COMSOL Multiphysics Models for Teaching Chemical Engineering Fundamentals:

Absorption Column Models and Illustration of the Two-Film Theory of Mass Transfer

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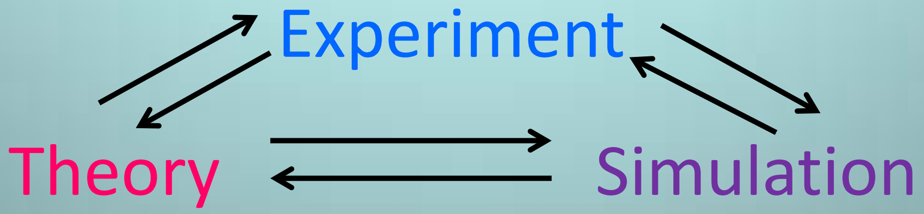
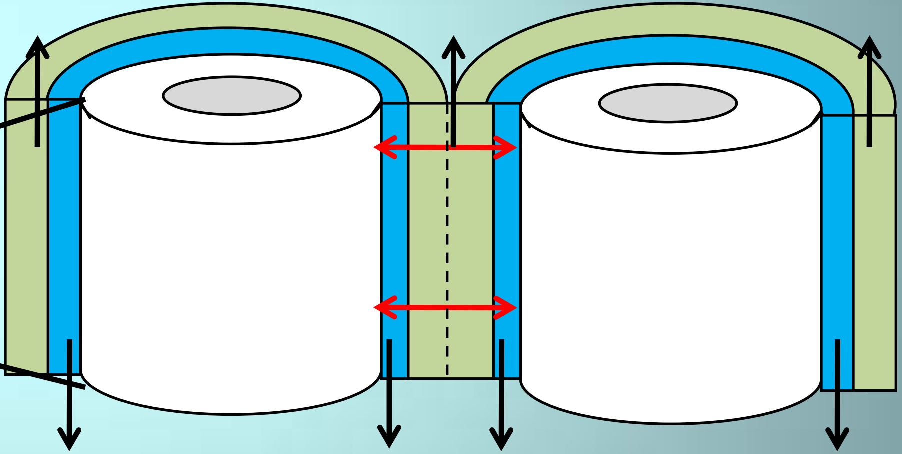

Experiment
Theory
Simulation

Packed Absorption Column

Removing CO_2 from air into water.
Water flowing downward,
gas flowing upward over packing.



Ignoring details and complexities of packing arrangement and flow patterns.

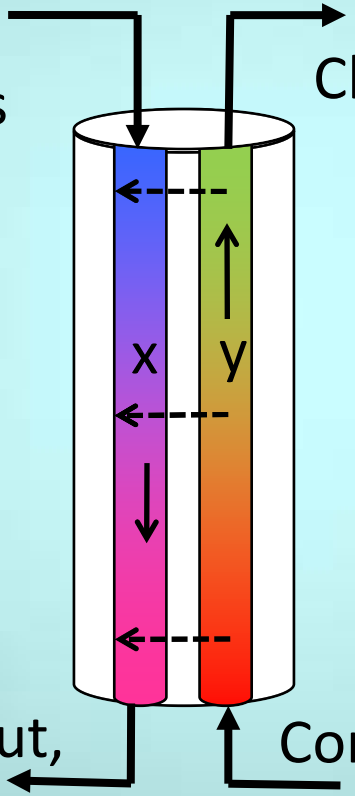
Absorption Analysis

CO_2 transferred from air to water

Water in, $x_t = 0$

Water flux, L_0 mol/m^{2}s

Cleaner air out, $y_t = 0.099$



$$-\frac{d}{dz}(Gy) = \frac{d}{dz}(Lx)$$

Contaminated water out,

$x_b = 0.000126$

Contaminated air in, $y_b = 0.185$

Air flux, G_0 mol/m^{2}s

Traditional Analysis

Lump all complexities of convection and diffusion into $K_y a$ – overall gas phase mass transfer coefficient

$$-\frac{d}{dz}(Gy) = \frac{d}{dz}(Lx) = K_y a\left(y - ye\right)$$

Driving force for mass transfer assumed to be (y-ye)

Henry's law gives ye as function of x (equilibrium line)

$$ye\,P = H\,x$$

If not dilute, gas and liquid fluxes vary

$$G = G_0\left(\frac{1}{1-y}\right)$$

$$L = L_0\left(\frac{1}{1-x}\right)$$

Traditional Analysis

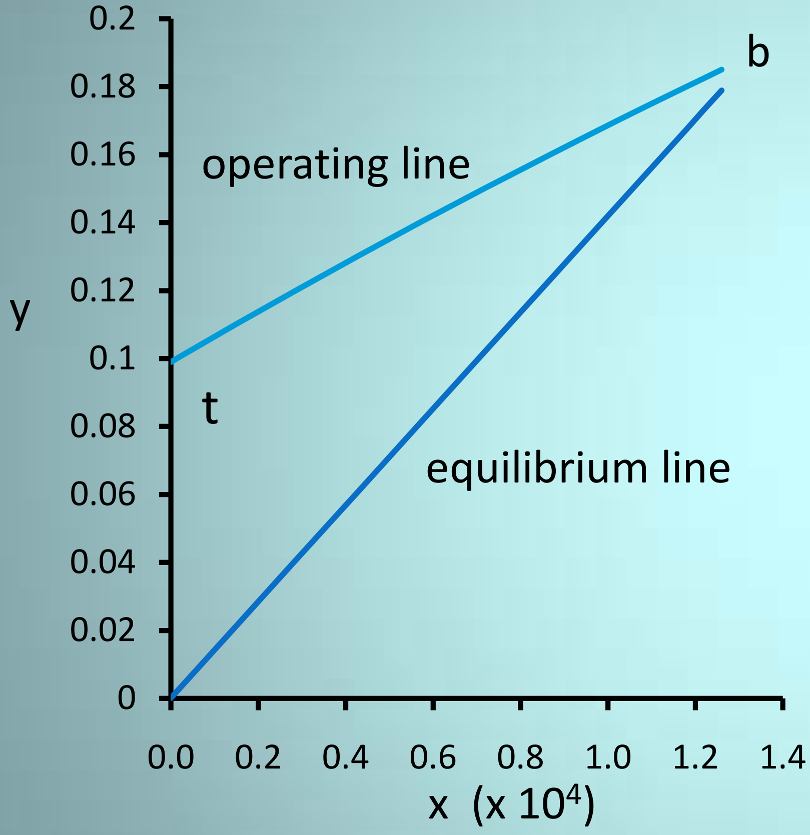
$$y = \frac{\left(\frac{y_b}{1-y_b}\right) + \frac{L_0}{G_0}\left(\frac{x}{1-x} - \frac{x_b}{1-x_b}\right)}{1 + \left(\frac{y_b}{1-y_b}\right) + \frac{L_0}{G_0}\left(\frac{x}{1-x} - \frac{x_b}{1-x_b}\right)}$$ (operating line)

$$0 = -\frac{G_0}{(1-y)^2}\frac{dy}{dz} - K_y a(y - ye)$$

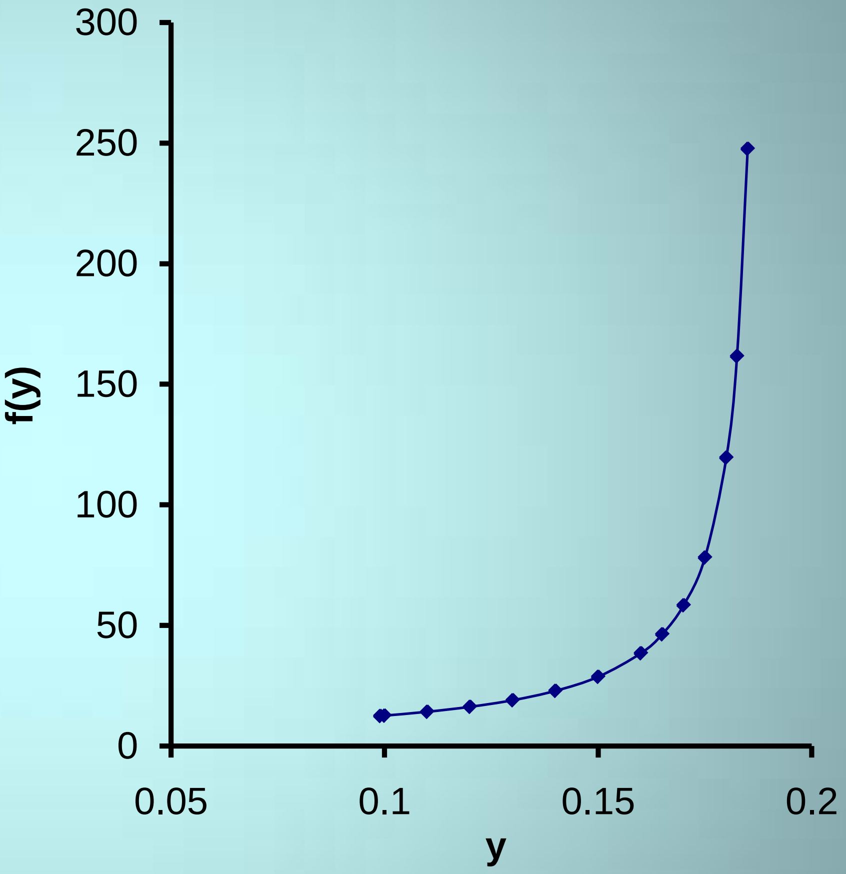
$$Z = \int_0^Z dz = \frac{G_0}{K_y a}\int_{y_b}^{y_t} \frac{dy}{(1-y)^2(y-ye)}$$

$$K_y a = \frac{G_0}{Z}\int_{y_b}^{y_t} \frac{dy}{(1-y)^2(y-ye)}$$

Traditional Analysis



$$f(y) = \frac{1}{(1-y)^2(y-ye)}$$



integrate graphically

$$K_y a = \frac{G_0}{Z}\int_{y_b}^{y_t}\frac{dy}{(1-y)^2(y-ye)}$$

MATLAB Analysis

```
% run_absorber.m
global L0 G0 xb yb yt H
H=1420;Z = 1.372;S = 0.00456;
L0 = 1.06*1000/60/18/S;
G0 = 1.42*1000/(100^3*60*0.022415)/S;
yb = 0.185; yt = 0.099;
OPTIONS=[];
xb = fzero(@xbofy,0.0001,OPTIONS,yt)
NTU = quadv(@funy,yt,yb)
HTU = Z/NTU
Kya = G0/HTU*3600
```

Evaluates $$\int_{y_b}^{y_t} \frac{dy}{(1-y)^2(y-ye)}$$

```
%xbofy.m
%mass balance used to find xb, outlet liquid
%phase mole fraction
function f = xbofy(x,y)
global L0 G0 xb yb yt H
f=y-(yb/(1-yb)+L0/G0*(-x/(1-x)))/(1+yb/(1-yb)+L0/G0*
(-x/(1-x)));
```

MATLAB Analysis

```
% funy.m
% function to integrate to get NTU
function f = funy(y)
global L0 G0 xb yb yt H
OPTIONS=[];
x=fzero(@xofy,0.00001,OPTIONS,y);
ye=H*x;
f = 1/((1-y)^2*(y-ye));
```

Finds x for every y and ye at every x

```
%xofy.m
%finds x at every y for operating line
function f = xofy(x,y)
global L0 G0 xb yb yt H
f=y-(yb/(1-yb)+L0/G0*(x/(1-x)-xb/(1-xb)))/(1+yb/(1-
yb)+L0/G0*(x/(1-x)-xb/(1-xb)));
```

```
>> run_absorber
xb = 1.2597e-004
NTU = 3.3846
HTU = 0.4054
Kya = 2.0563e+003
```

COMSOL Analysis

Gas and liquid phases treated separately in the same geometry

2-D axial symmetry with mapped mesh using actual dimensions

(1-D and 3-D also work well but 2-D-as gives the best visual results)

Equations

$$\nabla \bullet (-Dg\nabla cg) = R - \vec{u} \bullet \nabla cg \qquad \nabla \bullet (-Dl\nabla cl) = R - \vec{u} \bullet \nabla cl$$

$$R = -K_y a\,(1 - y)\,(y - ye) \qquad R = K_y a\,(y - ye)$$

Expressions

$vg = vg_0 / (1-y)$

$y = (cg\ R\ T) / P$

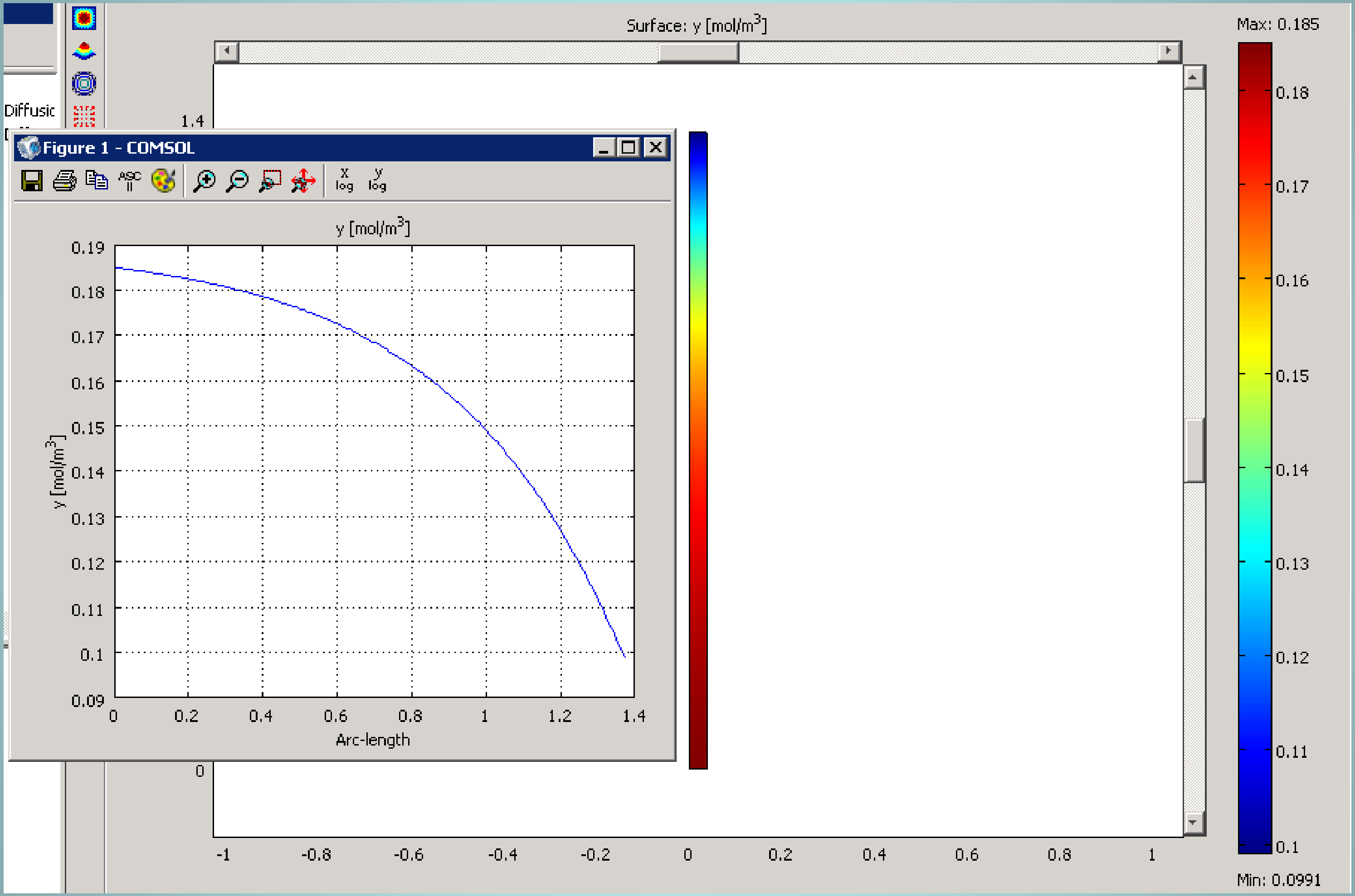
$x = (cl\ MW)/(\rho)$

$ye = H\ x$

Boundary Conditions

Insulation and symmetry, fixed inlet concentrations, convective flux at outlets

COMSOL Analysis



Using $K_y a$ from traditional analysis we can reproduce the experimental results. Alternatively, $K_y a$ that best fits the data can be obtained using the parametric solver.

Advantages of COMSOL Analysis

- More straightforward and easier to use than MATLAB or traditional graphical analysis
- Gives colorful, visual representation of concentration profile
- Additional post processing can provide a wide variety of information with little or no further effort
- Heat effects, variable mass transfer coefficients, and chemical reactions can be included easily

Two-Film Theory

Overall resistance is described as sum of individual resistances

$$\frac{1}{K_y a} = \frac{1}{k_y a} + \frac{H}{k_x a}$$

interfacial area

Equilibrium at interface , $y P = H x$

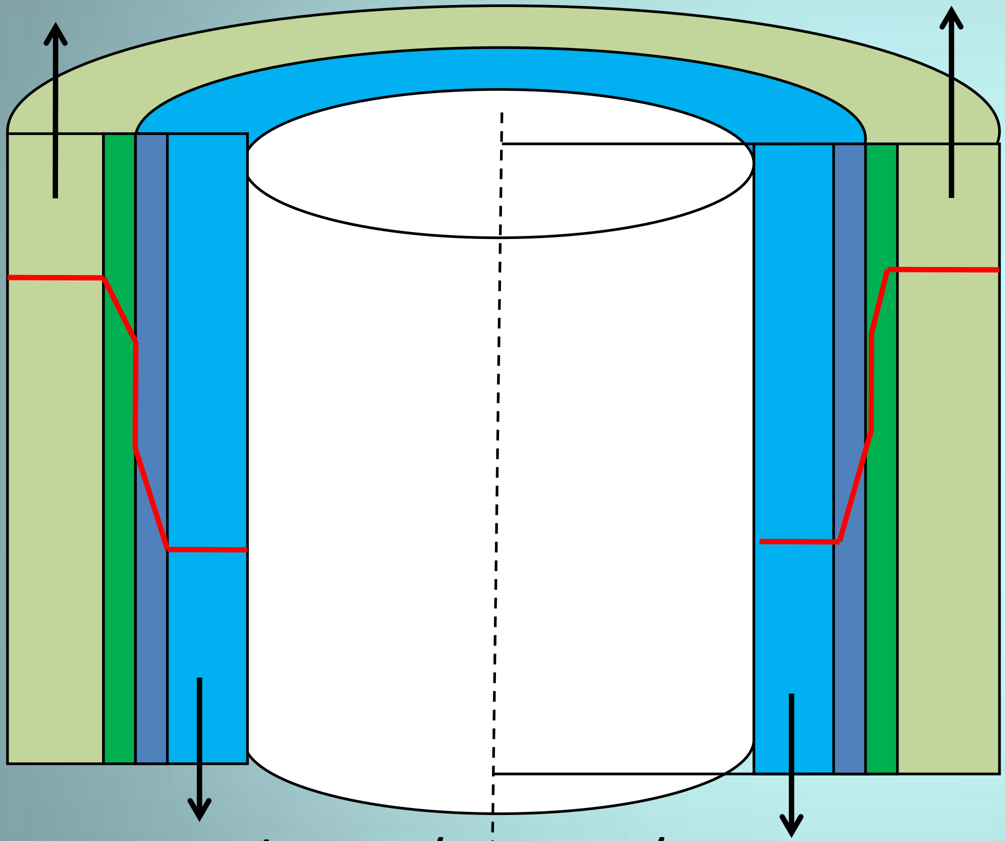
Flux across the interface = $k_x (x_i – x) = k_y (y – y_i)$

Each film considered to be a stagnant layer of a given thickness with mass transfer described by molecular diffusion only

Flux across the interface = $(D_l / t_l) (c_{li} – c_l) = (D_g / t_g) (c_g – c_{gi})$

$k_{cl} = D_l / t_l = k_x MW / \rho$ and $k_{cg} = D_g / t_g = k_y RT/P$

Explicit Two-Film Model



$$k_c = D / t = D_{eff} / t_{eff}$$

$$D_{l\ eff} = t_{l\ eff}\ k_x a\ MW / \rho\ a$$

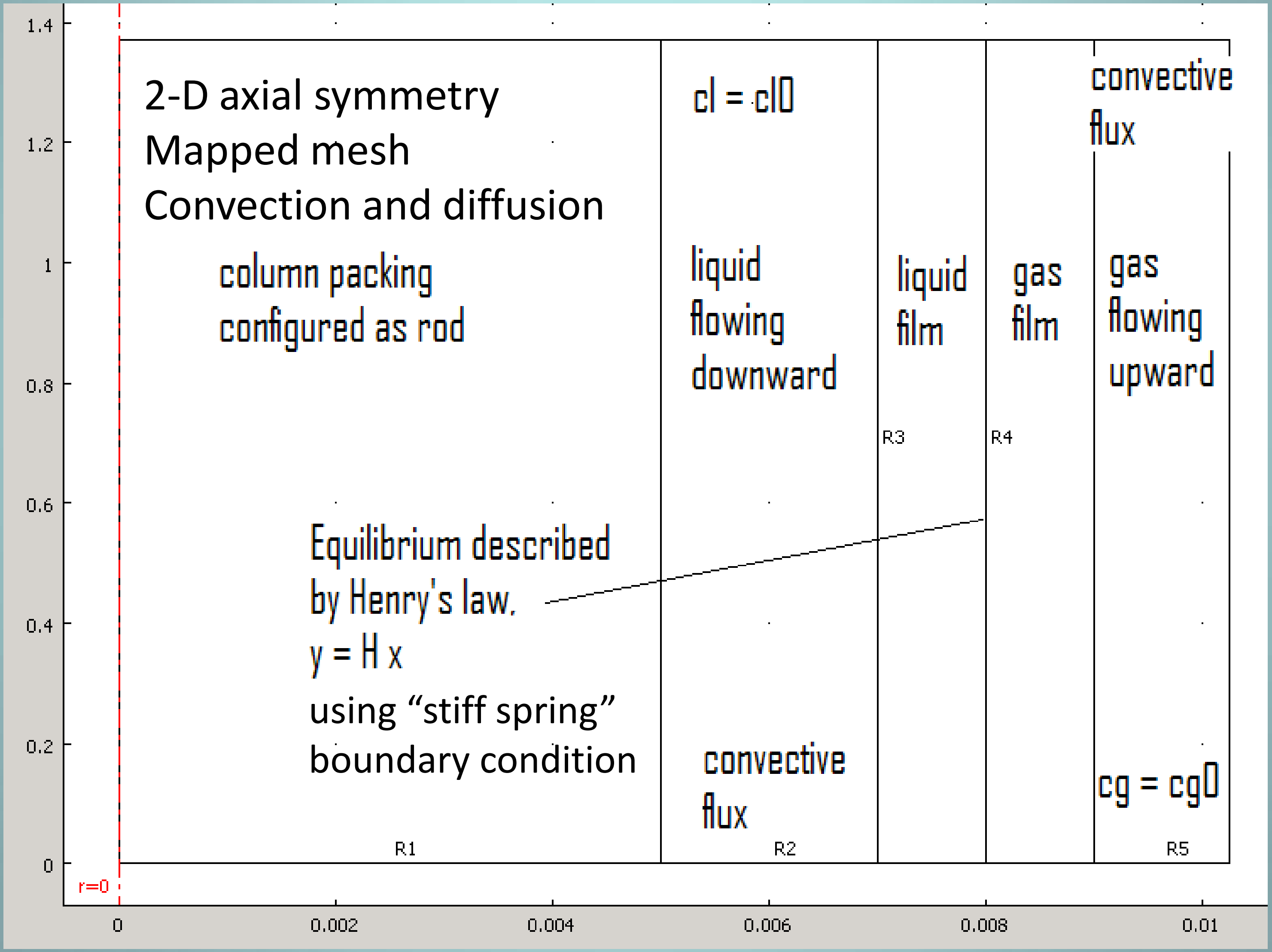
$$D_{g\ eff} = t_{g\ eff}\ k_y a\ RT/P\ a$$

Column modeled as inert rods, coated by a liquid layer flowing down surrounded by a gas layer flowing up.

Rod number and layer thicknesses are set to provide required velocities and flow rates – only study one rod.

Between each flowing layer and the interface is a stagnant film with mass transfer governed by molecular diffusion. Film layers set at arbitrary effective thickness. Effective diffusivities evaluated using $k_x a$ and $k_y a$ obtained from traditional analysis.

Explicit Two-Film Model



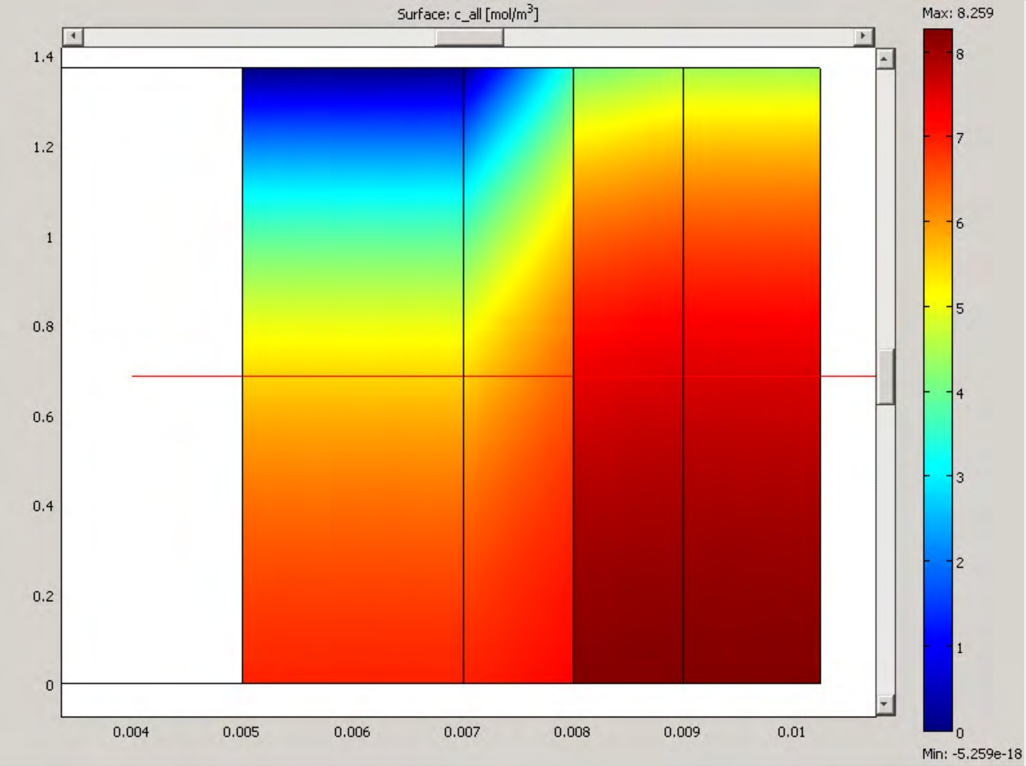
2-D axial symmetry

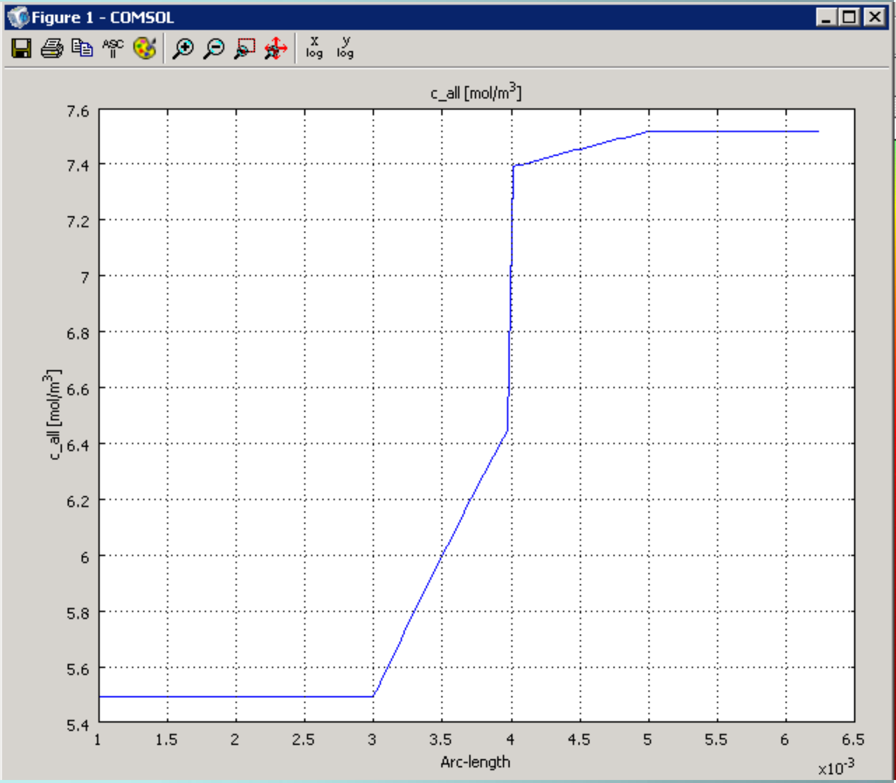
Mapped mesh

Convection and diffusion

using “stiff spring” boundary condition

CO_2 Absorption

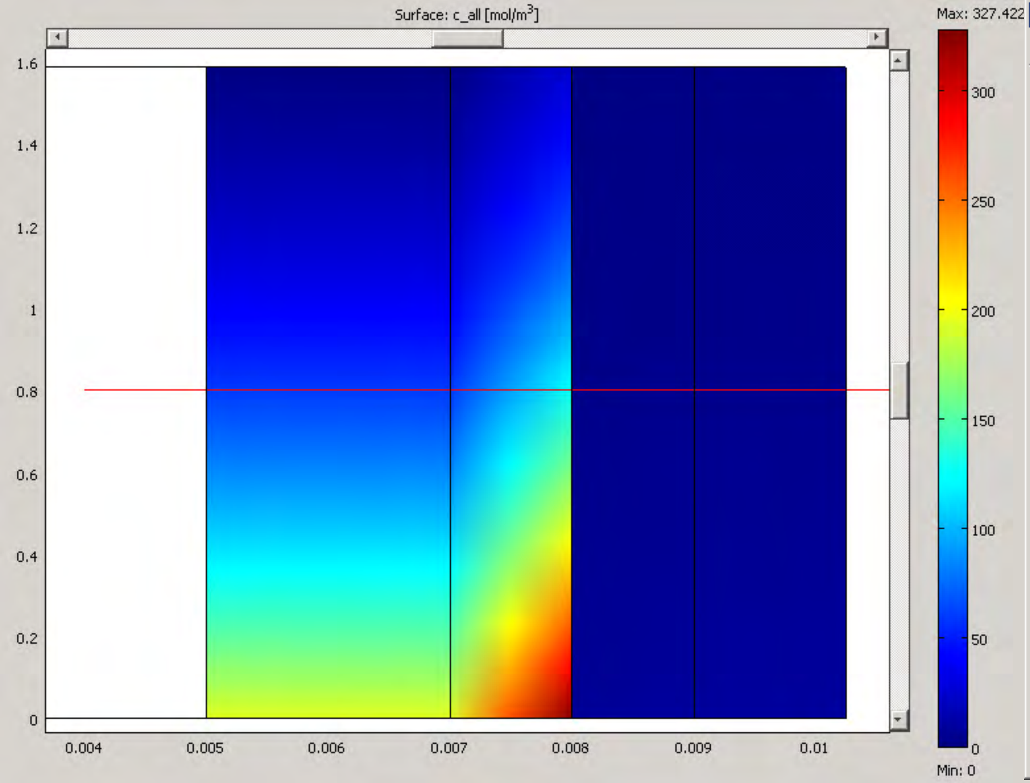


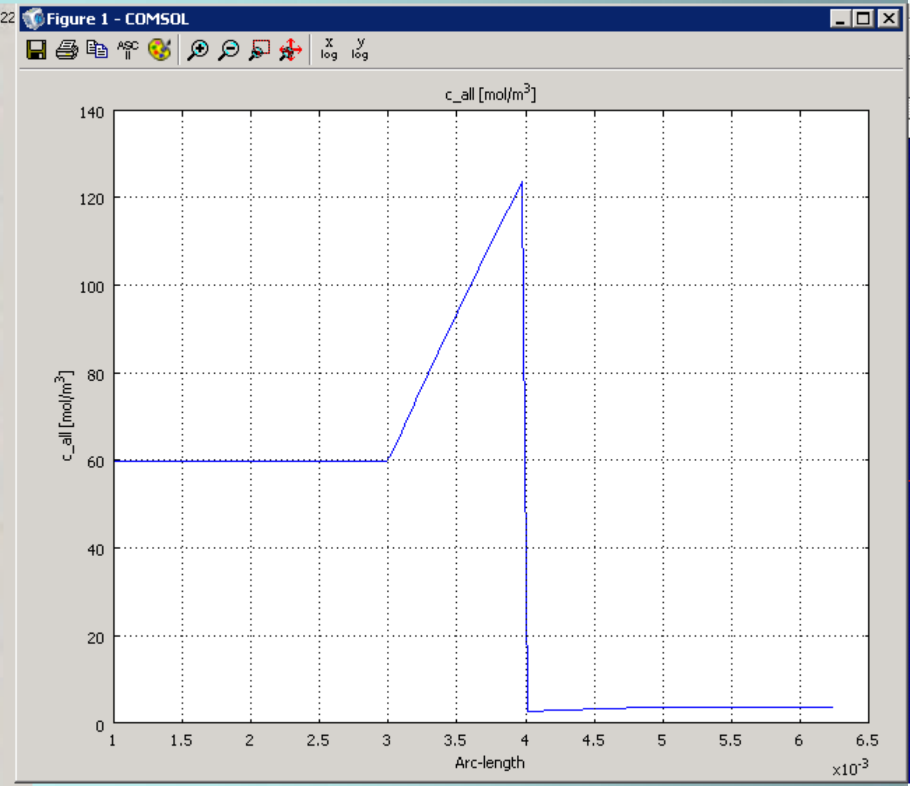


Results agree with those from experiments and simple model.

$y = 1420\,x$

SO_2 Absorption





Results agree with experiments from the literature and simple model.

y = 27 x

Illustrating Mass Transfer Coefficient Definition and Dependence

k_x “measured” in the model by determining flux across the membrane:

$$\text{Flux across the interface} / (x_i - x) = k_x$$

This value of k_x can be seen to agree with k_x from traditional analysis used to define $D_{l\ eff}$

$$k_{cl} = D_l / t_l = D_{l\ eff} / t_{l\ eff} = k_x\, MW / \rho$$

Assuming the interfacial area, a, is constant, the liquid film thickness decreasing with water flow rate explains the mass transfer increase.

Water Rate L/min	$k_x a$ mol/m^{3}s	k_x mol/m^{2}s	t_l m x10^5
0.53	508	0.76	13.15
1.06	916	1.37	7.28
1.58	1028	1.54	6.49
2.11	1172	1.76	5.69

Implementation in Lab Course

Currently using these absorber models in our senior laboratory course.

Comparing test scores and report content of students who use the models to those who do not.

Assessing improvement in student attitudes and learning.

Previously made assessment of models for heat exchanger, gas permeation and fluid flow.

Expected Results

Student Comments on Heat Exchanger Lab Simulation

- "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"

Acknowledgements

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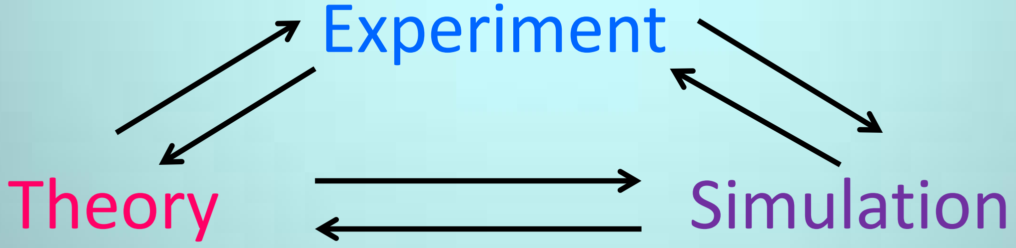

Experiment

Theory

Simulation