Process synthesis of advanced NH_3 and MeOH plants with gas switching reforming (GSR)

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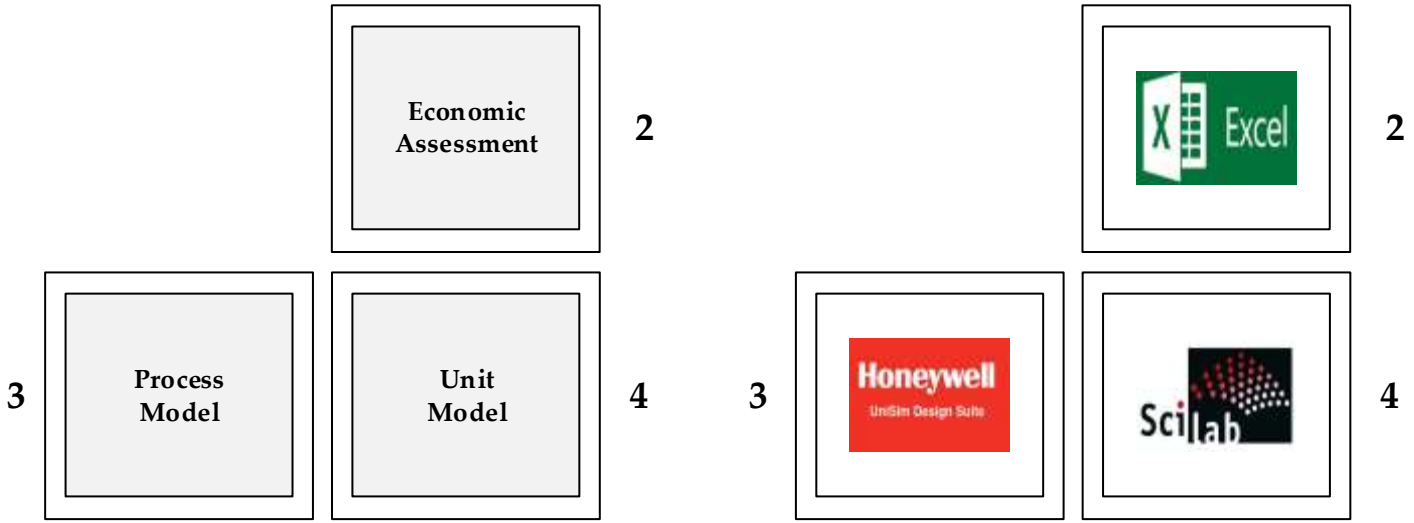
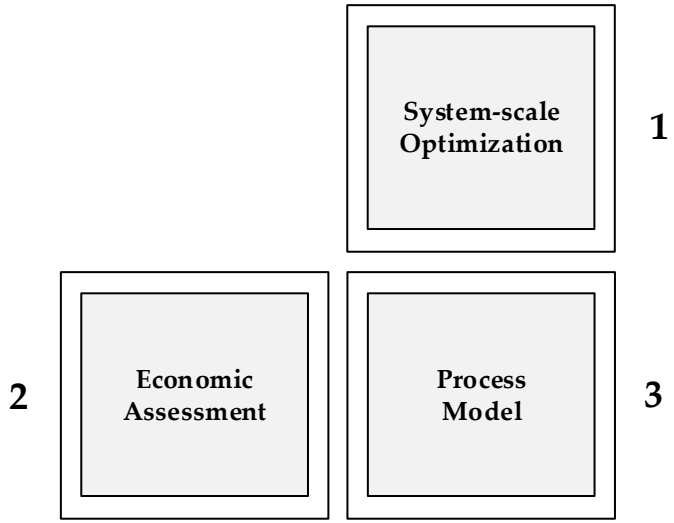
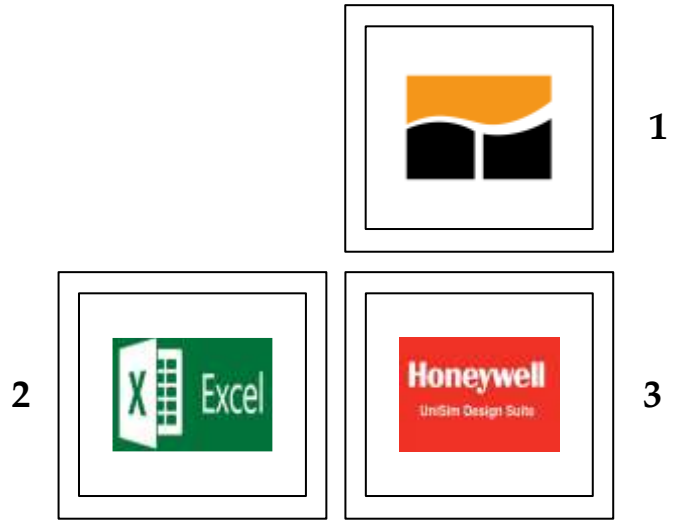
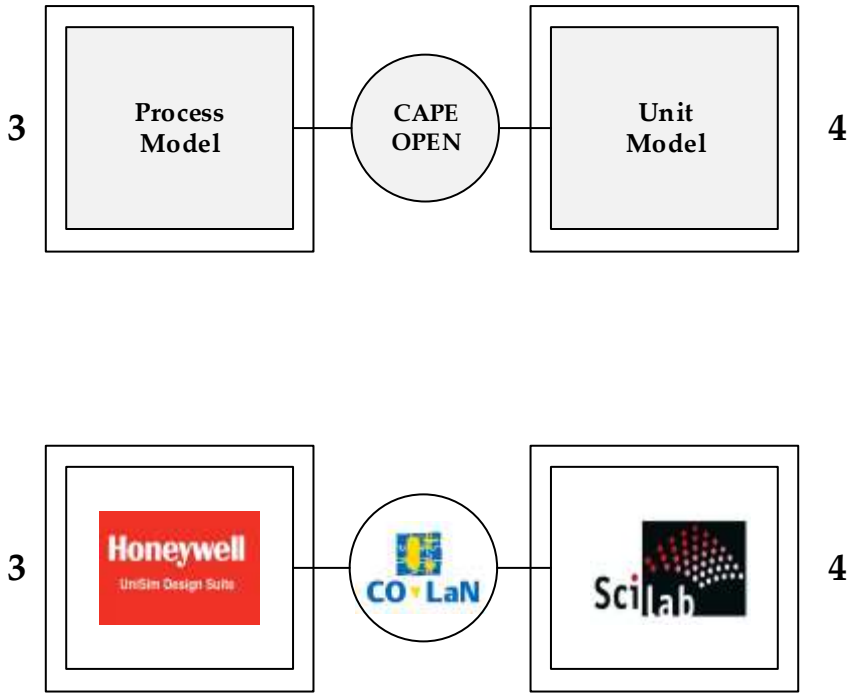

Economic Assessment
2
Excel
2
3
Process Model
Unit Model
4
3
Honeywell
UniSim Design Suite
Scilab
4

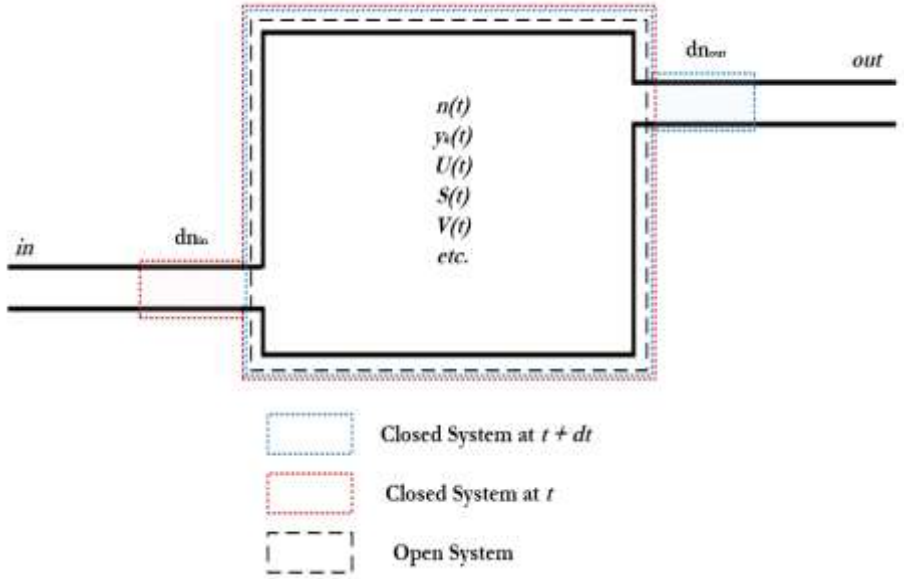

System-scale Optimization
1
2
Economic Assessment
Process Model
3

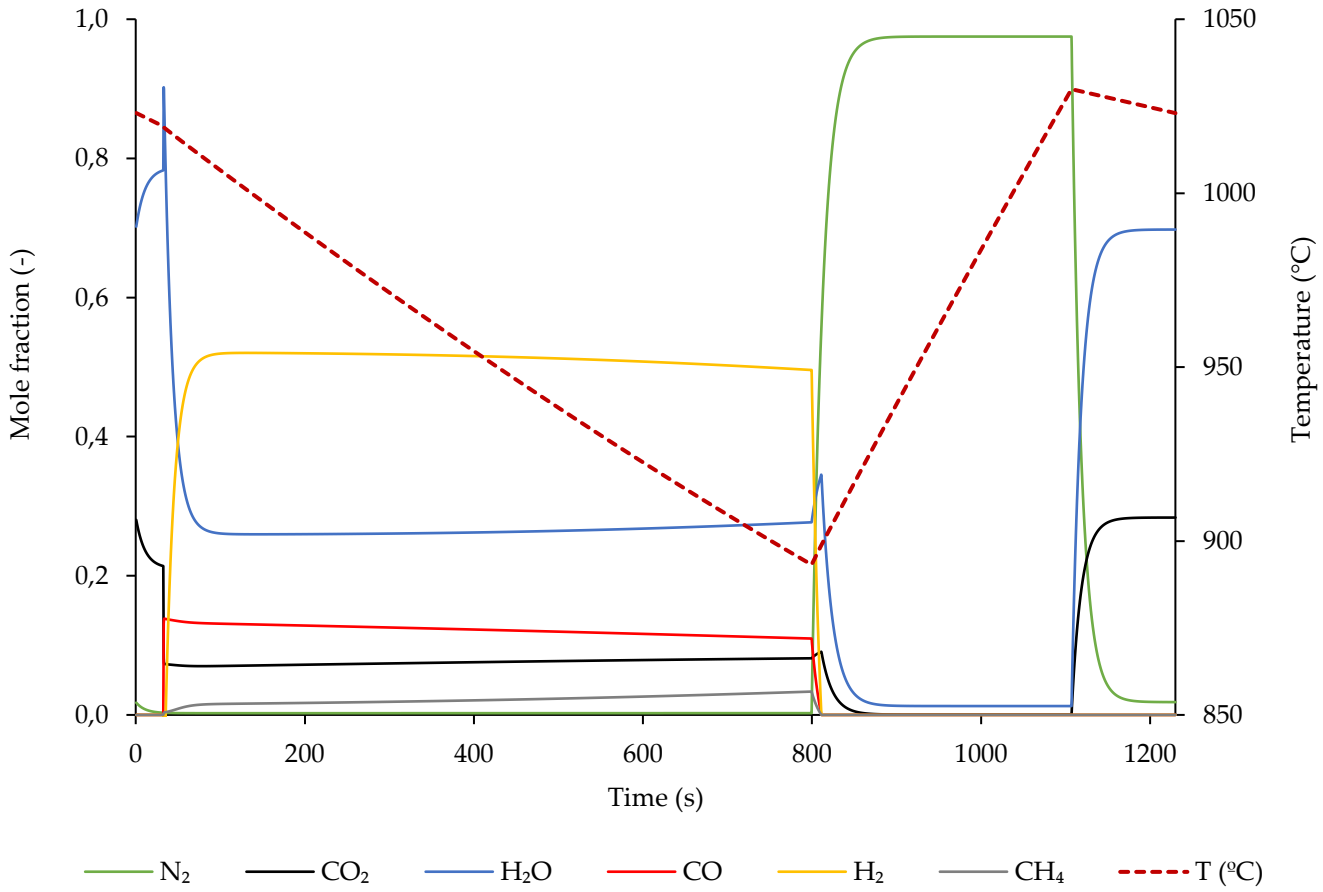

1
2
Excel
Honeywell
UniSim Design Suite
3


3
Process Model
CAPE OPEN
Unit Model
4
3
Honeywell
UniSim Design Suite
CO-LaN
Scilab
4

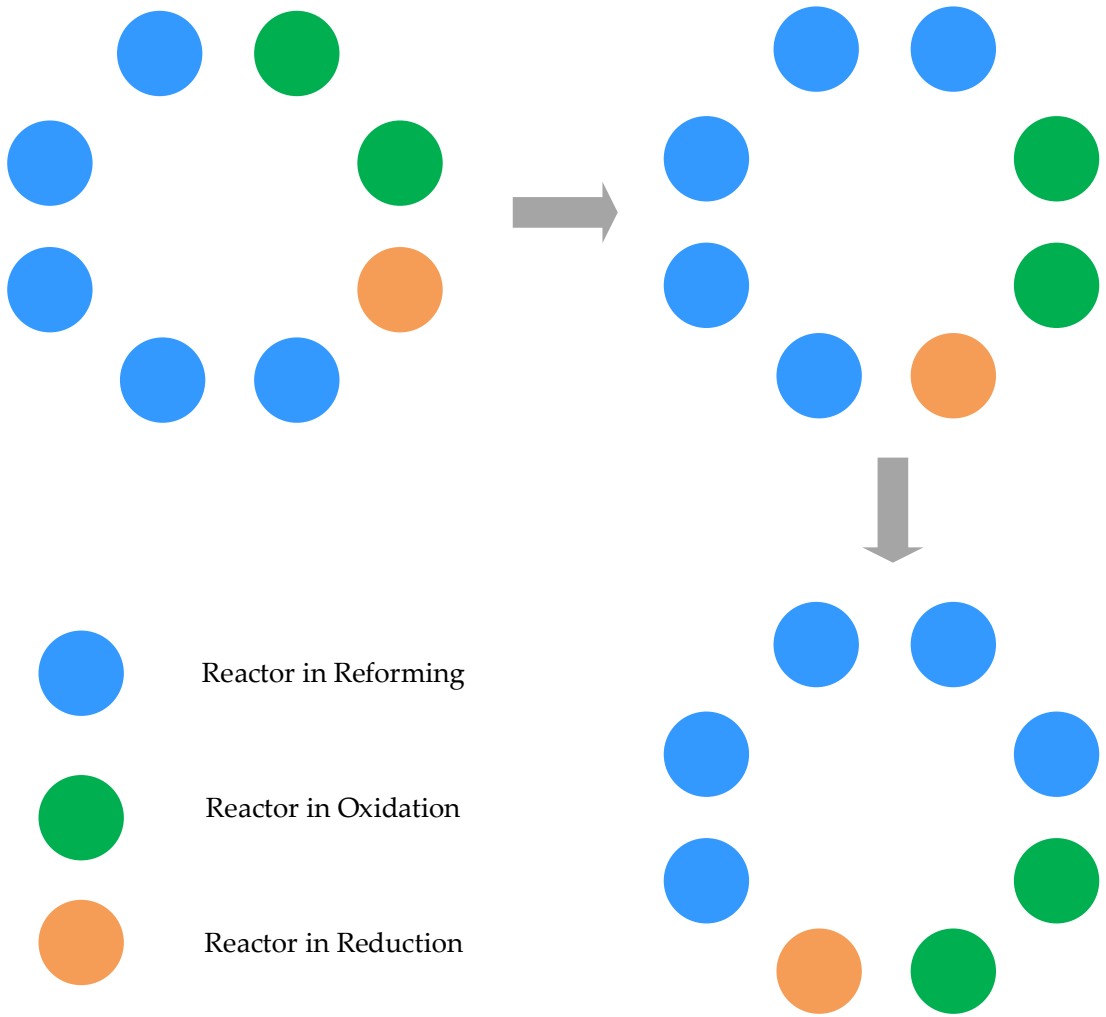
GSR reactor

Mass Balance	$\frac{dn_k}{dt} = F_{in} y_{in,k} + F_{out} y_{out,k} + \sum_{r=1}^{R} \upsilon_{r,k} \xi_r$
Energy Balance	$\frac{dT}{dt} = \frac{-F_{in} \sum_k y_{in,k} \int_{T_{in}}^{T} c_{p,k} dT + \sum_{r=1}^{R} \xi_r (-\Delta H_{r,T})}{\sum_k n_k \, c_{p,k}}$
Outlet flow	$F_{out} = F_{in} + \sum_{R}^{k \in gases} \upsilon_{k,r} \xi_r + \frac{P V_{gas}}{R T^2} \dot{T}$

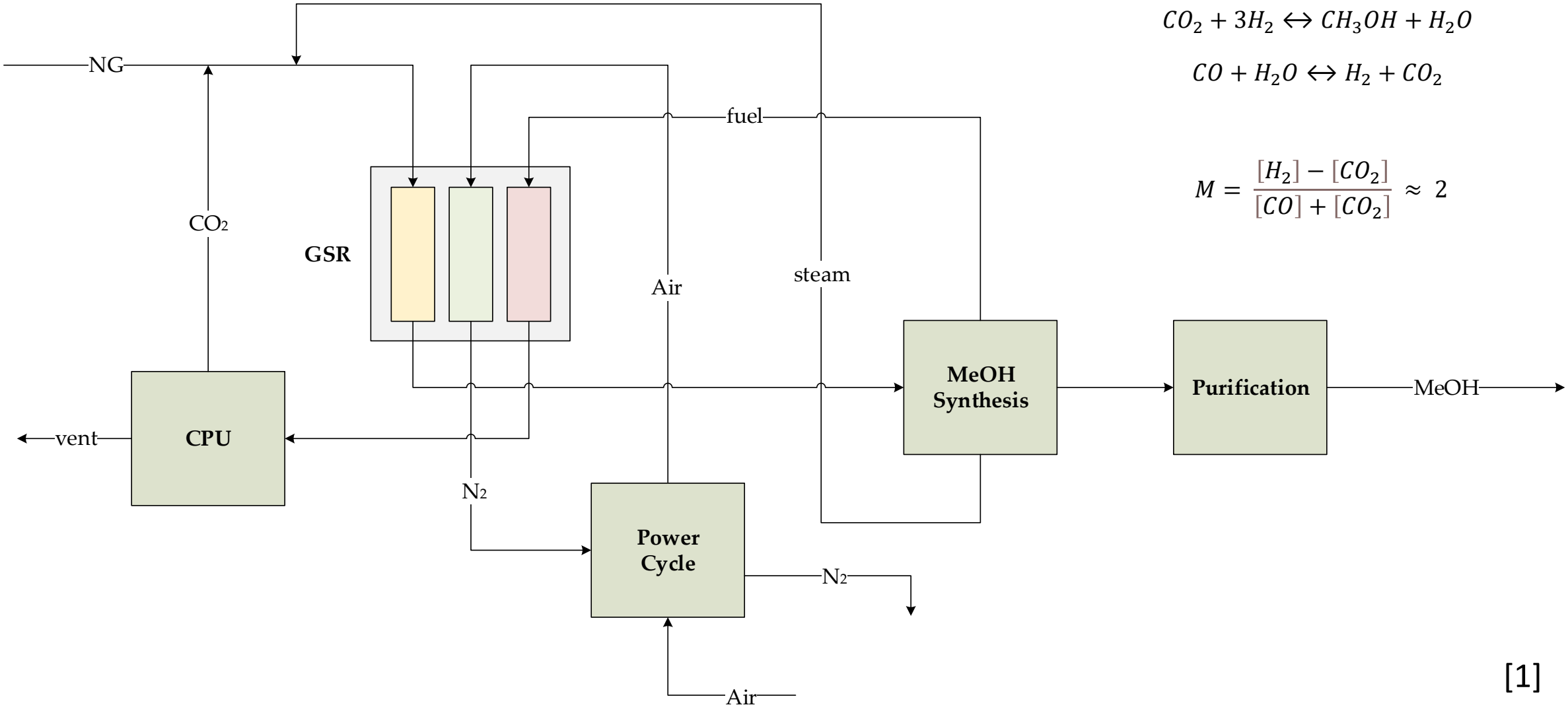



1,0
0,8
0,6
0,4
0,2
0,0
Mole fraction (-)
0
200
400
600
800
1000
1200
Time (s)
1050
1000
950
900
850
Temperature (°C)
N2
CO2
H2O
CO
H2
CH4
T (ºC)

GSR cluster


Reactor in Reforming
Reactor in Oxidation
Reactor in Reduction

GSR-MeOH



$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$$

$$CO + H_2O \leftrightarrow H_2 + CO_2$$

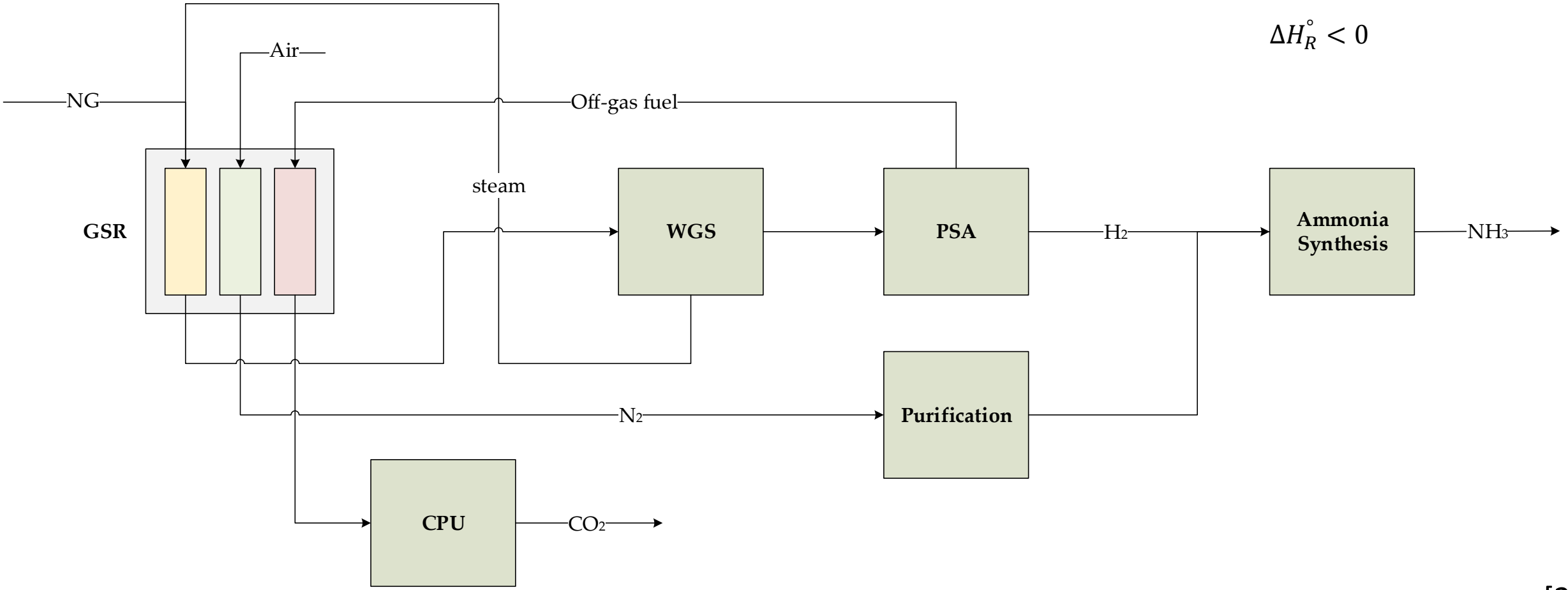
$$M = \frac{[H_2] - [CO_2]}{[CO] + [CO_2]} \approx 2$$

[1]

GSR-NH_3

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

$$\Delta H_R^{\circ} < 0$$



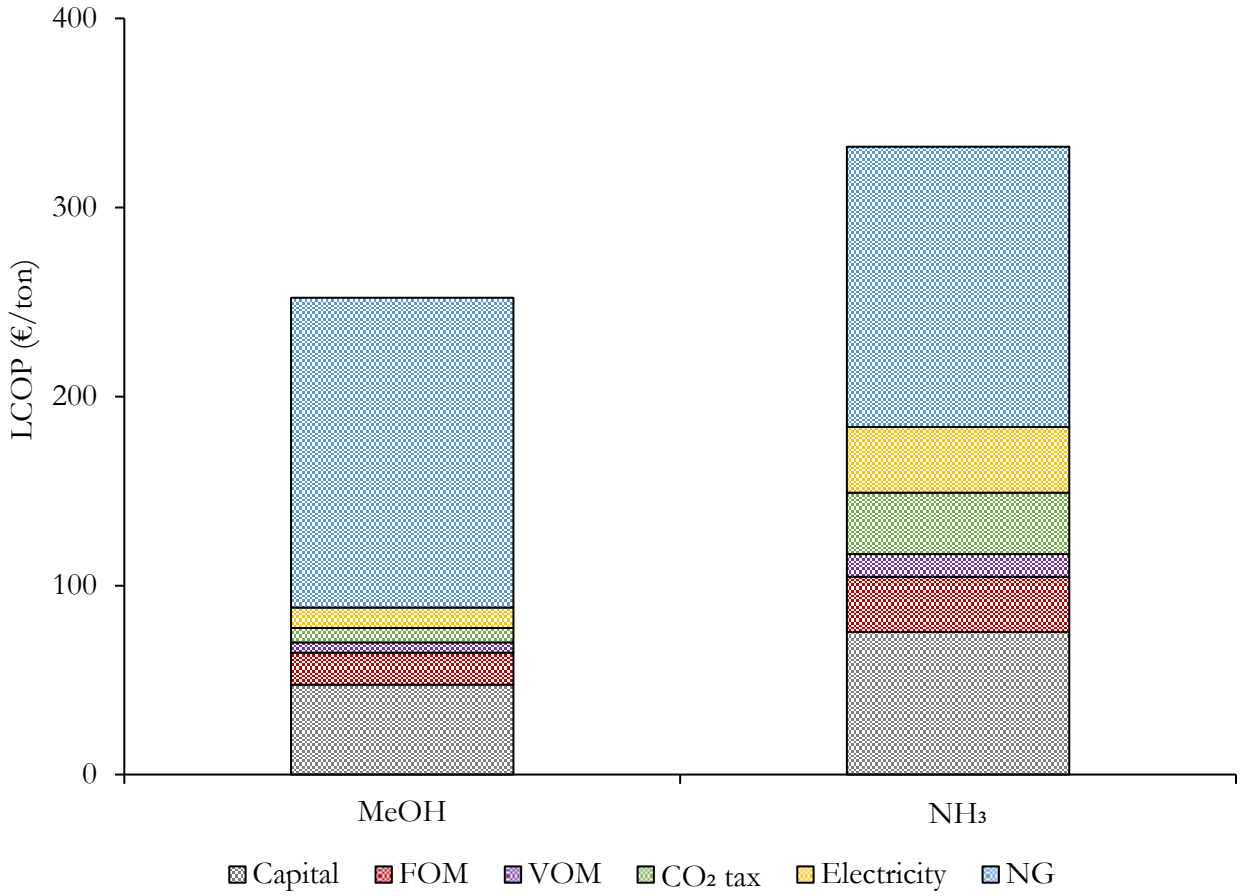
[2]

CAPE-OPEN unit

1. getFeedProp
2. getParameter
3. setProduct

Input	Output
Air	N_2
Fuel	Reduction gases
Natural gas	Syngas
nº of reactors	fl. velocities

Results


400
300
200
100
0
LCOP (€/ton)
MeOH
NH3
Capital
FOM
VOM
CO2 tax
Electricity
NG

[3]

Conclusions

- CAPE-OPEN Unisim Design – Scilab unit operation
- Transient gas switching reforming (GSR) model connected to stationary plant
- GSR model can be specified in process flowsheet
- Research output: 7 (9)

References

[1] C. Arnaiz del Pozo, S. Cloete and Á Jiménez Álvaro, "Techno-economic assessment of long-term methanol production from natural gas and renewables" *Energy Conversion and Management.* 2022, vol. 266, pp. 115785.

[2] C. Arnaiz del Pozo and S. Cloete, "Techno-economic assessment of blue and green ammonia as energy carriers in a low-carbon future" *Energy Conversion and Management.* 2022, vol. 255, pp. 115312.

[3] Carlos Arnaiz del Pozo, Schalk Cloete, and Ángel Jiménez Álvaro. Standard Economic Assessment (SEA) Tool. Available from: https://bit.ly/3hyF1TT .