Teaching gPROMS to 18 year olds – Why, What and How

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Summary

The Department of Chemical Engineering at UCL is introducing gPROMS to its students as one of the main simulation tools in the undergraduate programme. In the past, the tool has only been used in the fourth year of studies, however, from 2014-15, gPROMS is being introduced as early as in Year 1.
The initial introduction to gPROMS is given to enable the students to do dynamic modelling and simulation of very simple processes. The feedback from both staff and students has been very positive, and the Year 1 students seem to cope better with gPROMS than the Year 4 students.

Lectures		
Part A: STEADY STATE SYSTEMS	**Part B:** DYNAMIC SYSTEMS	**Part C:** OPTIMISATION
1. Introduction to Modelling of Steady State Systems 2. Process Flowsheeting with Recycle 3. Flash Calculations 4. Equation Solving Methods	5. Introduction to Modelling of Dynamic Systems 6. Differential Equation Models	7. Linear Programming
Part D: COMPUTATIONAL TOOLS		
8. GAMS (General Algebraic Modelling System): for Parts A and C **9. gPROMS** (general Process Modelling System): for Part B		

CENG105P Computational Modelling and Analysis

The aim in this module is to provide the core computational and modelling skills that underpin studies in chemical engineering with emphasis on the modelling and analysis of systems through integration of computation, modelling theory and engineering practice.

The followings are highlighted in this module:

- Development of mathematical models for Chemical Engineering process design and simulation.
- Basic theoretical knowledge of numerical methods: nonlinear equations, differential equations and optimisation.
- Tools for design and simulation including the gPROMS and GAMS.

Upon completion of this module students will be expected to:

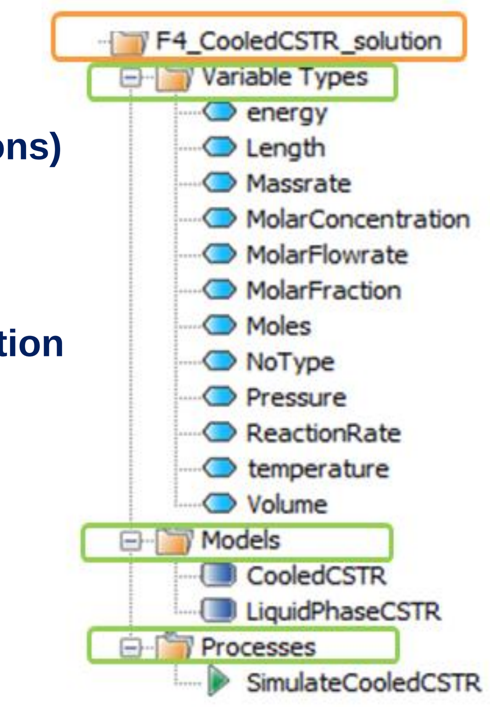
- ✓ Have knowledge of, and be able to use, a range of modelling strategies, computational methods and tools for process design and simulation.
- ✓ Have an understanding of numerical methods for the solution of simple sets of algebraic and differential equations and of linear programming problems.
- ✓ Understand the role of the computational tools in building management strategies.

Lecture (2hr)

An Introduction to gPROMS

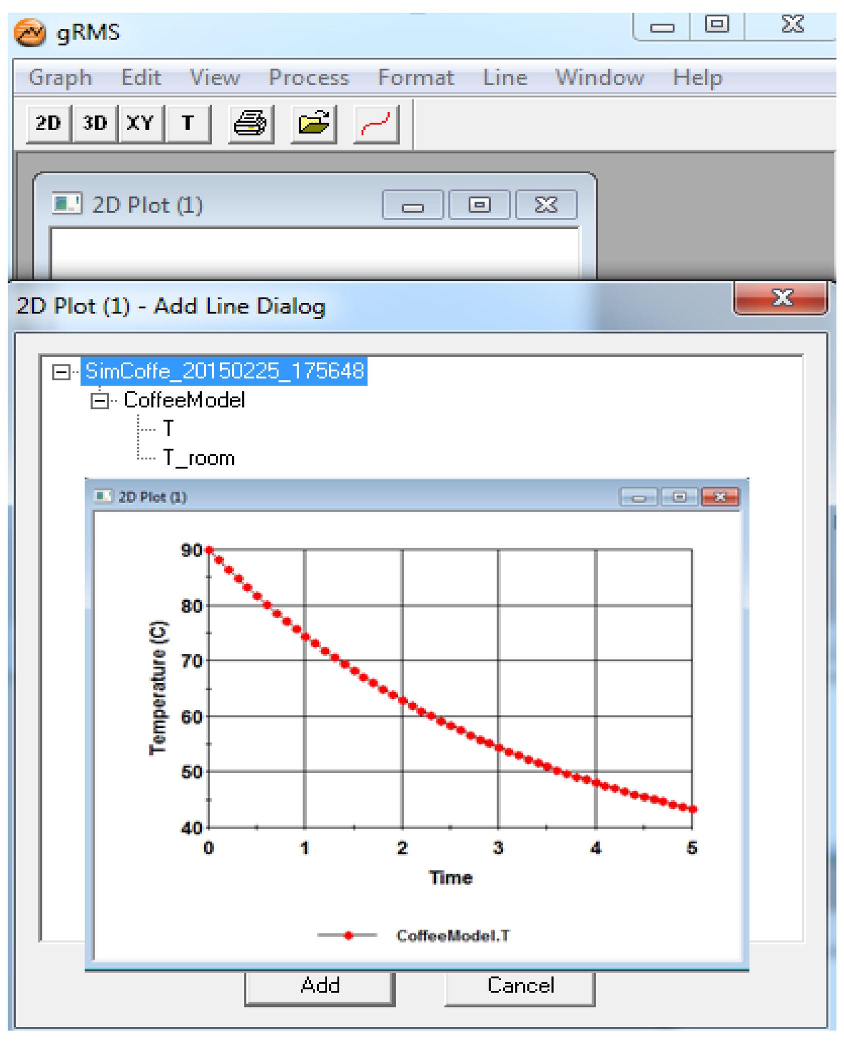
- ❖ The gPROMS ModelBuilder environment
- ❖ First-principles mathematical modelling in gPROMS

  - ➢ **Variable types**
  - ➢ **Models (Equations)**
    - **Parameters**
    - **Variables**
    - **Equations**
  - ➢ **Process/Simulation**
    - **Unit**
    - **Set**
    - **Assign**
    - **Initial**
    - **Schedule**



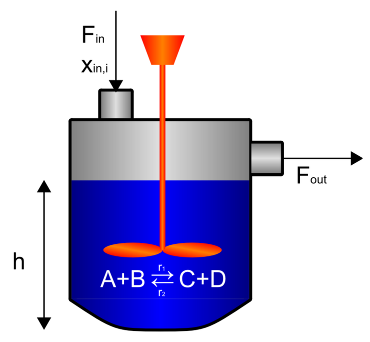
Note: Arrays were not included in this lecture!

- ❖ Running a simulation and viewing the result using gRMS



Tutorial (2hr)

Continuous Stirred Tank Reactor (CSTR)



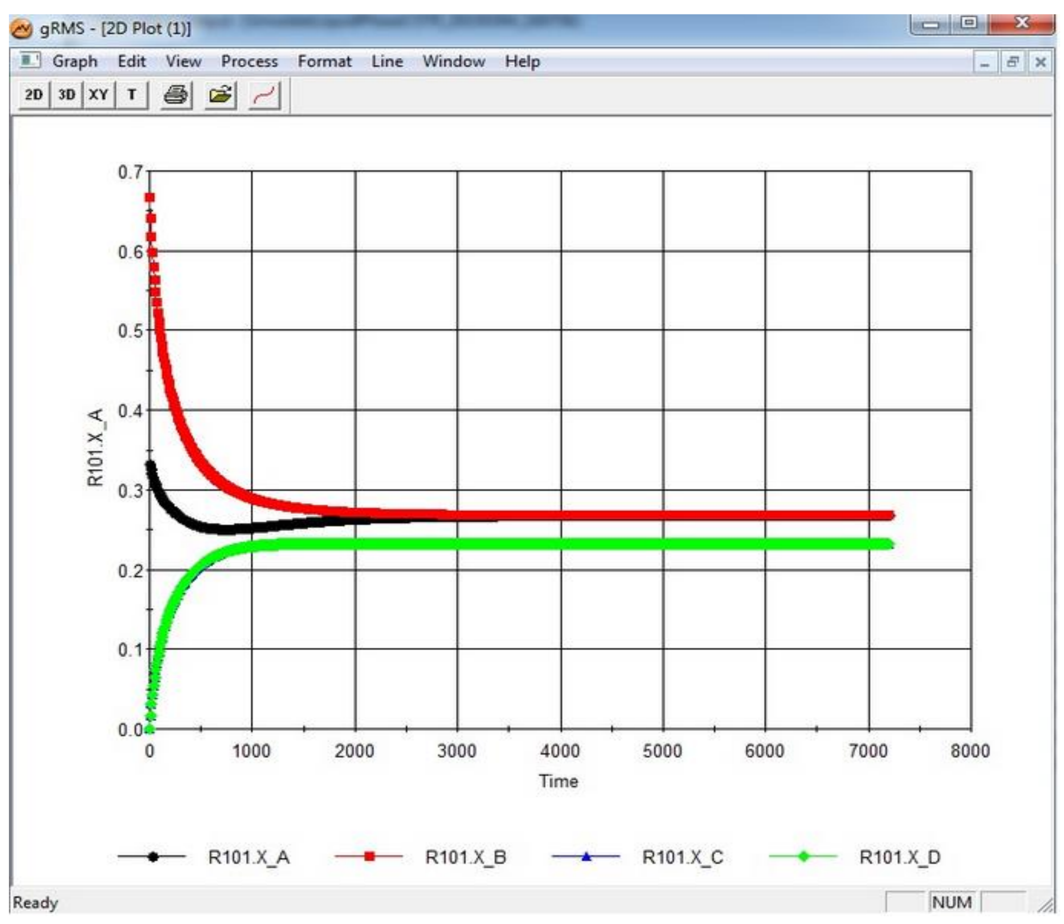
$$A + B \Leftrightarrow C + D$$

We want to simulate the first two hours of the dynamic operation of a Continuous Stirred Tank Reactor (CSTR) used to carry out the above reaction:

Eqn.	Description	Equation
1	Molar balance of components:	$\frac{\partial N_i}{\partial t} = F_{in}X_{in,i} - F_{out}X_i + V(v_{A,Fw}r_{Fw} + v_{A,Rv}r_{Rv})$ $\forall i = A,B,C,D$
2	Reaction rates	$r_{Fw} = k_{0,Fw}e^{\frac{-E_{a,Fw}}{RT}}(C_A^{\alpha_{A,Fw}} \times C_B^{\alpha_{B,Fw}} \times C_C^{\alpha_{C,Fw}} \times C_D^{\alpha_{D,Fw}})$ $r_{Rv} = k_{0,Rv}e^{\frac{-E_{a,Rv}}{RT}}(C_A^{\alpha_{A,Rv}} \times C_B^{\alpha_{B,Rv}} \times C_C^{\alpha_{C,Rv}} \times C_D^{\alpha_{D,Rv}})$
3	Total holdup:	$N_T = (N_A + N_B + N_C + N_D)$
4	Total volume	$V = \left(\frac{N_A}{\rho_A} + \frac{N_B}{\rho_B} + \frac{N_C}{\rho_C} + \frac{N_D}{\rho_D}\right)$
5	Molar fractions:	$N_i = X_i N_T$
6	Molar concentrations	$N_i = C_i V$
7	Liquid level	$V = Ah$
8	Outlet flowrate	$F_{out} = \begin{cases} \alpha(h - h_p) & \text{if } h > h_p \\ 0 & \text{if } h \le h_p \end{cases}$

The reactor is initially loaded with 10 m^3 of A and B. The molar fraction of A in the initial mixture is half that of B, *i.e.* $x_B(0)=2x_A(0)$. The reactor operating temperature and the initial temperature of the reactor mixture at 65°C.

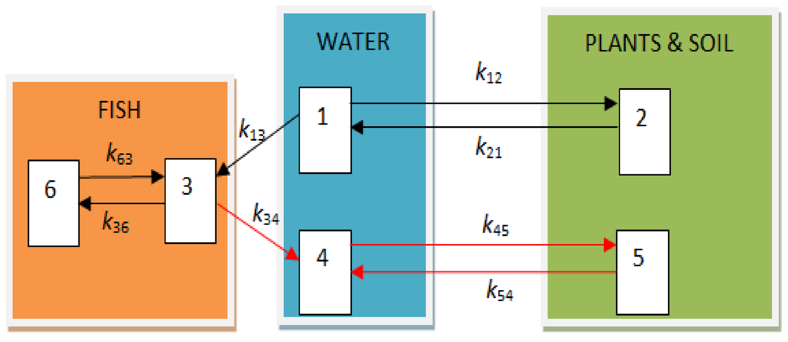
The input to the reactor is a stream that contains 50% A and 50% B, with a flowrate of 1 *kmol*·s^{-1} at a temperature of 65°C.



Coursework (13% of mark)

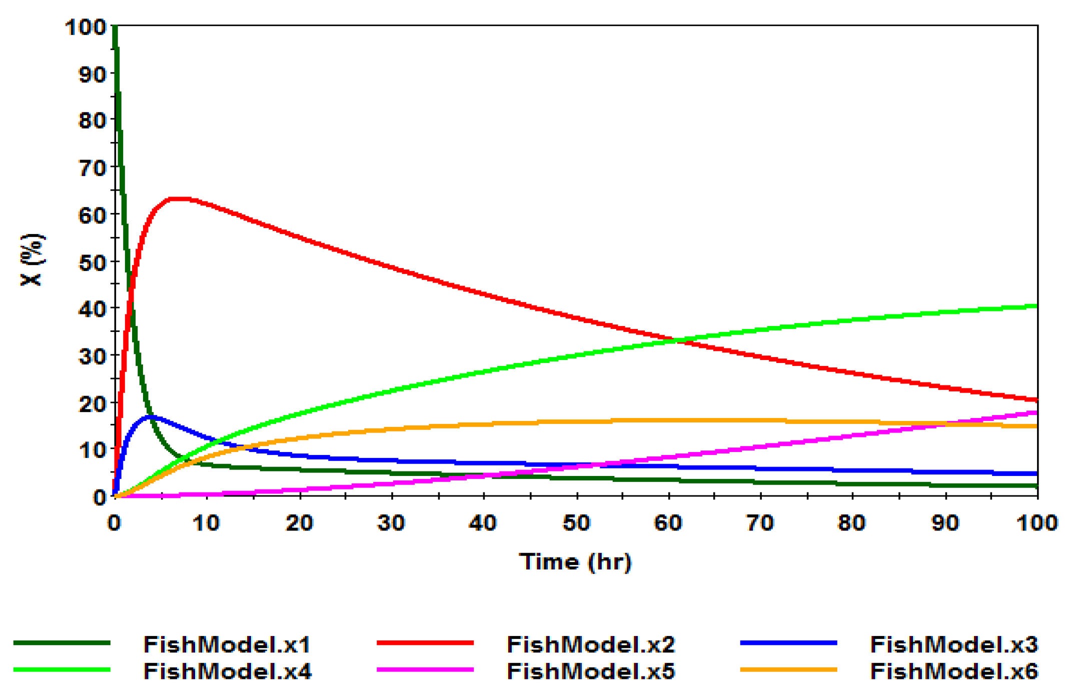
Compartmental model

The transport of agrochemicals from land to water, and the accumulation of these chemicals in water, plants, soil and fish, is represented by Ordinary Differential Equations (ODEs).



1: insecticide in water
2: insecticide in plants and soil
3: insecticide in fish
4: metabolite in water
5: metabolite in plants and soil
6: insecticide stored in fish

Description	Equation
Ordinary Differential Equations (ODEs) corresponding to the change of chemical (x) in different compartment s(i)	$dx_1/dt = k_{21}x_2 - k_{12}x_1 - k_{13}x_1$
	$dx_2/dt = k_{12}x_1 - k_{21}x_2$
	$dx_3/dt = k_{13}x_1 + k_{63}x_6 - k_{36}x_3 - k_{34}x_3$
	$dx_4/dt = k_{34}x_3 - k_{45}x_4 + k_{54}x_5$
	$dx_5/dt = k_{45}x_4 - k_{54}x_5$
	$dx_6/dt = k_{36}x_3 - k_{63}x_6$
Values of the transfer coefficient parameters (h^{-1})	$k_{12} = 0.388$, $k_{21} = 0.0515$, $k_{13} = 0.136$, $k_{36} = 0.067$, $k_{63} = 0.0254$, $k_{34} = 0.0788$, $k_{45} = 0.0068$, $k_{54} = 0.001$

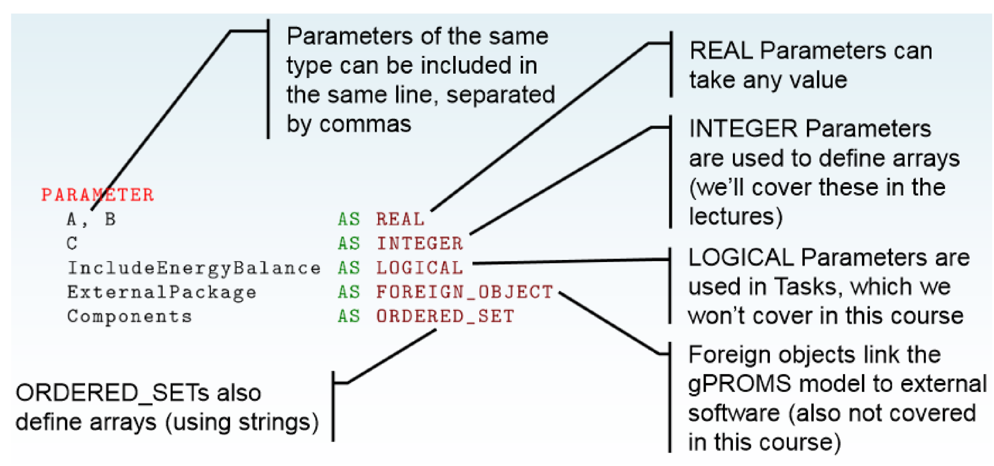


Online Material

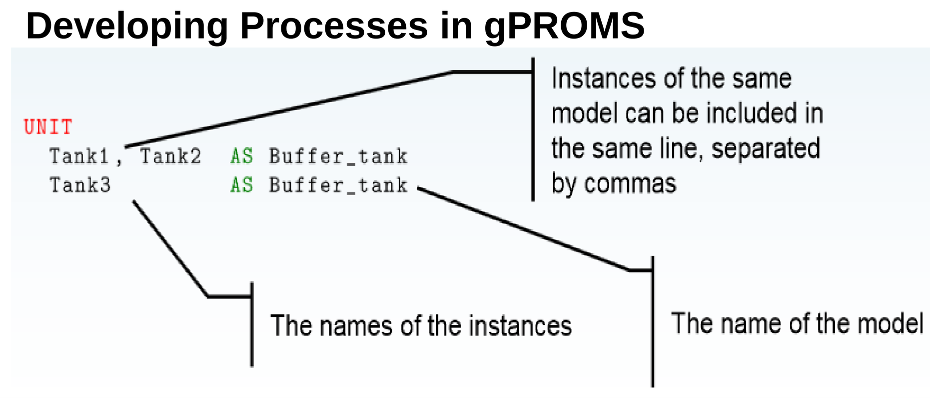
Due to the time limitation during the lectures, it is impossible to deliver all the concepts comprehensively and in a detailed manner. Online material is therefore used to provide extensive information to the students beyond what can be covered during the lecture or tutorial.

❖ **Examples of online material:**

- ➢ **Developing Models in gPROMS**



- ➢ **Developing Processes in gPROMS**



gPROMS for first year students

Using gPROMS as a modelling and simulation tool for first year students can potentially be challenging, however, depends on how the use of the tool is introduced and implemented, and has the potential of being quite exciting for them.

The background knowledge of the students in mathematical modelling and process engineering must be considered, and the computational tool introduced accordingly. At UCL, the main aim in Year 1 is to enable the students to solve simple mathematical models associated with chemical processes. In subsequent years, they will learn how to deal with more complicated problems in both modelling and optimisation.

Our experience confirms that the main challenge is not gPROMS itself, but the students' understanding of mathematical modelling. The feedback shows that the students are enjoying the challenge.

Student feedback

A very good initiative to introduce all the existing technology to 1st year students to broaden their scope of knowledge.

It was introduced in a very good way. The lecture slides and the information given was more than adequate, and was really helpful.

Best lecturer material in terms of teaching, step by step and very coherent.

Dr Molaei was extremely helpful. He answered all my questions and helped me improve my understanding of the coursework.

The tutorial was good as it applied the basic skills we learnt in the lecture. This was very helpful and again had an easy to follow structure.

More lecture or tutorial have to be taught. And the way to identify error in gProms should be introduced

I would recommend to have more tutorials, because practice makes perfection. One tutorial can be almost irrelevant.