Bringing modelling to life: current research in an introductory MSc modelling course

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Stefan Trapp, Massimo Rolle and Luca Vezzaro

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Department of Environmental Engineering

How do you take newly enrolled MSc students who have little experience with models…

…and bring them to research standard in an **introductory** modelling course?

I have taken a course in numerical methods?	Yes 21	No 41
I have taken a course in PDES	Yes 14	No 48
I have some basic background in statistics	Yes 60	No 2
I know how to fit a straight line to a set of data	Yes 51	No 11

Environ. Sci. Technol. **2010,** *44,* 7622–7627

Evaluation of Bioaugmentation with Entrapped Degrading Cells as a Soil Remediation Technology

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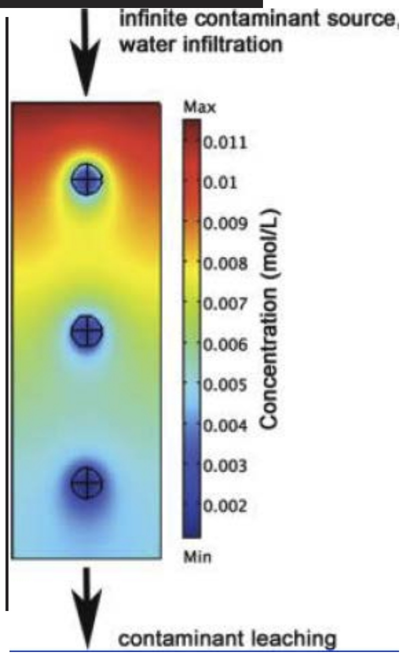
Soil augmentation with microbial degraders immobilized on



12104 Modelling of Environmental Processes and Technologies

10 ECTS course

Compulsory General Competence Course for all MSc in Environmental Engineering students (60-90 students).

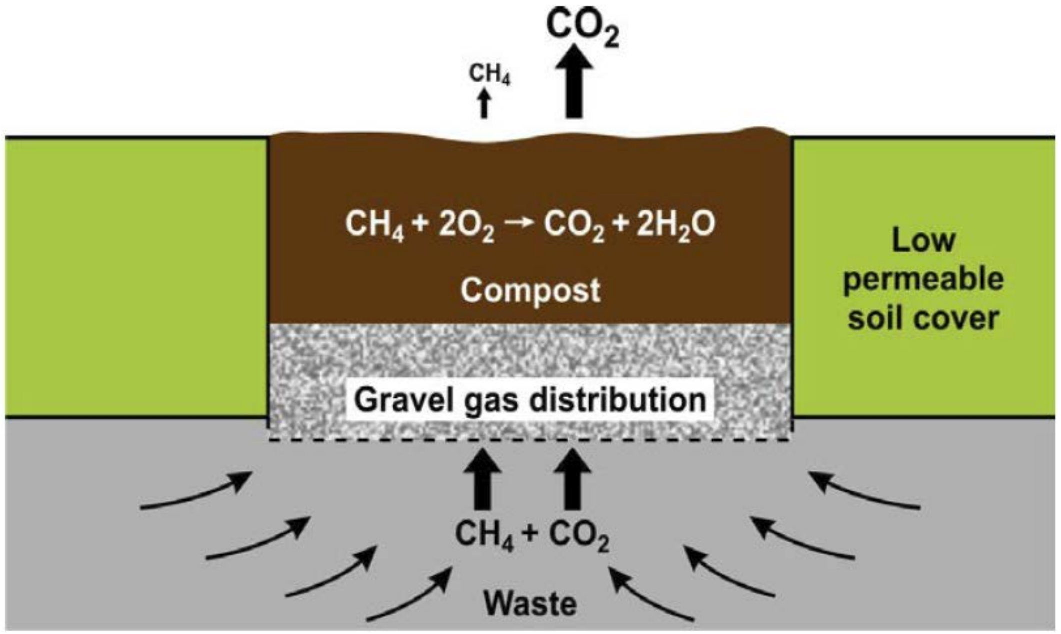
Typically first course taken in MSc at DTU

The curriculum contains 5 main elements:

- Models based on analytical solutions and programming
- Statistics
- Ordinary differential equations
- Partial differential equations
- Model parameter estimation, sensitivity and uncertainty analysis.

The central element of the course is 5 assignments which are new every year and address current research being conducted at the Department.

MATLAB, COMSOL Multiphysics, PHREEQC

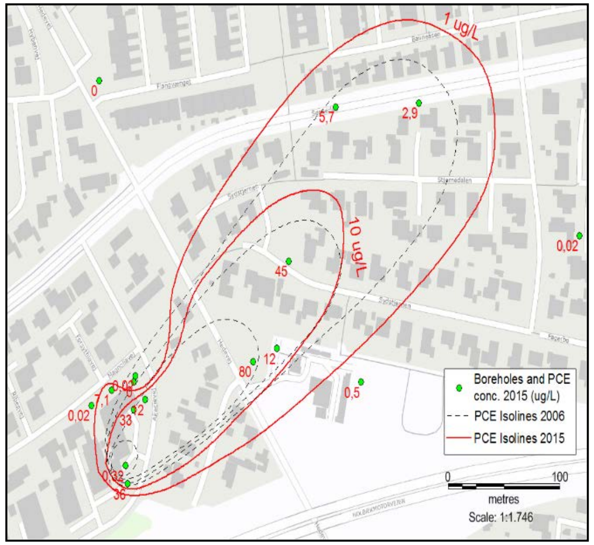


Landfill biobarriers
(Analytical solutions)

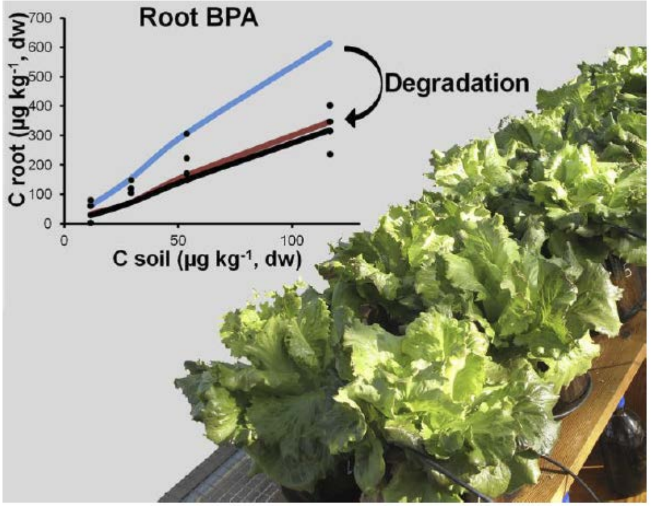
2016 Assignments: 2-3 weeks each, first assignment given on day 1

DTU

Analytical solutions programming



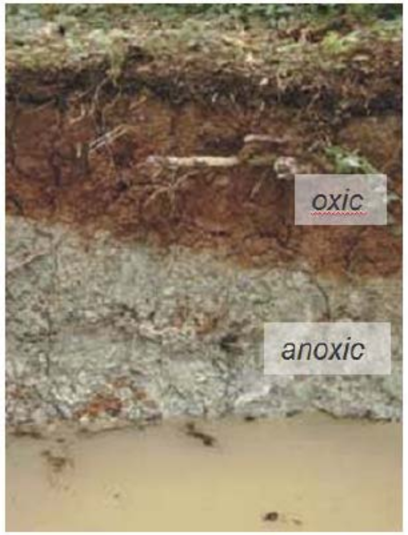
Ordinary differential equations



Partial differential equations

Statistics

Aqueous geochemical modelling

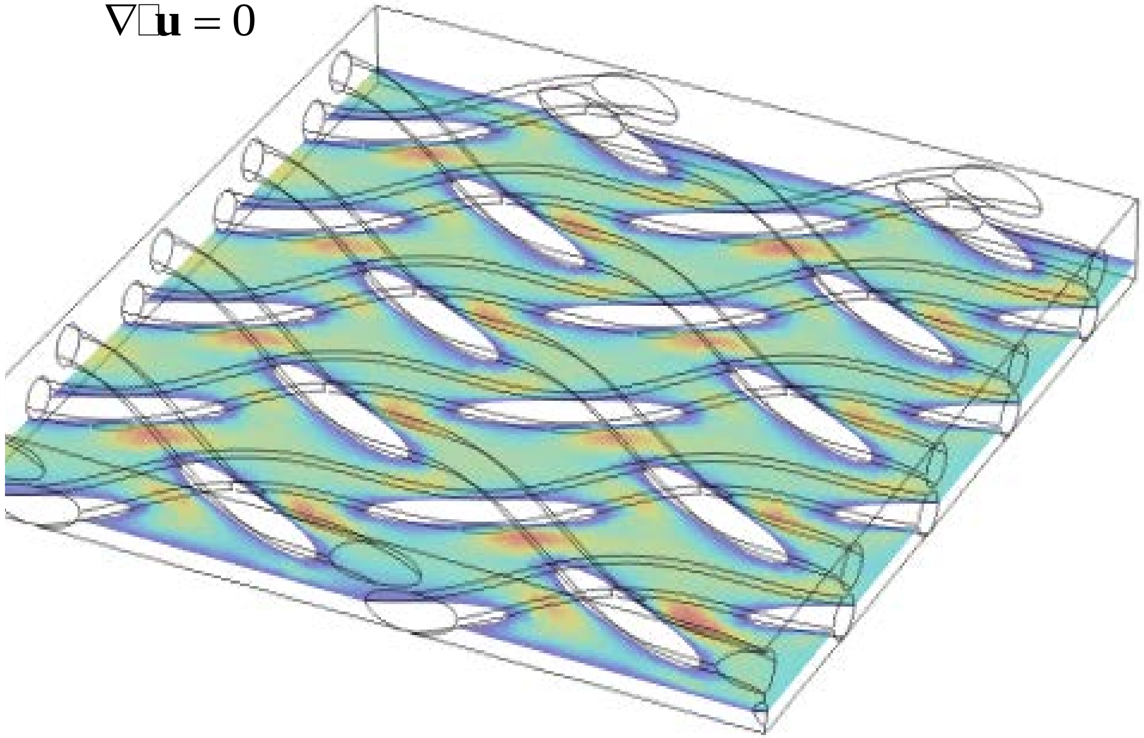


Model parameter estimation sensitivity and uncertainty analysis

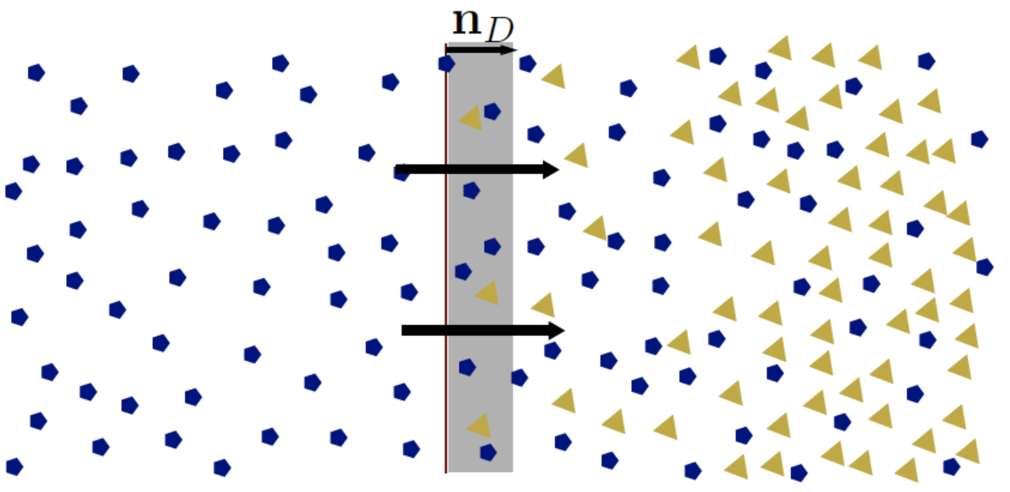
Example assignment

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}(\nabla \cdot \mathbf{u}) = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0$$



$$n\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{J}c) - \nabla \cdot (\tau n D_o \nabla c) = 0$$



1. If the membrane permeability A is 4 ml/(min cm^2 bar), calculate the water flux $\mathbf{J}$, assuming complete mixing in the feed and draw solution and support layer with $c_F = 1 \times 10^{-6}$ mol/L and $c_D = 1 \times 10^{-3}$ mol/L . Assume that there is no fluid pressure gradient across the membrane ($p_D - p_F = 0$). The water temperature is 25°C.

12. The effect of a broader mesh grid can be analyzed to examine the impact of changes in mesh design. Change the spacer distance to 3 mm, redo questions 10 and 11 for this spacer grid and comment on the difference.

Selection of Assignment topics

- Pick problems from current work
  Time spent developing assignments is time invested in your own research.

- Couple assignments to work of PhD teaching assistants
  If they are going to teach, get them to teach on their own work

- We never invest in new assignments unless we can see a potential spin-off.

Warning: The assignments are 'open' problems

Expectation management is critical

12104 - Assignment 4

Due date: 08:00 Friday 8 Nov 2016

Submission:

** One electronic copy of your assignment response, submitted to the assignments menu under campusnet for the course.*

** One electronic copy of the model input files you used to generate your results. Submit via campusnet as above.*

** A declaration stating the individual contributions of each student to the work*

Format

** You do not need to submit a report. You should answer each question clearly and concisely. Provide adequate documentation so that the reader can determine how you obtained your answer.*

***Important**: this is a real **research** assignment, so be careful not to use too much of your time. You could spend much more time than is available for this assignment, so judge carefully when it is time to stop! The assignment gets progressively more difficult. The last questions are part of a current PhD project!*

Benefits of new assignments

Many people look at a problem and this provides new insight

The students are extremely good at finding deficiencies in problems and holes in solution approaches.

The development of a new assignment forces the lecturer to simplify the problem sufficiently so it can be done, sharpening their own understanding of the problem.

The use of current and new problems each year means that the course is ‘alive’

Each year is different and so staff are heavily engaged in the course.

Green roofs
(parameter estimation)

Course → research and products

12104 - Assignment 1
Due date: 21:00 Friday 21 Sept 2012

Submission:
** One electronic copy of your assignment response, submitted to the assignments menu under campusnet for the course.*
** One electronic copy of the model input files you used to generate your results. Submit via campusnet as above.*
** One paper copy of your assignment response.*
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Part 1: Mixing of groundwater discharge into rivers.
Philip Binning

This assignment is based on a current project being carried out by DTU with the consulting company Orbicon for the Danish EPA and a DTU MSc by Mette Fjendbo Petersen.

Contaminated sites can impact surface water bodies via groundwater discharge. Indeed, they can be an important contributor to the total contaminant load in a stream. For example, at Grindsted stream on Fyn, MSc student Mette Fjendbo Petersen has estimated that 370 kg/yr sulfonamides (used in the production of anti-bacterial drugs) leach into the stream from the Grindsted works (see figure 1). To determine the impact of the contaminants, it is important to calculate the concentration in the stream. This assignment provides a variety of methods to do this.

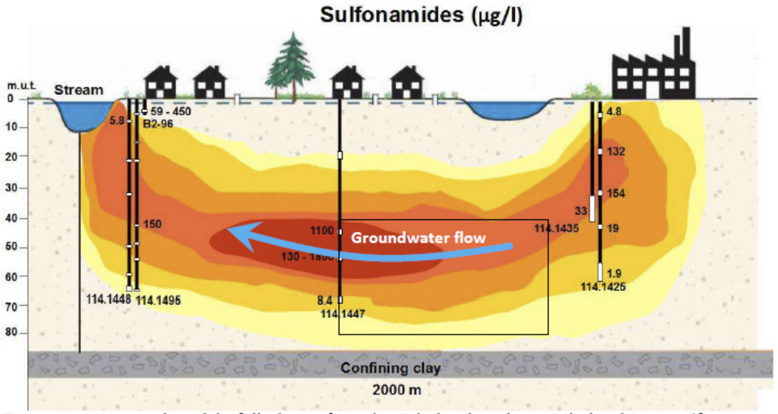

Figure 1. Conceptual model of discharge from the Grindsted works to Grindsted Stream (from [*Petersen*, 2012]).

Journal of Contaminant Hydrology 172 (2015) 71–83

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journal homepage: www.elsevier.com/locate/jconhyd

Dilution and volatilization of groundwater contaminant discharges in streams

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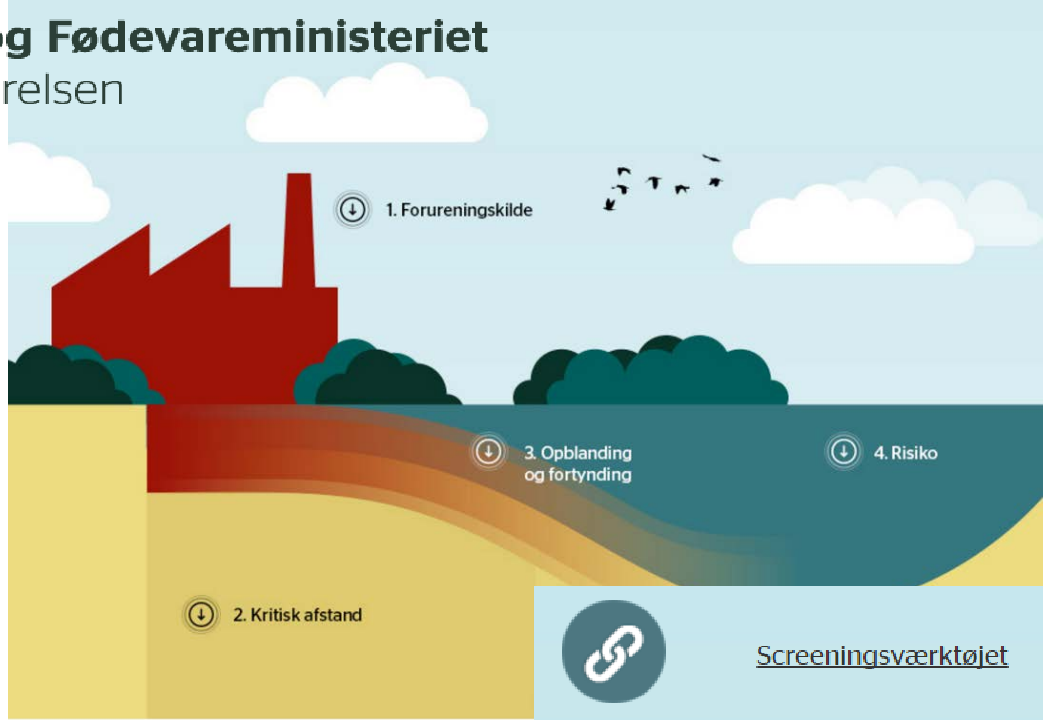
Miljø- og Fødevareministeriet
Miljøstyrelsen



Flipped learning

Flipped learning leads to motivated students!

1. Assignment

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Design of Reverse Osmosis (RO) membranes

This assignment is based on work currently being carried out at DTU Environment for the company Aquaporin by PhD student Fynn Aschmoneit under the supervision of Claus Helix-Nielsen

Aquaporin A/S is a global cleantech company located in Kongens Lyngby, Denmark (www.aquaporin.dk). Aquaporin wishes to revolutionize water purification through the use of industrial biotechnological techniques. Reverse Osmosis (RO) is a proven technology and widely applied as the final step in many water treatment processes in order to turn polluted water into drinkable or reusable water. The Aquaporin Inside™ technology allows RO membranes to have both improved water flux and higher rejection rates. All Aquaporin's RO products are made from flat sheets and supplied as spiral wound modules adhering to industry standards. Currently, Aquaporin delivers tap water RO membranes with increased water flux. High rejection tap water as well as brackish water and seawater RO membranes are under development.

Figure 1: *Aquaporin Inside RO Tap Water unit (picture and text above from www.aquaporin.dk)*

2. Tutorials

12104 - Tutorial PDEs 04

Flow past a cylinder

This tutorial is intended to familiarize students with turbulent flow and its modelling with Comsol Multiphysics.

We will construct a model of the Karmen Vortex Street, shown in figure 1. This is a classical experiment in fluid mechanics and helps understand the phenomenon of turbulence. It can, for example be observed in the flow of air over obstacles like windmills (figure 2).

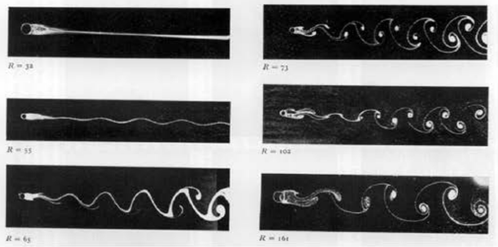


Figure 1. *Experimental investigation of flow stability, and its dependence on Reynolds number: The Karman Vortex Street pattern changes with higher Reynolds number.* http://hmf.enseeiht.fr/travaux/CD0102/travaux/optmfn/gpfmho/01-02/grp6/images/allees.jpg

Figure 2. *Turbulent wakes downstream of windmills. These wakes decrease the energy output of the windmill park. The wakes are formed when water vaporizes in the low pressure region downwind of the windmills. (https://ing.dk/artikel/eons-nye-vindmoller-stjaeler-vind-fra-dong-97227)*

3. Lectures

Navier Stokes equations

$$\rho \mathbf{g} - \nabla p + \mu \nabla^2 \mathbf{v} = \rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right]$$

$$\nabla \cdot \mathbf{v} = 0$$

Incompressible, Newtonian fluids

4 equations in 4 unknowns p, u, v, w

Some vector notation

$$\nabla^2 \mathbf{v} = \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \\ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \\ \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \end{pmatrix} \qquad (\mathbf{v} \cdot \nabla) \mathbf{v} = \begin{pmatrix} u \frac{\partial u}{\partial x} \\ v \frac{\partial v}{\partial y} \\ w \frac{\partial w}{\partial z} \end{pmatrix}$$

$$\nabla^2 \mathbf{v} = \nabla \cdot \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right)$$

Here tensor notation is employed!

4. Readings

Fluid Mechanics

Eighth Edition

Frank M. White

University of Rhode Island

Adapted by

Professor Rhim Yoon Chul

School of Mechanical Engineering, Yonsei University

Mc Graw Hill Education

Typical day: 1 hr

1-2 hrs

< 1hr

Tutorials

12104 - Tutorial PDEs 03

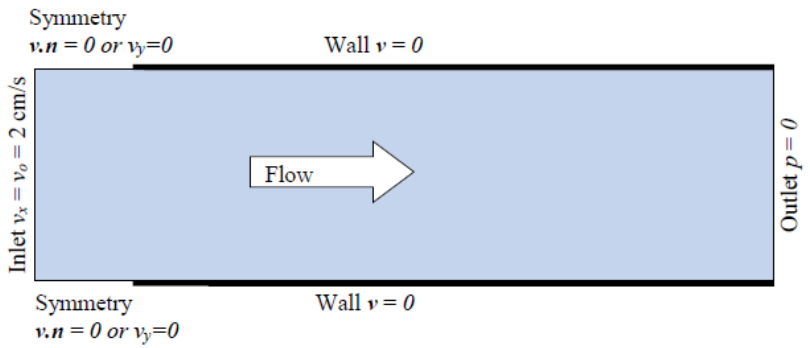
Poiseuille flows describe the condition where flow is occurring between parallel plates or in a pipe, and the velocity profile has reached a steady state condition, with zero flow on the walls and a maximum flow in the middle of the pipe or channel.

It is one of the few examples where the Navier Stokes equations can be solved exactly. Here we solve the Navier-Stokes equations for the parallel plate problem using Multiphysics and compare with an analytical solution.

The Navier Stokes equation is given by:

$$\rho\left[\frac{\partial \mathbf{v}}{\partial t}+(\mathbf{v}\cdot\nabla)\mathbf{v}\right]=-\nabla p+\rho\mathbf{g}+\mu\nabla^2\mathbf{v}$$

We solve the equation on the domain shown below, with boundary conditions noted:



The plates are separated by 0.02 m, the entrance section (with symmetry boundaries) is 0.01 m long and the outlet is 0.05 m from the inlet. The fluid is not water and has a viscosity of 0.01 kg/(m s) and a density of 1000 kg/m^3.

Solve the problem in Comsol Multiphysics, and answer the following questions:

1. Determine at what y distance the velocity profile can be considered fully developed for the flow between 2 parallel plates with uniform inlet velocity. Include a figure showing the velocity in the channel as a function of y at several values of x. Explain your answer.
2. Determine the pressure gradient for fully developed flow. Compare with the theoretically obtained value.
3. Compare the analytical and simulated velocity profiles. Does the model produce good results?

12104 - Tutorial PDEs 03 Toolbox

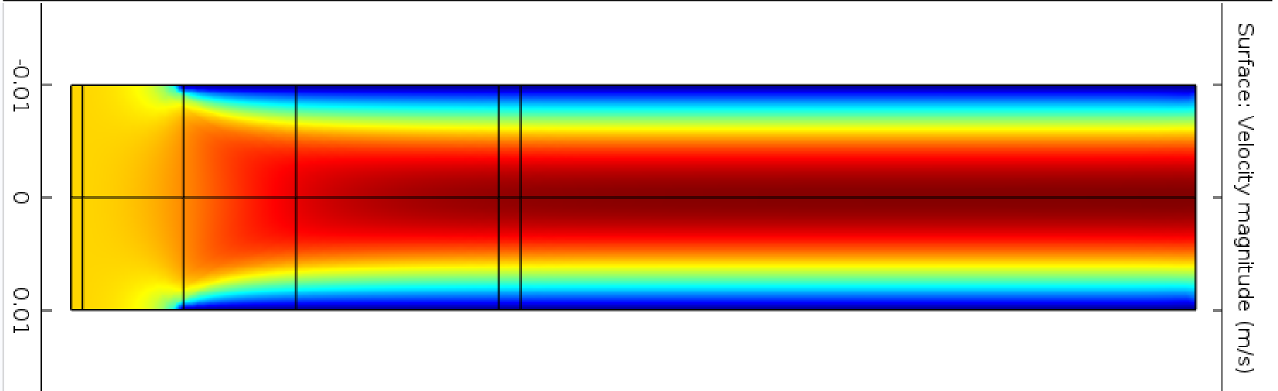
1 Start multiphysics and set up your model

1. Start COMSOL Multiphysics 5.2.
2. Click on the Model Wizard button [Model Wizard].
3. Select 2D when asked to 'Select Space Dimension'.
4. In the 'Select Physics' page, click on the triangle next to 'Mathematics' and 'Fluid Flow'. Select 'Single-Phase flow -> Laminar flow' and press the 'Add' button.
5. Press the green right arrow 'Study' button.
6. Select 'Stationary' in the 'Select Study' and press the done button.

2 Geometry

1. In the Model Builder window, right click on the 'Geometry 1' item and select 'Rectangle'. In the Rectangle window, type in 0.02m for the width and 0.05m for the height.
2. Press the 'Build Selected' button [Build Selected].
3. Use the 'Geometry -> Bezier Polygon' to add 4 lines across the whole width of the rectangle at y=0.001, 0.01, 0.02, 0.04

12104 - Tutorial PDES 03 - Solution



What do we expect from the students?

Aim is NOT to educate modelling experts

- Inspiration
- Exposure to techniques
- Modelling Experience

Leaching of antioxidants from pipes
(Analytical solutions)

Staffing

- 4 Academic staff
- 2 post-docs
- 2 PhD students
- 3 MSc teaching assistants

Groups

Group size = 4 students

Assigned groups on day 1

Free groups for assignments 2-5

Formula:
1-2 DTU students (old + young)
1 Guest student
1-2 International MSc students

Aim: Integration of new students

More than half keep assigned groups after Assignment 1

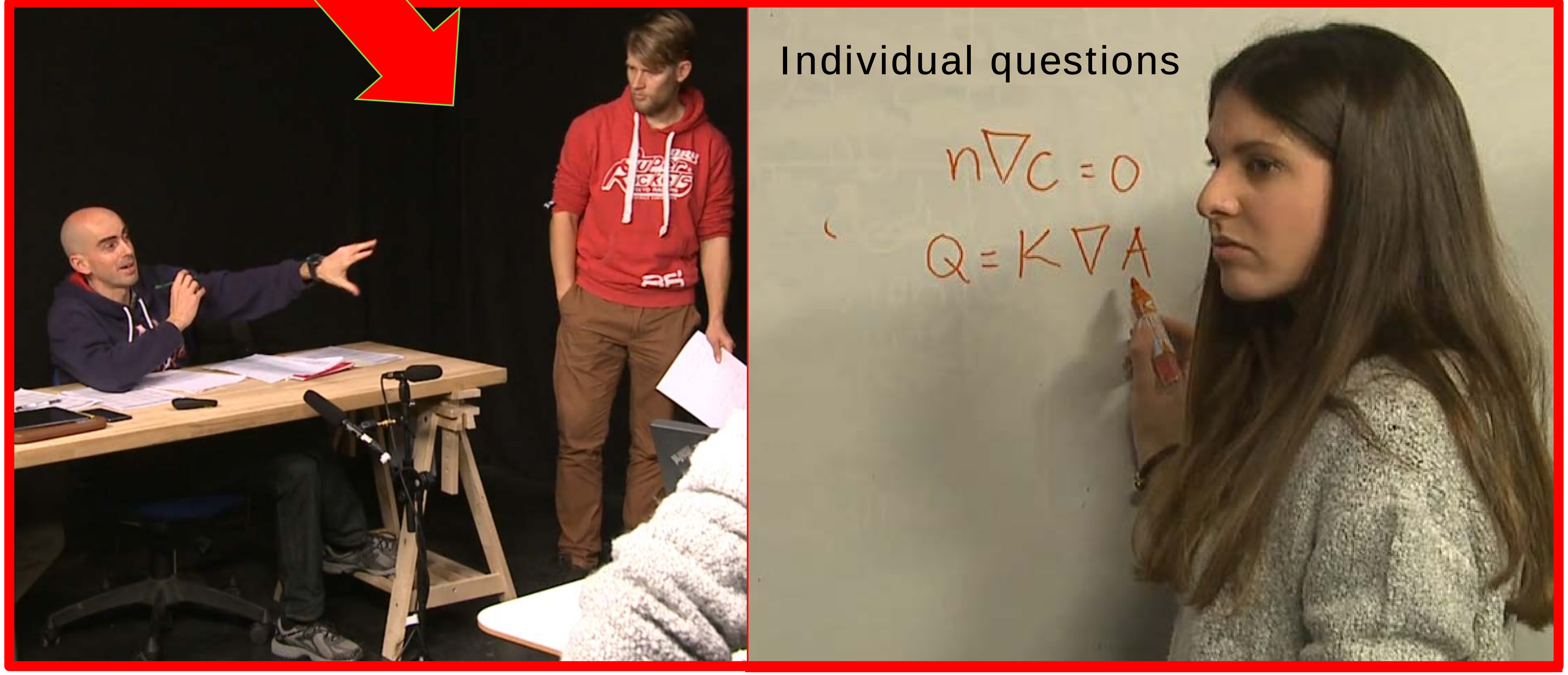
Students very positive about group assignment process

Exam

1. 5 Assignment submissions
2. Videotaped oral exam

Overall Evaluation
(Exam used to check assignment grades)

External examinar reviews selected videos



Evaluations

A good course

Helt enig	23		34,33%
	27		40,30%
	11		16,42%
	4		5,97%
Helt uenig	2		2,99%

Workload

Meget mindre	0		0,00%
	5		7,46%
	23		34,33%
	30		44,78%
Meget større	9		13,43%

I learned alot

Helt enig	27		40,30%
	23		34,33%
	10		14,93%
	7		10,45%
Helt uenig	0		0,00%

Student feedback

The course is very interesting because the assignments have to do with real projects

Cooll that the assignments are made new every year

This course is great, and very challenging

Class is very dynamic

Group formation at the beginning

The tempo of the course was too fast to really understand

Getting filmed at the exam seems nerve-wracking

Discussion

- Is the course cost effective? Could you get the same result with less resources?

- Teaching approach: There are many ways to teach modelling. Are we doing it right?
  Our focus is on inspiration/experience.
  But you could base course on fundamentals (e.g. Mass, Energy, Momentum equations)

- Grading of all those assignments. It is a big task to grade 5 open ended assignments.
  How can it be done effectively?

How we will do it:

1. 5 minutes in a group of 3. Write down your thoughts.
2. Swap with neighbours. 5 minutes to reflect and add to neighbours document.
3. Discussion in plenum

Discussion

- I am happy see that you don't find it difficult to find topics for discussions. Especially because we have decided to extend the format for "presentations" a little bit and allocate 35 minutes for each topic. This will allow for *both* a presentation of the case (~ 15 minutes) *and* activities involving the participants. Activities could be organized as individual reflections and/or discussions in groups and/or plenum– where "provocative questions" will be an ideal starting point.
- As an alternative to a 15 + 20 min. structure (presentation + activities), some activities could be imbedded in the presentation part.
- An active session host may help with facilitating discussions – however, you are very welcome to run it yourselfJ.