Teaching Chemical Engineering Fundamentals with COMSOL Multiphysics®

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William M. Clark
Chemical Engineering Department
Worcester Polytechnic Institute

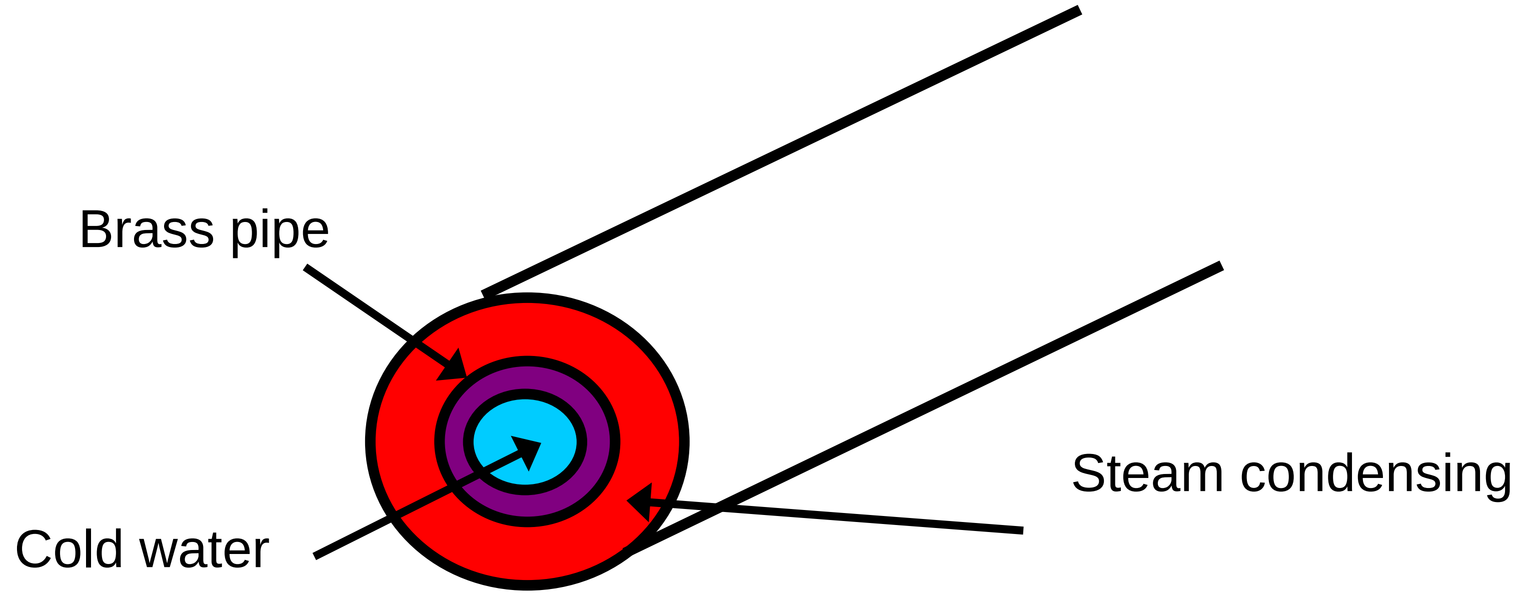
Confucius

- I hear and I forget.
- I see and I remember.
- I do and I understand.

h ? γ ?

(What would Confucius do to understand heat transfer and activity coefficients?)

Double Pipe Heat Exchanger Lab



- Measure Ts, Ps, flow rates.
- Determine U_o, h_o, h_i.
- Explain h_i dependence on water rate.

Traditional Analysis

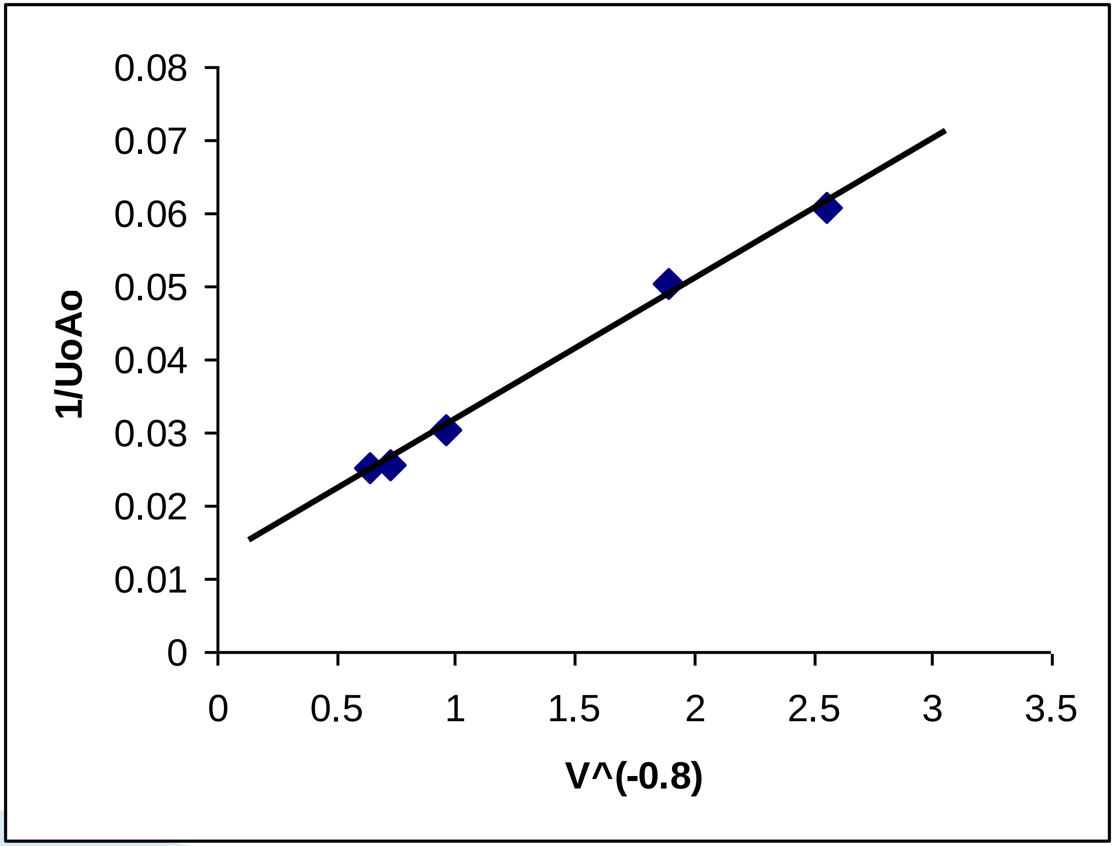
Empirical and Complex

$$q = U_o A_o \Delta T_{LM}$$

$$\frac{1}{U_o A_o} = R_i + R_w + R_o = \frac{1}{h_i A_i} + \frac{W_t}{k_p A} + \frac{1}{h_o A_o}$$

$$\frac{1}{U_o A_o} = C_1 (V)^{-0.8} + C_2$$

h_i and h_o obtained from C_1 and C_2 (slope and intercept)



The Problem

- Tedious.
- T ↓ but h_i ↑ when water rate ↑ .
- Why? No physical insight.
- What is h_i anyway?
- $q = h\,A\,\Delta T$ doesn't describe the process.

A Potential Solution

- As a pre-lab exercise, solve:

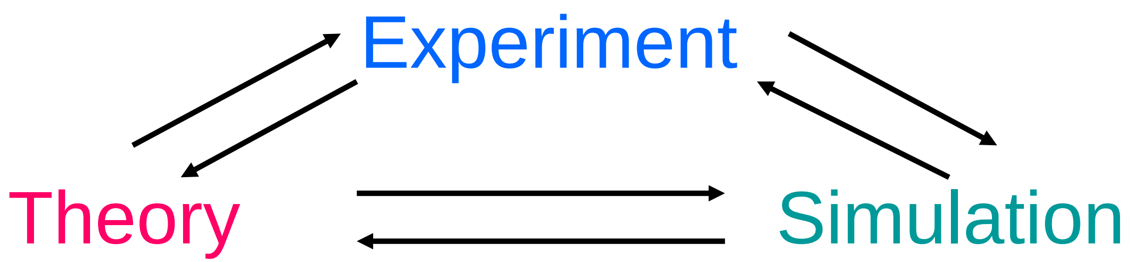
$$q = -\nabla \bullet \left(k \nabla T\right) + \rho\, C_P\, \mathbf{u} \bullet \nabla T$$

$$\rho \mathbf{u} \bullet \nabla \mathbf{u} = -\nabla \mathrm{p} + \mu \nabla^2 \mathbf{u}$$

to give visual representation of the temperature and velocity profiles.

- Integrate along boundaries to evaluate average (measured) temperature, velocity, and heat flux.

Reinforcing Fundamentals with Simulations in the Laboratory

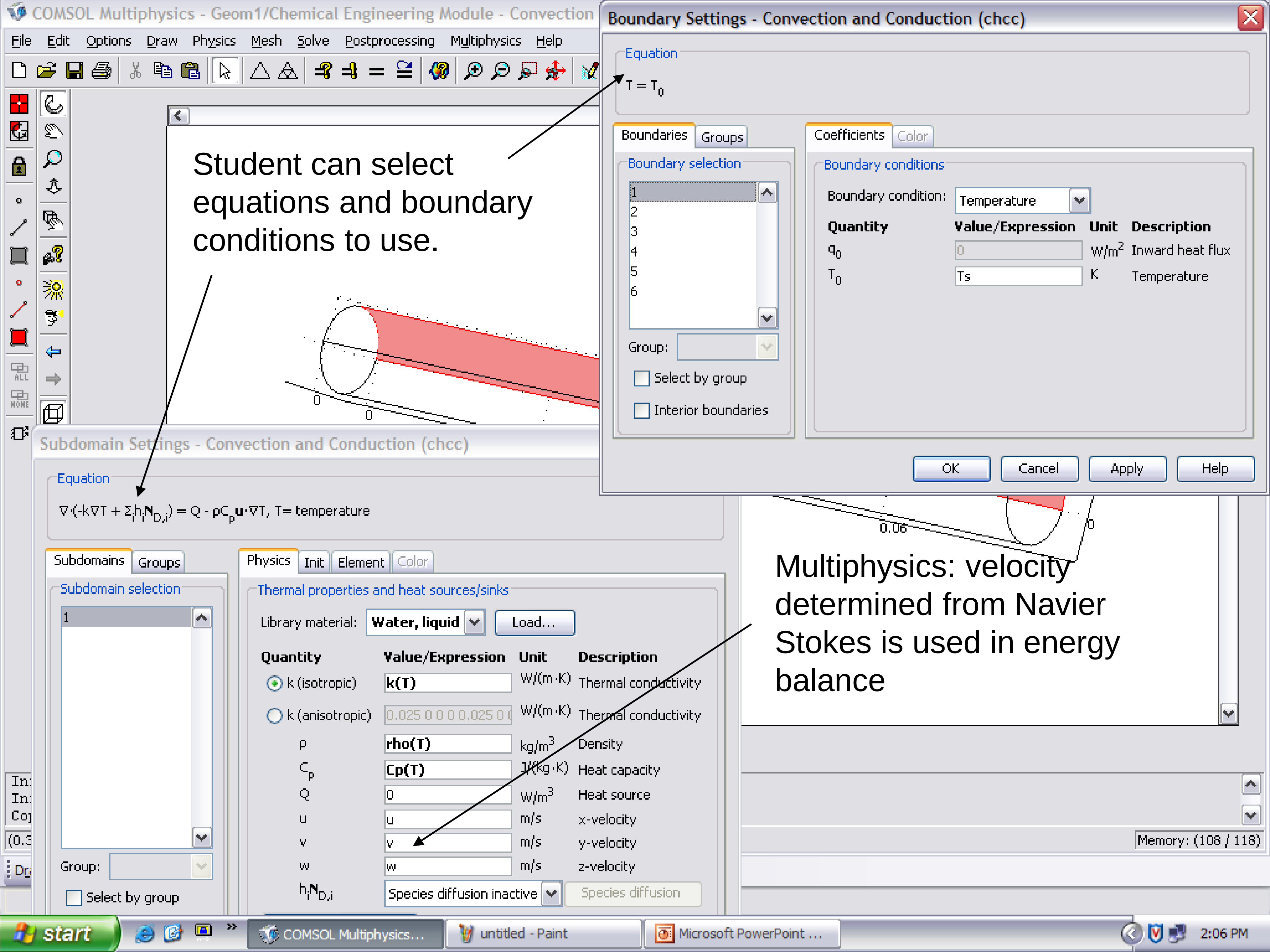


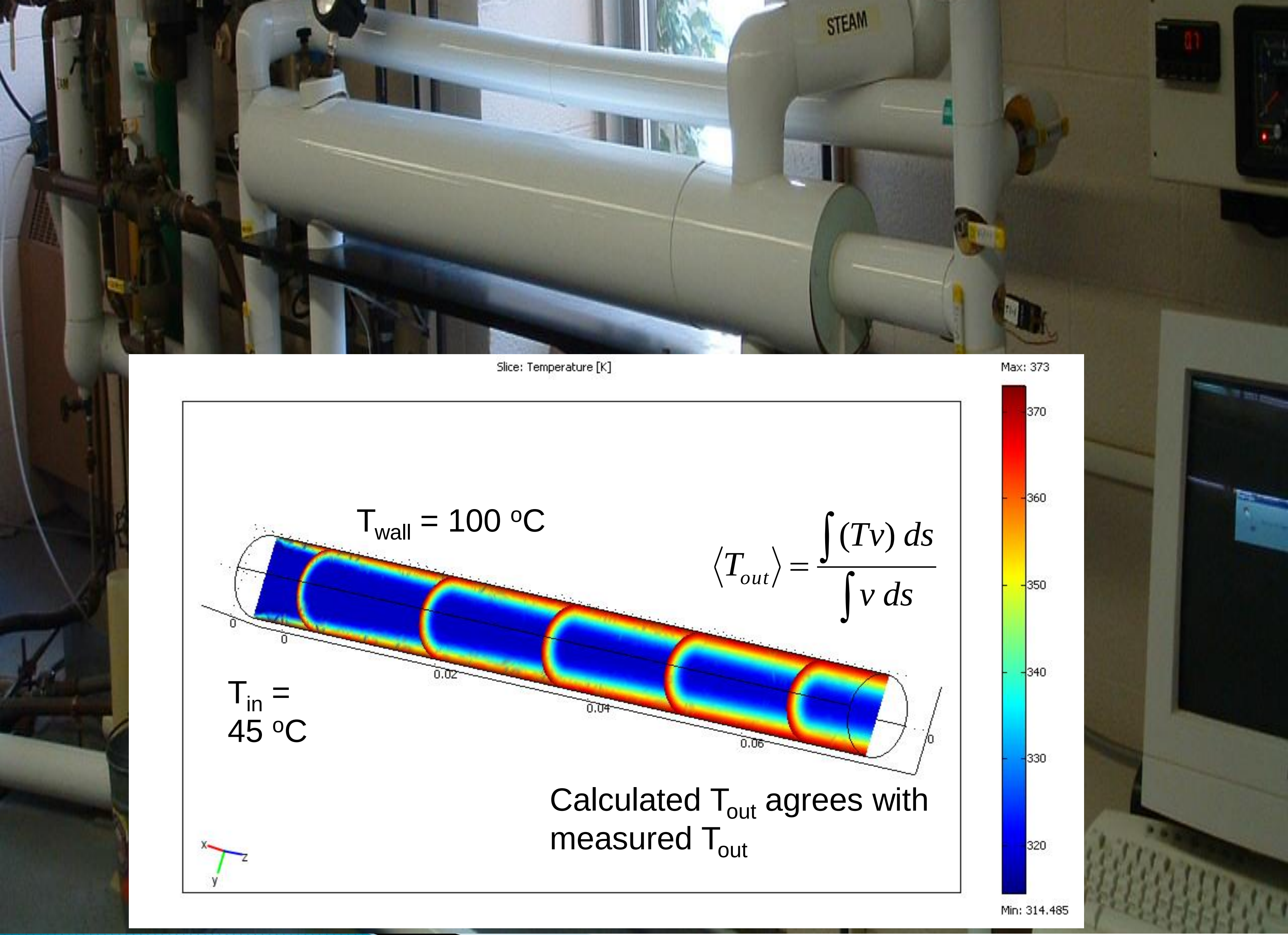
- Combining simulation with experiment and theory makes the physical process and the mathematics "come alive".

- Visualizing the details of the pressure, temperature, and velocity profile lets the student "see inside the equipment".

COMSOL Multiphysics® at Worcester Polytechnic Institute

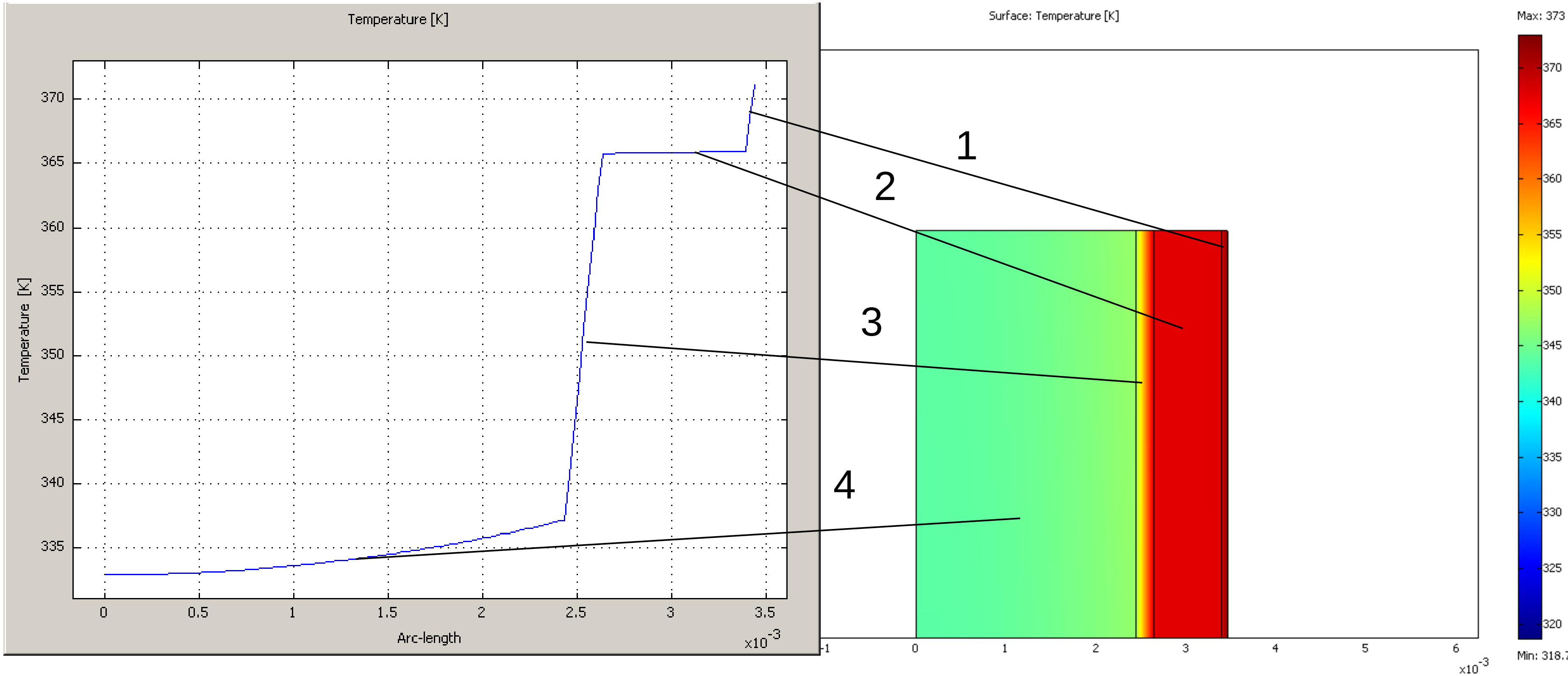
- Finite Element Software Solves Differential Equations in Specified Geometry.
- Research Modeling Tool, e.g. fuel cells, lab-on-a-chip biosensors, packed bed reactors.
- Featured Modeling Tool in "Applied Mathematics in Chemical Engineering" Course (numerical techniques, how to develop models).
- Reinforcing Fundamental Concepts in Undergraduate Courses (using developed models to gain physical understanding).


Student can select equations and boundary conditions to use.
Multiphysics: velocity determined from Navier Stokes is used in energy balance
COMSOL Multiphysics - Geom1/Chemical Engineering Module - Convection
Boundary Settings - Convection and Conduction (chcc)
Equation
T = T0
Boundaries
Groups
Boundary selection
Group:
Select by group
Interior boundaries
Coefficients
Color
Boundary conditions
Boundary condition: Temperature
Quantity
Value/Expression
Unit
Description
q0
W/m2
Inward heat flux
T0
Ts
K
Temperature
OK
Cancel
Apply
Help
Subdomain Settings - Convection and Conduction (chcc)
∇·(-k∇T + Σihi ND,i) = Q - ρCp u·∇T, T= temperature
Subdomains
Groups
Subdomain selection
Physics
Init
Element
Color
Thermal properties and heat sources/sinks
Library material: Water, liquid
Load...
k (isotropic)
k(T)
W/(m·K)
Thermal conductivity
k (anisotropic)
0.025 0 0 0 0.025 0
Density
rho(T)
kg/m3
Heat capacity
Cp(T)
J/(kg·K)
Heat source
W/m3
x-velocity
y-velocity
z-velocity
m/s
Species diffusion inactive
Species diffusion
Memory: (108 / 118)
start
COMSOL Multiphysics...
untitled - Paint
Microsoft PowerPoint ...
2:06 PM



STEAM
Slice: Temperature [K]
Max: 373
370
360
350
340
330
320
Min: 314.485
0
0
0.02
0.04
0.06
0
x
y
z
T_{wall} = 100 ^oC
T_{in} =
45 ^oC
$$\langle T_{out} \rangle = \frac{\int (Tv)\, ds}{\int v\, ds}$$
Calculated T_{out} agrees with
measured T_{out}

Simulation Results Illustrate Temperature Profile and Resistance to Heat Transfer



1 = condensed steam, 2 = brass pipe, 3 = boundary layer, 4 = turbulent bulk

(heat exchanger now arranged vertically with axial symmetry)

$$h = \frac{q}{A\,\Delta T}$$

Student Comments

- "I liked that it was visual, hands-on, and self-paced"
- "taught me outlet T versus flow rate"
- "good visualization that could not be achieved through a book…much better than just equations"
- **"the meaning of inside and outside heat transfer coefficients … how boundary layers provide the most resistance to heat transfer"**
- "more heatx type prelabs or similar reports"
- "liked the heat exchanger pre-lab module, opportunity for feedback"

Assessment

- 1st Implementation offered "optional" simulations – American students didn't use them.
- Students reported a perceived increased in understanding in subsequent "required" implementations.
- Compared pre and post quizzes and final written and oral laboratory reports of students who used the simulations against control groups who did not – there was no significant difference in critical thinking among these groups. Attributed to small sample size and confounding issues (variations in students and multiple paths to learn the material).

Assessing Impact of Simulations on Understanding using Concept Inventories

- Force Concept Inventory (FCI) developed by Hestenes et al. revealed robust misconceptions.
- Mazur found that even Harvard University physics students had misconceptions and weak physical understanding – began a revolution to teach concepts.
- Concept inventories have been developed and used to measure understanding of fluid mechanics, thermodynamics, heat transfer and other engineering fundamentals.

Example CI Question

Fluid Mechanics Concept Inventory (FMCI) developed by Martin et al.

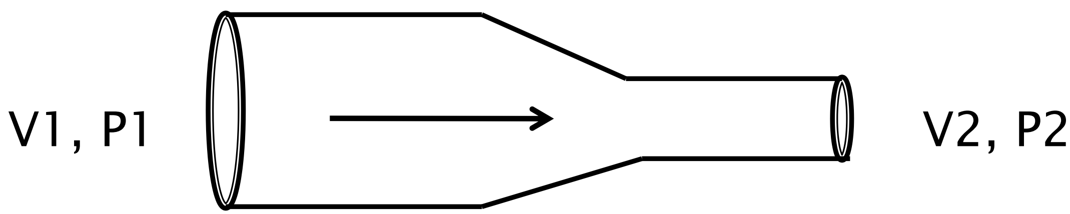


FIGURE 1. CONVERGING PIPE.

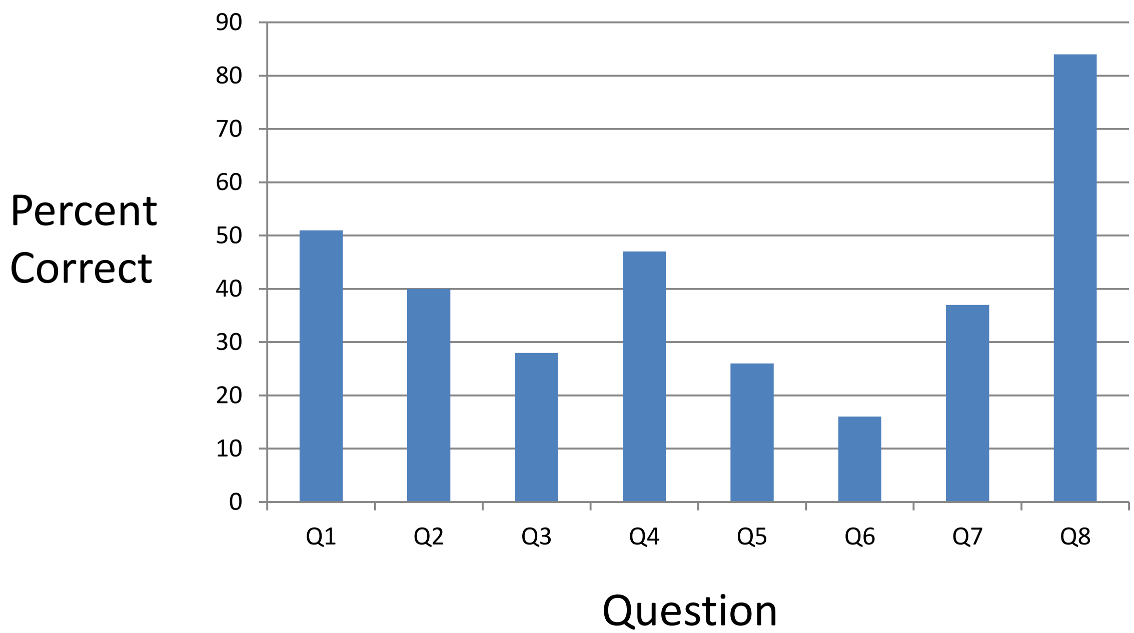
Water flows through a pipe and enters a section where the cross sectional area is smaller as shown in Figure 1. Select the letter of the correct statement about the change in pressure (P) and the average velocity (V).

A. P2 is less than P1 and V2 is greater than V1
B. P2 is less than P1 and V2 is less than V1
C. P2 is greater than P1 and V2 is less than V1
D. P2 is equal to P1 and V2 is greater than V1

Typical Results

Chemical Engineering Sophomores,
University of Cape Town. 24 % correct

Chemical Engineering Seniors,
Worcester Polytechnic Institute. 28 % correct



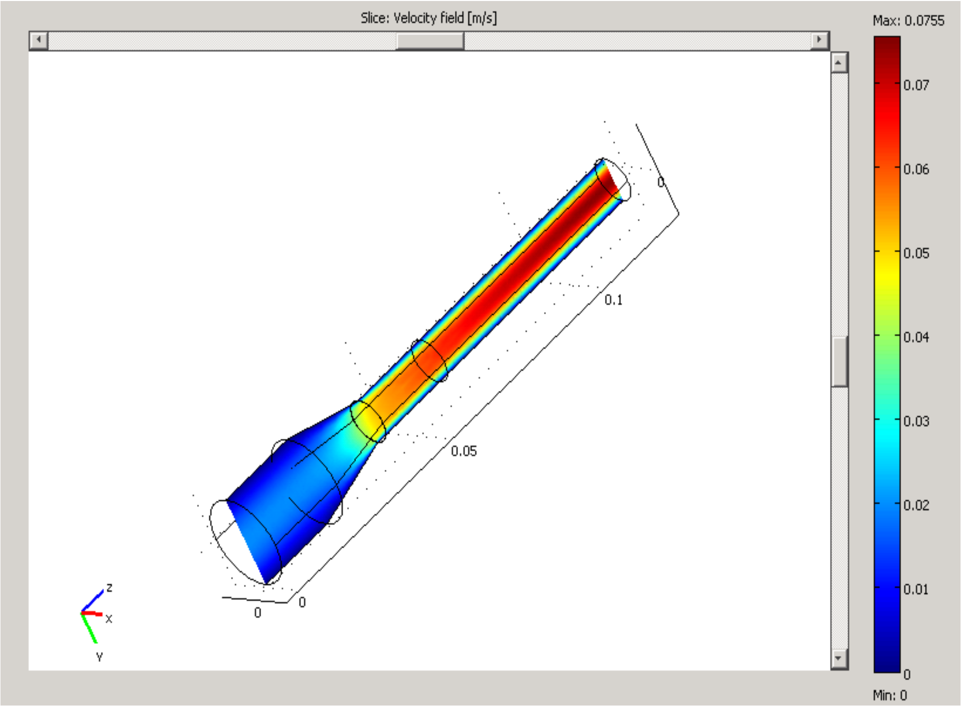
Eight Questions from FMCI as online HW on day 2 of class

Consistent with norms among major universities.

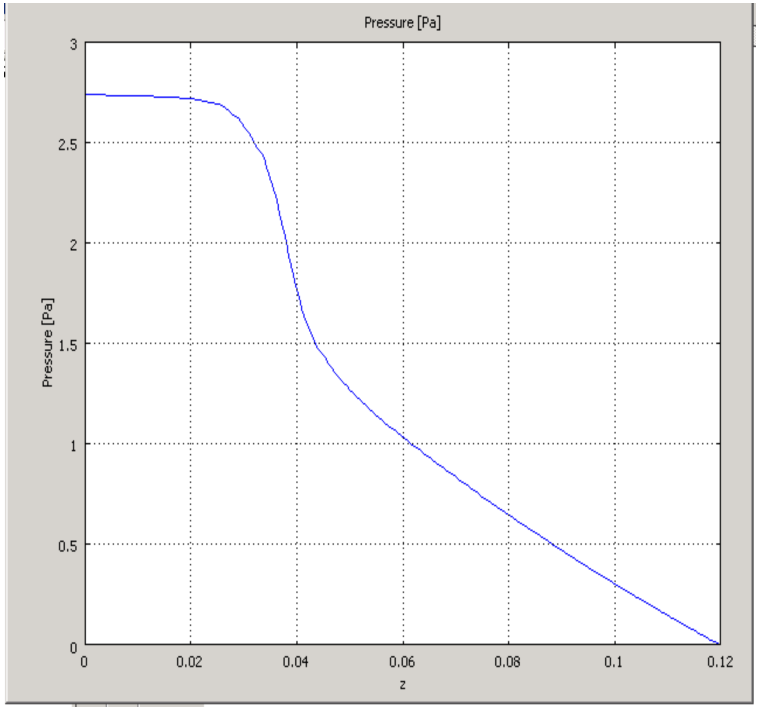
Can Computer Simulation Correct Misconceptions?

- Built simulations of fluid flow situations with COMSOL Multiphysics®.
- Homework assignments required students to study the simulations via a tutorial and answer quiz questions online.
- Repeated 8 question FMCI diagnostic as online homework within three days of studying the simulations.
- Repeated 8 question FMCI on paper 6 weeks later.

Example Simulation



Velocity field in converging pipe



Pressure along centerline of converging pipe

Students encouraged to experiment with different inlet conditions, fluid properties, etc. and study pressure and velocity profiles in different locations, etc.

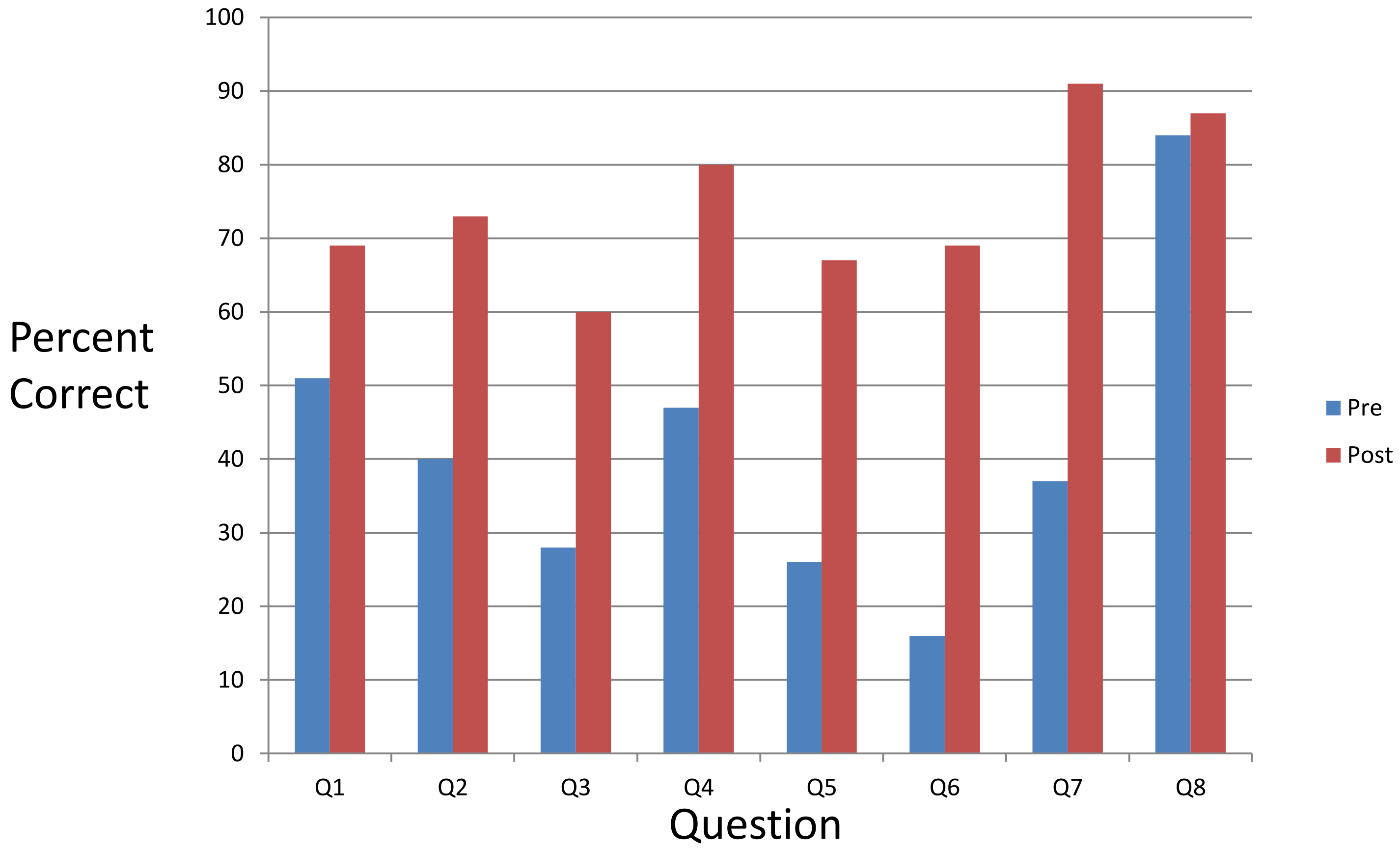
Example Online Quiz Question

Assuming we have fully developed laminar flow of water with V_{avg} = 0.04 m/s, the Hagen–Poiseuille (Equation 4) result for the pressure drop over the last 0.06 m of our converging pipe (D = 0.01 m here) would be:

a: 0.554 Pa
b: 0.763 Pa
c. 0.911 Pa
d. 1.051 Pa

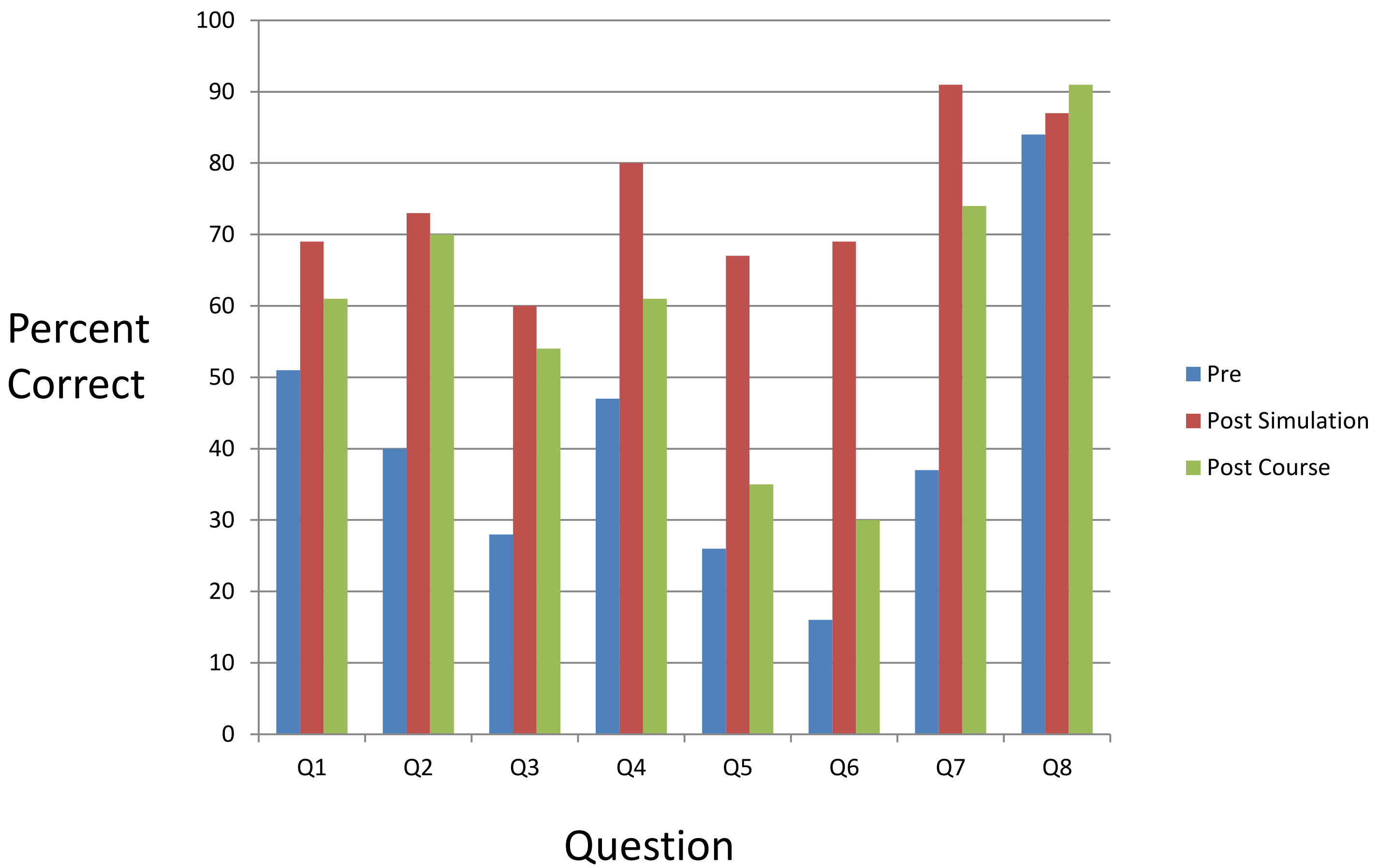
Students "measured" the pressure drop and compared to H–P result.

Pre / Post Assessment



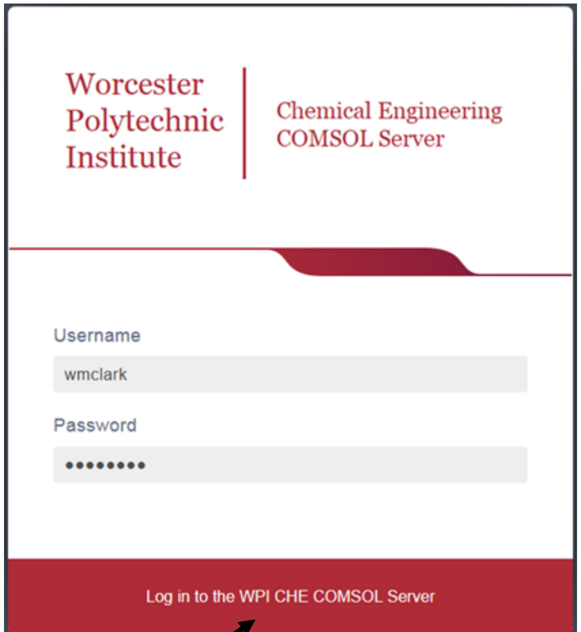
FMCI Results for 46 students

Repeated 8 Question FMCI 6 Weeks Later

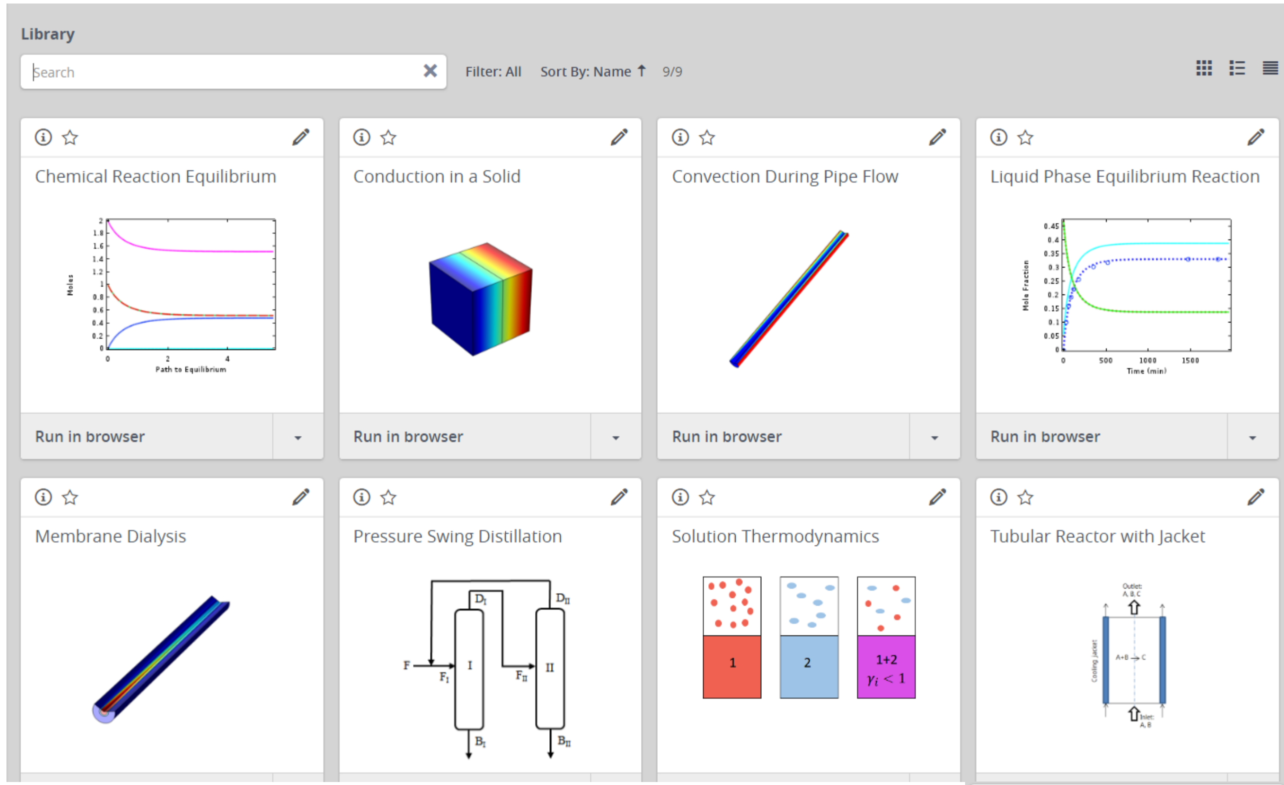


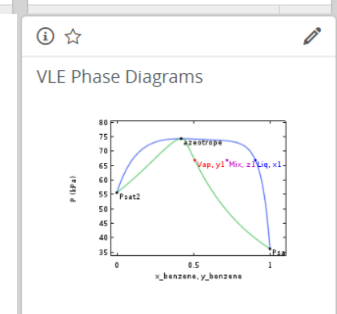
COMSOL SERVER^{TM} AND APPS

Apps are self contained learning modules. No need to learn COMSOL software.



Click here



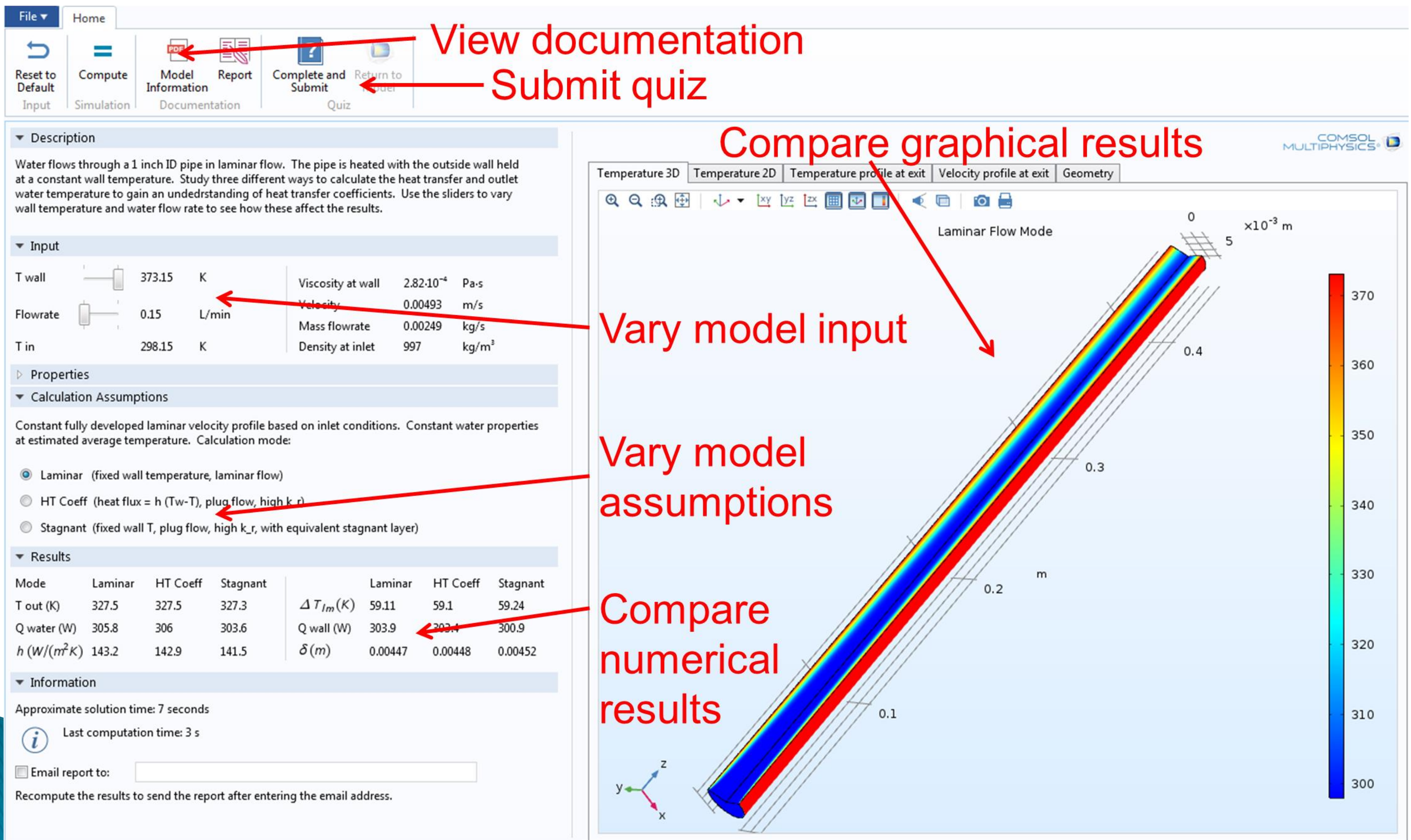


http://comsol-server.wpi.edu/app-lib

User Name: Guest01, Guest02, …Guest99

Password: Gibbs

COMSOL App



View documentation
Submit quiz
Compare graphical results
Vary model input
Vary model assumptions
Compare numerical results
File
Home
Reset to Default
Compute
Model Information
Report
Complete and Submit
Return to Model
Input
Simulation
Documentation
Quiz
Description
Water flows through a 1 inch ID pipe in laminar flow. The pipe is heated with the outside wall held at a constant wall temperature. Study three different ways to calculate the heat transfer and outlet water temperature to gain an undedrstanding of heat transfer coefficients. Use the sliders to vary wall temperature and water flow rate to see how these affect the results.
Input
T wall 373.15 K
Flowrate 0.15 L/min
T in 298.15 K
Viscosity at wall 2.82·10⁻⁴ Pa·s
Velocity 0.00493 m/s
Mass flowrate 0.00249 kg/s
Density at inlet 997 kg/m³
Properties
Calculation Assumptions
Constant fully developed laminar velocity profile based on inlet conditions. Constant water properties at estimated average temperature. Calculation mode:
Laminar (fixed wall temperature, laminar flow)
HT Coeff (heat flux = h (Tw-T), plug flow, high k_r)
Stagnant (fixed wall T, plug flow, high k_r, with equivalent stagnant layer)
Results
Mode Laminar HT Coeff Stagnant
T out (K) 327.5 327.5 327.3
Q water (W) 305.8 306 303.6
h (W/(m²K) 143.2 142.9 141.5
Laminar HT Coeff Stagnant
ΔT_lm(K) 59.11 59.1 59.24
Q wall (W) 303.9 303.4 300.9
δ(m) 0.00447 0.00448 0.00452
Information
Approximate solution time: 7 seconds
Last computation time: 3 s
Email report to:
Recompute the results to send the report after entering the email address.
COMSOL MULTIPHYSICS
Temperature 3D
Temperature 2D
Temperature profile at exit
Velocity profile at exit
Geometry
Laminar Flow Mode
×10⁻³ m
0
5
0.4
0.3
0.2
0.1
m
370
360
350
340
330
320
310
300
z
y
x

Built-in Quiz Emailed to Grader

▾ Question 7

Considering the equation Q = h A (Delta T), increasing flow rate has the main effect of:

- ○ increasing Q by increasing the driving force for heat transfer.
- ○ increasing Q by increasing the heat transfer area.
- ◉ increasing Q by increasing the heat transfer coefficient, h.
- ○ no significant effect.

▾ Question 8

Considering the equation Q=mCp(Tout -Tin), what happens to Tout if m doubles while Q increases less than twofold?

- ○ the senario described is not possible.
- ○ Tout will increase, because the velocity increases.
- ◉ Tout will decrease, because there is more material to heat.
- ○ Tout will remain unchanged because it does not depend on the mass flow rate.

▾ Grade and Submit Quiz

Enter your name: Sally Student

When you click the Submit Quiz button your grade and the correct answers will be shown below and sent to the grader.

Email of grader: wmclark@wpi.edu [Submit Quiz]

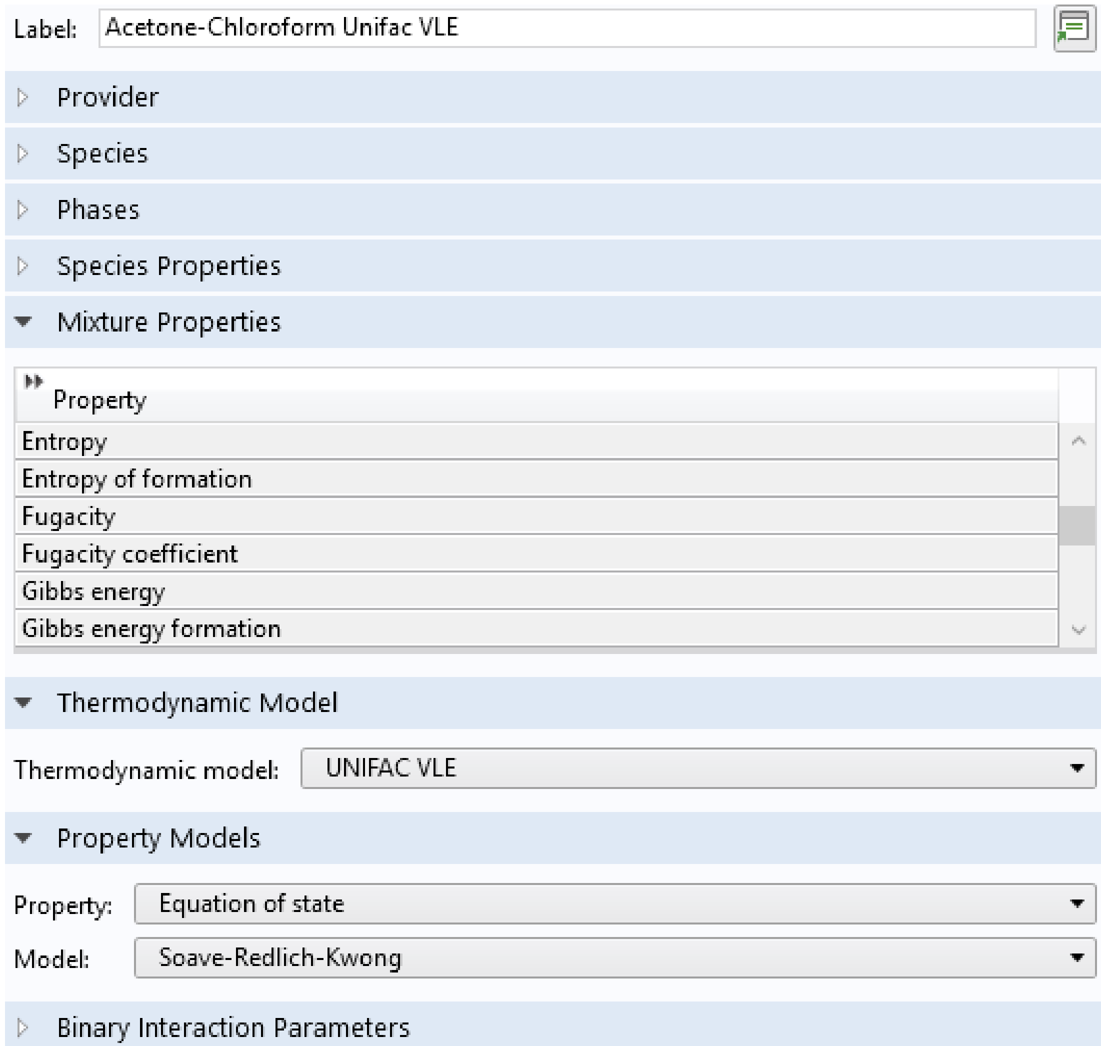
Maximum Points 8 Correct Answer Sequence 2_3_3_4_2_1_3_3

Your Points 8

Compared Apps to Tutorials

- Both were effective for reviewing fundamentals for UO lab class.
- Apps were easier to use via access from any web browser.
- Most students preferred apps, but some preferred manipulating the pre-built COMSOL models using the software directly.

COMSOL Thermodynamics Feature

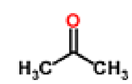
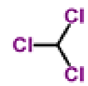


Solution Thermodynamics App

▾ Input

Temperature 298.15 K   Pressure 101.325 kPa

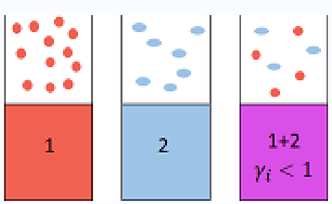
- ○ Hypothetical Ideal Solution A(1)-B(2)
- ○ Benzene(1)-Toluene(2)
- ○ Benzene(1)-Heptane(2)
- ○ 2-Butanone(1)-Toluene(2)
- ○ Ethanol(1)-Heptane(2)
- ○ Ethanol(1)-Water(2)
- ○ Ethanol(1)-Chloroform(2)
- ◉ Acetone(1)-Chloroform(2)
- ○ Chloroform(1)-1-4-Dioxane(2)

	Acetone	Chloroform
Formula	$(CH_3)_2CO$	$CHCl_3$
Structure		
Molecular weight	58.08	119.37
Normal boiling point, °C	56.05	61.15
H-bond donors	0	0
H-bond acceptors	1	0

Mixture properties

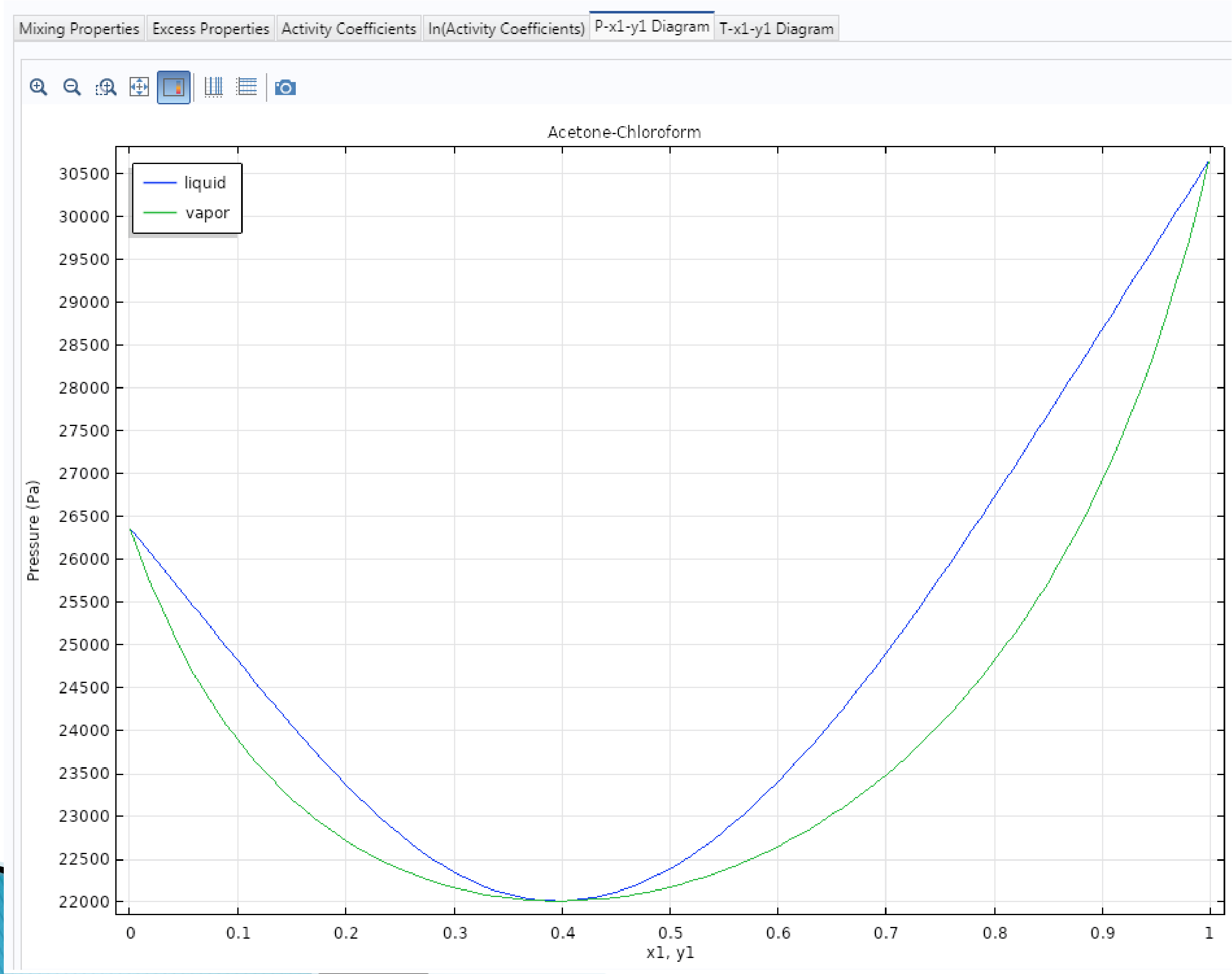
- ○ No prediction. Please make a mixture property prediction and click compute.
- ○ Ideal or nearly ideal, G_excess near zero, activity coefficients near one, no azeotrope.
- ○ Small positive deviations, G_excess > 0, activity coefficients > 1, azeotrope is unlikely.
- ○ Large positive deviations, G_excess >> 0, activity coefficients >> 1, minimum boiling azeotrope.
- ○ Small negative deviations, G_excess < 0, activity coefficients < 1, azeotrope is unlikely.
- ◉ Large negaitive deviations, G_excess << 0, activity coefficients << 1, maximum boiling azeotrope.

▾ Results



Correct. Acetone-chloroform mixtures display large negative deviations from Raoult's law. Chloroform is weakly polar giving rise to dipole-dipole interactions similar to hydrogen bonds. Apparently the interaction of chloroform with acetone is stronger than with itself. The escaping tendenies for the species from the mixture are less than those from the pure liquids. The P-x curve goes below both vapor pressures. Minimum pressure and maximum temperature azeotropes occur.

Solution Thermodynamics App



Chemical Equilibria App

$C_2H_4 + H_2O \rightleftharpoons C_2H_5OH$

Gas phase reaction reaches equilibrium at the specified conditions.
Try to maximize conversion without causing condensation.

Input

System conditions

Temperature 450 K

Pressure 20 bar

Initial composition

	C_2H_4	H_2O	C_2H_5OH	N_2	Total
Moles	1	1	0	0	2
Mole Fraction	0.5	0.5	0	0	

Calculation Assumptions

Results

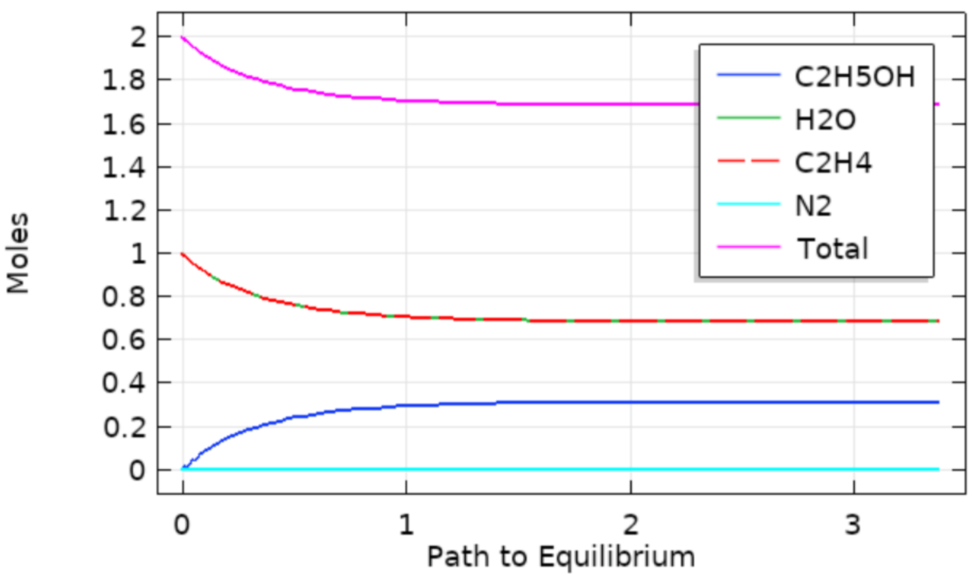
Species values

	C_2H_4	H_2O	C_2H_5OH	N_2	Total
Moles	0.686	0.686	0.314	0	1.69
Mole Fraction	0.407	0.407	0.186	0	
$\hat{\phi}_i$	0.986	0.903	0.846		

Reaction values

ΔH^0	$-4.698 \cdot 10^4$	J/mol
ΔG^0	$1.096 \cdot 10^4$	J/mol
K	0.0535	
Conversion	31.4	%

Mole Fraction | Moles | H Balance | C Balance | O Balance | Pure Fugacity | Mixture Fugacity



Calculation Assumptions

Fugacity Coefficients

- (●) Mixture Fugacity Coefficients
- ( ) Ideal Solution of Gases
- ( ) Ideal Gas Mixture

ΔH^0

- (●) Function of T
- ( ) Constant

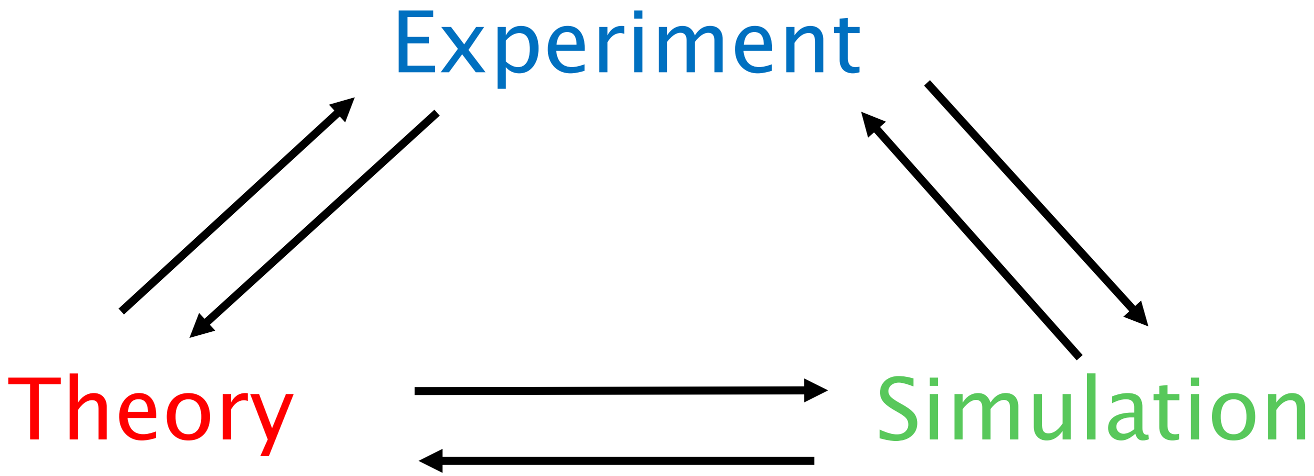
Conclusions

- COMSOL Multiphysics® simulations are useful as virtual experiments and pre-lab exercises particularly because they provide visual representation of detailed results.
- Student satisfaction and perceived learning improvement were positive.
- Simulations proved to have a positive short term effect especially for problems that benefit from visualization.
- Simulations may also have a positive longer term effect.

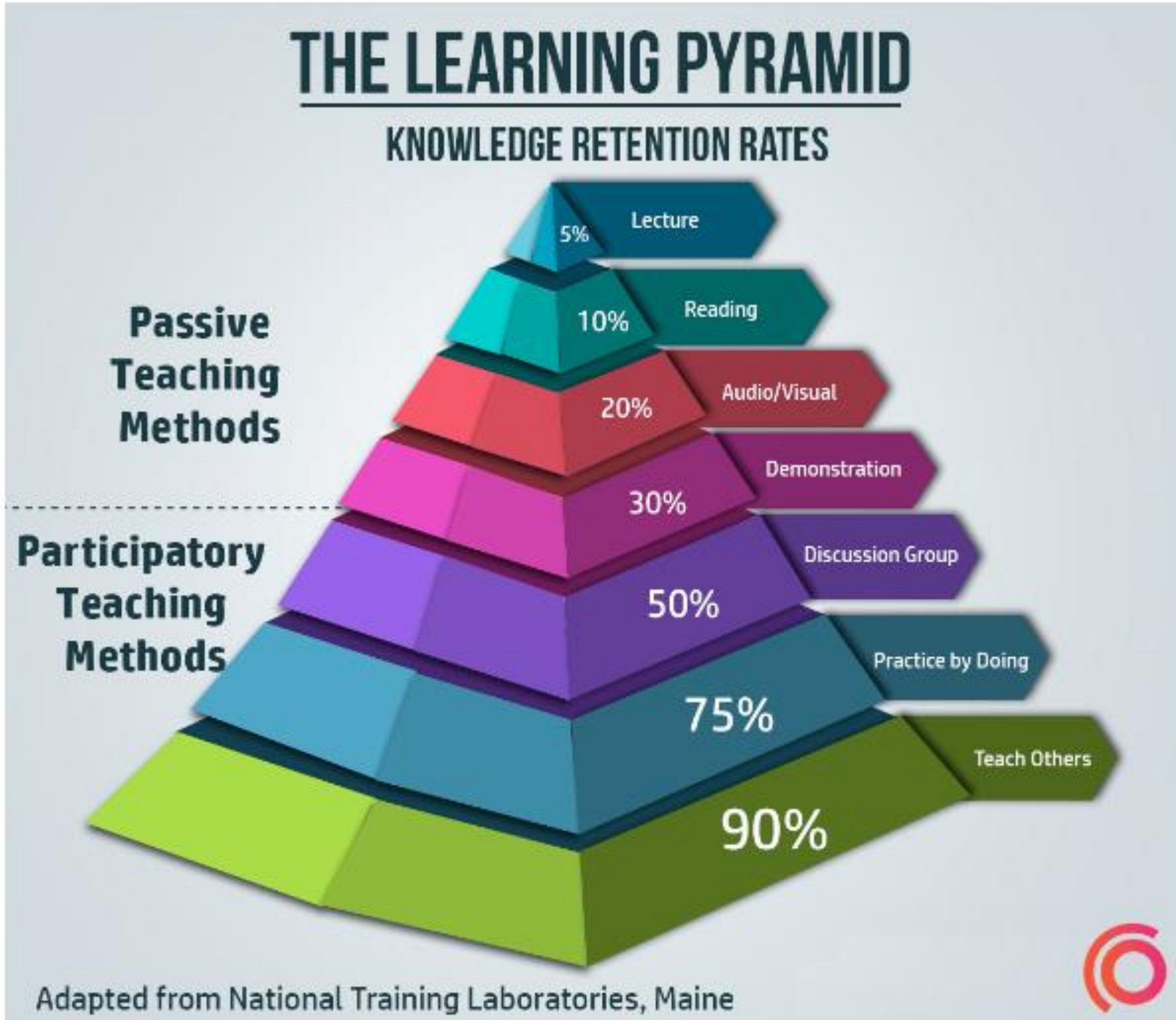
Conclusions

- COMSOL Server is a convenient way to deliver online learning materials.
- New thermodynamic feature is very useful.
- Chemical engineering application library at http://comsol-server.wpi.edu/app-lib

Questions ?



Extra Slides



Where does running a computer simulation fall?

Questions 6 – visual

6. Two very long plates, with a layer of water between them, are pulled in opposite directions as shown in Figure 4. There is no imposed pressure gradient in the direction of flow and the velocities in the water are laminar and due only to the motion of the plates. Select the letter that best represents the velocity profile (distribution of the velocity of the water with distance) inside the water layer.

Students did poorly before and after the course, but did well after the simulation.

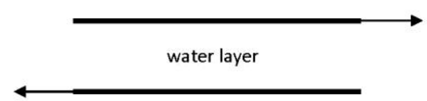
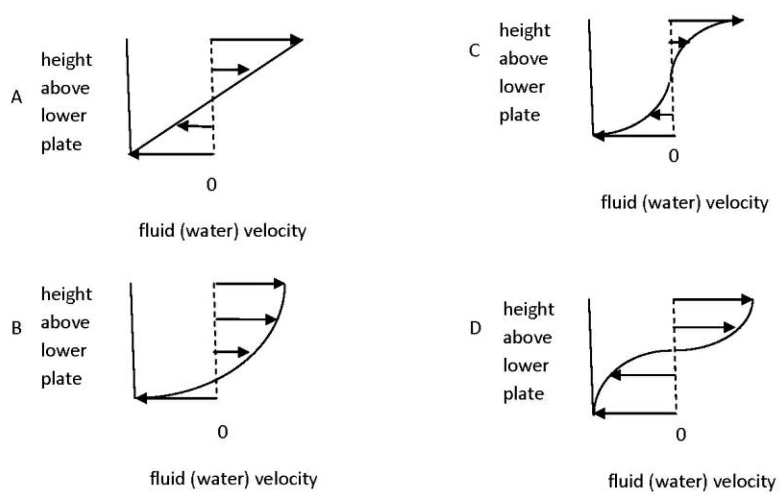


Figure 4. Water layer between two moving plates.



Comparing Models with Tutorials to Apps

- 66 Unit Ops lab students used apps to review heat transfer fundamentals and used pre-built COMSOL models and detailed tutorials to review fluid flow fundamentals.
- Both groups showed improvement between pre and post diagnostic tests. They improved about the same amount.
- Apps took slightly longer to produce than models with associated tutorials.
- Apps with built-in quizzes were convenient self-contained learning modules deliverable to any browser.

Comparing Models with Tutorials to Apps

Table 2. Student satisfaction survey response (%).

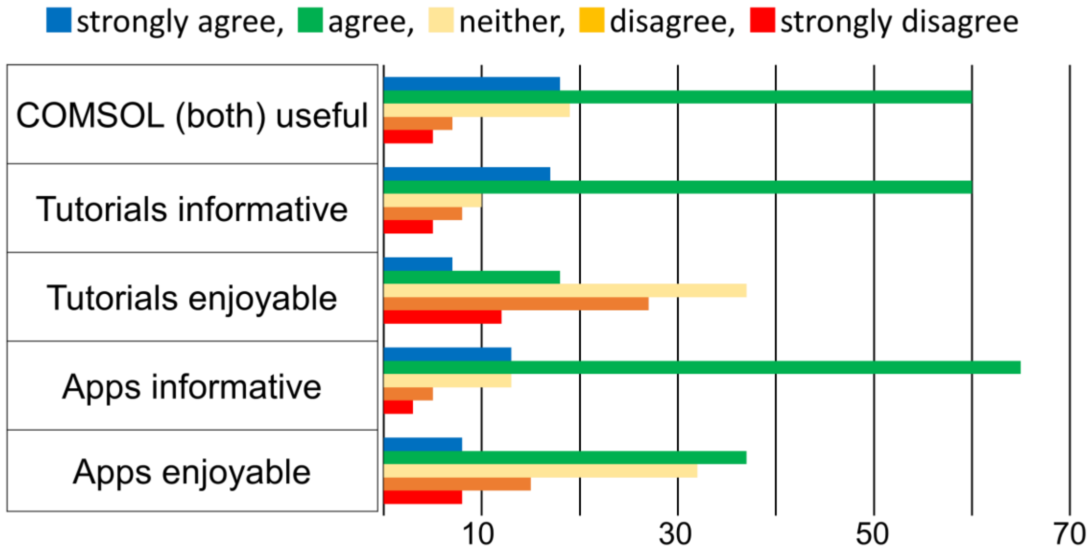


Table 3. Student preference survey response (%).