The 6th International Supercritical CO_2 Power Cycles Symposium
March 27 - 29, 2018, Pittsburgh, Pennsylvania

Design of SC-CO_2 Brayton cycles using MINLP optimization within a commercial simulator

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ABSTRACT

The off-design modeling, simulation and optimization have been served as an important and effective tool in the SC-CO_2 Brayton cycle technology assessment. Cycle layout improvement has been noticed as a potential solution to increase the Brayton cycle efficiency, yet no quantified comparison has been carried out to explain which configuration is more promising since each of them has been assessed in different conditions and hypothesis.

The purpose of this study is to provide an easily handled methodology of optimization where a large quantity of Brayton cycle layouts are reviewed and automatically optimized. In this paper, the notion of superstructure is introduced and calculations are performed in the commercial simulator ProsimPlus. All equipment that can be potentially selected as well as their interconnections are represented in the superstructure.

The optimizer MIDACO (Mixed Integer Distributed Ant Colony Optimization) applied in this paper not only enables the optimization of conventional continuous process parameters but also the flowsheet topology. By formulating this problem as the Mixed Non-Linear programming (MINLP) optimization, a global optimal layout of SC-CO_2 Brayton cycle along with optimized process specifications have been found for the two superstructures studied.

INTRODUCTION

Supercritical CO_2 (SC-CO_2) Brayton cycles have emerged as a promising solution to achieve high efficiency in a variety of applications operating with different temperature levels: fossil-thermal, nuclear and solar-thermal applications [1-4]. Numbers of projects are currently under development worldwide in order to explore both its fundamental aspects as well as some technical limitations emerging from the crucial components such as turbo-machinery and heat exchanger [5].

Optimization is one of the key features which guarantees the future practical deployment of innovative technology. It highlights the potential of technologies and can also guide further improvements in practical operation. Current studies of SC-CO_2 Brayton cycle have been devoted to maximize the cycle efficiency by using parametric optimization where the decision variables are continuous process parameters (temperature, flowrates, pressures, etc.) and the flowsheet topology (cycle layout) has always been kept fixed [1, 6].

However, cycle layout improvement is also a potential strategy to increase Brayton cycle efficiency. Defining an optimal-synthesis task is thus necessary to search for a competitive layout among many different cycle layouts or even explore new layouts. In another word, the configuration of SC-CO_2 Brayton cycle needs to be optimized and this task encompasses the selection of the technical components as well as their interconnections. More precisely, according to Floudas [7], the optimization-based process synthesis approach consists of introducing a superstructure in which all equipment that can be potentially selected (in the final flowsheet) are available as well as equipment interconnections.
In this work, a superstructure optimization of a SC-CO_2 Brayton cycle is brought out. The modelling and optimization environment used in this paper is the commercial process simulator (ProsimPlus) interfaced with a metaheuristic optimizer (MIDACO). The process layouts are addressed as integer variables and the conventional process parameters (temperature, pressure etc.) are treated as continuous variables. The simultaneous optimization of both types of variables is classed as a mixed-integer nonlinear programming (MINLP) problem [7].

The main advantage of the proposed strategy is that the superstructure can be graphically represented in the simulator meaning that the optimization problem can be easily adapted if additional constraints (e.g., new restriction on some variables, or new cost function developed) need to be added.
This paper is structured as follows: first the main modeling strategy and the formulation of the synthesis problem are introduced. The second part provides the results of applied methodology in superstructure Brayton cycle application where two superstructures are constructed and optimized.

METHODOLOGY

The aim of this work is to propose a methodology for a MINLP superstructure optimization of SC-CO_2 Brayton cycle. A commercial process simulator (ProSimPlus) coupled with an optimizer (MIDACO) enables practitioners to optimize any superstructure with personalized conditions.
The process synthesis performed in this paper can be described as two main levels. Firstly, the superstructure modeling with interconnection identification is carried out. Then by employing an external optimizer MIDACO linked with the process simulator ProSimPlus, both continuous (e.g. process specifications) variables and discrete integer variables (decision variables) are optimized.

1. Superstructure modeling

The MINLP superstructure optimization firstly requires to postulate a set of process alternatives, represented by a superstructure [7-8]. The development of a superstructure depicting a SC-CO_2 Brayton cycle integrates alternative collection, insight-based synthesis and combinatorial synthesis approaches [9]. The first two methods consist in listing the known processing Brayton cycle configurations based on previous experiences and in using engineering insights to include new solutions and exclude infeasible or not-convenient alternatives. The combination of different switches (multipath logical switches denoted SW) permits to enlarge the searching space (beyond usual configurations), which may include innovative design

solutions.
Furthermore, the process simulator environment enables practitioners to choose any component available in the simulator during the superstructure generation. As for the thermodynamic package, the accurate Span-Wagner equation of state has been chosen in ProSimPlus simulator to predict the properties of pure CO_2 [10]. This step of modeling is guaranteed by ProSimPlus that can be interfaced with Refprop [11].

2. Optimization strategy

a. Master interface ProsimPlus

The predefined communication interface implemented in ProSimPlus makes possible to select external optimizers. The communication between simulator and optimizer is guaranteed by an external dynamic library (.dll) which is linked with the external algorithm along with a wrapper generated by ProSimPlus.
Once established, the link permits the external optimizer to receive automatically the value of the objective function as well as constraints generated by the simulation loop. Then the latter calculates the new values of the continuous and integer variables to be optimized, Figure 1.

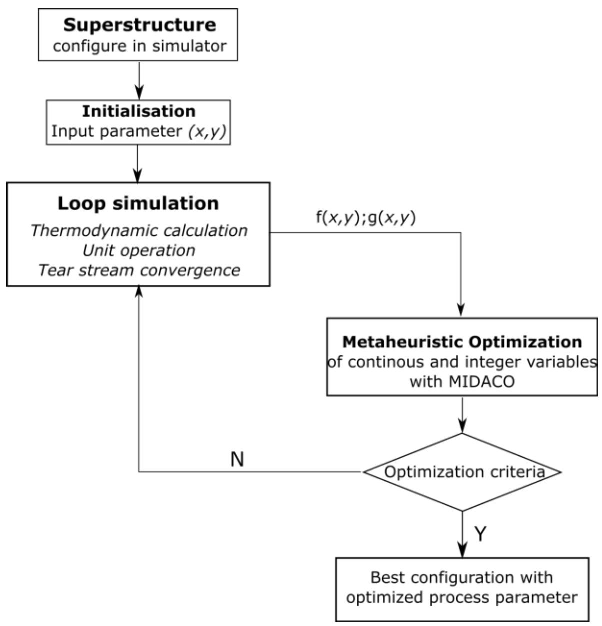


Figure 1 Block diagram

b. Metaheursitic optimizer MIDACO

The motivations of using the metaheuristic optimizer MIDACO developed by Schüler et al. [12], are its black-box and stochastic probabilistic nature. The first property allows to optimize non-convex MINLP problem without explicit expression of the objective and constraint functions. Furthermore, the search for the optimal solution also relies on several points simultaneously and the results are not initialization dependent. Secondly, the stochastic nature of the metaheuristic optimizer makes it possible to selectively search a much smaller fraction of the solution space and thus to reduce the computational time efforts [9, 12].

c. Specification

Table 1 *Hypothesis and Values of fixed process variables used in the MINLP optimization*

Hypothesis and Equipment data	
Tit turbine inlet temperature (K)	893.15
Tit turbine inlet temperature after reheating (K)	893.15
Tpinch (K)	≥10
Turbine isentropic efficiency	0.9
Compressor isentropic efficiency	0.89
Pressure drop in every component (% of inlet pressure)	1
Bounds of variables	
Minimal stream temperature (K)	304.35
Maximal stream temperature (K)	893.15
Minimal component inlet pressure (MPa)	3.3
Maximal component outlet pressure (MPa)	30

Optimal design of the SC-CO_2 Brayton cycle implies the determination of numerous variables among continuous and integers, such as equipment temperature, pressure, existence of recuperators and interconnection flows. Other variables are classified as fixed and calculated variables and are associated with hypotheses imposed by the modeler, Table 1. The calculated variables are process variables estimable from the application of mass and energy balances on process units, once specified or determined values of fixed and optimized variables [10]. For example, the last turbine outlet pressure can be deduced from the Brayton cycle inlet pressure and all the pressure losses. Meanwhile, for the different mixers, it is also suggested to consider sometimes that the two streams have the same pressure before entering the mixers. The specification of these variables involves logical rules since their values vary with the process layout (i.e. are dependent on integer variables). Such a method is simple to apply, yet it reduces the number of variables and constraints associated.

d. Objective function

In this study, the cycle efficiency is seen as an indicator of the energy performance:

$$\eta = \text{Cycle efficiency (\%)} = \frac{\text{TurbinePower(MW)} - \text{Compressorwork(MW)}}{\text{Thermal flux of HeatSource(MW)}} \times 100 \qquad [1]$$

An optimal design matches an energy system that produces electricity with a cycle efficiency as high as possible. The superstructure optimization problem is then expressed as:

$$\begin{gathered} Min\ \varphi\,(x, y) = -\eta\ \ (x \in R^{\,n_{con}}, y \in Z^{n_{int}}) \qquad [2] \\ s.t.\, h(x) = 0 \\ g(x) \geq 0 \\ x_{min} \leq x \leq x_{max} \\ y_{min} \leq y \leq y_{max} \end{gathered}$$

where h(x) is the vector of equality constraints and g(x) represents the vector of inequality constraints.

x are continuous optimized variables (operational temperature and/or pressure in key features) and y are integer optimized variables (logical switches of different levels).

RESULTS AND DISCUSSION

1. Superstructure I for SC-CO_2 Brayton cycle

A first superstructure (SS1) is constructed as an illustration the methodology. The relevance of superstructure SS1 that models a SC-CO_2 Brayton cycle (*Figure 2*) can be illustrated by the possible topology changes in: heat source & electricity production part and heat integration part. Three path switches are involved. From left to right, the first logical switch *SW1* alternates between a Brayton cycle with and without reheating. The second and third switches *SW2 and SW3* determine the existence of an extra heat recuperator meanwhile they select the flow that will be heated in this recuperator.

The 8 (=2^3) structural alternatives included in this first superstructure could not seem very sophisticated but they involve 10 variables (including 3 integer variable y_1, y_2, y_3) to be optimized in this non-convex MINLP problem. Inequality constraints are also considered for the minimal pinch in each recuperator (R1, R2).

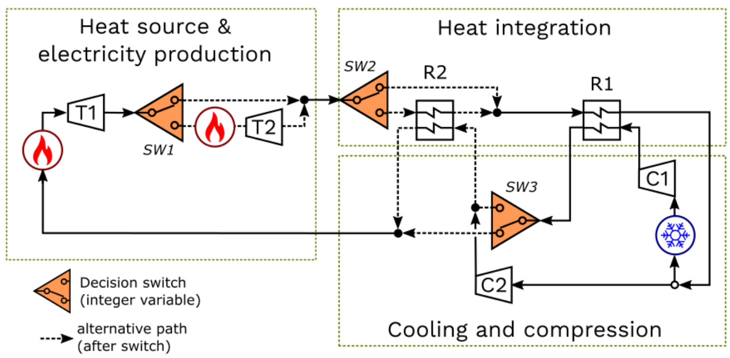


Figure 2 Superstructure I for SC-CO_2 Brayton cycle (2^3=8 structural alternatives)

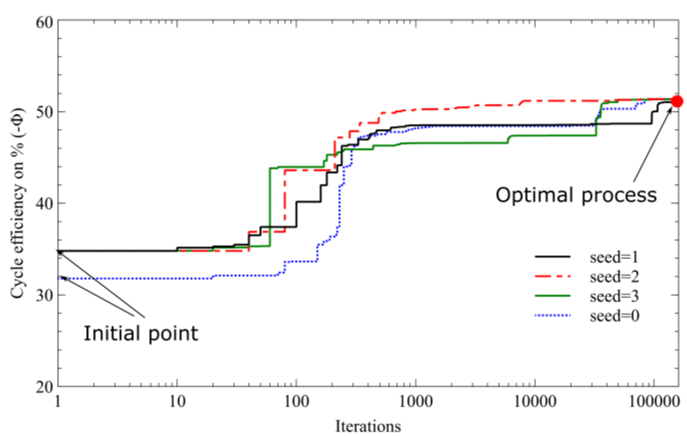


Figure 3 Optimization progress of four runs with different random seeds, for SS1

Four different optimization runs were carried out using four different pseudo random numbers (seed) in MIDACO, Figure 3. Note that each random seed leads to a different profile of optimization and let the optimizer generating and evaluating different populations.

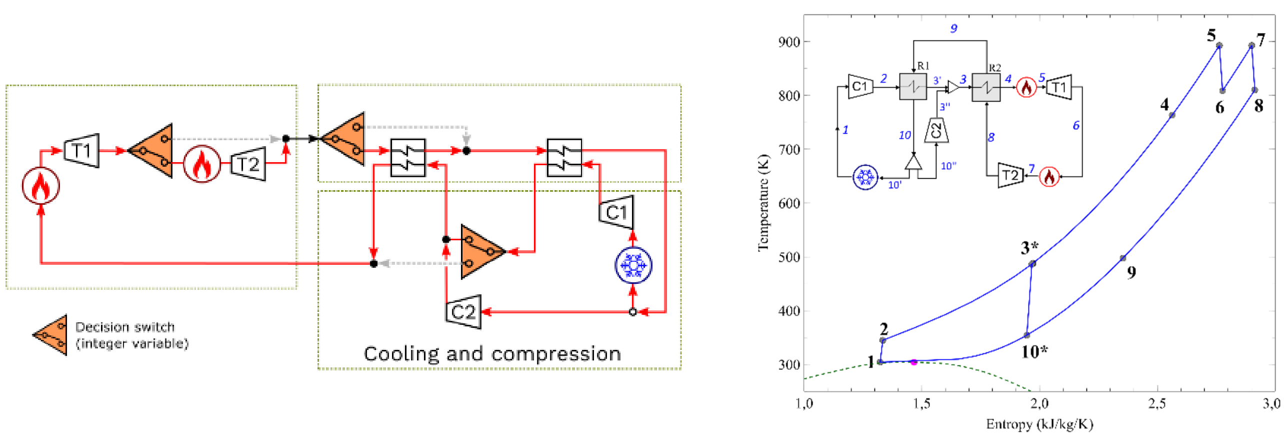
Moreover, after 6 hours of calculation (generation up to 160,000 generations), the structural and design result of the best individual is identical (i.e., identical set of [x,y] shows in Table 2), which also confirms that this layout is the best known solution for the defined optimization problem.

It has also been noted that some seeds have evolved more quickly towards better individuals than the others. For instance when seed 2 and seed 3 are selected, optimization ends after about 75, 000 iterations, which halved the entire evaluation time. It is thus recommended to launch several seeds for an optimization problem.

Table 2 Results for superstructure optimization SS1 of SC-CO_2 Brayton cycle

Results	Variable range	
Objective function (%)		51.38
Integer variables		{1; 1; 1}
P_{in} compressor (MPa)	$x_1 \in [3.3 - 10]$	7.50
$T_{cooling}$ (K)	$x_2 \in [304.35 - 373.15\,]$	304.35
Flow to Recompression (%)	$x_3 \in [10^{-5} - 0.5]$	0.34
P_{out} compressor (MPa)	$x_4 \in [3.3 - 30]$	30.00
Ratio main turbine (-)	$x_6 \in [1 - 5]$	1.92
T_{R1} cold side out (K)	$x_5 \in [304.35 - 893.15\,]$	495.03
T_{R2} hot side out (K)	$x_7 \in [304.35 - 893.15\,]$	504.56
Constraints (all respected)		
g_1, ΔT on R1 hot end (K)	≥ 10	
g_2, ΔT on R1 cold end (K)	≥ 10	
g_3 , ΔT on R2 cold end (K)	≥ 10	
g_4 , ΔT on R2 hot end (K)	≥ 10	
g_5 , ratio of main compressor (-)	≥ 1	

For the continuous process variables such as main cooling temperature ($T_{cooling}$) and the outlet compressor pressure (P_{out} compressor), their optimal value reaches respectively the lower and upper bound stipulated in this study. Table 2 indicates that at the optimum, the cooling temperature tends to 304.35 K while the optimal compressor outlet pressure reaches 30 MPa. This trend is rather logical the higher the average temperature of heat absorption and the lower the average temperature of heat release, the greater the cycle efficiency can be achieved.



a) optimal configuration y=[1,1,1]

b) Temperature-entropy diagram

Figure 4 Process synthesis result: optimal flowsheet for the SC-CO_2 Brayton cycle

The optimal process layout with cycle net efficiency as high as 51.4 % is composed of two compressors, two recuperators, and one reheat (thus two turbines), Figure 4(a). Compared with the initial proposal of SC-

CO_2 Brayton cycle by Feher and Angelino, [13] and [14], the optimal process configuration has an enforced heat integration. Figure 4(b) indicates that all the exchangers have reached a minimal accepted thermal pinch (10 ± 0.5 K on their hot end). It can be concluded that the efficiency can be further improved by relaxing the constraint on minimal pinch. Furthermore, entropy loss is avoided at mixer since stream 3' and 3'' have the identical temperature and pressure (iso-entropy) before mixing.

2. Superstructure II for SC-CO_2 Brayton cycle in pulverized coal-fired power plant application

While in the first superstructure SS1, the heat source serves only for heat addition at a constant temperature, in the case of a pulverized coal-fired power plant, the flue gas leaving the boiler can preheat a fraction of cold SC-CO2 at high pressure [6]. This consideration is compulsory for a state of art boiler design to reduce the flue gas temperature (to around 110°C) before emission to the atmosphere.

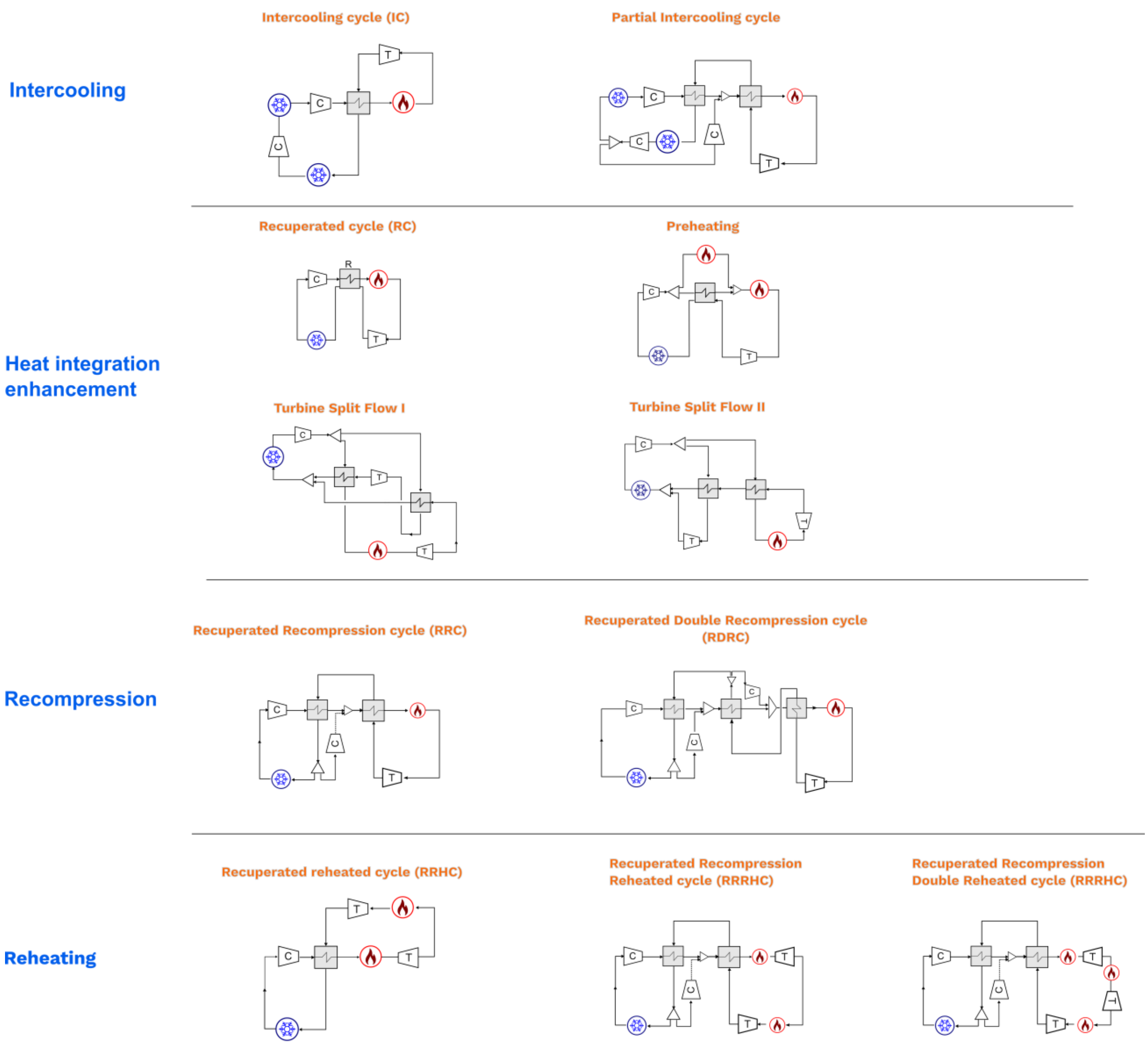


Figure 5 Extraction of interesting configuration from literature [6] and [15]

A second superstructure (SS2) was constructed in order to possibly include this SC-CO2 preheating section as mentioned in the study of Mecheri and LeMoullec [6], Figure 5 (Preheating). It has been illustrated that as for the coal-fired power application, the flue gas temperature could get up to over 530-550 °C. Adding a split of CO_2 preheated by the flue gas could help to recover this unexploited energy [6].

Another particularity of this superstructure is to take into account, as much as possible, the known configurations of a SC-CO_2 Brayton cycle. In a review conducted by Crespi et al. [15] concerning SC-CO_2 Brayton cycle, a list of 42 different stand-alone Brayton cycle configurations is proposed. The construction of this second superstructure (SS2) has taken 11 of them into account, listed in Figure 5.

Together with the combination of logical switches and flow splitters, SS2 represents over 1000 layouts of SC-CO_2 Brayton cycle at once. This large searching space will lead to an advanced process structural optimization with a global view and some innovative design solutions may occur.

The energy efficiency is considered as the objective function and a total of 21 variables are optimized among which 5 are discrete integer variables (note that there are switches of multi-level). One equality constraint along with 7 inequality constraints have also been considered, Table 3.

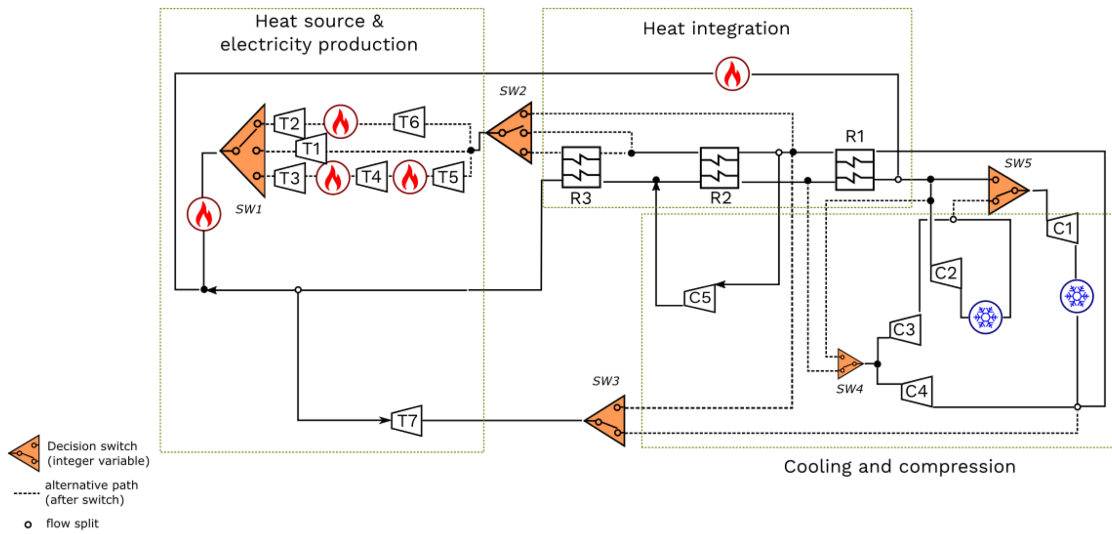


Figure 6 Superstructure II for SC-CO_2 Brayton cycle ($2^7 * 3^2 = 1152$ structural alternatives)

Table 3 List of optimized variables and their bounds considered in SS2

Optimized continuous variables x	Bounds
P_{in} compressor C1 (MPa)	$x_1 \in 3.3 - 10$
$T_{cooling}$(K)	$x_2 \in 304.35 - 373.15$
Flow to Recompression C4 (%)	$x_3 \in 10^{-6} - 0.5$
P_{out} compressor C1 (MPa)	$x_4 \in 3.3 - 30$
Flow to recompression C3 (%)	$x_5 \in 10^{-6} - 0.5$
P_{out} compressor C2/MPa	$x_6 \in 3.3 - 30$
T_{R1}cold side out (K)	$x_7 \in 304.35 - 893.15$
Flow to recompression C5 (%)	$x_8 \in 10^{-6} - 0.5$
T_{R2} hot side out (K)	$x_9 \in 304.35 - 893.15$
T_{R3} hot side out (K)	$x_{10} \in 304.35 - 893.15$
P_{out} compressor C5/MPa	$x_{11} \in 3.3 - 30$
Ratio turbine T2 (-)	$x_{12} \in 1 - 5$
Ratio turbine T3 (-)	$x_{13} \in 1 - 5$
Ratio turbine T4 (-)	$x_{14} \in 1 - 5$
(1-Flow Split to T7)/%	$x_{15} \in 10^{-6} - 0.5$
Flow split to flue gas economizer (%)	$x_{16} \in 10^{-6} - 0.5$
Optimized integer variables y	
SW1	$y_1 \in \{1, 2, 3\}$
SW2	$y_2 \in \{1, 2, 3\}$
SW3	$y_3 \in \{1, 2\}$
SW4	$y_4 \in \{1, 2\}$
SW5	$y_5 \in \{1, 2\}$

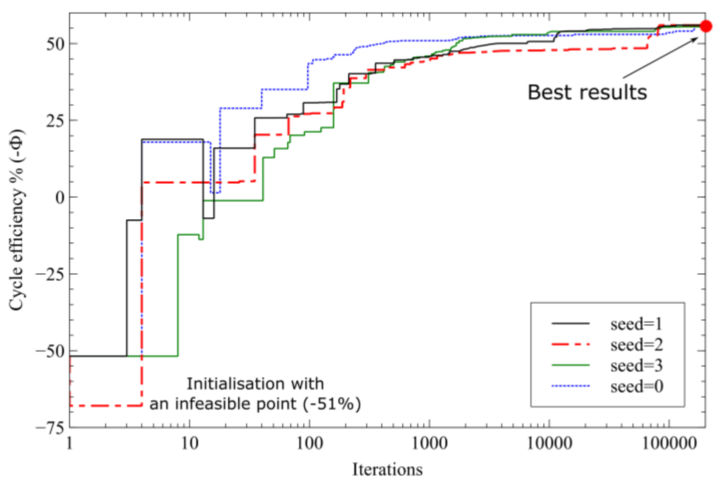


Figure 7 Optimization progress of four runs with different random seeds, for SS2

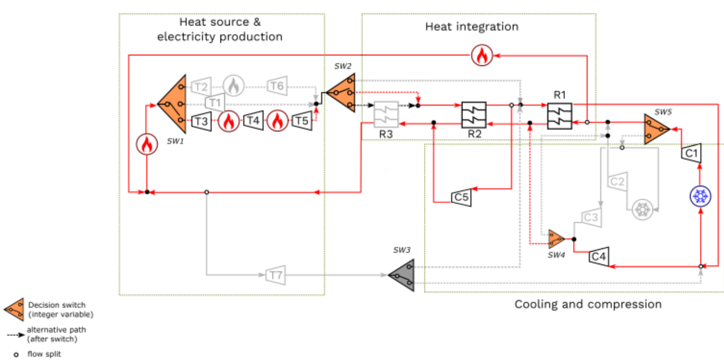
After 60 hours of calculation (up to 200,000 iterations), 4 optimizations with different seeds are completed. Two promising structural result are achieved: y= {3 2 1 1 1} which reaches a net efficiency of 55.58% (Figure 8 c); and y= {1 2 1 1 1} which has a cycle efficiency of 55.99% (Figure 8 a).

Table 4 Results for superstructure optimization SS2 of SC-CO_2 Brayton cycle

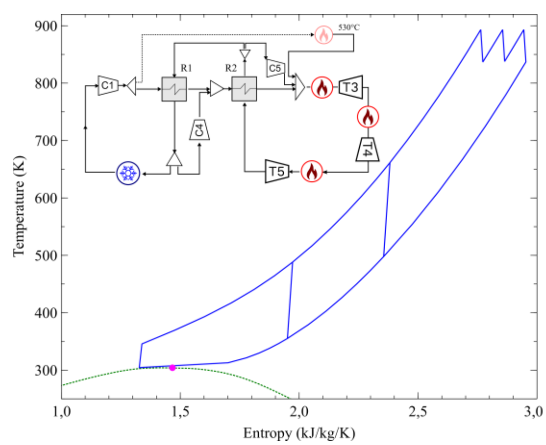
Results	Variable range	Case I	Case II
Objective function (%)		55.99%	55.57%
Integer variables	$\{y_1\ y_2\ y_3\ y_4\ y_5\}$	{1 2 1 1 1}	{3 2 1 1 1}
Pin (C1)/ MPa	$x_1 \in [3.3 - 10]$	7.60	7.62
Tcooling /°C	$x_2 \in [304.35 - 373.15\ ]$	304.35	304.35
Flow to recompression C4/%	$x_3 \in [10^{-5} - 0.5]$	0.30	0.30
P_{out} compressor C1/ MPa	$x_4 \in [3.3 - 30]$	30.00	29.92

Flow to recompression C3/%	$x_5 \in [10^{-5} - 0.5]$	-	-
P_{out} compressor C2/MPa	$x_6 \in [3.3 - 30]$	-	-
T_{R1} cold side out (K)	$x_7 \in [304.35 - 893.15\,]$	486.69	486.22
Flow to recompression C5/%	$x_8 \in [10^{-5} - 0.5]$	0.077	0.084
T_{R2} hot side out (K)	$x_9 \in [304.35 - 893.15\,]$	496.25	495.92
T_{R3} hot side out	$x_{10} \in [304.35 - 893.15\,]$	877.95	883.20
Pout C5/MPa	$x_{11} \in [3.3 - 30]$	3.79	3.77
Turbine ratio T2/(-)	$x_{12} \in [1 - 5]$	-	1.84176
Turbine ratio T3 (reheating)/(-)	$x_{13} \in [1 - 5]$	1.53	-
Turbine ratio T4 (reheating)/ (-)	$x_{14} \in [1 - 5]$	1.53	-
(1-Split to T7)/%	$x_{15} \in [10^{-5} - 0.5]$	10^{-5}	10^{-5}
Flow of CO2 pass to flue gas exchanger%	$[10^{-5} - 0.5]$	5.04	5.33
Constraints (all respected)			
g_1, ΔT on R1 hot end (K)		≥ 10	≥ 10
g_2, ΔT on R1 cold end (K)		≥ 10	≥ 10
g_3, ΔT on R2 cold end (K)		≥ 10	≥ 10
g_4, ΔT on R2 hot end (K)		≥ 10	≥ 10
g_5, ΔT R3 hot end (K)		≥ 10	≥ 10
g_6 on ratio of main compressor (-)		≥ 1	≥ 1
g_7 on flue gas g_8 $Q_{flue\ gas}$=9% of Q_{boiler} (equality constraint)		$\leq 1e^{-5}$	$\leq 1e^{-5}$

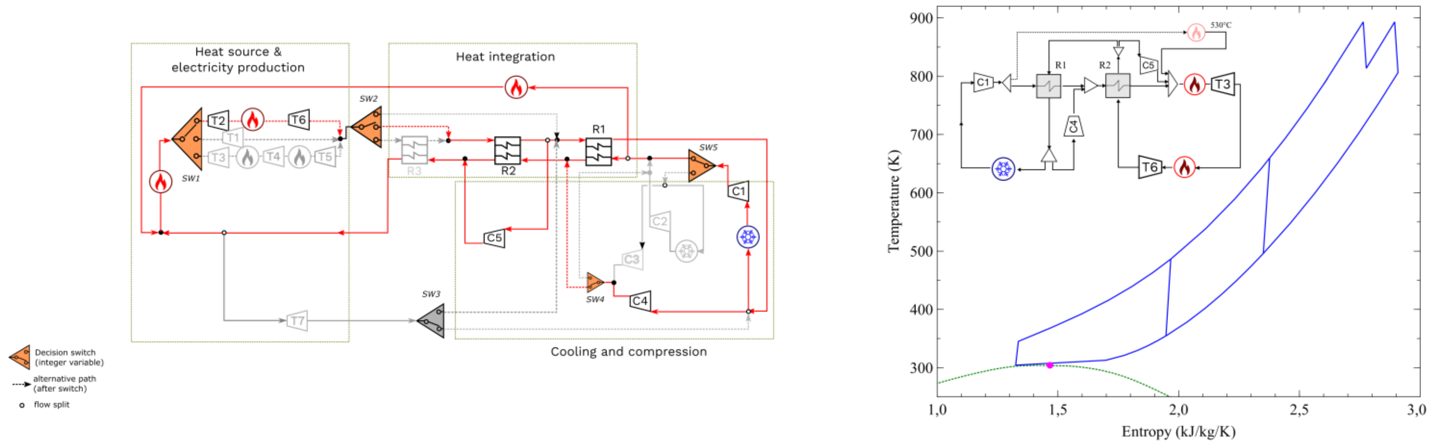
Table 4 lists the optimal process conditions of the best two configurations. It has been noticed that both configurations have similar key feature conditions though an additional reheating exists in the Case I. In the further techno-economic study, the removal of this extra turbine is expected.



a) optimal configuration y={12111}



b) Temperature-entropy diagram



c) optimal configuration y={32111}

d) Temperature-entropy diagram

Figure 8 *Process synthesis result: optimal flowsheet for the SC-CO_2 Brayton cycle*

It has been noticed that for the hypothesis considered (Table 1), the intercooling or partial intercooling (C2 and C2) are not recommended by optimization. This result is consistent with the study of Bennett et al. [16], where they demonstrated that the configuration without intercooling was more advantageous when the compressor inlet temperature was rather low (less than 50°C). In this study, the result is automatically retrieved.

CONCLUSION

In this work, the optimization of a superstructure that depicts a SC-CO_2 Brayton cycle has been presented. This approach makes it possible to systematically study numerous configurations under the same modelling environment and hypotheses. This paper illustrates how the simulator enables to manage the entire Mixed Non Linear Programming (MINLP) optimization, where the optimizer MIDACO searches simultaneously both continuous variables (process variables) and the discrete integer variables (process layout).
This study highlighted that the commercial process simulator ProSimPlus was very flexible and useable in many other applications since any unit operation that is available in the simulator can be used to design the superstructure. In a sensitivity study, the lower and upper bound of each variable can be easily adapted depending on the expressed design hypotheses.
It has been noticed that in the case of SS2, it is nearly impossible to find manually any feasible condition for both simulation and optimization. The proposed methodology can be thus seen as an automatic tool in technology evaluation.

For the two studied superstructures, the obtained results on the SC-CO_2 Brayton cycle are the best known optimal designs. As for a simple Brayton cycle superstructure design, the configuration of recuperated recompression Brayton cycle achieves an efficiency of 51.4 %. The superstructure SS2 enables to review larger amount of cycle configuration, where the best cycle efficiencies rise up to 56.0% and 55.6%. The most promising Brayton cycle has been found to be a double recompression-preheating-reheating layout. However, given that the preheating might be difficult when other heat sources are applied, additional optimization shows that SS2 without preheating (under the some optimization condition) can reach a cycle efficiency of 52.1%.
Furthermore, the decision making of practical systems requires the knowledge of LCOE (levelized cost of electricity), the established techno-economic cost functions are currently being taken into account. This study is expected to show the compromise between economic and energy efficient, which would lead to different promising SC-CO2 Brayton cycle configurations.

ACKNOWLEDGEMENTS

Authors would like to thank Prosim Company for their advice and technical support. They have contributed in the reversal communication establishment between ProSimPlus and external solver MIDACO.

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