POLITECNICO
MILANO 1863

Thermodynamic Optimization of heat recovery ORCs for heavy duty Internal Combustion Engine: pure fluids vs. zeotropic mixtures

4th International Seminar on ORC Power Systems

September 13th - 15th, 2017
Politecnico di Milano - Milan, Italy

Roberto Scaccabarozzi

Michele Tavano
Costante Mario Invernizzi
Emanuele Martelli
emanuele.martelli@polimi.it

Motivations

Great diffusion of internal combustion engine, mainly in the transport sector

Main advantages of **recovering the waste heat**:

- Increasing **power generation** and **efficiency**
- Reducing **carbon footprint** and **fossil fuel consumption**

The **technical and economic feasibility** increases with engine **size** and for engines running mainly at **constant load**, like for power production and large naval engines

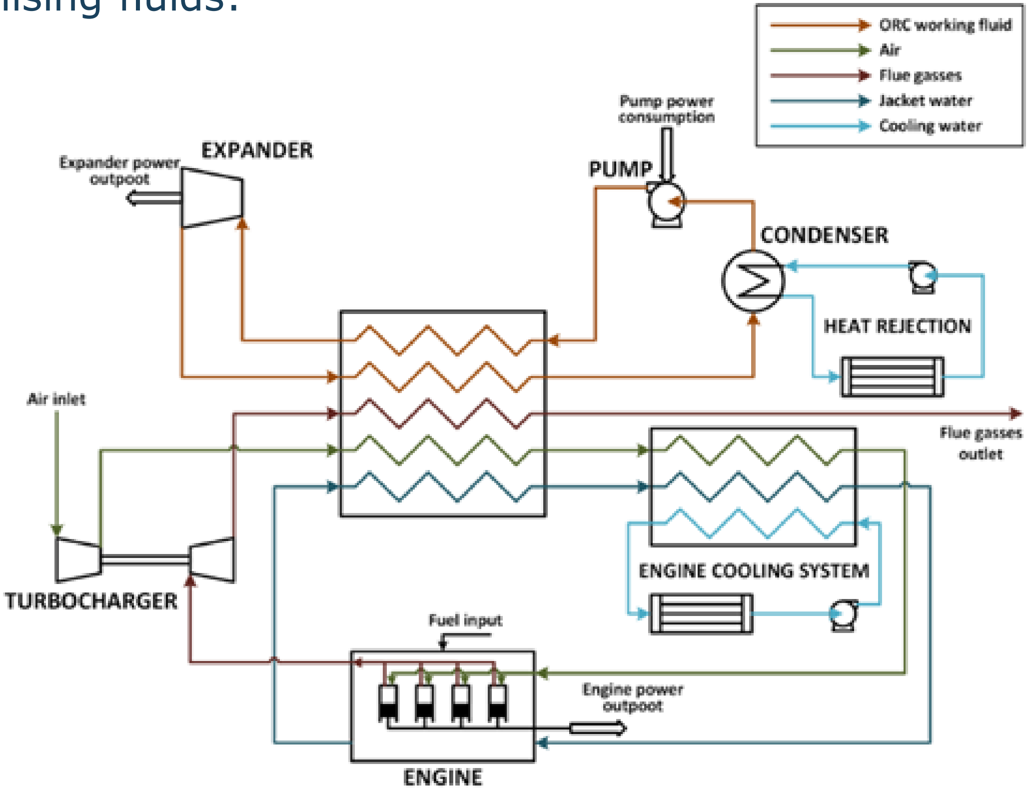
Lacking of a systematic study of the ORC considering:

- The optimal **working fluid** selection
- The optimization of the **heat integration** with all the possible heat sources
- The optimization of the **cycle variables**

Objectives

1. Performing a systematic **thermodynamic optimization** of heat recovery ORCs for internal combustion engines
2. Devising an ad hoc **optimization approach**
3. Screening a large number of promising fluids:
   - **Conventional** and **recently developed** fluids (HFE, HCFO, HFO)
   - **Binary zeotropic mixtures**
4. Selecting optimal **operative conditions** and cycle configuration

Economic and operational aspects, which require also the optimization of the heat exchanger configuration, are **not considered** in this work



Challenges

- Extremely **large number** of possible fluids and mixtures → Need of **fluid selection criteria**
- **Several heat sources** available:
  - Exhaust gas
  - Scavenge air
  - Jacket water
- **Several possible arrangements** of the heat exchangers → Need of considering the heat integration between the three hot streams and the cycle

Fluid selection

Selection criteria:

- Optimal **heat integration** with the hot flue gas stream (critical temperature close to flue gas inlet temperature)
- **Condensation pressure** at ambient temperature higher than 0.03 bar (preferably above atmospheric)
- **Thermo-chemical stability** (preferably up to the flue gas inlet temperature)
- Low **environmental impact** (GWP, ODP, ALT)
  - No CFC, HCFC, PFC
- **Measured** fluid **property data** and **validated Equation of State** (NIST, REFPROP V9.1)

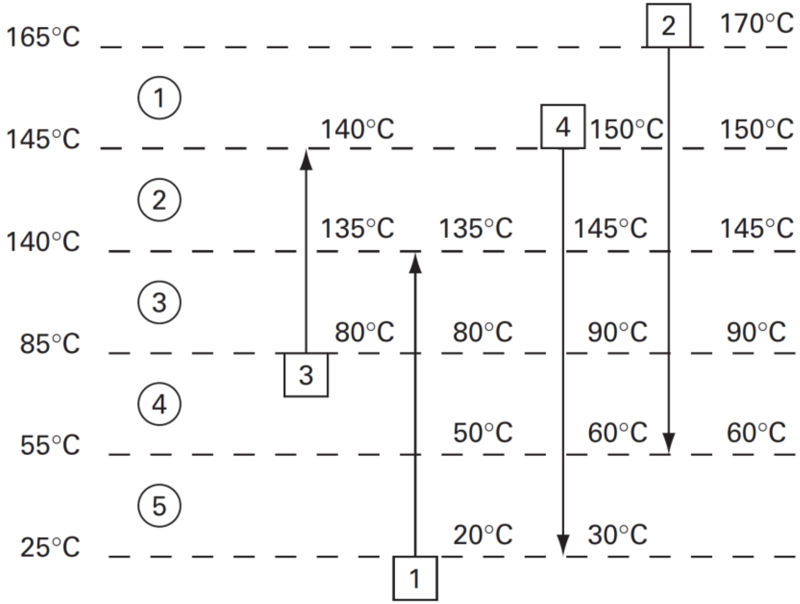
  - OR -

  Available Equation of State **parameter estimation method** (Lemmon 2001)

Heat Integration

The heat integration algorithm is the **energy targeting** method proposed by Maréchal and Kalitventzeff based on the “heat cascade”:

- **No restriction** regarding the possible matching of the flows
- The heat transfer is performed in a **multi-flow heat exchanger**
- **Linear bihavior** of the streams (disctretization)
- Streams are divided into **temperature intervals**
- Heat transfer can occur between any hot and cold stream with **$\Delta T \geq \Delta T_{min}$**
- The variables are the **ORC mass flow rate** and cooling water
- The constraints are the **energy balance** of each temperature interval
- The objective function is the **maximum energy efficiency** (recovered power)



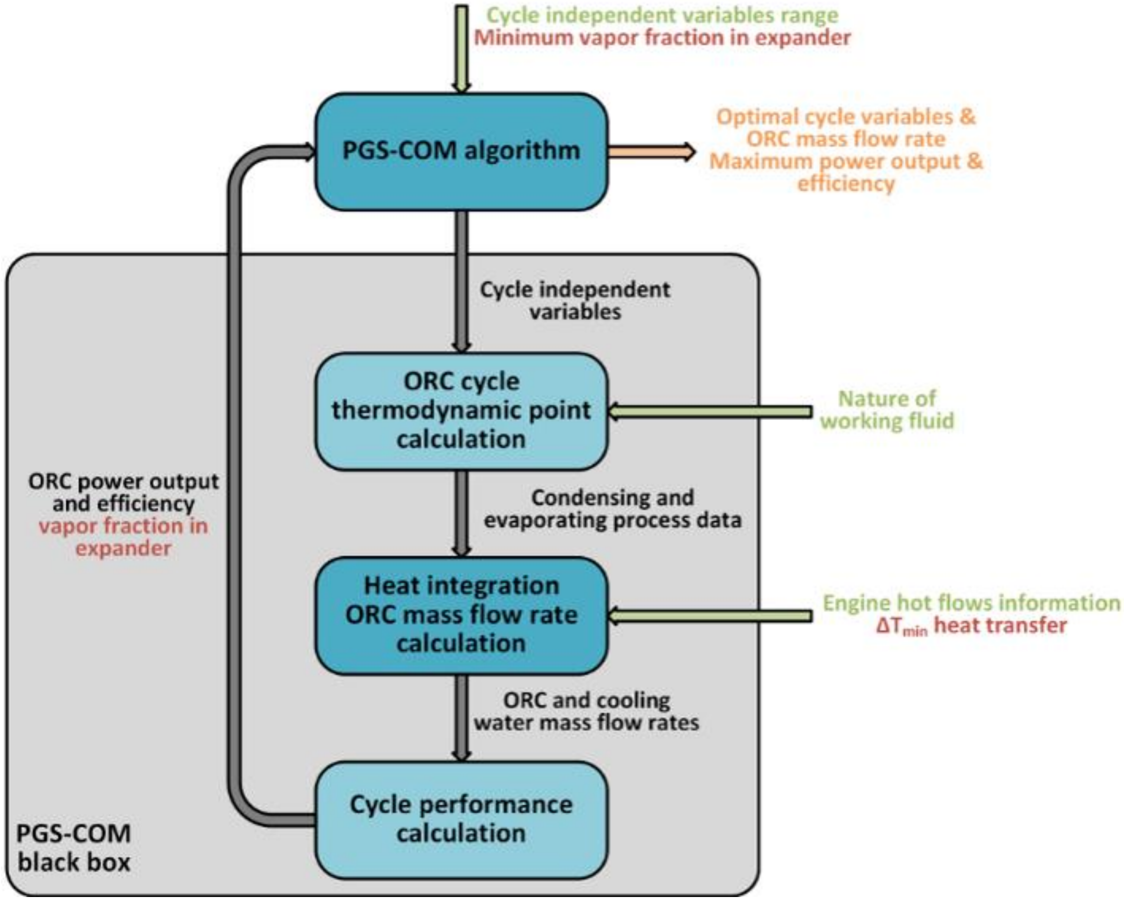
Cycle optimization problem

Optimization problem: (performed for each fluid/mixture selected)

- **Objective function:**
  - **Maximum mechanical/electric power** generated by the heat recovery ORC
- **Independent optimization variables:**
  - Evaporating pressure
  - Condensing pressure
  - Turbine inlet temperature
  - Mass flow rate of ORC
  - Composition (only for mixtures)
- **Nonlinear constraints:**
  - Minimum vapor fraction in the expansion greater than 0.88
  - Minimum temperature difference in each heat exchanger grater or equal to 5°C
- **Key Assumptions:**
  - Set of hot streams made available by an internal combustion engine
  - Temperature of the available heat sink
  - Ideal behavior of the ORC cycle components

Optimization algorithm

- At the upper level, **PGS-COM** (evolutionary) optimizes the independent **cycle variables and the composition** (mixtures)
- **REFPROP** evaluates the **thermodynamic properties** of the fluids
- The energy targeting optimizes the **ORC and cooling water mass flow rates**
- The ORC mechanical power and efficiency are returned to PGS-COM as **output of the optimized black-box** function



Heat recovery applications

Two large Diesel engines of the same size (10 MW), but with **opposite features**:

- **Man S60-MC6**: two-stroke with P_{el}=10.2 MW and T_{fg}=245°C
- **Wärtsilä 46DF**: four-stroke with P_{el}=10.3 MW and T_{fg}=354°C

Different exhaust temperatures allows assessing the effects of this parameter on the optimal fluid selection, cycle configuration and ORC efficiency

Flow	Feature	Units of measurement	Man S60-MC6	Wärtsilä 46DF
	Cycle type	-	Two-stroke	Four-stroke
	Power output	kW	10 200	10 305
	Efficiency (full load)	%	49.59	45.33
Exhaust gas	Mass flow rate	kg/s	26.53	19.00
	Thermal power	kW	3 607	4 892
	Temperature range	°C	245 - 120	354 - 120
Scavenge air	Mass flow rate	kg/s	26.00	18.40
	Thermal power	kW	3 970	3 789
	Temperature range	°C	198 - 48	253 - 50
Jacket water	Mass flow rate	kg/s	21.06	23.16
	Thermal power	kW	1 490	1 653
	Temperature range	°C	80 – 63	91 - 74

Pure fluids results

Man S60-MC6 (T_{fg}=245°C):

- HCFO-1233zde
  - Trans-critical cycle configuration with isentropic expansion
  - Non-flammable* GWP=1 ODP=0
- HFE-245fa2
  - Trans-critical cycle configuration with dry expansion and large regenerator
  - Non-flammable* GWP=812 ODP=0
- HFO-1336mzz
  - Trans-critical cycle configuration with dry expansion and large regenerator
  - Non-flammable* GWP=2 ODP=0

Fluid	W_{out} ORC	η_{exe}	Turbine inlet temperature	Turbine inlet pressure	N° of expander stages
	kW	%	°C	bar	-
HCFO-1233zde	1 802.5	75.71	196.31	38.61	2
HFE-245fa2	1 795.9	75.44	197.86	36.17	2
HFO-1336mzz	1 790.1	75.19	195.38	30.52	2
Novec^{TM} 649	1 687.6	70.89	178.46	19.06	2

*directly coupled with the flue gasses

Pure fluids results

Man S60-MC6 (T_{fg}=245°C):

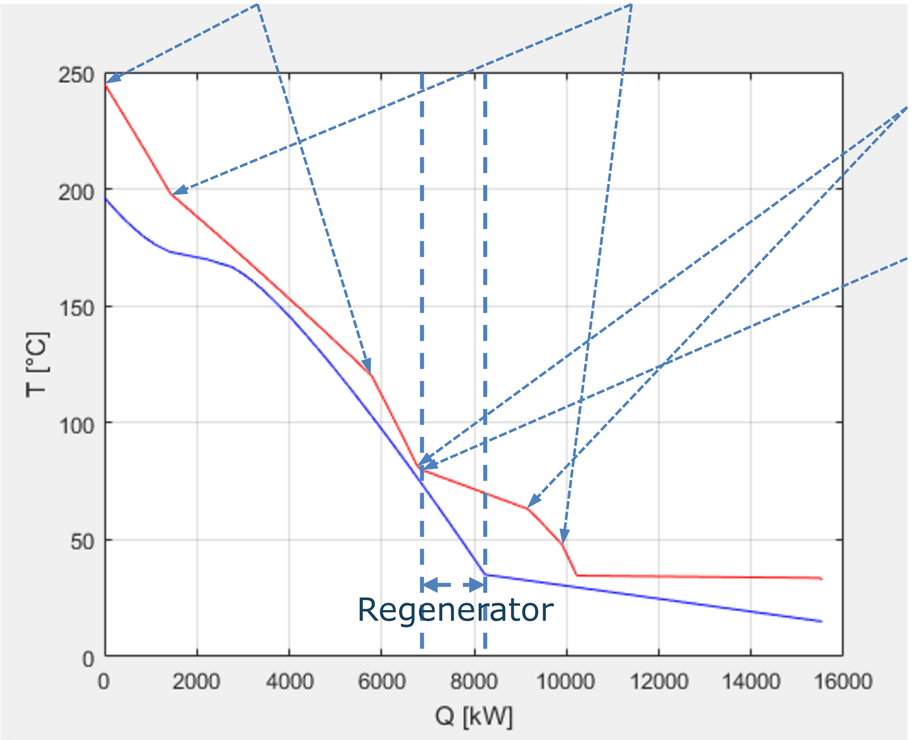
- HCFO-1233zde

Exhaust gas in-out

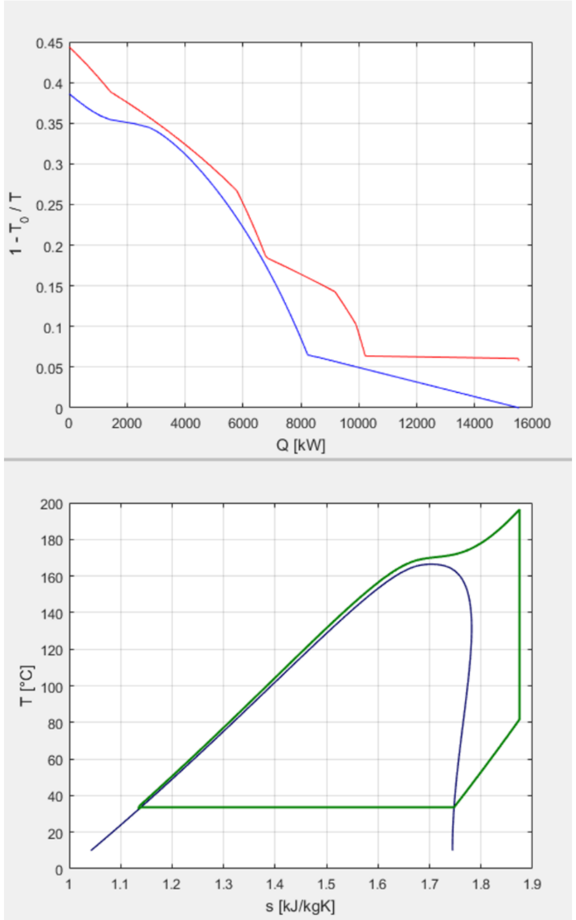
Scavenge air in-out

Jacket water in-out

ORC turbine out



Regenerator



Pure fluids results

Wärtsilä 46DF (T_{fg}=354°C):

- Cyclopentane
  - Sub-critical cycle configuration with isentropic expansion and sub-atmospheric condensing pressure
  - Flammable toxic GWP=11 ODP=0
- Ammonia
  - Trans-critical cycle configuration with wet expansion
  - Flammable toxic GWP=0 ODP=0
- HCFO-1233zde
  - Trans-critical cycle configuration with isentropic expansion
  - Non-flammable* GWP=1 ODP=0

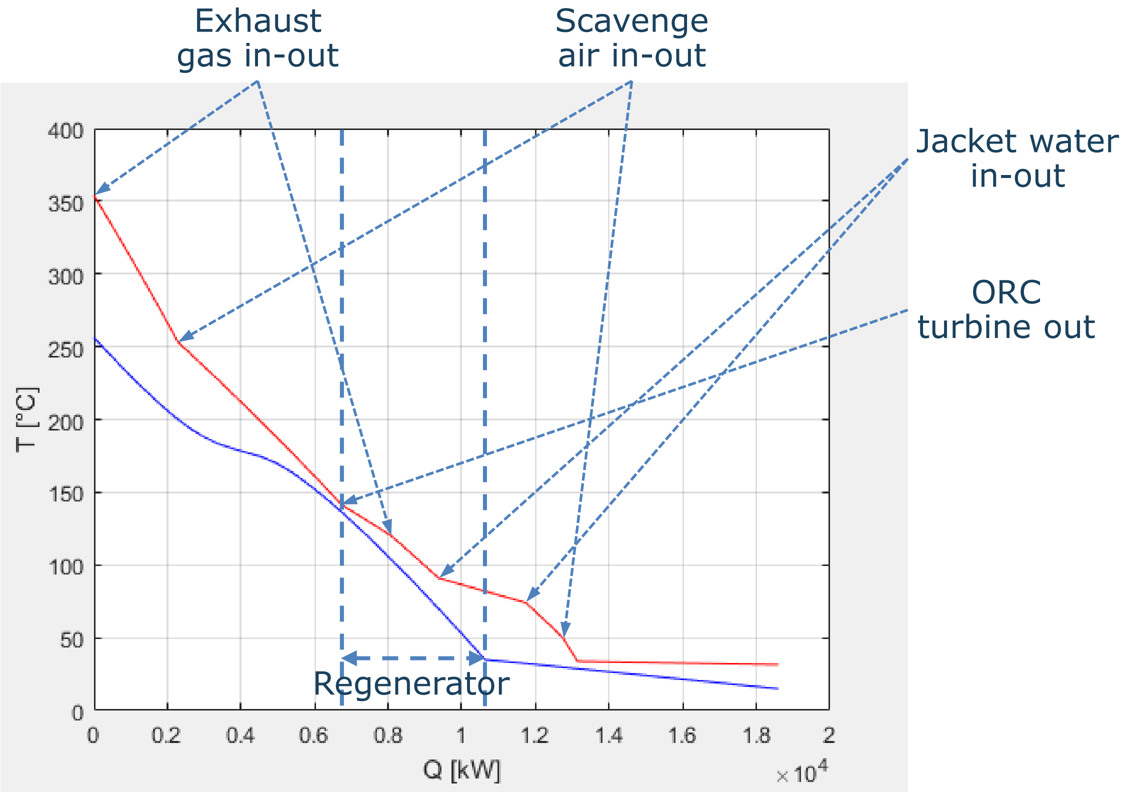
Fluid	W_{out} ORC	η_{exe}	Turbine inlet temperature	Turbine inlet pressure	N° of expander stages
	kW	%	°C	bar	-
Cyclopentane	2 456.5	73.82	235.54	42.70	2
Ammonia	2 443.1	73.42	325.00	166.93	4
HCFO-1233zde	2 420.2	72.73	256.34	43.56	2
Novec™ 649	2 244.4	67.45	226.85	19.78	2

*directly coupled with the flue gasses

Pure fluids results

Wärtsilä 46DF (T_{fg}=354°C):

- HCFO-1233zde

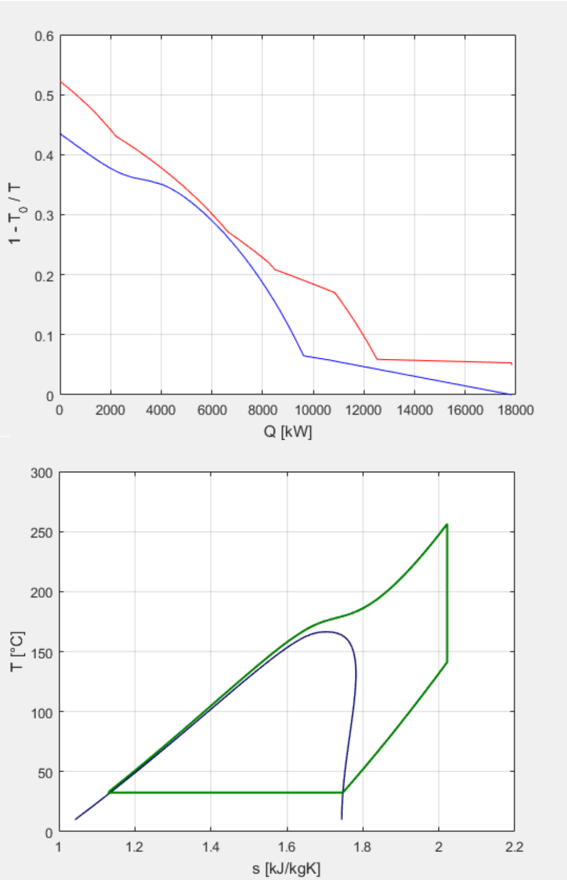


Exhaust gas in-out

Scavenge air in-out

Jacket water in-out

ORC turbine out



Mixtures results

Man S60-MC6 (T_{fg}=245°C):

- HCFO-1233zde/HFC-134a (90/10 wt%)
  - Trans-critical cycle configuration
  - Non-flammable* $GWP_{HFC\text{-}134a}=1430$
- HFO-1336mzz/HFC-134a (97/3 wt%)
  - Trans-critical cycle configuration
  - Non-flammable* $GWP_{HFC\text{-}134a}=1430$
- Isobutane/Pentane (56/44 wt%)
  - Trans-critical cycle configuration
  - Flammable GWP<20

Fluid (Weight fraction wt%)		W_{out} ORC kW	η_{exe} %	Turbine inlet temperature °C	Turbine inlet pressure bar	N° of expander stages -
HCFO-1233zde (90)	HFC-134a (10)	1867.8	78.45	206.85	42.17	2
HFO-1336mzz (97)	HFC-134a (3)	1827.5	76.76	195.07	31.55	2
Isobutane (56)	Pentane (44)	1694.7	71.18	170.02	38.60	2

*directly coupled with the flue gasses

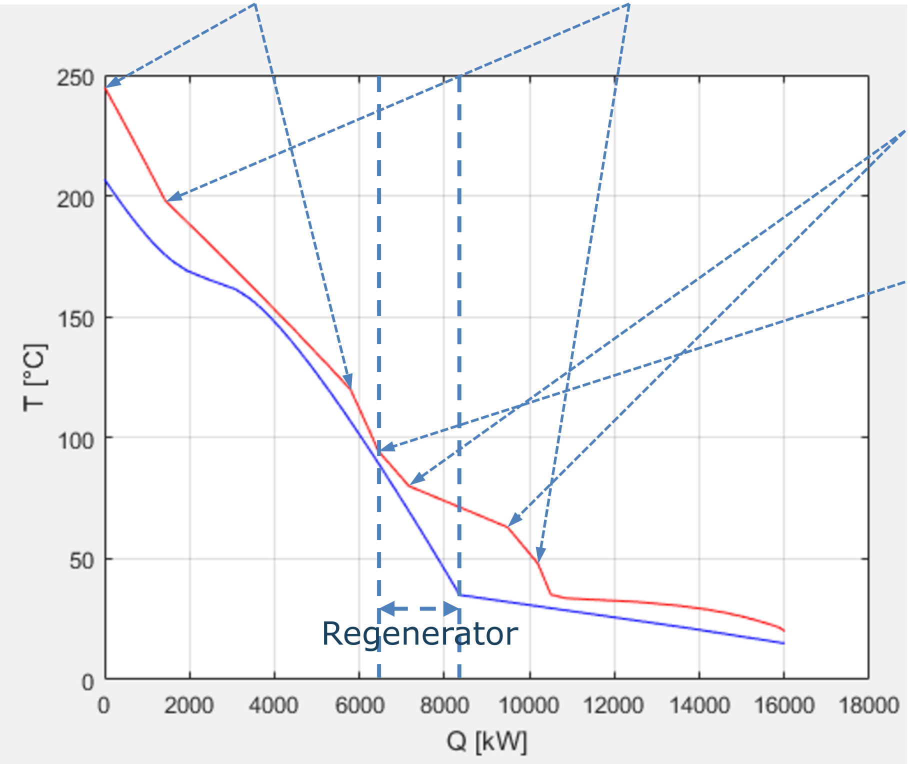
Mixtures results

Man S60-MC6 (T_{fg}=245°C):

- HCFO-1233zde/HFC-134a (90/10 wt%)

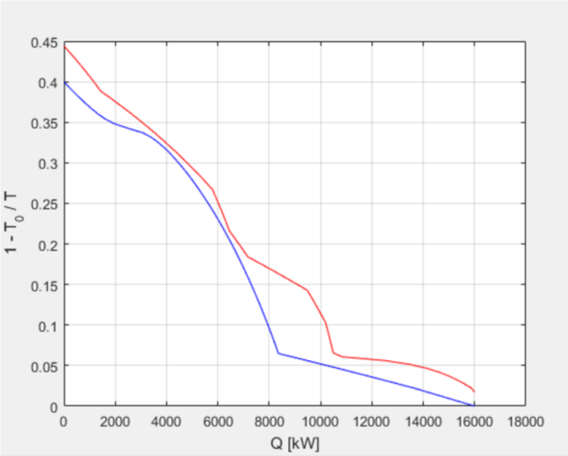
Exhaust gas in-out

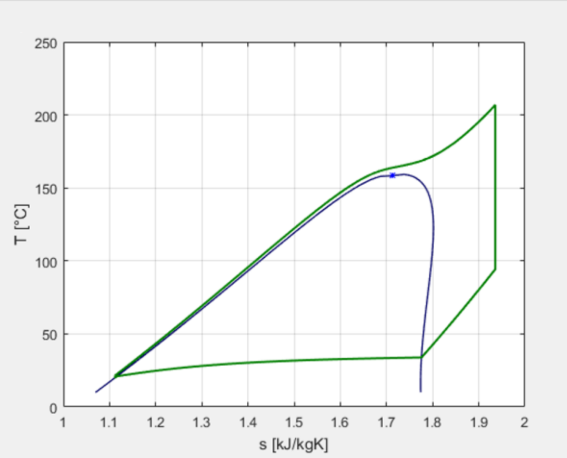
Scavenge air in-out



Jacket water in-out

ORC turbine out





Mixtures results

Wärtsilä 46DF (T_{fg}=354°C):

- Cyclopentane/Cis-Butene (82/18 wt%)
  - Trans-critical cycle configuration
  - Flammable
- Cyclopentane/Heptane (78/22 wt%)
  - Sub-critical cycle configuration
  - Flammable
- Ammonia/Water (98/2 wt%)
  - Trans-critical cycle configuration
  - Flammable

Fluid (Weight fraction wt%)		W_{out} ORC kW	η_{exe} %	Turbine inlet temperature °C	Turbine inlet pressure bar	N° of expander stages -
Cyclopentane (82)	Cis-Butene (18)	2 540.4	76.35	233.78	47.04	2
Cyclopentane (78)	Heptane (22)	2 528.9	76.00	235.26	36.44	2
Ammonia (98)	Water (2)	2 523.2	75.83	324.86	165.34	4

Comparison: Pure fluid vs. Mixtures

		Man S60-MC6				Wärtsilä 46DF		
		W_{out} ORC kW	η_{exe} %	$\eta_{II\ ICE+ORC}$ %		W_{out} ORC kW	η_{exe} %	$\eta_{II\ ICE+ORC}$ %
Pure fluid	HCFO-1233zde	1 802.5	75.71	58.36	Cyclopentane	2 456.5	73.82	56.13
	HFE-245fa2	1 795.9	75.44	58.33	Ammonia	2 443.1	73.42	56.07
	HFO-1336mzz	1 790.1	75.19	58.30	HCFO-1233zde	2 420.2	72.73	55.97
Mixtures (wt%)	HCFO-1233zde (90) + HFC-134a (10)	1 867.8	78.45	58.68	Cyclopentane (82) + Cis-Butene (18)	2 540.4	76.35	56.50
	HFO-1336mzz (97) + HFC-134a (3)	1 827.5	76.76	58.48	Cyclopentane (78) + Heptane (22)	2 528.9	76.00	56.45
	Isobutane (56) + Pentane (44)	1 694.7	71.18	57.83	Ammonia (98) + Water (2)	2 523.2	75.83	56.43

Conclusion

Pure fluids:

- **Super-critical cycles** can reach a **better thermodynamic matching** with the linear temperature profile of the hot flue gases (Lorentz cycle)
- **HCFO-1233zde** appears to be a promising fluid both the engines analyzed, in particular with the low-temperature exhaust gasses
  - Relatively low critical temperature (**trans-critical** cycle configuration)
  - High molar mass (small **enthalpy drop** and **number of expander stages**)
  - **Condensing pressure** higher than the atmospheric one
- Another promising pure fluid is **Novec^{TM} 649**
  - **Trans-critical** cycle configuration with **sub-atmospheric condensing pressure**
  - Close to maximum **efficiency**
  - Small **enthalpy drop** and **volumetric ratio**
  - Non-flammable
  - Low environmental impact (GWP = 1 ODP=0)

Conclusion

Mixtures:

- The use of optimized mixtures leads to an increase of the **recovered mechanical power of around 3 percentage points**
- The **advantage** of mixtures compared to pure fluids is **lower** than the values reported in the literature because the optimal cycle is trans-critical (the **temperature glide** can be exploited only in condensation)
- The little efficiency advantage is likely not sufficient to compensate the **reduction of heat transfer coefficient** which affects mixtures

Future works:

- Complete the analysis with a **techno-economic** analysis of ORCs using **HCFO-1233zde** and **Novec^{TM} 649**
- Apply the optimization methodology to **other heat recovery applications** (e.g., low grade heat)

Thanks for your attention