Using gPROMS in undergraduate teaching

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Summary

The Department of Chemical Engineering at UCL has used gPROMS in its undergraduate programme for nearly a decade, both for design projects and for research projects. The main use is in a compulsory MEng design module entitled **CENGM011 Advanced Process Modelling and Design** which accounts for ¼ of the fourth and final MEng year.
The class size has increased every year and currently counts 48 undergraduate students.
The students perceive this module to be quite challenging, but also the most relevant to their chemical engineering degrees.

CENGM011 Intended learning outcomes

On completion of the module, the students will be expected to be:

- able to develop computational models for complex plant items;
- able to use a contemporary tool for modelling process dynamics;
- able to develop control strategies for process plants;
- able to evaluate alternative control strategies on the basis of numerical simulations;
- aware of contemporary tools for advanced process design.

Modelling and use of gPROMS → Mathematical model from first principles → Disturbances and control alternatives → Open loop responses (gPROMS) → Closed loop responses (gPROMS)

TERM 1 | TERM 2

CENGM011 Advanced Process Modelling and Design

The module runs over two terms of 11 weeks each. Term 1 is also taken by MSc students on a separate module.
Term 1 covers the use of gPROMS as well as general modelling concepts, particularly related to distillation and absorption columns, through a series of lectures and cluster room tutorials. The assessment is based on three pieces of individual coursework as well as one 2 hr gPROMS exam taken in a computer cluster room.
Term 2 is spent on a design project where the students work in teams of six to produce a report which analyses the dynamics and control of one main unit each from a given plant based on gPROMS models that they develop from first principles using Modelbuilder.
Throughout the term, several intermediate reports and one oral presentation are assessed by both students (peer assessment) and tutors.

Term 1 – Lectures

1. Introduction and Modelling I
2. gPROMS I – simple models
3. gPROMS II – composite models
4. Modelling II – column modelling
5. gPROMS III – operating procedures
6. *READING WEEK*
7. Modelling III – model verification
8. gPROMS IV – debugging
9. Modelling IV – model assumptions
10. Modelling in industry (guest lecture)
11. Introduction to design project

Term 2 – Design brief

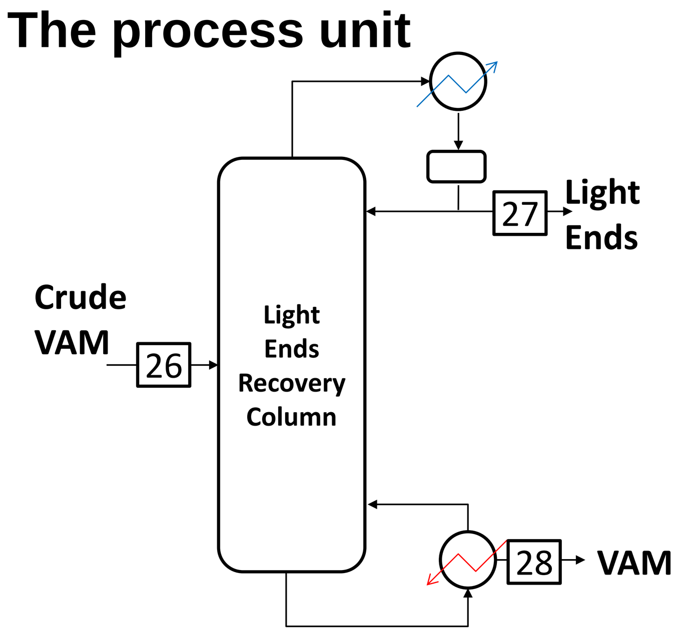
"You should produce a report providing evidence that the plant can satisfactorily reject all expected disturbances.

At least three disturbances and three alternative control schemes should be considered with a recommendation as to which scheme is the preferred option and why.

The conclusions should be based on a working simulation of the plant using the dynamic simulation package gPROMS."

The Design Project

The process unit



Specifications	
Operating Pressure (bar)	1.15
Design Pressure (bar)	2.15
Design Temperature (K)	373
Number of Stages	20
Feed Stage	5
Condenser Duty (MJ/hr)	-1023
Reboiler Duty (MJ/hr)	1062
Reflux Ratio	7.3
Column Diameter (m)	0.61
Column Height (m)	12.81
Tray Type	Sieve
Tray Spacing (m)	0.61
Vessel Material	Carbon Steel

The model assumptions

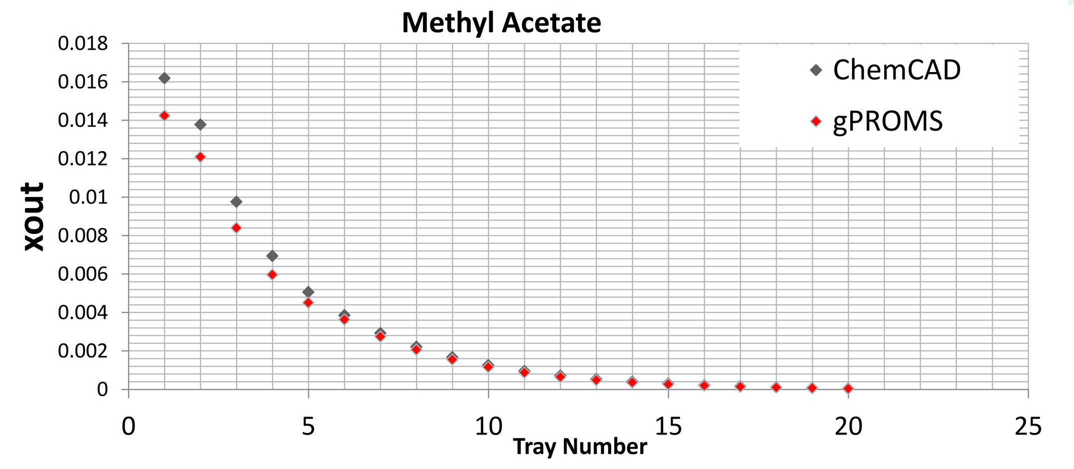
1. No chemical reaction
2. Constant pressure
3. Vapour holdup neglected
4. Ideal mixture with constant relative volatilities
5. Prefect mixing
6. Equimolar overflow
7. Linear tray hydraulics
8. Downcomer dynamics ignored
9. Total condenser with no sub-cooling
10. No condenser accumulation
11. Equilibrium stage kettle reboiler
12. Negligible heat losses from the column
13. Constant specific heats and negligible heats of mixing

The main disturbances

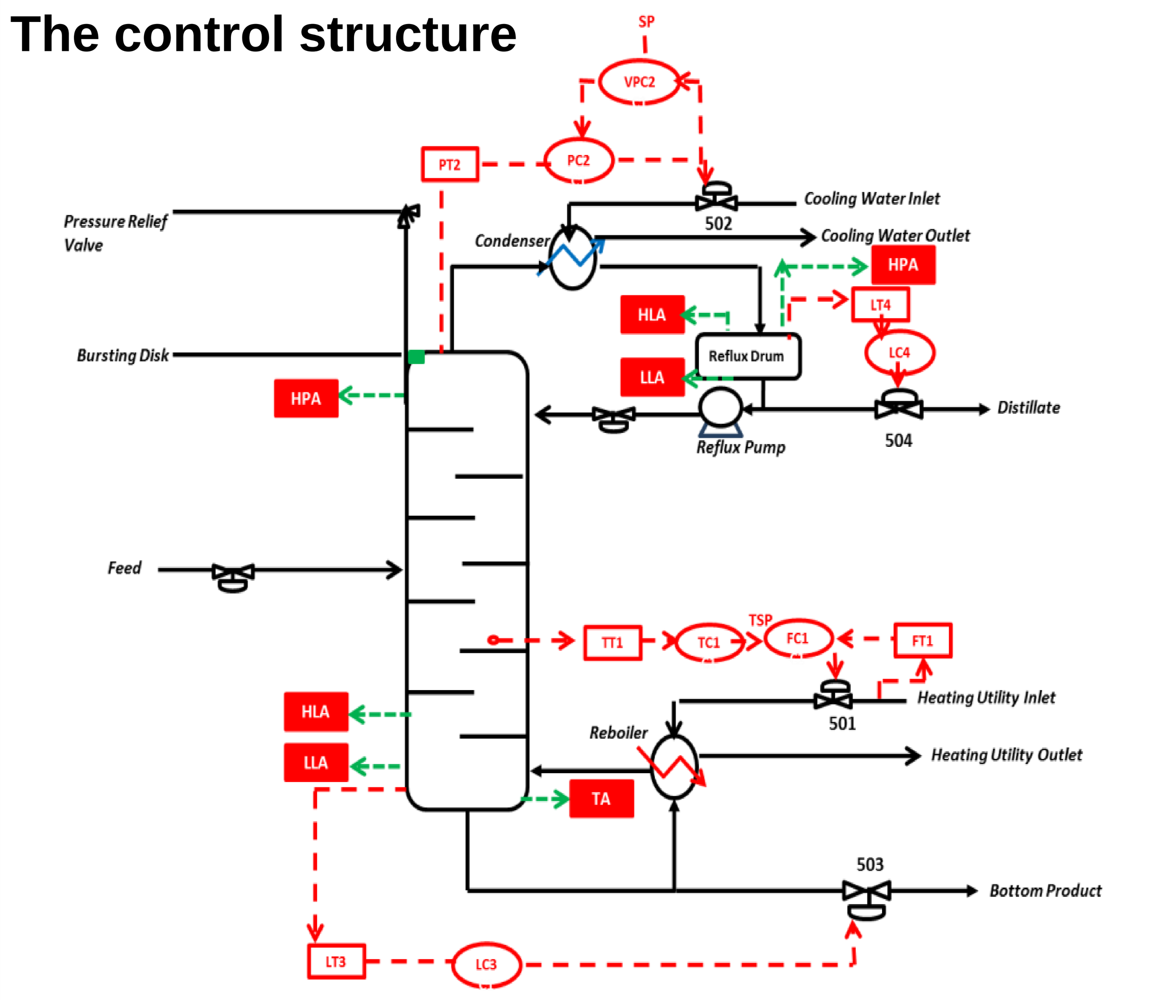
a) Feed flow rate
b) Reboiler duty
c) Condenser duty

The model equations and model verification

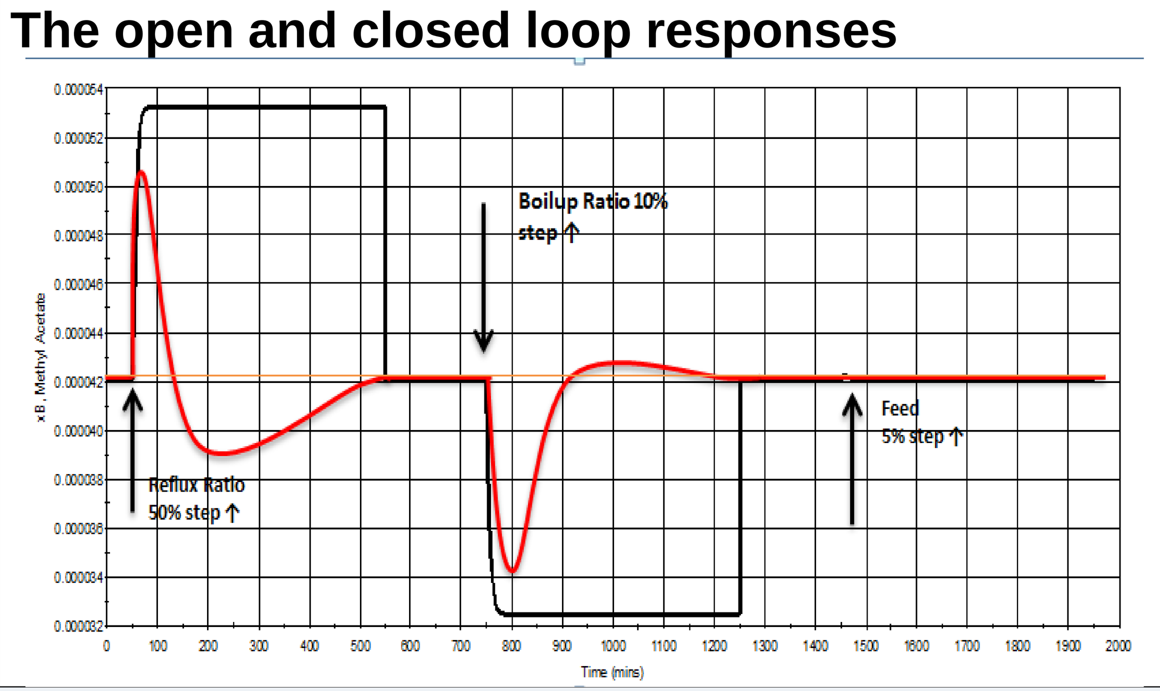
Eqn.	Description	Equation
	VLE	
1	Constant relative volatility	$y_i = \frac{a_i x_i}{\sum_{i=1}^{NC} a_j x_j} \quad \forall\, i = 1, \dots, \mathrm{NC}$
	Tray Model	
2	Component material balance	$\frac{dM_i}{dt} = F z_i + L_{in} x_{i,in} + V_{in} y_{i,in} - L_{out} x_{i,out} - V_{out} y_{i,out} \quad \forall\, i = 1, \dots, NC$
3	Component molar holdup	$M_i = M_{Tot} * x_{out,i} \quad \forall\, i = 1, \dots, NC$
4	Total molar holdup	$M_{Tot} = \sum_{NC}^{I} M_i$
5	Vapour flow rate (Equimolar overflow)	$V_{out} = V_{in}$
6	Linear tray hydraulics	$L_{out} = F_{out}^0 + (M_{Tot} - {M_{Tot}}^0)/\tau$
7	Energy balance	$\frac{dU}{dt} = F \mathrm{h}_f + L_{in} {\mathrm{h}_{in}}^L + V_{in} {\mathrm{h}_{in}}^V - L_{out} {\mathrm{h}_{out}}^L - V_{out} {\mathrm{h}_{out}}^V$
8	Energy holdup	$U = M_{Tot} {\mathrm{h}_{out}}^L - Pv$
	Physical Properties Model	
30	Pure component liquid enthalpy	${\mathrm{h}_i}^{0,L} = \left[A_{i,1}(T - T_{ref}) + \frac{A_{i,2}}{2}(T^2 - T_{ref}^2) + \frac{A_{i,3}}{3}(T^3 - T_{ref}^3)\right] \quad \forall\, i = 1, \dots, NC$
31	Reduced temperature	$T_{i,r} = T_{i,c}/T \quad \forall\, i = 1, \dots, NC$
32	Heat of vaporisation	$\Delta H_i^{vap} = B_{i,1}(1 - T_{r,1})^{B_{i,2}} \quad \forall\, i = 1, \dots, NC$
33	Pure component vapour enthalpy	$\Delta H_i^{vap} = B_{i,1}(1 - T_{r,1})^{B_{i,2}} \quad \forall\, i = 1, \dots, NC$
34	Liquid specific enthalpy	$\mathrm{h}^L = \sum_{i=1}^{Nc} {\mathrm{h}_i}^{0,L} x_i$
35	Vapour specific enthalpy	$\mathrm{h}^V = \sum_{i=1}^{Nc} {\mathrm{h}_i}^{0,V} y_i$



The control structure



The open and closed loop responses



Student feedback

I found the first half of the course useful as I learnt more about first principles modelling and dynamics of familiar unit operations.

When first using gPROMS it was incredibly difficult. However, in hindsight, it makes more sense and has definitely helped to consolidate technical knowledge.

Although gPROMS is a versatile software with easy to understand syntax, getting it to do what you want it to do is not.

gPROMS has usually very understandable error messages, but some would be VERY puzzling.

Guest lecture was good, it let us see the importance of industrial process modelling from another perspective.

The lecturers were very helpful and the course was challenging, interesting and enjoyable.

One of the best taught courses over the 4 year MEng program.

All in all I feel I have learned many skills that will be useful in the work place.

gPROMS for undergraduate students

Using a tool such as gPROMS in a final year undergraduate module can be challenging, particularly for weaker students who find computational work difficult.

The main challenge, however, is not gPROMS, but a lack of fundamental process understanding and appropriate modelling skills. Modelling must therefore be taught either before, or in parallel with, the use of gPROMS.

The students also need to develop an understanding of the implications of different modelling assumptions and of the need for proper model verification.

Extensive use of tutorials and cluster room support is essential.

Assessment of individual computational course work may be difficult when students collaborate extensively. An individual exam can be used to better gauge understanding, even for gPROMS coding.

Self- and peer assessment further develops the students' understanding of technical writing in terms of clear and accurate presentation.

UCL Best Design Prize

Process Systems Enterprise are sponsoring the annual award for the best individual contribution to the design project.

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