King Saud University
Chemical Engineering Department

CHE 401: Computational Techniques

Catalog Data: (2 Credit Hour – 3 Contact Hour (2+1))

(Mathematical formulation of chemical engineering problems. Numerical methods of particular interest to chemical engineers. Application of softwares such as IMSL and MATLAB to the solution of chemical engineering problems using computer).

Prerequisite: CHE 201, CHE 302

Textbooks:

1. B. W. Bequette, *Process Dynamics Modeling, Analysis, and Simulation*, Prentice Hall, 1998.
2. S. K. Gupta, *Numerical Methods for Engineers*, New Age International Publishers Limited-Wiley Eastern Limited, New Delhi, 1995.

References:

1. A. Constantinides and N. Mostoufi, *Numerical Methods for Chemical Engineers with MATLAB applications*, Prentice Hall, 1999.
2. S. C. Chapra and R. P. Canale, *Numerical Methods for Engineers*, 4th Edition, McGraw Hill, 2002.
3. M. B. Cutlip and M. Shacham, *Problem Solving in Chemical Engineering with Numerical Methods*, Prentice Hall, 1999.
4. J. B. Riggs, *An Introduction to Numerical Methods for Chemical Engineers*, 2nd Edition, Texas Tech University Press, 1994.
5. W. F. Ramirez, *Computational Methods for Process Simulation*, 2nd Edition, Butterworth, 1997.
6. O. T. Hanna and O. C. Sandall, *Computational Methods in Chemical Engineering*, Prentice Hall, 1995.
7. T. F. Edgar, D. M. Himmelblau, and L. S., Lasdon, *Optimization of Chemical Processes*, 2nd Edition, McGraw Hill, 2001.

Goal:

The course is aimed at providing basic skills of mathematical modeling and numerical solution of problems commonly encountered in chemical engineering design and analysis. Students are exposed to modeling and solution of steady state and unsteady state lumped parameter systems and steady state

distributed parameter systems. Students get hands on practice of using softwares to apply numerical methods for solving problems on computer. Basic principles of optimization of linear constrained and nonlinear unconstrained problems are also introduced.

Topics to be covered:

1. introduction to the course. Basic definitions, various types of process models and the corresponding type of resulting equations. (2 classes)

2. General Process Modelling – Mass and energy balance equations, constitutive relationships. Modeling examples of lumped parameter and distributed parameter systems. Non-dimensionalization of model equations. (4 classes)

3. Numerical Methods: Solution of the system of linear algebraic equations. (5 classes)

4. Solution of nonlinear algebraic equations – single variable and multi-variable cases. (4 classes)

5. Function approximation and curve fitting. (4 classes)

6. Numerical differentiation and integration techniques. (2 clases)

7. Solution of ordinary differential equations – IVPs & BVPs. Explicit and implicit methods, PC and Ruge-Kutta methods for IVPs and finite difference technique for BVPs. (5 classes)

8. Introduction to optimization methods – single variable and multi variable optimization, linear programming technique. (2 classes)

Class requirements:

1. Homework assignments
2. Mid-term exams
3. Class quizzes
4. Final Exam

Computer usage:

Students get hands on practice in the computer lab on the use of Fortran programs and software packages (e.g., MATLAB, IMSL) to apply various numerical techniques for problem solving.

Laboratory Project: None

Assessment of course goals:

Through homework, class quizzes, mid-term and final exams
(Homework 10%, Quizez 10%, Mid-terms 30%, Final exam 50%)

Contribution to course goals:

Engineering science: 1½ credit hours
Engineering Design: ½ credit hours
Mathematics or Basic Sciences: 0 credit hours

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