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DESIGN OPTIMIZATION OF A HEAT RECOVERY ORC FOR A NOVEL BIOMASS TO METHANOL PLANT

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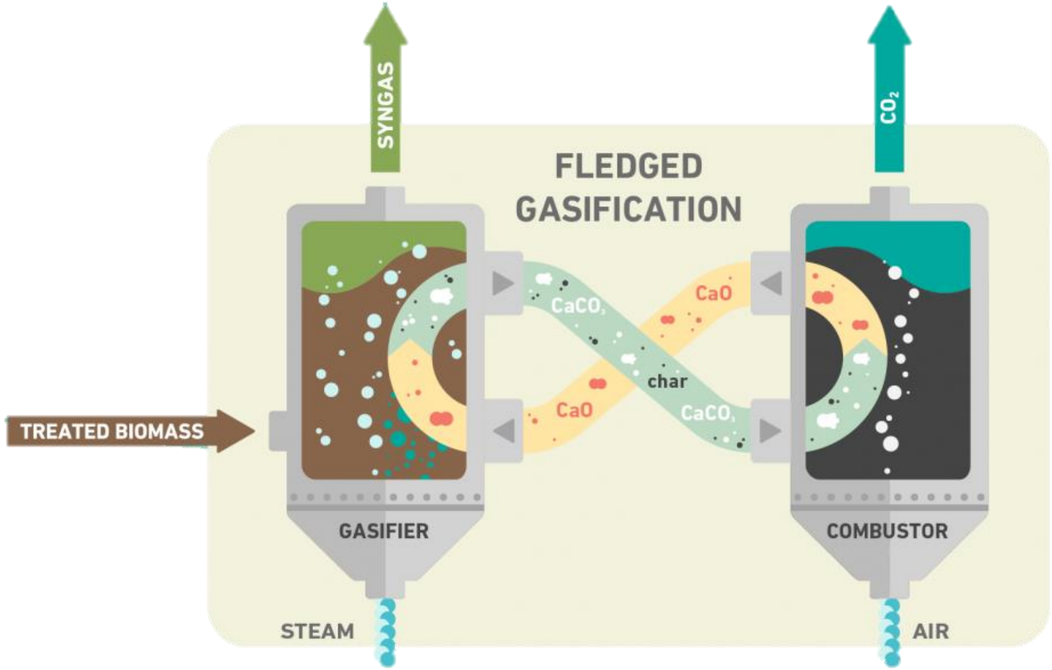
Introduction

Novel biomass to methanol plant

Flexible “sorption-enhanced” gasification reactor (SEG)



Gasification concept based on indirect gasification in a dual fluidized bed system using a CaO-rich bed material

Preliminary design optimization

Process layout

ORC fluid selection and parameters (thermodynamic evaluation)

ORC design and heat exchanger network (techno-economic evaluation)

Biomass to Methanol+Electricity plant layout

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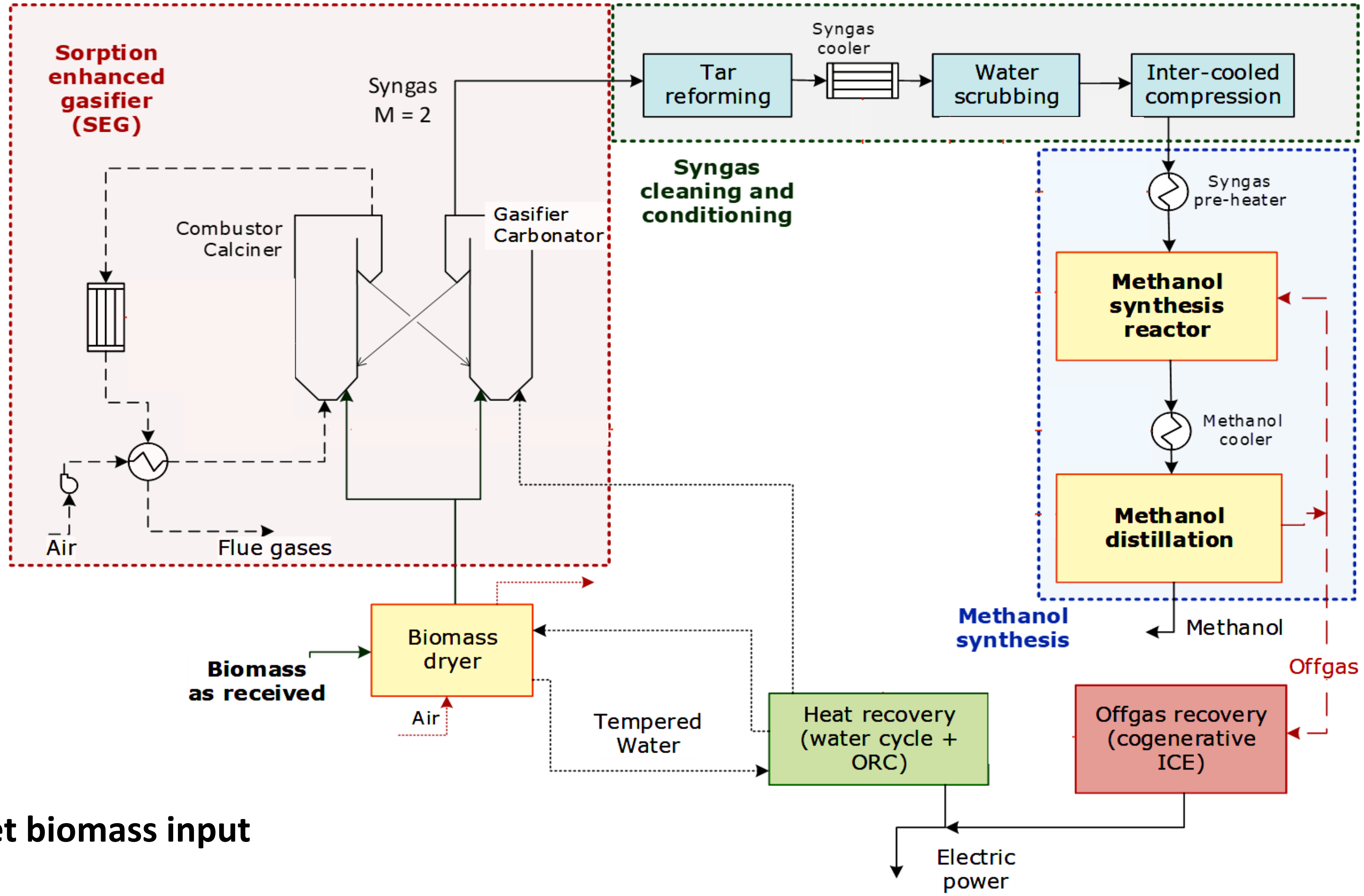

10 MW_{LHV} wet biomass input

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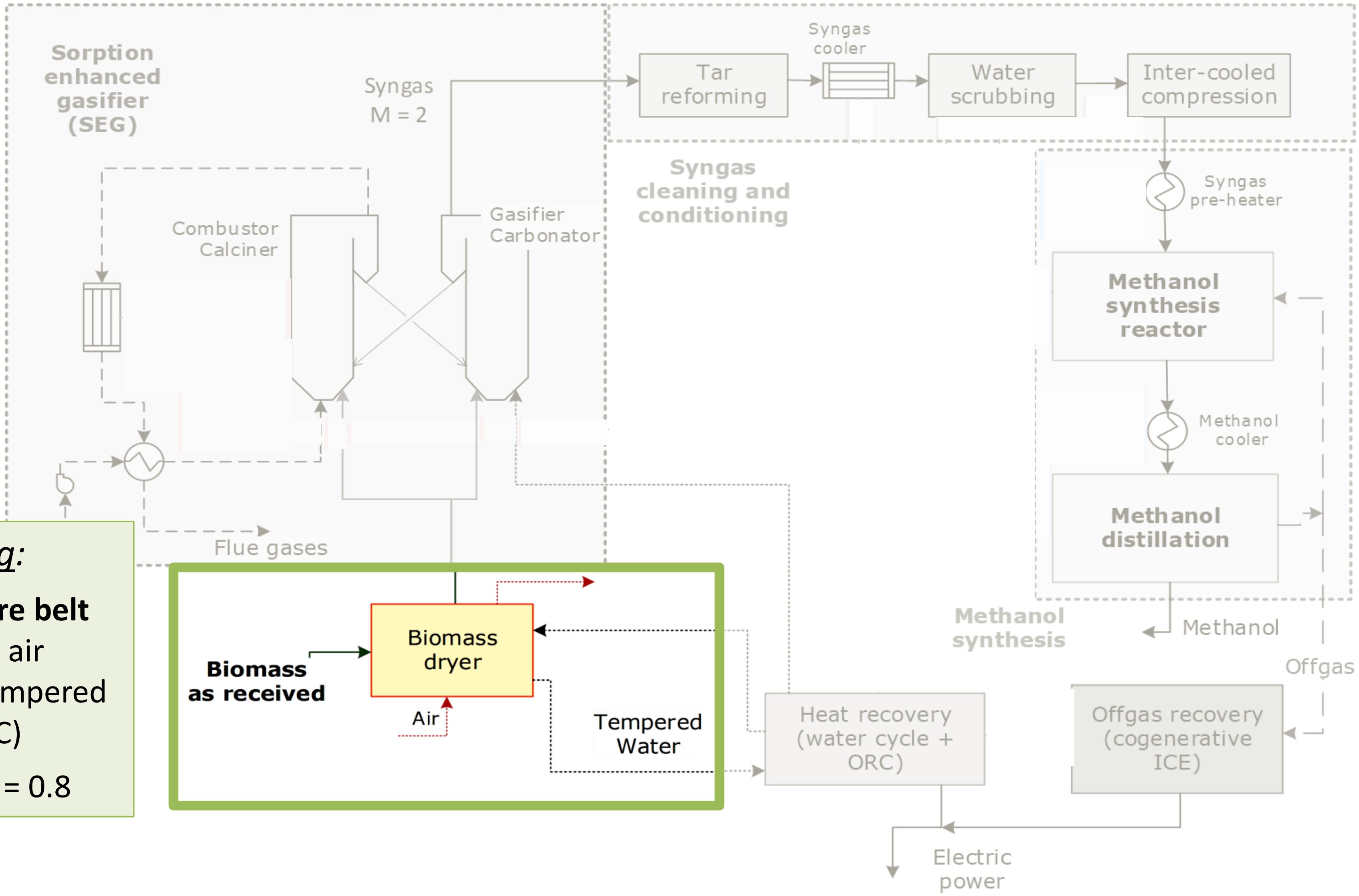
Biomass to Methanol+Electricity plant layout

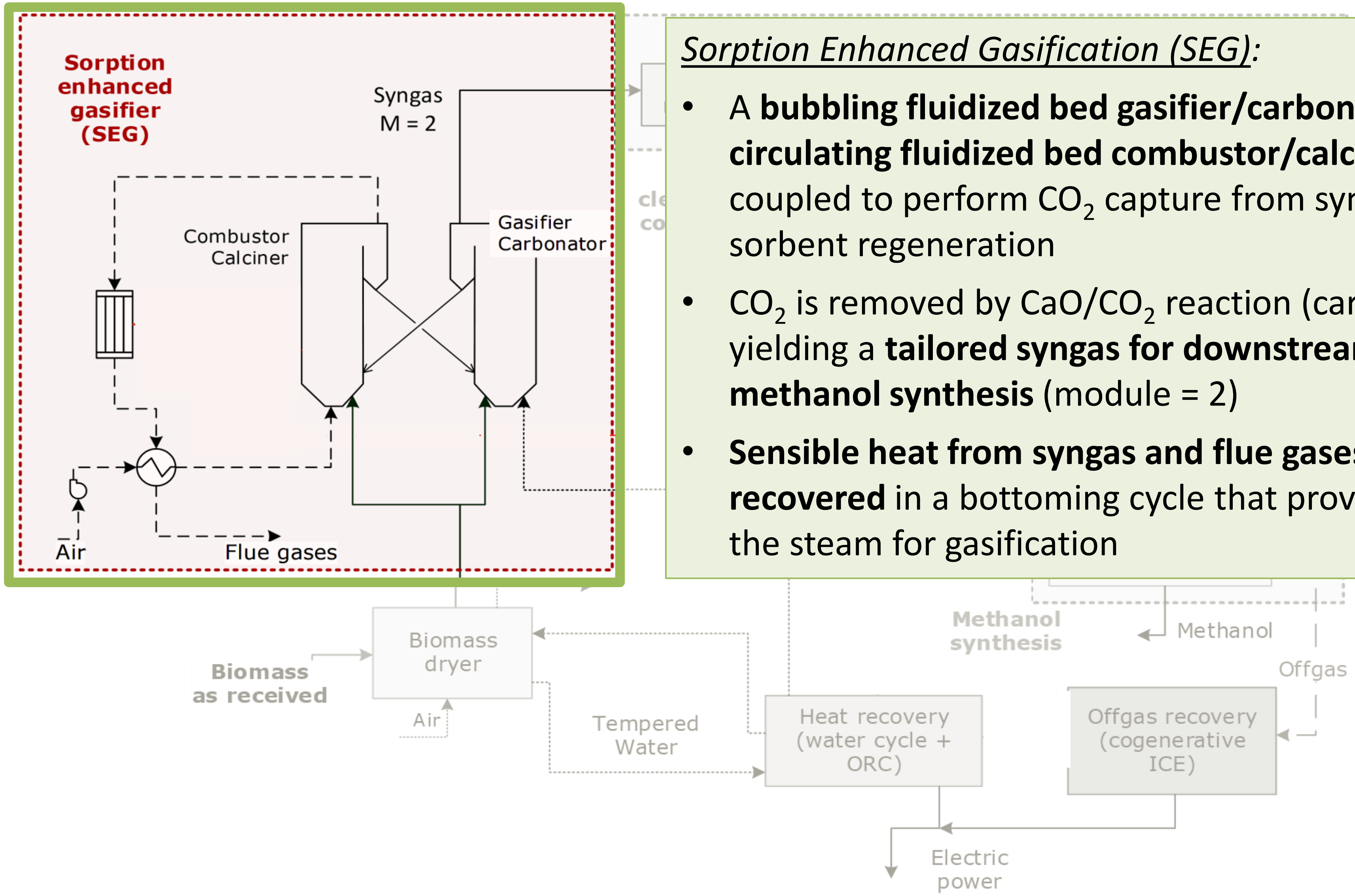


Biomass drying:

Low-temperature belt dryer heated by air preheated by tempered water (78-120 °C)

Dryer efficiency = 0.8

Biomass to Methanol+Electricity plant layout



<u>Sorption Enhanced Gasification (SEG):</u>

- A **bubbling fluidized bed gasifier/carbonator** and a **circulating fluidized bed combustor/calciner** are coupled to perform CO_2 capture from syngas and sorbent regeneration
- CO_2 is removed by CaO/CO_2 reaction (carbonation) yielding a **tailored syngas for downstream methanol synthesis** (module = 2)
- **Sensible heat from syngas and flue gases is recovered** in a bottoming cycle that provides also the steam for gasification

Biomass to Methanol+Electricity plant layout

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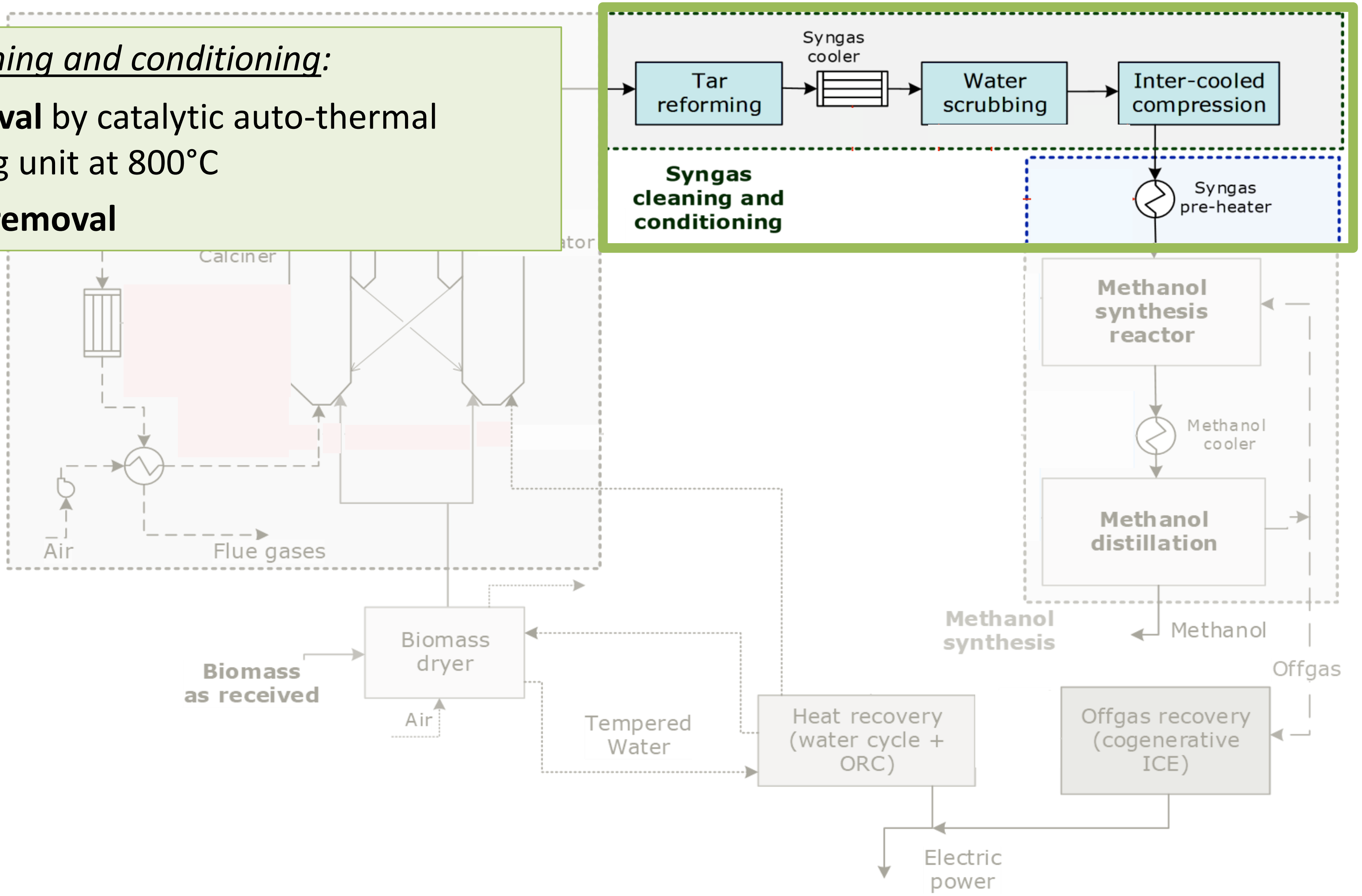
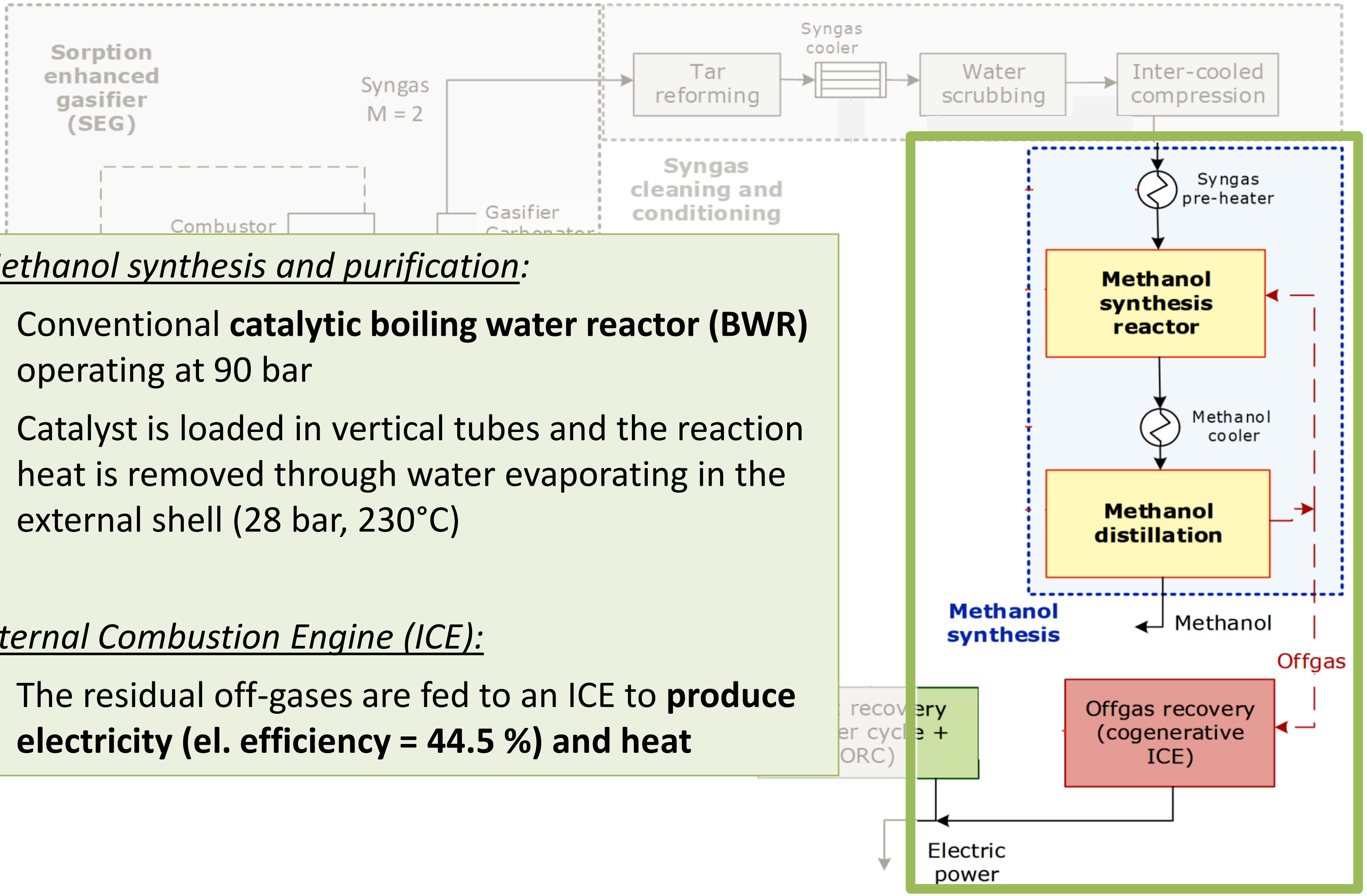
Syngas cleaning and conditioning:

- **Tar removal** by catalytic auto-thermal reforming unit at 800°C
- **Sulphur removal**



Biomass to Methanol+Electricity plant layout



Methanol synthesis and purification:

- Conventional **catalytic boiling water reactor (BWR)** operating at 90 bar
- Catalyst is loaded in vertical tubes and the reaction heat is removed through water evaporating in the external shell (28 bar, 230°C)

Internal Combustion Engine (ICE):

- The residual off-gases are fed to an ICE to **produce electricity (el. efficiency = 44.5 %) and heat**

Preliminary simulation results

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Performances indexes

- **Gasifier island**

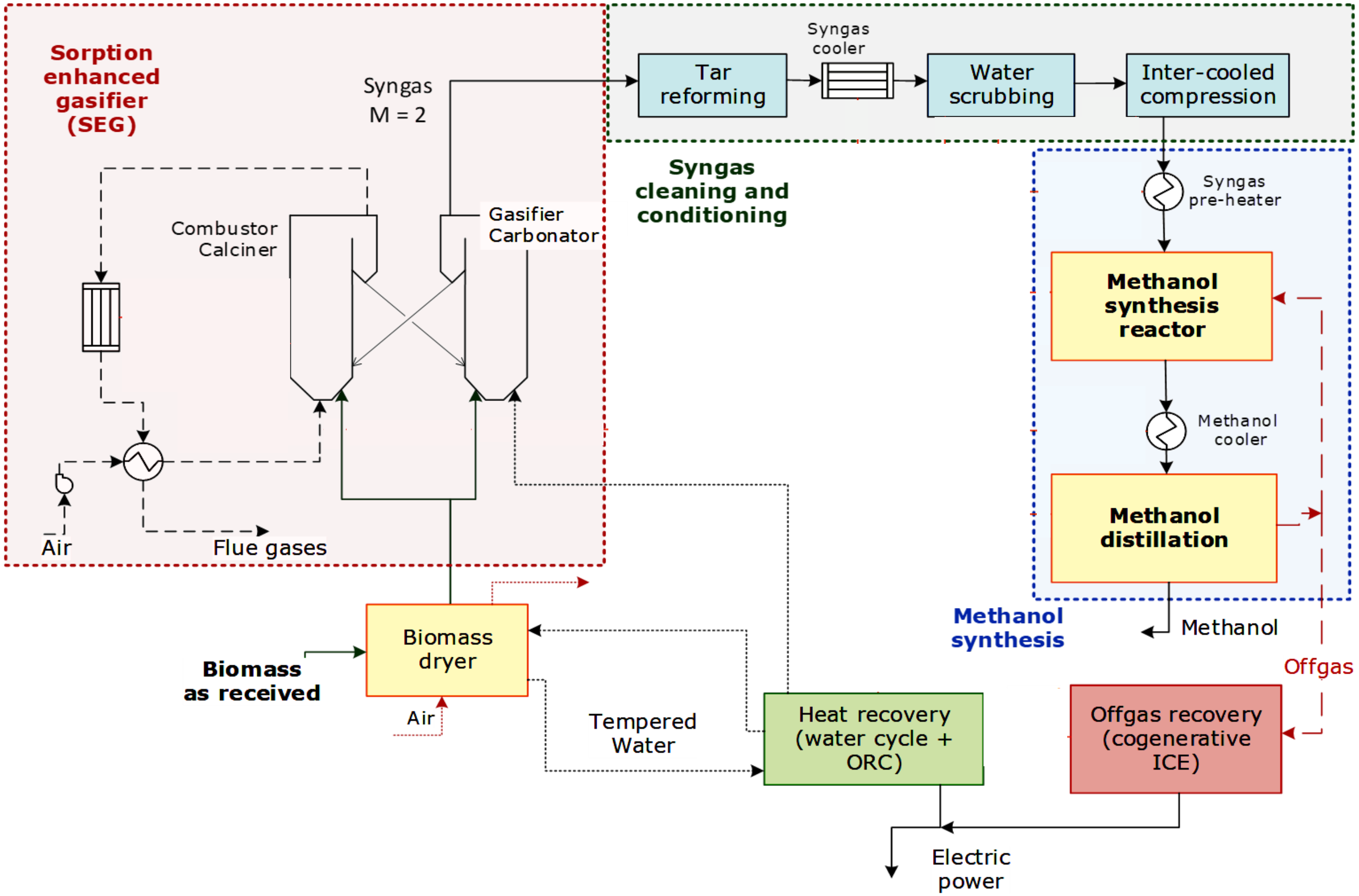
$$CGE_{gasif} = \frac{G_{syngas} LHV_{syngas}}{G_{biomass} LHV_{biomass}}$$

- **MeOH synthesis island**

$$CGE_{MeOH} = \frac{G_{MeOH} LHV_{MeOH}}{G_{syngas} LHV_{syngas}}$$

Dryer		
Biomass thermal input to the plant (LHV)	**10**	**MW_{th}**
Biomass thermal input after drying (LHV)	10.88	MW_{th}
Dryer heat input	1.05	MW_{th}
SEG		
Syngas production (wet)	0.84	kg/s
Syngas heating value (LHV wet)	8.99	MJ/kg
Gasifier cold gas efficiency (CGE_{gasif})	**69.32**	**%**
Syngas compressors		
Compressor consumption	0.68	MW_{el}
Methanol synthesis		
MeOH production rate	0.28	kg/s
MeOH chemical power (LHV basis)	5.56	MW
Syngas to MeOH conversion efficiency (CGE_{MeOH})	**78.46**	**%**
Biomass to MeOH conversion efficiency	**55.55**	**%**

Heat integration study



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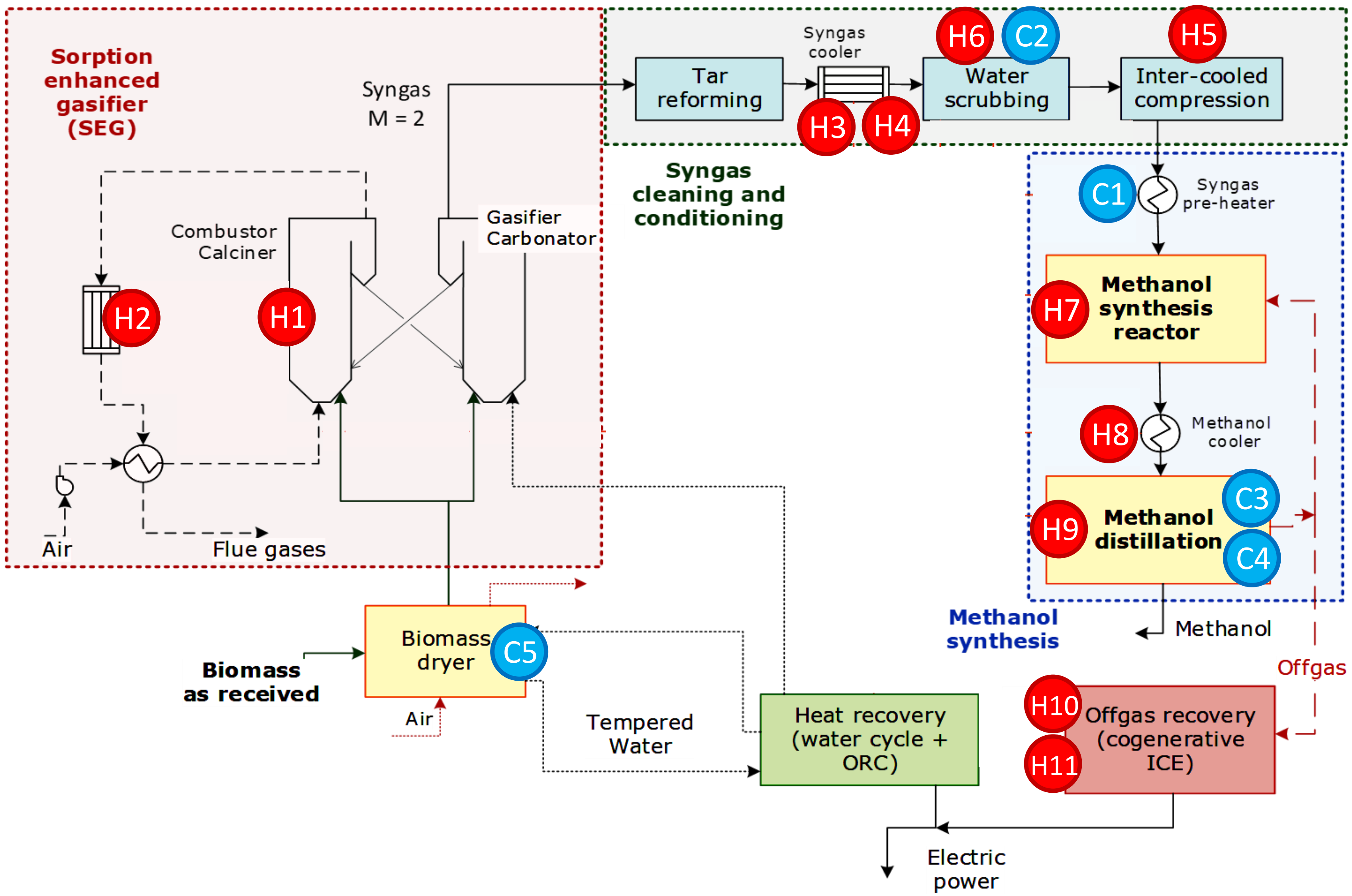

Heat integration study

Hot streams	Heat	Inlet temperature	Outlet temperature	Name	Constraints
SEG combustor	193.28 kW	910 °C	910 °C	H1	Only evaporators
SEG flue gases	1319.06 kW	910 °C	300 °C	H2	NO superheaters
Syngas cooler HT	1016.72 kW	800 °C	340 °C	H3	NO syngas preheaters
Syngas cooler LT	528.82 kW	340 °C	80 °C	H4	
Compressor intercoolers	681.76 kW	122 °C	40 °C	H5	
Scrubber cooler	1037.19 kW	78 °C	25 °C	H6	
MeOH reactor	659.49 kW	265 °C	265 °C	H7	MP evaporator
MeOH cooler	1575.64 kW	265 °C	40 °C	H8	
Condenser 2nd column	609.69 kW	73 °C	73 °C	H9	
ICE flue gases	151.69 kW	360 °C	110 °C	H10	
ICE hot water	48.18 kW	94 °C	87 °C	H11	
Total	**7821.51 kW**				

Cold streams	Heat, kW	Inlet temperature	Outlet temperature	Name	Constraints
Syngas preheat	1058.50 kW	43 °C	254 °C	C1	
Scrubber heater	22.50 kW	25 °C	220 °C	C2	
Reboiler 1st column	50.07 kW	81 °C	81 °C	C3	NO syngas coolers, flue gases, reactors
Reboiler 2nd column	589.20 kW	82 °C	109 °C	C4	NO syngas coolers, flue gases, reactors
Biomass dryer	1309.66 kW	78 °C	120 °C	C5	
Total	**2768.0 kW**				

Steam network	Mass flow rate	Temperature	Pressure
Steam to gasifier	0.4335 kg/s	170 °C	1.5 bar
Total th. power	**228.9 kW**		

Heat integration study

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The gross energy available from process waste heat and purification off-gases is **78 % of the biomass thermal power (LHV)**, of which 17 % must be provided to dryer

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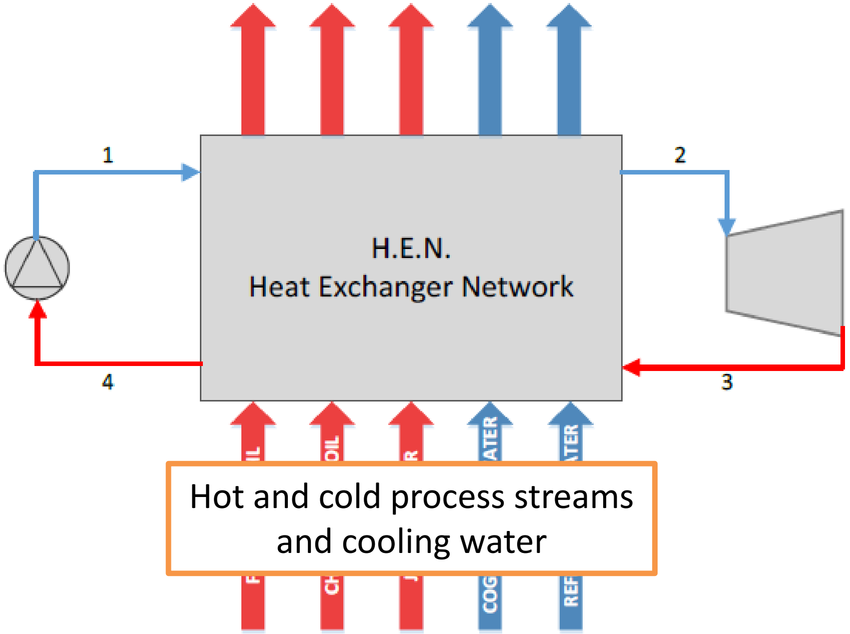
Methodology for heat integration study



Objectives:

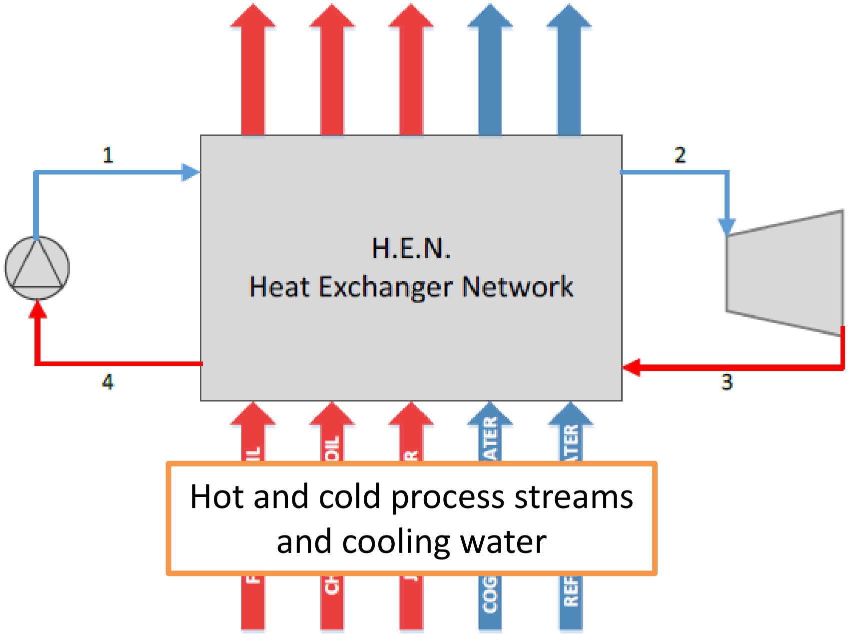
- Optimize the **heat integration** between hot and cold process streams as well as ORC design and steam network
- Optimize the layout of the **ORC + steam network** considering:
  - Multiple heat sources available
  - Steam users (gasifier, MeOH reactor)
  - Technical limits (metal dusting, required MeOH reactor cooling steam, etc.)

Methodology[1,2]:

- Combination of **two superstructures** (for Rankine cycles and for HEN synthesis)
- **Simultaneous design of ORC and HEN**, considering energy efficiency and capital costs (i.e., targeting the minimum Total Annual Cost, rather than just efficiency) → TECHNO-ECONOMIC OPTIMIZATION
- Challenging MINLP problem

1. Martelli, E., Elsido, C., Mian, A., & Marechal, F. (2017). Comput. Chem. Eng., vol. 106: p. 663-689
2. Elsido, C., Martelli, E., & Grossmann, I.E. (2019). Comput. Chem. Eng., vol. 128: p. 228-245

Methodology for heat integration study



Mathematical model:

Binary decision variables:

- Activation of the heat exchanger between each hot stream and each cold stream in each stage of the HEN
- Activation of each ORC and steam network stream

Continuous variables:

- Heat exchanged
- Temperatures at hot end of each stage of the HEN
- Temperature difference for each heat exchanger
- Areas of the heat exchangers
- Mass flow rate of each ORC and steam network stream

Objective function: **Minimize**: *Total Annual Cost*

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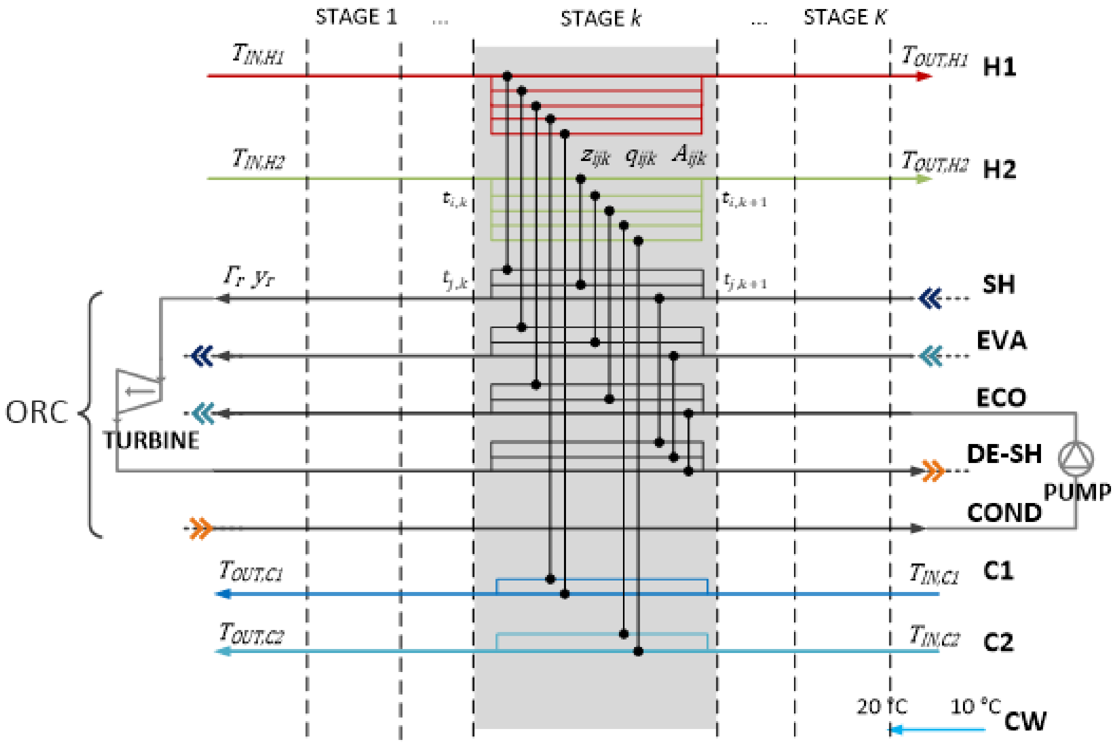

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Methodology for heat integration study

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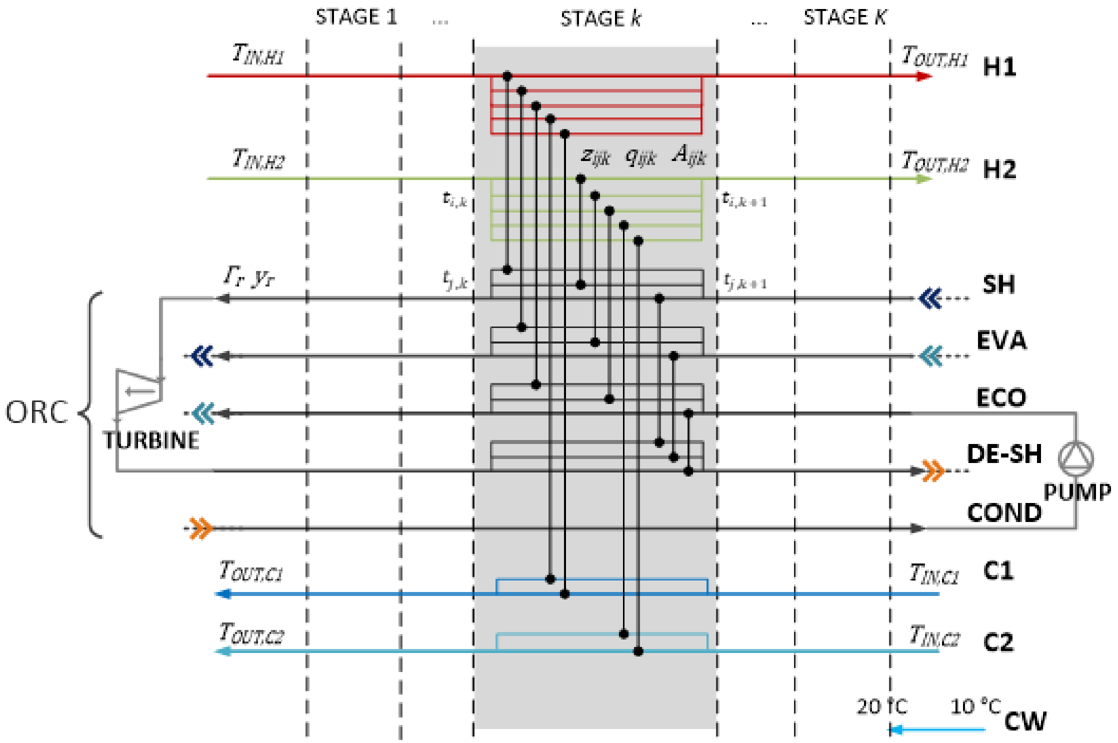

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Objective function: **Minimize**: *Total Annual Cost*

Methodology[1,2]:

Nonconvex Mixed Integer NonLinear Programming (MINLP) problem:

- modelled with **GAMS**
- solved using **ad-hoc bilevel decomposition algorithm**, employing CPLEX to solve the master level Mixed Integer Linear Program (MILP) and BARON for the lower level NonLinear Program (NLP)

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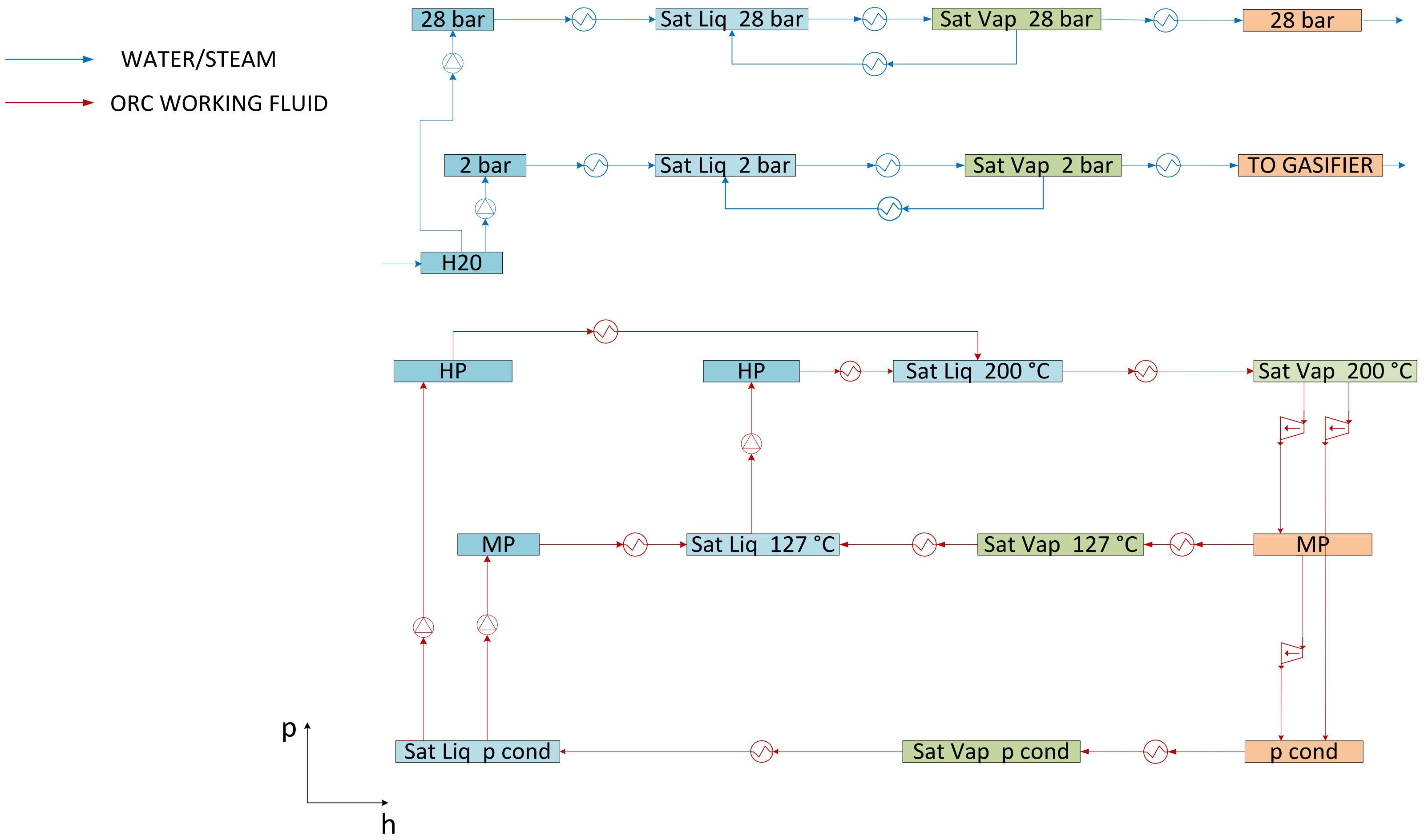
ORC + steam network superstructure



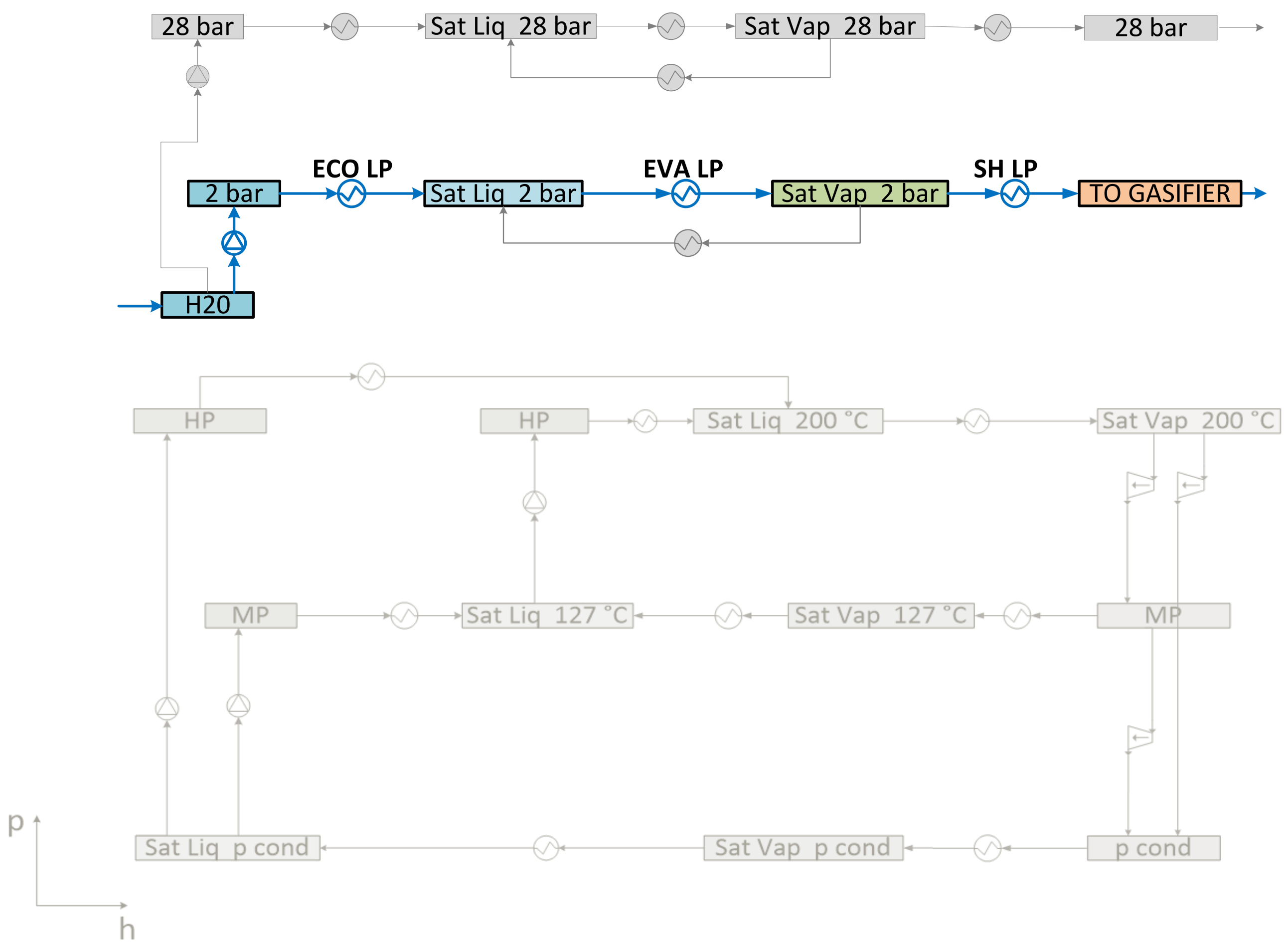
"*p-h* superstructure"

Superstructure of all considered alternative configurations:

- ORC with one level of evaporation and two levels of condensation
- Steam network with two different pressure levels

ORC + steam network superstructure

Steam network with low-pressure **(LP) level**



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Superstructure of all considered alternative configurations:

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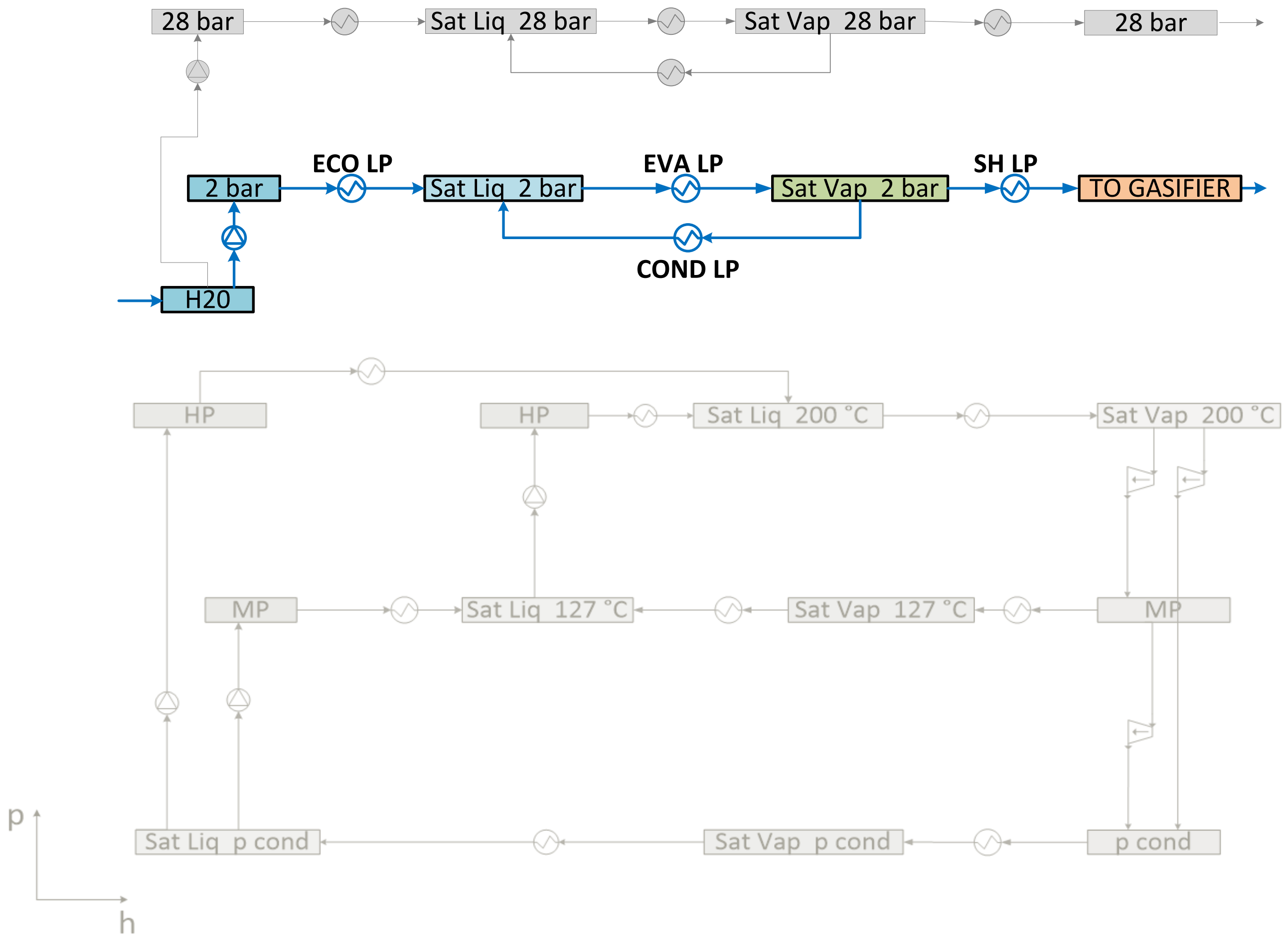
ORC + steam network superstructure

Steam network with low-pressure level and **evap-cond loop**



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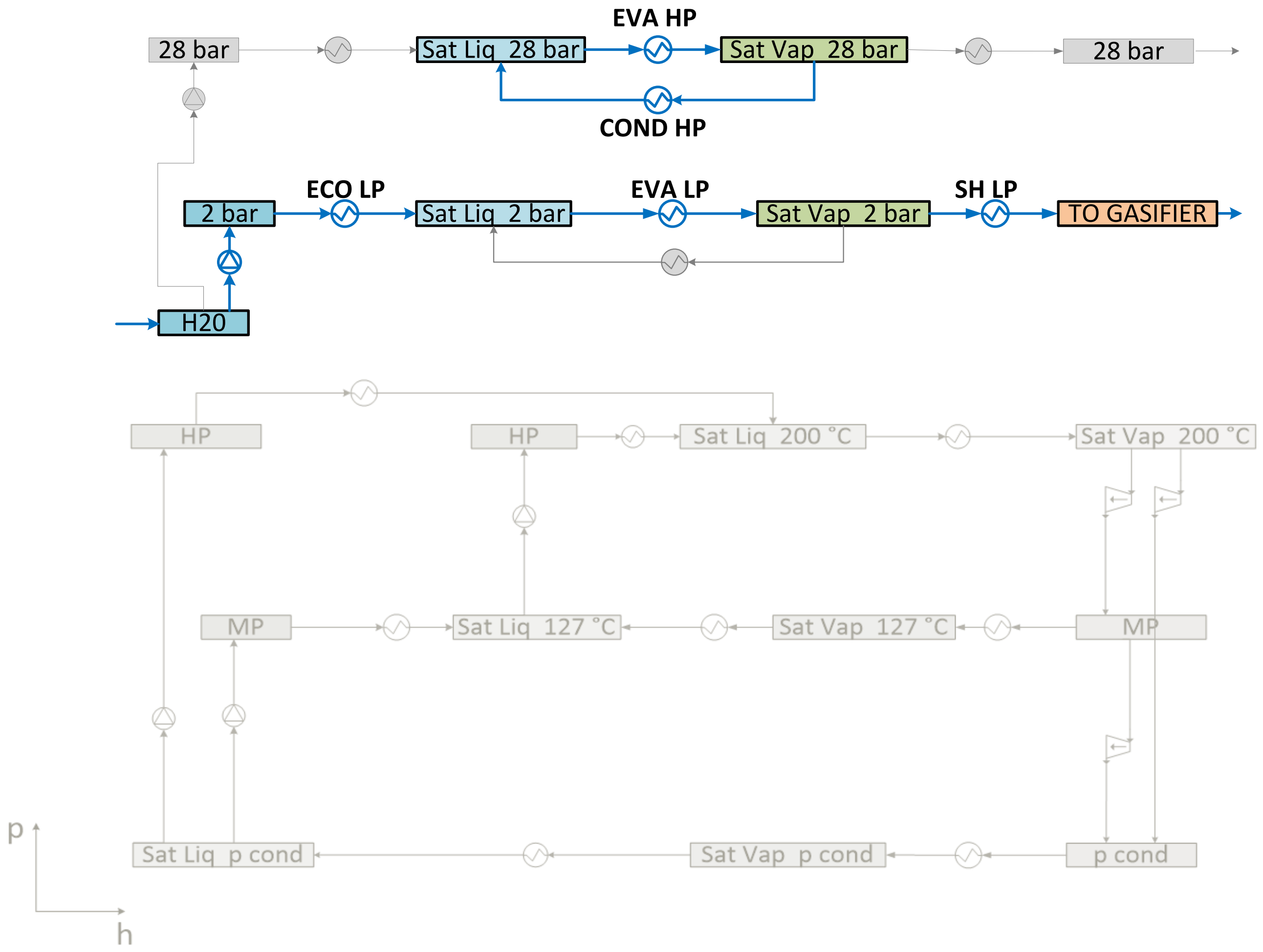
ORC + steam network superstructure

Steam network with low-pressure level and **HP level evap-cond loop**



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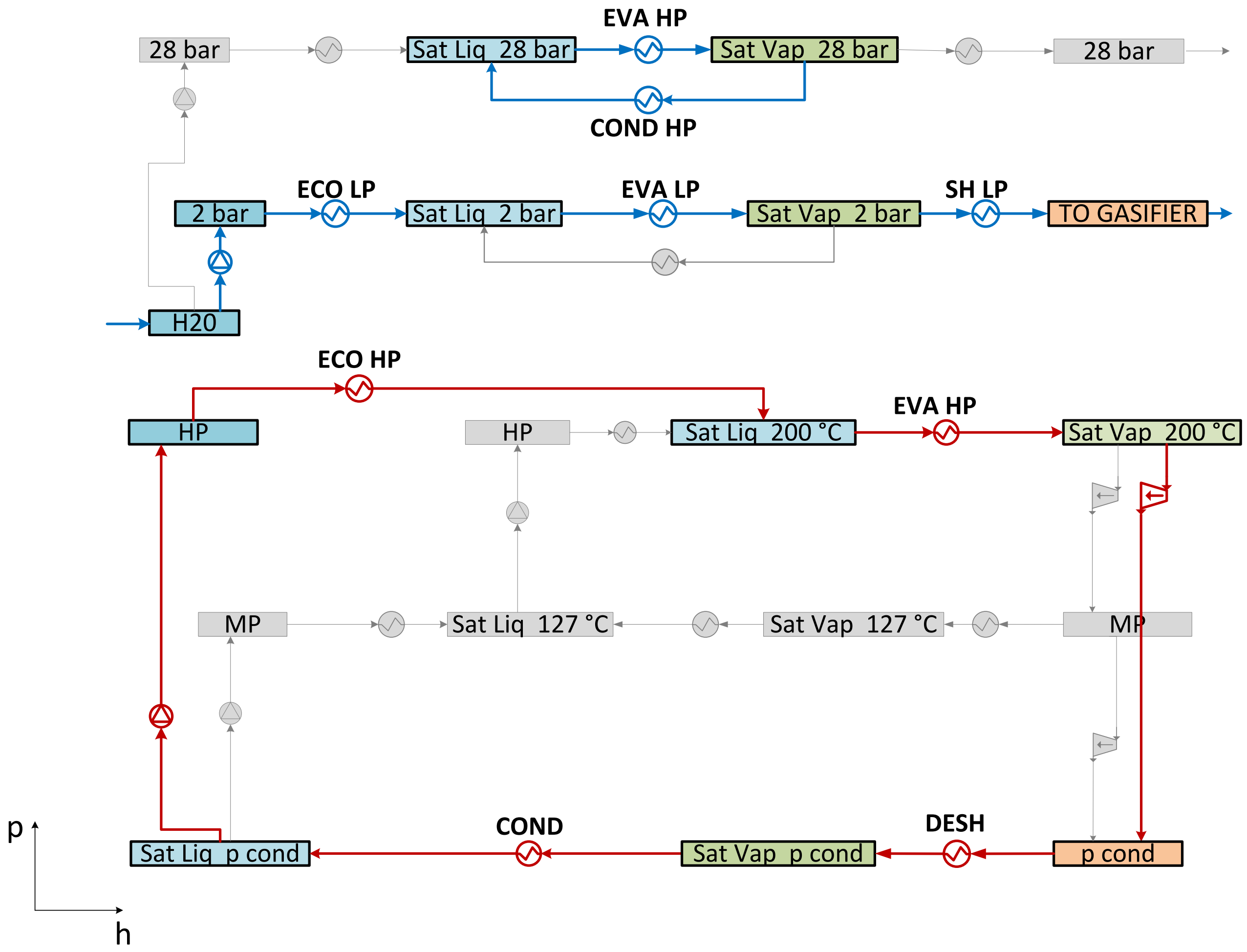
ORC + steam network superstructure

Steam network with low-pressure level and HP level evap-cond loop

ORC with one level of pressure



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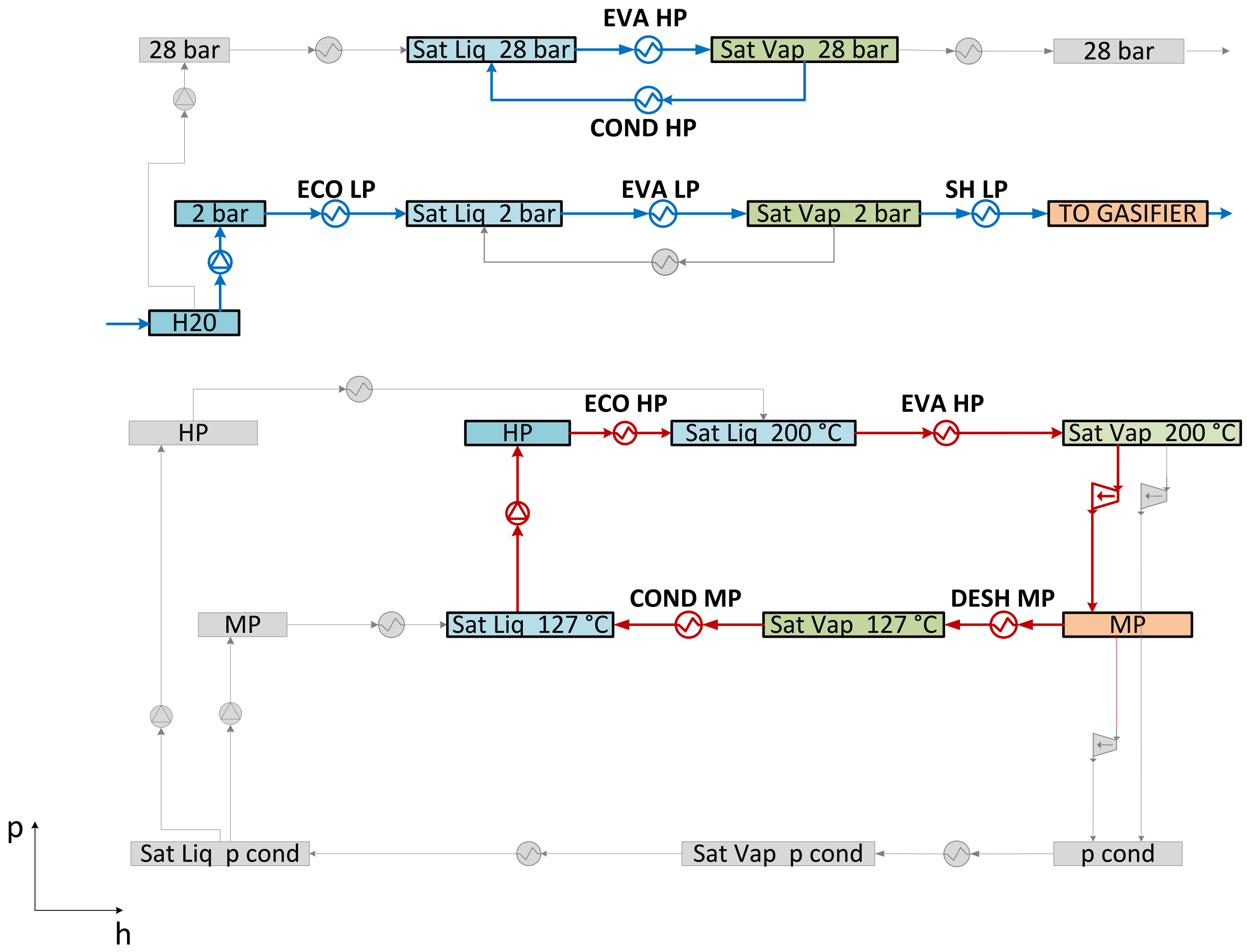
ORC + steam network superstructure

Steam network with low-pressure level and HP level evap-cond loop

ORC with one level of pressure and **back-pressure** turbine



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Superstructure of all considered alternative configurations:

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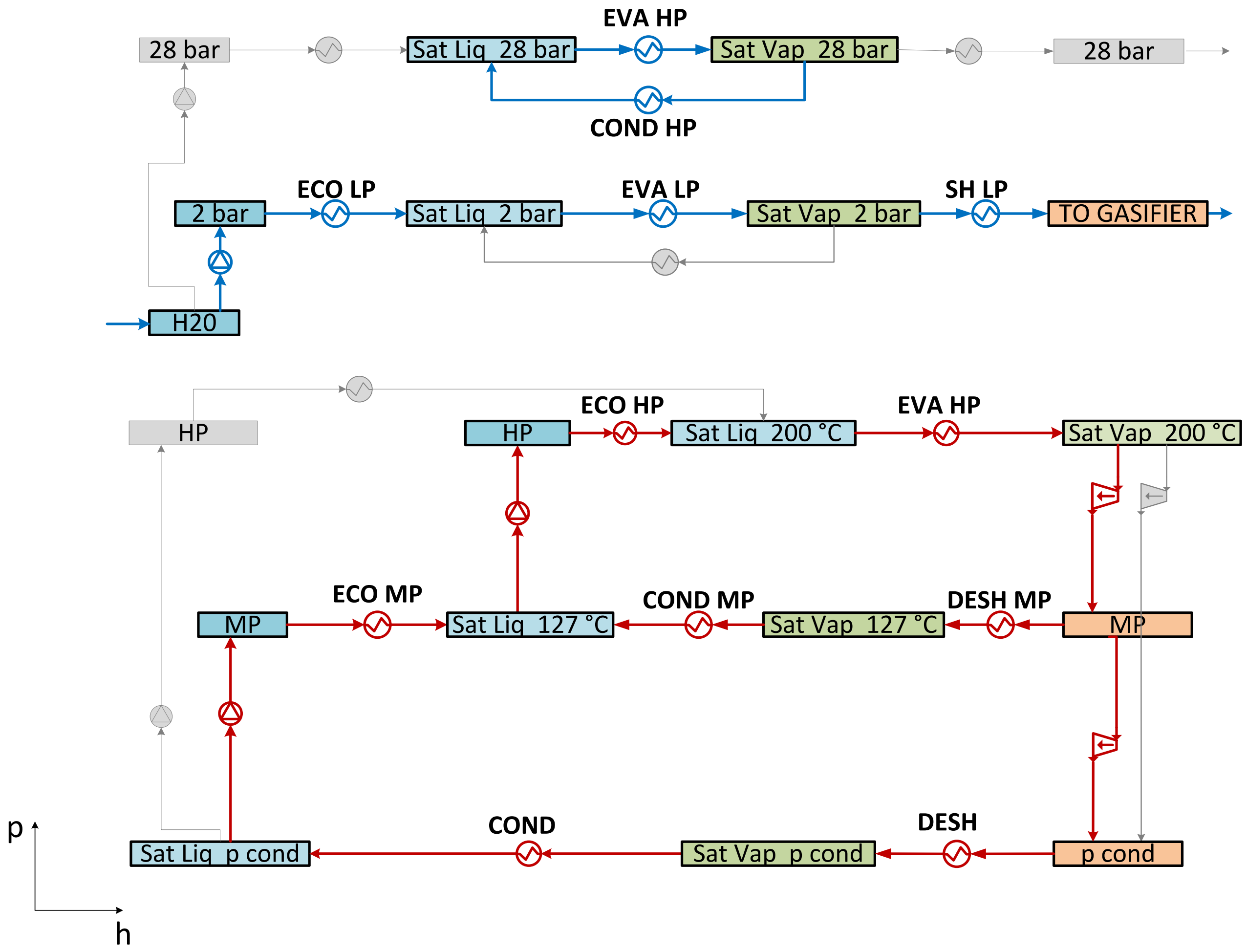
- Steam network with two different pressure levels

ORC + steam network superstructure

Steam network with low-pressure level and HP level evap-cond loop

ORC with **two levels of condensation**



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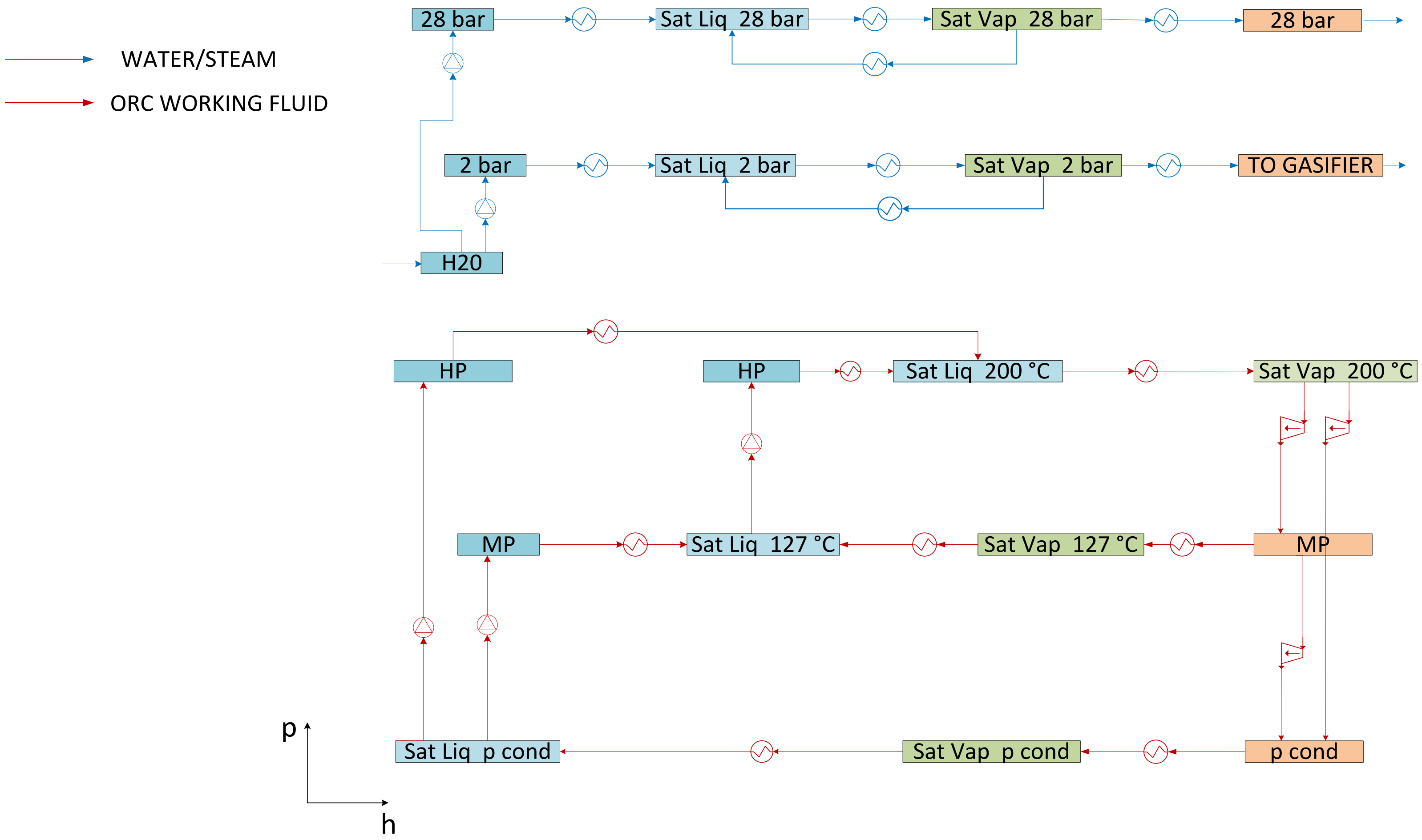
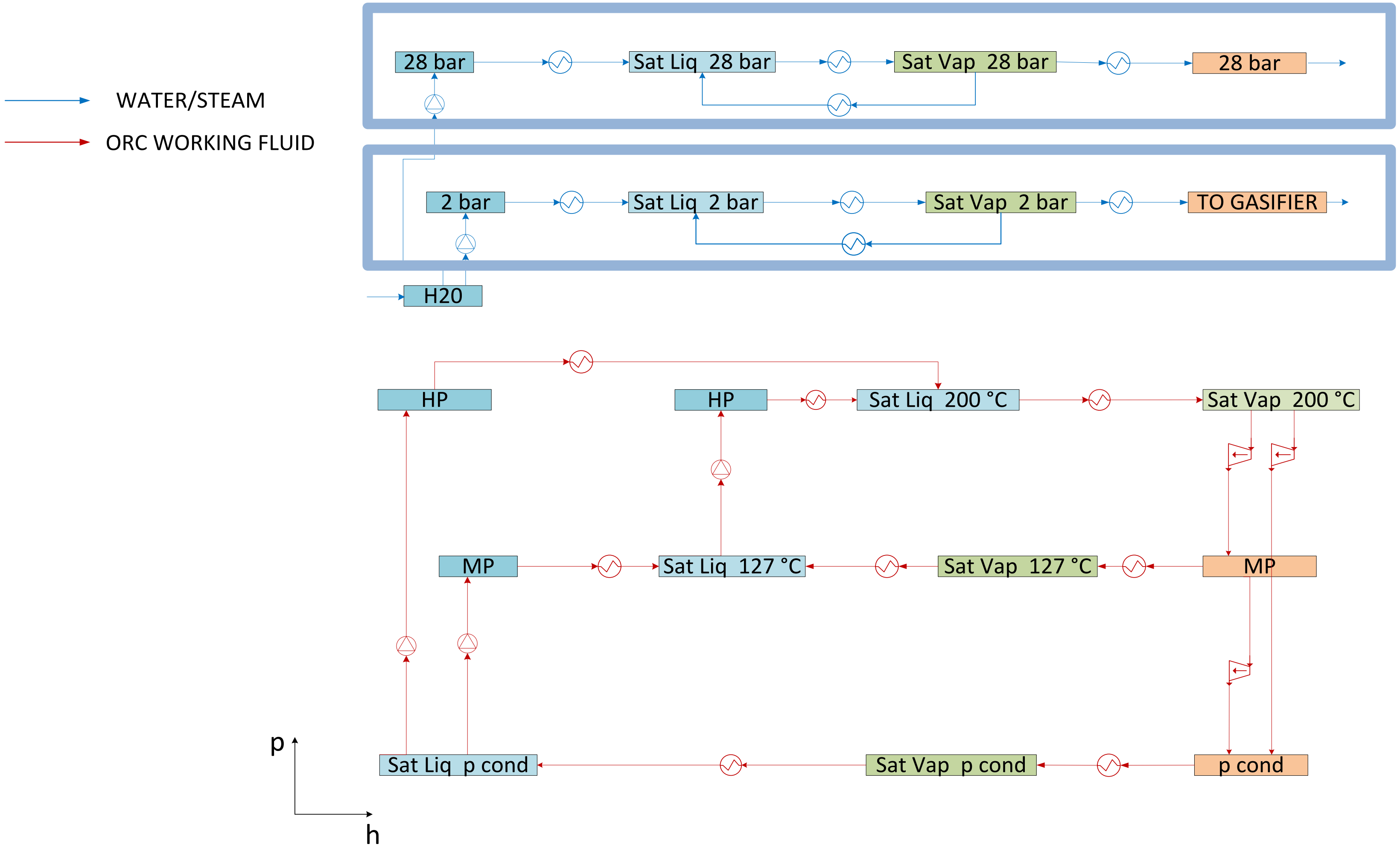
ORC + steam network superstructure



ORC + steam network superstructure

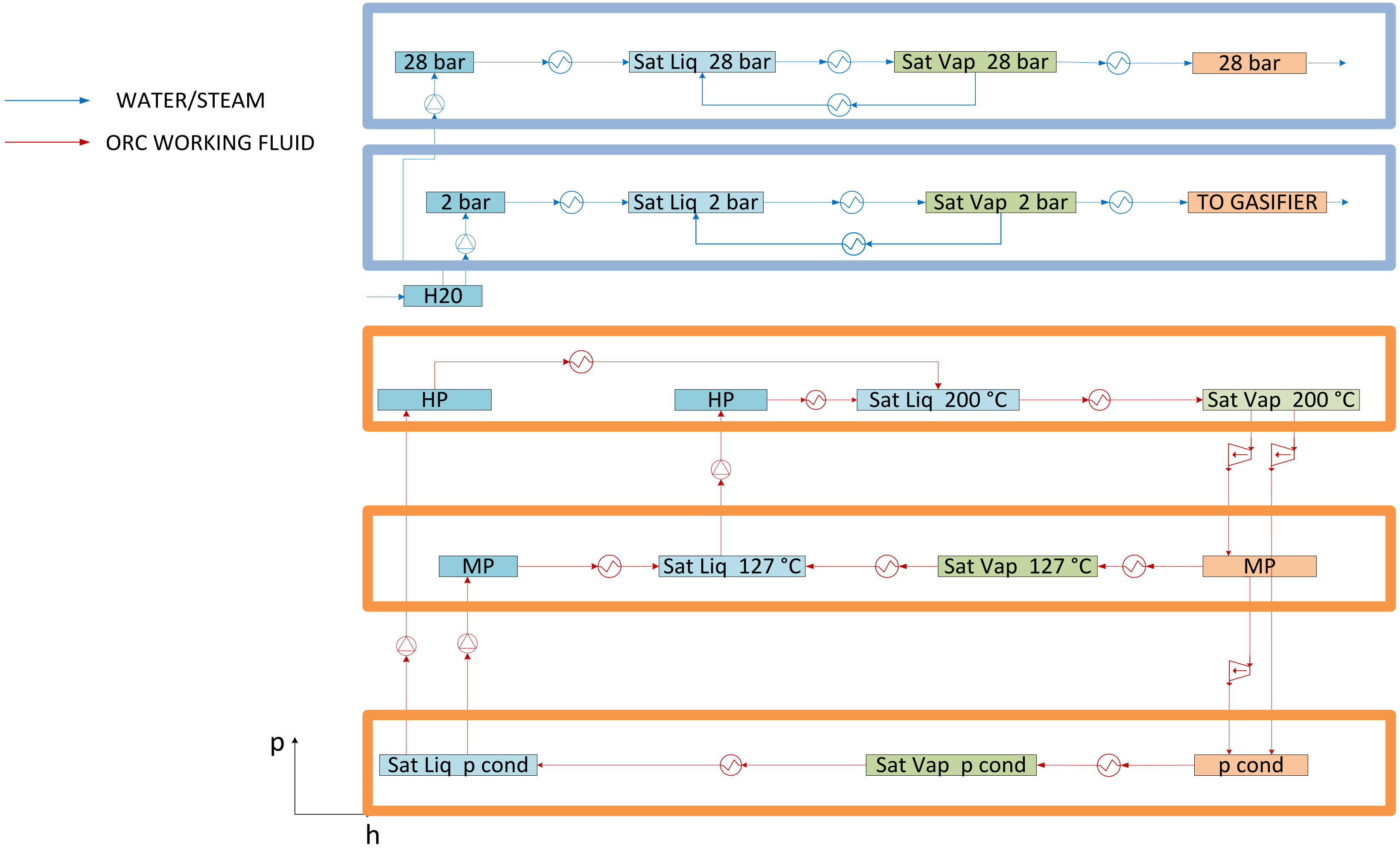


HP level @28 bar (230 °C)
(MeOH reactor at 265 °C)

LP level @ 2 bar (120 °C)

- boilers purification unit
- Steam to gasifier

ORC + steam network superstructure



HP level @28 bar (230 °C)
(MeOH reactor at 265 °C)

LP level @ 2 bar (120 °C)
- boilers purification unit
- Steam to gasifier

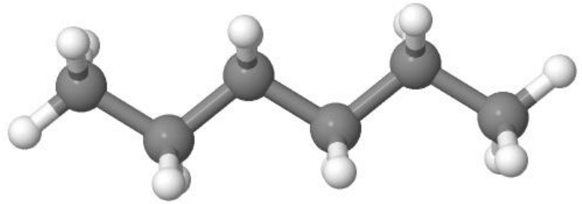
ORC HP level: max temperature 200 °C

ORC MP condensation temperature = 127 °C
- Biomass dryers
- LP steam loop

Condenser temperature = 30 °C

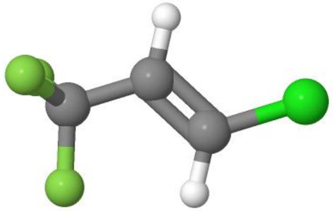
ORC working fluid selection

Hexane



- Alkane commonly used for WHR applications
- Hexane critical temperature = **235 °C** → sub-critical ORC and efficient high-temperature heat recovery
- High molecular complexity → **dry expansion**
- GWP = 5-6
- Pressure levels: 18.03 bar (HP level), 4.68 bar (MP level), and 0.25 bar (LP level)

R1233zde



- New generation hydrofluoroolefin (HFO)
- R1233zde critical temperature = **166 °C** → supercritical HP level with the given superstructure
- High molecular complexity → **dry expansion**
- GWP = 1, near-zero flammability
- Pressure levels: 30 bar (HP level, supercritical), 18.03 bar (MP level), and 1.55 bar (LP level)

Techno-economic optimization

Two scenarios

- Low electricity price = 50 $/MWh
- High electricity price =100 $/MWh

Cost models for Heat Exchangers

Bare module cost of the heat exchanger between hot stream *i* and cold stream *j:*

$$C_{HX} = c_{ref}\left(\frac{A_{ij}}{A_{ref}}\right)^{f}$$

where: A_{ij} heat exchanger area, c_{ref} specific area cost at the reference area A_{ref}, f scale-law exponent

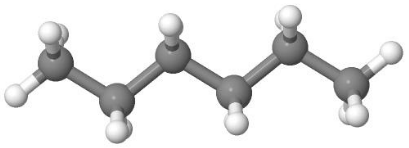
Data for the techno-economic optimization

Parameter	Value
Isentropic efficiency of turbines	0.8
Hydraulic efficiency of pumps	0.8
Mechanical/electrical efficiency of turbines and pumps	0.9
Specific investment cost for turbines at ref. size of 4000 kW, $/kW	430
Scale factor for turbine cost	0.67
Specific cost for heat exchangers at ref. size (external area) of 500 m^2, $/$m^2$	400
Scale factor for heat exchanger cost	0.6
Annualization factor, 1/year	0.15
Equivalent operating hours, h/year	7,884
Multiplication factor for costs due to engineering, procurement & construction	1.5

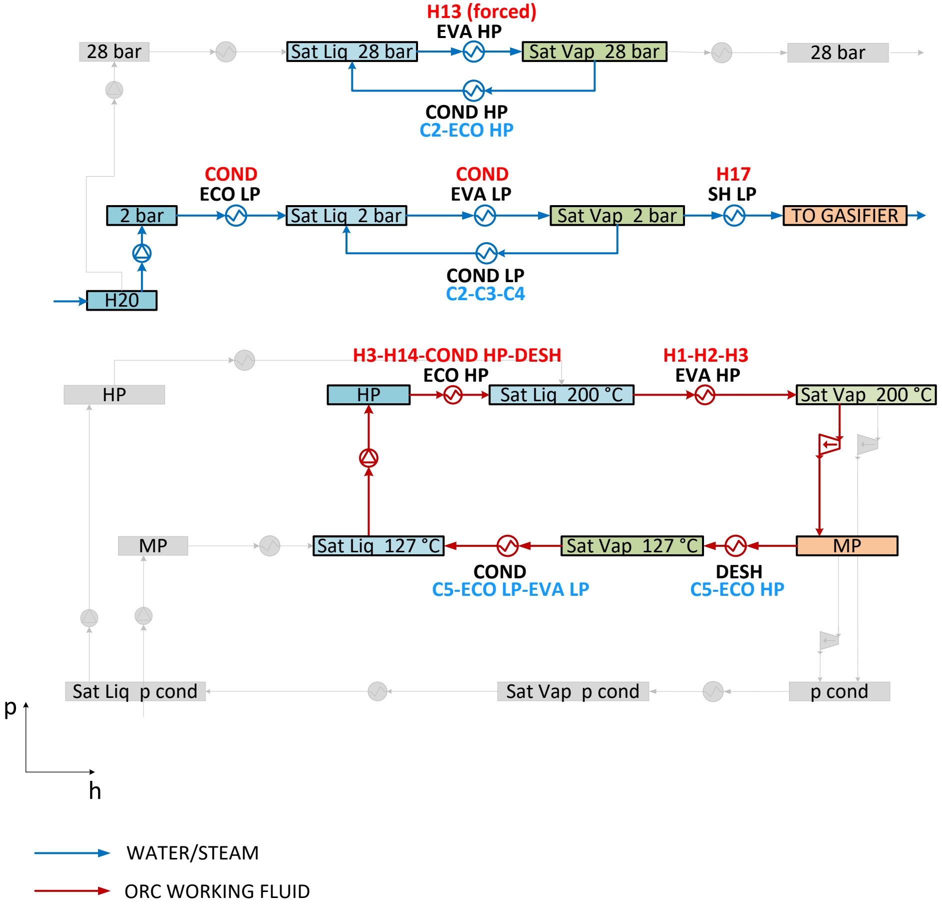
Parameter	Value
Conv. heat transfer coef. of flue gases/syngas (process streams), W/m^2K	60-80
Conv. heat transfer coef. of SEG combustor (radiative), W/m^2K	150
Conv. heat transfer coef. of liquid water, W/m^2K	5,000
Conv. heat transfer coef. of boiling water, W/m^2K	50,000
Conv. heat transfer coef. of superheated steam, W/m^2K	600
Conv. heat transfer coef. of condensing steam, W/m^2K	10,000
Conv. heat transfer coef. of liquid and boiling organic fluids, W/m^2K	1,500
Conv. heat transfer coef. of superheated organic fluids, W/m^2K	1,000
Conv. heat transfer coef. of condensing organic fluids, W/m^2K	3,000
Cooling water pumping and auxiliaries' cost, $/kW	3

Results

Hexane



Optimization results - Hexane	Energy target (maximum power output)	Electricity price = 50 $/MWh	Electricity price = 100 $/MWh
Mass flow rate ORC HP evap. level, kg/s	11.618	0.00	10.436
Mass flow rate ORC MP cond. level, kg/s	9.106	0.00	10.436
Mass flow rate ORC LP cond. level, kg/s	2.512	0.00	0.00
Mass flow rate HP st. network (evap/cond), kg/s	0.364/0.364	0.364/0.364	0.364/0.364
Mass flow rate LP st. network (evap/cond), kg/s	0.757/0.323	0.724/0.291	0.724/0.291
Regenerative ORC (Yes/No)	-	-	Yes
ORC net electric power output, kW	602.40	0.00	346.53
ORC net electric efficiency	16.84%	-	9.83%
Plant net electric efficiency	7.70%	-	4.43%
Number of heat exchangers	-	19	25
Cost of heat exchangers, k$	-	659.47	1,175.17
Cost of machinery, k$	-	0.00	525.65
TAC (ORC, steam network and HEN), k$/year	-	109.59	-7.23
LCOE (ORC, steam network and HEN), $/MWh	-	-	96.96



Results

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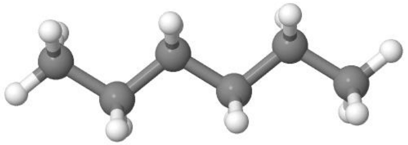

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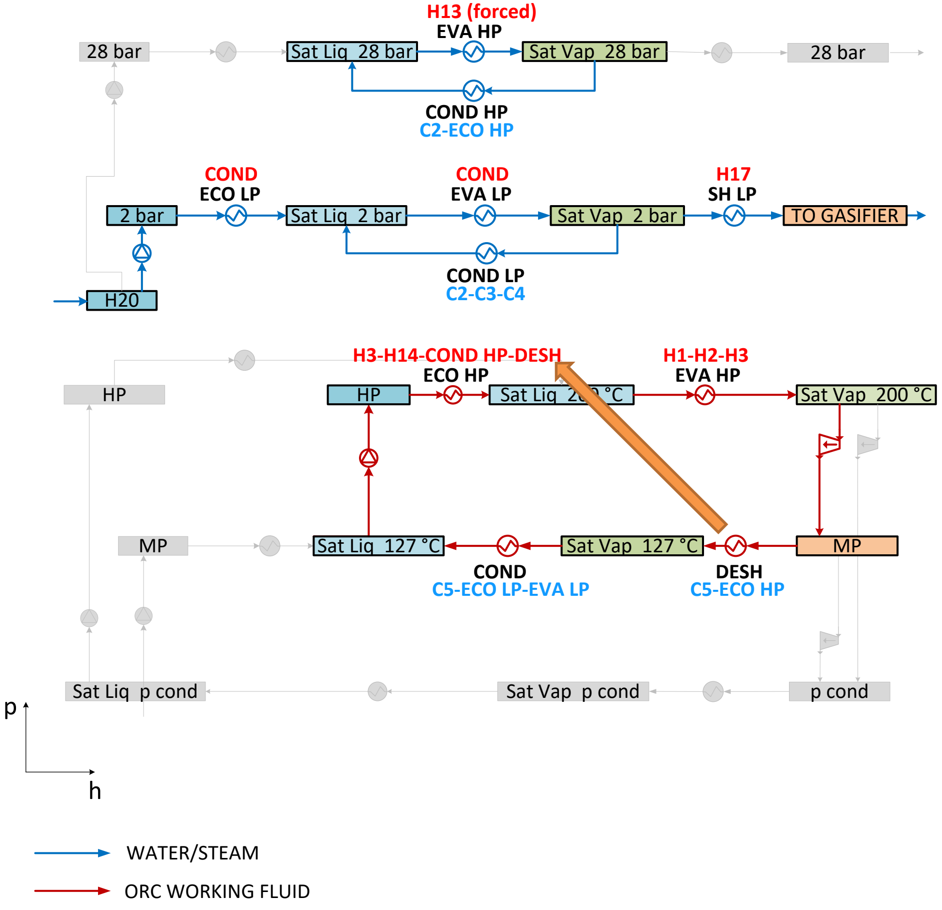
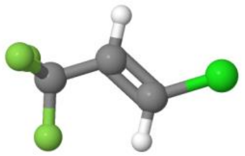
Mass flow rate ORC MP cond. level, kg/s	9.106	0.00	10.436
Mass flow rate ORC LP cond. level, kg/s	2.512	0.00	0.00
Mass flow rate HP st. network (evap/cond), kg/s	0.364/0.364	0.364/0.364	0.364/0.364
Mass flow rate LP st. network (evap/cond), kg/s	0.757/0.323	0.724/0.291	0.724/0.291
Regenerative ORC (Yes/No)	-	-	Yes
ORC net electric power output, kW	602.40	0.00	346.53
ORC net electric efficiency	16.84%	-	9.83%
Plant net electric efficiency	7.70%	-	4.43%
Number of heat exchangers	-	19	25
Cost of heat exchangers, k$	-	659.47	1,175.17
Cost of machinery, k$	-	0.00	525.65
TAC (ORC, steam network and HEN), k$/year	-	109.59	-7.23
LCOE (ORC, steam network and HEN), $/MWh	-	-	96.96

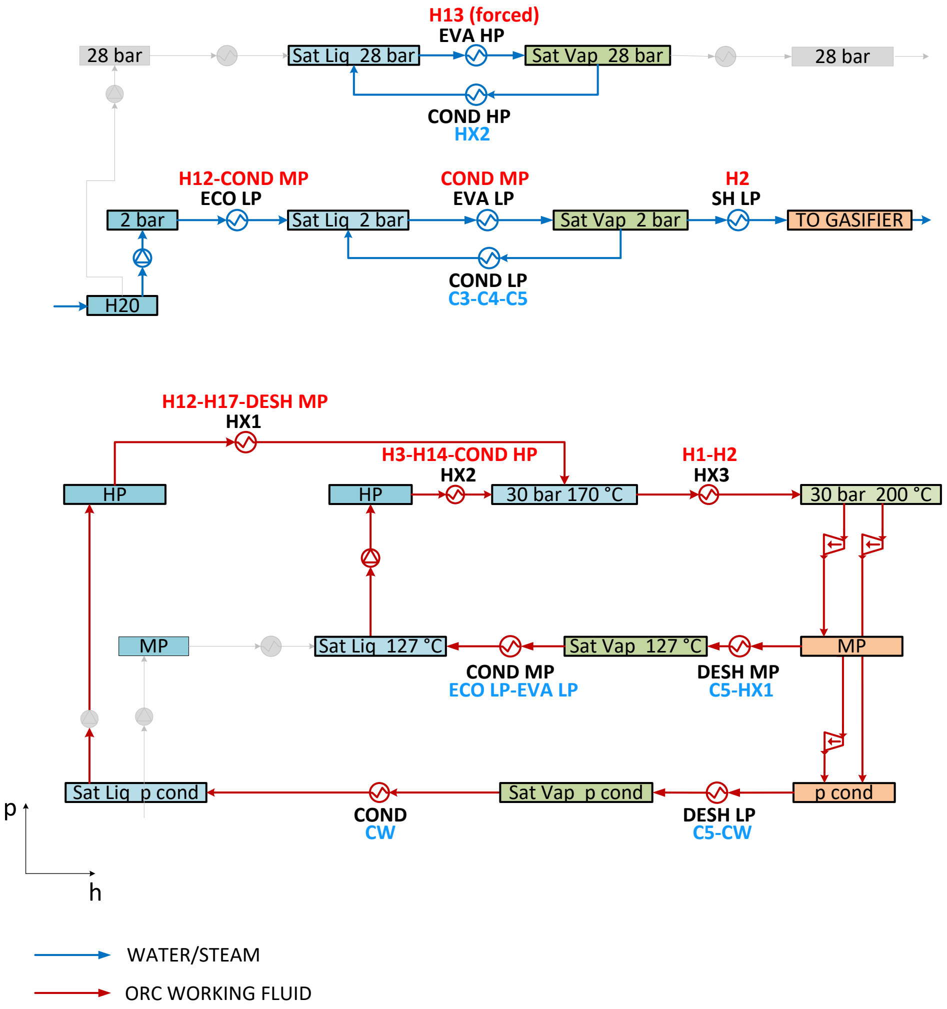


Results

R1233zde

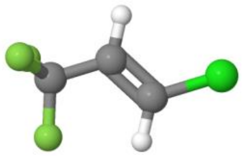


Optimization results – R1233zde	Energy target (maximum power output)	Electricity price = 50 $/MWh	Electricity price = 100 $/MWh
Mass flow rate ORC HP evap. level, kg/s	30.773	0.00	23.044
Mass flow rate ORC MP cond. level, kg/s	24.294	0.00	17.906
Mass flow rate ORC LP cond. level, kg/s	6.479	0.00	5.138
Mass flow rate HP st. network (evap/cond), kg/s	0.364/0.364	0.364/0.364	0.364/0.364
Mass flow rate LP st. network (evap/cond), kg/s	0.996/0.563	0.724/0.291	0.890/0.456
Regenerative ORC (Yes/No)	-	-	Yes
ORC net electric power output, kW	519.46	0.00	401.76
ORC net electric efficiency	14.26%	-	10.12%
Plant net electric efficiency	6.64%	-	5.14%
Number of heat exchangers	-	19	30
Cost of heat exchangers, k$	-	659.47	1,572.21
Cost of machinery, k$	-	0.00	730.79
TAC (ORC, steam network and HEN), k$/year	-	109.59	39.78
LCOE (ORC, steam network and HEN), $/MWh	-	-	112.09



Results

R1233zde



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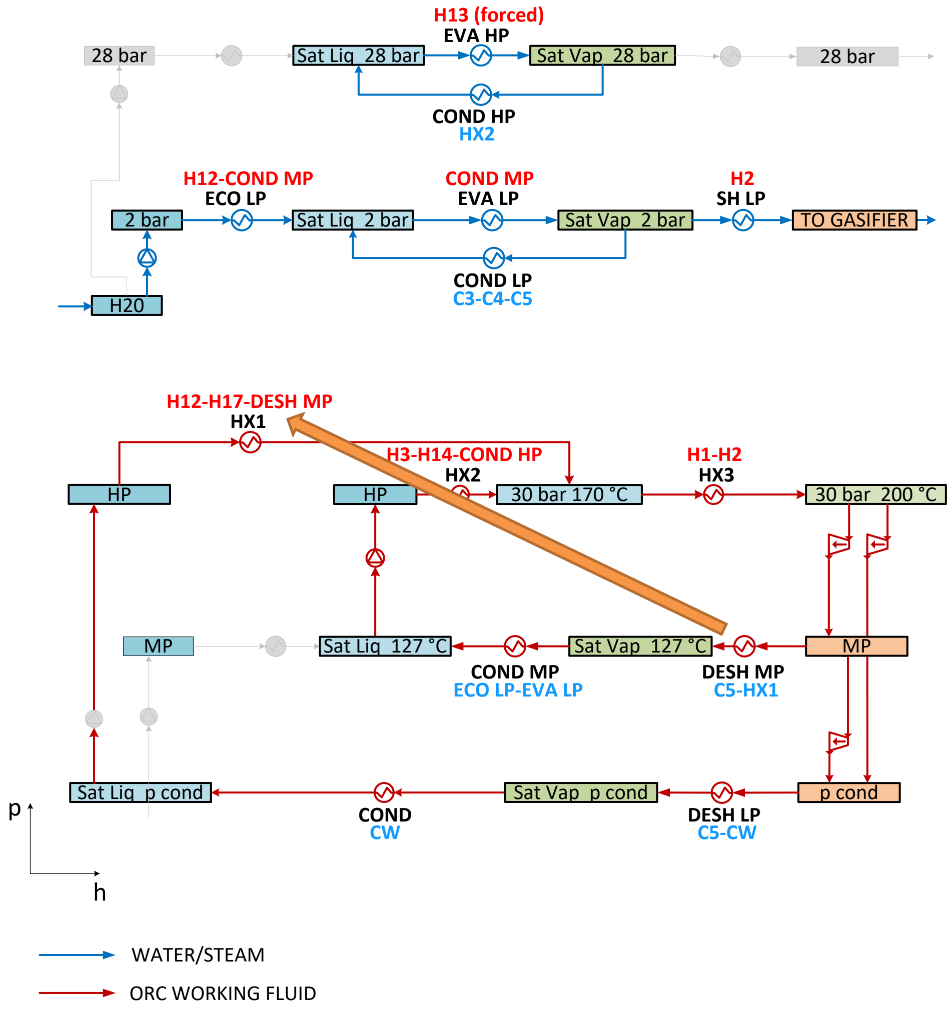

Conclusions

- This preliminary study on a **novel biomass to methanol production plant** showed that the use of a heat recovery ORC is economically advantageous **only for high electricity prices**
- Assumption: **Nth-of-a-kind (NOAK) analysis:** low contingencies, installation & engineering costs, etc.
- The techno-economic optimization, performed considering hexane and R1233zde as candidate fluids, shows that a **back-pressure ORC using hexane** is the best option in terms of costs
- The economic-optimal ORC designs are noticeably **less efficient than the energy target** estimates due to the need of limiting the investment costs of the equipment units
- Due to **hexane flammability**, extra costs (not considered here) in terms of investment and operating costs might appear to meet regulatory requirements and safety provisions
- **Future works** will address the optimization of the pressure and temperature levels of the ORC and the comparison with other working fluids

THANK YOU FOR YOUR ATTENTION!

ANY QUESTIONS?

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