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Optimal Integration of Organic Rankine Cycles with Heat Exchanger Networks Using Intermediate Heat Transfer Fluids

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In recent years, different methodologies and mathematical models have been proposed for the optimal integration of Organic Rankine Cycles (ORC) into Heat Exchanger Networks (HEN) for the recovery of low-grade heat. Most of these works have been focused on the optimization of the ORC configuration or its operational parameters and assume a direct heat exchange between the working fluid and the process streams. However, in many industrial applications a direct heat exchange between the working fluids and the process streams is undesirable due to logistics, controllability or safety reasons and an intermediate heat recovery loop (HRL) using heat transfer fluids (HTFs) is preferred. This work proposes a novel stage-wise superstructure for the optimal integration of ORCs into HENs through the use of intermediate HTFs. These HRLs can be located between the ORC and the hot or cold streams. In this work the objective function will be the net power generated by the ORC from the waste heat. A case study from the literature is presented to demonstrate the methodology and the results are compared with the case of the direct heat exchange between working fluid and process streams. The novelty of the formulation lies on the integration of the ORC into the background process using HTFs while simultaneously performing the synthesis of the HEN and the optimization of the operating parameters of the HRLs.

1. Introduction

The industrial sector amounts to almost the 30 % of the Final Energy Consumption worldwide (IEA, 2019). For the last five decades, Process Integration (PI) has been one methodology to increase the efficiency of industrial processes decreasing their energy consumption (Klemeš et al., 2018). From mainly graphical methods like the Pinch Analysis (Linnhoff and Flower, 1978) to increasingly complex mathematical models based on mathematical programming, the success of PI has been undeniable (Klemeš and Kravanja, 2013), even though significant amounts of waste heat from industrial processes remain. According to Forman et al. (2016) around 30 % of the energy supplied to industrial processes is released through a heat carrier (gas or liquid) unused to the environment as industrial waste heat. It is clear that a reduction in this waste heat will have a significant impact on decreasing the CO_2 emissions of the industrial sector and increasing its competitiveness (O'Rielly and Jeswiet, 2015). Recently, waste heat recovery technologies have been studied in order to harness the unexploited potential of the waste heat (Huang et al., 2017). Organic Rankine Cycles (ORCs) are one of the most promising technologies (Mahmoudi et al., 2018).

Lately, different studies exploring simultaneously the integration of ORCs into the background processes and the synthesis of the HENs have been presented. The work by Desai and Bandyopadhyay (2009) presented a graphical approach using the Grand Composite Curves and other tools of Pinch Analysis for the exploration of ORC integration opportunities. Later, a work by Chen et al. (2014), developed a mathematical programming approach to the simultaneous integration of ORCs into the background processes and the synthesis of the accompanying HEN. The work is an extension of the stage-wise superstructure model for the synthesis of HENs by Yee and Grossmann (1990) , also known as SYNHEAT model, and in it, Chen et al. (2014) pursued the maximization of the Net Power generated from the waste heat and used the Peng Robinson Equations of State (PR-EOS) to calculate, separately from the optimization model, the thermophysical properties of the working fluid. Chen et al. (2014) also considered the latent heat of evaporation and condensation of the working fluid

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and rightfully proved its influence on the model results. The model used a simple ORC configuration and it allowed the heat exchange between the working fluid and the process streams in all stages of the superstructure. More recently Yu et al. (2017a) presented a 2-Step mathematical formulation based on the Duran-Grossmann model for Heat Integration (Duran and Grossmann, 1986) that includes the optimization of the ORC configuration (turbine bleeding, regeneration and superheating) and its operating conditions (e.g. temperatures and/or pressure levels) integrating the PR-EOS on the model. In this formulation, the first step optimizes the net power generated from the system including a penalty term for additional hot utility consumption, and in the second step the HEN is generated using the transhipment model (Papoulias and Grossmann, 1983). Similarly, Kermani et al. (2018) presented an extended generic superstructure including additional ORC configurations while presenting different objective functions. Kermani et al. (2018) divide the problem in two steps. The first step optimizes the operating conditions (temperatures, pressure, reheating temperatures and working fluid) depending on the objective function using a genetic Algorithm (GA). Then a MILP solver is used to optimize the ORC configuration. Finally, the HEN can be generated afterwards using a modified formulation of the sequential synthesis methodology developed by Floudas and Grossmann (1987). In all cases, they only considered the direct heat exchange between the working fluid and the process streams. A work by Chen et al. (2016), explored a mathematical programming approach for the integration of ORCs for waste heat recovery in a refinery using HTFs. They developed a superstructure where waste heat from hot streams was recovered using one or more HRLs using HTFs. The temperatures and mass flow for the fluids in the HRLs were variables to be optimized by the model. The evaporator and condenser temperatures of the working fluids were optimized using an iteration algorithm. As the problem didn't consider cold streams, the synthesis of the HEN wasn't studied. A recent work by Yu et al. (2017b) explored hot water as an HTF for ORC heat integration and similar to his other work, it used the Duran-Grossmann model and the PR-EOS to optimize the ORC operating conditions. The HEN was then generated using the transhipment model.

In this paper, an extension of the SYNHEAT model is presented for the integration of ORC in HEN using HTFs. To the best of the authors' knowledge, no previous formulation allows the indirect integration of ORCs into the background processes using HRLs, while simultaneously performing the synthesis of the HEN and the optimization of the operating parameters of the HRLs. The ORC operating parameters are defined in advance and the properties of the working fluid are calculated independent of the optimization model using the PR-EOS. The model allows the exchange of heat between the hot and cold streams and between the hot and cold streams and the HTFs in the HRLs. The heat exhausted by the condenser of the ORC can be used to heat the cold streams through the cold HRL. A known example from the literature is presented to illustrate the methodology and the results compared with the case for the direct heat exchange between working fluid and process streams.

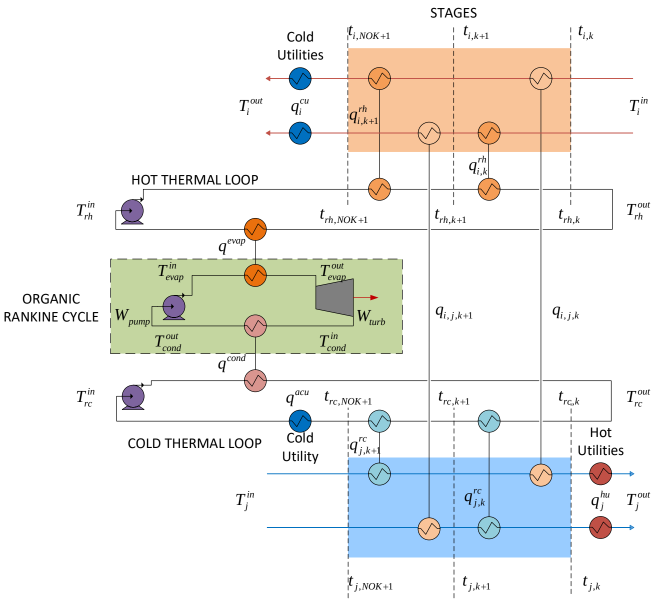

Figure 1: Simplified schematic representation of the model superstructure

2. Methodology

The developed superstructure is represented in Figure 1. The direct heat exchange between cold and hot utilities takes place inside the stages of the superstructure. Additionally, the hot streams can also exchange heat with the HTF at the hot thermal loop which then can exchange heat with the working fluid at the evaporator of the ORC. The working fluid leaves the evaporator as a saturated vapour at the predefined evaporation temperature and it is expanded in the turbine generating electricity. The expanded fluid at a superheated state is cooled in the condenser where it exchanges heat with the HTF at the cold thermal loop. The working fluid leaves the condenser as a saturated liquid at the condensation temperature and it is then pumped back to the evaporator pressure to restart the cycle. The HTF at the cold thermal loop can be used to heat the cold streams or release its energy to the cold utility. Hot and cold utilities are used at the hot and cold ends of the superstructure to supply/remove the remaining energy required to achieve the target temperatures of the process streams. In case that stream splits are necessary, the mixing of the fluids will be isothermal.

2.1 Mathematical formulation

Eq(1) and Eq(2) represent the overall energy balances of the process streams with the additional terms for the heat exchange between the process streams and the HRLs added, where F_i and F_j are the heat capacity rates of the streams. Eq(3) and Eq(4) describe the energy supplied and rejected from the ORC system as the results of energy balances on the HRLs on one side and the ORC evaporator and condenser on the other. In these equations, the terms $cp_{w(l)}$ and $cp_{w(g)}$ refer to the average specific heat capacities of the working fluid in its liquid and gas phase and the lambda terms λ_{evap} and λ_{cond} represent the specific latent heats of vaporization of the working fluid at the evaporator and condenser. The mass flow rates of the HTFs inside the hot and cold HRLs are $\dot{m}_{rh}$ and $\dot{m}_{rc}$. The specific heat capacities cp_{rh} and cp_{rc} refer to the hot and cold HTFs. Eq(5) and Eq(6) are the stage energy balances for each process stream and each HRL. Eq(7) calculates the utility demands of the cold HRL and the process streams. The expressions presented in Eq(8) and Eq(9) represent the temperature assignments and logical constraints at the first and last stage of the superstructure for the process streams and the HTFs at the HRLs. Eq(10) provide additional logical conditions for the temperatures at the extremes of the HRLs. Eq(11) describe the monotonicity of the temperatures of the process streams and HTFs inside the superstructure. Eq(12) to Eq(14) provide generic expressions for logical constraints to the heat transfer duties ($q_*^\dagger$) and approach temperatures at the hot and cold ends ($dt1_*^\dagger$ and $dt2_*^\dagger$) of all possible heat exchangers in the superstructure, as represented in Figure 1.The binary variables $z_*^\dagger$ represent the existence or absence of a particular heat exchanger. Terms Γ and Ω represent arbitrary big numbers in the Big-M formulations. Eq(15) and Eq(16) guarantee that the minimum approach temperature is maintained inside the ORC evaporator and condenser. Eq(17) calculates the power consumed by the pump and generated in the turbine in the ORC as a function of the mass flow of working fluid and its specific enthalpy changes Δh_{pump} and Δh_{turb} inside of them. The enthalpy changes are calculated using the PR-EOS using the property tables and methods presented by Poling et al. (2001) and used by Chen et al. (2014).

$$\sum_{j\in CP}\sum_{k\in ST} q_{i,j,k} + \sum_{k\in ST} q_{i,k}^{rh} + q_i^{cu} = F_i\left(T_i^{in} - T_i^{out}\right) \tag{1}$$

$$\sum_{i\in HP}\sum_{k\in ST} q_{i,j,k} + \sum_{k\in ST} q_{j,k}^{rc} + q_j^{hu} = F_j\left(T_j^{out} - T_j^{in}\right) \tag{2}$$

$$q^{evap} = \sum_{i\in HP}\sum_{k\in ST} q_{i,k}^{rh} = cp_{rh}\dot{m}_{rh}(T_{rh}^{out} - T_{rh}^{in}) = \dot{m}_w\left(cp_{w_{(l)}}\left(T_{evap}^{out} - T_{evap}^{in}\right) + \lambda_{evap}\right) \tag{3}$$

$$q^{cond} = \sum_{j\in CP}\sum_{k\in ST} q_{j,k}^{rh} + q^{acu} = cp_{rc}\dot{m}_{rc}(T_{rc}^{out} - T_{rc}^{in}) = \dot{m}_w\left(cp_{w_{(g)}}\left(T_{cond}^{in} - T_{cond}^{out}\right) + \lambda_{cond}\right) \tag{4}$$

$$\sum_{j\in CP} q_{i,j,k} + q_{i,k}^{rh} = F_i\left(t_{i,k} - t_{i,k+1}\right),\ \sum_{i\in HP} q_{i,j,k} + q_{j,k}^{rc} = F_j\left(t_{j,k} - t_{j,k+1}\right) \tag{5}$$

$$\sum_{i\in HP} q_{i,k}^{rh} = cp_{rh}\,\dot{m}_{rh}\left(t_{rh,k} - t_{rh,k+1}\right),\ \sum_{j\in CP} q_{j,k}^{rc} = cp_{rc}\,\dot{m}_{rc}\left(t_{rc,k} - t_{rc,k+1}\right) \tag{6}$$

$$q^{acu} = \dot{m}_{rc}\,cp_{rc}\left(t_{rc,NOK+1} - T_{rc}^{in}\right),\quad q_i^{cu} = F_i\left(t_{i,NOK+1} - T_i^{out}\right),\ q_j^{hu} = F_j\left(T_j^{out} - t_{j,1}\right) \tag{7}$$

$$T_i^{in} = t_{i,1},\quad t_{j,NOK+1} \geq T_j^{in} \tag{8}$$

$$t_{rh,1} = T_{rh}^{out},\quad t_{rh,NOK+1} = T_{rh}^{in},\quad t_{rc,1} = T_{rc}^{out},\quad t_{rc,NOK+1} \leq T_{rc}^{out} \tag{9}$$

$$T_{rh}^{out} \geq T_{rh}^{in},\quad T_{rc}^{out} \geq T_{rc}^{in} \tag{10}$$

$$t_{i,k} \geq t_{i,k+1}\,, \qquad t_{j,k} \geq t_{j,k+1}\,, \qquad t_{rh,k} \geq t_{rh,k+1}\,, \qquad t_{rc,k} \geq t_{rc,k+1} \tag{11}$$

$$q_*^\dagger - \Omega z_*^\dagger \leq 0 \qquad * \in \{i, j, (i,k), (j,k), (i,j,k)\}\,,\ \dagger \in \{cu, hu, rc, rh, evap, cond, acu\} \tag{12}$$

$$\Delta T_{min} \leq dt1_*^\dagger \ \leq \Delta T_{Hot-End} + \Gamma\left(1 - z_*^\dagger\right) \tag{13}$$

$$\Delta T_{min} \leq dt2_*^\dagger \ \leq \Delta T_{Cold-End} + \Gamma\left(1 - z_*^\dagger\right) \tag{14}$$

$$\Delta T_{min} \leq dt3^{evap} \ \leq \left(T_{rh}^{in} + \frac{mw\ cpw_{(l)}\left(T_{evap}^{out} - T_{evap}^{in}\right)}{cp_{rh} m_{rh}}\right) - T_{evap}^{out} + \ \Gamma(1 - z^{evap}) \tag{15}$$

$$\Delta T_{min} \leq dt^{cond} \ \leq T_{cond}^{out} - \left(T_{rc}^{out} - \frac{mw\ cpw_{(g)}\left(T_{cond}^{in} - T_{cond}^{out}\right)}{cp_{rc} m_{rc}}\right) + \ \Gamma(1 - z^{cond}) \tag{16}$$

$$W_{pump} = \dot{m}_w \Delta h_{pump,is} / \eta_{pump} = \dot{m}_w \Delta h_{pump}, \qquad W_{turb} = \eta_{turbine} \dot{m}_w \Delta h_{turb,is} = \dot{m}_w \Delta h_{turb} \tag{17}$$

2.2 Objective Function

In this formulation, the objective is to maximize the net power generated by the ORC without increasing the utility consumption of the system in comparison with the standalone HEN. This case can be described with Eq(18) and the additional constraints in Eq(19). The utility requirements of the standalone HEN ($q_j^{hu}(HEN)$ and $q_i^{cu}(HEN)$) can be calculated beforehand using Pinch Analysis or the Problem Table Algorithm. As simplification, the electricity required to pump the HTFs inside the HRLs will not be considered.

$$\max W_{net} = W_{turb} - W_{pump} \tag{18}$$

$$\sum_{j \in CP} q_j^{hu} \leq \ \sum_{j \in CP} q_j^{hu}\,(HEN), q^{acu} + \sum_{i \in HP} q_i^{cu} \leq \ \sum_{i \in HP} q_i^{cu}\,(HEN) \tag{19}$$

3. Case Study

The case study is taken from Chen et al. (2014) and 3 hot streams and 4 cold streams are available (Table 1). Between process streams and between the process streams and the utilities, a $\Delta T_{min} = 20\ °C$ will be used with a minimum utility consumption of 244.131 kW (Hot Utility) and 172.596 kW (Cold Utility) for the stand-alone HEN according to Pinch Analysis (Figure 2). The working fluid is n-Hexane and its thermophysical properties are calculated using the PR-EOS and the procedures explained by Poling et al. (2001). The working fluid temperatures at the end of the evaporation and condensation processes are set to 186.5 °C (P_{evap} = 1,450 kPa) and 73 °C (P_{cond} = 116 kPa). The HTF in both HRLs is Dowtherm A by the Dow Chemical Company with an average specific heat capacity in the liquid form of 2.16 kJ/kg°C. Isentropic efficiencies in pump and turbine are $\eta_{turbine} = 0.8$ and $\eta_{pump} = 0.65$. The results for different minimum approach temperatures between the HTFs and the process streams or working fluid ($\Delta T_{min,HTF}$) are summarized in Table 2. Expected savings on annual CO_2 emissions at full operation compared with the case of no ORC are calculated using the emission factor of the German electricity mix for 2019, which is 401 g/kWh (Umweltbundesamt, 2020). The model is implemented in GAMS (version 25.1.1) and the global solver BARON with an optimality gap of 1 % will be used to solve the MINLP. The optimization was performed on a Windows machine with an Intel(R) Core(TM) i7-6600U 2.60 GHz CPU and 12 GB RAM. In total, the model consists of 373 equations with 402 variables (86 integer variables). CPU solution times for the different runs were consistently around 1,200 s.

Table 1: Data for Process Streams (Chen 2014)

Hot Streams	T_{in}(°C)	T_{out}(°C)	F(kW/°C)	Cold Streams	T_{in}(°C)	T_{out}(°C)	F(kW/°C)
H1	353	313	9.802	C1	224	340	7.179
H2	347	246	2.931	C2	116	303	0.641
H3	255	80	6.161	C3	53	113	7.627
HU	377	377		C4	40	293	1.690
				CU	20	30	

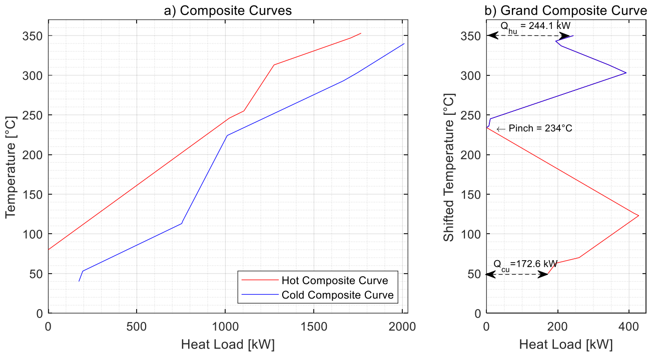

Figure 2: a) Composite Curves and b) Grand Composite Curve of the Case Study. (ΔT_{min} = 20 °C)

As expected the net power generated by the ORC decrease with higher $\Delta T_{min,HTF}$. This is analogue to an increase in the pinch temperature, decreasing the number of process streams that are available for heat exchange and limiting the amount of energy that they are capable of supply or accept. At $\Delta T_{min,HTF}$ = 25 °C none of the process streams is able to supply or receive energy from the ORC System. At $\Delta T_{min,HTF}$ = 5 °C and $\Delta T_{min,HTF}$ = 10 °C the ORC is able to supply energy to the cold streams decreasing the amount of energy that is exhausted to the cold utility at the cold HRL. In comparison with the direct heat integration between the ORC and the process streams as developed by Chen et al. (2014), the use of HTFs decrease the amount of energy available for the heat exchange and the net power generated is lower. For the case study with a $\Delta T_{min,HTF}$ = 10 °C and ΔT_{min} = 20 °C the net power generated 27.68 kW is 42 % lower than the 47.97 kW generated with direct ORC integration. The design for this case is presented in Figure 3.

Table 2. Optimization results at different $\Delta T_{min,HTF}$

$\Delta T_{min,HTF}$ (°C)	W_{net} (kW)	W_{turb} (kW)	W_{pump} (kW)	M_w (kg/s)	Q_{evap} (kW)	Q_{cond} (kW)	Q_{acu} (kW)	CO_2 Savings (t/y)
5	30.34	31.79	1.45	0.44	229.71	199.36	142.26	106.58
10	27.68	29	1.33	0.4	209.55	181.87	144.92	97.23
15	22.8	23.89	1.09	0.33	172.6	149.8	149.8	77.56
20	17.02	17.84	0.82	0.25	128.87	111.85	111.85	59.79
25	0	0	0	0	0	0	0	0

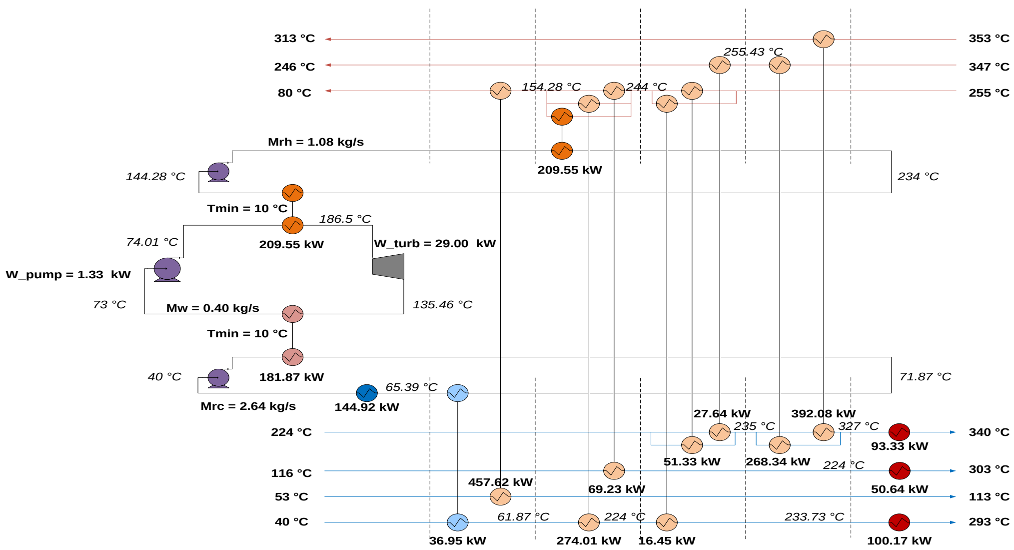

Figure 3: HEN with Integrated ORC for the case $\Delta T_{min,HTF}$ = 10 °C and ΔT_{min} = 20 °C .

4. Conclusions

In this work a novel superstructure for the optimal integration of ORCs into HENs using intermediate HTFs was presented. The superstructure based on the SYNHEAT model allows the energy exchange between the process streams and the working fluid at the ORC through the use of HRLs where an intermediate HTF circulates. On industrial cases, this formulation allows to design systems where the physical location of the ORC is distant to the process streams or where for safety and/or controllability reasons, a direct exchange between the working fluid and the process streams is undesirable. The formulation also can be extended to consider more complex objective functions like the total annual cost (TAC) or to account for the pumping cost at the HRLs.

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