THERMO-ECONOMIC ANALYSIS OF ZEOTROPIC MIXTURES AND PURE WORKING FLUIDS IN ORGANIC RANINKE CYCLES FOR WASTE HEAT RECOVERY

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ABSTRACT

We present a thermo-economic analysis of an Organic Rankine Cycle (ORC) for waste heat recovery. A case study for a heat source temperature of 150 °C and a subcritical, saturated cycle is performed. As working fluids R245fa, isobutane, isopentane and the mixture of isobutane and isopentane are considered. The minimal temperature difference in the evaporator and condenser as well as the mixture composition are chosen as variables in order to identify the most suitable working fluid in combination with optimal process parameters under thermo-economic criteria.

In general, cost-effective systems show a high minimal temperature difference $\Delta T_{PP,C}$ at the pinch-point of the condenser and a low minimal temperature difference $\Delta T_{PP,E}$ at the pinch-point of the evaporator. In case of R245fa, the design parameters $\Delta T_{PP,E} = 1$ K and $\Delta T_{PP,C} = 13$ K lead to minimal costs of 56.8 €/GJ. Choosing isobutane as working fluid leads to the lowest costs per unit exergy with 52.0 €/GJ ($\Delta T_{PP,E} = 1.2$ K; $\Delta T_{PP,C} = 14$ K). Considering the major components of the ORC, specific costs range between 1150 €/kW$_{el}$ and 2250 €/kW$_{el}$. For the mixture isobutane/isopentane, a mole fraction of 90 % isobutane leads to lowest specific costs per unit exergy. Despite an increased efficiency an overcompensation of the additional expenses for the heat exchange equipment is not achieved compared to isobutane. The pure working fluid is 3.3 % more cost-effective. A sensitivity analysis for the ORC system using isobutane as working fluid shows high sensitivity of the costs per unit exergy to the costs of process integration and the isentropic efficiency of the turbine.

1. INTRODUCTION

Organic Rankine Cycle (ORC) systems for waste heat recovery have a high growth potential (Tchanche *et al.*, 2011). Numerous investigations are performed in order to maximize the efficiency of such power plants by working fluid selection with respect to the heat source temperature. Particularly, the use of zeotropic fluid mixtures is a promising optimisation approach due to a good glide match of the temperature profiles at phase change. In this context, Angelino and Colonna di Paliano (1998) show for a low-temperature application that mixtures of natural hydrocarbons (n-butane/n-hexane) lead to an efficiency increase of 6.8 % compared to the pure working fluid n-pentane. Other case studies for geothermal heat sources prove the potential of zeotropic mixtures as working fluids in ORC systems (Demuth, 1981; Iqbal *et al.*, 1976). For subcritical cycles an increase in efficiency by up to 16 % is obtained compared to pure working fluids, like isobutane or isopentane. More recent investigations include sensitivity analyses for crucial parameters (Borsukiewicz-Gozdur and Nowak, 2007; Wang and Zhao, 2009; Chen *et al.*, 2011; Garg *et al.*, 2013; Dong *et al.*, 2014; Lecompte *et al.*, 2014; Shu *et al.*, 2014). In addition, Heberle *et al.* (2012b) show high second law efficiencies for mixture compositions which lead to an good match of the temperature profiles at

condensation. However, these concentrations show a significant increase in heat exchange capacity. Similar results are obtained by Andreasen *et al.* (2014) considering pure components and their zeotropic mixtures as working fluids for subcritical and transcritical cycles in case of a low-temperature heat source. For a heat source temperature of 120 °C, mixtures of propane and higher boiling natural hydrocarbons as well as isobutane/isopentane show high first law efficiency for the subcritical cycle. At the same time, an increase of the heat exchange capacity for the condenser is presented, which is an indicator for the requirement of high heat transfer areas. Angelino and Colonna di Paliano (2000) compare an equimolar mixture of n-butane/n-hexane and pure n-pentane as ORC working fluids in a case study for waste heat recovery. Fan power savings of the air-cooling system of 49 % by using the zeotropic mixture are determined. However, an additional heat transfer area of 73 % is required. Weith *et al.* (2014) have recently shown for a waste heat recovery unit that the use of a siloxane mixture leads to an efficiency increase of 3 % compared to the most efficient pure component. In consequence, a 14 % higher heat transfer area of the evaporator is determined for the zeotropic mixture.

The described dependence suggests a thermo- or exergo-economic analysis of ORC systems in order to evaluate the increased power output and the additionally required heat exchange area for fluid mixtures. Existing thermo-economic analyses of ORC systems are focused on pure working fluids (Tempesti and Fiaschi, 2013; Astolfi *et al.*, 2014; Heberle and Brüggemann, 2014). Regarding small-scale waste heat recovery ORC units, Quoilin *et al.* (2011) determine specific investment costs for 8 working fluids in the range of 2136 €/kW and 4260 €/kW. For an electric capacity between 30 kW and 120 kW, Imran *et al.* (2014) considered different plant schemes and working fluids. In this context, specific investment costs in the range of 3556 €/kW and 4960 €/kW are obtained. Quoilin *et al.* (2013) indicate specific investment costs between 8000 €/kW and 1000 €/kW for an ORC waste heat recovery module in the range of 10 kW and 7500 kW electrical power output. In case of an geothermal resource, Heberle *et al.* (2012a) identify isobutane as a cost-efficient working-fluid compared to isopentane. The lowest specific costs are obtained for a minimal temperature difference of 3 K in the evaporator and 7 K in the condenser.

Under the consideration of zeotropic mixtures as potential ORC working fluids, we provide a thermo-economic analysis of waste heat recovery ORCs. In order to clarify if an efficiency increase overcompensates the additional heat transfer requirements. A case study is performed for a heat source temperature of 150 °C. In this context, a second law analysis for the ORC working fluids R245fa, isobutane and isopentane as well as for the zeotropic mixture isobutane/isopentane is conducted. Based on processes parameters the required heat exchange equipment is designed. Finally, the specific costs for the generated electricity are calculated. Depending on the working fluid composition and the minimal temperature difference in the condenser and evaporator, the most cost-efficient system is identified.

2. METHODS

2.1 Exergy analysis

For the exergy analysis, steady-state simulations are performed using the software Cycle Tempo (Woudstra, N. and van der Stelt, T.P., 2002). Fluid properties are calculated by RefProp Version 9.1 (Lemmon, E.W. *et al.*, 2013). Process simulations are conducted for a subcritical and saturated cycle. The scheme of the module and the corresponding *T,s*-diagram in case of a pure working fluid is illustrated in Figure 1.

The present case study is conducted for a low-temperature waste heat source of 150 °C. As a heat transfer medium pressurized water is assumed (p_{HS} = 6 bar). The mass flow and the outlet temperature of the heat source are chosen according to a thermal heat input of 3 MW. For the analysis, an air-cooled system is considered. R245fa, isobutane and isopentane as well as the zeotropic mixture isobutane/isopentane are examined as ORC working fluids. For the considered mixture, the composition is varied in discrete steps of 10 mole-%. The temperature difference in the evaporator and condenser is chosen as independent design variables in order to identify the most cost-efficient

process parameters. The analysis is conducted neglecting pressure and heat losses in the pipes and components. In Table 1 the boundary conditions for the cycle simulations are shown.
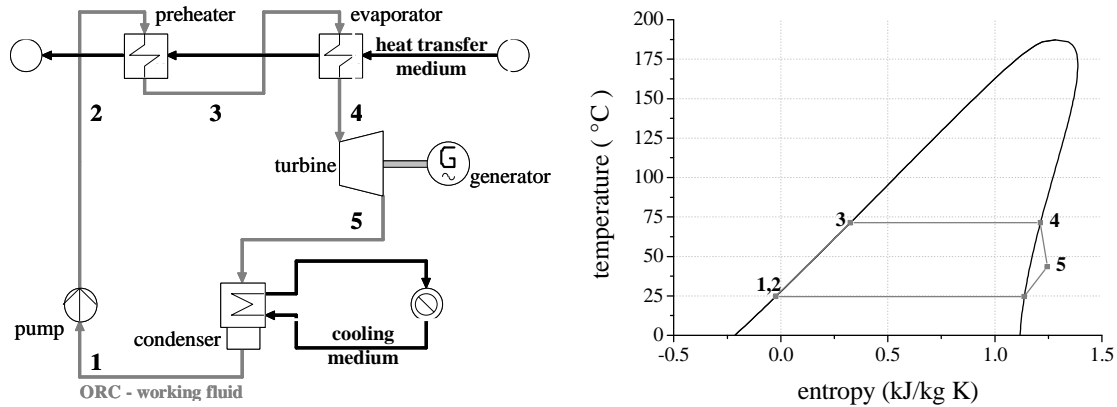

Figure 1: Scheme of ORC system and corresponding *T,s*-diagram for the working fluid isopentane

Table 1. Boundary conditions assumed for the second law analysis

parameter	
mass flow rate of heat source $\dot{m}_{HS}$	10 kg/s
outlet temperature of heat source $T_{HS,in}$	80 °C
inlet temperature of cooling medium $T_{CM,in}$	15 °C
temperature difference of cooling medium ΔT_{CM}	15 °C
maximal ORC process pressure p_2	$0.8 \cdot p_{crit}$
isentropic efficiency of feed pump $\eta_{i,P}$	75 %
isentropic efficiency of turbine $\eta_{is,T}$	80 %
efficiency of generator η_G	98 %

To evaluate the cycle efficiency, the net second law efficiency η_{II} of the ORC is calculated by

$$\eta_{II} = \frac{\left| P_G + P_{Pump} + P_{Fans} \right|}{\dot{E}_{HS}} = \frac{P_{net}}{\dot{m}_{HS} \cdot e_{HS}} \tag{1}$$

where P_G and P_{Pump} correspond to the power of the generator and the pump. P_{Fans} is related to the power of the air cooler fans. The exergy flow of the heat source $\dot{E}_{HS}$ is obtained by multiplying the specific exergy e_{HS} with the mass flow rate $\dot{m}_{HS}$. The specific exergy could be calculated by

$$e_{HS} = h - h_0 - T_0(s - s_0) \tag{2}$$

where the subscript 0 corresponds to the reference state ($T_0 = 15$ °C and $p_0 = 1$ bar). Corresponding to (Bejan et al., 1996), the exergy analysis is extended by an exergy balance for each component *k* of the system

$$\dot{E}_{F,k} = \dot{E}_{P,k} + \dot{E}_{L,k} + \dot{E}_{D,k} \tag{3}$$

where $\dot{E}_F$ and $\dot{E}_P$ describe the exergy flow rate of the fuel and the product. The exergy flow rate $\dot{E}_L$ includes heat losses to the surrounding or exergy that leaves the system in a physical way, like exhaust gases. Here $\dot{E}_L = 0$, due to neglected heat losses. The exergy flow rate $\dot{E}_D$ represents the exergy destruction rate associated to irreversibilities. Exemplarily, the exergy destruction rate of the preheater can be calculated as

$$\dot{E}_{D,PH} = \dot{m}_{ORC} T_0 \left[(s_3 - s_2) - \frac{h_3 - h_2}{T_{m,PH}} \right] \tag{4}$$

where $T_{m,PH}$ corresponds to the thermodynamic mean temperature of the heat source in the preheater.

2.2 Component design and economic analysis

For the major components of the ORC module, the purchased equipment costs (PEC) are estimated based on cost data of Turton *et al.* (2003). Purchased equipment costs C_0 based on ambient operating conditions and a carbon steel construction are calculated in US $ depending on parameter Y:

$$\log_{10} C_0 = K_1 + K_2 \log_{10}(Y) + K_3 \left(\log_{10}(Y) \right)^2 \tag{5}$$

where Y represents the capacity or size of a component. The parameters K_1, K_2 and K_3 are listed in Table 2. To convert the PEC in Euro a conversion ratio of 0.815 is considered. Due to maximal ORC pressures below 35 bar, additional cost factors depending on system pressure are not considered.

Table 2. Equipment cost data used for Equation (5) according to Turton *et al.* (2003)

component	Y; unit	K_1	K_2	K_3
Pump (centrifugal)	kW	3.3892	0.0536	0.1538
Heat exchanger (floating head)	m^2	4.8306	-0.8509	0.3187
Heat exchanger (air cooler)	m^2	4.0336	0.2341	0.0497
Turbine (axial)	kW	2.7051	1.4398	-0.1776

By setting the corresponding Chemical Engineering Plant Cost Index (CEPCI$_{2001}$) of 397 into relation to the value of 2014 with 575, the inflation and the development of raw material prices are taken into account Turton *et al.* (2003). For the costs $C_{tot,ORC}$ of the major components of the ORC power plant the PEC are summarized. The total investment costs of the power plant are calculated by multiplying $C_{tot,ORC}$ by the factor $F_{costs} = 6.32$. According to Bejan *et al.* (1996) this parameter represents additional costs like installation, piping, controls, basic engineering and others. The heat exchange area A is determined for the shell and tube heat exchanger in counter flow. Therefore, the overall heat transfer coefficient U_{tot} of each heat exchanger is calculated by

$$\frac{1}{U_{tot}} = \frac{1}{\alpha_o} + \frac{1}{\alpha_i} \frac{r_o}{r_i} + \frac{r_o \ln(r_o / r_i)}{\lambda_t} \tag{6}$$

where α_o represents the heat transfer coefficient at the outside of the tube, respectively, the shell side and α_i corresponds to the heat transfer coefficient at the inside of the tube. The inner and outer radius of the tube are represented by r_i and r_o. The thermal conductivity of the tube corresponds to λ_t. The outer diameter of the tubes is 20 mm and the wall thickness of the tube is 2 mm. In order to calculate the required diameter of the shell and the number of tubes, the maximal flow velocities of 1.5 m/s for liquid flows and 20 m/s for gaseous flows are assumed according to chapter O1 of the VDI Heat Atlas (VDI-GVC, 2010). In general, the ORC working fluid is led inside the tubes. Regarding the tube layout, a squared pitch and a pitch to diameter ratio of 1.22 are assumed. The considered heat transfer correlations for the calculation of α_i, depending on phase state and flow configuration are listed in Table 3. In case of the preheater and the evaporator, the method of Kern (1950) is applied for the shell side (α_o). For the air-cooled condenser a tube bank staggered arrangement is applied. In this context, a cross-flow heat exchanger with finned tubes is considered and the following design parameters are assumed: fin height of 3 mm, a fin thickness of 0.3 mm, a fin spacing of 2 mm and a transversal tube pitch of 60 mm. The air-side heat transfer coefficient is determined by the method of Shah *et al.* (2003). For all considered heat exchangers, the heat transfer surface is finally calculated by

$$\dot{Q} = U_{tot} A F_{LMTD} \Delta T_{log} \tag{7}$$

where ΔT_{log} is the logarithmic mean temperature difference. In general, the logarithmic mean temperature difference correction factor F_{LMTD} is equal 1 for condensation and boiling heat transfer. In this study, the simplifying assumption of $F_{LMTD} = 1$ is also met for single phase heat transfer.

Table 3. References for the considered heat transfer correlations

heat exchanger	tube side
preheater	(Sieder and Tate, 1936)
evaporator (pure working fluid)	(Steiner, 2006)
evaporator (zeotropic mixture)	(Schlünder, 1983)
condenser (pure working fluid)	(Shah, 1979)
condenser (zeotropic mixture)	(Bell and Ghaly, 1973; Silver, 1964)

2.3 Exergy costing

The thermo-economic analysis combines thermodynamic and economic aspects. In this context, the product of the energy conversion as well as each component can be evaluated according to the cost formation process. For the presented analysis, the method by Tsatsaronis and Winhold (1985), also known as exergo-economic method, is used. The exergy costing converts an exergy stream $\dot{E}$ to a cost stream $\dot{C}$, by multiplying the exergy with corresponding average costs per unit of exergy, respectively, specific costs c. In this context, a system of equations is set up consisting of the cost balance for each component k of system (Bejan *et al.*, 1996), (Heberle *et al.*, 2012a):

$$\dot{C}_{P,k} = \dot{C}_{F,k} - \dot{C}_{D,k} + \dot{Z}_k \tag{8}$$

The cost streams $\dot{Z}_k$ describe the costs of the k-th component depending on operation and maintenance $\dot{Z}_{O\&M}$ and capital investment $\dot{Z}_{CI}$. In order to calculate the described cost streams the economic boundary conditions listed in Table 4 are assumed.

Table 4. Economic parameters for the calculation of the cost streams $\dot{Z}_k$

parameter	
lifetime	20 years
interest rate *ir*	4.0 %
annual operation hours	7500 h/year
Cost rate for operation and maintenance	$0.02 \cdot \dot{Z}_{CI}$
Costs for process integration C_{PI}	$0.2 \cdot C_{tot,ORC}$
Power requirements of the air-cooling system	5 kW$_e$/MW$_{th}$
Electricity price €/kWh	0.08 €/kWh

The selected optimization criteria for the system is the minimization of the costs per unit exergy of the total system $c_{P,tot}$. In this study, the generated electricity is considered as the product of the system and the $\dot{E}_{P,tot}$ correspond to the power output of the generator. In this context, the auxiliary power requirements are covered by electricity from the grid. Alternatively, the net power output of the system can be considered in the denominator of Equation (9). The exergy rate of the fuel $\dot{E}_{F,tot}$ represents the exergy rate of the waste heat source transferred to the ORC system.

$$c_{P,tot} = \frac{\dot{C}_{P,tot}}{\dot{E}_{P,tot}} = \frac{(c_{F,tot} \dot{E}_{F,tot} + \sum_k \dot{Z}_k)}{\dot{E}_{P,tot}} \tag{9}$$

In addition, the specific investment costs *SIC* are calculated:

$$SIC = \frac{C_{tot,ORC}}{P_{net}}$$ (10)

3. RESULTS AND DISCUSSION

3.1 Identification of cost-efficient design parameters

For each working fluid the minimal costs per unit exergy $c_{p,tot}$ are identified depending on the minimal temperature difference ΔT_{PP} in the evaporator and condenser. In order to vary the minimal temperature difference, the corresponding upper and lower ORC pressure is adapted. In Figure 2, the resulting specific costs of the product are shown exemplarily for R245fa. The most cost-efficient design parameters for this ORC working fluid are $\Delta T_{PP,E} = 1$ K and $\Delta T_{PP,C} = 13$ K. For these parameters, costs per unit exergy of 56.8 €/GJ are obtained. Considering a minimal temperature difference between 0.5 K and 6 K for the evaporator and 8 K and 14 K for the condenser, the maximum costs per unit exergy of 60.0 €/GJ are calculated ($\Delta T_{PP,E} = 6$ K; $\Delta T_{PP,C} = 8$ K). In general, the cost minimum is a compromise between rising power output and increasing costs with decreasing minimal temperature difference in the heat exchangers. The results show that the condenser is crucial for the total PEC. Due to the highest amount of transferred thermal energy combined with the lowest logarithmic mean temperature difference, the highest heat transfer areas and component costs are obtained for the condenser. Therefore, the most cost-effective parameters show a low ΔT_{PP} for the evaporator and a high value in case of the condenser.
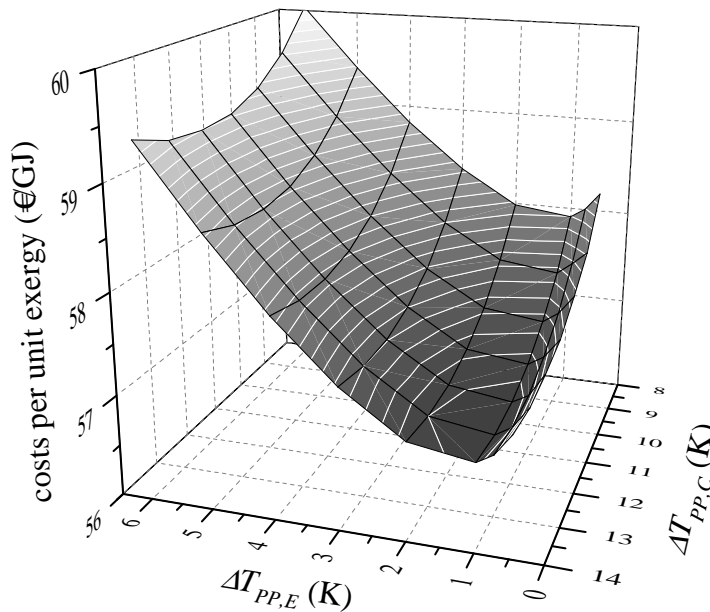
Figure 2: Costs per unit exergy for R245fa as ORC working fluid depending on minimum temperature difference in the evaporator and condenser

3.2 Comparison of ORC working fluids

Power output, heat transfer area and, therefore, capital investment costs for the ORC modules may considerably vary due to the working fluid selection and the corresponding fluid properties. In this context, Figure 3a illustrates the costs per unit exergy for the pure ORC working fluids isopentane, isobutane and R245fa as function of the minimum temperature difference in the condenser. For

$\Delta T_{PP,E}$, always the most cost-effective parameter is shown. In Figure 3b specific costs of the product are shown for selected mole fractions of the zeotropic mixture isobutane/isopentane.

Isobutane is identified as the most cost-effective working fluid for the considered case study with costs per unit exergy of 52.0 €/GJ. The corresponding design parameters are $\Delta T_{PP,E} = 1.2$ K and $\Delta T_{PP,C} = 14$ K. R245fa and isopentane lead to 9.2 % and 15.0 % higher costs per unit exergy (see Table 4). Although, these alternative pure working fluids show optimal design parameters with a lower minimum temperature difference, the power output is 10.8 % and 14.6 % lower. Net second law efficiency is between 1.0 % and 3.0 % lower compared to isobutane. The total heat exchange area differs only slightly and is 0.3 % lower for R245fa and 2.1 % higher for isopentane.
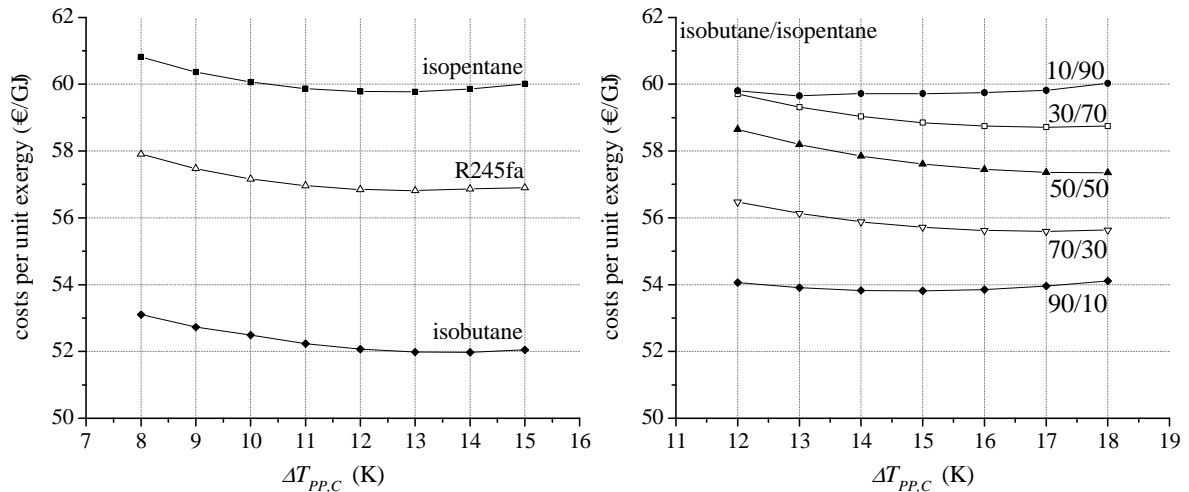

Figure 3: Costs per unit exergy for the pure ORC working fluids (**3a**) and for the zeotropic mixture isobutane/isopentane (**3b**) depending on the minimum temperature difference in the condenser

Regarding the mixture isobutane/isopentane, a mole fraction of 90 % isobutane leads to the lowest costs. In case of $\Delta T_{PP,E} = 2$ K and $\Delta T_{PP,C} = 15$ K specific costs of 53.8 €/GJ are obtained. However, the costs per unit exergy are 3.5 % higher compared to the most efficient component isobutane. This is due to a 5.5 % lower power output. At same time the total heat exchange area is only 3.6 % lower for 90/10 compared to isobutane.

Table 4. Selected ORC parameters for the most-effective cycles depending on fluid selection

parameter	isobutane	R245fa	isopentane	isobutane/isopentane
A_{PH} (m^2)	173.2	100.0	90.8	108.1
A_E (m^2)	123.1	118.1	118.6	112.8
A_C (m^2)	747.1	821.7	856.0	785.0
P_G (kW)	387.8	345.9	331.0	366.4
P_{Pump} (kW)	60.1	21.6	12.1	41.4
$\Delta T_{PP,E}$ (K)	1.2	1.0	1.0	2.0
$\Delta T_{PP,C}$ (K)	14.0	13.0	13.0	15.0
η_{II} (%)	30.3	30.0	29.4	30.0
SIC (€/kW)	1161.9	1270.1	1336.23	1203.0
$c_{p,tot}$ (€/GJ)	52.0	56.8	59.8	53.8

3.3 Sensitivity analysis for selected boundary conditions

In order to identify the most cost-important parameters of the estimated boundary conditions, Figure 4 illustrates the costs per unit exergy as function of interest rate, turbine efficiency, costs for process

integration, costs for operation and maintenance and *F*-factor. The specific costs per unit exergy show the highest sensitivity for the isentropic efficiency of the turbine and the costs for process integration.
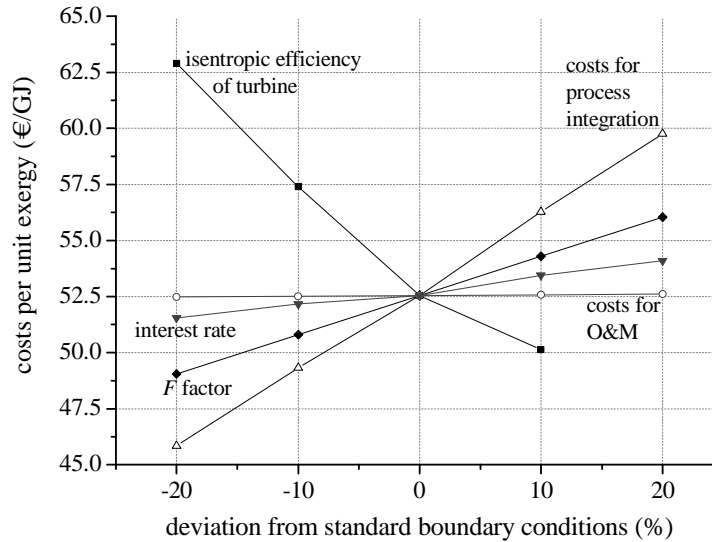

Figure 4: Cost per unit exergy as function of selected parameters for the working fluid isobutane

4. CONCLUSIONS

A thermo-economic case study for waste heat recovery by ORC is conducted. Cost-efficient design parameters concerning the temperature difference at the pinch point are identified in the case of pure working fluids and mixtures. In general, low minimum temperature differences in the evaporator and high values in the condenser are suitable for a cost-efficient ORC system. Isobutane as a working fluid leads to the most cost-effective ORC ($\Delta T_{PP,E}$ = 1.2 K; $\Delta T_{PP,C}$ = 14 K). Regarding the considered mixture isobutane/isopentane, a mole fraction of 90 % isobutane leads to the lowest costs per unit exergy. The economic parameters show a high sensitivity with respect to the estimated isentropic efficiency of the turbine and the costs for process integration. For further work, a variation of the heat source temperature and the heat exchanger design will be considered. In the context of a reliable estimation of the turbine efficiency, a detailed turbine model will be implemented in the analysis.

NOMENCLATURE

A	heat transfer area	(m^2)
c	costs per unit exergy	(€/GJ)
C	costs	(€)
$\dot{C}$	cost rate	(€/h)
e	specific exergy	(kJ/kg)
$\dot{E}$	exergy flow	(kW)
F	cost factor	(-)
h	specific enthalpy	(kJ/kg)
K	constant	(-)
$\dot{m}$	mass flow	(kg/s)
p	pressure	(bar)
P	power	(kW)
r	radius	(m)
s	specific entropy	(kJ/(kgK))
SIC	specific investment costs	(€/kW)
T	temperature	(°C)
U	overall heat transfer coeff.	(W/(m^{2}K))

Y	capacity/size parameter	(kW) or (m^2)
$\dot{Z}$	cost rate	(€/h)
α	heat transfer coefficient	(W/(m^{2}K))
ΔT	temperature difference	(K)
η	efficiency	(%)

Subscript

C	condenser	*log*	logarithmic
CI	capital investment	*m*	mean
CM	cooling medium	*net*	net
D	destruction	*o*	outer
E	evaporator	*out*	outlet
F	fuel	*O&M*	operation and
G	generator		maintenance
HS	heat source	*P*	product
i	inner	*PH*	preheater
is	isentropic	*PP*	pinch point
II	second law	*Pump*	pump
K	k-th component	*t*	tube
L	loss	*tot*	total
$LMTD$	logarithmic mean temperature difference	*0*	reference state

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