

**PROBABILISTIC TECHNIQUE FOR SOLVING COMPUTATIONAL PROBLEM:
APPLICATION OF ANT COLONY OPTIMIZATION (ACO) TO FIND THE BEST
SUPERCRITICAL CO₂ (sCO₂) BRAYTON CYCLE CONFIGURATION**

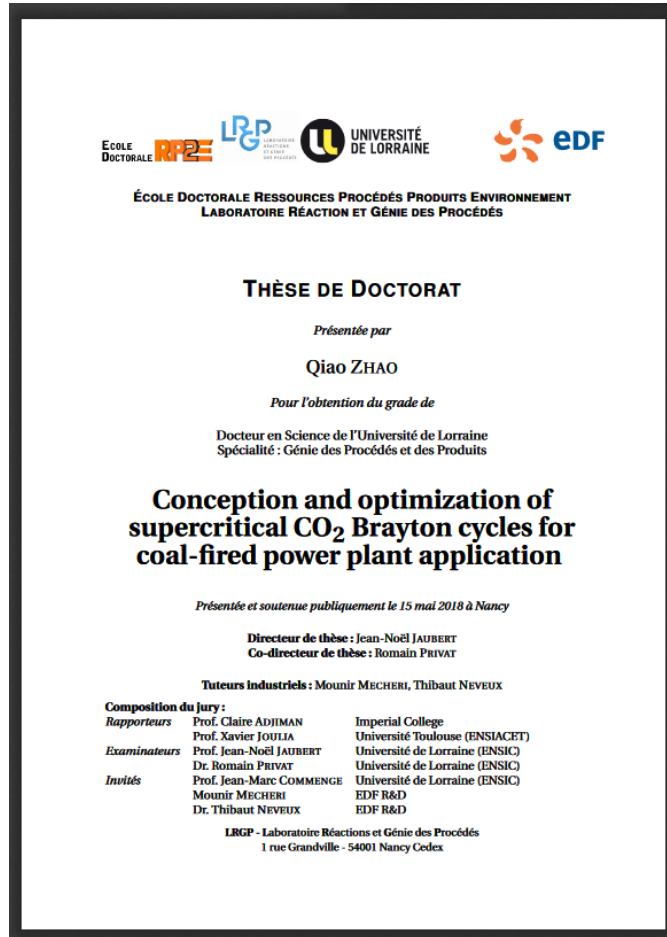
2019-sCO2.eu-147



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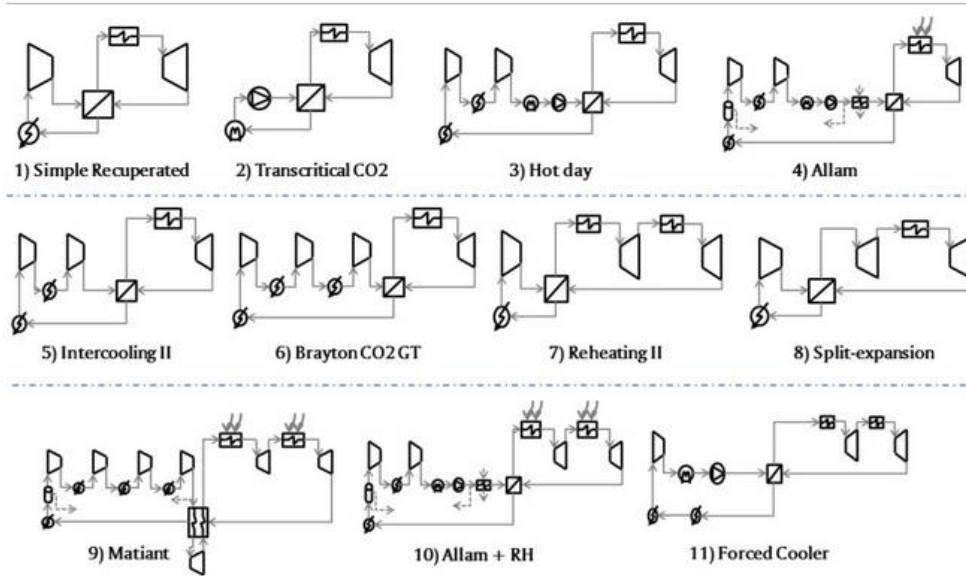
The results of this study are extracted from the PhD performed by Qiao ZHAO (EDF & LRGP) from 2015 to 2018

http://docnum.univ-lorraine.fr/public/DDOC_T_2018_0080_ZHAO.pdf

Outline

1. Introduction and context
2. Objectives
3. Methodology
4. Results
5. Conclusions and Perspectives

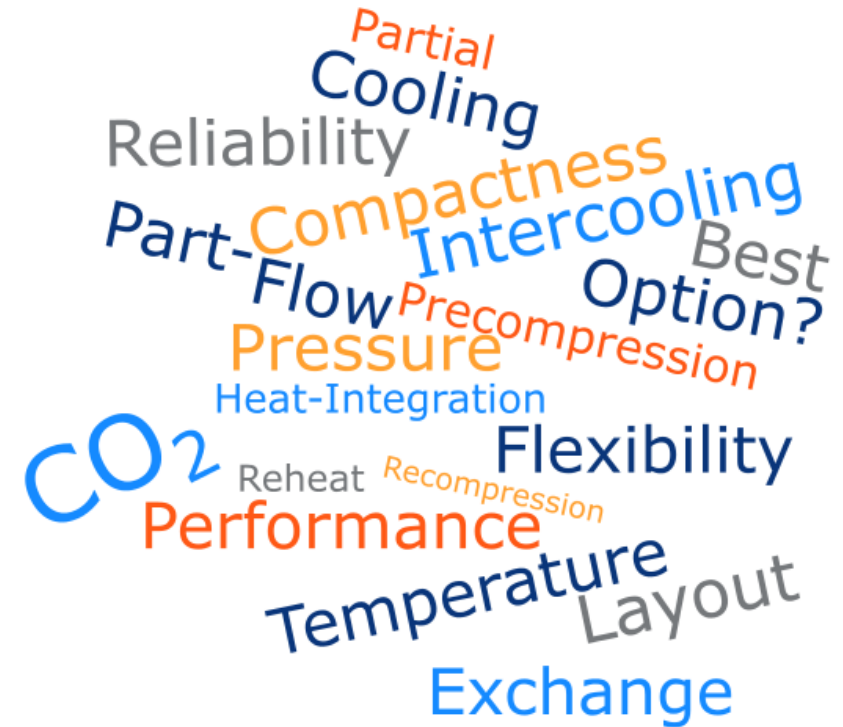
Many many cycle configurations [5] ...



Source : [Crespi et al. 2017](#)

...and many parameters :

Max./min temperature and pressure, number of reheat, intercooling, part-flow ratios...



?

Sensitivity analysis:



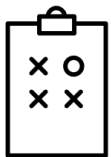
Step by step "hand" calculations/runs



Non-automatic cycle layout modification

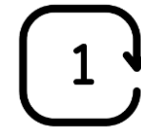


Manpower time consumption

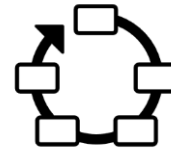


Low number of studied cases
(risk of missing optimal solution)

Computational optimization:



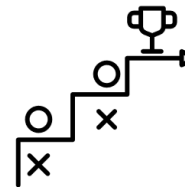
One initial interaction (setting and rules)



Automatic cycle layout modification and simulation runs



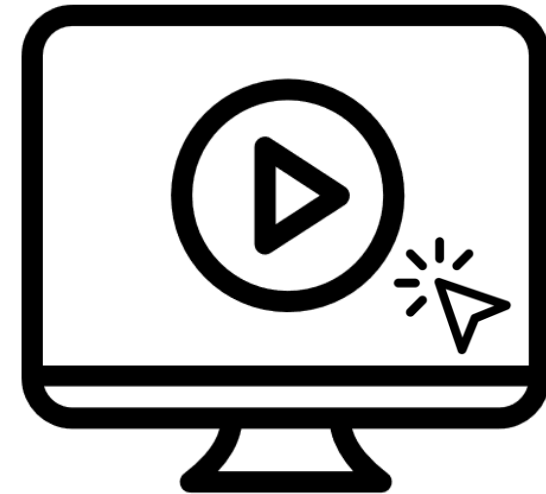
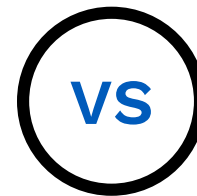
Computer time consumption



Computer pre-selection of best cases
among high number of possibilities

Introduction and Context

Code approach VS Commercial existing software



- ✓ Very specific to a given problem and methodology (accurate and refined)

- ✓ Existing tools and data
- ✓ No need for code skills

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Objectives of the PhD performed by Qiao ZHAO, 2015-2018 [4]:

- ✓ Check the best thermodynamic model for modeling CO₂, particularly near the critical point (comparison with available experimental data)
- ✓ Model and optimize a simple sCO₂ Brayton cycle layout
- ✓ Create and optimize a superstructure using both “commercial process software” and “solver”
- ✓ Perform a multi-objective optimization : energy & economic optimization



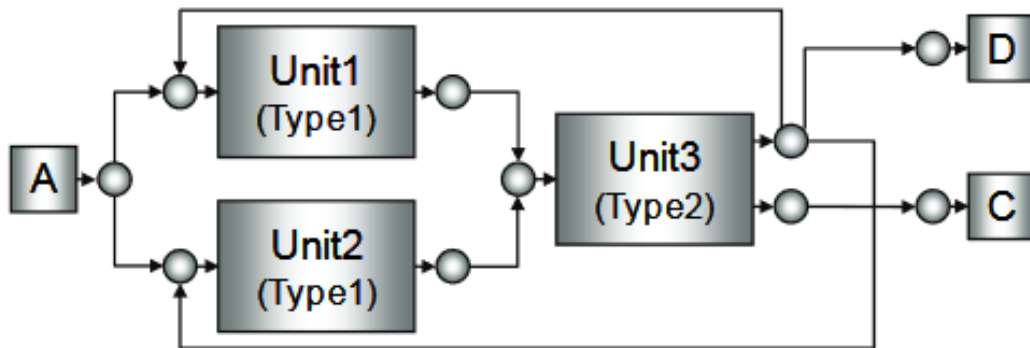
Objectives of this paper:

- ✓ Explain the global methodology used in the PhD (superstructure, optimization routine,...)
- ✓ Give the main assumptions and parameters of the study
- ✓ Share the main results and lessons learned
- ✓ Outline the perspectives

Outline

1. Introduction and context
2. Objectives
3. **Methodology**
 - Concept of Superstructures
 - Non-Linear optimization (definitions, optimization parameters and details)
 - Optimization routine
 - Problem definition and studied cases
4. Results
5. Conclusions and Perspectives

How to enable automatic switch between cycle architecture ?



The superstructure can easily be created in the Process Simulation Software, by using "split" modules (concept of "switch")

Strongly non-linear problem



Optimization parameters: seed concept, objective function,

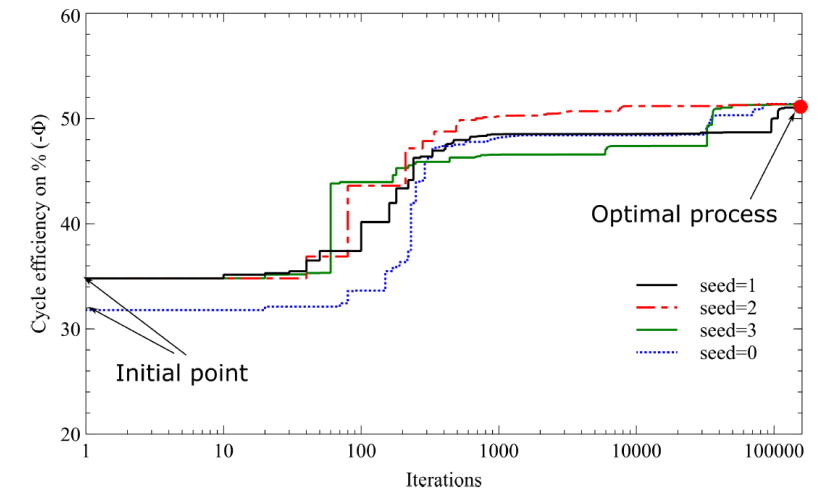
- ❑ **Non-linear problem** → can't be solved with classic/basic optimization methods (like gradient...)
 - Mixed Integer NonLinear Programming (MINLP) approach combined with meta-heuristic optimization technique : Mixed Integer Ant Colony Optimization (MIDACO) solver

MIDACO® solver

- ✓ Probabilistic technique
- ✓ Can be applied to continuous (NLP), discrete/integer (IP) and mixed integer (MINLP) problems...
- ✓ Single or Multi-objective optimization
- ✓ Suitable for equality or inequality constraints

Seed concept (randomness)

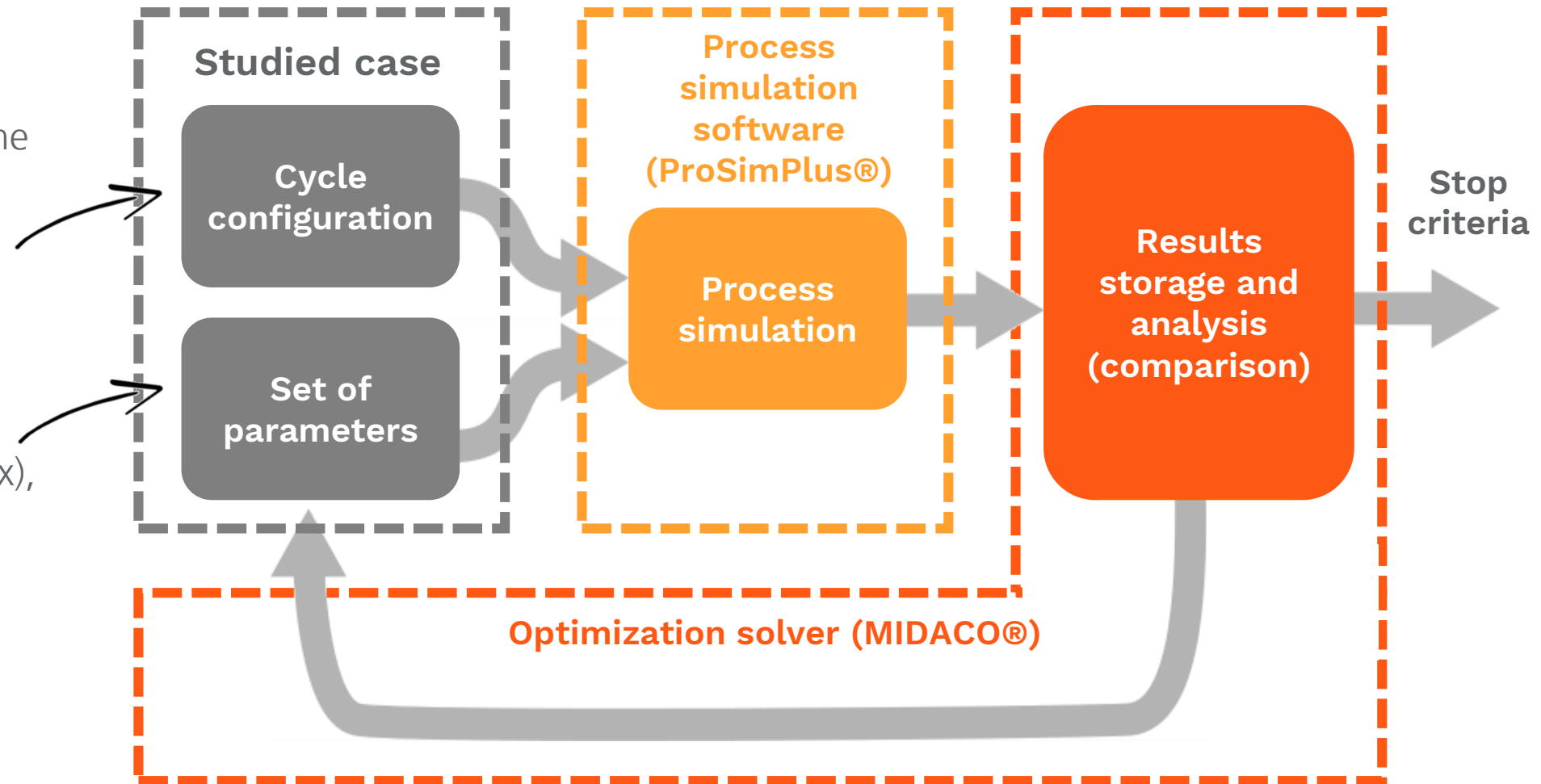
- ✓ Randomness of the initial ant colony population is controlled by a pseudo-random number generator called "seed"
- ✓ More promising strategy to execute several short runs of with different random seeds than performing only one very long run



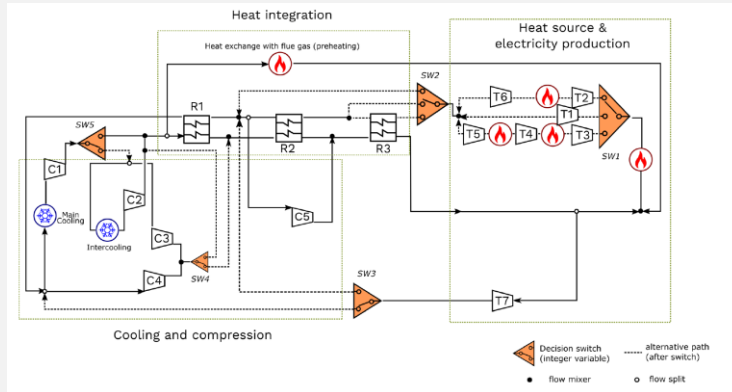
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One initial interaction by the **user** to specify:

- ✓ Cycle architectures to be studied
- ✓ Operating conditions, boundaries (min and max), parameters values...



Superstructure



- ❑ Three “2-paths switches” and four “flow splits”
- ❑ Two “3-paths switches”
→ $2^{(3+4)} \times 3^2 = 1\,152$ alternatives
- ❑ 32 unit operations (incl. splitters and mixers)

Variables and bounds

- ❑ Main compressor inlet pressure (3.3 to 10 MPa)
- ❑ Compressors’ outlet pressure (3.3 to 30 MPa)
- ❑ Cooling temperature (31 to 100°C) – (~87 to 212°F)
- ❑ Part flow rates (0 to 0.5)
- ❑ Heat exchanger cold and hot side outlet temperature (31 to 620°C)
- ❑ Turbine ratios (1 to 5)

Assumptions, fixed parameters

- ❑ Turbine inlet temperature = 620°C (1148°F)
- ❑ CO₂ flowrate before main cooling (kg/s) = 6000
- ❑ Minimum-Tpinch (K) = 10 (if relevant)
- ❑ Turbine is. efficiency (-) = 0.9
- ❑ Compressor is. efficiency (-) = 0.89
- ❑ Pressure drop in every component (% of inlet pressure) = 1

See more in the thesis report [4]

Case 1 : Mono-objective function

Search for best performance (cycle net efficiency) in a given frame

→ Technical constraints such as minimal pinch value (10K) to avoid theoretical results with “infinite heat exchanger surface)

Case 2 : Multi-objective functions

Search for:

1. Lowest electricity production cost (LCEO)
2. Lowest investment costs (CAPEX)
3. Best performance (cycle efficiency)

→ **Relaxing of technical constraints**

↘ Optimization result = initialization of ↗

See more details (formulas, economic hypotheses) in the thesis report [4]

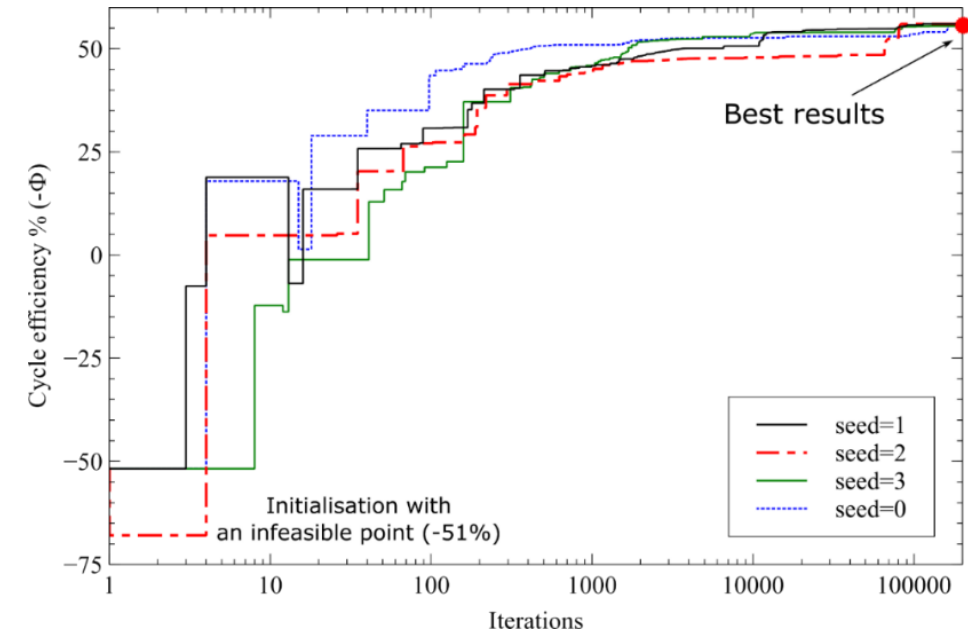
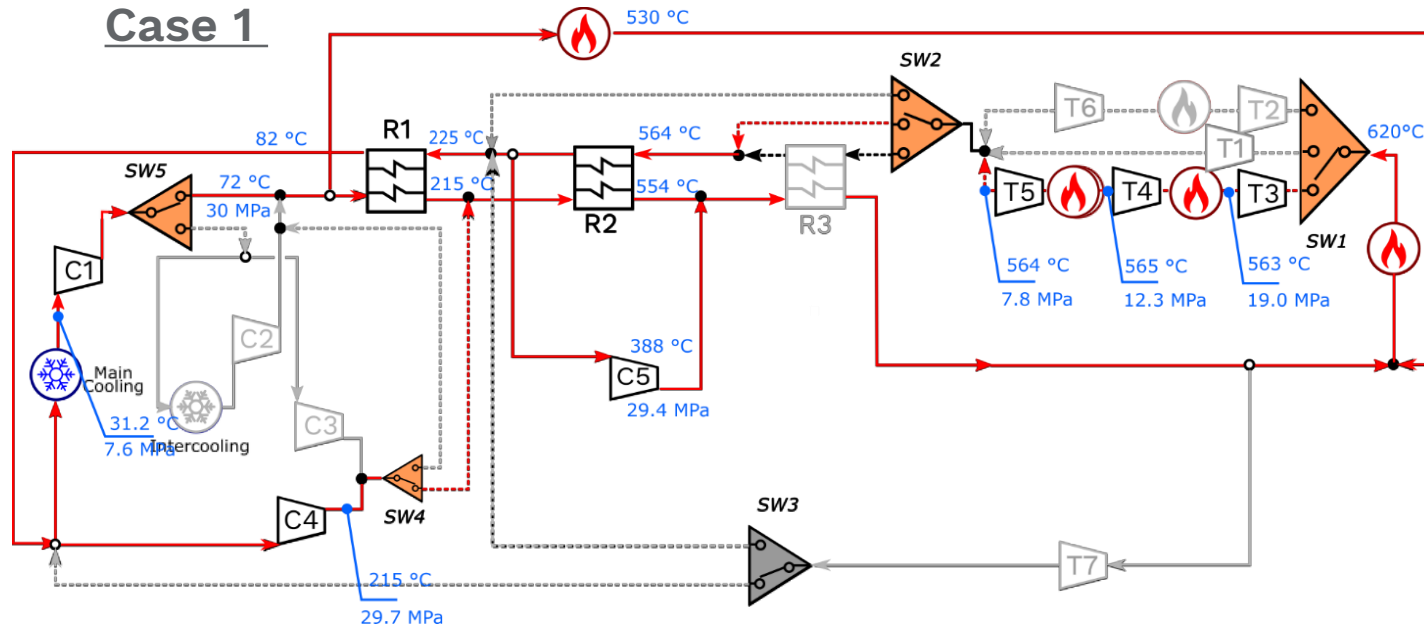
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 - Mono-objective optimization results
 - Multi-objective optimization results
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Results

Mono-objective results: performance & energy maximization

Case 1



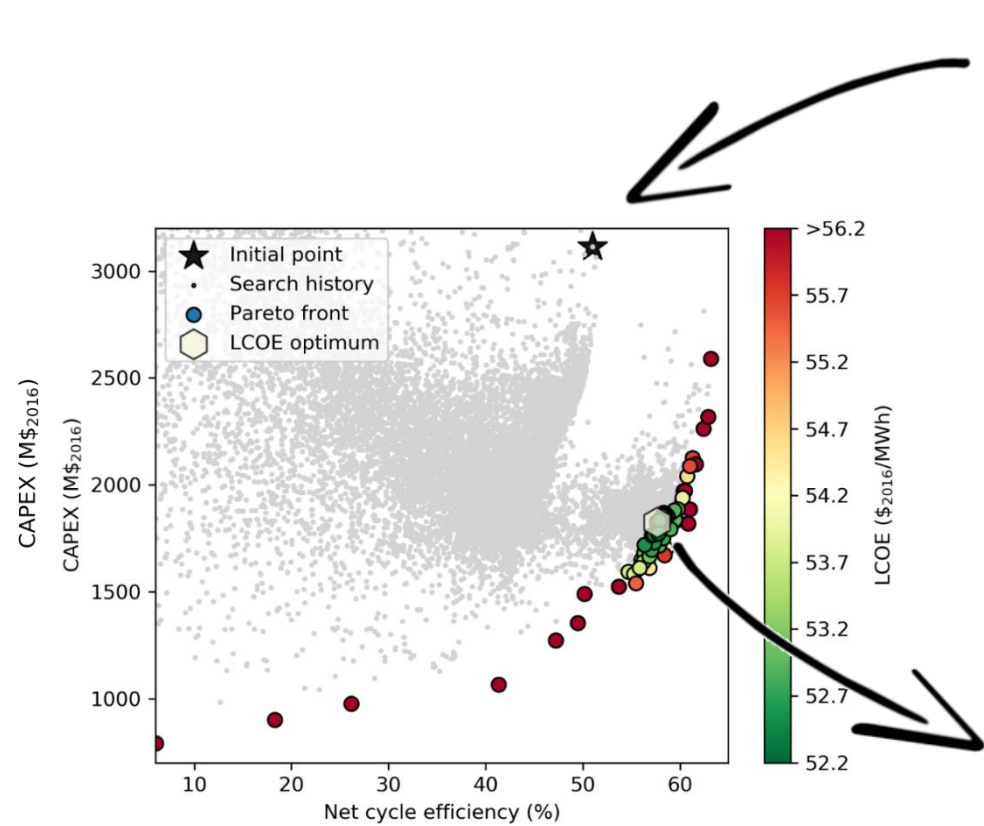
$\eta = 51\%$

Double reheating-double recompression-
preheating cycle

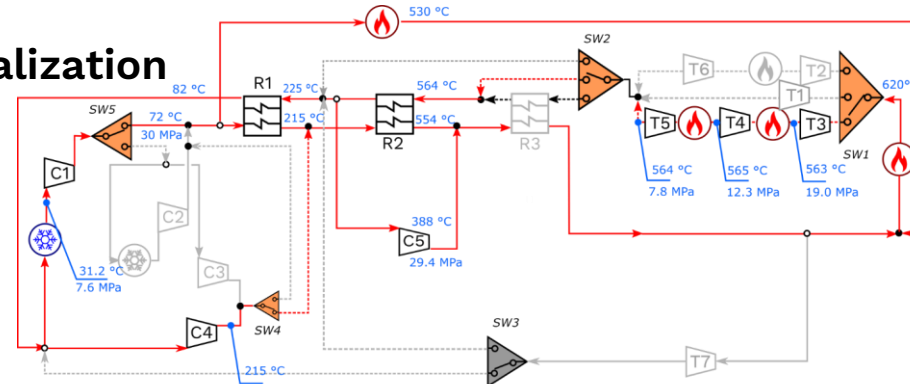
→ Initialization of next case

Results

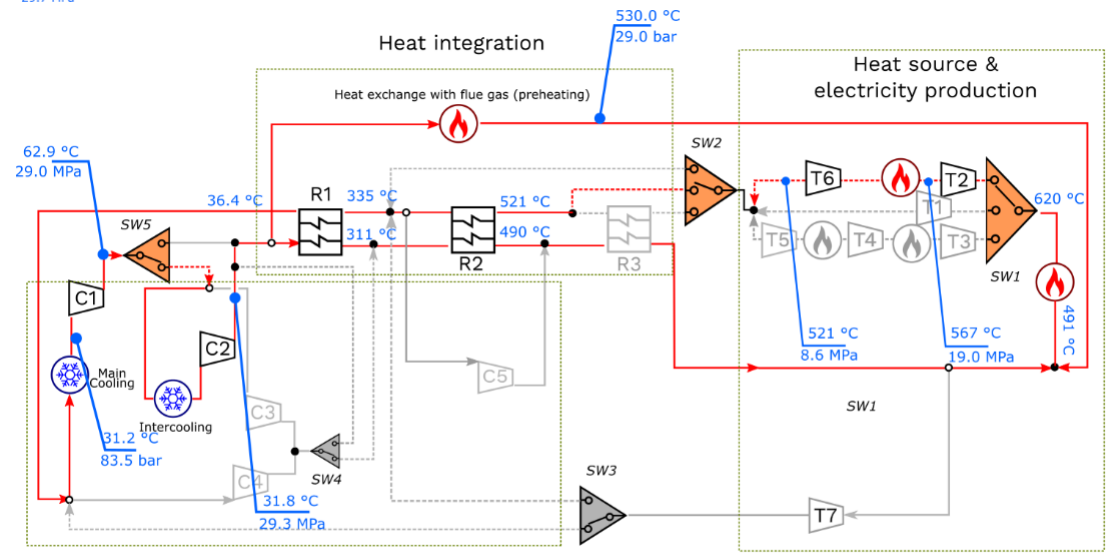
Multi-objective results: Cost of electricity & Investment costs & Performances



Initialization



New solution



$\eta = \sim 57\%$

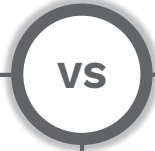
Single reheat - intercooling -
no recompression-preheating cycle

Decision switch (integer variable) alternative path (after switch)
flow mixer flow split

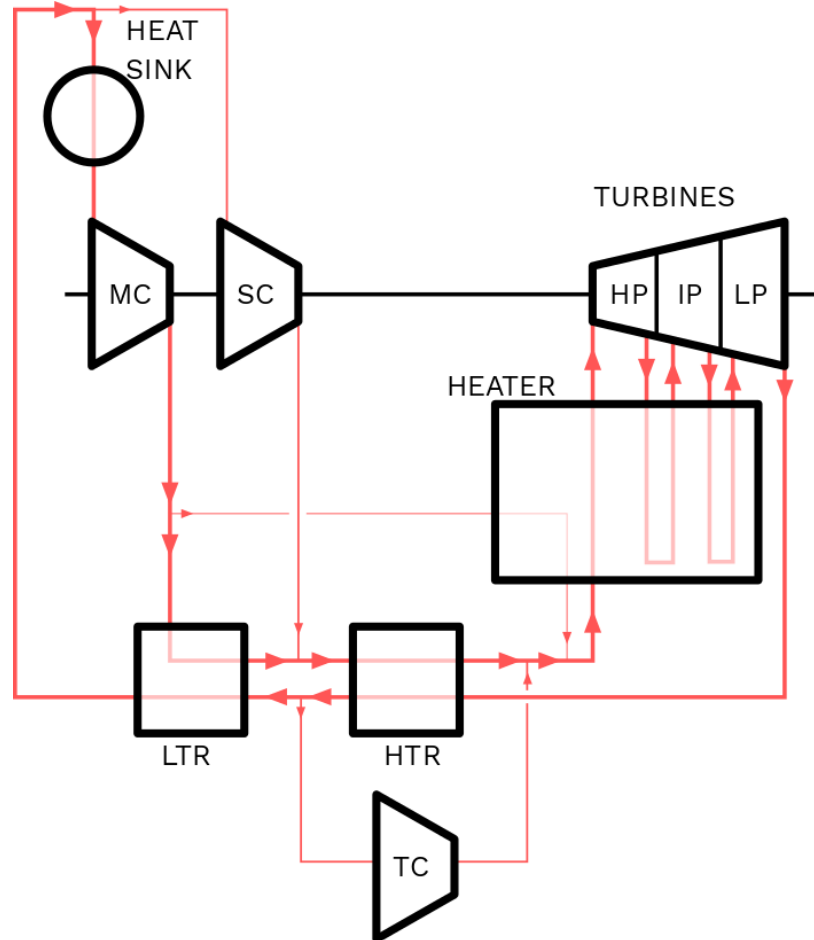
Results comparison



Mono-objective



Multi-objective



30 MPa

2

10 K

10 K

2

7.8 MPa

51 %

3,124 M\$

61 \$/MWh

0	Intercooling	1
	C. pressure outlet	29.3 MPa
2	Recompression	0
	LTR pinch	5K
	HTR pinch	24K
	# of Reheat	1
	LP-Turbine outlet pressure	8.6 MPa
	Net. Eff.	57 %*
	CAPEX	1,826 M\$
	LCOE	52.3 \$/MWh

1

29.3 MPa

0

5K

24K

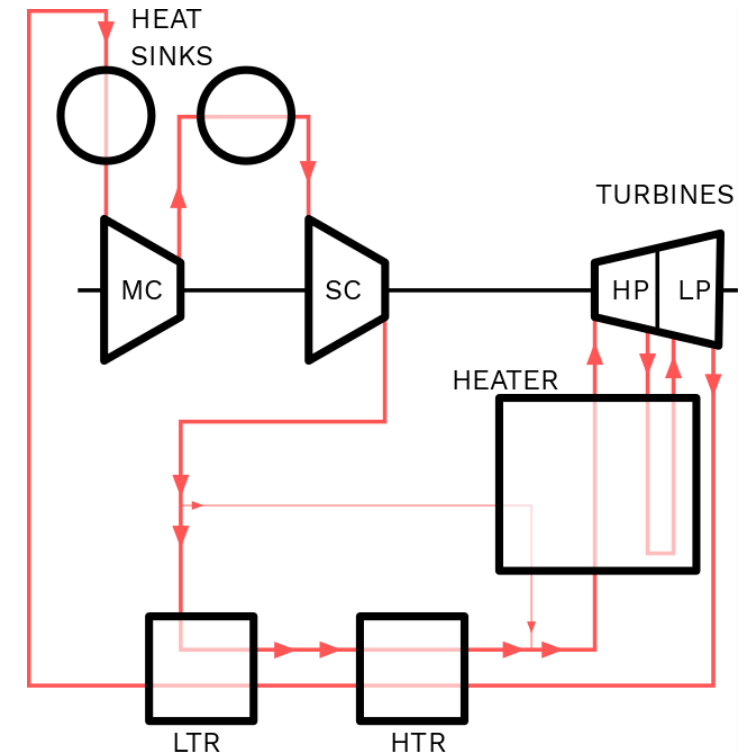
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8.6 MPa

57 %*

1,826 M\$

52.3 \$/MWh



*thanks to very low LTR pinch value

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- ✓ Successful coupling of “commercial software” and “optimization solver”
- ✓ Interesting and Encouraging results
- ✓ Impact of the objective function and hypotheses
- ✓ List of advantages and drawbacks of this method



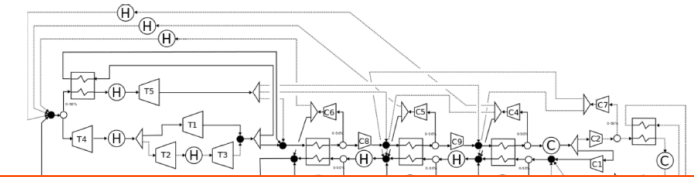
- Check, benchmark and refine the economic models
- Improve the CPU consumption time (several opportunities like meta-models...)
- Improve the reliability of calculation: inclusion of uncertainties, variability...
- Extension of the methodology to other applications
- Comparison of different stochastic/probabilistic optimization methodologies



Cycle selection and design – methodology 2/2

Optimization driven design with 2 approaches

1. « classic design » by simulation based on expertise learn and understood the design drivers
2. global optimization tool based on MINLP optimizer coupled with a cycle superstructure sure to not miss a good solution and explore out of the box ideas



Overview of Process Synthesis methods

	Superstructure with global NLP [1]	Superstructure with global MINLP [2]	Ab-initio [3]
Synthesis approach / search space	Superstructure (given set of alternatives)	Superstructure (given set of alternatives)	Library of unit operations (ab-initio, no superstructure)
System modelling	Equation-oriented	Simulator-based	Simulator-based
Optimization	Monotonic Basin Hopping + local NLP Programming (AMPL + KNITRO solver)	MINLP solved by Ant Colony Optimization Graphical (Commercial process simulator + MIDACO solver)	Evolutionary Programming + local NLP Programming (In-house simulator + SLSQP solver)

[1] Ramirez-Santos et al (2016), Journal of Membrane Science 566, 346-366
 [2] Zhao et al (2017) Computer Aided Chemical Engineering 43, 767-772
 [3] Neveux (2018), Chemical Engineering Science 185, 209-22

12th European Congress of Chemical Engineering (ECCE12) – sept. 15th/16th 2019 by Dr. Thibaut NEVEUX

Comparison of process synthesis methods: case study of the design of membrane separation processes

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12th European Congress of Chemical Engineering (ECCE 12)



123 - Machine Learning Based Design of a Supercritical CO₂ Concentrating Solar Power Plant
 Nabil, Tahar; Le Moullec, Yann; Le Coz, Adrien
 EDF R&D China

Thank you for your attention

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Acknowledgement

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