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 4\textsuperscript{th} year

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

The solution, using COCO to building competence in the curriculum

• introduce flow sheeting in 1\textsuperscript{st} year, add practice to theory
• In 2\textsuperscript{nd} year, use flow sheet tools to add practice to pumping, heat exchange, flash, thermodynamic and distillation phenomena – basic competence
• in 3\textsuperscript{rd} year, combine the skills to build flow sheeting skills and study a process.
structure of the chemical engineering curriculum

8 semesters over 4 years

<table>
<thead>
<tr>
<th></th>
<th>Semester 1</th>
<th>Semester 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st year</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1st quarter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd quarter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3rd quarter</td>
<td></td>
<td>Flowsheet application</td>
</tr>
<tr>
<td>4th quarter</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2nd year</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Block 1</td>
<td>Block 2</td>
<td>Block 3</td>
</tr>
<tr>
<td>Project 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Theory+tutorial</td>
<td>Theory+tutorial</td>
<td>Practice/Project</td>
</tr>
<tr>
<td>3rd year</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Block 1</td>
<td>Block 2</td>
<td>Block 3</td>
</tr>
<tr>
<td>Project 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4th year</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Design preparation - ASPEN</td>
<td>Process Design</td>
<td>Lab Project</td>
</tr>
</tbody>
</table>

Process Modelling & Optimisation Group
what we teach

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

How we use COCO

• Teaching:
  o build a flow sheet with single reaction, splitters, recycle
  o Competency test on concepts

• Practice:
  o project...
  o alternative routes of methane conversion
  o using fixed conversion reactors, compound splitters, recycle, heaters
  o Look at the energy of each process
Teaching COCO to first year students

• The audience
  o no programming background (poor at spreadsheets)
  o no process or unit operation background
  o poor practical engineering knowledge

• The challenge
  o 150 students, hands on, follow me demonstration
  o avoid plug and play and copying the flow sheet without thought
  o to gain understanding and appreciate the value

• The plan
  o each student entering engineering MUST have a laptop
$n - C_7H_{14} \rightleftharpoons C_6H_{11}CH_3 + H_2, \ \Delta H^{400^\circ C}_{\text{rxn}} = 35673 \text{ J/mol}$

Table 1: Octane numbers of heptane and cyclohexane

<table>
<thead>
<tr>
<th>compound</th>
<th>RON</th>
<th>MON</th>
<th>BP</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>0</td>
<td>0</td>
<td>98</td>
</tr>
<tr>
<td>methylcyclohexane</td>
<td>104</td>
<td>84</td>
<td>101</td>
</tr>
<tr>
<td>toluene</td>
<td>124</td>
<td>112</td>
<td>111</td>
</tr>
</tbody>
</table>

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

Template with
- property pack
- reaction pack
implementation – 1st year

\[ n - C_7H_{14} \leftrightarrow C_6H_{11}CH_3 + H_2, \quad \Delta H_{rxn}^{400^\circ C} = 35673 \text{ J/mol} \]
implementation – 1st year

\[ n - C_7H_{14} \rightleftharpoons C_6H_{11}CH_3 + H_2, \quad \Delta H_{\text{rxn}}^{400^\circ C} = 35673 \text{ J/mol} \]
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, ...
Vinyl Chloride Monomer project

\[ \text{C}_2\text{H}_4 + \text{Cl}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2 \] (direct chlorination)

\[ \text{C}_2\text{H}_4 + 2 \text{HCl} + \frac{1}{2} \text{O}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2 + \text{H}_2\text{O} \] (oxy-chlorination)

\[ \text{C}_2\text{H}_4\text{Cl}_2 \rightarrow \text{C}_2\text{H}_3\text{Cl} + \text{HCl} \] (EDC decomposition)

Path 1: Hydro-chlorination
Path 2: Direct Chlorination → EDC Decomposition → Easy distillation
Path 3: Oxy-chlorination → Single-stage Flash → EDC Decomposition → Easy distillation
Path 4: Oxy-chlorination → Single-stage Flash → Difficult distillation → EDC Decomposition → Easy distillation
Path 5: Hydro-chlorination → EDC Decomposition → Easy distillation

Heat of reaction
Heat duties
Distillation
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**

\[
\begin{align*}
C_6H_5CH_2CH_3 & \rightleftharpoons C_6H_5CHCH_2 + H_2, \quad \Delta H^\circ_{298} = 117.6 \text{ kJ/mol} \\
C_6H_5CH_2CH_3 & \rightarrow C_6H_6 + C_2H_4, \quad \Delta H^\circ_{298} = 105.4 \text{ kJ/mol} \\
C_6H_5CH_2CH_3 + H_2 & \rightarrow C_6H_5CH_3 + CH_4, \quad \Delta H^\circ_{298} = 105.4 \text{ kJ/mol} \\
2H_2O + C_2H_4 & \rightarrow 2CO + 4H_2, \quad \Delta H^\circ_{298} = -54.6 \text{ kJ/mol} \\
H_2O + CH_4 & \rightarrow CO + 3H_2, \quad \Delta H^\circ_{298} = 210.2 \text{ kJ/mol} \\
H_2O + CO & \rightarrow CO_2 + H_2, \quad \Delta H^\circ_{298} = -41.2 \text{ kJ/mol}
\end{align*}
\]
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 understanding 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

4th year:
• no need for ASPEN training
• No need for unit operation development
• transition, design preparation and design project no longer limited by ASPEN competency issues.

SUCCESS!!!!
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
The projects

The design of a simplified Terephthalic Acid (TPA) Plant

- PX = para-xylene
- S = Solution
- TPA = Terephthalic Acid

Off-gases: 4 mole% O₂, 96% N₂

O₂, N₂, H₂O(v) → Condenser → H₂O(l)

105°C, 5.5 atm

Air @ 25°C, 6.0 atm → Reactor → Para-xylene(l)

3 kg S / kg feed → Reactor feed

Recycle (l): PX, S

TPA(s) → PX, TPA, S → Separator

The design of a syngas to methanol plant

P = 50 atm
T = 50°C
Flow rate = 5 kmol/s
 mole fractions
CD₂ = 0.387
CD = 0.06697
H₂ = 0.641
N₂ = 0.00287
Water = 0.0022
Methanol = 0

Methanol column

0.992 MeOH

Methanol
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
  o students very competent with regard plant operations
  o 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
Conversion of Olefins to distillates (PetroSA)

- Multi-phase adiabatic process model
- H2, 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
Research

Carbon black furnace model
Research

Carbon black furnace model
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