PSE ACADEMIC

PSE Academic Teaching Highway (PATH)

A proposal for process modelling course material

Background

Modelling is increasingly important to the process industries due to:

- Increased competition that requires more detailed models for design and operational decision support
- New product and process development, which is not covered by standard library models

Developing course material that prepares undergraduate students for the needs of industry is not straightforward. At the same time, modelling has become less prevalent in the academic curriculum. Modelling competes with new topics within the broadening scope of chemical engineering. There is a need for effective, open curriculum materials to teach process modelling in chemical engineering.

What is PATH?

PATH stands for PSE Academic Teaching Highway, an initiative to help bridge the gap between industry and academia with regards to process modelling. PATH is the result of discussions with PSE's Academic Advisory Board, a group including experts from industry and academia. The Academic Advisory Board helped establish the goals, structure and content of the PATH initiative.

PATH Benefits

- Modular approach to allow for added flexibility
- Reviewed by PSE's Academic Advisory Board with members from industry and academia
- Material is supplied under the Creative Commons license as Attribution-NonCommercial-ShareAlike license
  - Ready to use or alter as desired following the license
  - Potentially self-evolving and improving material
- Material is designed to be software agnostic as much as possible (hands-on examples are based on gPROMS)
- PSE customers that have Teaching licenses will get
  - Free access to the PATH material
  - Free access to how-to videos for gPROMS (registration required)

To find out more, go to:
www.psenterprise.com/academic/path

Who is this for?

The PATH material is aimed at undergraduate chemical engineering classes on process modelling (flowsheeting and first-principles models, i.e. balance equations and constitutive equations).

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Available Modules

Lumped modelling

Introduction into modelling, assumptions, DOF, mass & energy balances, generic modelling (4 modules*)

Distributed modelling

Partial differential equations, boundary conditions, DOF, methods, order, numerical solution (2 modules*)

Separation & reaction

Types of separation, separation factors, equilibrium, reaction kinetics, parameter estimation (3 modules*)

Basic control

Introduction into control, P & PI control, MV, CV, pairing, basic tuning, disturbances (1 module*)

Debugging

Introduction into debugging, general techniques, divide and conquer, hypothesizing (1 module*)

Flowsheeting basics

Sources, sinks, connections, building a flowsheet, recycles, dialogue boxes, adjust blocks (1 module*)

Flowsheeting: physical properties

Right/wrong choice effect, equations of state, activity models, SAFT, verifying choice (1 module*)

Flowsheeting: optimisation

Intro optimisation, defining the problem, solving the optimisation problem (1 module*)

Formulated products

(hands-on predominantly)

Several unit ops incl. milling, spray drying, granulation and tablet disintegration.

*1 module is roughly 45 minutes of class material

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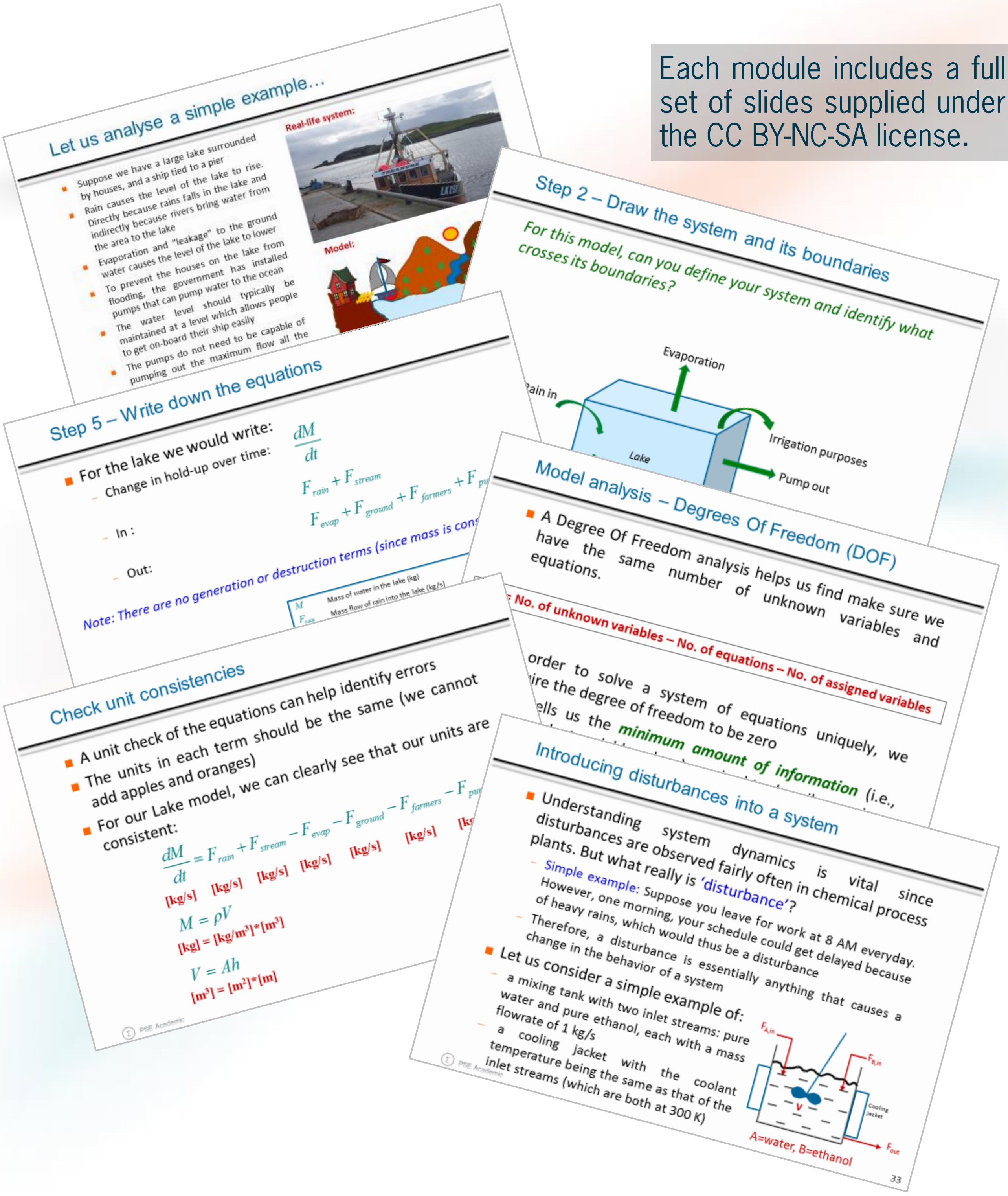
Examples of PATH Teaching Materials

Each module includes a full set of slides supplied under the CC BY-NC-SA license.



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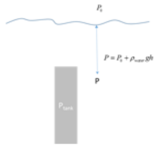
Examples of PATH Teaching Materials

Each module includes optional home assignments. Home assignments are designed to be software agnostic and are supplied as editable documents under the CC BY-NC-SA license.

Home assignment: Lumped models – a diving tank model

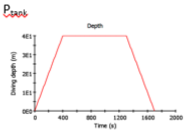
Scuba divers use air from a tank on their back to breath under water. Although the volume flow of air is fairly constant during a dive, the *mass* flow of air used in each breath is dependent on the depth the diver is at. This is because the pressure on the body of the diver increases with depth and to breath in, the pressure of the air coming in must be a little above the pressure of the surroundings. If the pressure is higher the density is higher and for the same volume flow that means the mass flow is higher.

A fanatic modeler and scuba diver wants to find out how much air he will have left in his tank after a nice pre-scheduled dive.



Derive the equations for a model of the scuba diving tank. Assume the following:

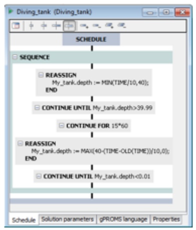
- Tank has a volume of 18 liters
- Initial pressure in the tank, P_{tank}, at the start of the dive is 210 bar
- We assume we can use the ideal gas law to determine:
  - the density of the air that the scuba diver is breathing in as a function of the surrounding pressure, P
  - the density of gas inside the tank at the pressure in the tank, P_{tank}
- Assume a constant volume flow of 30 liter per minute
- Assume the following values (R_{gas} is 8.314 J/(molK), g is 9.81 m/s²):
  - Temperature: 293 K
  - Molecular weight of air: 29 g/mol
  - Pressure of atmosphere, P_0: 1 bar
  - Density of water: 1000 kg/m³



- Assuming the following dive profile (see example of one way to implement this in a gPROMS model below):
  - Dive at constant rate from surface to 40 m at a rate of 0.1 m/s
  - Stay at 40 meters for 15 minutes
  - Return to surface at a rate of 0.1 m/s

How much will the diver have left in his tank at the end of his dive?

Example of gPROMS code to include diving schedule:



Note molar density is calculated as follows:

$$\rho_{mole} = \frac{P}{R_{gas}T}$$

Where ρ_{mole} is the density in mole/m³, P the pressure in Pa, R_{gas} the gas constant in J/(mol K) and T the temperature in K.

Figure of scuba diver taken from: https://pixabay.com/en/scuba-diving-diver-diving-147683/

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Hands-on session

Background

In this exercise we will develop a model of a gas storage tank. The tank is normal buffer to keep production constant. The tank has a safety system that releases th in case the pressure gets above 10 bar. Over a day the tank heats up due to sola changes in the surrounding temperature. This affects the pressure in the tank. In we will try to find what the flow rate into the tank needs to be to meet production of the product while maintaining a pressure in the tank of at least 8 bar.

Exercise 1

Creating a lumped model of a gas storage tank

Objectives

By the end of the exercise, you will know how to:

- Take advantage of the gML Basics library
- Build a model from scratch
- Write equations using the gPROMS language
- Run a dynamic simulation

Things to do

1. Open gPROMS ProcessBuilder 1.2.0 from the Windows start menu by clicking on the ProcessBuilder icon. When it opens, load the *gML Basics* library by clicking this icon on the menu toolbar.
2. Create a new project file by going to the menu *File > New*. Save the newly created project under a different name. Make sure the name is highlighted in the project tree and go to the menu *File > Save as...* Choose an appropriate location and name for the file, e.g. *Gas_Tank.gPJ*

   Concept > gPROMS ProcessBuilder project tree. ProcessBuilder uses a Windows Explorer-like "project tree" structure to organise the different sections of the model description. To open an entity, navigate to it, by expanding the tree if necessary, and then double-click it. It will open in the workspace to the right.
3. Cross-reference the *gML Basics Interface* library by right-clicking on the project name, clicking on the *Properties*, and then in the *Cross-references* tab selecting the library of interest as shown in the following picture:

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Modules include hands-on, computer lab exercises. The optional exercises are supplied as editable documents with flowsheet templates where appropriate. Exercises use gPROMS platform products. They are supplied according to the terms of the PSE Academic license agreement.

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