

PSE Academic Workshop Agenda: Hands-on Session

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Goal: To introduce some of the material developed for academic institutions by PSE

- The material has been designed to:
 - Familiarise undergraduate students with the fundamental principles of mathematical modelling
 - Equip students with the knowledge to use these tools for process design, control, operations and optimisation
- Format:
 - Slides and exercises available for review
 - Bring a laptop if you want to run the exercises (USB sticks with software and examples will be provided)

- ***Sample modules*** covered during the workshop:
 - *Mathematical modelling of lumped models*
 - Introduction to the importance of modelling and simulation
 - Basics of developing customised models
 - Implementation of simple examples and hands-on assignments
 - *Custom modelling of distributed systems*
 - Fundamental concepts of developing complex distributed models
 - Introduction to numerical solutions
 - Includes interesting examples and home assignments
 - *Introduction to flowsheeting*
 - Creating your own flowsheets and simulating these processes
 - Scheduling operating procedures

Some ideas of material covered

What are mathematical models used for?

- Models help us develop a better scientific understanding of the behavior of a system

How do models help?

Safety: Models to accurately measure the effect of control rods, pressure, temperature at several points inside a nuclear reactor under various operating conditions

Economy: Financial models for homeowners rely on to decide whether to invest in a new house

Let us analyse a simple example...

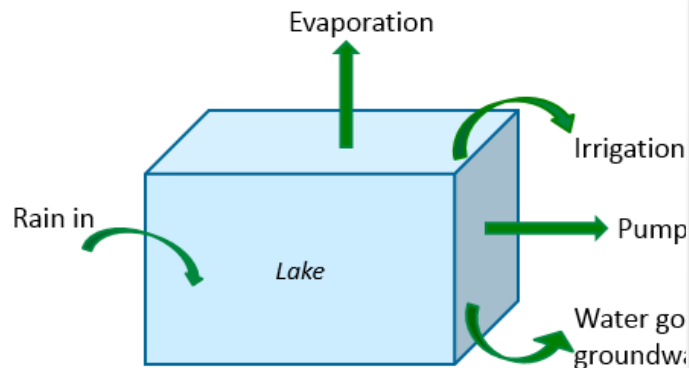
- Suppose we have a large lake surrounded by houses
- Rain causes the level of the lake to rise

Real-life system:



Step 2 – Draw the system and its boundaries

For this model, can you define your system and its boundaries? What crosses its boundaries?



Step 5 – write down the equations

- The basis of (most) models are the balance equations
- Balance equations are “keeping track” of conserved properties
- We almost always start with the mass balance
- We track what we call the hold-up, the amount held inside the system
- The general form of a balance is:

$$\text{Change in hold-up over time} = \text{in} - \text{out} + \text{generation} - \text{destruction}$$

Change in hold-up over time is typically called accumulation

Some ideas of material covered



Model analysis – Degrees Of Freedom (DOF)

- A Degree of freedom analysis helps us find out if we have “*enough*” or too much information to solve a particular problem

$$\text{DOF} = \text{No. of unknown variables} - \text{No. of equations} - \text{No. of assigned variables}$$

- In order to solve a system of equations require the degree of freedom to be zero
- This tells us the minimum amount of independent variable values) required to de state of a system

Numerical software available for modeling

- Analytical software: Mathcad, Maple, Maxima, ...
- Spreadsheets: Excel, Lotus
- Matrix Algebra tools: Matlab, Scilab, Octave
- Flowsheeting tools: Aspen, HYSYS, PRO/II, ChemCad, Unisim, gPROMS ProcessBuilder
- Equation-Oriented tools: ACM, Modelica, gPROMS ProcessBuilder, gPROMS ModelBuilder, ...
- General software languages: Fortran, C++, Java, Python, ...

Thank you

