

Application of Numerical Problem Solving in Chemical Engineering Coursework

Presenters: Robert P. Hesketh, Rowan University; Michael B. Cutlip, University of Connecticut



The image shows a dark blue banner for Polymath software. On the left, a light blue box contains a snippet of Polymath code: `CB0=1.5`, `d(x)/d(w)=-rA/FA0`, `delH=-40000`, `logP=a-b`, `(C+TC)`, and `-2.38173`. To the right of this box is the **polymath** logo in white, with the word `s o f t w a r e` in a smaller font below it. Above the logo, a navigation menu lists `home | overview | order | manuals | support | demos`. At the bottom right, the website URL `http://www.polymath-software.com/` is displayed.

```
CB0=1.5
d(x)/d(w)=-rA/FA0
delH=-40000
logP=a-b
(C+TC)
-2.38173
```

home | overview | order | manuals | support | demos

polymath
s o f t w a r e

<http://www.polymath-software.com/>

Polymath **Software** problem-solving capabilities include

- **Linear Equations** - up to **264** simultaneous equations
- **Nonlinear Equations** - up to **300** simultaneous nonlinear and 300 additional explicit algebraic equations
- **Differential Equations** - up to **300** simultaneous ordinary differential and 300 additional explicit algebraic equations
- **Data analysis and Regression** - up to 200 variables with up to 1000 data points for each, with capabilities for **linear, multiple linear, and nonlinear regressions** with extensive statistics plus polynomial and spline fitting with interpolation and graphing capabilities

Integration of POLYMATH with Fogler's chemical reaction engineering textbook

Example 6-2 Membrane Reactor

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = -r_A - k_c C_B$$

$$\frac{dF_C}{dV} = r_C$$

$$r_A = -k \left(C_A - \frac{C_B C_C}{K_{BQ}} \right)$$

Isothermal Reactor Design: Molar Flow Rates Chapter 6

TABLE E6-2.1 POLYMATH PROGRAM

Differential equations

- 1 $d(F_A)/d(V) = r_A$
- 2 $d(F_B)/d(V) = -r_A - k_c C_B$
- 3 $d(F_C)/d(V) = r_C$

Explicit equations

- 1 $K_c = 0.05$
- 2 $F_t = F_A + F_B + F_C$
- 3 $k = 0.7$
- 4 $C_{t0} = 0.2$
- 5 $r_A = -k C_{t0} \left((F_A/F_t) - C_{t0}/K_c (F_B/F_t) (F_C/F_t) \right)$
- 6 $k_c = 0.2$

Calculated values of DEQ variables

	Variable	Initial value	Final value
1	Cto	0.2	0.2
2	Fa	10.	3.995179
3	Fb	0	1.832577
4	Fc	0	6.004821
5	Ft	10.	11.83258
6	k	0.7	0.7
7	Kc	0.05	0.05
8	kc	0.2	0.2
9	ra	-0.14	-0.0032558
10	V	0	500.

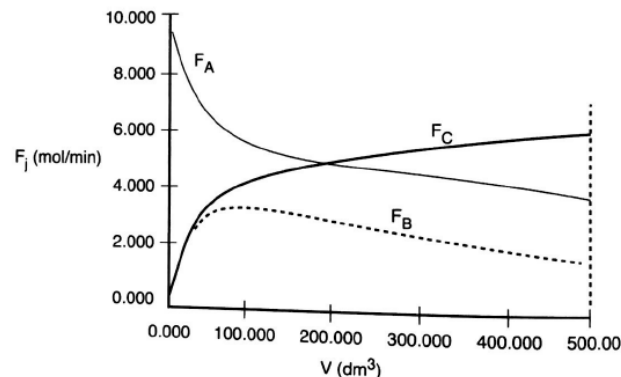
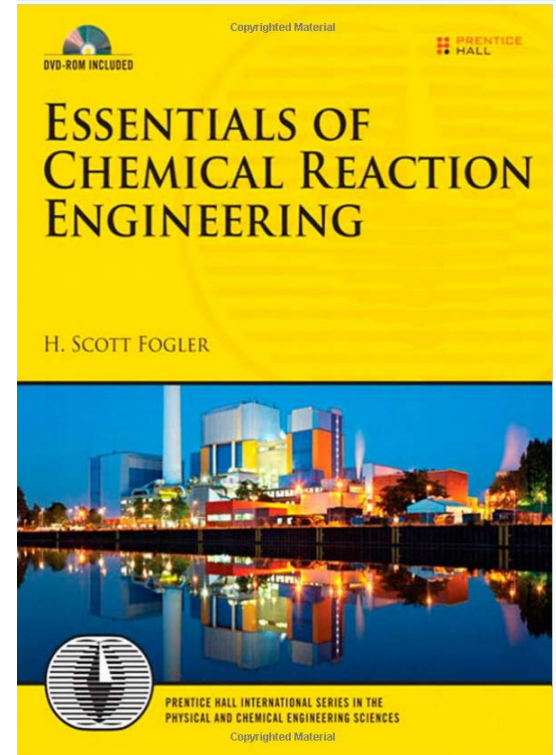


Figure E6-2.1 Polymath solution.

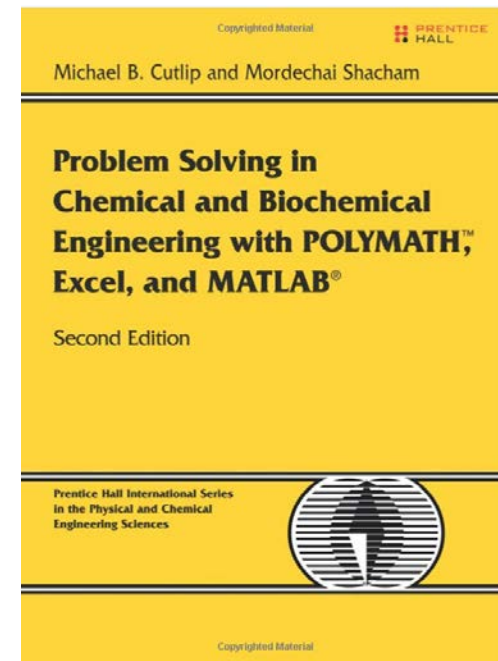


Integration already
accomplished! No extra
work required.

How do you integrate POLYMATH into your course?

Start with examples from POLYMATH Text

- Thermodynamics,
- Fluid Mechanics,
- Heat Transfer,
- Mass Transfer,
- Chemical Reaction Engineering,
- Phase Equilibria and Distillation,
- Process Dynamics and Control,
- Biochemical Engineering

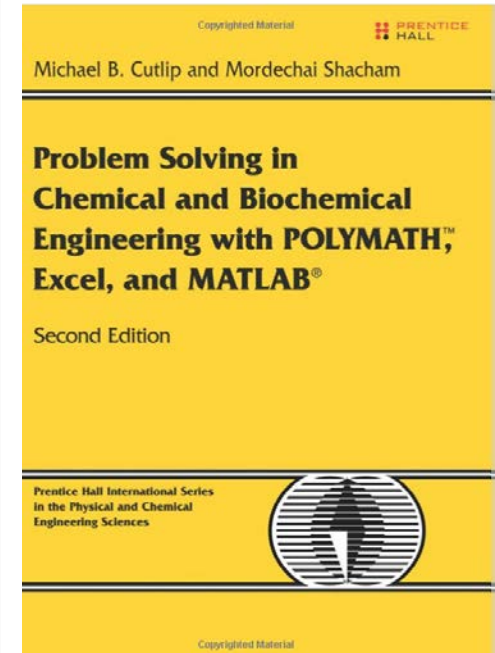


Polymath Text: Fluids Course

Table I-3 Problems in Fluid Mechanics

NO.	PROBLEMS IN FLUID MECHANICS	PAGE
4.2	EXCEL—CALCULATION OF THE FLOW RATE IN A PIPELINE	110
5.2	MATLAB—CALCULATION OF THE FLOW RATE IN A PIPELINE	165
8.1	LAMINAR FLOW OF A NEWTONIAN FLUID IN A HORIZONTAL PIPE	283
8.2	LAMINAR FLOW OF NON-NEWTONIAN FLUIDS IN A HORIZONTAL PIPE	289
8.3	VERTICAL LAMINAR FLOW OF A LIQUID FILM	291
8.4	LAMINAR FLOW OF NON-NEWTONIAN FLUIDS IN A HORIZONTAL ANNULUS	294
8.5	TEMPERATURE DEPENDENCY OF DENSITY AND VISCOSITY OF VARIOUS LIQUIDS	297
8.6	TERMINAL VELOCITY OF FALLING PARTICLES	299
8.7	COMPARISON OF FRICTION FACTOR CORRELATIONS FOR TURBULENT PIPE FLOW	301
8.8	CALCULATIONS INVOLVING FRICTION FACTORS FOR FLOW IN PIPES	303
8.9	AVERAGE VELOCITY IN TURBULENT SMOOTH PIPE FLOW FROM MAXIMUM VELOCITY	306
8.10	CALCULATION OF THE FLOW RATE IN A PIPELINE	307
8.11	FLOW DISTRIBUTION IN A PIPELINE NETWORK	309
8.12	WATER DISTRIBUTION NETWORK	313
8.13	PIPE AND PUMP NETWORK	315
8.14	OPTIMAL PIPE LENGTH FOR DRAINING A CYLINDRICAL TANK IN TURBULENT FLOW	317
8.15	OPTIMAL PIPE LENGTH FOR DRAINING A CYLINDRICAL TANK IN LAMINAR FLOW	320
8.16	BASEBALL TRAJECTORIES AS A FUNCTION OF ELEVATION	322
8.17	VELOCITY PROFILES FOR A WALL SUDDENLY SET IN MOTION—LAMINAR FLOW	325
8.18	BOUNDARY LAYER FLOW OF A NEWTONIAN FLUID ON A FLAT PLATE	328
10.15	DIFFUSION AND REACTION IN A FALLING LAMINAR LIQUID FILM	438

21 Problems in fluids



Example Schedule of Topics for ChE Fluids (2 credit hour)

Chemical Engineering Fluid Mechanics Schedule of Topics → Spring 2016 → Revised 3/18/2016

TOPIC LIST & COURSE SCHEDULE (TENTATIVE)

Tuesday 08:00 AM - 10:45 AM ROW 340 (Double Period)

Friday 08:00 AM - 9:15 AM ROW 340 (Single Period)

All Chapter and section references are to the *Never* text unless referenced otherwise.

Polymath: Nonlinear Equation Solver (NLE)

Polymath: Differential Equation Solver (DEQ) & COMSOL

Date	Topics
January 19 Tuesday	<p>Introduction to Course, Objectives, Syllabus</p> <p>Team Problem Solving, Inductive Topic Order</p> <p>Chemical Engineers $\rho g = \gamma$ Mechanical Engineers (eqn 2.7)</p> <p>Fluids Lab 1: Introduction to Fluids Experiments</p> <p>Chapter 2 Fluid Statics Sections 2-2.2, 2.6, 2.7 and Chapter 5 Elementary Fluid Dynamics</p> <p>(Also review Felder & Rousseau Section 3.1-3.4 Fluid Pressure, Hydrostatic Head, Manometers)</p>
22 Friday	<p>Fluid Flow without accounting for friction</p> <p>Review of Intro to Fluids Lab</p> <p>Chapter 2 & Chapter 5 - The Bernoulli Equation - Neglecting Friction</p> <p>Felder & Rousseau 7.7 Mechanical Energy Balances, eqn 7.7-1</p> <p>3.5 Unsteady-State Mass Balances</p>
26 Tuesday	<p>3.5 Unsteady-State Mass Balances (continued)</p> <p>3.4.1 Average Velocity</p> <p>Applications of Unsteady-State Mass Balances and Bernoulli's Equation</p> <p>Tank Drainage Problem</p> <p>Fluids Lab 2: Tank Drainage & Siphon Experiments</p>
29 Friday	<p>Applications of Bernoulli's Equation continued</p> <p>5.5 Diffusers and Sudden Expansions</p>
February 2 Tuesday	<p>Fluids Lab 3:</p> <p>F1-15 Bernoulli's Theorem - Venturi</p> <p>F1-17 Orifice and Free Jet Flow</p> <p>Pressure Drop in Pipes: Hagen-Poiseuille</p> <p>Computer Lab: Introduction to POLYMATH Laboratory</p>
5 Friday	<p>5.8.3 Venturi, and Restrictions on the Use of the Bernoulli Equation</p> <p>5.8.1 & 5.8.2 Pitot tube</p>
9 Tuesday	<p>Chapter 6 Viscous Flow in Pipes</p> <p>Incompressible Flow in Pipes and Channels</p> <p>Figure 6.10 - Friction Factor Charts</p> <p>6.1 Reynolds Number (Re) and viscosity</p> <p>Cutlip & Shacham 8.7 Comparison of Friction Factor Correlations for Turbulent Pipe Flow</p> <p>Cutlip & Shacham 8.8 Calculations Involving Friction Factors for Flow in Pipes</p>
12 Friday	<p>6.5 Pipe Flow Problems - finding friction factor Example problems: simple piping</p> <p>Standard Steel Pipe Properties: Appendix A.2 page 598</p> <p>Standard Tube Properties: Cutlip & Shacham p 699, Chemical Engineer's Handbook has both</p>
16 Tuesday	<p>Fluids Lab 4:</p> <p>Pressure Drop in Pipeline Elements: Hagen-Poiseuille</p> <p>F1-22 Energy Losses in Bends and Fittings</p> <p>Osborne-Reynolds Demonstration</p> <p>Computer Lab - Excel</p>

19 Friday	<p>6.8 & 6.9 Minor Pressure Losses, Frictional Losses in Pipeline Elements Perry's p 6-16</p> <p>(See Table 6-4 for turbulent, Table 6-5 for laminar)</p> <p>Review for Exam 1</p> <p>Cutlip & Shacham 8.10 Calculation of the Flow Rate in a Pipeline</p> <p>Cutlip & Shacham 8.14 Optimal Pipe Length for Draining a Cylindrical Tank in Turbulent Flow</p> <p>Cutlip & Shacham 8.14 Optimal Pipe Length for Draining a Cylindrical Tank in Laminar Flow</p>
23 Tuesday	<p>6.13 Terminal Velocities Solid Objects and Spheres</p> <p>Fluids Lab 5:</p> <p>Lab: Measurement of Terminal Velocities</p>
26 Friday	Exam 1: Chapters 2 and 5
March 1 Tuesday	Terminal Velocity Continued
4 Friday	<p>6.2 Laminar and Turbulent flow</p> <p>6.3 Laminar Flow Velocity Profiles</p> <p>Entrance Region and Fully Developed Flow</p>
8 Tuesday	<p>6.10.3 Turbulent Flow in Noncircular Channels</p> <p>6.10.2 Seal Leaks</p> <p>6.12 Economic Pipe Diameter, Economic Velocity</p>
11 Friday	<p>Introduction to Pipe Flow Rate Measurements: orifice, venturi and rotameter</p> <p>Permanent and Temporary Pressure Losses</p> <p>How to purchase a Flowmeter</p> <p>5.8 - Bernoulli Equation</p> <p>Perry's 10-6 to 10-20 Measurement of Flow</p>
14-19	Spring Break
22 Tuesday	<p>Chapter 7: Mass, Energy, and Momentum Balances</p> <p>7.2 Momentum Balance - Typical Forces: gravity, Pressure and Wall Shear Stress</p> <p>Fluids Lab 6: Flowmeters</p> <p>Rotameter - Variable Area Flowmeter, Venturi, Orifice, Pitot tube</p>
25 Friday	Good Friday: No Classes
29 Tuesday	<p>7.3 Momentum Balances Applications: Flow Through a Nozzle (Example 7.5), U-Bend in piping, Reducing Elbow, Jet Ejector Pump (7.3.5)</p> <p>Macroscopic Control Volume: Pressure drop and Wall Stress</p>
April 1 Friday	<p>Microscopic Control Volume - Derivation of laminar flow velocity profile</p> <p>Examples of the Momentum Balances: Alphaterm in Bernoulli Equation & Diameter of a Free Jet</p>
5 Tuesday	<p>Examples of the Momentum Balance Continued: Impinging jet, Orifice Plate, Sudden Expansion</p> <p>7.4 Relative velocities & Trolley Example</p> <p>Review for Exam 2</p> <p>Impact of a Jet Videos (See the Force of water)</p>
8 Friday	Exam 2: Chapter 6 and 5.8: Pipe Flow, Fittings & Valves, and Flowmeters
12 Tuesday	<p>Examples of the Momentum Balance Continued: Rotameter (also see Chapter 6 in Darn), 6.10.3 Turbulent flow in Noncircular Channels</p> <p>Fluids Lab 7: Aspirator laboratory</p>
15 Friday	7.5 Starting and Stopping Flows: Water Hammer
19 Tuesday	7.7 Introduction to Angular Momentum
22 Friday	Chapter 9: Dimensionless Numbers and Dimensional Analysis
26 Tuesday	Chapter 9: Dimensionless Numbers and Dimensional Analysis (continued)
29 Friday	Review for Comprehensive Final Exam
May	<p>Final Exam 3 May 2016</p> <p>CHEM-ENGINEER-FLUID-MECHANICS Benketh, Robert Paul T-0800-1000 ROWAN-340 (Exam)</p> <p>Go out and design a fluid transport system for your parent's fountain and pond</p>

Adv. ChE Fluids (2 cr)

Tentative Schedule of Topics ¶

Process Fluid Transport CHE06-309-2-2016¶

Polymath: Nonlinear Equation Solver (NLE)¶

Polymath: Differential Equation Solver (DEQ) & COMSOL¶

Date:¶	Proposed Topics for Section 1: Wednesday (double period) - Friday (single period)¶
September 9/2/16¶ Friday¶	Course Introductions¶ Review of fluid Mechanics: Statics and Bernoulli¶ Chapter 3.3 Pumps and Gas-Moving Equipment - Geankoplis¶ Chapter 10: Centrifugal Pumps - FMChE¶
9/7/16¶ Wednesday¶	Centrifugal Pumps (continued)¶
9/9/16¶ Friday¶	Centrifugal Pumps (continued)¶
9/14/16¶ Wednesday¶	Centrifugal Pumps: NPSH¶ Complex Flow Networks C&S2 nd 8.11 and FMChE pages 213-214¶
9/16/16¶ Friday¶	Complex Flow Networks C&S2 nd 8.11 and FMChE pages 213-214 (continued)¶
9/21/16¶ Wednesday¶	Single Pump Lab: Standard Pump Curve¶ POLYMATH - C&S 6.1 & 6.5 (If new to POLYMATH review POLYMATH Introduction)¶
9/23/16¶ Friday¶	Chapter 10: Introduction to Positive Displacement Pumps (Syringe and Squirt Gun) - FMChE¶
9/28/16¶ Wednesday¶	Review Chapter 7 The Momentum Balance sections through 7.2 and Geankoplis 2.8¶ Macroscopic Momentum Balance Pipe Flow¶ Laminar Flow Between Parallel Plates Geankoplis 2.9C¶
9/30/16¶ Friday¶	Laminar Flow Between Parallel Plates Geankoplis 2.9C (continued)¶ Momentum Balance Derivation for Laminar flow in a pipe C&S2 nd 8.1 Geankoplis 2.9B¶ Chapter 20 Computational Fluid Dynamics - FMChE¶
October 10/5/16¶ Wednesday¶	Comsol Fluids Computer Lab - Introduction Flow Between Parallel Plates¶ Exam 1: Pumps and Complex Flow Networks¶
10/7/16¶ Friday¶	Momentum Balance Derivation for Laminar flow in a pipe (continued)¶
10/12/16¶ Wednesday¶	C&S2 nd 8.3 Vertical Laminar Flow of a Liquid Film - Newtonian fluid¶ Geankoplis 2.9C¶ Comment on Laminar Flow in an Annulus¶ Navier-Stokes Equations: Geankoplis 3.6-3.7, 3.8B and Chapter 15: Two and Three Dimensional Fluid Mechanics - FMChE¶ Flow Between two coaxial Cylinders, Fluid flow in a rotating cylinder, Geankoplis 3.8C Flow Between two coaxial Cylinders, Fluid flow in a rotating cylinder, Geankoplis 3.8C¶
10/14/16¶ Friday¶	Comsol Fluids Computer Lab - Rotational Flows (Bring your LAPTOP to class)¶
10/19/16¶ Wednesday¶	Geankoplis 3.5 Non-Newtonian Fluids¶ Non-Newtonian Fluids - Flow between parallel plates - powerlaw fluid & Bingham Plastics¶ Non-Newtonian Fluids - Flow in a horizontal pipe - powerlaw fluid & Bingham Plastics¶ C&S2 nd 8.2 Non-Newtonian laminar flow in a horizontal pipe ¶ Geankoplis 3.5H Non-Newtonian laminar flow in a horizontal pipe¶

10/21/16¶ Friday¶	Non-Newtonian Fluid Flow Continued¶ Chapter 13 Non-Newtonian Fluid Flow in Circular Pipes - FMChE¶ C&S2 nd 8.3 Vertical Laminar Flow of a Liquid Film - Non-Newtonian fluid¶ C&S2 nd 8.4 Laminar Flow of Non-Newtonian Fluids in a Horizontal Annulus¶
10/26/16¶ Wednesday¶	Geankoplis 3.5E Laminar Flow of time-Independent Non-Newtonian fluids¶ Comsol Fluids Computer Lab - Non-Newtonian Flows¶
10/28/16¶	Geankoplis 3.1C Flow in Packed Beds¶
11/1/16¶	Chapter 12 Gas-Liquid Flows
Wednesday¶	Fluidized Bed Experiment ¶
December, 12/2/16¶ Friday¶	Gas-Liquid Flows Continued¶ Compressible Gas Flows Chapter 8 FMChE and Geankoplis 2.11¶ Nozzle Choking, 8.3 FMChE¶
12/7/16¶ Wednesday¶	Mixing¶ Geankoplis 3.4 Agitation and Mixing of Fluids and Power Requirements and Chapter 19 Mixing - FMChE¶ POLYMATH and COMSOL Quizzes¶
12/9/16¶ Friday¶	Geankoplis 3.4 Agitation and Mixing of Fluids and Power Requirements and Chapter 19 Mixing - FMChE¶ continued¶ Evaluations¶ Review for final¶
12/14/16¶ Wednesday¶	Comprehensive Final Exam 6:00-10:00 AM-ROWAN 340¶
Finals Week¶	14-20 December¶
¶	Go out and make your holiday process fluid transport toys - They make great gifts!¶

Polymath: Nonlinear Equation Solver (NLE)

Polymath: Differential Equation Solver (DEQ) & COMSOL

Typical Fluids Problems

ChE Course	Problem Name	Numerical Method Illustrated	Equations
Fluids	Unsteady-state tank drainage using a siphon tube (similar to POLYMATH text 8.14) <i>C&S8-14soln.pdf</i>	Solution of an first order ordinary differential equation (DEQ)	$\frac{dh_T}{dt} = v_{out} \frac{A_{out}}{A_{tank}}$ $v_{out} = f(h_T)$
	Calculations involving Friction Factors for Flow in Pipes (POLYMATH Text 8.7) and <i>pipeflow homework frictionfactorcalcsoln.pdf</i> <i>Excel Tutorial Solver Add-Ins rev4.pdf</i>	Solution of a system of simultaneous nonlinear algebraic equations (NLE)	$\frac{\Delta P}{\Delta L} = 2f_F \frac{\rho v^2}{D}$ $f_F = f(\varepsilon/D, Re)$ $Re = \rho v D / \mu$
Advanced Fluids	NonNewtonian fluid flow through a pipe (POLYMATH Text 8.2c) <i>NonNewtonian C&S 8.2 solutions & comsol.pdf</i> NonNewtonian fluid flow through an annulus (POLYMATH Text 8.4) <i>NonNewtonian C&S8.4 polymath&comsol & 3.8-8 solutions 2017.pdf</i>	Solution of 2 simultaneous first order ordinary differential equations with split boundary value conditions and comparison with solution using COMSOL which is an advanced finite element program	$\frac{d(r\tau_{rx})}{dr} = -\frac{dP}{dx}r$ $\tau_{rx} = -K \left(\frac{dv_x}{dr} \right) \left(\left \frac{dv_x}{dr} \right \right)^{(n-1)}$

What about models that are formulated as integrals?

- Previous *state of the art* numerical methods where based on evaluating integrals
 - Trapezoidal rule
 - Simpson's Rule
- Many textbooks present models only as integrals

Packed Towers: Gas Absorption

Traditional Approach using **integrals**

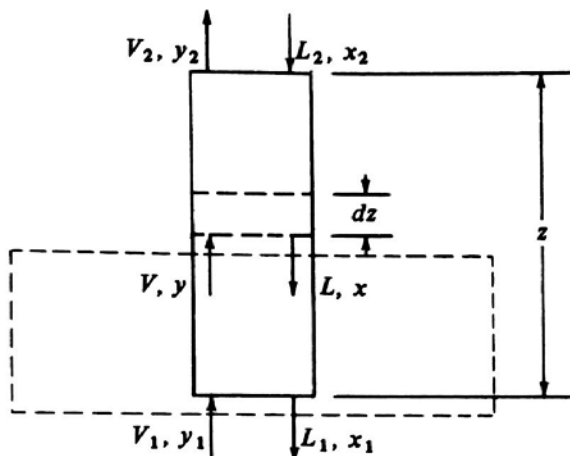


FIGURE 10.6-9. Material balance for a countercurrent packed absorption tower.

5. Design method for packed towers using mass-transfer coefficients. For absorption of A from stagnant B , the operating-line equation (10.6-5) holds. For the differential height of tower dz in Fig. 10.6-9, the moles of A leaving V equal the moles entering L :

$$d(Vy) = d(Lx) \quad (10.6-10)$$

where V = kg mol total gas/s, L = kg mol total liquid/s, and $d(Vy) = d(Lx)$ = kg mol A transferred/s in height dz m. The kg mol A transferred/s from Eq. (10.6-10) must equal the kg mol A transferred/s from the mass-transfer equation for N_A . Equation (10.4-8) gives the flux N_A using the gas-film and liquid-film coefficients:

$$N_A = \frac{k'_y}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai}) = \frac{k'_x}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL}) \quad (10.4-8)$$

where $(1 - y_A)_{iM}$ and $(1 - x_A)_{iM}$ are defined by Eqs. (10.4-6) and (10.4-7). Multiplying the left-hand side of Eq. (10.4-8) by dA and the two right-side terms by $aS dz$ from Eq. (10.6-9),

$$N_A dA = \frac{k'_y a}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai}) S dz = \frac{k'_x a}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL}) S dz \quad (10.6-11)$$

where $N_A dA$ = kg mol A transferred/s in height dz m (lb mol/h).

Equating Eq. (10.6-10) to (10.6-11) and using y_{AG} for the bulk gas phase and x_{AL} for the bulk liquid phase,

Dropping the subscripts A , G , and L and integrating, the final equations are as follows using film coefficients:

$$\int_0^z dz = z = \int_{y_2}^{y_1} \frac{V dy}{\frac{k'_y a S}{(1 - y)_{iM}} (1 - y)(y - y_i)} \quad (10.6-17)$$

$$\int_0^z dz = z = \int_{x_2}^{x_1} \frac{L dx}{\frac{k'_x a S}{(1 - x)_{iM}} (1 - x)(x_i - x)} \quad (10.6-18)$$

Derive model using Plug Flow Assumption: Create Differential Equations

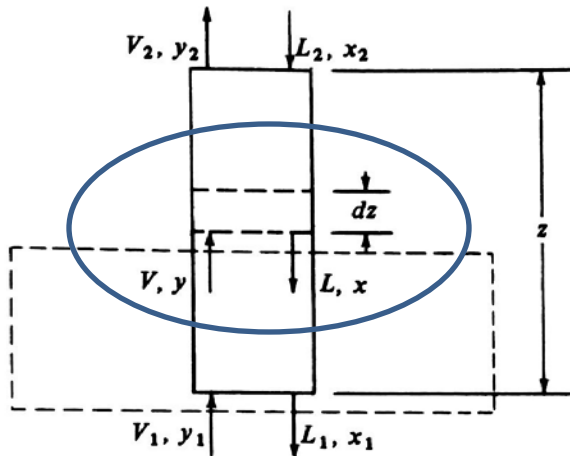


FIGURE 10.6-9. Material balance for a countercurrent packed absorption tower.

$$\frac{d(Vy_{AG})}{dz} = -\frac{k'_y a S}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai})$$

$$\frac{d(Lx_{AL})}{dz} = -\frac{k'_x a S}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL})$$

5. Design method for packed towers using mass-transfer coefficients. For absorption of A from stagnant B, the operating-line equation (10.6-5) holds. For the differential height of tower dz in Fig. 10.6-9, the moles of A leaving V equal the moles entering L :

$$d(Vy) = d(Lx) \quad (10.6-10)$$

where V = kg mol total gas/s, L = kg mol total liquid/s, and $d(Vy) = d(Lx)$ = kg mol A transferred/s in height dz m. The kg mol A transferred/s from Eq. (10.6-10) must equal the kg mol A transferred/s from the mass-transfer equation for N_A . Equation (10.4-8) gives the flux N_A using the gas-film and liquid-film coefficients:

$$N_A = \frac{k'_y}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai}) = \frac{k'_x}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL}) \quad (10.4-8)$$

where $(1 - y_A)_{iM}$ and $(1 - x_A)_{iM}$ are defined by Eqs. (10.4-6) and (10.4-7). Multiplying the left-hand side of Eq. (10.4-8) by dA and the two right-side terms by $aS dz$ from Eq. (10.6-9),

$$N_A dA = \frac{k'_y a}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai}) S dz = \frac{k'_x a}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL}) S dz \quad (10.6-11)$$

where $N_A dA$ = kg mol A transferred/s in height dz m (lb mol/h).

Equating Eq. (10.6-10) to (10.6-11) and using y_{AG} for the bulk gas phase and x_{AL} for the bulk liquid phase,

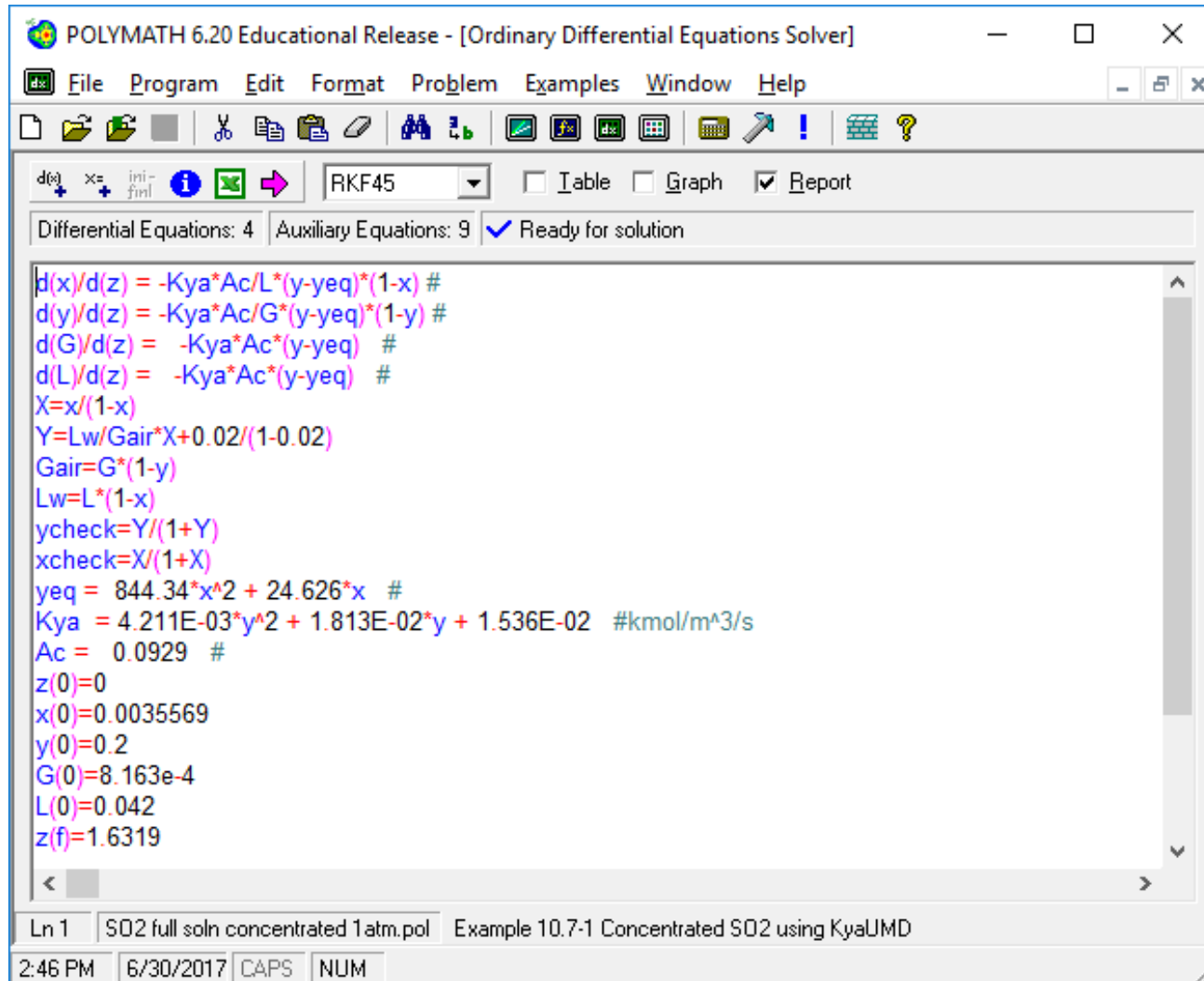
$$d(Vy_{AG}) = \frac{k'_y a}{(1 - y_A)_{iM}} (y_{AG} - y_{Ai}) S dz \quad (10.6-12)$$

$$d(Lx_{AL}) = \frac{k'_x a}{(1 - x_A)_{iM}} (x_{Ai} - x_{AL}) S dz \quad (10.6-13)$$

Since $V' = V(1 - y_{AG})$ or $V = V'/(1 - y_{AG})$,

$$d(Vy_{AG}) = d\left(\frac{V'}{(1 - y_{AG})} y_{AG}\right) = V' d\left(\frac{y_{AG}}{1 - y_{AG}}\right) = \frac{V' dy_{AG}}{(1 - y_{AG})^2} \quad (10.6-14)$$

Polymath Absorber Model



POLYMATH 6.20 Educational Release - [Ordinary Differential Equations Solver]

File Program Edit Format Problem Examples Window Help

d(x) x= ini- RKF45 Iable Graph Report

Differential Equations: 4 Auxiliary Equations: 9 Ready for solution

```
d(x)/d(z) = -Kya*Ac/L*(y-yeq)*(1-x) #
d(y)/d(z) = -Kya*Ac/G*(y-yeq)*(1-y) #
d(G)/d(z) = -Kya*Ac*(y-yeq) #
d(L)/d(z) = -Kya*Ac*(y-yeq) #
X=x/(1-x)
Y=Lw/Gair*X+0.02/(1-0.02)
Gair=G*(1-y)
Lw=L*(1-x)
ycheck=Y/(1+Y)
xcheck=X/(1+X)
yeq = 844.34*x^2 + 24.626*x #
Kya = 4.211E-03*y^2 + 1.813E-02*y + 1.536E-02 #kmol/m^3/s
Ac = 0.0929 #
z(0)=0
x(0)=0.0035569
y(0)=0.2
G(0)=8.163e-4
L(0)=0.042
z(f)=1.6319
```

Ln 1 SO2 full soln concentrated 1atm.pol Example 10.7-1 Concentrated SO2 using KyaUMD

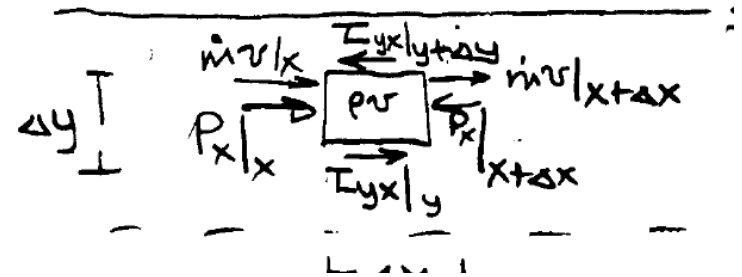
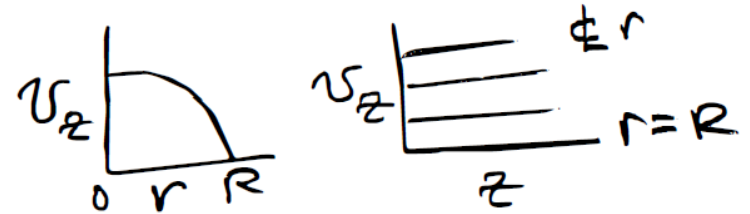
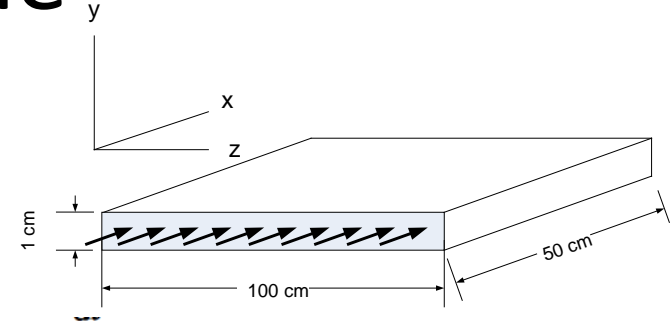
2:46 PM 6/30/2017 CAPS NUM

POLYMATH is a learning tool

- Students need to derive the model equations
- Then enter them into POLYMATH
- POLYMATH is not a “canned” program in which the equations are hidden such as in COMSOL and ASPEN
- The next slides give an example of using POLYMATH with a problem in Fluids

Newtonian Fluid Flow Between Parallel Plates Example

- Figures showing flow
- Graphs with expected behavior
- Control Volume – shell balance
- Derivation
- Simplifications: steady-state etc.



$$\frac{d(\rho r)}{dt} = - \frac{\partial(\rho r v)}{\partial x} - \frac{\partial P_x}{\partial x} - \frac{\partial (T_{yx})}{\partial y}$$

Analytical Solution

- Newtonian Fluid

$$\tau_{yx} = -\mu \frac{\partial v_x}{\partial y}$$

$$\frac{\partial (\tau_{yx})}{\partial y} = - \underbrace{\frac{\partial P_x}{\partial x}}_{\text{this is a constant}}$$

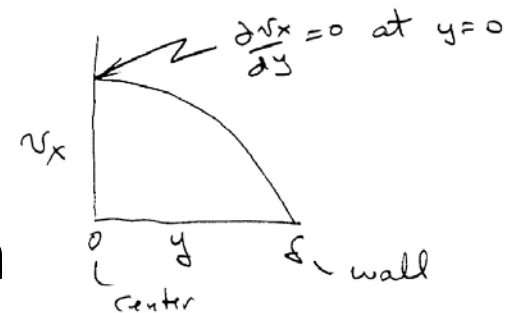
- Boundary Conditions

$$\triangleright y = 0 \quad v_x = \max \quad \tau_{yx} = 0$$

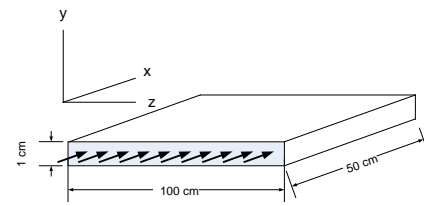
$$\triangleright y = \text{wall} \quad v_x = 0 \quad \tau_{yx} = \max$$

- Integrate Twice: Analytical Solution

$$\triangleright v_x = -\frac{dP}{dx} \left(\frac{\delta^2}{2\mu} \right) \left[1 - \left(\frac{y}{\delta} \right)^2 \right]$$



Numerical Solution

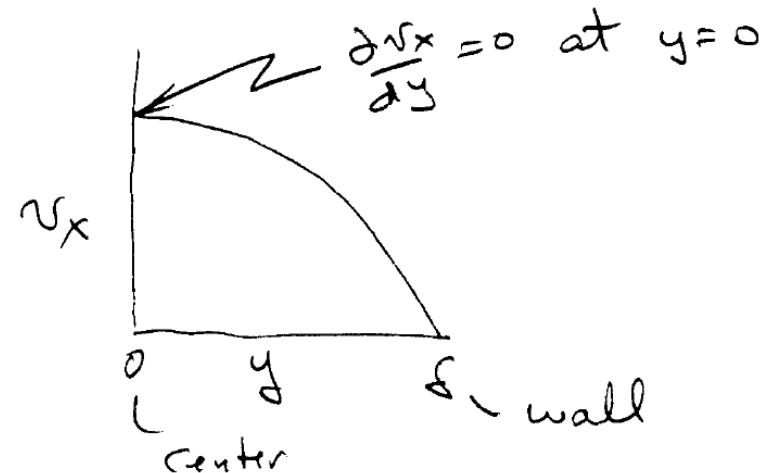


- Newtonian Fluid

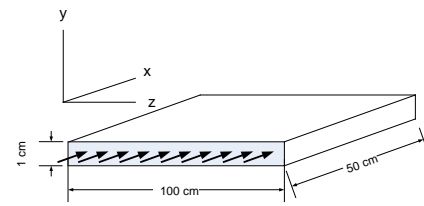
$$\tau_{yx} = -\mu \frac{\partial v_x}{\partial y}$$

$$\frac{\partial (\tau_{yx})}{\partial y} = - \underbrace{\frac{\partial P_x}{\partial x}}_{\text{this is a constant}}$$

- Two coupled ODE's :
Split Boundary Condition
- Then manipulate two ODE's so they can be solved using the POLYMATH Differential Equation Solver (DEQ)

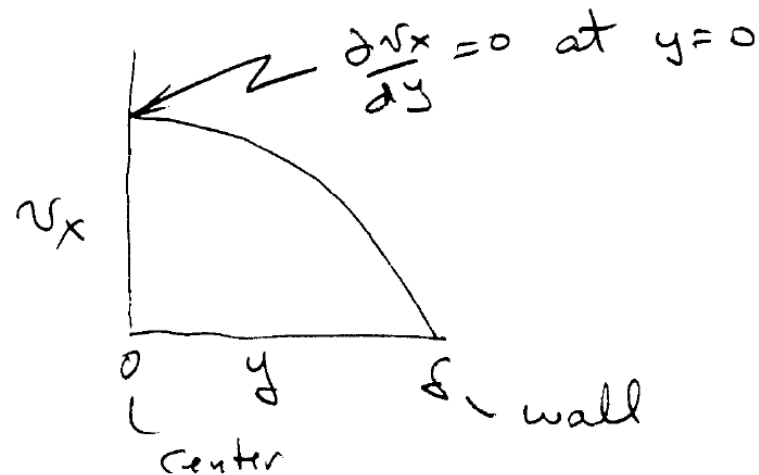


Required manipulation to solve 2 ODE's with split Boundary conditions



$$\tau_{yx} = -\mu \frac{\partial v_x}{\partial y} \quad \longrightarrow \quad \left(\frac{\partial v_x}{\partial y} \right) = \frac{\tau_{yx}}{-\mu}$$

$$\frac{\partial (\tau_{yx})}{\partial y} = - \underbrace{\frac{\partial P_x}{\partial x}}_{\text{this is a constant}} \quad \longrightarrow \quad \left(\frac{\partial \tau_{yx}}{\partial y} \right) = - \frac{dP}{dx}$$

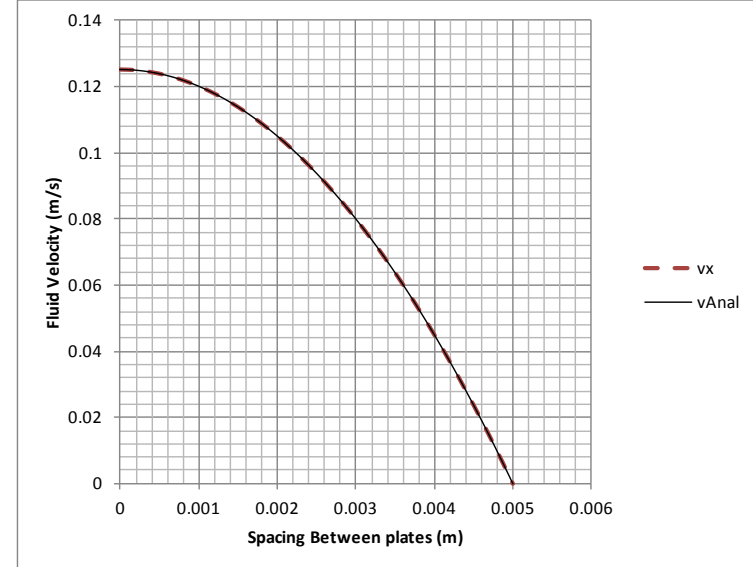


$$\begin{array}{lll} y = 0 & v_x = \max & \tau_{yx} = 0 \\ y = \text{wall} & v_x = 0 & \tau_{yx} = \max \end{array}$$

Integration starts at $y=0$ and both initial conditions must be known!

Solution is to guess v_x at $y = 0$ until at $y = \text{wall}$ $v_x = 0$

Solution



Differential Equations Solution #6

File Edit Help

POLYMATH Report Newtonian Fluid Flow Between 2 parallel plates
Ordinary Differential Equations 30-Jun-2017

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	delta	0.005	0.005	0.005	0.005
2	dPdx	100.	100.	100.	100.
3	mu	0.01	0.01	0.01	0.01
4	Re	62.5	1.9396E-13	62.5	1.9396E-13
5	rho	1000.	1000.	1000.	1000.
6	Tau	0	0	0.5	0.5
7	vAnal	0.125	0	0.125	0
8	vx	0.125	3.8793E-16	0.125	3.8793E-16
9	y	0	0	0.005	0.005

Differential equations

- $d(\text{Tau})/d(y) = d\text{Pdx}$
- $d(vx)/d(y) = -\text{Tau}/\mu$

Explicit equations

- $\rho = 1000$
- $\mu = 0.01$
- $\delta = 0.01/2$
- $\text{Re} = \rho \cdot \delta \cdot vx / \mu$
- $d\text{Pdx} = 100$
- $v\text{Anal} = d\text{Pdx} \cdot \delta^2 / 2 / \mu \cdot (1 - (y/\delta)^2)$

POLYMATH 6.20 Educational Release - [Ordinary Differential Equations Solver]

File Program Edit Format Problem Examples Window Help

RKF45

Differential Equations: 2 Auxiliary Equations: 6 Ready for solution

```

d(Tau) / d(y) = dPdx
d(vx) / d(y) = -Tau/mu
rho=1000
Re = rho*delta*vx/mu
delta = 0.01/2
vAnal = dPdx*delta^2/2/mu*(1-(y/delta)^2)
dPdx = 100
mu = 0.01
y(0) = 0
y(f) = 0.005
Tau(0) = 0
vx(0) = 0.125
    
```

Ln 6 parallel plates newtonian.pol Newtonian Fluid Flow Between 2 parallel plates

3:36 PM 6/30/2017 CAPS NUM

Trials using interpolation
after 3rd guess

v at center	v at wall
0.1	-0.025
0.5	0.375
0.1250	3.88E-16

Students are Confused

- **Question**

Why do I have to do trial & error for the initial velocity? Why not just plug-in the maximum velocity from the analytical solution?

- **Answer**

Your goal is always to compare a numerical solution to a simple analytical problem solution. This shows that the numerical solution method is correct.

- Then give students a more complex problem with one of the plates heated resulting in a temperature profile in the liquid. Now they must do the trial and error procedure.

Temperature Profile in liquid:

$$T = 5000 \frac{K}{m} y + 293.15K$$

$$\mu = \frac{196.99 \text{kg}}{m \text{ s}} \exp\left(-\frac{0.033}{K} T\right)$$

Heated Plates

POLYMATH 6.20 Educational Release - [Ordinary Differential Equations Solver]

Differential Equations Solution #11

POLYMATH Report Newtonian Fluid Flow Between 2 parallel heated plates with viscosity a function of T
30-Jun-2017

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	delta	0.005	0.005	0.005	0.005
2	dPdx	100.	100.	100.	100.
3	mu	0.01239085	0.0054301	0.01239085	0.0054301
4	Re	71.867551	0.03636595	88.835003	0.03636595
5	rho	1000.	1000.	1000.	1000.
6	T	293.15	293.15	318.15	318.15
7	Tau	0	0	0.5	0.5
8	vAnal	0.1008809	0	0.11817159	0
9	vx	0.1781	0.00003949	0.1781	0.00003949
10	y	0	0	0.005	0.005

Differential equations

- $d(\text{Tau})/d(y) = dPdx$
- $d(vx)/d(y) = -\text{Tau}/\mu$

Explicit equations

- $\rho = 1000$
- $T = 5000*y + 293.15$
- $\delta = 0.01/2$
- $\mu = 196.99*\exp(-0.033*T)$
- $Re = \rho*\delta*vx/\mu$
- $dPdx = 100$
- $vAnal = dPdx*\delta^2/2/\mu*(1-(y/\delta)^2)$

Initial conditions

$$y(0) = 0$$

$$y(f) = 0.005$$

$$T(0) = 293.15$$

$$T(f) = 318.15$$

$$vx(0) = 0.1781$$

$$vx(f) = 0.00003949$$

Trials using interpolation after 3rd guess

v at center	v at wall
0.125	-0.05306
0.12	-0.05806
0.180	0.001939
0.17806	3.95E-05

Fluid Velocity (m/s) vs Spacing Between plates (m)

Legend: -- Solution, — OldAnalytical with T