °C</th>
<th>$\dot{m}_c$ kg/s</th>
<th>$c_{p,c}$ kJ/(kg K)</th>
<th>$\eta_p$</th>
<th>$\eta_e$</th>
<th>$PP_{h,min}$ °C</th>
<th>$PP_{c,min}$ °C</th>
<th>$P_{1,min}$ bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>4.2</td>
<td>15</td>
<td>5</td>
<td>4.2</td>
<td>0.7</td>
<td>0.8</td>
<td>10</td>
<td>5</td>
<td>0.25</td>
</tr>
</tbody>
</table>

- Alongside the ORC variables ($T_1, p_r, \Delta T_{sh}, PP_h$) the effect of the number of $>\text{CH}_2$ groups on ORC performance is investigated for four fluid families

<table>
<thead>
<tr>
<th>$n$-alkanes</th>
<th>methyl alkanes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{CH}_3 - (\text{CH}_2)_n - \text{CH}_3$</td>
<td>$(\text{CH}_3)_2 - \text{CH} - (\text{CH}_2)_n - \text{CH}_3$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-alkenes</th>
<th>2-alkenes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{CH}_2 = \text{CH} - (\text{CH}_2)_n - \text{CH}_3$</td>
<td>$\text{CH}_3 - \text{CH} = \text{CH} - (\text{CH}_2)_n - \text{CH}_3$</td>
</tr>
</tbody>
</table>

- 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

150 °C
- $n$-propane: 35.2 kW
- 2-pentene: 136.7 kW
- 2-hexene: 219.0 kW

250 °C
- $n$-alkanes
- Methyl alkanes
- 1-alkenes
- 2-alkenes

350 °C
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

- \( n \)-butane \( C_n = 4 \)
- \( n \)-pentane \( C_n = 5 \)
- \( n \)-hexane \( C_n = 6 \)
Component sizing results: 250 °C, \( n \)-alkane

\( n \)-butane
\( C_n = 4 \)

\( n \)-pentane
\( C_n = 5 \)

\( n \)-hexane
\( C_n = 6 \)

Maximise evaporation pressure \( \rightarrow \) Minimise two-phase heat transfer
Minimise superheating \( \rightarrow \) Minimise vapour heat transfer
Pinch at preheater inlet \( \rightarrow \) Small temperature differences

Maximise power output

Maximum heat-transfer area
Component sizing results: 250 °C, \textit{n}-alkane

Maximise evaporation pressure \implies\ Minimise two-phase heat transfer
More superheating required \implies\ Larger superheater but high $\Delta T$
Pinch at preheater inlet \implies\ Small temperature differences

16% reduction in power output \quad 16% reduction in heat-transfer area
Component sizing results: 250 °C, $n$-alkane

- **$n$-butane**
  - $C_n = 4$

- **$n$-pentane**
  - $C_n = 5$

- **$n$-hexane**
  - $C_n = 6$

Reduced evaporation pressure $\rightarrow$ More two-phase heat transfer
No superheating required $\rightarrow$ No superheater required
Not pinched at preheater inlet $\rightarrow$ 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

Graphs showing SIC [GBP/W] for n-alkanes, methyl alkanes, 1-alkenes, and 2-alkenes at 150 °C, 250 °C, and 350 °C.
Minimising SIC can identify different optimal working fluids

- **Isobutane**
  - 4.03 £/W
  - $\dot{W}_n = 4.9\%$

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

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

- CAMD facilitates an integrated approach to working fluid and ORC system optimisation
- SAFT-$\gamma$ 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 $\rightarrow$ isobutane  SIC = 4.03 £/W
  - 250 °C heat source $\rightarrow$ 2-pentene  SIC = 2.22 £/W
  - 350 °C heat source $\rightarrow$ 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
Thank you for listening.

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