http://my.fit.edu/~jbrenner/che1012/CHE1102 OR Canvas/Files
name = fltech password = brenner
click on lecturenotess15
Then open coursepacks12.pdf to PP. 7, 8, 12
problems #32 & #44

Then open 232excel.xls
244excel.xls
& week3.pdf

week3.zip
&
week3notes2020.pdf

Oakdale Engineering Datafit
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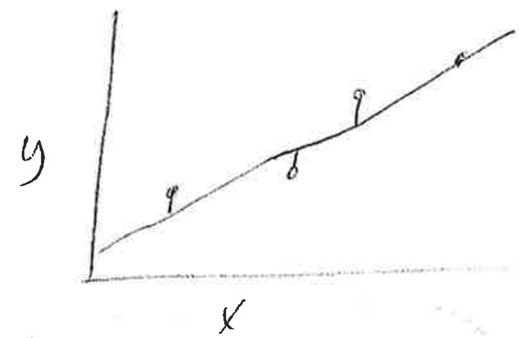
adding axis labels, etc.
Look under Chart Tools Design / Add Chart Element
or
" " Format

$$s = \left(\frac{\sum_{i=1}^{N} (X_i - \bar{X})^2}{(N-1)} \right)^{1/2}$$



$$\sum_{i=1}^{N} \left(y_{i,exp} - y_{i,calc} \right)^2$$

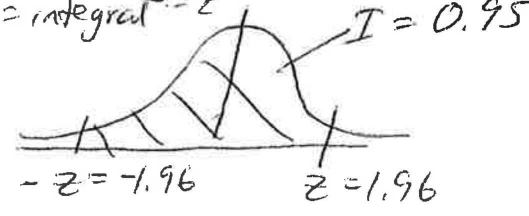
95% confidence interval on the mean of 1-dimensional data
Ex. color of paint in 2.19

$$\bar{X} \pm \frac{1.96\,(s)}{\sqrt{N}}$$

value of z such that

$$I = \int_{-z}^{z} \frac{1}{\sqrt{2\pi}} e^{-z^2/2}\, dz$$

I = integral



95% confidence interval in DataFit
on 2-dimensional data

	Value (Average value)	Error in slope or intercept: 95% t
a	6.536	da = 0.108
b	-4.206	db = 0.22966..

std. dev. in slope, a

$\bar{a} \pm \frac{1.96(S_a)}{\sqrt{N}}$

$\bar{b} \pm \frac{1.96(S_B)}{\sqrt{N}}$

Problem 2.31 - part of HW 4 (not HW 3)
Problem 2.32 + 44 = HW 3

Problem 2.31

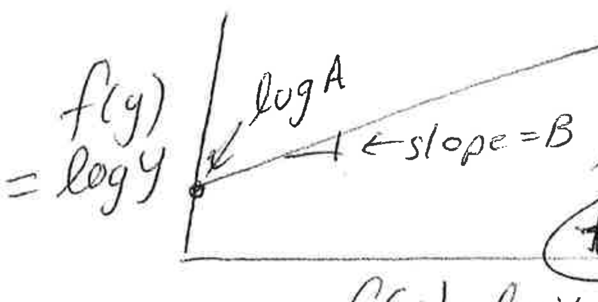
felderchapter2.tif
coursepacks12.pdf
or Handout from
1st class

Problem 2.44 page 12 of coursepacks12.pdf
31 page 7 " "
32 pages 7-8 " "

Problem 2.31
Goal is to transform nonlinear function into something that looks like $y = ax + b$

$y = Ax^B$ A, B unknown constants

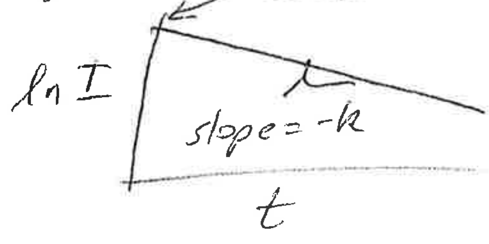
$\log y = \log(Ax^B) =$
$\log A + \log x^B =$



$\log y = \log A + B \log x$
$f(y) = y\text{-intercept} + \text{slope} * f(x)$

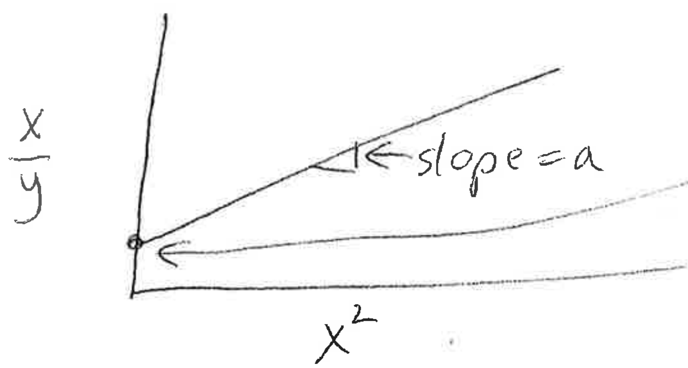
$\ln I = \ln I_0 - kt$

$I = I_0 e^{-kt}$
Radioactive decay



2.31 (G) $y = \left[ax + \frac{b}{x}\right]^{-1}$ $\frac{1}{y} = ax + \frac{b}{x}$

$\frac{x}{y} = ax^2 + b$



#32

95% conf. intervals

	(Average) Value	95% ± (error)
a	474.804	17.827
b	-0.213	1.847

Not necessary

DataFit
Define User Model
$y = \text{Slope} * x$
$y = ax + b$
in Excel
using Add Trendline

slope = 473 ± 8

slope = 474 ±
intercept = 0 ± 2

Error in intercept ≥ |Intercept|

∴ You don't need the y-intercept

Goal: Describe data with as few parameters as necessary

DataFit steps
Copy + paste data into DataFit
Solve Regression, OK, click model, OK
Results Detailed

For 2.32 when adding trendline
Click set intercept = 0 checkbox

Excel/watergasshiftequilibrium.xls and coursepacks12.pdf p. 54

HW 8 coursepacks12.pdf p. 73

HW 9 coursepacks12.pdf pp. 74-77 especially 76

Excel/terminalvelocityofsolidblank.xls to start problem

Excel/terminalvelocityofsolid.xls to check answer

HW 10 coursepacks12.pdf pp. 78-82 especially 82

Excel/numericintegrationtrapezoidalruleblank to start problem

Excel/numericintegrationtrapezoidalrule to check answer

$I = I_0 e^{-kt}$

$f(I) = \text{slope} * f(t) + \text{y-intercept}$

$f(I) = \ln I$

slope = $-k$

$f(t) = t$

$\ln I = \ln I_0 - kt$

2.316 $y = [ax + \frac{b}{x}]^{-1}$

$\frac{1}{y} = ax + \frac{b}{x}$

$\frac{x}{y} = ax^2 + b$

$f(y) = \frac{x}{y}$

← slope = a

← b = y-intercept

$f(x) = x^2$

http://my.fit.edu/~jbrenner/che11012/CHE1102/
name = fltech password = brenner

Click on lecturenotess12
Click on coursepacks12.pdf see p.12 Problem 2.44

In Excel

x	y
1.0	2.35
1.5	5.53
2.0	8.92
2.5	12.15
3.0	15.38

Today we will plot this data & fit it to a straight line $y = ax + b$

~~Better~~ Easier if you use Office 97, 2000, or 2003 or OpenOffice than if you use Office 2007 or higher (No longer toolbars or Chart Wizard)

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http://my.fit.edu/~jbrenner/www3265/datafit6.zip
datafitinstructions.txt datafitreadme.txt on How to do curve fitting step-by-step

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How to Plot

1) Insert Scatter plot (with no markers)
2) Right click on plot + Move Chart to its own worksheet
3) Click on upper left
Bold
Times New Roman
16 = font size
4) Delete gridlines
Delete legend if there is only 1 curve
5) Label axes with text + units if possible
6) Change your title to make it meaningful

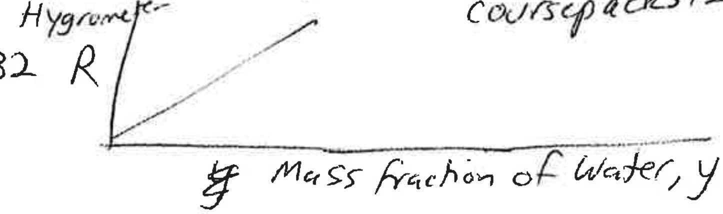
Chart Tools Layout
y-axis — rotated title

7) Click on each axis & add major & minor tick marks (For minor tick marks, make sure they don't count by ~~3~~ fours)
under Format Axis
8) Format Axis Number to appropriate # of decimal places

9) Right click on Data
Add Trendline
Click Display Equation on chart
For Problem 32, also click Set Intercept = 0

Homework 3 Problems 2.44, 2.32 → P. 12 of → pp. 7-8 of coursepacks12.pdf
Save 2.31 for HW 4

Problem 32



10) Edit equation to include errors & ±'s
11) Copy + paste x-y data into DataFit
12) Solve regression
$y = ax + b$ ← Click this for #44
13) Results Detailed
Check model plot
Fit Information error in a+b under 95% confidence intervals where it says 95% ±

95% Confidence Intervals

	Value (Average Value)		95% ± error in
a	Average slope		Error in slope
b	Average intercept		Error in intercept
a	6.536	±	.108
b	−4.206	±	.230

} From Problem 2.44

1) The first and only significant digit in the error is in the same decimal place as the last significant digit in the average value.

2) 5+, round up 4− ↓ round down

$a = 6.5 \pm 0.1$ ← Errors only have one significant figure

$b = -4.2 \pm 0.2$

PRINT

Page Setup for each sheet with a plot or that must be turned in on a test

Header + Footer

Custome Header

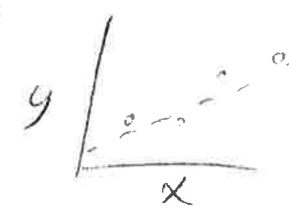
Name Problem # Wed 3-5

Change default printer to Black + White

SAVE

Hygrometer 1st linear fit with intercept

	Value	95% +/-
a	474.8	17.8
b	-0.21	1.85



$a = 470 \pm 20$

$b = 0 \pm 2$ — This is a waste.

The goal of curve fitting is to fit data with as few parameters as necessary.

Refit without any intercept.

Solve/Define User Model

New

Name your Model ID

$y = a * x$ ← your slope

Initial estimates default to 1. For linear curve fitting, you are guaranteed convergence to the right answer. Starting next week when do nonlinear curve fitting, there are no such guarantees. If you get Solution Failed. → Sign of divergence improve initial guess(es).

If you see your Model Plot doesn't fit the data, change your initial guess(es).

Solve

Find your newly defined model at the bottom of the list. Click OK to do fit.

Results Detailed

Check Model plot

Check Fit Information

	Value	95% ±
slope	473.08	7.53

COPY (473 ± 8) back to plot

(a) Use two-point linear interpolation to estimate the value of p^* at $T = 185°C$.

(b) Write a computer subroutine to estimate the vapor pressure of 1-chlorotetradecane for any temperature between 98.5°C and 215.5°C using two-point linear interpolation. The subroutine must determine which two tabulated temperatures bracket the given temperature, and apply the interpolation to estimate $p^*(T)$. Then write a main program to read and store the values of p^* and T given in the table and to generate a table of vapor pressures at temperatures $T = 100°C, 105°C, 110°C, \ldots, 215°C$, calling your subroutine to estimate p^* at each temperature. Check your program using the result of part (a).

2.30. Sketch the plots described below and calculate the equations for $y(x)$ from the given information. The plots are all straight lines. Note that the given coordinates refer to abscissa and ordinate values, not x and y values. [The solution of part (a) is given as an example.]

(a) A plot of $\ln y$ versus x on rectangular coordinates passes through (1.0, 0.693) and (2.0, 0.0) (i.e., at the first point $x = 1.0$ and $\ln y = 0.693$).

Solution: $\ln y = bx + \ln a \Longrightarrow y = ae^{bx}$

$$b = (\ln y_2 - \ln y_1)/(x_2 - x_1) = (0 - 0.693)/(2.0 - 1.0) = -0.693$$

$$\ln a = \ln y_1 - bx_1 = 0.693 + 0.693 * 1.0 = 1.386 \Longrightarrow a = e^{1.386} = 4.00$$

$$\Downarrow$$

$$\boxed{y = 4.00e^{-0.693x}}$$

(b) A semilog plot of y (logarithmic axis) versus x passes through (1, 2) and (2, 1).

(c) A log plot of y versus x passes through (1, 2) and (2, 1).

(d) A semilog plot of xy (logarithmic axis) versus y/x passes through (1.0, 40.2) and (2.0, 807.0).

(e) A log plot of y^2/x versus $(x - 2)$ passes through (1.0, 40.2) and (2.0, 807.0).

2.31. State what you would plot to get a straight line if experimental (x, y) data are to be correlated by the following relations, and what the slopes and intercepts would be in terms of the relation parameters. If you could equally well use two different kinds of plots (e.g., rectangular or semilog), state what you would plot in each case. [The solution to part (a) is given as an example.]

(a) $y^2 = ae^{-b/x}$.

Solution: Construct a semilog plot of y^2 versus $1/x$ or a plot of $\ln(y^2)$ versus $1/x$ on rectangular coordinates. Slope $= -b$, intercept $= \ln a$.

(b) $y^2 = mx^3 - n$

(c) $1/\ln(y - 3) = (1 + a\sqrt{x})/b$

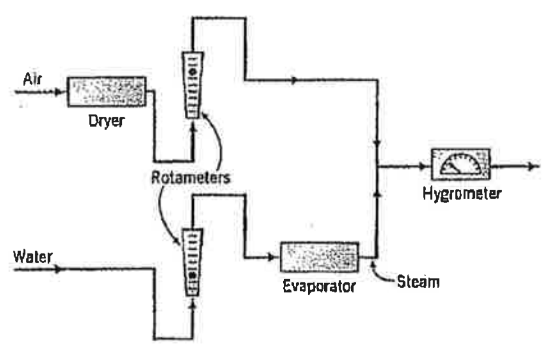
(d) $(y + 1)^2 = [a(x - 3)^3]^{-1}$

(e) $y = \exp(a\sqrt{x} + b)$

(f) $xy = 10^{[a(x^2+y^2)+b]}$

(g) $y = [ax + b/x]^{-1}$

2.32. A **hygrometer**, which measures the amount of moisture in a gas stream, is to be calibrated using the apparatus shown here:



7

Steam and dry air are fed at known flow rates and mixed to form a gas stream with a known water content, and the hygrometer reading is recorded; the flow rate of either the water or the air is changed to produce a stream with a different water content and the new reading is recorded, and so on. The following data are taken:

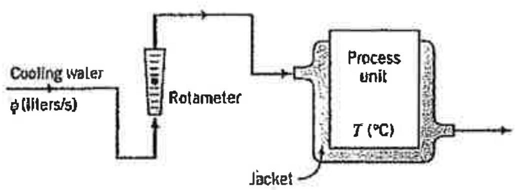
Mass Fraction of Water, y	Hygrometer Reading, R
0.011	5
0.044	20
0.083	40
0.126	60
0.170	80

$\frac{3}{20}$ × .021 .091 = × .3 .006

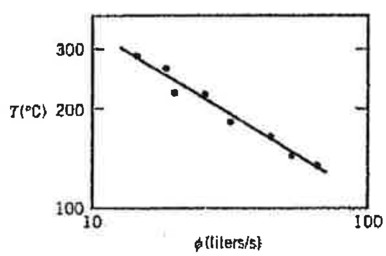
(a) Draw a calibration curve and determine an equation for $y(R)$. $R(y)$

(b) Suppose a sample of a stack gas is inserted in the sample chamber of the hygrometer and a reading of $R = 43$ is obtained. If the mass flow rate of the stack gas is 1200 kg/h, what is the mass flow rate of water vapor in the gas?

2.33. The temperature in a process unit is controlled by passing cooling water at a measured rate through a jacket that encloses the unit.



The exact relationship between the unit temperature T(°C) and the cooling flow water flow rate ϕ (L/s) is extremely complex, and it is desired to derive a simple empirical formula to approximate this relationship over a limited range of flow rates and temperatures. Data are taken for T versus ϕ. Plots of T versus ϕ on rectangular and semilog coordinates are distinctly curved (ruling out $T = a\phi + b$ and $T = ae^{b\phi}$ as possible empirical functions), but a log plot appears as follows:



A line drawn through the data goes through the points ($\phi_1 = 25, T_1 = 210$) and ($\phi_2 = 40, T_2 = 160$).

(a) What is the empirical relationship between ϕ and T?

(b) Using your derived equation, estimate the cooling water flow rates needed to maintain the process unit temperature at 85°C, 175°C, and 290°C.

(c) In which of the three estimates in part (b) would you have the most confidence and in which would you have the least confidence? Explain your reasoning.

2.34. A chemical reaction A → B is carried out in a closed vessel. The following data are taken for the concentration of A, C_A(g/L), as a function of time, t(min), from the start of the reaction:

8

*2.44. Write a computer program to fit a straight line $y = ax + b$ to tabulated (x, y) data, assuming that no more than 100 data points will be taken in any one run. Your program should read in and store the data, evaluate the slope a and intercept b of the best line through the data using Equations A.1-3 through A.1-5 in Appendix A, then print out the measured values of x and y and calculated values of $y(= ax + b)$ for each tabulated value of x.

Test your program by fitting a line to the data in the following table:

x	1.0	1.5	2.0	2.5	3.0
y	2.35	5.53	8.92	12.15	15.38

2.45. The rate at which a substance passes through a semipermeable membrane is determined by the *diffusivity* $D(\text{cm}^2/\text{s})$ of the gas. D varies with the membrane temperature $T(K)$ according to the *Arrhenius equation*:

$$D = D_0 \exp(-E/RT)$$

where D_0 = the *preexponential factor*
E = the *activation energy* for diffusion
R = 1.987 cal/(mol·K)

Diffusivities of SO_2 in a fluorosilicone rubber tube are measured at several temperatures, with the following results:

T (K)	$D(\text{cm}^2/\text{s}) \times 10^6$	
347.0	1.34	← (so that $D = 1.34 \times 10^{-6} \text{cm}^2/\text{s}$)
374.2	2.50	
396.2	4.55	
420.7	8.52	
447.7	14.07	
471.2	19.99	

(a) What are the units of D_0 and E?
(b) How should the data be plotted to obtain a straight line on rectangular coordinates?
(c) Plot the data in the manner indicated in part (b), and determine D_0 and E from the resulting line.
*(d) Write a computer program or spreadsheet to read in the (T, D) data and to calculate D_0 and E using the method of least squares (Appendix A.1). Then run the program and print out the results.

*Computer problem.