



UNIVERSITY
OF PETROLEUM
& ENERGY STUDIES

MODELING, OPTIMIZATION, CONTROL AND DESIGN: SOME THOUGHTS

***SANTOSH K. GUPTA
DEPARTMENT OF CHEMICAL ENGINEERING
UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
DEHRADUN 248007***



UNIVERSITY
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TEXTBOOKS (USE ONLY CLASSIC TEXTS) :

LIST OF TOP 30 IN THE WORLD

**CODES (MATLAB, ASPEN-HYSIS, HTRI,
POLYMERPLUS, etc.**

SOLUTIONS MANUALS

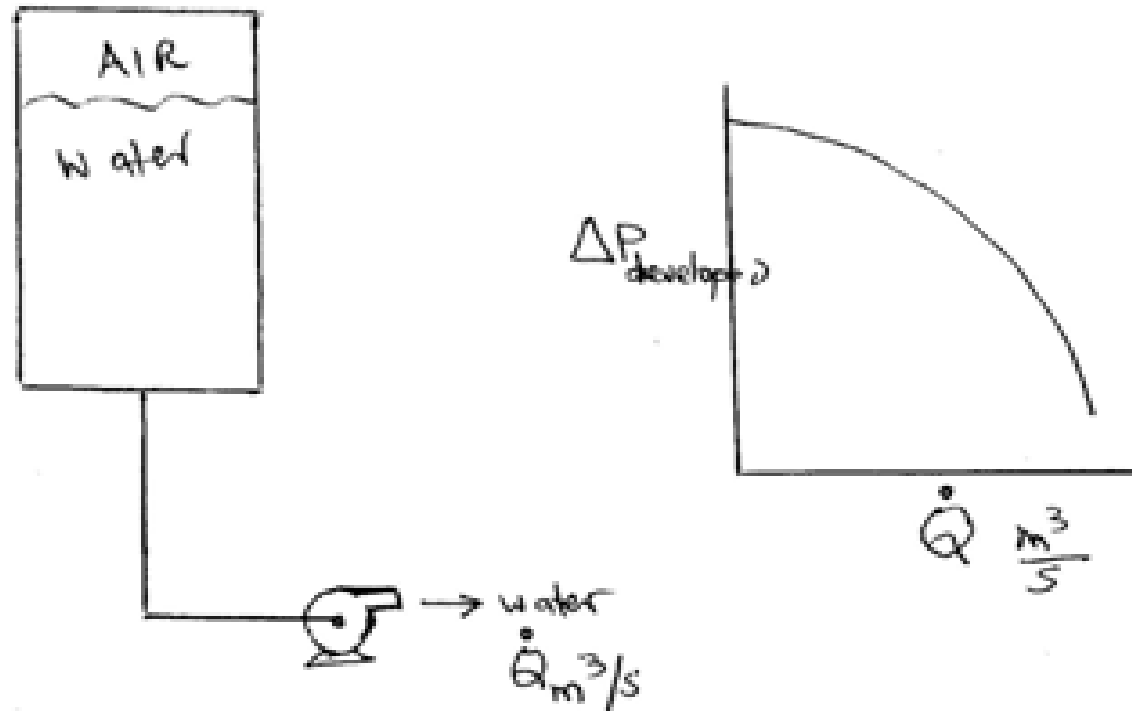
***OFTEN AVAILABLE ON-LINE THESE
DAYS, e.g., OF SMITH AND VAN NESS)***

**JOURNAL ACCESS HELPS BUT VERY
EXPENSIVE**

Rs 70,000/YR ScienceDirect

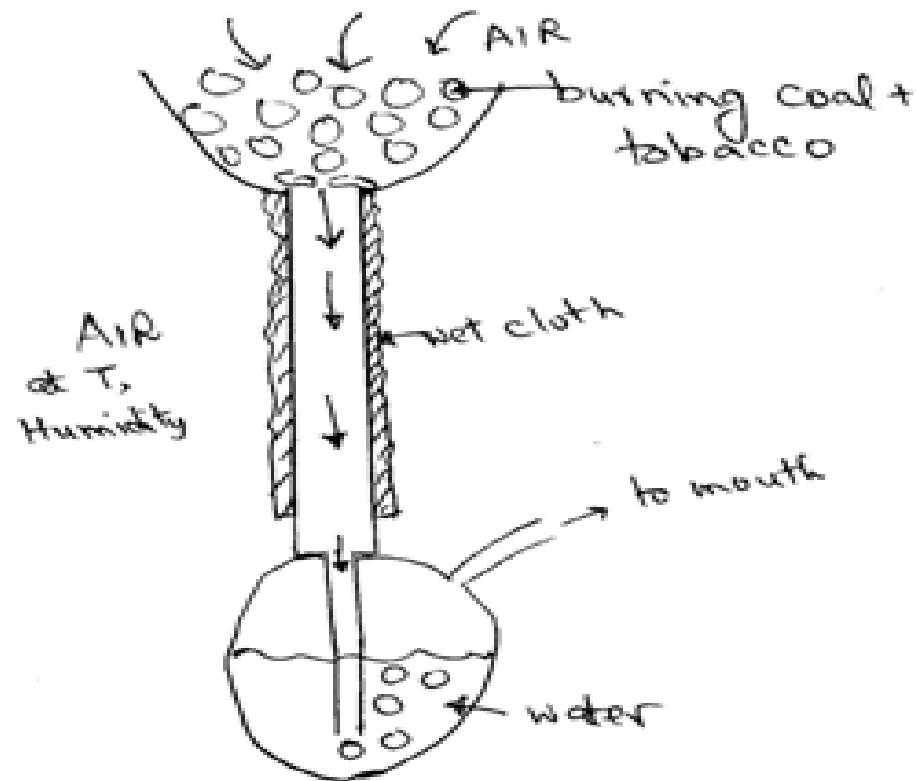
CHALLENGING TEACHING (SOME CHALLENGE PROBLEMS)

- **BREAST FEEDING: CENTRIFUGAL PUMP CONNECTED TO A SEALED TANK WITH WATER AND SOME AIR AT THE TOP**



SOME CHALLENGE PROBLEMS...continued

- HOOKAH PROBLEM IN TRANSPORT PHENOMENA



MPDE 813

Chemical Engineering Computing

Instructors:

Dr. Santosh K. Gupta (skgupta@ddn.upes.ac.in; skgupta@iitk.ac.in)

Office: Room EH 281

X: 361; Call: +91 95542 72320

Text

Gupta, Santosh K.; **Numerical Methods for Engineers**, New Age Intl. Publishers, New Delhi, 2nd Ed., 2010

References:

Carnahan, B.; Luther, H. A. and Wilkes, J. O.; **Applied Numerical Methods**, Wiley, New York, 1969 (a bit outdated now – yet a classic when it first came out)

Finlayson, B. A.; **Nonlinear Analysis in Chemical Engineering**, McGraw Hill, New York, 1980 (a bit at an advanced level – errata is quite long)

Lapidus, L. and Seinfeld, J. H.; **Numerical Solutions of ODEs**, Academic Press, New York, 1971

Davis, M. E.; **Numerical Methods and Modelling for ChE**, Wiley, New York, 1984 (short, yet good presentation)

Chapra, S. C. and Canale, R.; **Numerical Methods for Engineers**, 5th Ed., 2005, Chapter 1 (softcover edition available)

Topics:

(MATLAB and Use of Spreadsheets will be done in MPDE 814)

1. Linear Algebraic Equations (3 lectures).
2. Eigenvalues, Eigenvectors, Stability, Faddeev-Leverrier Method (2 lectures).
3. Solutions of Nonlinear Algebraic Equations: Successive Substitutions and Newton-Raphson; Multiplicity of Solutions; Singularity Theory (4 lectures).
4. Solutions of Ordinary Differential Equations-Initial Value Problems (ODE-IVPs): Stiffness; Explicit and Implicit Methods; Runge-Kutta Methods; Stability; Accuracy, Gear's package for ODE-IVPs; DDASSL package for DAEs (8 lectures).
5. Solutions of Ordinary-Differential Equations-Boundary Value Problems (ODE-BVPs): Finite Difference; Orthogonal Collocation; Orthogonal Collocation on Finite Elements; Galerkin Finite Elements; Shooting Methods (17 lectures).
6. Solutions of Partial Differential Equations: Finite Difference; *Collocation*; *Finite Elements* (10 lectures).

Prerequisites:

Exposure to programming, MATLAB

Grading (BOTH EXAMS ARE OPEN TEXTBOOK-AND-NOTES):

One 2 hr Mid Term Exam	20 %
One 3 hr Final Exam	50 %
Labs, impressions, attendance, assignments	30 %

Attendance:

Attendance in lectures is *mandatory*.

H. W. and Solutions:

Solutions will be available in a file in my office about a week after they are assigned. These **can** be taken out for photocopying.

Mobiles: MUST be switched off (or in silent mode) during the Lectures.

Assignment Problems (from the text)

(Problems in boldface are to be done in MPDE 814)

Assn 1

Q. 1.1, 2, 3, 4, 6, 8, 10, **13, 15, 18** (make a single general program *yourself* for the Jacobi, GS and SOR methods, and solve; print out values at each iteration)

Read only: 1.9

Q. 2.1, 2, 4

Assn 2

Q. 3.3, 4 (single-variable NR; make a single general program *yourself* and solve using the SRK, o-RK, PR and vdW equations of state; print out values at each iteration), 8, 18 (multi-variable NR; use a MATLAB code and solve; print out values at each iteration), 22, 28 (as for Problem 3.18)

READ only: 3.7 (flash), 3.19 (compressors), 3.25, 3.27

Assn 3

Q 4.12, 19, 24, 25 (use a spline-fit code in MATLAB), 27, 33, 34

Assn 4

Q. 5.2, 4, 7 (use a 4th order RK code in MATLAB), 21 (use a code in MATLAB), 23, 28 d (use a Gear code in MATLAB)

Assn 5

Q. 6.2, 3 (c), 7 (use your Gauss Seidel program made in Assignment 1 to solve the algebraic equations), 14, 26 (OC), 36 (don't compare),

7.1 (FD, use a Gear code in MATLAB, after reduction)

Try (formulate only) 6.41 (GFE-ODE)

Read only: 6.18

Systems Analysis and Optimization

Lecture Schedule

- Single-variable optimization

Simultaneous search, Sequential search,
Dichotomous sequential search, Fibonacci search,
Golden-section search

- Multi-variable optimization without constraints

Direct methods

- alternate variable search
- Box complex
- Steepest ascent/descent

Indirect methods

Newton's

Marquardt-Levenberg

Broyden

Davidon-Fletcher-Powell

BFGS

• Multivariable optimization *with constraints*

- Lagrangian multipliers (and Kuhn-Tucker formulation)

- Penalty functions

Genetic algorithm, Simulated annealing and Multi-objective optimization

SGA, NSGA-II, Jumping Gene, Altruistic adaptations

SA, NSSA, Jumping Gene adaptations

Pontryagin's principle and Variational calculus

SQP and its variants (*time permitting*)

TEXTBOOKS

- G. S. G. Beveridge and R. S. Schechter, *Optimization, Theory and Practice*, McGraw Hill, New York, 1970 (Intl. Edn. was available, but is now *out of print*; an excellent text).
- Asgar Hussain and K. Gangaiah, *Optimization Techniques for Chemical Engineering*, MacMillan, Delhi, 1976.
- T. F. Edgar, D. M. Himmelblau and L. S. Lasdon, *Optimization of Chemical Processes*, 2nd Ed., McGraw Hill, New York, 2001 (Intl. Edn. is available).
- M. M. Denn, *Optimization by Variational Principles*, McGraw Hill, New York, 1969.

- **W. H. Ray and J. Szekeley, *Process Optimization*, Wiley, New York, 1973 (Well written).**
- **G. V. Reklaitis, A. Ravindran and K. M. Ragsdell, *Engineering Optimization*, Wiley, New York, 1983.**
- **K. Deb, *Optimization for Engineering Design: Algorithms and Examples*, Prentice hall of India, New Delhi, 1995 (Excellent text but at a more elementary level, ME oriented).**
- **A. E. Bryson and Y.-C. Ho, *Applied Optimal Control*, Hemisphere, New York, 1975.**



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Process Control (Theory and Lab) **Textbooks**

B. W. Bequette, *Process Dynamics--Modeling, Analysis and Simulation*, Prentice Hall, Englewood Cliffs, NJ, 1998.

W. L. Luyben, *Process Modeling, Simulation and Control for Chemical Engineers*, 2nd Ed., McGraw Hill, 1990.

B. A. Ogunnaike and W. H. Ray, *Process Dynamics, Modeling and Control*, Oxford University Press, UK, 1994.

BASICS OF INSTRUMENTATION, PROCESS DYNAMIC AND CONTROL (6)

Feedback Control Loop–The Five Elements
Closed Loop Dynamics
Terminologies and Symbols

CONVENTIONAL CONTROL DESIGN (6)

Degrees of Freedom and Control
Single Loop Control
PID Control Algorithms
Tuning of PID Controllers

INTRODUCTION TO MODERN CONTROL ALGORITHMS (9)

Multi-variable Control and Controller Design
Model Predictive Control; IMC, DMC

Control Design for Non-Linear Systems

Concepts of Robust Control

Plant-wide Control

CONTROL HARDWARE (6)

Measurement of Process Parameters

Level, Temperature, Pressure, Composition,

Measuring Instruments and Their Selection,

Data Sheets–Performance Related Parameters

for Instrumentation

Control Loop Hardware

Transmitters, Transducers, Pneumatic System,

Hydraulic System, Electronic System

Final Control Elements

Control Valves–Types, Selection and Sizing,

Inherent and Installed Characteristics,

Dynamic Behavior, Actuators

CONTROL PRACTICE–GENERIC CASE STUDIES (12)

Centrifugal Compressor/Steam Turbine Control

Fired Heaters/Boiler Control

Distillation Column Control (CDU also)

Process Shutdown and Emergency Shutdown Systems

Reactor Control

Catalytic Packed Bed Reactors

Solution Polymerization

FCCU Control

OVERVIEW OF DCS AND SCADA (3)

**Definition, Application and Architecture,
Performance Specification**

P&IDs AND CONTROL (3)

**Read a Simple P&ID, Identify Control Loop Details,
Read and Interpret a Detailed P&ID, Case Studies
Specific to Hydrocarbon Industry**

LAB COMPONENT

ASPEN: Introduction to ASPEN, Process Simulation in ASPEN Hysys/Plus, Petroleum Refinery Simulation in ASPEN Hysys/Plus, User Defined Functions in ASPEN Hysys/Plus

MATLAB: Introduction to MATLAB, Simulation of Separation Processes, Reactors and Entire Plants in MATLAB



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Process Design, Simulation and Flow Sheeting

COURSE DESCRIPTION

Conceptual Design, Process Synthesis and Design Alternatives (2)

Design under Uncertainty, Design under Safety (9)

Plant Location and Plant Layout (6)



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Definition and Objectives of Flow Diagrams:

**Purpose of Process Flow Diagram (PFD),
Piping & Instrumentation Diagram (P&ID) (4)**

**Development of PFD: Features of Process
Simulation Software, Contents of PFD,
Evolution of PFD from Simulation Results (4)**

**Generic Symbology and Numbering Systems:
Symbols: Equipment, Piping, Valve, Specialty
Items, Control Valves, other**



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Instrument Hardware, Numbering, Tags and Notations: Flow Directions, Origins of Lines, Special Notes (4)

Understanding and Developing P&ID:

Guidelines on Steps in Evolving a P&ID, Development of a Simple Basic P& ID, Piping Specification and Line Designation Valves – Type and Application, Instruments-- Development of Control Loops, Need and Location of Measuring Depiction of DCS and



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RTU in P&ID, Incorporation of Miscellaneous Information in P&ID–Slops, Elevations, Introduction to PDS: Software for making 2-D and 3-D Layouts, etc. (4)

Thermodynamic and Physical Properties Calculation Facility (3)

Methods of Solution of the Model Equations:

Sequential Modular and Simultaneous Equation-Solving Approaches, Recycle



Calculations, Partitioning and Tearing of Algorithms, Mathematical Tools (2)

Introduction to Commercial Simulators (ASPEN PLUS, HYSYS, etc.), their Architecture, Utility and Limitations (3)

Text books

- i) G. Towler and R. K. Sinnott, *Chemical Engineering Design*, Elsevier, Oxford, UK, 2???**



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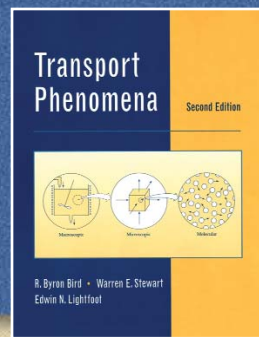
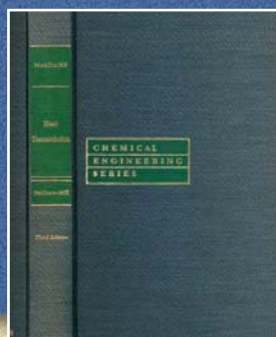
S. Thakore and B. Bhatt, *Introduction to Process Engineering Design*, Tata McGraw Hill, New Delhi, India, 2008.

W. D. Seider, J. D. Seader, D. R. Levin and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis and Design*, 3rd Ed.; Wiley, New York, 2009.

B. V. Babu, *Process Plant Simulation*, Oxford University Press, New Delhi, 2004.

THANK YOU

30 Authors and Their Groundbreaking Chemical Engineering Books



The literature of chemical engineering has defined the discipline, with an impact as powerful as any of the profession's engineering accomplishments. The authors of these books have created a major part of the heritage and shared experience of all chemical engineers.

AIChE's Centennial Celebration Committee has identified a selection of authors who have given these important chemical engineering books to the profession.

R. BYRON BIRD
WARREN E. STEWART
EDWIN N. LIGHTFOOT



From left, Bird, Stewart and Lightfoot in 2001, with leather-bound 2nd Editions — and 62nd printings — of *Transport Phenomena*.

TRANSPORT PHENOMENA

Publisher: Wiley
First edition: 1960
Latest edition: 2008 (2nd- Revised; 62 1st-edition printings between 1960 and 2001)

DONALD R. COUGHANOWR
PROCESS SYSTEMS ANALYSIS AND CONTROL (with Lowell Koppel)
Publisher: McGraw-Hill
First edition: 1965
Latest edition: 2008 (3rd)

RICHARD M. FELDER
RONALD W. ROUSSEAU



Richard Felder and Ronald Rousseau

ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES
Publisher: Wiley
First edition: 1978
Latest edition: 2000 (3rd)

H. SCOTT FOGLER



ELEMENTS OF CHEMICAL REACTION ENGINEERING
Publisher: Prentice Hall
First edition: 1986
Latest edition: 2005 (4th)

PHILIP H. GROGGINS*
UNIT PROCESSES IN ORGANIC SYNTHESIS

Publisher: McGraw-Hill
First edition: 1935
Latest edition: 1952 (4th)

DAVID M. HIMMELBLAU
BASIC PRINCIPLES AND CALCULATIONS



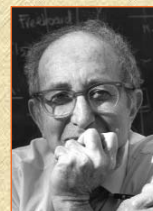
IN CHEMICAL ENGINEERING
Publisher: Prentice Hall
First edition: 1962
Latest edition: 2003 (7th)

OLAF A. HOUGEN*
KENNETH WATSON*
CHEMICAL PROCESS PRINCIPLES, VOL. 1: MATERIAL AND ENERGY BALANCES
Publisher: Wiley
Published: 1943

CHEMICAL PROCESS PRINCIPLES, VOL. 2: THERMODYNAMICS
Publisher: Wiley, Chapman & Hall
First edition: 1947
Latest printing: 1949 (5th)

CHEMICAL PROCESS PRINCIPLES, VOL. 3: KINETICS & CATALYSIS
Publisher: Wiley
First edition: 1947
Latest printing: 1949 (3rd)

OCTAVE LEVENSPIEL



CHEMICAL REACTION ENGINEERING
Publisher: Wiley
First edition: 1962
Latest edition: 1998 (3rd)

WARREN K. LEWIS*



INDUSTRIAL STOICHIOMETRY (with Arthur Radasch)
Publisher: McGraw-Hill
First edition: 1923
Latest edition: 1937 (3rd; with Edward R. Gilliland as co-author)

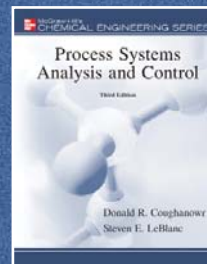
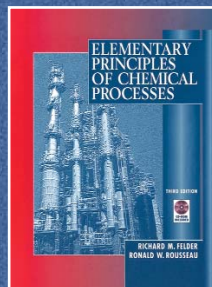
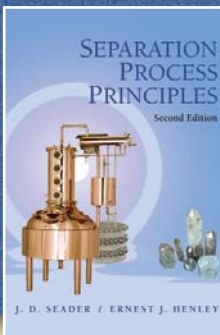
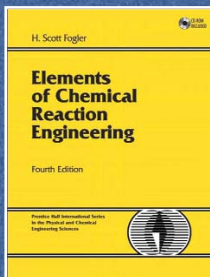
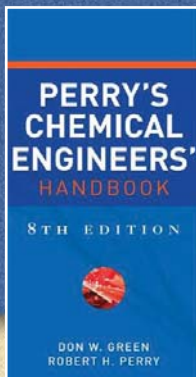
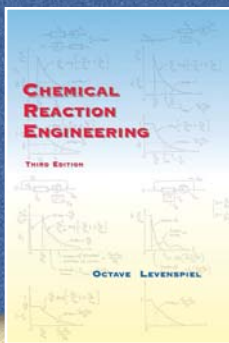
WARREN K. LEWIS*
WILLIAM H. McADAMS*
WILLIAM H. WALKER*



PRINCIPLES OF CHEMICAL ENGINEERING
Publisher: McGraw-Hill
First edition: 1923
Latest edition: 1937 (3rd; with Edward R. Gilliland as co-author)

Portrait of William H. Walker, William Haynes Portrait Collection, Courtesy of Chemical Heritage Foundation Collections.

WILLIAM H. McADAMS*
HEAT TRANSMISSION
Publisher: McGraw-Hill Series in Chemical Engineering
First edition: 1933
Latest edition: 1954 (3rd)



WARREN McCABE*

ELEMENTS OF CHEMICAL ENGINEERING

(with Walter L. Badger)
Publisher: McGraw-Hill
First edition: 1931
Latest edition: 1936 (2nd)

UNIT OPERATIONS OF CHEMICAL ENGINEERING (with Julian Smith and Peter Harriott)

Publisher: McGraw-Hill
First edition: 1956
Latest edition: 2004 (7th)

DONALD F. OTHMER*



KIRK-OTHMER ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY (with Raymond Kirk)
Publisher: Wiley Blackwell
First edition: 1947
Latest edition: 2001 (5th)

Donald Othmer, Othmer Collection, Courtesy of Chemical Heritage Foundation Collections.

JOHN H. PERRY*

CHEMICAL ENGINEERS' HANDBOOK (AKA "PERRY'S HANDBOOK")

(with Robert H. Perry)
Publisher: McGraw-Hill
First edition: 1934
Latest edition: 2007 (8th)

CLARK ROBINSON*

ELEMENTS OF FRACTIONAL DISTILLATION

Publisher: McGraw-Hill Books / Blatter Press
First edition: 1922
Latest edition: 1939 (3rd)

STANLEY I. SANDLER



CHEMICAL, BIOCHEMICAL, AND ENGINEERING THERMODYNAMICS
Publisher: Wiley
First edition: 1977
Latest edition: 2006 (4th)

J. D. (BOB) SEADER



SEPARATION PROCESS PRINCIPLES

(with Ernest J. Henley)
Publisher: Wiley
First edition: 1998
Latest edition: 2005 (2nd)

WARREN D. SEIDER



INTRODUCTION TO CHEMICAL ENGINEERING AND COMPUTER CALCULATIONS

(with Alan L. Myers)
Publisher: Prentice Hall
Published: 1976

THOMAS SHERWOOD*

ABSORPTION AND EXTRACTION

Publisher: McGraw-Hill
First edition: 1937
Latest edition: 1952 (2nd; co-authored with Robert L. Pigford)

APPLIED MATHEMATICS IN CHEMICAL ENGINEERING (with Charles Reed)

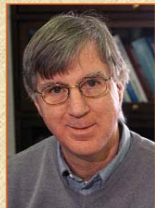
Publisher: McGraw-Hill
First edition: 1939
Latest edition: 1957 (4th; with Harold S. Mickley as senior author)

NORRIS SHREVE*

CHEMICAL PROCESS INDUSTRIES

Publisher: McGraw-Hill Professional
First edition: 1945
Latest edition: 1991 (5th)

MICHAEL SHULER



BIOPROCESS ENGINEERING: BASIC CONCEPTS

(with Fikret Kargi)
Publisher: Prentice Hall
First edition: 1992
Latest edition: 2002 (2nd)

JOE MAUK SMITH*

INTRODUCTION TO CHEMICAL ENGINEERING THERMODYNAMICS

Publisher: McGraw-Hill
First edition: 1949
Latest edition: 2001 (6th)
(Hendrick C. van Ness became co-author with the 1959 second edition)

ROBERT E. TREYBAL*

MASS TRANSFER OPERATIONS

Publisher: McGraw-Hill
First edition: 1955
Latest edition: 1980 (3rd)

FRANK VILBRANDT*

CHEMICAL ENGINEERING PLANT DESIGN

Publisher: McGraw-Hill
First edition: 1934
Latest edition: 1959 (4th)

RALPH T. YANG



GAS SEPARATION BY ADSORPTION PROCESSES

Publisher: Imperial College Press
Published: 1986
Latest reprint: 1997

FRED ZENZ

FLUIDIZATION AND FLUID-PARTICLE SYSTEMS (with Donald F. Othmer)

Publisher: Reinhold
Published: 1960

**Indicates Foundation Age recognitions (i.e., engineers who had attained the equivalent of AIChE Senior Member status during or prior to World War II).*

First editions of many of these groundbreaking books will be on display at the Chemical Heritage Foundation's Othmer Library of Chemical History — during AIChE's 2008 Centennial Annual Meeting in Philadelphia (see pg. 23 for information).

More for your reading list:
Learn more about chemical engineering highlights of the past 100 years at AIChE's Centennial Web site: www.aiche.org/100/