

화학공정설계에서의 Simulation의 응용

정 연 수
한국과학기술연구원
화학공정연구실

Process Flowsheeting

the use of computer aids to perform steady-state heat and mass balancing, sizing, and costing calculations for a chemical process

Process Design

1. Synthesis

- developing a flowsheet structure

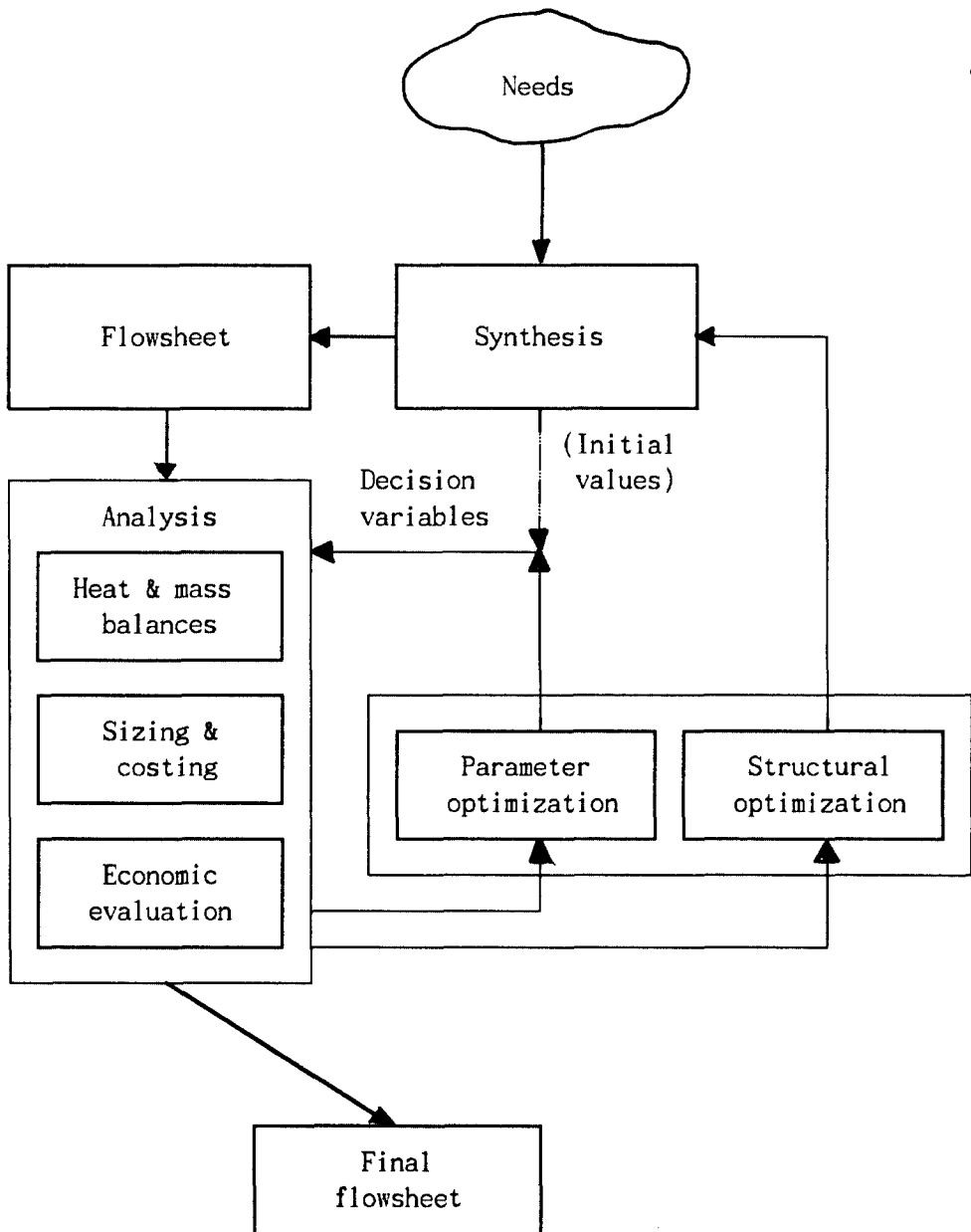
2. Analysis

- solving heat and mass balance
- sizing and costing equipments
- evaluating the worth of flowsheet

3. Optimization

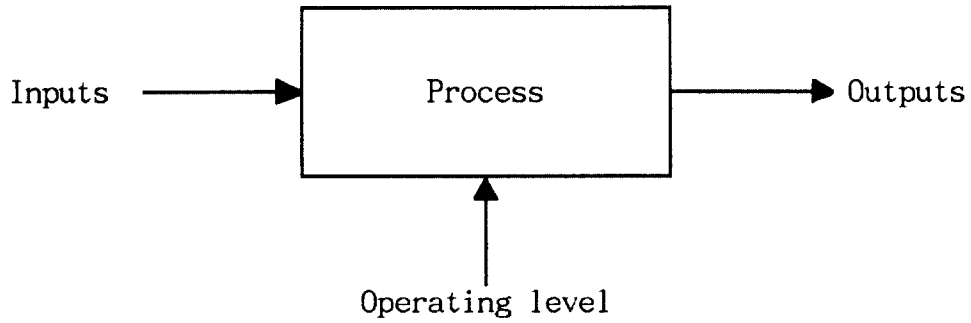
- parameter optimization
- structural optimization

Process Design

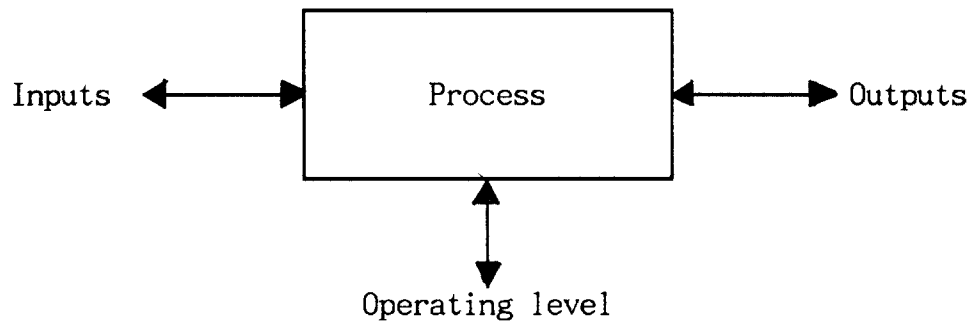


Design Calculations

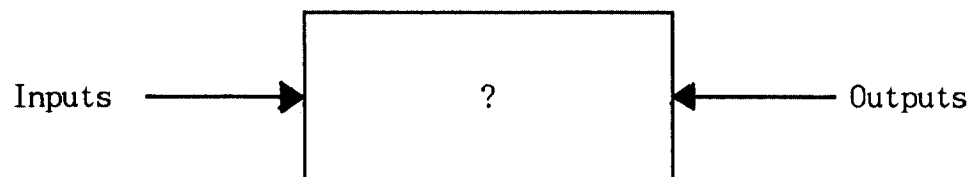
1. Simulation



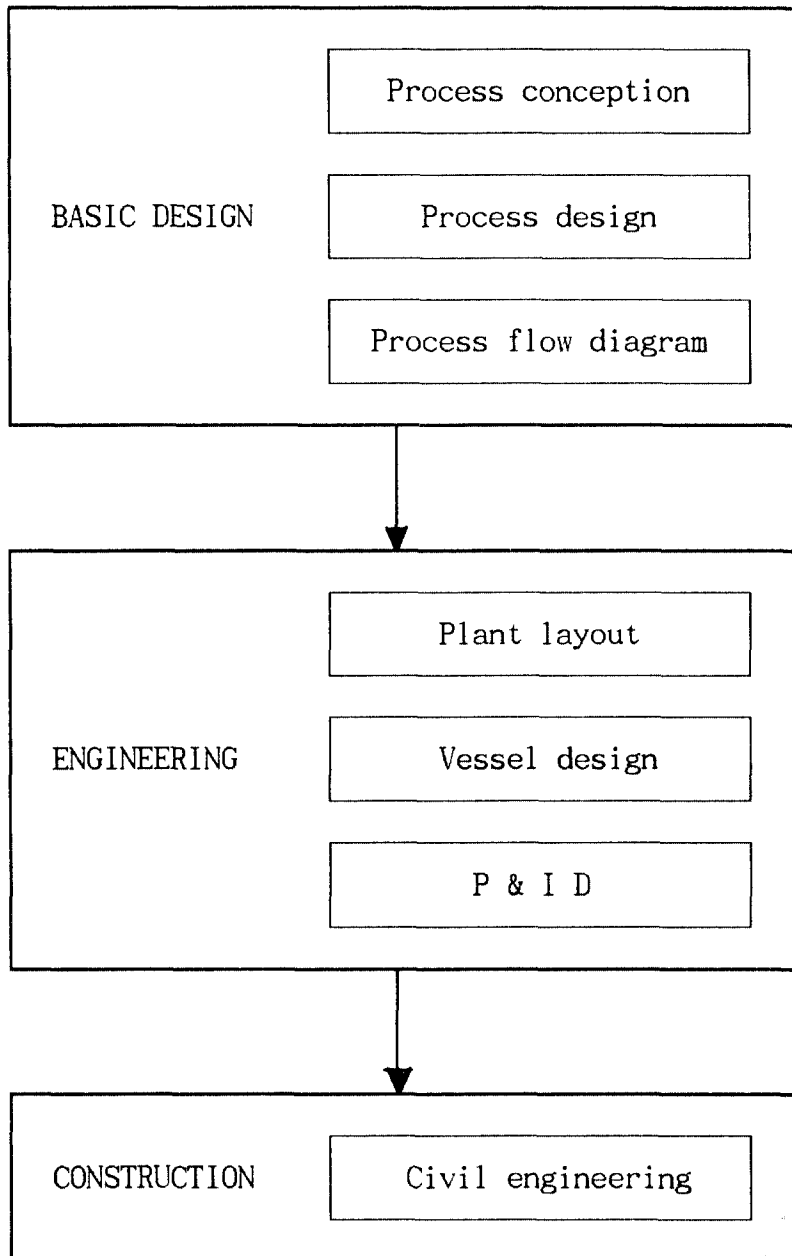
2. Analysis



3. Synthesis



The Total Plant Design Project



Advantages for Flowsheeting System

- . aid in flowsheet and data input
- . consistent solution for repeated calculations

Disadvantages

- . no answer for an ill-suited or
an ill-defined system

Human's Role in Flowsheeting

Flowsheeting systems are man-made and as such contain 'bugs' which the user may be unaware of, or all-too-aware of.

And, these 'bugs' may lead to incorrect answers or no answers.

History of Process Flowsheeting

- 1955 ~ 1959 :

- . primitive computer technology
- . no language such as FORTRAN
- . design calculations only for single units
- . Kelloggs - Flexible Flowsheet Program

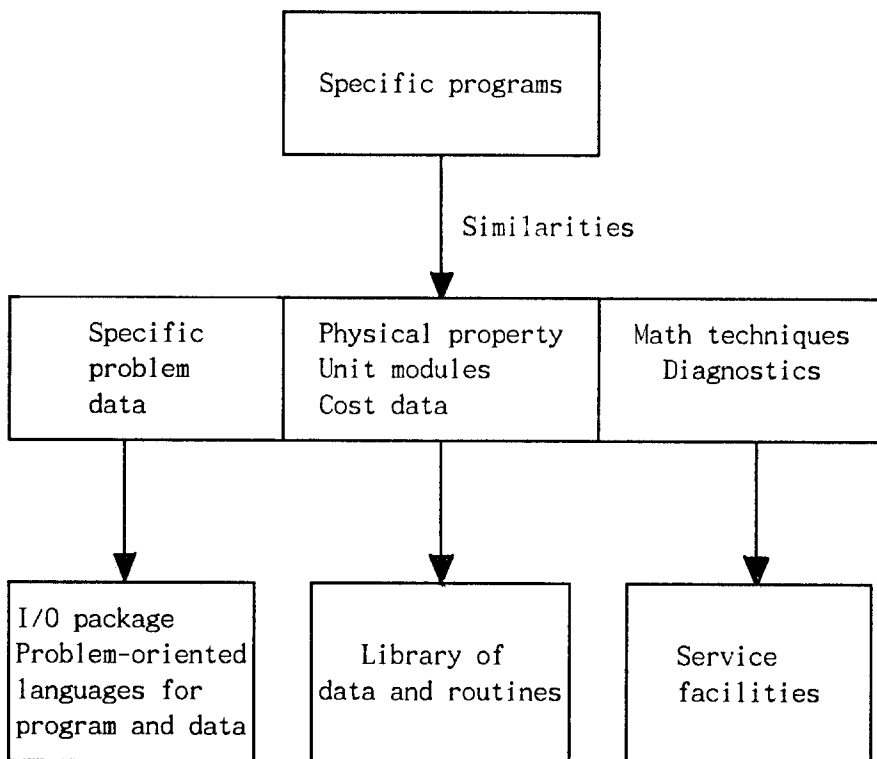
- 1960 ~ 1964

- . several simulators
- . high level language ~ FORTRAN
- . modular fashion
- . rigorous physical property calculations

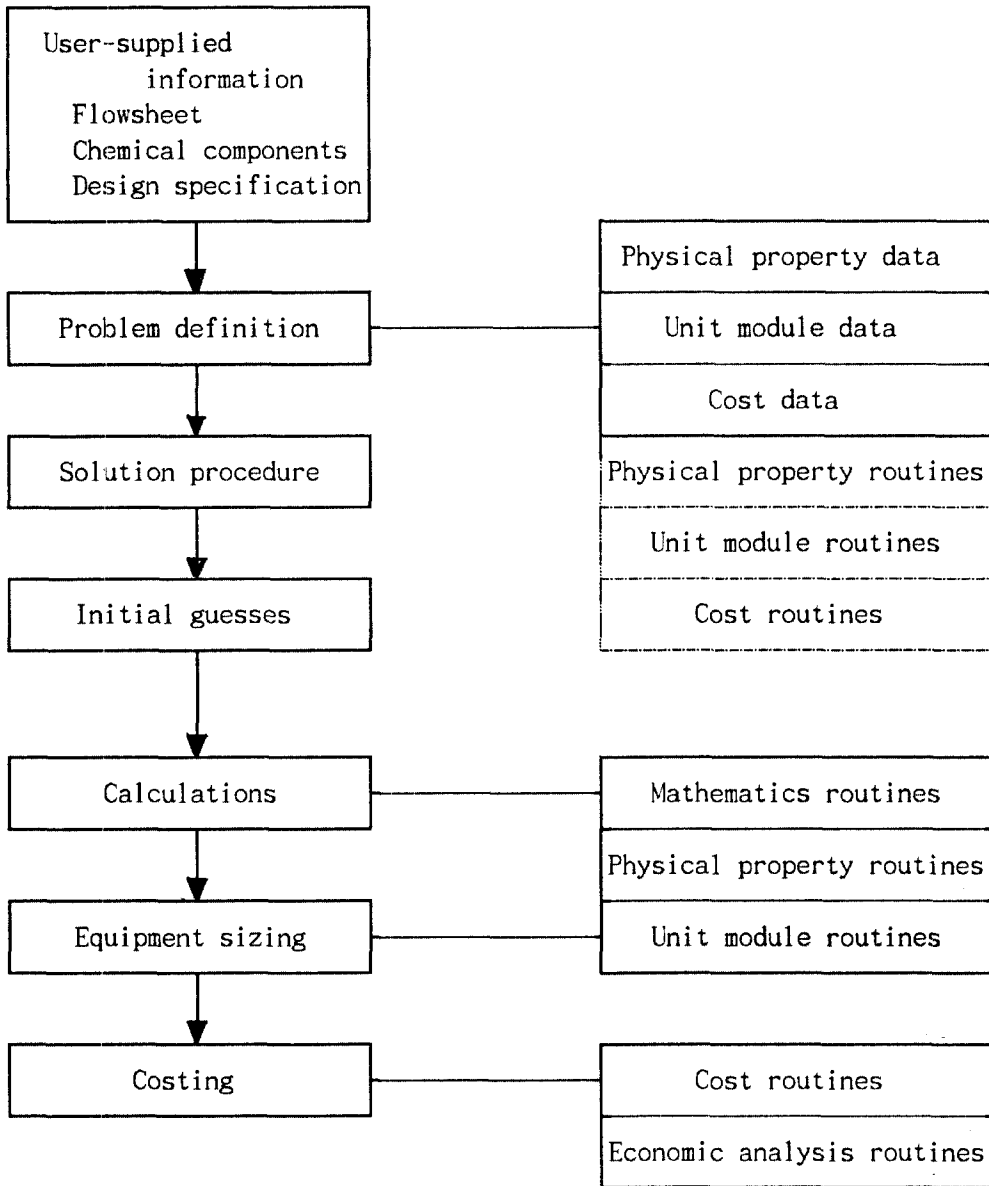
- 1965 ~ 1969

- . proving and weeding-out time
- . large scale computer power available
- . prove flowsheeting programs useful
- . fast, reliable enough to be practical
for even moderately large process
- . special purpose program

Motivation for Development of General Purpose Flowsheeting Programs



Developing a Simulation Model



Simulation Methods

1. Sequential modular approach

- . calculate the output stream values of a unit given its input stream values and the unit parameter values
- . rigid structure, straight solution algorithm
- . no good for general design specifications

2. Equation-oriented approach

- . flowsheet = a collection of simultaneous nonlinear equations
- . gather full set of equations and solve it
- . flexible structure
- . complex solution algorithm
- . good for any kind of design calculations

Commercially Available Simulators

1. ASPEN PLUS

- . Sequential modular approach
- . steady-state simulation only
- . one of the most popular packages in process flowsheeting

2. SpeedUp

- . Equation-oriented approach
- . steady-state and dynamic simulation
- . unique dynamic simulator commercially available