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DECARBONISATION THROUGH INNOVATION

Energy, environmental and economic analysis of the integration of high temperature heat pumps into amine regeneration process

Manuele Gatti[1], Giammarco Gioco[2], Luca Molinaroli[1,*], Mario Primato[2], Paola Starace[2]

1 Dipartimento di Energia, Politecnico di Milano, Via Raffaele Lambruschini 4/A, 20156, Milano, Italy
2 ENI Spa, Via Felice Maritano 26, 20097, San Donato Milanese (MI), Italy

Abstract

This paper presents a numerical investigation of the integration of a high temperature heat pump into an amine regeneration process, with the aim of enhancing energy efficiency and reducing environmental impact (i.e. CO_2 emissions) via the electrification of steam supply. Several system configurations are systematically explored, involving different heat pump architectures and working fluids. The architectures considered include a simple configuration based on a standard reverse cycle and one employing mechanical recompression of steam. For refrigerant selection, a set of candidates working fluids is extracted from the Refprop 10.0 database by filtering them based on critical temperature, normal boiling point, and Global Warming Potential. For each combination of system architecture and working fluid, a thermodynamic optimization of the heat pump working cycle conditions is carried out using a Particle Swarm Optimization algorithm. This approach enables the identification of optimal design thermodynamic parameters while ensuring compliance with a set of thermodynamic and technical constraints. The result of this phase is the identification of the most suitable refrigerant for each configuration. Following the thermodynamic analysis, a techno-economic and environmental assessment is performed, comparing the performance of the proposed heat pump integration with that of a conventional combustion boiler-based heat supply system. The results demonstrate that, under the specific constraints of the case study, the integration of a high-temperature heat pump can lead to equivalent primary energy savings in the range 31.6 to 36.6%, reductions in CO_2 emissions from 26.8 to 32.0%, and OPEX saving is within 2.16M€/y to 2.71 M€/y, resulting in simplified payback between time between 0.87 years and 4.00 years. Overall, the high-temperature heat pump emerges as a key enabling technology for the transition toward more sustainable industrial thermal systems.

Keywords: High temperature heat pump; Indutrial process; Particle Swarm Optimization

1. Introduction

In 2020 the European Commission approved the European Green Deal, a set of initiatives that aim to achieve climate neutrality in Europe by 2050 [1]. Within this framework, the industrial sector, which is responsible for approximately 25% of the final primary energy consumption, must undergo a profound transformation, especially in how the heat is supplied to its processes. Indeed, while fossil-fuel boilers are the current reference technology, High Temperature Heat Pumps (HTHPs) are emerging as the next generation technology for heat supply decarbonization, especially in the low-to-medium temperature range (i.e. sink temperature below 200 °C) [2-3].

Recent reviews have established the thermodynamic potential of HTHPs related to the high energy performance, to the possible integration with renewable energy sources (HTHP has intrinsic capability of electrifying the supply of heat), and to the possibility of recovering and upgrading low temperature waste heat. Jiang et al. [4] highlighted the rapid progress of laboratory and industrial-scale applications, identifying low-

* Corresponding author. Tel.: +39-02-23993872
E-mail address: luca.molinaroli@polimi.it

GWP refrigerants and larger temperature lifts as central trends. Adamson et al. [5] further demonstrated that advances in transcritical and cascade cycles can extend operational boundaries and improve the COP through better process integration. From a techno-economic standpoint, Bergamini et al. [6] confirmed that vapor compression HTHPs can thermodynamically and economically compete with natural gas boilers, achieving high COPs and substantial primary energy savings, particularly when using natural refrigerants such as ammonia or water. Lastly, Bless et al. [7] found that the use of HTHPs to generate steam can lead to significant energy and greenhouse gas emission savings, especially when using electricity from a high penetration of renewables grid, as well as to be highly cost-competitive provided that a suitable heat source for waste heat recovery is available. Although there is a consensus regarding the potentially superior performance of HTHPs, the identification of general integration strategies remains limited. This is because several alternative configurations for integrating an HTHP into an industrial process exist, and the optimal scheme and operating conditions are strongly case-specific. Consequently, the most suitable integration scenario is determined through a detailed techno-economic analysis of the industrial process characteristics, including thermal demand profile, temperature requirements, and operational constraints [8].

The present paper contributes to this discussion by examining the integration of an HTHP into an amine regeneration process. Two different configurations of HTHP are considered and their potential benefits in terms of energy savings, economic performance, and CO_2 emission reduction are assessed. The analysis ultimately identifies the most advantageous solution able to fulfil the industrial process need as well as to deliver the greatest improvements with respect to a fossil fuel boiler, i.e, the reference heating technology.

2. Amine regeneration process description

The industrial process analysed in the present study is the regeneration process of an amine solution, a typical unitary process in the oil and gas industry in which amine is used as an acid gas (e.g., CO_2) removal from a process stream and is thermally regenerated in a stripper column via a reboiler heated by external steam. The plant configuration is shown in Fig. 1, where information about mass flow rate and temperature of the different streams is also available. For regeneration, the rich amine is heated up to 130 °C, and in the baseline configuration this is carried out using a stream of saturated steam at 313 kPa (saturation temperature equal to 135 °C) supplied by a 14 MW (useful thermal power) natural gas boiler. After regeneration, the lean amine flow leaves the regeneration column and passes first through a recuperative heat exchanger, that cools it down to 110 °C while preheating the rich amine, and then through a dry cooler that rejects heat to the environment allowing for further cooling the solvent before suppling it to the absorber (not shown).

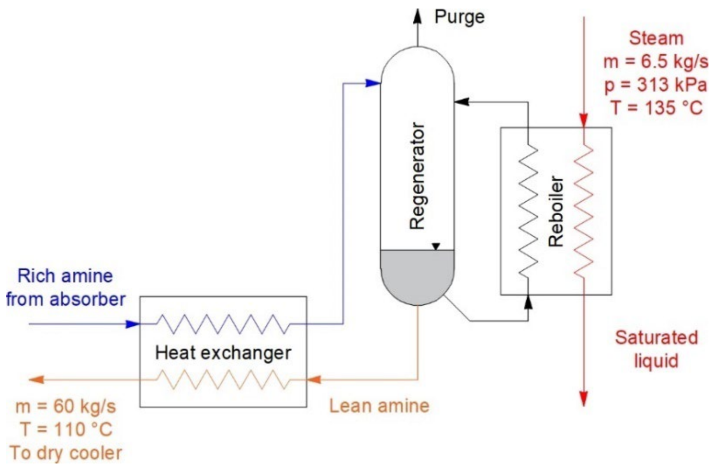

Figure 1. Scheme of the industrial process for which decarbonization of reboiler heat supply by HTHP has been analysed.

To integrate the high temperature heat pump, the lean amine stream leaving the recuperative heat exchanger is used as cold heat source, while for the hot heat sink two options are analysed, as shown in Fig. 2. In Scenario 01 (left), the heat pump is integrated to directly heat the amine flow, while in Scenario 02 (right) steam produced by the heat pump is used as heat carrier to regenerate the amine solution. It is worth mentioning that, as shown in Fig. 2, while in the first scenario the heat pump consists of a traditional vapour compression cycle, in the second scenario it consists of a vapour compression cycle coupled with steam compressor (in cascade, vapour compression cycle bottoming the steam compressor) since the steam is produced at 100 kPa in the condenser sink of the bottoming heat pump and is then compressed up to the delivery pressure with a two stage Mechanical Vapor Recompression configuration (featuring water injection after each stage to achieve greater efficiency). In this scenario, since saturated water at 100 kPa is needed at the inlet of the condenser, an additional heat exchanger coupling saturated water at the reboiler outlet and the rich amine at the regenerator inlet is used to improve the useful heat recovery in the process (liquid water is subcooled while the amine flow is further preheated). This additional heat recovery results in 910 kW reduction in the heat duty of the heat pump. Scenario 02 is more complex as it involves more equipment units, but it allows a better heat integration and takes advantages from the application of steam compression in the region above 100 °C.

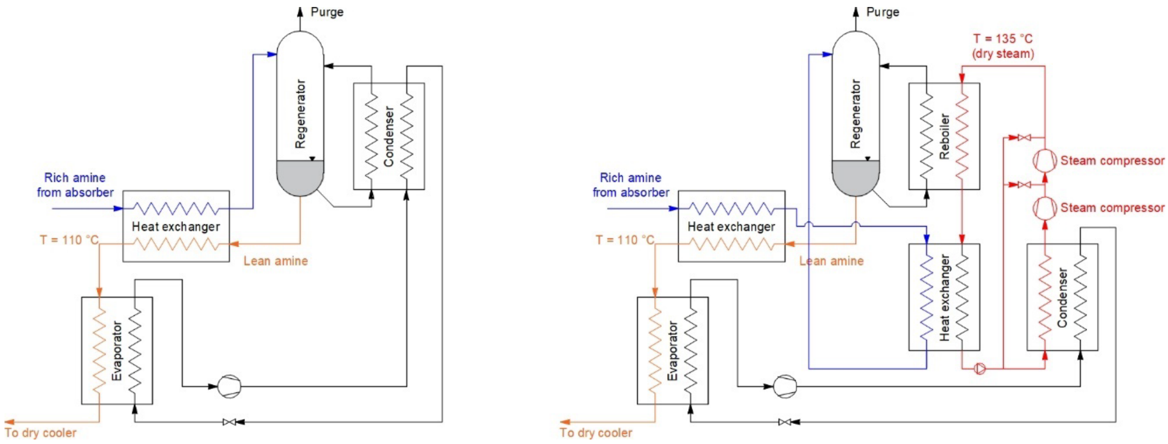

Figure 2 – Scenarios for HTHP integration: direct heat of amine flow (left, Scenario 01) and steam production (right, Scenario 02).

3. High temperature heat pump design

To design the HTHP to be integrated into the industrial process, a simulation framework inspired by Vieren et al. [8] is implemented in the Matlab 2024 environment [10]. The framework consists of a thermodynamic model of HTHP which is coupled to a global optimization routine. The thermodynamic model performs the thermodynamic design of the HTHP, i.e. it computes all the operational parameters for each working fluid (mass flow rate, pressure, temperature and enthalpy, while satisfying the first law balances) given the heating capacity, the working conditions of the evaporator (evaporating temperature, superheating, saturation temperature drop) and the working conditions of the condenser (condensing temperature, subcooling, saturation temperature drop). The thermophysical properties of each fluid are computed using Refprop 10.0 [11]. The optimization routine finds the HTHP design that maximizes the COP bounding the thermodynamic parameters within physically-based ranges (e.g. non-negative superheating, non-negative pressure drop, etc.) as well as constraining their final values so that a minimum pinch-point temperature difference is obtained in each heat exchanger, which is a simple way to consider the real-size effect without detailing the heat exchanger geometrical features. To this task, a global optimization routine such as the Particle Swarm Optimization algorithm is used to deal with possible local maxima. The heat pump technical assumptions, together with the solution-space of the abovementioned parameters, are reported in Table 1, where the pressure drop range is expressed as saturation temperature drop, i.e. the way typically used in vapour compression systems. It is worth specifying that the compressor efficiency is the global one, i.e. it accounts for the electro-mechanical efficiency of the heat pump motor.

Table 1. Solution space and constraints for the parameters of the optimization framework

Parameter	Range
T_{EVAP} [°C]	0 - 110
ΔT_{SH} [K]	0 - 100
Δp_{EVAP} [K]	0.5 - 5
T_{COND} [°C]	130 – (T_{CRIT}-1)
ΔT_{SC} [K]	0 - 100
Δp_{COND} [K]	0.5 - 5

Constraints / Assumptions	Value
η_{COMP} [-]	0.70
$\Delta T_{PP,EVAP}$ [K]	3
$\Delta T_{PP,COND}$ [K]	3
$\Delta T_{SAT,STEAM,COMP}$ [K]	< 20

Before optimizing the thermodynamic design of the HTHP, a refrigerant screening is carried out to select the working fluids that meet the following criteria:

- The critical temperature should be greater than 150 °C, i.e. 15 K higher than the temperature of the supplied steam in the baseline scenario, avoiding transcritical cycle arrangements and guaranteeing the refrigerant condensation. This is motivated considering that, depending on the scenario, the hot heat sink consists of amine or water streams undergoing evaporation, and, therefore, the temperature is nearly constant in the cold side of the condenser. Consequently, condensation should provide the best T-Q matching and the most thermodynamically favorable process.
- The working fluid saturation pressure at 50 °C should be higher than atmospheric pressure. This arises from the need to avoid sub-atmospheric operation in the evaporator, with 50 °C identified as a reasonable evaporation temperature based on preliminary calculation from T-Q profile of the lean amine stream supplying waste heat to the evaporator.
- Finally, to comply with current environmental standards and regulations, only refrigerants with ODP = 0 and GWP < 150 are considered.

Once the refrigerants are screened, the optimization routine is applied to identify, for each of them, the best HTHP design. The final results, for some of the most promising refrigerants, are summarized in Table 2, which reports the selected working fluid, the COP, the compression ratio, and the compressor discharge temperature of the best-performing heat pump for both scenarios. The final decision is a multi-objective evaluation that qualitatively considers not only the COP but also the practical feasibility of the heat pump, accounting for the need to split compression into multiple stages for high pressure ratios and avoiding excessively high compressor discharge temperatures that could be challenging for its safe operation and would have special requirements for lubricant oil and materials. Overall, R601 (pentane) is chosen as working fluid in both scenarios as it allows keeping the maximum temperature after the compressor below 180 °C with high COP.

Table 2. COP, pressure ratio and compressor discharge temperature of the optimal design of the HTHP for some selected refrigerants (7 out of 15 screened) in the two configurations considered.

Refrigerant	Scenario 01			Scenario 02		
	COP [-]	p_{RATIO} [-]	T_{DIS} [°C]	COP [-]	p_{RATIO} [-]	T_{DIS} [°C]
R1234ze(Z)	3.02	5.43	185.82	3.14	3.49	163.17
R600 (Butane)	3.00	4.65	173.64	3.16	3.12	154.47
R601b (N-pentane)	3.01	4.78	161.43	3.16	3.16	161.04
R1336mzz(Z)	3.12	6.62	167.79	3.22	4.05	150.16
R601a (Isopentane)	3.19	5.76	166.16	3.24	3.62	149.29
R601(Pentane)	3.23	6.29	168.50	3.25	3.85	151.01
Acetone	3.35	8.49	218.79	3.22	4.68	186.94

4. Energy, environmental and economic analysis

Finally, the energy, environmental and economic benefits arising from the integration of the HTHPs into the amine regeneration process are assessed comparing it to the baseline natural gas boiler figures of merit.

For each scenario, energy consumption, Scope 1 and Scope 2 CO_2 emissions as well as the CAPEX and OPEX are assessed. For the latter, the costs associated to O&M, to fuel or electricity consumption and the price of CO_2 emission allowances (equivalent to a carbon tax according to the EU emission trading system) are accounted for. The assumptions used to perform the energy analysis are: annual equivalent working hours equal to 8000 h/y; boiler efficiency equal to η_{BOILER} = 0.90; dry cooler electric power equal to 1% of heat rejected and primary energy conversion factor (Fuel/Electricity) equal to 2.5. Those used for the environmental analysis are: CO_2 emission factor equal to 0.280 t_{CO2}/MWh_{LHV} for boiler fuel and 0.744 t_{CO2}/MWh_{EL} for electricity. Finally, those used for the economic analysis are: CAPEX (total investment cost), specific to heat supplied equal to 52 €/kW for boiler and 200-600 €/kW for HTHP; yearly operation and maintenance cost (O&M cost) equal to 4% of CAPEX per year; OPEX specific costs equal to 35 €/MWh_{LHV} for fuel, 75 €/MWh_{EL} for electricity and 70 €/t_{CO2} for CO_2 emissions.

It should be noted that, with respect to the economic assessment, a precise value for the HTHP CAPEX is difficult to estimate when a conceptual or pre-feasibility study, such as the one done in this study, is performed. Therefore, a range of values is reported based on the cost range reported in the IEA Annex 58 report indicating, for this application, a heating-capacity-based specific investment cost between 200 €/kW and 600 €/kW [9].

The results are reported in Table 3 and show that, compared to the boiler, the adoption of HTHP leads to significant benefits from the energy, environmental and economic point of view in both scenarios, with an advantage for the HTHP configuration of Scenario 02. Overall, the reduction in primary energy consumption ranges from 31.6% to 36.6%, that in fossil CO_2 emissions ranges from 26.8% to 32.0% (but could be even more significant if a greater share of renewables is considered in the electricity mix to further reduce the CO_2 intensity of the grid, e.g. in Italy the average CO_2 emission factor is currently 0.270 t_{CO2}/MWh_{EL}), while the OPEX saving is within 2163k€/y to 2712 k€/y, resulting in discounted payback time between 0.87 years and 4.00 years, depending on the HTHP configuration and on the CAPEX. It should be noted that the reported result accounts only for the cost of the heat pump itself, without including expenditures associated with auxiliary components (balance of plant) or EPC services. In addition, the estimated payback period may differ substantially depending on the availability and nature of applicable financial support or incentive schemes.

Table 3. Results of the energy, environmental and economic analysis

Parameter	Scenario		
	Baseline	Scenario 01	Scenario 02
Energy analysis			
$\dot{Q}_{PROCESS}$ [kW]	14000 kW	14000 kW	13090 kW
$\dot{Q}_{BOILER}$ [kW_{LHV}]	15556	0	0
Electric Power (Heat pump) [kW]	0	4333	4023
Electric Power (Dry cooler) [kW]	116	37	34
Boiler primary energy consumption [MWh_{LHV}/y]	124444	0	0
Electric energy consumption [MWh_{EL}/y]	928	34961	32457
Annual primary energy saving [MWh/y]	0	39363 (31.6%)	45623 (36.6%)
Environmental analysis			
CO_2 emissions fuel[t_{CO2}/y]	34844	0	0
CO_2 emissions electricity [t_{CO2}/y]	691	26011	24148
Annual CO_2 emissions saving [t_{CO2}/y]	-	9524 (26.8%)	11387 (32.0%)
Economic analysis			
CAPEX [k€]	722	2800 - 8400	2618 - 7854
Annual O&M cost [k€/y]	28.89	112 - 336	104.72 - 314.16
Annual Fuel costs [k€/y]	4355.56	0	0
Annual Electricity costs [k€/y]	69.62	2622.10	2434.26
Annual CO_2 emissions ETS costs [k€/y]	2487.45	1820.77	1690.36
Total Annual OPEX [k€/y]	6914.52	4554.83 - 4778.83	4229.32 - 4438.76
Annual OPEX saving[k€/y]	-	2386.69 - 2162.69	2712.19 - 2502.75
Simplified payback time [y]	-	0.87 - 4.00	0.70 - 3.15

5. Conclusions

In the present study, the integration of HTHPs in an amine regeneration process is assessed. First, an heat integration analysis of the process is done to identify the stream to be used as heat source at the evaporator of the HTHP. Then, the cycle schemes are assessed resulting in two candidate configurations: the traditional vapour compression cycle, in which the condenser rejects heat directly to the amine flow, and the vapour compression cycle coupled with steam compressor, in which steam is produced and supplied to the process heat exchanger. Then, a numerical optimization framework allowing heat pump optimal thermodynamic design is developed and applied to the case study under analysis. A screening of the potential working fluids with specific constraints for the case study under analysis is carried out with the aim of limiting the number of refrigerants to be used in the heat pump. For both scenarios, the most performing HTHPs is chosen with a multicriteria approach identifying pentane as one of the best working fluids for this application. Finally, the energy, environmental and economic benefits arising from the HTHP integration into the process are assessed. The findings show saving of primary energy within 31.6% to 36.6%, of greenhouse gas emission within 26.8% to 32.0% and economic saving within 2162.69 k€/y to 2712.19 k€/y, leading to a simplified payback time between 0.87 years to 4 years, with better results for the configuration entailing steam compressor. Overall, the HTHP emerges as a key enabling technology for the transition toward more sustainable industrial thermal systems. It is worth noting that this work is representative of an industrial case study and, therefore, the findings are valid only under the context and techno-economic assumptions associated with it. Consequently, although the method employed for the analysis is of general validity and applicable to other industrial case studies, it is not possible to generalise the specific results to other scenarios without performing additional simulations requiring specific assumptions and inputs on a case-by-case basis.

Nomenclature

GWP	Global warming potential [-[
ODP	Ozone depletion potential [-]
T_{COND}	Condensing temperature [K]
T_{EVAP}	Evaporating temperature [K]
Δp_{COND}	Saturation temperature drop due to pressure drop in the condenser [K]
Δp_{EVAP}	Saturation temperature drop due to pressure drop in the evaporator [K]
$\Delta T_{PP,COND}$	Pinch point temperature difference in the condenser [K]
$\Delta T_{PP,EVAP}$	Pinch point temperature difference in the evaporator [K]
$\Delta T_{SAT,STEAM,COMP}$	Saturation temperature increase in the steam compressor [K]
ΔT_{SC}	Subcooling temperature difference [K]
ΔT_{SH}	Superheating temperature difference [K]
η_{COMP}	Global efficiency of the compressor [-]

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