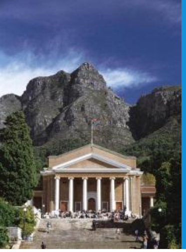
The use of CAPE-OPEN tools, COCO, Chemsep, in the teaching of undergraduate students at universities in southern Africa.

Klaus Möller



Outline

Teaching at University of Cape Town

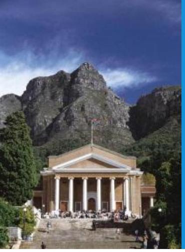
- Conceptual idea
- Curriculum change
- Implementation
- Engineering Council accredited design course
- Use of TEA and ChemsepThermo

Teaching at Eduardo Mondlane University, Maputo, Mozambique

Research

- GTL: Custom thermo, Scilab UO
- Carbon black furnace, thermo, Scilab, Gibbs

The future



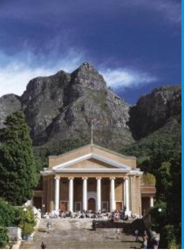
Conceptual idea:
4 year chemical engineering degree

ASPEN used in 4th year

- **licenses too costly**
- **not possible to share across 4 years (500+ students)**
- **want to retain ASPEN for final year design**
  - problems with application and understanding
  - insufficient time to become skilled at flow sheeting
  - competency hurdles student nightmare

The solution, using COCO to building competence in the curriculum

- **introduce flow sheeting in 1st year, add practice to theory**
- **In 2nd year, use flow sheet tools to add practice to pumping, heat exchange, flash, thermodynamic and distillation phenomena – basic competence**
- **in 3rd year, combine the skills to build flow sheeting skills and study a process.**



structure of the chemical engineering curriculum

8 semesters over 4 years

Semester 1	Semester 2

1st year

1st quarter	2nd quarter	3rd quarter	4th quarter
			Flowsheet application

2nd year

Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8
Project 1				Project 2			

Block 4:

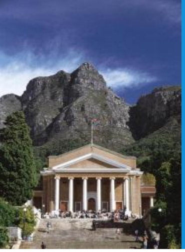
Theory+tutorial	Theory+tutorial	Practice/Project

3rd year

Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8
Project 1				Project 2 : Technical Engineering evaluation			

4th year

Design preparation - ASPEN	Process Design	Lab Project



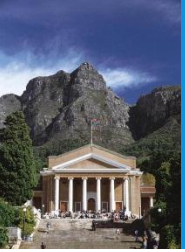
implementation – 1st year

what we teach

- **Mass balances, single reactions, recycle**
- **looking at temperatures and energy requirements**

How we use COCO

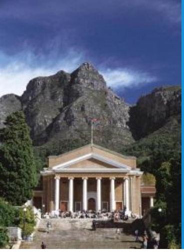
- **Teaching:**
  - build a flow sheet with single reaction, splitters, recycle
  - Competency test on concepts
- **Practice:**
  - project...
  - alternative routes of methane conversion
  - using fixed conversion reactors, compound splitters, recycle, heaters
  - Look at the energy of each process



implementation – 1st year

Teaching COCO to first year students

- **The audience**
  - no programming background (poor at spreadsheets)
  - no process or unit operation background
  - poor practical engineering knowledge
- **The challenge**
  - 150 students, hands on, follow me demonstration
  - avoid plug and play and copying the flow sheet without thought
  - to gain understanding and appreciate the value
- **The plan**
  - each student entering engineering MUST have a laptop



implementation – 1st year

$$n - C_7H_{14} \rightleftarrows C_6H_{11}CH_3 + H_2, \quad \Delta H_{rxn}^{400^\circ C} = 35673\, J/mol$$

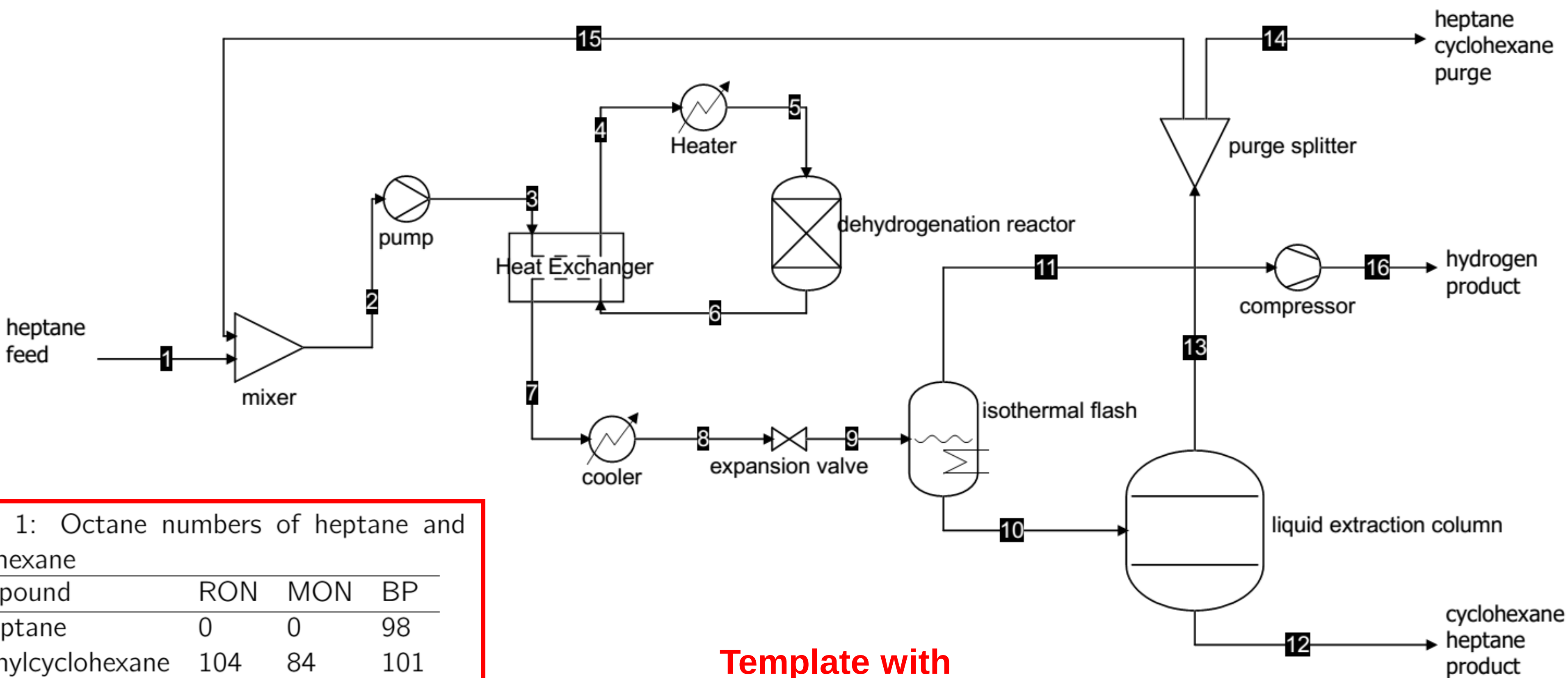


Table 1: Octane numbers of heptane and cyclohexane

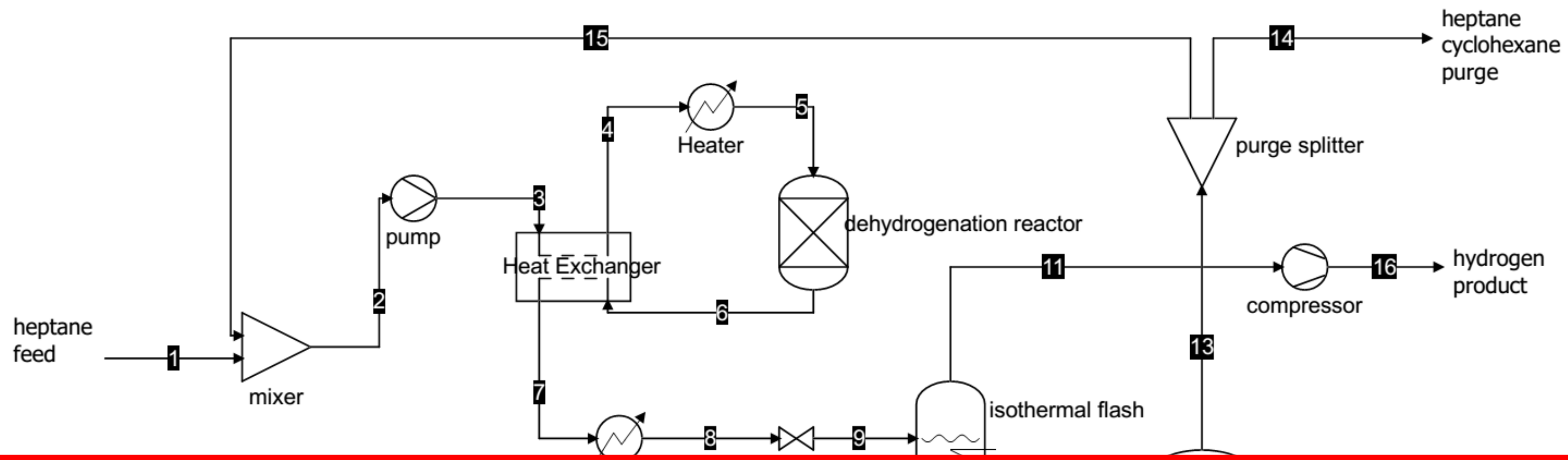
compound	RON	MON	BP
n-heptane	0	0	98
methylcyclohexane	104	84	101
toluene	124	112	111

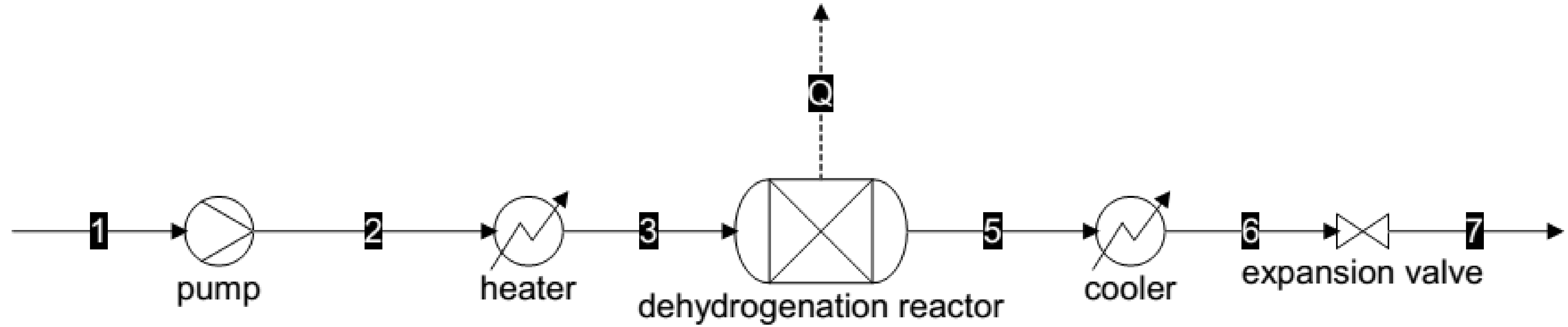
RON = Research Octane Number
MON = Motor Octane Number
BP = Boiling Point in C at 760mmHg

Template with
- **property pack**
- **reaction pack**

implementation – 1st year

$$n-C_7H_{14} \rightleftarrows C_6H_{11}CH_3 + H_2, \quad \Delta H_{rxn}^{400^\circ C} = 35673\, J/mol$$





implementation – 1st year

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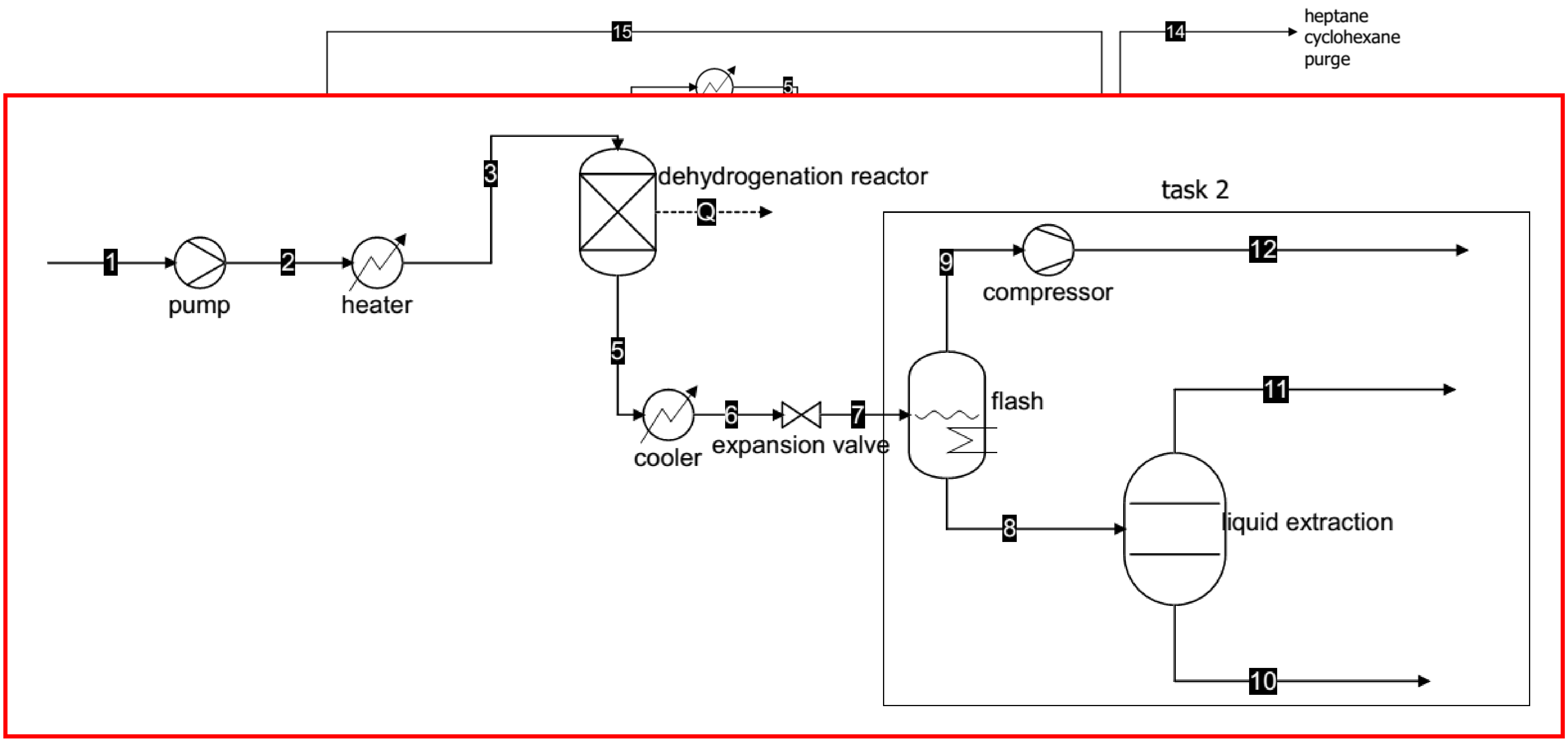

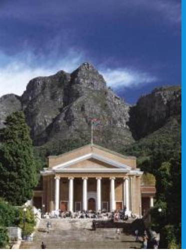

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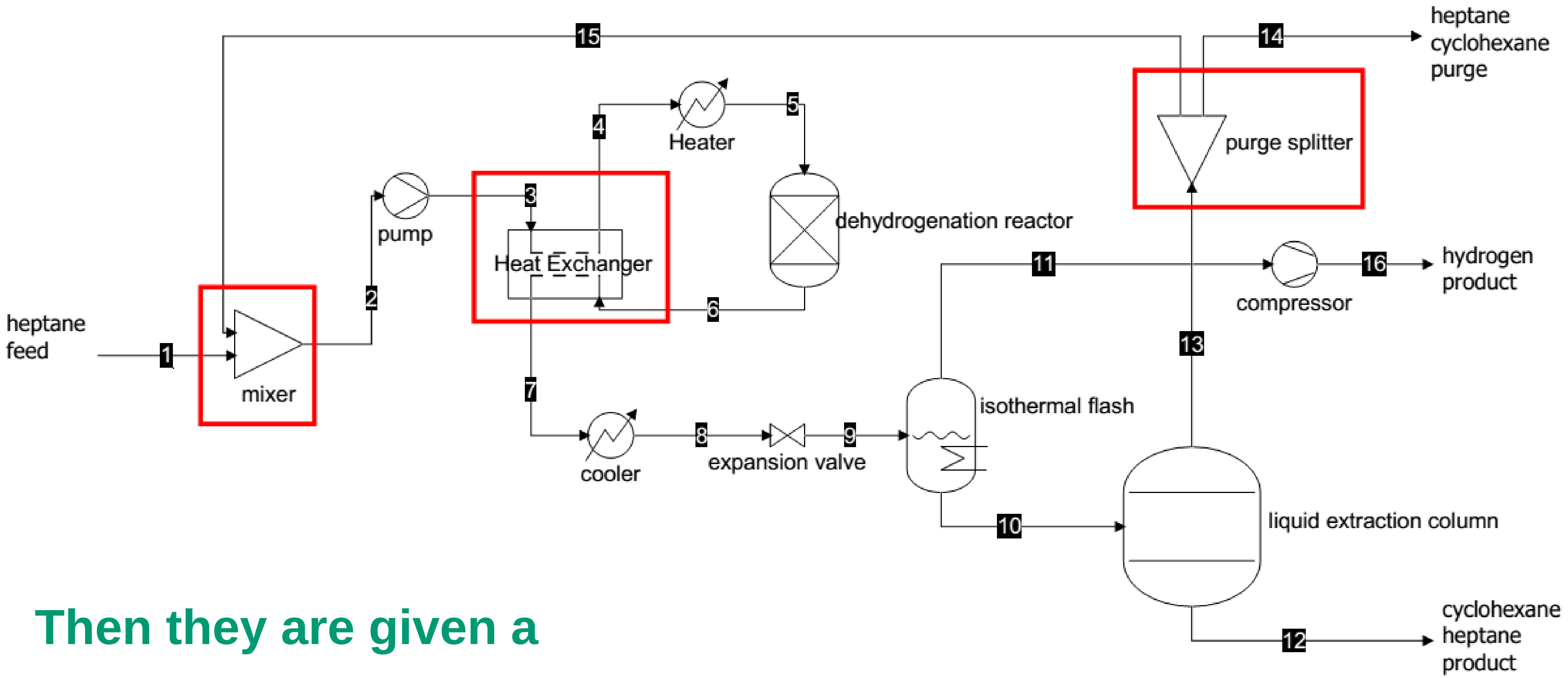
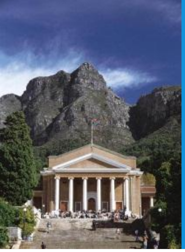


Then they are given a

- **Test**
- **project to carry out**



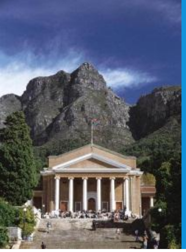
implementation – 2nd year

what we teach

- **flow systems, heat systems, thermodynamics of processes**
- **recycle systems, energy balances,**
- **single reaction systems, separation systems**

How we use COCO/chemsep

- **learn to build a property pack**
- **learn to build a reaction pack**
- **flash calculations**
- **Gibbs reactor**
- **fixed conversion reactor**
- **heat of reaction**
- **Distillation using chemsep, McCabe-Thiele, stage efficiency, ...**



implementation – 2nd year

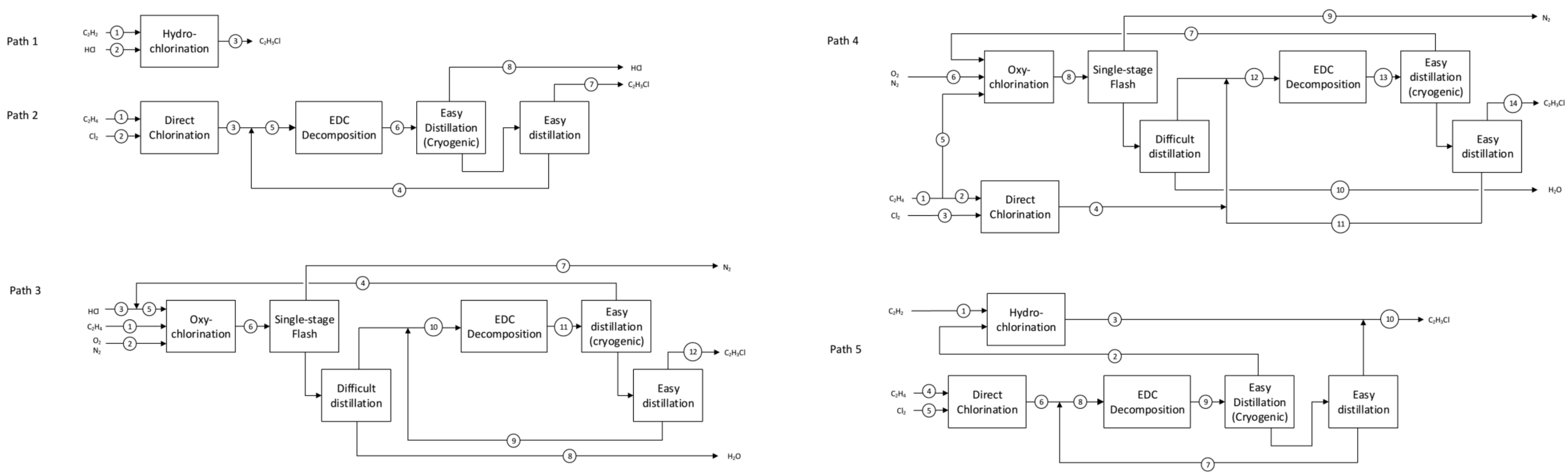
Vinyl Chloride Monomer project

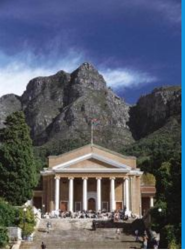
$$C_2H_4 + Cl_2 \longrightarrow C_2H_4Cl_2 \qquad \text{(direct chlorination)}$$

$$C_2H_4 + 2\,HCl + \tfrac{1}{2}\,O_2 \longrightarrow C_2H_4Cl_2 + H_2O \qquad \text{(oxy-chlorination)}$$

$$C_2H_4Cl_2 \longrightarrow C_2H_3Cl + HCl \qquad \text{(EDC decomposition)}$$

Heat of reaction
Heat duties
distillation





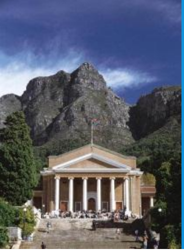
implementation – 3rd year

what we teach

- solid-fluid systems, mass transfer
- adiabatic reactors, phase thermodynamics, complex separations
- process control, dynamics

How we use COCO

- Multiple reactions, pressure drop, catalyst material, adiabatic
- Multi-stage reactors
- Flow sheets with recycle and make-up mixer
- Flow sheets with distillation sequences



Styrene monomer plant

$$C_6H_5CH_2CH_3 \rightleftarrows C_6H_5CHCH_2 + H_2, \quad \Delta H_R^{298} = 117.6\,kJ/mol \qquad (1)$$

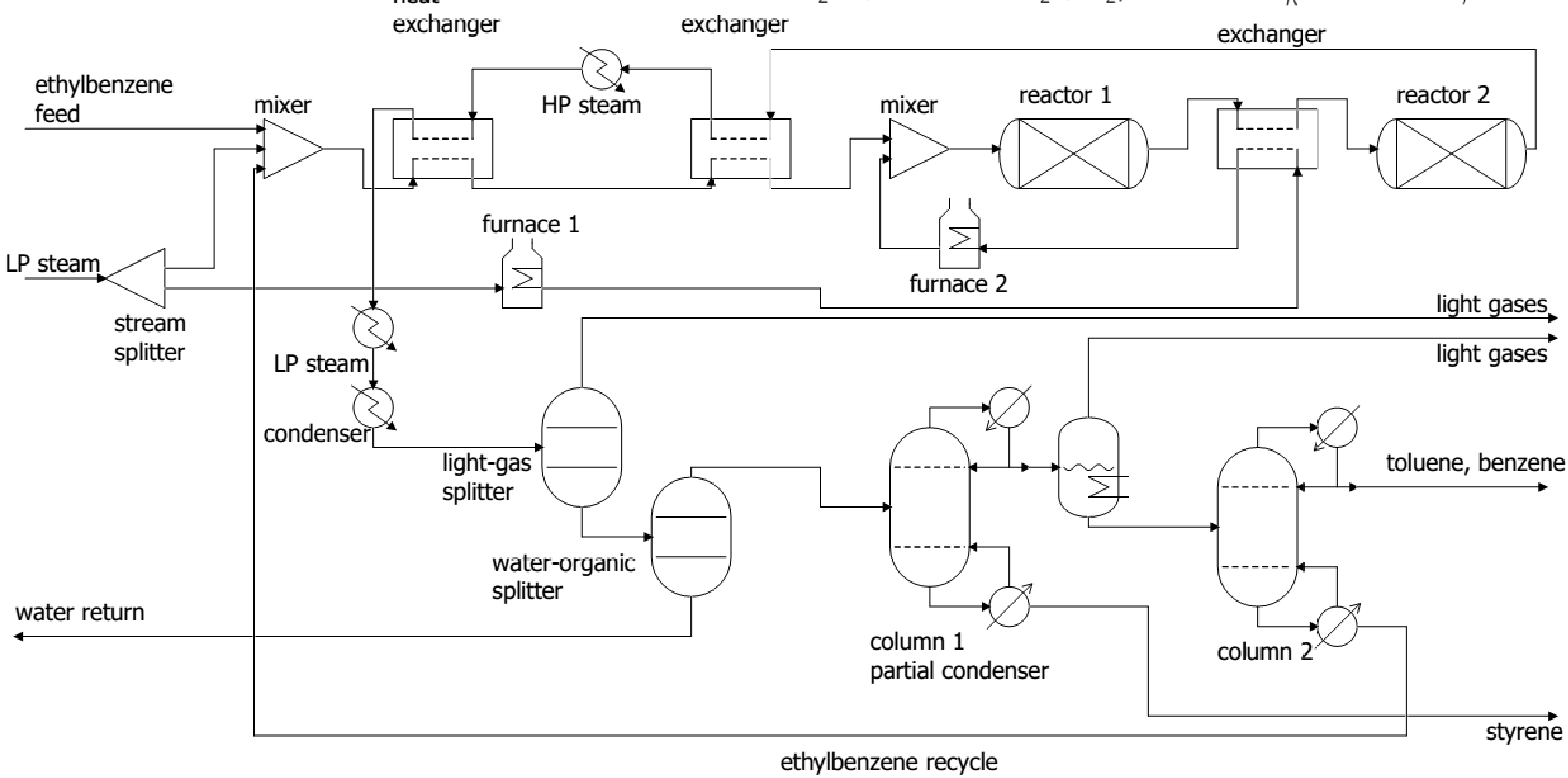
$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4, \quad \Delta H_R^{298} = 105.4\,kJ/mol \qquad (2)$$

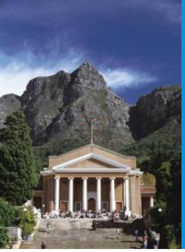
$$C_6H_5CH_2CH_3 + H_2 \rightarrow C_6H_5CH_3 + CH_4, \quad \Delta H_R^{298} = 105.4\,kJ/mol \qquad (3)$$

$$2H_2O + C_2H_4 \rightarrow 2CO + 4H_2, \quad \Delta H_R^{298} = -54.6\,kJ/mol \qquad (4)$$

$$H_2O + CH_4 \rightarrow CO + 3H_2, \quad \Delta H_R^{298} = 210.2\,kJ/mol \qquad (5)$$

$$H_2O + CO \rightarrow CO_2 + H_2, \quad \Delta H_R^{298} = -41.2\,kJ/mol \qquad (6)$$





COCO/Chemsep a great success
Student development, ASPEN preparation

1st year:

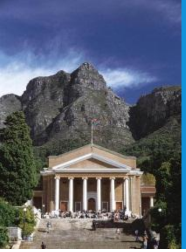
- **explore chemical engineering calculations**
- **Students highly motivated,**
- **COCO easily applied although the understanding is lacking**

2nd year:

- **develop own flowsheet**
- **better physical undertanding of flow systems, Pressure, temperature, valves, pumps,**

3rd year:

- **complex reaction and separations system design**
- **recycle and heat integration**
- **economics and “optimisation”**
- **concepts and applications make students ASPEN ready**



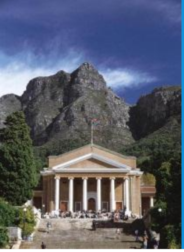
COCO/Chemsep a great success
Student development, ASPEN preparation

4^{th} year:

- no need for ASPEN training
- No need for unit operation development
- transition, design peparation and design project no longer limited by ASPEN competency issues.

SUCCESS!!!!

3^{rd} years at work



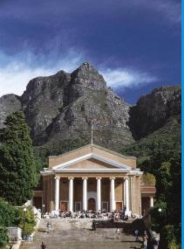
University of Eduardo Mondlane, Maputo, Mozambique Chemical Engineering Masters programme teaching

This is part of a SASOL sponsored MSc programme on petroleum refining

- **The audience: Chemical engineering and geological engineering**
- **The challenge:**
  - They are not well trained in computer usage
  - They have very old poorly maintained laptops
  - Home language is Portuguese
  - small classes – 10-15 (lucky)
  - poor facilities
  - course runs entirely paperless, wifi!!!!!!

How it runs

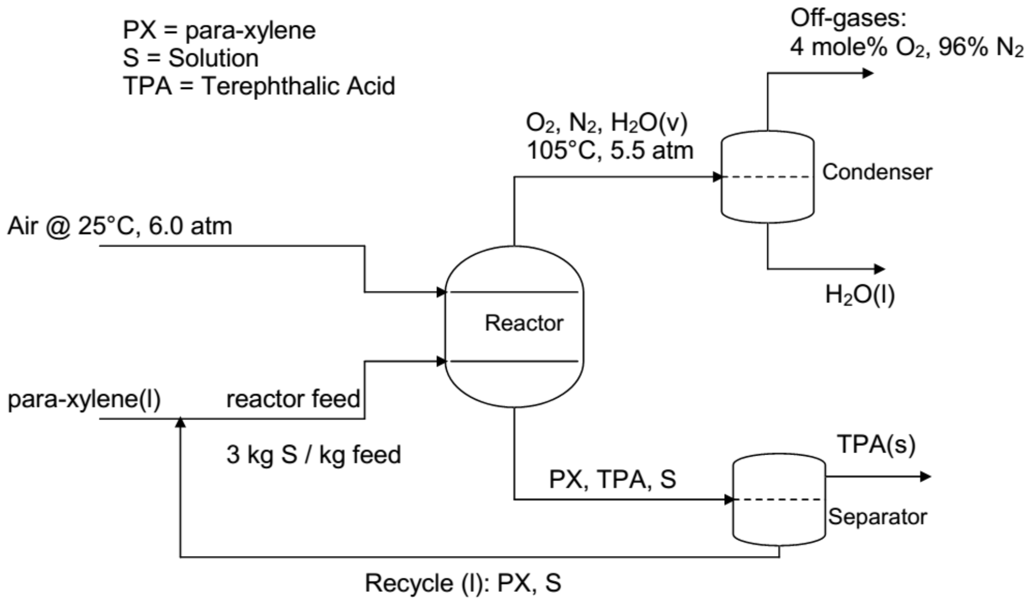
- **2 week intense programme (with much hand waving)**
- **about 8 hours a day of lectures and one-on-one contact**
- **1 test, 2 projects**



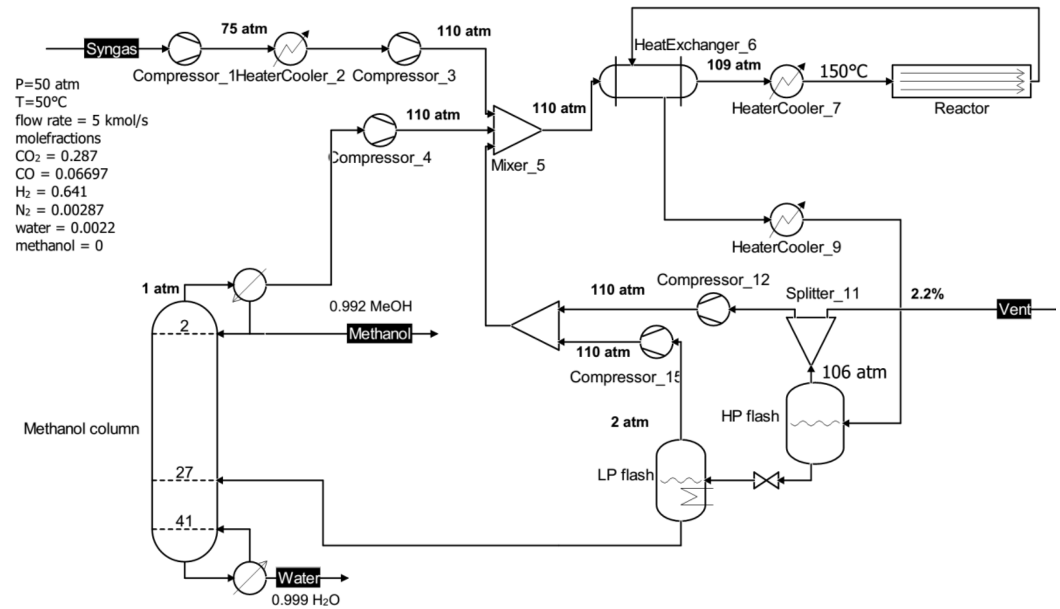
University of Eduardo Mondlane, Maputo, Mozambique
Chemical Engineering Masters programme teaching

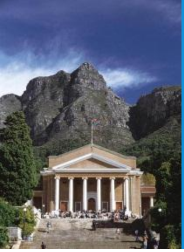
The projects

The design of a simplified Terephthalic Acid (TPA) Plant



The design of a syngas to methanol plant





University of Eduardo Mondlane, Maputo, Mozambique
Chemical Engineering Masters programme teaching

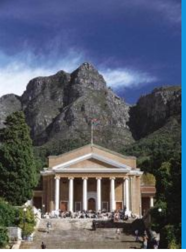
Has it worked

- **has run in 2017/2018**
- **First group spent 1 month on SASOL secunda plant**
- **Are using COCO/ASPEN to carry out some of the analysis**
- **Feedback I have from engineers on the plant**
  - students very competent with regard plant operations
  - Students have good simulation skills

YES, it has

Other initiatives using the same model not yet successful

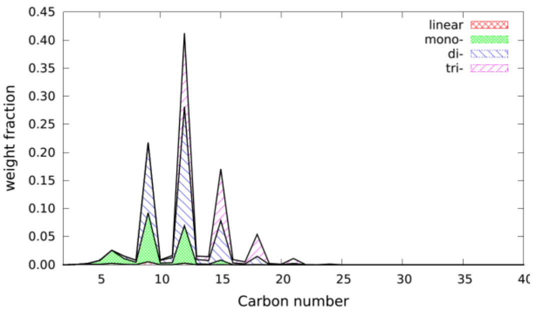
- **Universities with chemical engineering in Kenya and Tanzania**

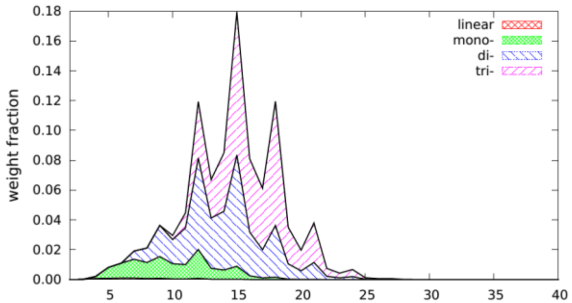


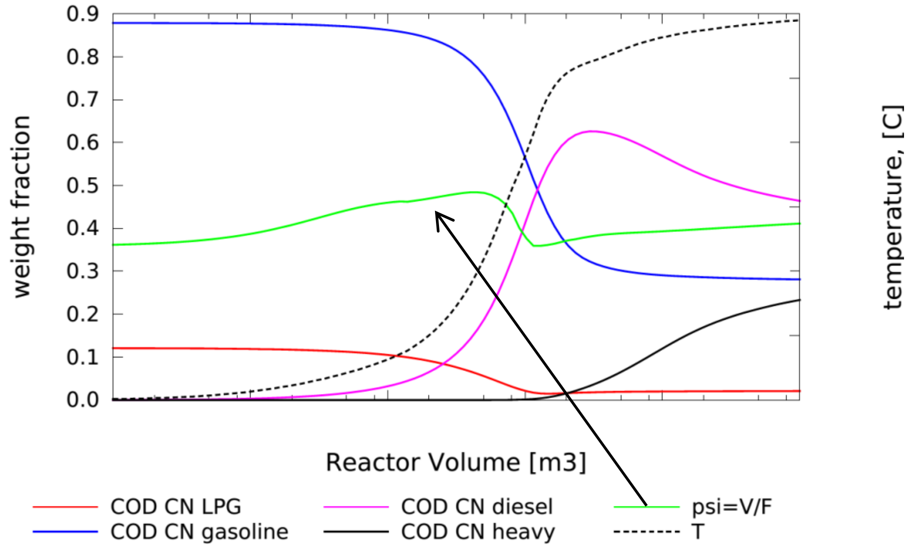
Research

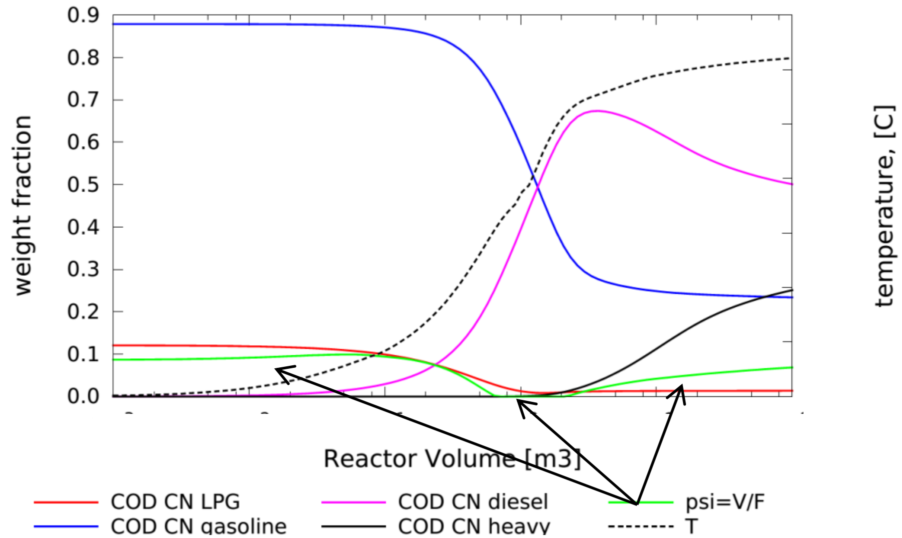
Conversion of Olefins to distillates (PetroSA)

- **Multi-phase adiabatic process model**
- **H_2, C1-C40, olefins and parafins, with linear, mono-branched, di-branched and tri-branched species, thousands of reactions including reversibility**
- **custom thermo and VLE engine**
- **seconds-few minutes on laptop**
- **Needs a wrapper for ASPEN**

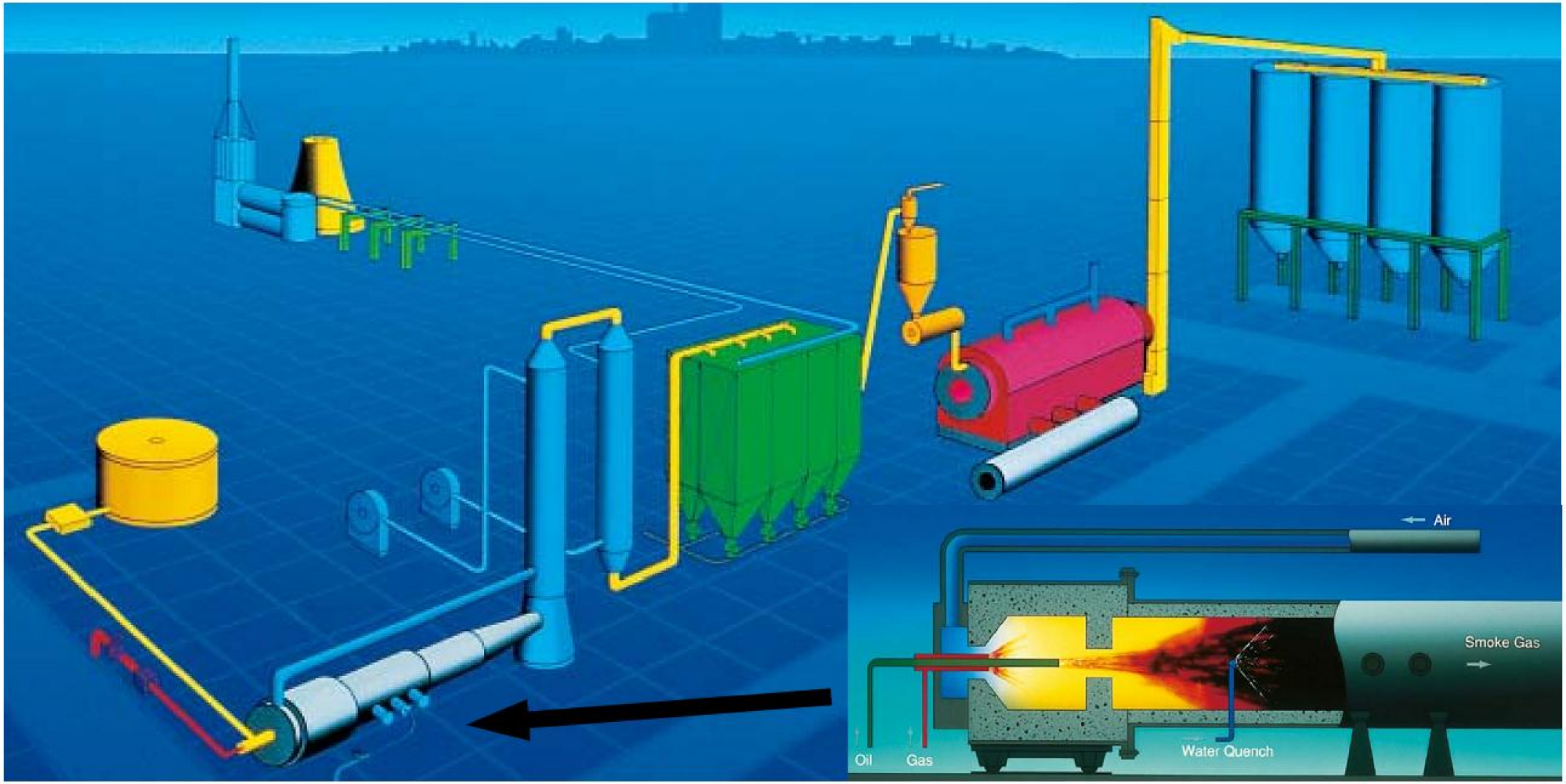








Carbon black furnace model



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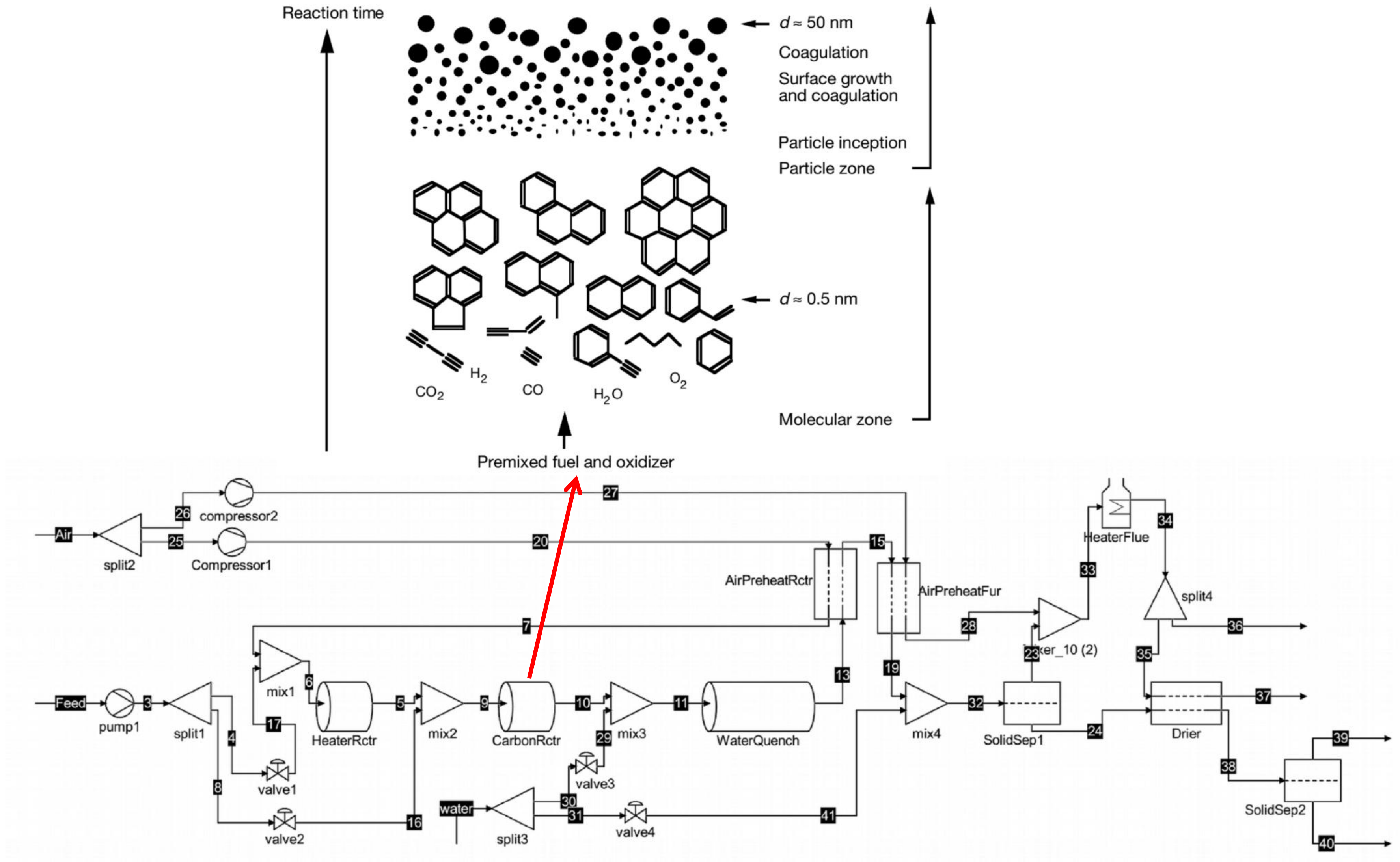

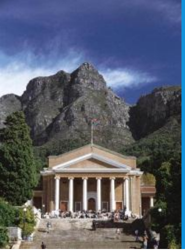

Summary Remarks

Teaching with Cape Open/COCO/Chemsep

- **great success**
- **Students also use TEA, COPP , ScilabUO**

Research

- **On Going**
- **Bigger challenges**

Future

- **Tools and knowledge great asset to resource limited countries**
- **More teaching, more usage and more Cape open based solutions needed**