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Exergy based methodology for optimized integration of vapor compression heat pumps in industrial processes

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ABSTRACT

Industrial processes may use heat pumps to recover low-grade heat or to combine heating and cooling needs. In many cases, this technology leads to reduced energy consumption and greenhouse gases emissions. In this paper, a methodology, based on exergy analysis of heat sources and heat sinks, helping in optimizing industrial heat pumps design is presented. The optimization variables are: the refrigerant choice (pure fluid, azeotropic mixture, non azeotropic mixture), the thermodynamic state of the refrigerant (subcritical, supercritical) and the architecture of the heat pump (single heat pump, heat pump in reverse series). The heat pump is modeled in Modelica language: "pinch" method is used to model the heat exchangers and the compressor model is based on an isentropic efficiency assumption. The objective function is the maximization of the heat pump system exergy efficiency. Genetic algorithm is used to perform the optimization. The methodology is applied on a case study of an industrial process where a fluid is heated from 60° C to more than 120° C, and industrial effluents are available at 50° C.

1. INTRODUCTION

In recent decades, research on the recovery of low grade heat from industrial wastes by the integration of heat pumps has received great attention (Laue, Lehmann, & Milbitz, 1990; Silva & Rosa, 1993; Smolen & Budnik-Rodz, 2006). The energetic analysis based only on the first law of the thermodynamics is not adapted to design optimal heat pump because the energy balance treats all forms of energy as equivalent and generally provide no information about internal losses. However, the exergy method is an alternative to find the usable work of a process and is particularly adapted to find the irreversibilities of a multi-component system (Kotas, 1995). The number and type of working fluids and the efficiency of compressors, expanders and heat exchangers give to the thermodynamic cycle of heat pump an infinite number of degrees of freedom. Thus, a mathematical model for steady-state simulation based on the exergy analysis has been developed in order to design the optimal vapor compression heat pump in accordance with the studied industrial process.

The thermodynamic properties of a selection of working fluids, presented on the Table 1, have been implemented with the NIST database. Natural refrigerants, HFCs and one HFO have been selected for the investigation. Seven of them (R-717, R-718, R-744, R-143a, R-152a, R-41, R-32) are "dry" fluids and the others (R-1234yf, R-134a, R-227ea, R-245ca, R-245fa) are "wet" fluids. Some of the HFCs have a GWP higher than 2500 and will be probably prohibited the coming years by the last revision of the European regulation named "F-Gas" (*Proposal for a regulation of the European Parliament and of the Council on fluorinated greenhouse gases*, 2013) and by the new agreement between USA and China in order to reduce the high-GWP HFCs (Clodic, Pan, Devin, Michineau, & Barrault, 2013). Consequently, a GWP limit constraint is set avoiding that the optimization model chooses one of those fluids. However, they can be blended with others refrigerants to have an acceptable environmental impact. The properties of refrigerant mixtures are calculated with explicit mixture models in Helmholtz energy equation of state (Lemmon, 2004). Therefore, the model can simulate heat pump thermodynamic cycles integrated in a process, with

pure refrigerants, azeotropic refrigerant mixtures and non azeotropic refrigerant mixtures. The choice of the working fluids is essential to achieve good cycle performance. It depends on the operating conditions, *i.e.* heat source and heat sink temperature level and profile. One of the advantages of non azeotropic mixtures is the possibility to reduce heat exchangers irreversibilities by matching the temperature glide of refrigerant with the temperature glide of the medium (air, water...) (Venkatarathnam, Mokashi, & Murthy, 1996).

Moreover, the thermodynamic cycle of the heat pump can be subcritical, transcritical or supercritical. Those different regimes of the working fluid can be investigated. The transcritical cycles are particularly adapted to deliver heat at high temperature level because the pressure ratios have a favorable influence on the transcritical compressor efficiency (Angelino, 1994).

In order to study several possibilities to integrate efficient heat pump system adapted to the studied industrial process, the heat pump architecture is not defined *a priori*. In addition to the cycle regime and the refrigerant optimization, cascading heat pumps may be investigated by the optimizer allowing to recover the low-grade heat source and provide heat to the heat sink by stage, while using different working refrigerants adapted to the temperature levels for each heat pump.

The model has been developed using the Modelica language. The optimization is performed by a genetic algorithm integrated in OMOPTIM (Murr, Thieriot, Zoughaib, & Clodic, 2011) tool which handles easily Modelica models. In this present paper, the optimal designs are presented as a function of the source and sinks profiles.

 Table 1: Basic thermodynamic and environmental properties of the selected fluids with their safety group (ASHRAE Handbook, Volume Refrigeration, 2009; Order, 2013; Walter et al., 2008)

Refrigerants	Critical pressure	Critical Temperature	GWP	Туре	Safety
	(MPa)	(°C)	100-Year		group
R-717	11.33	132.25	<1	Natural refrigerant	B2L
R-718	22.06	373.95	<1	Natural refrigerant	A1
R-744	7.38	30.98	1	Natural refrigerant	A1
R-32	5.78	78.11	716	HFC	A2L
R-41	5.90	44.13	_	HFC	_
R-134a	4.06	101.06	1300	HFC	A1
R-143a	3.76	72.71	3800	HFC	A2L
R-152a	4.52	113.26	132	HFC	A2
R-227ea	2.92	101.75	2900	HFC	A1
R-245ca	3.92	174.42	560	HFC	_
R-245fa	3.64	154.05	820	HFC	B1
R-1234yf	3.38	94.70	4	HFO	A2L

2. HEAT PUMPS CLASSIFICATION

Vapor compression heat pumps cycle can be one of the following three ones: subcritical vapor compression cycle, transcritical vapor compression heat pump cycle and supercritical vapor compression cycle. Each of them has its particularities. Figure 1 represents the evolution of the temperatures versus heat in both heat exchangers of the heat pump for the three cycles and three industrial processes situations. The situation (a) is a process where the heating needs and the cooling needs take place at almost constant temperature (e.g. condensation, evaporation or high mass flow rate). In the situation (c), the heating and cooling needs are typical of liquid or gas cooling and heating. The situation (b) is a mixture between the situation (a) and (b) where the cooling needs take place at almost constant temperature.

2.1 Subcritical cycle (see Appendix 1)

A subcritical vapor compression heat pump consists of 4 mains parts: evaporator (evaporation 1-2' and superheating 2'-2), compressor (2-3), condenser (desuperheating 3-4', condensation 4'-4'' and subcooling 4''-4) and an expansion valve (4-1) at subcritical pressures. The superheating ΔT_{SH} (2'-2) is required to protect the compressor by making sure the refrigerant is fully evaporated at the compressor inlet. The ΔT_{SH} parameter can be controlled by the expansion valve. Generally it is fixed between 3°C and 8°C (Meunier, Rivet, & Terrier, 2010). The subcooling ΔT_{SC} (4''-4) is also a parameter which can be controlled by adjusting the active charge of the heat pump (Jensen & Skogestad, 2007). The refrigerant choice changes the heat pump behavior. For pure refrigerants or azeotropic

mixtures, the subcritical vapor compression heat pump has no temperature glide on the two HEXs. These heat pumps are adapted for processes with low temperature lift (van de Bor & Infante Ferreira, 2013), since the exergy losses at the HEXs are minimized (LALLEMAND, 2014). On the other hand, as shown in Figure 1 using non azeotropic mixtures causes temperature glide during the condensation or evaporation and reduces the exergy destruction when the glide of heat source and heat sink are matching the refrigerant one.

2.2 Transcritical cycle (see Appendix 1)

A transcritical vapor compression heat pump consists of an evaporator (evaporation at subcritical pressure 1-2' and super-heating 2'-2), compressor (2-3), gas cooler (gas cooling at supercritical pressure 3-4) and expansion valve (4-1). Here, the sub-cooling does not exist because the saturation line of the refrigerant is under the gas cooling curve but the active charge defines the high pressure of the cycle, which has a significant impact on the performance of a transcritical vapor compression heat pump (Cho, Ryu, Kim, & Kim, 2005). As shown in Figure 1, when the refrigerant is a pure fluid or an azeotropic mixture, those heat pumps presents less exergy losses for high glide heat sinks and small glide heat sources. For high glide heat sinks and heat sources, a non azeotropic mixture may be expected to match better the different glides.



Figure 1: Diagram $(\Theta; \dot{Q})$ presenting the HEXs of three vapor compression heat pumps cycles, for three applications processes (a, b and c), the HEXs are considered in counter flow

3. EXERGY ANALYSIS AT STEADY STATE OF VAPOR COMPRESSION HEAT PUMP

3.1 Heat pump model

The method used to model the heat pump behavior in steady state is commonly called "Pinch" method. It consists to define the minimum temperature difference between the refrigerant and the medium, in the heat exchangers. Depending on the flow arrangement of the heat exchangers (cross, parallel or counter flow), the thermodynamic region of the pinch exists at different locations. For the parallel flow heat exchangers, the pinch point is always located at the outlet. For the cross flow heat exchangers, the pinch point is located between the inlet cold fluid and the outlet hot fluid. While, the counter flow heat exchanger has two possible pinch points: one at the inlet cold fluid and another one, located at area depending if the heat exchanger is an evaporator, a condenser or a gas cooler. The different possible locations of the two pinch point is located at the vapor saturation of the refrigerant. For the gas cooler, the second pinch point is located at the vapor saturation of the refrigerant. For the gas cooler, the refrigerant temperature curve inflexion during its cooling. The definition of pseudocritical temperature T_{pc} is the temperature at which the specific heat reaches a maximum for a given pressure (Yu, Lin, Lin, & Wang, 2012).



Figure 2: Possible Pinch point locations for the counter flow heat exchangers

3.2 Fluid properties implementation

The refrigerants, water and air properties have been implemented in the heat pump model by using the Helmholtz equations of states for each fluid (pure or mixture), based on the NIST database. The functions that are used are:

- P_{sat} function of T and X
- T_{sat} function of P and X
- s function of P, h and X
- s function of P, T, and X
- h function of P, T and X
- h function of P, Q and X
- T function of P, h, and X
- T function of P, Q and X
- ρ function of P, h and X

3.3 Assumptions

The following assumptions are made for the heat pump model:

- Each component of the cycle is analyzed as a control volume at steady state
- There are not heat exchange between each component with its surroundings
- There are no pressure drops through the heat exchangers
- The heat exchangers are counter flow ones
- The compressor (volumetric technology) operates adiabatically with an isentropic efficiency of 65% and a volumetric efficiency of 70%
- The expansion through the valve is a throttling process
- Kinetic and potential energy effects are negligible

3.4 Exergy analysis

Exergy analysis is a methodology for the analysis, design and improvement of thermodynamic systems and is a useful tool for reaching the goal of more efficient energy-resource use. The irreversibility of a process is the sum of all of the exergy destructions of all the streams in the system.

Exergy destructions, which are obtained from exergy balances, for each of the heat pump components, can be expressed as follows:

$$\zeta_{comp} = \dot{e}_{fl_{in}} - \dot{e}_{fl_{out}} + \dot{W}_{in} \tag{1}$$

$$\zeta_{exp} = \dot{e}_{fl_{in}} - \dot{e}_{fl_{in}} \tag{2}$$

$$\zeta_{HEXS} = \dot{e}_{fl_{in}} - \dot{e}_{fl_{out}} + \dot{e}_{me_{in}} - \dot{e}_{me_{out}}$$
(3)

It can be shown that the exergy efficiency of each component is equal to:

$$\eta_{comp} = \frac{\dot{e}_{fl_{in}} - \dot{e}_{fl_{out}}}{\dot{W}_{in}} \tag{4}$$

$$\eta_{exp} = \frac{e_{fl_{out}}}{e_{fl_{in}}} \tag{5}$$

$$\eta_{HEXS} = \frac{\dot{e}_{c_{out}} - \dot{e}_{c_{in}}}{\dot{e}_{h_{out}} - \dot{e}_{h_{in}}} \tag{6}$$

Because of the possible variation of the source and sink temperatures, the average temperature is defined as the ratio between enthalpy variation and the entropy variation (Meunier, Rivet, & Terrier, 2010):

$$\dot{s} = \frac{h_{out} - h_{in}}{s_{out} - s_{in}} \tag{7}$$

The exergy efficiency of the heat pump can be defined as

$$\eta_{HP} = 1 - \frac{\sum \zeta}{\dot{W}_{in}} \tag{8}$$

$$\eta_{HP} \left(T_0 = \tilde{T}_{c_{me}} \right) = \left(1 - \frac{\tilde{T}_{c_{me}}}{\tilde{T}_{h_{me}}} \right) * \frac{\dot{Q}_{HEX}^{HP}}{\dot{W}_{in}}$$
(9)

And the exergy efficiency of the system of two heat pumps in inverted series can be defined as:

$$\eta_{HP} = 1 - \frac{\sum \zeta}{\dot{W}_{in_1} + \dot{W}_{in_2}}$$
(10)

3.5 Optimization strategies

The model presented can be used to determine the performance and the compressor size of a heat pump by using as input the process characteristics. In order to optimize the integration of the industrial heat pump in a process, numerical optimization is used. When the heat pump uses a pure refrigerant, the optimization is based on a thermodynamic analysis (for a certain fluid) and when the heat pump is using a refrigerant mixture a metaheuristic optimization is associated to the thermodynamic optimization.

3.5.1 Thermodynamic optimization

The thermodynamic optimization consists to minimize the exergy losses of each component. This leads to determine the thermodynamic cycle of the heat pump that have the best matching curve at the heat exchangers (low pressure and high pressure). The best matching appears when there is a double pinch at each heat exchanger. Indeed, as shown at figures 1 and 2, the area between the hot and cold curve at each heat exchanger is minimal when the double pinch is observed. For the subcritical heat pump the double pinch is obtained by varying the subcooling ΔT_{SC} at the condenser and the superheat ΔT_{SH} at the evaporator. The figure 3 and 4 shows the evolution of the exergy efficiency of the heat pump using the R134a and the R1234yf for ΔT_{SC} and ΔT_{SH} variations. The process is defined by a source of air of 2kg/s at 25°C and a sink of air of 1kg/s at 25°C. The objective of the heat pump is to heat the sink from 25°C to 65°C. The pinch temperature for both heat exchangers is equal to 5 K.



Figure 3: Subcooling optimization (SH=5°C)

Figure 4: Superheating optimization (SC=2°C)

By comparing the results of the simulation for both optimizations, the subcooling optimization has more impact on exergy losses and energy performances. For the next simulations, the superheating optimization will not be considered and the superheating will be fixed at 5° C.

For the transcritical heat pump, the double pinch in the gas cooler is obtained by a variation of the high pressure. By the same exergy and energy analysis, the double pinch allows having the most efficient heat pump.

3.5.2 Metaheuristic optimization

A metaheuristic optimization is necessary for the heat pumps using refrigerant mixtures, because the number of possibilities is high due to the refrigerants combinations and compositions (Appendix 1). A genetic algorithm has been used to optimize the mass ratio of each refrigerant composing the mixtures created by the model.

4. RESULTS

An industrial process has been studied to determine the most efficient heat pump by using the methodology presented. The process characteristics are:

- Temperature inlet of the heat source (low grade energy) = 50° C
- Temperature inlet of the heat $sink = 60^{\circ}C$
- Temperature outlet of the heat sink (needs of the process) = 120° C

The mass flow rate of the low-grade energy and the needs of the process are not fixed in order to study different scenarios. The heat capacity flow rate ratio has been defined in that way:

$$\xi = \frac{(\dot{m} * Cp_i)_{Source}}{(\dot{m} * Cp_i)_{Sink}}$$
(11)



For different ratios, Figure 5 presents the optimization results for each heat pump types:

Figure 5: Optimal results in term of COP, for heat pumps with ΔT_{SC} optimized for all subcritical cycles, $\Delta T_{SH} = 5^{\circ}C$ for all cycles and the high supercritical pressure optimized for the transcritical cycle.

The optimization results show that there is an optimal solution for each heat capacity flow rate ratio. When the heat capacity flow rate ratio is less than 1 the subcritical heat pump with a non azeotropic refrigerant mixture is better than other heat pumps. It is due to the glide of source and sink temperatures, as it is shown in the figure 1, process (c). However when the heat capacity flow rate ratio is more than 1 the transcritical heat pump is the best choice. This is due to the source glide temperature, which decreases with the increase of the heat capacity flow rate ratio, as it is shown in the figure 1, process (b).

5. Conclusions

In this article, a steady state heat pump model and an optimization methodology to obtain the best integrated heat pump in an industrial process have been presented. The subcooling and the active charge are optimization variables, which have a real impact on the exergy efficiency and energy performance of the heat pumps. Moreover, the optimization results have shown that it is possible to have a COP higher than 3.5 for very high temperature processes (120°C) with an important glide sink temperature. The transcritical heat pumps using the R-32 as working fluid has the best performance for calorific ratios higher than 1. This type of heat pump may present a real economic advantage for the drying processes where the heat source are effluents with an important value of latent heat while heat sink is dry air that has to be heated to high temperatures.



Appendix 1: Heat pump systems modelling

NOMENCLATURE

COP	coefficient of performance		
Ср	specific heat capacity	(J/kg.K)	
GWP	global warming potential		
h	specific enthalpy	(J/kg)	
HEX	heat exchanger		
HFC	hydro fluorocarbon		
HFO	hydro fluorocarbon olefin		
Ν	number	(-)	
Р	pressure	(Pa)	
Ż	calorific	(W)	
S	specific entropy	(J/kg.K)	
Т	temperature	(K)	
$ ilde{T}$	average temperature	(K)	
Ŵ	power	(W)	
Х	mass fraction	(-)	
Greek symbols			
Δ	difference of quantities	(-)	
ζ	exergetic losses	(W)	
η	efficiency	(-)	
ξ	heat capacity flow rate ratio	(-)	
ρ	density	(kg/m³)	
Θ	Carnot temperature	(-)	
Subscript			
0	reference		
C	cold		
comp	compressor		
exp fl	fluid		
h	hot		
in	inlet		
m	mixture		
max	maximum		
me	medium		
min	minimum		
out	outlet		
рс	pseudocritical		
sat	saturation		
sc	subcooling		
sh	superheating		

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