The use of Cape Open tools in research at the University of Cape Town.

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October, 2019

Outline

Background

Research topics involving CO

- **SCC conversion-energy model**
  - Riser reactor
  - Integration of the energy
- **Carbon black furnace**
  - Preheat stage Gibbs reactor
  - Carbon formation Gibbs reactor
- **GTL: COCO**
  - Air supplied ATR-FT recycle system
  - ATR-Reformer air based energy coupling

Summary

- Work is ongoing

Background

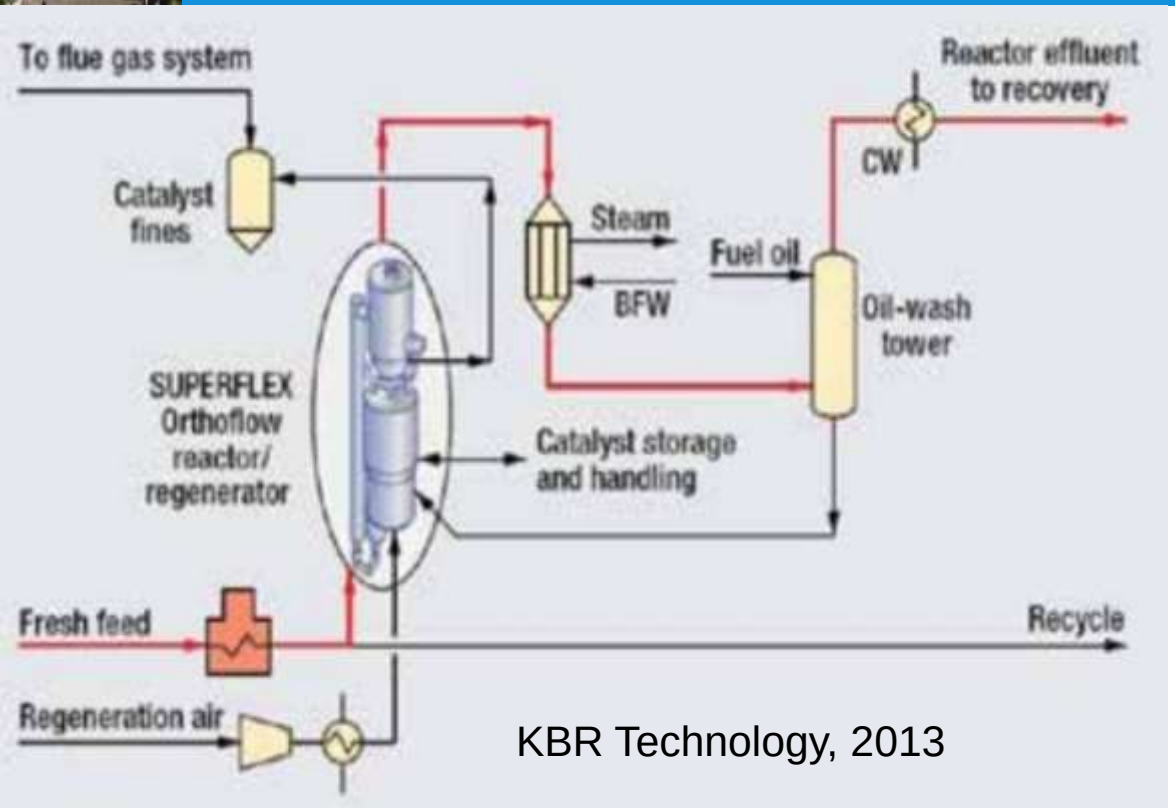
COCO, Scilab and Cape Open tools used for

- **Teaching**
- **Research**

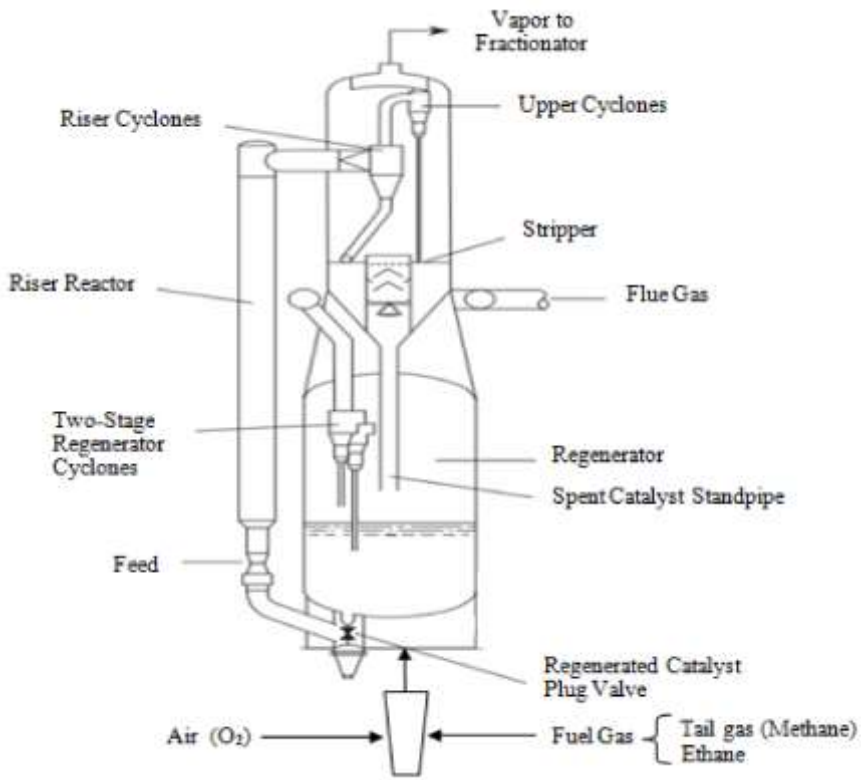
The presentation is about the ongoing research work

- **Advantages**
  - Simple flexible platform, fast prototyping, integrates well
  - There is prior knowledge
- **Limitations**
  - Database, performance
  - Often study anomalous systems or systems with large number of species
  - Need for extensive customisation, compromises needed (nice to have versus the thesis must be completed on time)
  - We are still not experts

SCC (superflex catalytic cracking)



Schematic flow diagram for a SCC unit



Operational details of the SCC unit

Some notes

- Energy integration
- Catalyst:fuel ratio >> 10
- Products used for regeneration, heating
- Catalyst is the energy carrier
- T>>600C
- Products: target light olefins and aromatics

SCC – reactions and NG

Reaction families that occur in the SCC

Reaction Class	Specific Reaction
1. Cracking :	
• **Paraffin cracked to olefins and smaller paraffins;**	$C_{10}H_{22} \rightarrow C_4H_{10} + C_6H_{12}$
• **Olefins cracked to smaller olefins;**	$C_9H_{18} \rightarrow C_4H_8 + C_5H_{10}$
• **Aromatic side-chain scission;**	$ArC_{10}H_{21} \rightarrow ArC_5H_9 + C_5H_{12}$
• **Naphthenes (cycloparaffins) cracked to olefins and smaller compounds**	Cyclo-$C_{10}H_{20} \rightarrow C_6H_{12} + C_4H_8$
2. Isomerization:	
• **Olefin bond shift;**	1-$C_4H_8 \rightarrow$ trans-2-C_4H_8
• **Normal olefin to iso-olefin;**	n-$C_5H_{10} \rightarrow$ iso-C_5H_{10}
• **Normal paraffin to isoparaffin;**	n-$C_4H_{10} \rightarrow$ iso-C_4H_{10}
3. Hydrogen transfer:	
• **Cycloaromatization: Paraffin and olefins are converted to aromatics and paraffins.**	Naphthene + olefin → aromatic + paraffin
4. Transalkylation/alkyl-group transfer	$C_6H_4(CH_3)2 + C_6H_6 \rightarrow 2\ C_6H_5CH_3$
5. Cyclization of olefins to naphthenes	$C_7H_{14} \rightarrow CH_3$-cyclo-$C_6H_{11}$
6. Dehydrogenation	n-$C_8H_{18} \rightarrow C_8H_{16} + H_2$
7. Dealkylation	Iso-C_3H_7-$C_6H_5 \rightarrow C_6H_6 + C_3H_6$
8. Condensation: to produce multiple- ring aromatics.	Ar-CH = CH_2 + R1CH=CHR2 → Ar-Ar + 2H

NG (Temane, Mozambique)

Component	Mass (Wt %)
Methane	0.00
Ethane	0.03
Propane	0.70
i-Butane	1.36
n-butane	3.2
Neo-Pentane	0.11
i-Pentane	4.07
n-Pentane	4.58
Benzenes	0.16
Hexanes	12.66
Heptane	26.44
Toluene	0.36
Octane	26.22
Xylene	0.60
Nonane	9.38
Decane	5.07
Undecane	2.87
Dodecane	1.52
Tridecane	0.67

SCC – Feed, measured products

FEED to SCC

Flow Hydrogen	0.0 kg / h
Flow Oxygen	0.0 kg / h
Flow Nitrogen	0.0 kg / h
Flow Carbon dioxide	0.0 kg / h
Flow Methane	0.0 kg / h
Flow Ethylene	0.0 kg / h
Flow Ethane	3.0 kg / h
Flow Propylene	0.0 kg / h
Flow Propane	70.0 kg / h
Flow 1,3-butadiene	0.0 kg / h
Flow 1-butene	0.0 kg / h
Flow N-butane	456.0 kg / h
Flow Isoprene	0.0 kg / h
Flow 1-pentene	0.0 kg / h
Flow N-pentane	1692.0 kg / h
Flow 1-hexene	0.0 kg / h
Flow N-hexane	2537.0 kg / h
Flow 1-heptene	0.0 kg / h
Flow N-heptane	846.0 kg / h
Flow 1-octene	0.0 kg / h
Flow N-octane	2537.0 kg / h
Flow 1-nonene	0.0 kg / h
Flow N-nonane	846.0 kg / h
Flow N-decane	507.0 kg / h
Flow N-undecane	287.0 kg / h
Flow N-dodecane	152.0 kg / h
Flow N-tridecane	67.0 kg / h
Flow Benzene	0.0 kg / h
Flow Toluene	0.0 kg / h
Flow M-xylene	0.0 kg / h
Flow Pyrene	0.0 kg / h
Flow Water	0.0 kg / h

Products, Coke(=pyrene) added as 4wt%

	Hydrogen	282.94
	Methane	226.35
	Ethylene	949.88
	Ethane	303.15
	Propylene	2879.95
	Propane	181.89
measured lumped species	all C4s	1123.69
	all C5s	642.68
	all C6s+Bz	964.03
	all C7s+Tol	321.34
	all C8s+Xyl	964.03
	N-nonane	321.34
	N-decane	217.26
	N-undecane	123.28
	N-dodecane	65.68
	N-tridecane	28.29
coke →	Pyrene	404.20

Matrix method – COCO fixed conversion

$$\begin{vmatrix} F_{out,1} \\ F_{out,2} \\ \vdots \\ F_{out,i} \\ \vdots \\ F_{out,n} \end{vmatrix} = \begin{vmatrix} F_{in,1} \\ F_{in,2} \\ \vdots \\ F_{in,i} \\ \vdots \\ F_{in,n} \end{vmatrix} + \begin{vmatrix} \eta_{1,1} & \eta_{1,2} & \cdots & \cdots & \cdots & \eta_{1,m} \\ \eta_{2,1} & \eta_{2,2} & & & & \vdots \\ \vdots & & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & \vdots \\ \eta_{n,1} & \cdots & \cdots & \cdots & \cdots & \eta_{n,m} \end{vmatrix} \times \left(\begin{vmatrix} X_1 \\ X_2 \\ \vdots \\ X_j \\ \vdots \\ X_m \end{vmatrix} \cdot \begin{vmatrix} F_{in,i} \\ F_{in,j} \\ \vdots \\ F_{in,k} \\ \vdots \\ F_{in,m} \end{vmatrix} \right)$$

Products Feed Stoichiometric matrix Conversion x reference Extent of reaction

$$X = \frac{\left(\eta^T \times \eta\right)^{-1} \left[\eta^T \left(F_{out} - F_{in}\right)\right]}{F_X}$$

inversion possible to get extent of reaction
IF reactions are independent

Missing species, lumped species

Least squares method used

$$\Psi(X) = \sum \epsilon_i^2$$

$$\epsilon_i = F_{out,i}^{measured} - F_{out,i}^{model}$$

- Error based on species
- Cannot fit uniquely for more conversions (extents) than there are reactions

When there are lumps

$$\epsilon_i = F_{out,lump1}^{measured} - \sum_{j=lump1} F_{out,j}^{model}$$

- Works as long as the number of errors > number of equations
- More species measured (lump=species) than equations

Fixed conversion reactor – to use in COCO

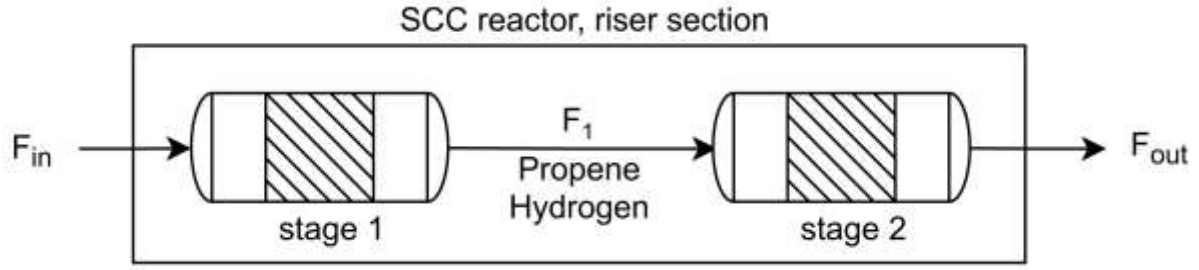
Need to regress data to obtain product species

Approach 1

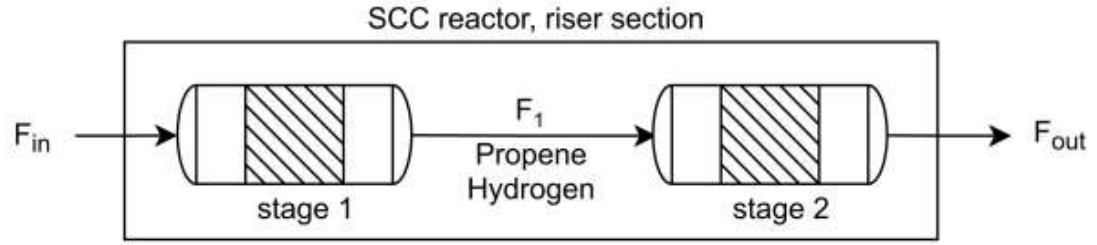
- **Use elementary reactions**
- **System does not solve uniquely,**
- **complicated by series reaction steps**

Approach 2

- **Premise: It does not matter what happens inbetween, as long as the input and output are correctly represented, this ensures**
  - Mass balance correct
  - Energy correctly accounted for
- **2 stage reactor system**



SCC - Two stage riser section



Feed converted to propene + H2

Reaction i	Stage 1 Reactions
Reaction 1	$C_2H_6 \rightarrow 2/3C_3H6 + H_2$
Reaction 2	$C_3H_8 \rightarrow C_3H_6 + H_2$
Reaction 3	$C_4H_{10} \rightarrow 4/3C_3H_6 + H_2$
Reaction 4	$C_5H_{12} \rightarrow 5/3C_3H_6 + H_2$
Reaction 5	$C_6H_{14} \rightarrow 6/3C_3H_6 + H_2$
Reaction 6	$C_7H_{16} \rightarrow 7/3C_3H_6 + H_2$
Reaction 7	$C_8H_{18} \rightarrow 8/3C_3H_6 + H_2$
Reaction 8	$C_9H_{20} \rightarrow 9/3C_3H_6 + H_2$
Reaction 9	$C_{10}H_{22} \rightarrow 10/3C_3H_6 + H_2$
Reaction 10	$C_{11}H_{24} \rightarrow 11/3C_3H_6 + H_2$
Reaction 11	$C_{12}H_{26} \rightarrow 12/3C_3H_6 + H_2$
Reaction 12	$C_{13}H_{28} \rightarrow 13/3C_3H_6 + H_2$

All reactions parallel, easy to tune selectivity

Propene + H2 converted to all assumed products
N reactions < N measured species

Reaction i	Stage 2 Reactions
Reaction 1	$C_3H_6 + 3H_2 \rightarrow 3CH_4$
Reaction 2	$C_3H_6 \rightarrow 3/2C_2H_4$
Reaction 3	$C_3H_6 + 3/2H_2 \rightarrow 3/2C_2H_6$
Reaction 4	$C_3H_6 + H_2 \rightarrow C_3H_8$
Reaction 5	$C_3H_6 \rightarrow 1/16(C_4H_6 + 10C_4H_8 + C_4H_{10})$
Reaction 6	$C_3H_6 \rightarrow 1/20(C_5H_8 + 10C_5H_{10} + C_5H_{12})$
Reaction 7	$C_3H_6 \rightarrow 1/12(4C_6H_6 + C_6H_{12} + C_6H_{14}) + 11/12H_2$
Reaction 8	$C_3H_6 \rightarrow 1/14(4C_7H_8 + C_7H_{14} + C_7H_{16}) + 11/14H_2$
Reaction 9	$C_3H_6 \rightarrow 1/16(4C_8H_{10} + C_8H_{16} + C_8H_{18}) + 11/16H_2$
Reaction 10	$C_3H_6 + 1/6H_2 \rightarrow 1/6(C_9H_{18} + C_9H_{20})$
Reaction 11	$C_3H_6 + 3/10H_2 \rightarrow 3/10C_{10}H_{22}$
Reaction 12	$C_3H_6 + 3/11H_2 \rightarrow 3/11C_{11}H_{24}$
Reaction 13	$C_3H_6 + 1/4H_2 \rightarrow 1/4C_{12}H_{26}$
Reaction 14	$C_3H_6 + 3/13H_2 \rightarrow 3/13C_{13}H_{28}$
Reaction 15	$C_3H_6 \rightarrow 3/16C_{16}H_{10} + 33/16H_2$

Assumptions about the products made

SCC – regression, stage 2 conversions

Prediction of the data

i	name	Measured(kg/h)	Predicted(kg/h)
1	Hydrogen(!)	283	282.9
2	Methane	226.3	226.4
3	Ethylene	949.9	949.9
4	Ethane	303.1	303.2
5	Propylene	2879.9	2880
6	Propane	181.9	181.9
7	all C4s	1123.7	1123.7
8	all C5s	642.7	642.7
9	all C6s+Bz	964	964
10	all C7s+Tol	321.3	321.3
11	all C8s+Xyl	964	964
12	N-nonane	321.3	321.3
13	N-decane	217.3	217.3
14	N-undecane	123.3	123.3
15	N-dodecane	65.7	65.7
16	N-tridecane	28.3	28.3
17	Pyrene	404.2	404.2

Conversions

Conversion of reaction i

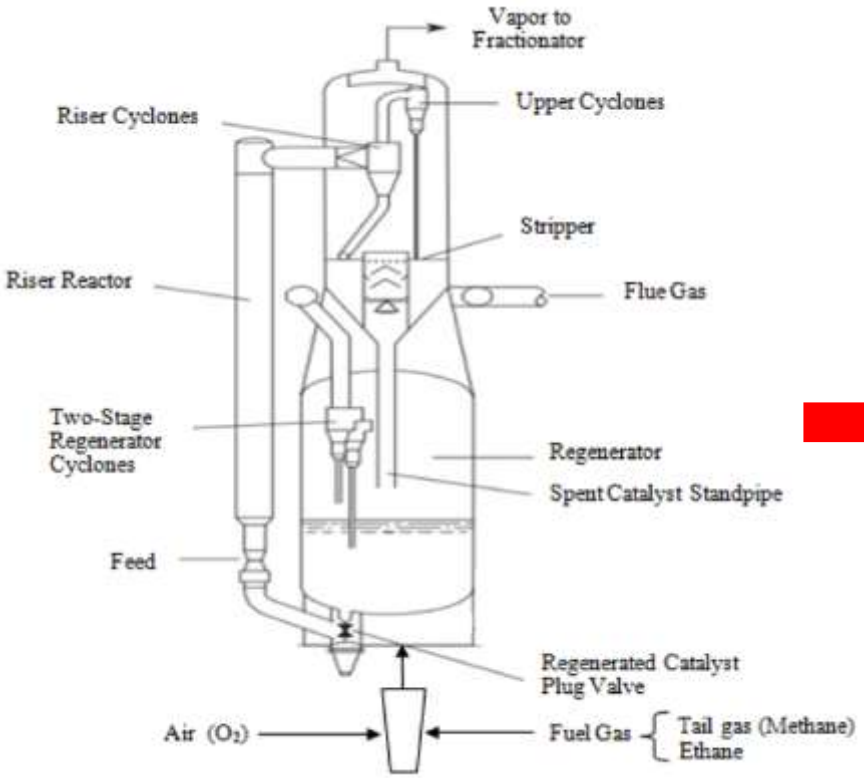
X(1)= 0.02022
X(2)= 0.09707
X(3)= 0.0289
X(4)= 0.01774
X(5)= 0.11483
X(6)= 0.06568
X(7)= 0.10304
X(8)= 0.03412
X(9)= 0.10187
X(10)= 0.03258
X(11)= 0.02189
X(12)= 0.01244
X(13)= 0.00663
X(14)= 0.00286
X(15)= 0.04583

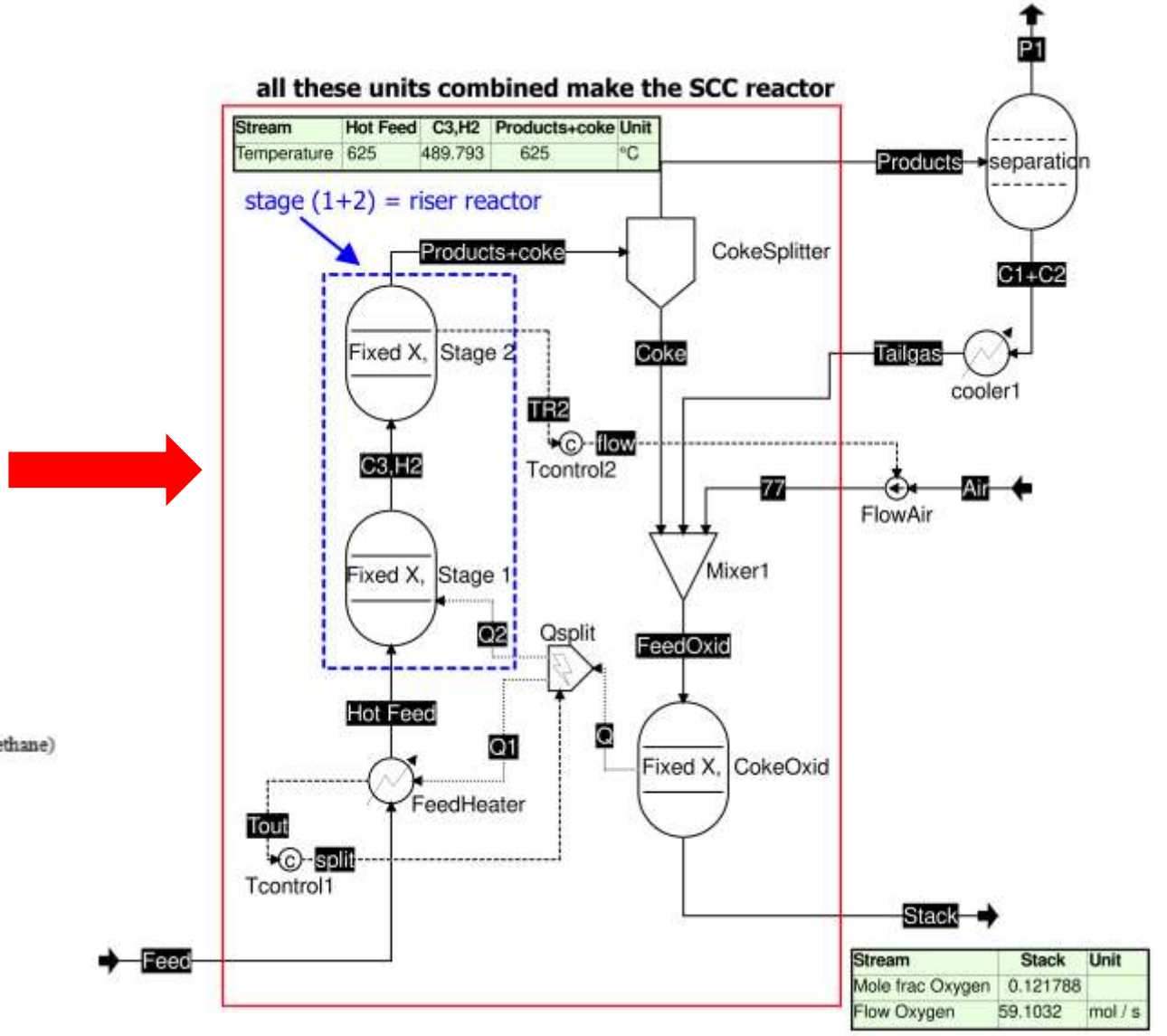
i	name	Mout(kg/h)
1	Hydrogen	283
2	Methane	226.3
3	Ethylene	949.9
4	Ethane	303.1
5	Propylene	2879.9
6	Propane	181.9
7	1,3-butadiene	90.3
8	1-butene	936.4
9	N-butane	97
10	Isoprene	52
11	1-pentene	535.6
12	N-pentane	55.1
13	1-hexene	168
14	N-hexane	172.1
15	1-heptene	55.7
16	N-heptane	56.8
17	1-octene	166.1
18	N-octane	169.1
19	1-nonene	159.4
20	N-nonane	161.9
21	N-decane	217.3
22	N-undecane	123.3
23	N-dodecane	65.7
24	N-tridecane	28.3
25	Benzene	623.9
26	Toluene	208.9
27	M-xylene	628.8
28	Pyrene	404.2

The unpacking of the lumped analysis

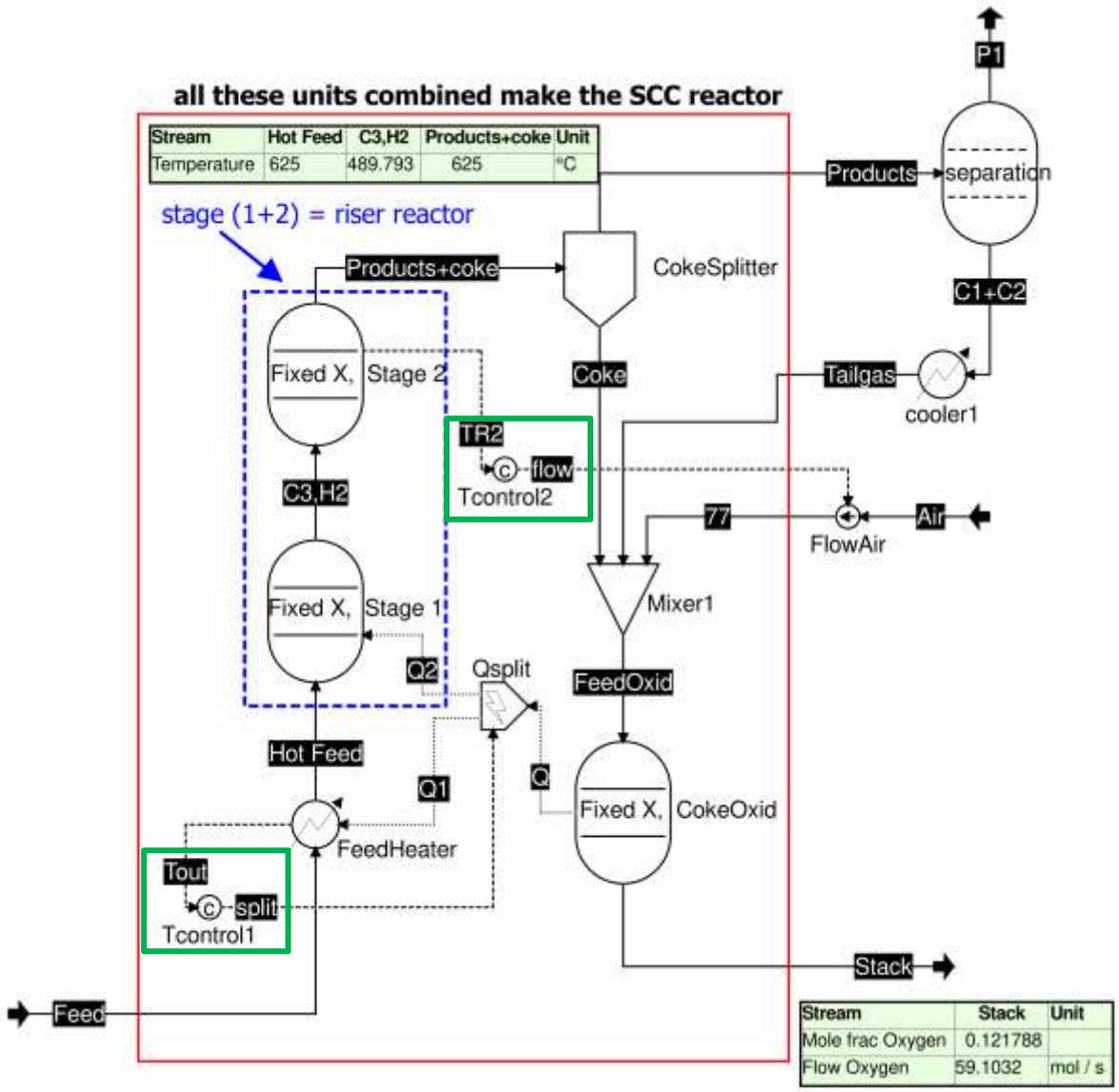
- Based on assumed product distributions
- Prior knowledge from the process

SCC – COCO


Vapor to Fractionator
Riser Cyclones
Upper Cyclones
Stripper
Riser Reactor
Flue Gas
Two-Stage Regenerator Cyclones
Regenerator
Spent Catalyst Standpipe
Feed
Regenerated Catalyst Plug Valve
Air (O2)
Fuel Gas
Tail gas (Methane) Ethane


all these units combined make the SCC reactor
Stream | Hot Feed | C3,H2 | Products+coke | Unit
Temperature | 625 | 489.793 | 625 | °C
stage (1+2) = riser reactor
Products+coke
CokeSplitter
Products
separation
P1
C1+C2
Coke
Tailgas
cooler1
Fixed X, Stage 2
TR2
flow
Tcontrol2
C3,H2
77
Air
FlowAir
Fixed X, Stage 1
Mixer1
Q2
Qsplit
FeedOxid
Hot Feed
Q1
Q
Fixed X, CokeOxid
FeedHeater
Tout
split
Tcontrol1
Stack
Feed
Stream | Stack | Unit
Mole frac Oxygen | 0.121788
Flow Oxygen | 59.1032 | mol / s

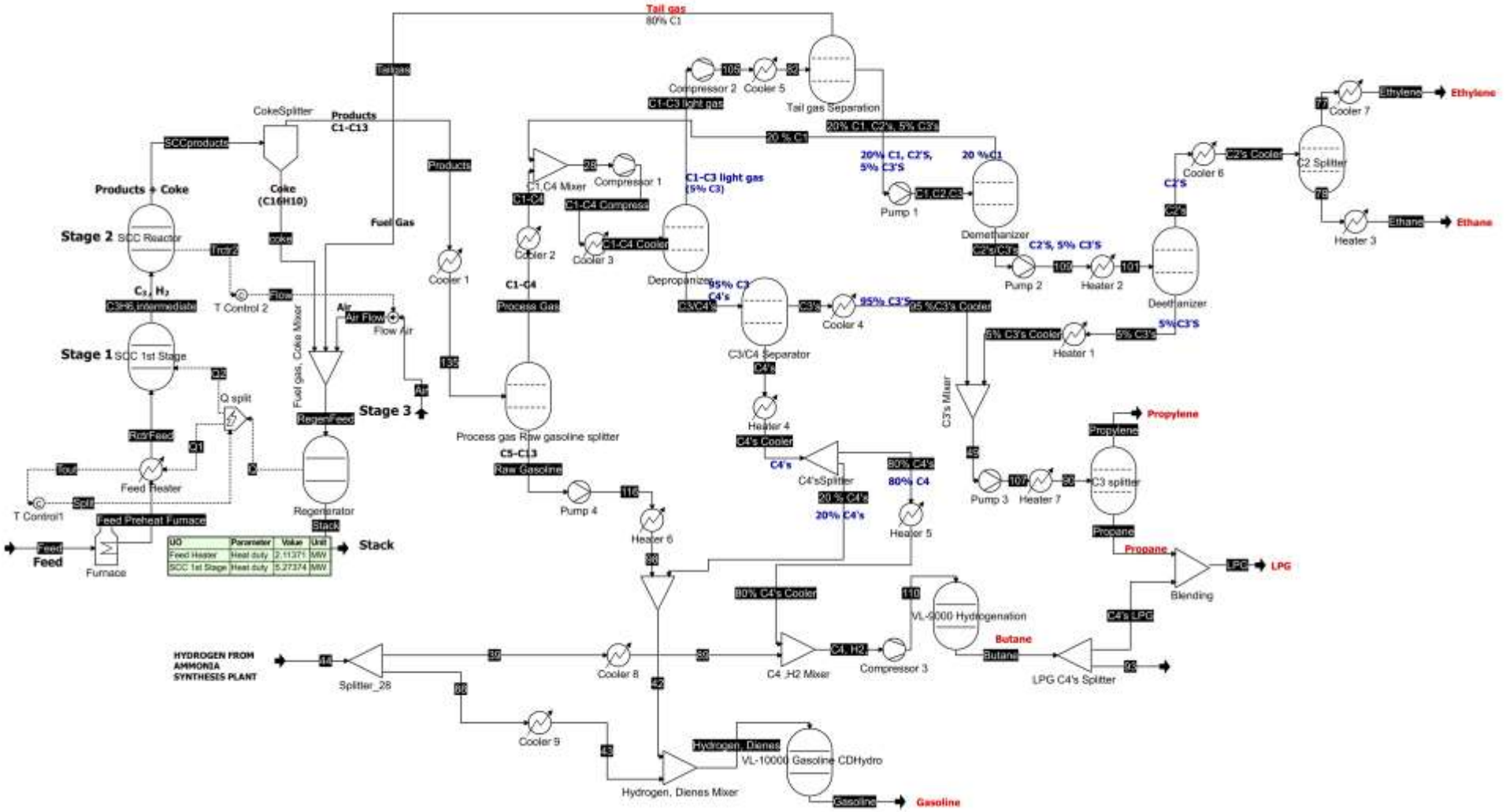
SCC – COCO, energy integration



The “circulating catalyst” as energy carried

- Catalyst:oil >20
- Assume near isothermal (T=625)
- Coke (pyrene) separated and combusted with tail gas
- Q preheat feed (Q1) and stage 1 (Q2)
- Stage 1 – Endothermic,
- Stage 2 – Exothermic
- TControl 1: Feed preheater via split (Q1=0.286Q)
- Tcontrol 2: Tout riser via air flowrate
- Tout,stage1 = 490C

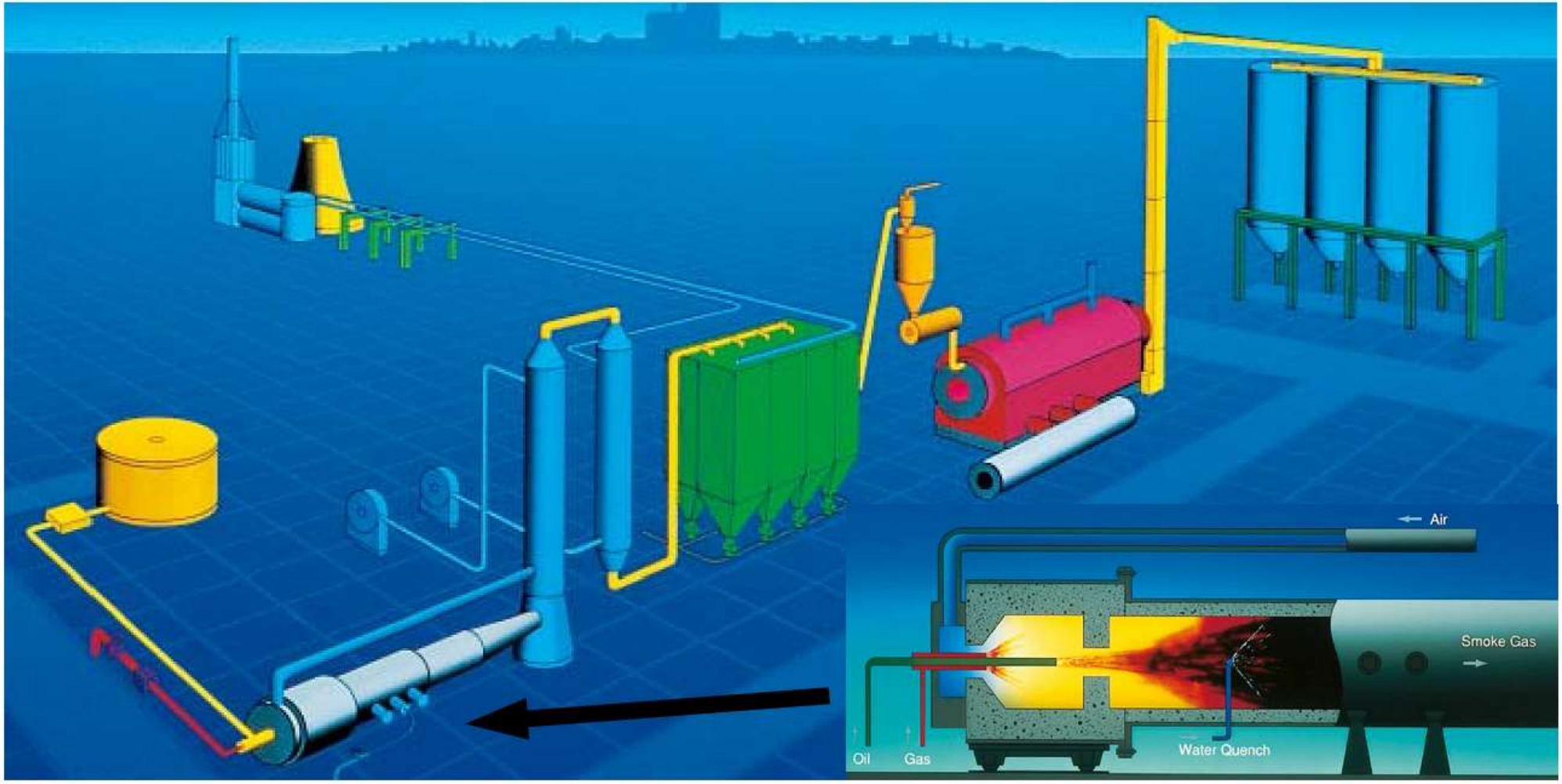
SCC – the whole flow sheet



MSc Thesis, University Eduardo Mondlane, Maputo, Mozambique

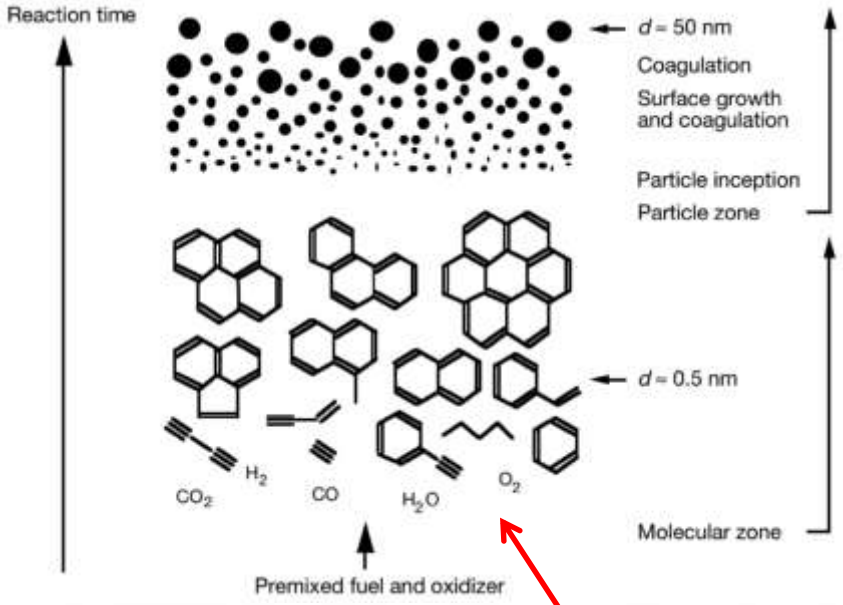
Carbon Black furnace simulations

Carbon black furnace model



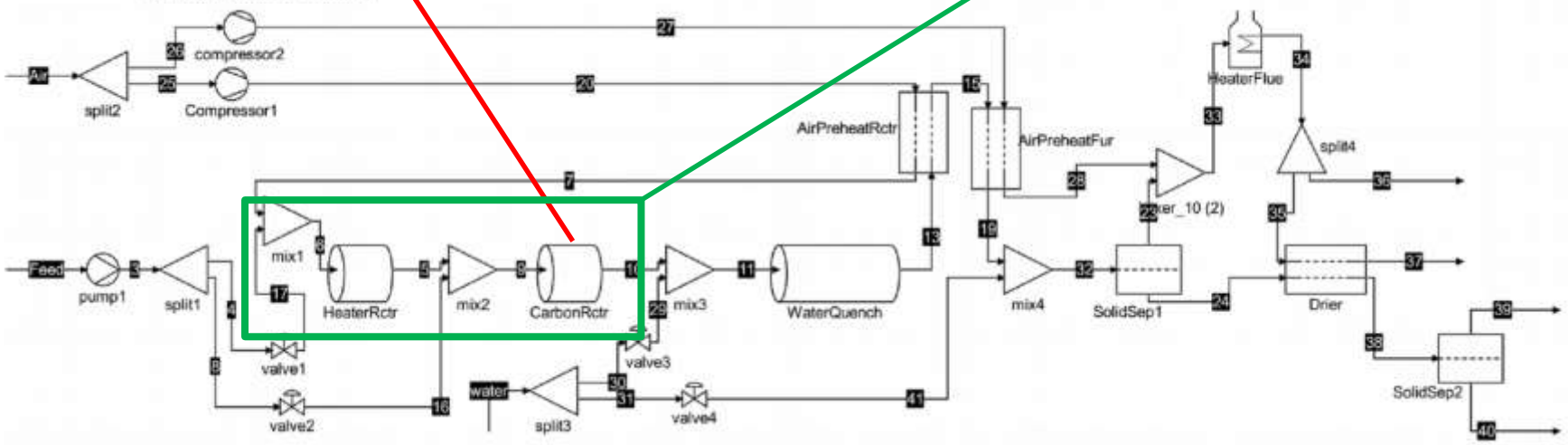
Carbon Black furnace simulations

Carbon black furnace model

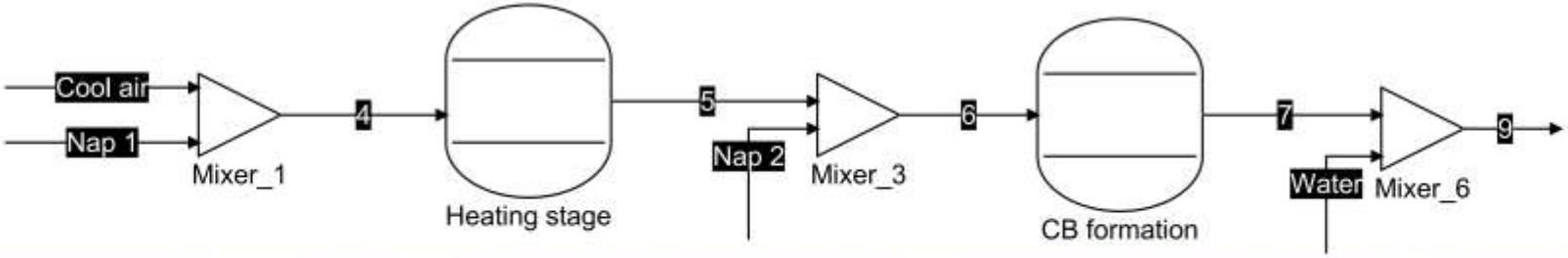


Focus on these two reactors

1. Combustion preheat (Gibbs)
2. Carbon Formation, Carbon solids (Gibbs)



Carbon Black – COCO and Gibbs



Stream	Cool air	Nap 1	4	5	Nap 2	6	7	Water	9	Unit
Pressure	1.97385	1	1	1	1.97385	1	1	1.97385	1	atm
Temperature	700	25	611.765	1660.21	20	1114.6	1315.33	25	714.71	°C
Flow rate	67	1	68	73.1711	4	77.1711	95.6012	33	128.601	mol / h
Mole frac Carbon dioxide	0	0	0	0.0409269	0	0.0388056	3.12585e-07	0	2.32373e-07	
Mole frac Carbon monoxide	0	0	0	0.0957391	0	0.0907767	0.294346	0	0.218815	
Mole frac Water	0	0	0	0.0363969	0	0.0345103	7.04314e-07	1	0.256608	
Mole frac Oxygen	0.21	0	0.206912	0.0852942	0	0.0808732	8.96192e-16	0	6.66223e-16	
Mole frac Hydrogen	0	0	0	0.0182696	0	0.0173226	0.137679	0	0.10235	
Mole frac Nitrogen	0.79	0	0.778382	0.723373	0	0.685879	0.553654	0	0.411582	
Mole frac Naphthalene	0	1	0.0147059	1.33356e-18	1	0.0518329	7.62535e-05	0	5.66863e-05	
Mole frac Pyrene	0	0	0	4.00069e-18	0	3.79332e-18	0.0142435	0	0.0105885	
Flow Carbon dioxide	0	0	0	2.99467	0	2.99467	2.98835e-05	0	2.98835e-05	mol / h
Flow Carbon monoxide	0	0	0	7.00533	0	7.00533	28.1399	0	28.1399	mol / h
Flow Water	0	0	0	2.6632	0	2.6632	6.73333e-05	33	33.0001	mol / h
Flow Oxygen	14.07	0	14.07	6.24107	0	6.24107	8.56771e-14	0	8.56771e-14	mol / h
Flow Hydrogen	0	0	0	1.3368	0	1.3368	13.1623	0	13.1623	mol / h
Flow Nitrogen	52.93	0	52.93	52.93	0	52.93	52.93	0	52.93	mol / h
Flow Naphthalene	0	1	1	9.75782e-17	4	4	0.00728992	0	0.00728992	mol / h
Flow Pyrene	0	0	0	2.92735e-16	0	2.92735e-16	1.3617	0	1.3617	mol / h

approximated as carbon black

Gibbs solutions oscillate

Carbon Black – Scilab-ipopt-ThermoImport

Gibbs minimisation

- **Ideal gases**

$$f(x) = min\left(\frac{G}{RT}\right)_{x_i} = \sum_i x_i\left(\frac{\Delta G^0_{f,i}}{RT}\right) + \sum_i x_i ln\left(\frac{y_i P}{P_0}\right)$$

$$g_i(x) = 0 = |a_{i,k}| \cdot x_i - A_k, \quad i = 1:n, k = 1:m$$

with m elements and n species and x_i moles of each species, $y_i = \frac{x_i}{\sum x_i}$.

- **Analytical derivatives**

$$\frac{\partial f}{\partial x_i} = \left(\frac{\Delta G^0_{f,i}}{RT}\right) + ln\left(\frac{y_i P}{P_0}\right)$$

$$\frac{\partial g_i}{\partial x_k} = a_{i,k}$$

- **Properties using ThermoImport**

Adiabatic operation

- **External loop, energy balance to get T and properties**
- **Maintains the simplicity of the minimisation**
- **Only few iterations (typically <5) needed.**

Carbon Black – Scilab-ipopt-ThermoImport

Gibbs minimisation, with solid carbon

- **Solid activity = 1, thus ln(activity)=0, f modified as follows, n=solid**
- **Ideal gases**

$$f(x) = min\left(\frac{G}{RT}\right)_{x_i} = \sum_i x_i\left(\frac{\Delta G^0_{f,i}}{RT}\right) + \sum_i x_i ln\left(\frac{y_i P}{P_0}\right), \quad y_i = \frac{x_i}{\sum_{i=1}^{n-1} x_i}, \quad y_n = \frac{1}{P_0}$$

$$g_i(x) = 0 = |a_{i,k}| \cdot x_i - A_k, \quad i = 1:n, k = 1:m$$

- **Analytical derivatives**

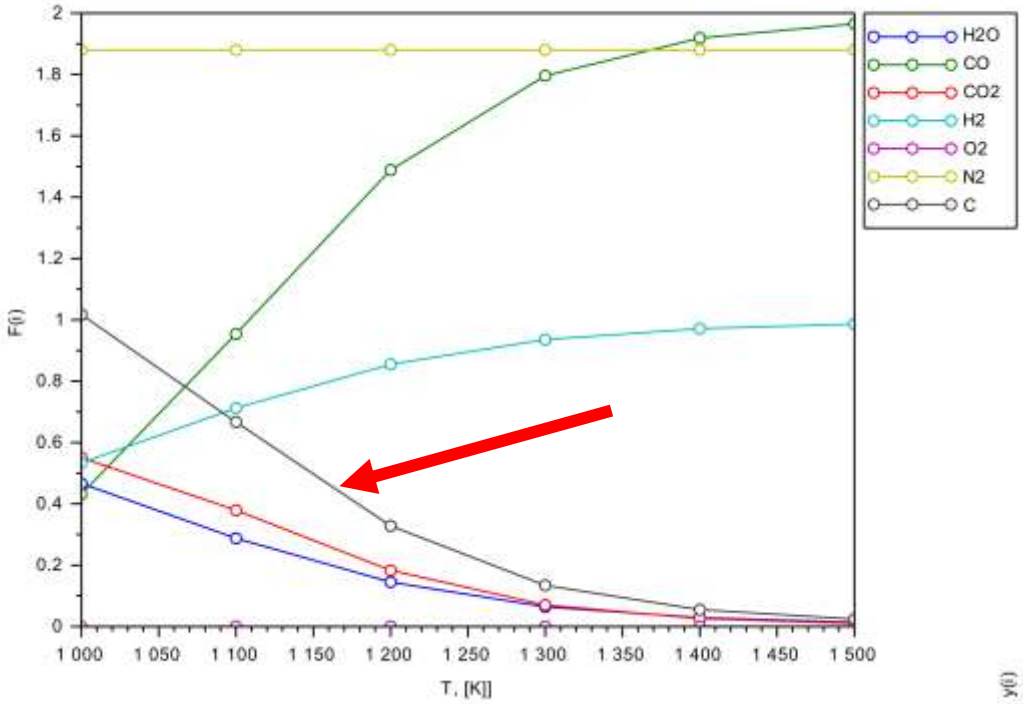
$$\frac{\partial f}{\partial x_i} = \left(\frac{\Delta G^0_{f,i}}{RT}\right) + ln\left(\frac{y_i P}{P_0}\right), \quad \frac{\partial f}{\partial x_n} = \left(\frac{\Delta G^0_{f,n}}{RT}\right)$$

$$\frac{\partial g_i}{\partial x_k} = a_{i,k}$$

- **Properties using ThermoImport**
- **Robust method**

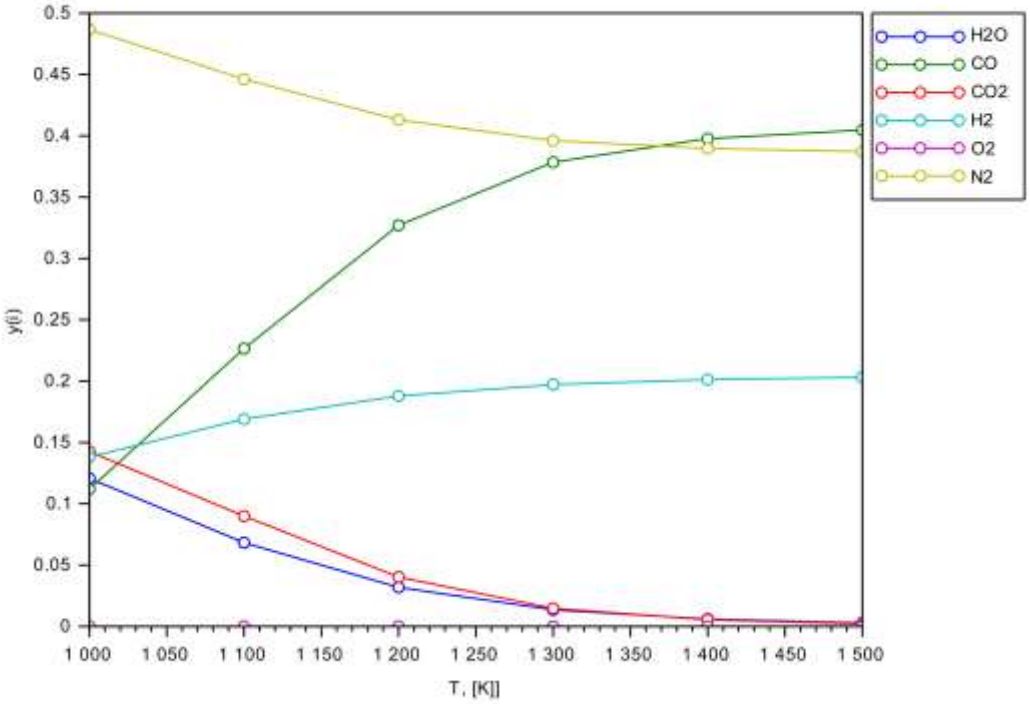
Need to build ScilabUnitOperation

Carbon Black – Scilab-Gibbs-test



Total flow rates including carbon

Total flow rates of gases only



Carbon Black – Scilab-Gibbs-test

Isothermal, 1000C

```
============================================================
IDEAL GAS CHEMICAL REACTION EQUILIBRIUM
Gibbs energy minimisation with IPopt solver
============================================================
T=1000.0 [C]   P=101325.0 [atm]
------------------------------------------
 i   species             moles    molefrac
------------------------------------------
 1   Carbon dioxide    10.0000     0.14493
 2   Water              4.0000     0.05797
 3   Carbon monoxide    0.0000     0.00000
 4   Oxygen             2.0700     0.03000
 5   Nitrogen          52.9300     0.76710
 6   Naphthalene        0.0000     0.00000
 7   Hydrogen           0.0000     0.00000
 8   Pyrene             0.0000     0.00000
------------------------------------------
total moles at equilibrium   69.000
------------------------------------------
lagrange multipliers
 1    37.741
 2    17.984
 3    15.380
 4    12.888
IPOpt iterations   23
============================================================
status = 0
iteration count = 23
cpu time        = 0.048000
number of objective function evaluation              = 24
number of gradient of objective function evaluation  = 24
number of constraint function evaluation             = 24
number of gradient of constraint function evaluation = 24
number of hessian function evaluation                = 0
dual infeasibility   = 0.000000
constraint violation = 0.000000
complementarity      = 0.000000
kkt error            = 0.000000
```

Adiabatic

```
============================================================
IDEAL GAS CHEMICAL REACTION EQUILIBRIUM
Gibbs energy minimisation with IPopt solver
============================================================
T=2480.3 [C]   P=101325.0 [atm]
------------------------------------------
 i   species             moles    molefrac
------------------------------------------
 1   Carbon dioxide    10.0000     0.14493
 2   Water              4.0000     0.05797
 3   Carbon monoxide    0.0000     0.00000
 4   Oxygen             2.0700     0.03000
 5   Nitrogen          52.9300     0.76710
 6   Naphthalene        0.0000     0.00000
 7   Hydrogen           0.0000     0.00000
 8   Pyrene             0.0000     0.00000
------------------------------------------
total moles at equilibrium   69.000
------------------------------------------
lagrange multipliers
 1  475638.285
 2  280065.038
 3  342714.174
 4  321146.851
IPOpt iterations    7
============================================================
status = 0
iteration count = 7
cpu time        = 0.017000
number of objective function evaluation              = 8
number of gradient of objective function evaluation  = 8
number of constraint function evaluation             = 8
number of gradient of constraint function evaluation = 8
number of hessian function evaluation                = 0
dual infeasibility   = 0.000000
constraint violation = 0.000000
complementarity      = 0.000000
kkt error            = 0.000000
```

Carbon Black – Scilab-Gibbs-test

Isothermal, 2480C

```
============================================================
IDEAL GAS CHEMICAL REACTION EQUILIBRIUM
Gibbs energy minimisation with IPopt solver
============================================================
T=2480.0 [C]   P=101325.0 [atm]
-----------------------------------------
 i   species             moles    molefrac
-----------------------------------------
 1   Carbon dioxide     6.6085     0.09326
 2   Water              3.6746     0.05186
 3   Carbon monoxide    3.3915     0.04786
 4   Oxygen             3.9285     0.05544
 5   Nitrogen          52.9300     0.74698
 6   Naphthalene        0.0000     0.00000
 7   Hydrogen           0.3254     0.00459
 8   Pyrene             0.0000     0.00000
-----------------------------------------
total moles at equilibrium   70.858
-----------------------------------------
lagrange multipliers
 1    20.259
 2    12.991
 3    16.416
 4    14.174
IPOpt iterations   15
============================================================
status = 0
iteration count = 15
cpu time        = 0.033000
number of objective function evaluation              = 16
number of gradient of objective function evaluation  = 16
number of constraint function evaluation             = 16
number of gradient of constraint function evaluation = 16
number of hessian function evaluation                = 0
dual infeasibility   = 0.000000
constraint violation = 0.000000
complementarity      = 0.000000
kkt error            = 0.000000
```

Adiabatic

```
============================================================
IDEAL GAS CHEMICAL REACTION EQUILIBRIUM
Gibbs energy minimisation with IPopt solver
============================================================
T=2480.3 [C]   P=101325.0 [atm]
-----------------------------------------
 i   species             moles    molefrac
-----------------------------------------
 1   Carbon dioxide    10.0000     0.14493
 2   Water              4.0000     0.05797
 3   Carbon monoxide    0.0000     0.00000
 4   Oxygen             2.0700     0.03000
 5   Nitrogen          52.9300     0.76710
 6   Naphthalene        0.0000     0.00000
 7   Hydrogen           0.0000     0.00000
 8   Pyrene             0.0000     0.00000
-----------------------------------------
total moles at equilibrium   69.000
-----------------------------------------
lagrange multipliers
 1  475638.285
 2  280065.038
 3  342714.174
 4  321146.851
IPOpt iterations    7
============================================================
status = 0
iteration count = 7
cpu time        = 0.020000
number of objective function evaluation              = 8
number of gradient of objective function evaluation  = 8
number of constraint function evaluation             = 8
number of gradient of constraint function evaluation = 8
number of hessian function evaluation                = 0
dual infeasibility   = 0.000000
constraint violation = 0.000000
complementarity      = 0.000000
kkt error            = 0.000000
```

ATR-SR-syngas-energy coupling

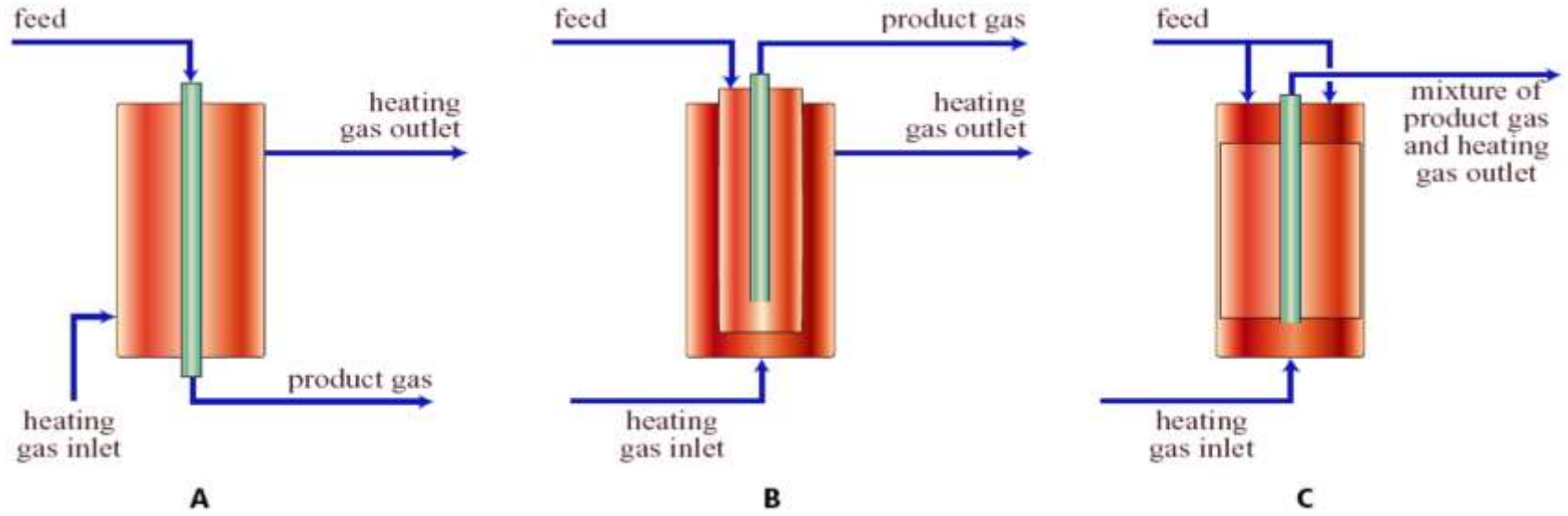
Objective:

- **Combined autothermal reforming and steam-reforming**
- **Using air as a oxygen source**
- **Energy coupling between the ATR and SR**
- **Maximising formation of Syngas for Methanol and ammonia production**
- **Sensitivity of the operating conditions of the ATR-SR on syngas and energy**

MSc

- **University Eduardo Mondlane, Maputo, Mozambique**

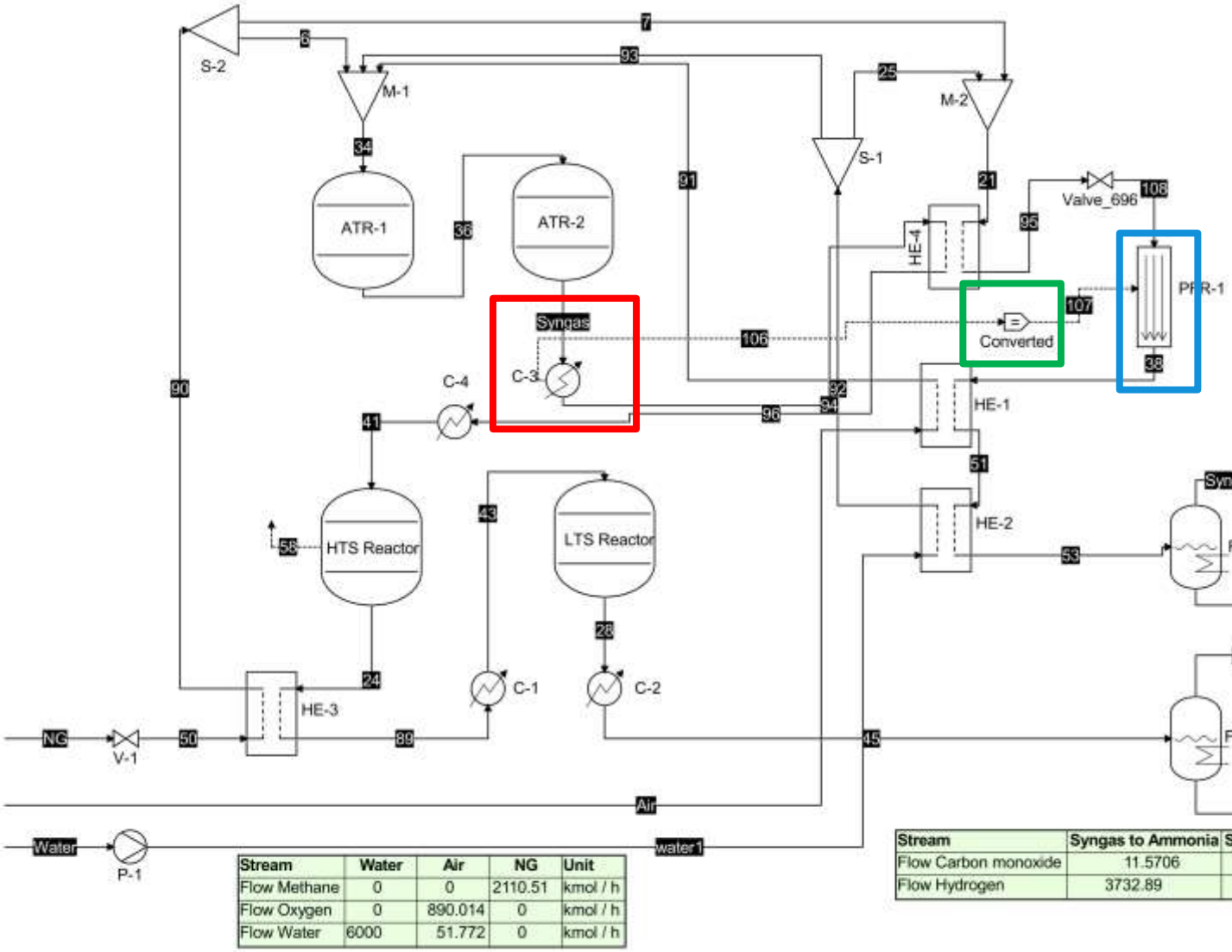
ATR-SR-syngas-energy coupling



Heat exchanged reformers

- A,B are standalone, while C is integrated
- C is the target, energy for the SR is supplied by the ATR
- Conceptual COCO design

ATR-SR-syngas-energy coupling



Stream	Water	Air	NG	Unit
Flow Methane	0	0	2110.51	kmol / h
Flow Oxygen	0	890.014	0	kmol / h
Flow Water	6000	51.772	0	kmol / h

Stream	Syngas to Ammonia	Syngas to Methanol Plant	Syngas	24	Unit
Flow Carbon monoxide	11.5706	416.019	936.12	228.61	kmol / h
Flow Hydrogen	3732.89	2186.95	2808.36	3515.87	kmol / h

- **Some limits**
  - Tout C-3 > Tmin SR
  - Sensitivity analysis: must ensure that heat coupling is automated
  - Tout, C-3 fixed
  - Q converted to W/m

Summary Remarks

Research

- On Going
- Good vehicle for process modelling
- Other languages, Fortran, OpenFoam,…
- We are not yet experts!

Acknowledgements

- The students at UCT and UEM