Breakup: L –T –P –C

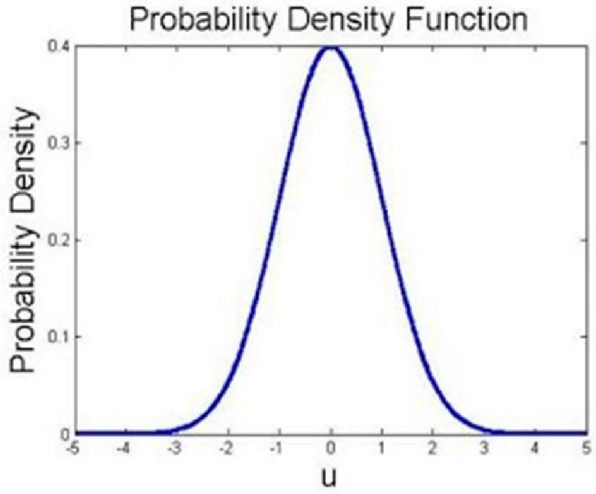
3 –1 –0 –4

Numerical Method for Chemical Engineers

CHE-S506

To solve problem that can not be solved exactly

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{u^2}{2}} du$$



Mathematical Problem

Analytical methods

Framing the problem **in a** well-understood form and calculating the exact solution.

* Solve the closed form equations on paper.
* Usually provide the most meaningful answer because we get an equation showing us exactly what happens with each variable.

But for complex systems the math can become too complicated.

Numerical methods

Find an approximate solution to a problem but may be simpler than an analytical approach.

Techniques for solving the same problem **with a** computer.

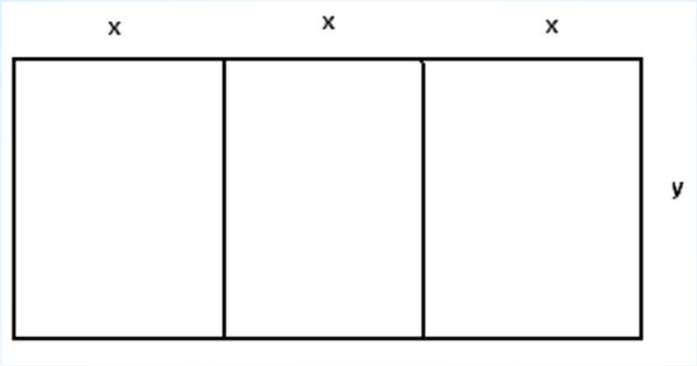
A **numerical** solution means making guesses at the solution and testing whether the problem is solved well enough to stop.

Graphical Method

Used to find an approximate solution to a problem by viewing an interpreting a graphical image accordingly.

Maximizing the area of a rectangular garden

Problem: A farmer needs 150 meters of fencing to fence three adjacent gardens.



a) What is the relationship between x and y?
b) Write the total area A of the three gardens as a function of x.
c) Find the value of x for which A is maximum.

Solution:

Formula for the perimeter
$150 = 6x + 4y$

The total area is
$A = 3xy$

Solve $150 = 6x + 4y$ for y.

$y = (75 - 3x) / 2$

Substitute y by $(75 - 3x) / 2$ in the formula for the area

$A(x) = 3x(75 - 3x) / 2$

$x > 0$ and $(75 - 3x) > 0$

Analytical Solution:

$A(x)$ is a quadratic function which may be written as

$A(x) = -(9 / 2)x^2 + (225 / 2)x$

For a quadratic function of the form $ax^2 + bx + c$

$x = -(225/2) / 2(-9/2) = 12.5$

Numerical Solution:

Solve the above inequalities to obtain the domain as the interval (0 , 25)

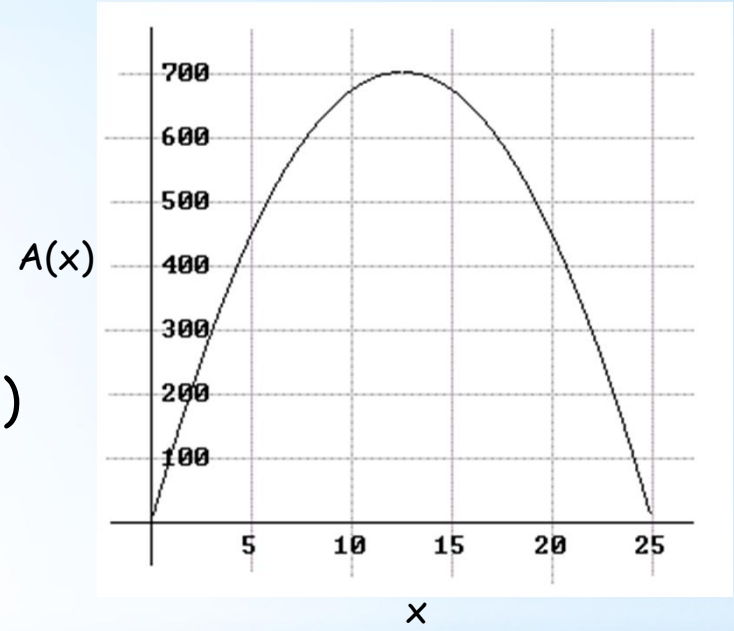
Check the convergence

$(Ai+1-Ai)/Ai \leq 0.0001$

Graphical Solution:

Plot the graph between x and A(x)

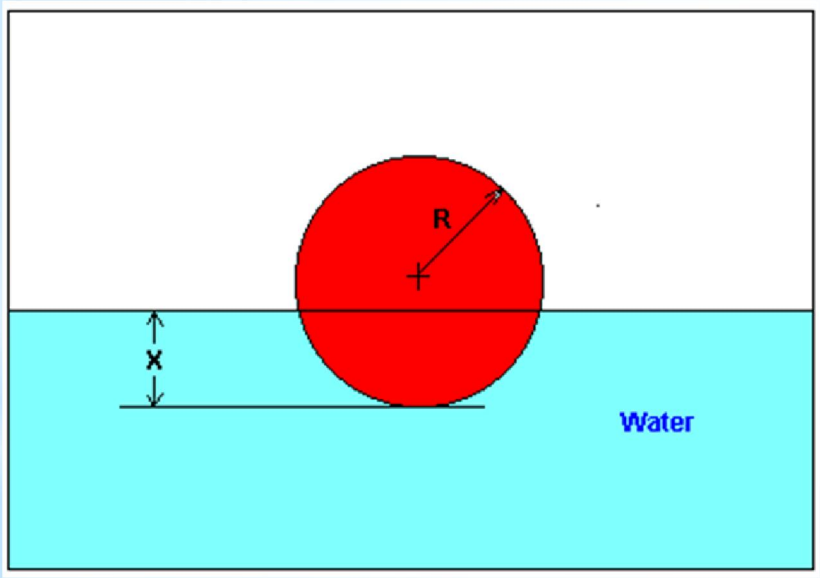
for interval (0 , 25)

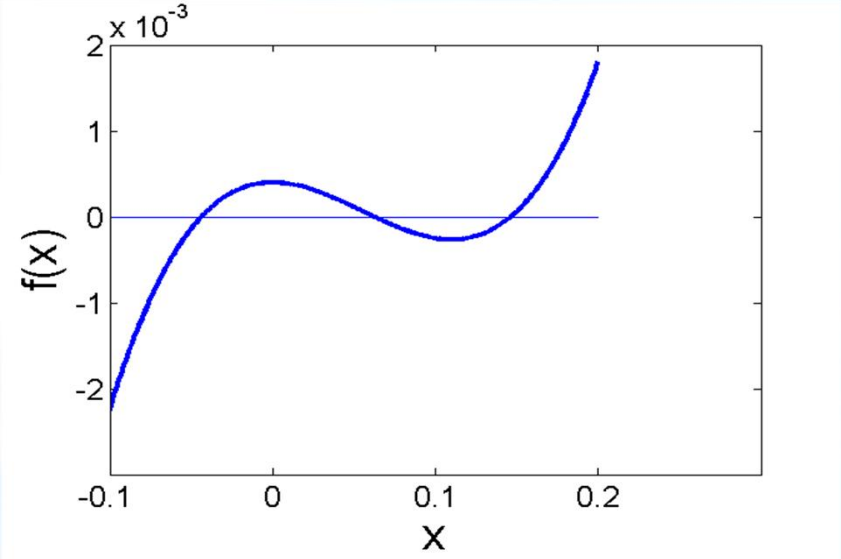


Nonlinear Equations

How much of the floating ball is under water?
Diameter=0.11m Specific Gravity=0.6

$$x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$$

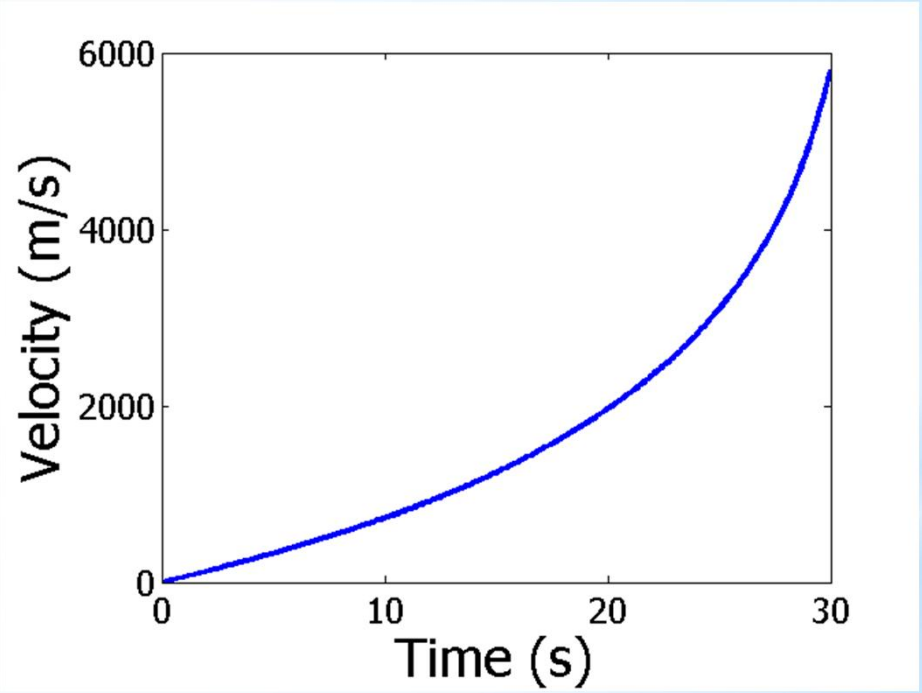




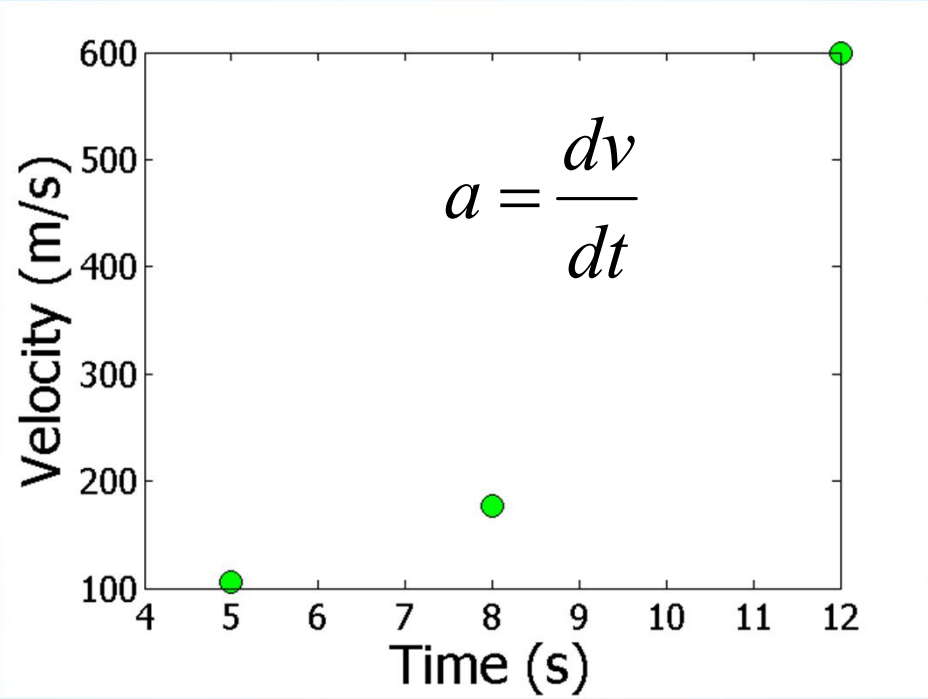
Differentiation

What is the acceleration at t=7 seconds?

$$v(t) = 2200 \ln\left(\frac{16\times10^4}{16\times10^4 - 5000t}\right) - 9.8t \qquad a = \frac{dv}{dt}$$



Time (s)	5	8	12
Vel (m/s)	106	177	600



What is Numerical Method?

Numerical method is an approach for solving complex mathematical problems using simple arithmetic operations.

It involves the formulation of model of physical situations that can be solved by arithmetic operations.

$$x^2 + y^2 + 4x - 2y = -1$$

The equation of a circle in the xy-plane is shown above. What is the radius of the circle?

A) 2

B) 3

C) 4

D) 9

Need of numerical method

Mathematical models are a central piece of science and engineering.

Some models have closed-form solutions, therefore they can be solved analytically.

Many models can not be solved analytically or the analytic solution is too costly to be practical.

All models can be solved computationally and the result may not be the exact answer but it can be useful..

Why are numerical methods used in Engineering?

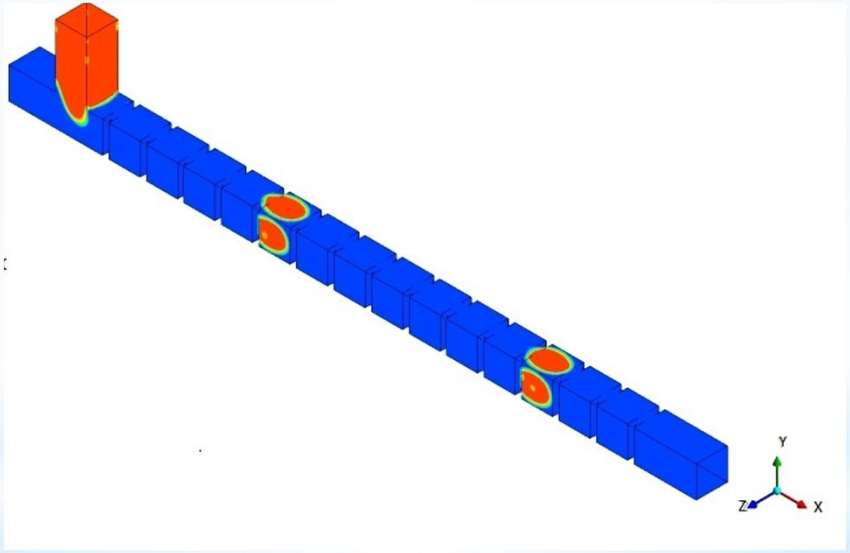
Engineers use mathematical modeling which includes various equations and data to describe and predict the behavior of systems.

Computers are widely used which give accurate results and are cheap and affordable to all.

Many software packages are available that can be used to solve the problems.

Aspen Plus	Hysys	ChemCAD
Design II	Pro II	Unisim
Winsim	Ansys	

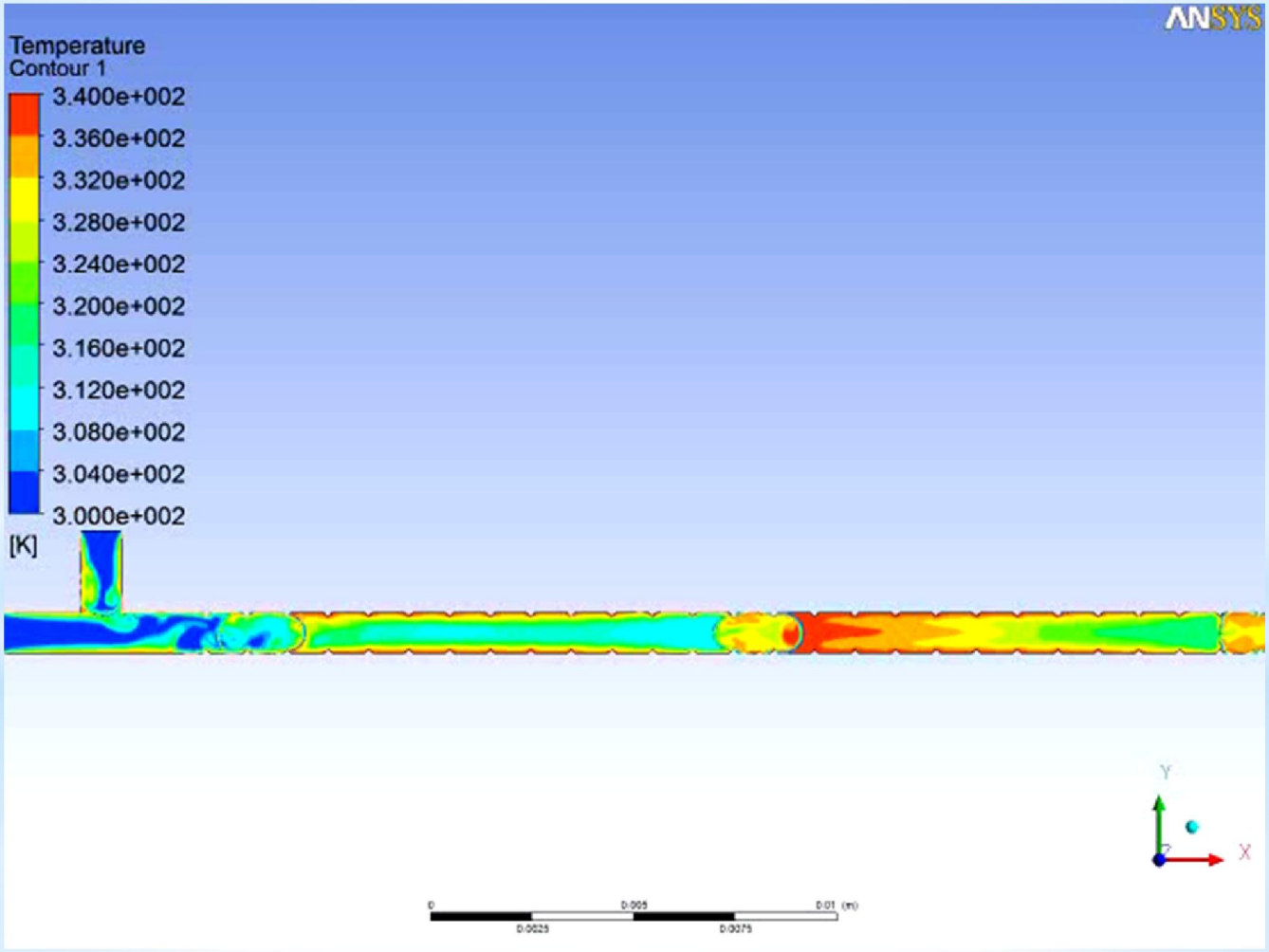
Numerical Simulation of liquid-liquid two phase flow



$$\nabla \bullet u = 0$$

$$\frac{\partial u}{\partial t} + \nabla \bullet (uu) = -(\nabla p) + \nabla \bullet [\mu(\nabla \vec{u} + \nabla \vec{u}^{T})] - \sigma \kappa_{n} \left[\frac{\phi_1 \rho_1 + \phi_2 \rho_2}{\frac{1}{2}(\rho_1 + \rho_2)} \right]$$

$$\rho C_p \frac{DT}{Dt} = k \nabla^2 T$$


ANSYS
Temperature
Contour 1
3.400e+002
3.360e+002
3.320e+002
3.280e+002
3.240e+002
3.200e+002
3.160e+002
3.120e+002
3.080e+002
3.040e+002
3.000e+002
[K]
Y
X

Syllabus of NMCP

Introduction to Numerical Method
- Approximations and errors in computation

Solution of Algebraic and Transcendental equations
- Bisection methods
- Regula-Falsi method
- Newton-Raphson methods
- Secant method

Solution of simultaneous Algebraic equations:
- Gauss elimination method
- Gauss Jordan method
- Jacobi Iteration method
- Gauss-Seidel iteration method

Interpolation and curve- fitting
- Graphical method
- Least Square method and curve fitting of data,
- Method of Moments,
- Cubic spline problems

Functions interpolation and extrapolation of techniques

Numerical differentiation

- Derivatives from difference tables

Numerical integration

- Newton Cotes Integration technique
- Trapezoidal rule
- Simpson's 1/3 rd and 3/8th rule
- Gaussian quadrature
- Double integration.

Ordinary differential equation

- Picard's method
- Euler's method
- Runge method
- Taylor series method
- Euler's modified iteration technique
- Runge-Kutta 4^{th} order technique

Solutions of ordinary differential equation (initial and boundary value problem)

Linear programming

- Simplex method
- Charne penalty method.
- Dual simplex

Text and References Books:

- S. K. Gupta, Numerical Methods for Chemical Engineers, New Age International
- S. Chapra and R. Canale, Numerical Methods for Engineers, McGraw Hill Education.
- B. S. Grewal, Numerical Methods in Engineering and science. Khanna Publishers
- S. S. Sastry, Introductory Methods of Numerical analysis, PHI learning.