SYSTEMATIC FLUID-SELECTION IN EARLY STAGES OF ORC DESIGN – A PRACTICAL ENGINEERING APPROACH

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ABSTRACT

The selection of a working fluid plays a major role in the design phase of organic Rankine cycles (ORC). Therefore, a suitable working fluid builds the foundation for a high power production in an ORC, which also leads to high cycle efficiencies and is hence one of the most significant selling arguments. But the selection of a working fluid should not only depend on the power output of the ORC. There are technical rules for example given by the legislator, which also have to be respected with highest priority.
For a quick evaluation of potential working fluids a selection procedure was developed. The method uses 23 criteria – in total – out of six main categories (*thermodynamical*, *procedural/ thermodynamical*, *safety*, *environmental*, *economical* and *chemical*), which should be considered with adequate priority related to the implementation of the ORC. During the first tests, not all of the criteria were evaluated, therefore, the process was improved with an accurate elaboration of the omitted criteria and by the integration of the working fluid mass flow directly into the selection process.
The procedure itself is divided into four main steps, the *pre-selection*, the *elimination process*, the *ranking process* and the *final fluid choice*. Such procedure requires the subdivision of the 23 criteria into elimination criteria (EC) and tolerance criteria (TC). An advantage of this disposition into a structured process in the early design phase of the ORC is the direct elimination of working fluids in the pre-selection- and elimination-phase. The application of the selection procedure into the design process leads also to a saving in development time and helps to make an educated decision.
This contribution deals with a comprehensive compilation of all 23 criteria deemed as relevant for the fluid selection and shows examples of fluid selections.

1. INTRODUCTION

With the perpetual increasing standards in the development of renewable energy technologies the ORC technology has to prove its own worth. To keep the competitive ability of ORCs the plant cost has to remain small while the power production and the electric cycle efficiency should increase.
Designing the cycle components as high-end equipment (e.g. pumps, fans and multistage turbines) surely leads to higher efficiencies but usually by acceptance of immensely rising plant cost.
The power production of an ORC depends also on the cycle design and the optimization of operation parameters as well as the selection of a suitable organic working fluid.
For industrial use, competitive systems must not exceed an upper boundary for the cost per installed kW of about 5000€ while the cycle efficiency should be as high as possible, which can partially be achieved by the selection of the most suitable working fluid.
However, a suitable working fluid has to combine a multitude of specific characteristics depending on the area of application and with respect to the manufacture's and the legislator's requirements. Quoilin et al. [6] observed, that commercial ORC power plants usually operate with common working fluids despite to the broad range of fluids, which have been analyzed and reviewed in numerous scientific fluid selection studies [1,2,3,4,5,7].

Hence, it might be of general interest to initiate a trend in the standardization of a working fluid selection procedure in the early design phase of ORCs without losing any kind of freedom in the individuality of the ORC plant design itself.
The recommendation for the integration of a structured procedure for the selection of organic working fluids into the ORC design phase was already expressed by Roedder et al. [8], where also the definition of the selection criteria with relation to earlier works from several authors and the development of the selection procedure is explained in more detail.
With the first application of the method by selecting a low temperature (LT) and a high temperature (HT) working fluid for a two stage ORC it was recognized that the integration of all criteria into the process workflow requires a more accurate revision.
In this work a revision of the suggested elimination criteria (EC) and tolerance criteria (TC) [8] is presented.
The present paper contains a short briefing about the selection method. The main focus is directed at additional criteria with respect to [8]. The significance of all criteria is then evaluated to compile a final version of the relevant elimination and tolerance criteria.

2. SYSTEMATIC APPROACH

The selection procedure itself is based on an evaluation method for the validation of technical systems [9], which provides a split of selection methods into partitions. A subdivision of the procedure enables a structured process, which increases the quality of the evaluation method that also depends strongly on the defined selection criteria. Hence it is important that the customer requirements are carefully included and explicitly considered while the criteria elaboration.
A split of the procedure into four main steps (the *pre-selection*, the *elimination*, the *ranking* and the *final fluid choice*) is evidentially practical for the evaluation of organic working fluids [8]. The suggested work flow ensures the elimination of working fluids in an early step of the method, which leads to a saving in time due to the rating of only passed fluids. A well-structured working instruction also leads to minimization of failures in the approach and hence carefulness for beginners and also advanced users in ORC design.

3. THE SELECTION PROCEDURE

The application of the procedure is demonstrated by selecting an organic working fluid for a custom designed single-stage HT-ORC for training intention and applied research. Due to the integration of an adjustable electric heating rod into the heat supplying thermo-oil cycle the system allows operation modes at different temperature levels. Using dry or isentropic fluids – where the turbine outlet condition is almost settled in the superheated area – enables the recovery of the excessive condensation heat by integration of a recuperator (R) behind the turbine (T).
After the selection of a suitable working fluid for the given HT-ORC (Figure 1) the design and the thermodynamical cycle calculation is performed with "EBSILON®Profesional" [12], a simulation tool for thermodynamic cycle calculations.

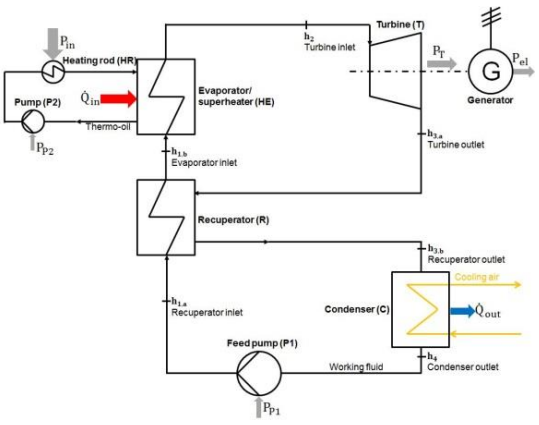

Figure 1: HT-ORC for training intention and applied research

If not indicated otherwise thermodynamic variables are calculated with the in "EBSILON®Professional" [12] integrated fluid properties calculator based on the "REFPROP-Database" – developed by the National Institute of Standards and Technology [11].
The "GESTIS Substance Database" [10] combines the information of data sheets about the risks of most fluids and standard properties (e.g. melting point etc.).

3.1 THE PLANT DESIGN

The thermo-oil cycle is designed with a 55kW heating rod (HR) and a circulation pump (P2) for supplying the HT-ORC with heat by transfer in the evaporator/superheater (HE). A 7,5kW synchro-generator (G) driven by a HT-turbine (T) feeds the primary power system. Improving the cycle efficiency by the recuperation of the condensation heat just conforms with the technical standard in the ORC technology.
Power plant components are designed for system operations up to a maximum temperature of 200°C, which fits the maximum main steam temperature at the turbine inlet $T_{h2} = 180°C$ and enables the design of favourable low priced components (e.g. brazed heat exchanger).
Condensing the fluid against the ambient condition favours the installation of an air cooled direct condenser, which omits the need of an additional cooling water cycle. Hence the condensing temperature is fixed at 35°C (T_{h4}).
Table 1 shows the assumed components efficiencies, which are required as input for a later cycle simulation and useful in the process of the selection procedure. With the currently available cycle conditions (also listed in Table 2) and with the assumed isentropic turbine efficiency given in Table 1 it is possible to calculate the fluid condition at the turbine outlet (equation 1).
But before starting detailed cycle calculations it is necessary to pre-select organic working fluids (see Table 3).

Table 1: Components efficiencies (η)

Component	Description		Value
Turbine	Isentropic efficiency	$\eta_{s,T}$	0.75
Feed pump	Isentropic efficiency	$\eta_{s,P}$	0.80
Generator	Electric efficiency	$\eta_{el,G}$	0.90
Heat exchanger	Component efficiency	η_{HE}	0.95

Table 2: Preliminary cycle conditions

Condition		Temperature [°C]
Turbine inlet	T_{h2}	180,0
Condenser outlet	T_{h4}	35,0

$$\eta_{s,turbine} = \frac{|h_3 - h_2|}{|h_{3,s} - h_2|} \quad (1)$$

3.2 PRE-SELECTION

The mean steam temperature (T_{h2}) at the turbine inlet of 180°C enables the use of high and low temperature working fluids.
Cyclopentane is indicated by Fischer et al. [3] as a proven high temperature working fluid and iso-Pentane investigated as low temperature working fluid [2]. Novec 649 is specified as an effective heat conducting working fluid with a high safety standard.
The comparison of the pre-selected fluids (Table 3) follows by involving EC and TC.

Table 3: Pre-selected working fluids

Name	Number	Molecular-formula	Substance class	Critical temperature	Critical pressure
				°C	bar
				T_c	p_c
Cyclopentane	1	C_5H_{10}	Cyclic alkanes	238,6	45,7
Iso-Pentane	2	C_5H_{12}	Branched alkanes	187,2	33,8
Novec 649	3	$C_6F_{12}O$	Branched ketones	168,7	18,7

3.3 ELIMINATION CRITERIA (EC)

For the elimination of potential working fluids each EC needs the specification of a fixed range of values (v_i) as described in [8]. The pre-selected working fluid can be eliminated directly via any EC by comparison of the fluid specific value with its specified range of values. It has to be rejected if it is

out of the defined range. An accurate explanation for the definition of the range of values is given as follows (Table 4):

Table 4: Definition of the Elimination criteria (EC) and range of value (v_i)

Elimination criterion	Reasoning for specified validity of value	Range of values (v_i)
C_1 **Boiling point (T_b)**	To prevent the vaporization of working fluids at general laboratory conditions (1,013bar) the boiling point temperature is restricted to temperatures below 35°C.	$35°C \leq T_b$
C_2 **Melting point (T_m)**	Permanent plant operation and a frozen fluid inside the plant should be avoided by the melting point criterion. The plant installation inside a permanent heated building allows a melting point with an upper boundary of $-1°C$.	$T_m \leq -1°C$
C_3 **Kinematic viscosity (ν)**	A very low viscosity leads to power losses and raises the pump wastage. A high viscosity has a negative effect on the pumpability of the fluid. Therefore, the viscosity can vary between a maximum and a minimum value, which is mostly given by the manufacturer of the fluid.	$0{,}3\frac{mm^2}{s} \leq \nu \leq 120\frac{mm^2}{s}$
C_4 **Thermo-stability (T_{max})**	Designing the plant for an operating temperature of about 200°C with additionally 20°C safety margin enables a maximum temperature of 220°C.	$220°C \leq T_{max}$
C_5 **Conden-sation pressure (p_{h3})**	According to the current state of technology the ORC systems should run safely with a vacuum up to 0,2bar. Fluids with a condensing pressure lower than 0,2bar depending on condensing Temperature (T_{h4}) are neglected.	$0{,}2bar \leq p_{h4}$
C_6 **Flamm-ability (T_{fl})**	The flammability of organic working fluids is a very important safety characteristic, which should contain a high safety-tolerance regarding the maximum of the heat source temperature – in this case 200°C. Therefore, only fluids with an ignition temperature of about 50°C above the temperature level of the heat source are recommended.	$250°C \leq T_{fl}$
C_7 **Toxicity (X_T)**	Substances which are harmful to health or dangerous to life are classified as hazardous substances according to the Globally Harmonised System (GHS) [13]. They have to be rejected. The "GESTIS Substance Database" [10] provides the information about the risks of most fluids.	$X_T = 0$ (none)
C_8 **Ozone depletion potential (ODP)**	Due to national or international prohibitions the consideration of working fluids with an ODP above zero would be wasted time.	ODP = 0 (none)
C_9 **Cost of the working fluid**	It should be noted that other criteria can be a much larger cost drivers than the cost of the substance itself (e.g. properties influencing component size & complexity, see e.g. C_{13}-C_{15}). Due to the small plant capacity, which minimizes the amount of the fluid, substance costs are not considered.	– not considered –

Table 5 contains the fluid specific values for the comparison with the defined range of value of the EC. If a fluid specific value does not match with the defined range, the fluid has to be rejected (fail / "0"). Otherwise fluids pass the elimination process and are marked with "1".

Table 5: Comparison of the fluid specific values with the defined range for the EC

				Cyclopentane		Iso-Pentane		Novec 649	
Elimination criteria (C_i)		**w_i**	**Range of value (v_i)**	**Value**	**e_i**	**Value**	**e_i**	**Value**	**e_i**
1	Boiling point	-	$35°C \leq T_b$	49	1	28	0	49	1
2	Melting point	-	$T_m \leq -1°C$	-94	1	-160	1	-108	1
3	Kinematic viscosity	-	$0{,}3 \leq \nu \leq 120$	5,32	1	0,34	1	1,74	1
4	Thermostability	-	$220°C < T_{max}$	276,9	1	226,9	1	226,9	1
5	Condensation pressure	-	$0{,}2bar \leq p_{h3}$	0.5	1	1.1	1	0.5	1
6	Flammability	-	$250°C \leq T_{fl}$	320	1	420	1	-	1
7	Toxicity	-	$X_T = 0$	-	1	-	1	-	1
8	Ozone depletion potential	-	$ODP = 0$	-	1	-	1	-	1
9	Cost of the working fluid	-	–	Not included		Not included		Not included	
Fail (0) / pass (1):				1		0		1	

3.4 TOLERANCE CRITERIA (TC)

Tolerance criteria (TC) are designated for the rating of the potential working fluids, which have passed the pre-selection and the elimination process. For the ranking process a weighting factor (w_i) needs to be defined for each TC. The weighting of a TC depends on its significance and should be considered with respect to the area of system application, scientific literature and manufactures acknowledgment. Table 6 contains the grading system for the TC weighting used as follows.
For the ranking of working fluids, ranges of values (v_i) have to be assigned to each TC with respect to the evaluation system shown in Table 7. The "top ranking" for the most suitable range is rated with four points and a just acceptable range is rated with one evaluation point. Outside the defined ranges fluids are evaluated with zero points.

Table 6: Grading system for the weighting factor (w_i)

Weighting-factor (w_i)	**Grading**
4	Essential
3	Important
2	Basic
1	Less Important

Table 7: Measurement for the suitability of the ranges (v_i)

Evaluation number (e_i)	**Suitability**
4	Top-ranking
3	Satisfyingly
2	Basic-ranking
1	Just acceptable
0	Out of range

After compiling the TC (see Table 8) and completing the preparation for the fluid ranking the specific values of the pre-selected working fluids have to be calculated and compared with the evaluated ranges (v_i) . Hence the working fluids are assigned with an evaluation number (e_i) for each TC with respect to the specified ranges.
In the ranking process, each fluid obtains a rating number (s_x) that depends on the achieved evaluation number (e_i) and the respective weighting factor (w_i). Therefore, the rating number or severity (s_x) for each fluid is defined as follows (equation 2):

$$s_x = \sum_{i=10}^{n} w_i \cdot e_i \qquad (2)$$

Table 8: Definition of the Tolerance criteria (TC) with weighting and range of values (v_i)

Tolerance criterion	Reasoning for specified range of values and weighting	e_i	Range of values (v_i)	
C_{10} **Enthalpy-slope ($\Delta h_{3,a-2}$)** $w_{10} = 2$	Working fluids with an enthalpy-slope of about $120\frac{kJ}{kG}$ in the region of superheated steam (turbine outlet to turbine inlet) are top ranked due to their high transfer of work, which can be converted by the turbine. Due to the direct influence on the cycle power production (equation 3) the enthalpy-slope is weighted as a basic criterion. $P_{el} = \Delta h_{3,a-2} \cdot \dot{m}_{Fluid}$ (3)	4	$120\frac{kJ}{kG} \leq \Delta h_{3-2}$	
		3	$60\frac{kJ}{kG} \leq \Delta h_{3-2} < 120\frac{kJ}{kG}$	
		2	$30\frac{kJ}{kG} \leq \Delta h_{3-2} < 60\frac{kJ}{kG}$	
		1	$10\frac{kJ}{kG} \leq \Delta h_{3-2} < 30\frac{kJ}{kG}$	
		0	$\Delta h_{3-2} < 10\frac{kJ}{kG}$	
C_{11} **Thermal conductivity (λ)** $w_{11} = 1$	For the first integration of the thermal conductivity (λ) into the procedure the top range is defined according to the thermal conductivity of water in its liquid phase ($1{,}013bar, 20°C$). For the comparison the fluid specific conductivity is calculated at the same condition. The thermal conductivity describes the ability of intermolecular heat transfer. Therefore, a high thermal conductivity is coupled to a favourable sizing of the heat exchangers. Due to the first consideration as tolerance criterion it is weighted as "less important".	4	$0{,}6\frac{W}{m \cdot K} \leq \lambda$	
		3	$0{,}3\frac{W}{m \cdot K} \leq \lambda < 0{,}6\frac{W}{m \cdot K}$	
		2	$0{,}1\frac{W}{m \cdot K} \leq \lambda < 0{,}3\frac{W}{m \cdot K}$	
		1	$0{,}001\frac{W}{m \cdot K} \leq \lambda < 0{,}1\frac{W}{m \cdot K}$	
		0	$\lambda < 0{,}001\frac{W}{m \cdot K}$	
C_{12} **Isobaric heat capacity (c_p)** $w_{12} = 1$	The benchmark for the isobaric heat capacity (c_p) is liquid water at 20°C and 1,013bar. For the comparison the liquid isobaric heat capacity (c_p) of the working fluid is required at the same condition. This criterion is weighted as "less important" because its implementation and significance in the process has to be evaluated in more detail.	4	$4{,}19\frac{kJ}{kg \cdot K} \leq c_p$	
		3	$3{,}00\frac{kJ}{kg \cdot K} \leq c_p < 4{,}19\frac{kJ}{kg \cdot K}$	
		2	$1{,}50\frac{kJ}{kg \cdot K} \leq c_p < 3{,}00\frac{kJ}{kg \cdot K}$	
		1	$0{,}50\frac{kJ}{kg \cdot K} \leq c_p < 1{,}50\frac{kJ}{kg \cdot K}$	
		0	$c_p < 0{,}50\frac{kJ}{kg \cdot K}$	
$C_{13.1}$ **Enthalpy of vaporization (E_v)** $w_{13.1} = 1$	With respect to cycle power, The enthalpy of vaporization – at main steam pressure – is coupled with the working fluid mass flow (C_{14}) and the supplied heat. For the considered application, an enthalpy of vaporization range at approximately $275\frac{kJ}{kg}$ allows system operation with a suitable working fluid mass flow $(0{,}2\frac{kg}{s})$ by given heat supply ($55kW$) until reaching the saturated steam area. Due to the negative as well as positive effects of high enthalpy ranges during vaporization – discussed in more detail by Roedder et al. [8] – the weighting equates "less important".	4	$250\frac{kJ}{kg} \leq E_v \leq 300\frac{kJ}{kg}$	
		3	$E_v < 250\frac{kJ}{kg}$	$300\frac{kJ}{kg} < E_v$
		2	$E_v < 150\frac{kJ}{kg}$	$400\frac{kJ}{kg} < E_v$
		1	$E_v < 50\frac{kJ}{kg}$	$500\frac{kJ}{kg} < E_v$
		0	-	
$C_{13.2}$ **Enthalpy of condensation (E_C)** $w_{13.2} = 2$	During condensation the entropy inside the system decreases, hence heat energy has to be extracted. For an efficient single stage cycle the condensing heat should be as small as possible because it is not of further use for the system. Due to its influence on the cycle efficiency the enthalpy of condensation is weighted as a "basic" criterion.	4	$E_c \leq 50\frac{kJ}{kg}$	
		3	$50\frac{kJ}{kg} < E_c \leq 100\frac{kJ}{kg}$	
		2	$100\frac{kJ}{kg} < E_c \leq 400\frac{kJ}{kg}$	
		1	$400\frac{kJ}{kg} < E_c \leq 1000\frac{kJ}{kg}$	
		0	$1000\frac{kJ}{kg} < E_c$	

C_{14} Working fluid mass flow ($\dot{m}_{Fluid}$)	For the power production, the working fluid mass flow should be as high as possible (see equation 3) but with increasing mass flow the volume flow increases too (equation 4). $\dot{V}_{Fluid} = \frac{\dot{m}_{Fluid}}{\rho}$ (4) Therefore, the working fluid mass flow needs an upper and a lower boundary. Its best available range for the present plant size is settled between $0{,}20\frac{kg}{s} \leq \dot{m}_{Fluid} \leq 0{,}25\frac{kg}{s}$. It should be possible to reach saturated steam condition by heating the fluid from 35°C (T_{h4}) up to 180°C ($\dot{Q}_{to}$) without involving the recuperation heat. The direct calculation of a mass flow requires the definition of the fluid condition at the turbine inlet (h_2) and after the feed pump ($h_{1,a}$) – without recuperator. Due to its direct influence on the cycle power production and also on the volume flow it is weighted relatively high.	4	$0{,}20\frac{kg}{s} \leq \dot{m}_{Fluid} \leq 0{,}25\frac{kg}{s}$	
		3	$\dot{m}_{Fluid} > 0{,}15\frac{kg}{s}$	$0{,}25\frac{kg}{s} < \dot{m}_{Fluid}$
		2	$\dot{m}_{Fluid} > 0{,}10\frac{kg}{s}$	$0{,}35\frac{kg}{s} < \dot{m}_{Fluid}$
		1	$\dot{m}_{Fluid} > 0{,}05\frac{kg}{s}$	$0{,}50\frac{kg}{s} < \dot{m}_{Fluid}$
$w_{14} = 3$		0	$\dot{m}_{Fluid} < 0{,}05\frac{kg}{s}$	$1{,}00\frac{kg}{s} < \dot{m}_{Fluid}$
C_{15} Density at the turbine outlet (ρ_3)	Due to the decreasing volume flow ($\dot{V}$) with increasing density (ρ) the plant size and cost remain small. Therefore, working fluids with a high density at the turbine outlet (ρ_3) are favoured due to their positive effect on the volume flow rate. Moreover a high fluid density can compensate the negative effect of a high working fluid mass flow on the volume flow.	4	$4{,}0\frac{kg}{m^3} \leq \rho_3$	
		3	$2{,}0\frac{kg}{m^3} \leq \rho_3 < 4{,}0\frac{kg}{m^3}$	
		2	$1{,}0\frac{kg}{m^3} \leq \rho_3 < 2{,}0\frac{kg}{m^3}$	
		1	$0{,}1\frac{kg}{m^3} \leq \rho_3 < 1{,}0\frac{kg}{m^3}$	
$w_{15} = 3$		0	$\rho_3 < 0{,}1\frac{kg}{m^3}$	
C_{16} Main steam pressure (p_{h2})	The main steam pressure depends on the turbine inlet temperature of the working fluid. It is a cycle variable which has direct influence on the cycle conduct (supercritical, subcritical, wet or superheated). As a reasonable simplification the main steam pressure is defined as equal to the evaporating pressure at the turbine inlet temperature (Table 2). Fluids with a pressure higher than 50bar are neglected.	4	$p_{h2} \leq 15\text{bar}$	
		3	$15\text{bar} < p_{h2} \leq 20\text{bar}$	
		2	$20\text{bar} < p_{h2} \leq 30\text{bar}$	
		1	$30\text{bar} < p_{h2} \leq 50\text{bar}$	
$w_{16} = 2$		0	$50\text{bar} < p_{h2}$	
C_{17} Heat transfer coefficient (α)	The heat transfer coefficient depends on the flow rate, the viscosity, the thermal conductivity, the geometric conditions of the cycle and the surface conditions. Hence the heat transfer coefficient can only be assumed for heat transferring components (e.g. evaporators, condensers or heat exchangers in general). The integration into the fluid selection process needs a more accurate analysis.		– not considered –	
$w_{17} = 1$				
C_{18} Global warming potential (GWP)	The global warming potential (GWP) of a fluid describes the negative effect after its release to the environment in contrast to carbon dioxide which has a GWP of "1". That means a substance with a GWP of "2" is assumed to affect global warming two times stronger than carbon dioxide. The GWP can be obtained from the "GESTIS Substance Database" [10].	4	GWP = 0 (none)	
		3	$0 < \text{GWP} \leq 100$	
		2	$100 < \text{GWP} \leq 500$	
		1	$500 < \text{GWP} \leq 1000$	
$w_{18} = 4$		0	$1000 < \text{GWP}$	
C_{19} Water pollution class (WGK)	• WGK1: light harmful • WGK2: harmful • WGK3: strong harmful	4	no WGK	
		3	WGK1	
		2	WGK2	
$w_{19} = 4$		0	WGK3	

C_{20} Gross thermal efficiency (η_g)	The gross thermal efficiency (η_g) can be evaluated with the help of the p,h-diagram. It is a quick method to consider the ratio of the external heat input to the isentropic expansion work at which the pump work and the irreversibilities in the turbine are neglected. For a detailed analysis the net thermal efficiency must be considered in a full performance analysis.	4	$14\% \leq \eta_g$
		3	$11\% \leq \eta_g < 14\%$
		2	$7\% \leq \eta_g < 11\%$
		1	$5\% \leq \eta_g < 7\%$
$w_{20} = 4$		0	$\eta_g < 5\%$
C_{21} Molecular weight (M)	Working fluids with high molecular weight (M) have a larger amount of mass per volume (equation 3), which has to be transported by the pump. Hence compressing heavy working fluids requires a larger energy input of the feed pump and leads to a negative effect on the net electric efficiency by an increased internal energy demand of the system. $m = M * n = [kg]$ (5)	4	$MW \leq 100 \frac{g}{mol}$
		3	$100 \frac{g}{mol} < MW \leq 250 \frac{g}{mol}$
		2	$250 \frac{g}{mol} < MW \leq 400 \frac{g}{mol}$
		1	$400 \frac{g}{mol} < MW \leq 550 \frac{g}{mol}$
$w_{21} = 2$		0	$550 \frac{g}{mol} < MW$
C_{22} Molecular complexity (MC)	A measurement for the complexity of a molecule can be the number of atomic bonds inside a molecule. For a user-friendly method of application the classification into cyclic, branched and single molecules is sufficient. Therefore, simple fluids with only one link should be classified as single molecules with strong interaction and not easily severable. Splitting branched molecules demand lesser energy due to their weakly cohesion and large contact surface. The cohesion inside a cyclic molecule-system is stronger than inside branched systems.	4	single structure
		3	cyclic structure
		2	branched structure
		1	–
$w_{22} = 1$		0	–

The fluid specific values for the comparison with the defined range of values (Table 8) are listed in Table 9, which also includes the calculation of the severity (s_x). The overall severity results in a maximum of 120 evaluation points in total. Iso-Pentane – although excluded during the elimination process – is also discussed in the ranking process.

Table 9: Comparison of the fluid specific values with the defined ranges for the TC (incl. ranking)

				Cyclopentane		Iso-Pentane		Novec 649	
Tolerance criteria (C_i)		**Unit**	**w_i**	**Value**	**e_i**	**Value**	**e_i**	**Value**	**e_i**
10	Enthalpy slope	$\left[\frac{kJ}{kg}\right]$	2	107,2	3	106,7	3	32,1	2
11	Thermal conductivity	$\left[\frac{W}{m \cdot K}\right]$	1	0,13	2	0,11	2	0,06	1
12	Isobaric heat capacity	$\left[\frac{kJ}{kg \cdot K}\right]$	1	1,79	2	2,25	2	1,10	1
13.1	Enthalpy of vaporization	$\left[\frac{kJ}{kg}\right]$	1	332,5	3	223,6	3	21,56	1
13.2	Enthalpy of condensation	$\left[\frac{kJ}{kg}\right]$	2	403,1	1	341,43	2	93,4	3
14	Working fluid mass flow	$\left[\frac{kg}{s}\right]$	3	0,093	1	0,095	1	0,313	3
15	Density (h_3)	$\left[\frac{kg}{m^3}\right]$	3	1,10	2	2,42	3	4,73	4
16	Main steam pressure	[bar]	2	5,8	4	14,6	4	17,6	3
17	Heat transfer coefficient	$\left[\frac{W}{m^2 \cdot K}\right]$	-	-	-	-	-	-	-
18	Global warming potential	[−]	4	-	4	3	3	1	3
19	Water pollution class	[−]	4	1	3	2	2	1	3
20	Gross thermal efficiency	[%]	4	12,84	3	13,08	3	13,01	3
21	Molecular weight	$\left[\frac{g}{mol}\right]$	2	70	4	72	4	316	2
22	Molecular complexity	[−]	1	cyclic	3	branched	2	branched	2
Severity (s_x) =				**83**		**79**		**82**	

3.5 FINAL FLUID CHOICE

Based on the working fluid ranking, Cyclopentane obtains the best severity (s=83) with only one evaluation point ahead of Novec 649 with s=82. Iso-Pentane (s=79) was already rejected during the elimination process because it evaporates at too low temperature level while ambient pressure. The close match of the ranking justifies the need of a detailed cycle simulation and the comparison of the net electric efficiency for the two remaining fluid.
The simulation with "EBSILON®Professional" [12] suggests the selection of Cyclopentane due to the higher net electric efficiency (12,7%) in contrast to Novec 649 (12,1%).

4. RESULTS

For the elimination of working fluids the cost of the working fluid itself (C_9) is excluded from the process due to the addition of much higher cost driver (C_{14} & C_{15}) into the ranking process.
The consideration of additional eight tolerance criteria (C_{11}; C_{12}; $C_{13.1}$; $C_{13.2}$; C_{14}; C_{17}; C_{21}; C_{22}) – compared to the earlier work of Roedder et al. [8] – was reviewed with respect to working effort and their utilization in the selection procedure.

In the presented work the thermal conductivity (C_{11}) was calculated with a simulation tool [12] that allows a simple integration into the selection procedure with only a slight demand of time.
The liquid isobaric heat capacity (C_{12}) – at ambient condition – is usually given by freeware substance-databases like "GESTIS" [10] or diverse other once or can also be calculated with any available calculation software and hence should be integrated into the rating process.
While using the p,h-diagram to consider the ratio of the external heat input to the isentropic expansion work – gross thermal efficiency (C_{20}) – the enthalpy of vaporization ($C_{13.1}$) and condensation ($C_{13.2}$) can also be achieved with nearly non additional work input.
For the integration of the heat transfer coefficient (C_{17}) an extensive calculation has to be performed. Hence it is the only TC, which is not considered in this work.
Due to heavy differences in the molecular weight (C_{21}) of working fluids and the increasing demand of energy consumed by the feed pump and hence its negative effect on the net electric efficiency the molecular weight should be included into the selection procedure.
The molecular complexity (C_{22}) is distinct in three categories with differences in their intermolecular cohesion, which is also confirmed by the thermostability of a working fluid (C_4) in the elimination process. Because it is not necessary to discuss criteria with the same meaning the molecular complexity can be omitted in favour of the thermostability. For the integration of the molecular complexity into the selection procedure the range of values needs a more complex classification.

5. CONCLUSIONS

In general, the integration of a standardized selection procedure into the early design phase of an Organic Rankine Cycle power plant is an assisting method, which pays of when several working fluids are to be considered.
The fluid selection is based on 21 criteria in total by exclusion of the working fluid cost (C_9) from the elimination process and the heat transfer coefficient (C_{17}) from the ranking process. It is shown that the ranking of the working fluid with the suggested tolerance criteria (C_{17} excluded) – leads to a representative result (see chapter 3.4), which is confirmed by a subsequent cycle simulation and the calculation of the net thermal efficiency.
In this work the integration of all reasonable criteria into the method was emphasized. Further investigations will be directed at a generalization of how to choose suitable weighting factors. It will also be necessary to show that the suggested method leads to customized results and shorter development times compared to a design process without application of an organized selection process ORC.

NOMENCLATURE

C	Criterion	$[-]$	$\dot{Q}$	Heat flow	$\left[\frac{kJ}{s}\right]$
e	Evaluation number	$[-]$	s	Rating number (severity)	$[-]$
EC	Elimination criterion	$[-]$	T	Temperature	$[°C]$
GHS	Globally Harmonised System	$[-]$	TC	Tolerance criterion	$[-]$
GWP	Global warming potential	$[-]$	v	Range of values	$[-]$
h	Specific enthalpy	$\left[\frac{kJ}{kg}\right]$	$\dot{V}$	Volume flow	$\left[\frac{m^3}{s}\right]$
HT	High temperature cycle	$[-]$	w	Weighting factor	$[-]$
LT	Low temperature cycle	$[-]$	X	Toxicity	$[-]$
$\dot{m}$	Mass flow	$\left[\frac{kg}{s}\right]$			
M	Molecular weight	$[-]$	α	Heat transfer coefficient	$\left[\frac{W}{m^2*K}\right]$
MC	Molecular complexity	$[-]$	η	Efficiency	$[-]$
ODP	Ozone depletion potential	$[-]$	λ	Thermal conductivity	$\left[\frac{W}{m*K}\right]$
p	Pressure	$[bar]$	ν	Kinematic viscosity	$\left[\frac{mm^2}{s}\right]$
P	Power	$[kW]$	ρ	Density	$\left[\frac{kg}{m^3}\right]$

REFERENCES

[1] Bao J., and Zhao L., 2013, A review of working fluid and expander selections for organic Rankine cycle, *Renewable and Sustainable Energy Reviews(24)*, pp. 325–342.

[2] Fischer J., Saleh B., Koglbauer G., Wendland M., 2007, Working fluids for low-temperature organic Rankine cycles, *Energy(32)*, pp. 1210–1221.

[3] Fischer J., Anh Lai N., Wendland M., Working fluids for high-temperature organic Rankine cycles, *Energy, 2011(36)*, pp. 199–211.

[4] Mohanraj M., Jayaraj S., and Muraleedharan C., 2009, Environmental friendly alternatives to halogenated refrigerants – A review, *International Journal of Greenhouse Gas Control(3)*, pp. 108–119.

[5] Papadopoulos A. I., Stijepovic M., and Linke P., 2010, On the systematic design and selection of optimal working fluids for Organic Rankine Cycles, *Applied Thermal Engineering(30)*, pp. 760–769.

[6] Quoilin S., Van Den Broek, Martijn, Declaye S., Dewallef P., and Lemort V., 2013, Techno-economic survey of Organic Rankine Cycle (ORC) systems, *Renewable and Sustainable Energy (22)*, pp. 168–186.

[7] Tchanche B.F., Papadakis G., Lambrinos G., Frangoudakis A., 2009, Fluid selection for a low-temperature solar organic Rankine cycle, *Applied Thermal Engineering (29)*, pp. 2468-2476.

[8] Rödder M., Neef M., Laux C., Priebe K.-P., 2015, Systematic fluid selection for organic Rankine cycles (ORC) and performance analysis for a combined high and low temperature cycle, *ASME-Paper GT2015-42432*, release in Proceedings of ASME Turbine Technical Conference and Exposition (TurboExpo), 15.-19. June 2015, Montreal, Canada

[9] Breiing A., and Knosala R., 1997, Bewerten technischer Systeme: Theoretische und methodische Grundlagen bewertungstechnischer Entscheidungshilfen, Springer, Berlin

[10] IFA Institut für Arbeitsschutz der Deutschen Gesetzlichen Unfallversicherung (German Social Accident Insurance), 2014, "GESTIS Information system on hazardous substances," www.dguv.de/ifa/gestis-database,

[11] Lemmon E. W., Huber M. L., McLinden M.O., 2013, "NIST Standard Reference Database 23, Fluid Thermodynamic and Transport Properties REFPROP, User's Guide," National Institute of Standards and Technology (NIST)

[12] Steag Energy Services, 2014, "*EBSILON®Professional* Program Documentation,"

[13] United Nations Organization, 2013, "Globally Harmonized System of Classification, Labelling and Packaging of Chemicals," GHS Rev.5, http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html.