Process Synthesis and Design Methodology

(Adapted from several Process Synthesis Lectures)

Process Design
Course Objectives

- By the end of this course, you will be able to
  - Design and size unit operations to accomplish a specific process step;
  - Integrate and arrange process units according to industrially accepted standards, hazards review procedures, and federal regulations to achieve an overall processing objective;
  - Build & simulate a process in ASPEN Plus®;
  - Estimate capital costs of unit ops, construction costs, product processing costs (raw materials, labor, and utilities), and process profitability; and
  - Optimize a process based on profit.

Engineering

- **Purpose** - To create new material wealth by chemical or biological transformation and/or separation of materials.

- **Design** – The creative activity whereby we generate ideas and translate them into equipment and processes for producing new materials or for significantly upgrading the value of existing materials.

Synthesis & Analysis

- #1 design problem → highly under-specified
- assumptions are absolutely necessary during the synthesis stage
  - Process units to use must be selected
  - Interconnection of process units must be selected
  - Operating conditions must be specified
- Synthesis is difficult because there are 10^4 - 10^9 unique ways of accomplishing the same goal. Hence, design tasks are very *open-ended*.

Synthesis & Analysis

- Design engineer desires to find the lowest alternative of the 10^4-10^9 possibilities, while still considering such intangibles as:
  - safety & environmental contraints
  - simplicity of start-up/operation/shut-down
- Use "rules-of-thumb" or *heuristics* to eliminate some alternatives from consideration, and to design a number of alternatives for comparison.
- More rigorous design calculations applied when a potentially profitable alternative is found.

Engineering Methodology

- Engineering Method – a solution strategy following successive refinements in the design, maintaining focus on the overall problem.
- The Engineering Method vs. the art of painting

Painting

- Starts with a pencil sketch, including only the most significant details of the painting.

Engineering Design

- Start with a pencil sketch, including only most significant details of processing plant.
- Seek most expensive parts of the process and significant economic trade-offs.

Painting

- Evaluate the preliminary drawing, and make modifications, using only gross outlines for subjects of the picture.

Engineering Design

- Evaluate initial guess of process, and generate potential alternatives that may lead to improvements.
- In such, generate a reasonable process design before adding significant detail.

Painting

- Adds color, shading and the details of the various gross outlines of objects.
- Major modifications made if warranted.

Engineering Design

- Use rigourous design & costing procedures for the most expensive equipment items.
- Improve material & energy balances via rigor.
- Add small, less expensive items necessary for operation but having little impact on plant cost.

Engineering Method

- A piece of artwork is finished when additional effort reaches a point of diminishing returns.
- i.e., little value is added from much additional effort.

Engineering Method

- There is never a single way to paint a *great* “Madonna and Child” or a landscape.
- Different process routes can be used to produce the same chemical or material at similar costs.

Engineering Method

- It is an “art” of judgment to know what level of detail to include in the various stages of developing a painting or a process.

Levels of Engineering Design

- Based on cost accuracy:
  - Order-of-Magnitude or Ratio Estimate
    - Based on similar previous cost data; ±40%
  - Study or Factored Estimate
    - Based on knowledge of major equipment items; ±25%
  - Preliminary, Budget Authorization, or Scope Estimate
    - Based on sufficient data to permit budgeting; ±12%
  - Definitive or Project Control Estimate
    - Based on almost complete data, but prior to completion of drawings and specifications; ±6%
  - Detailed or Contractor's Estimate
    - Based on complete engineering drawings, specifications, site surveys; ±3%

Definitions

- expensed engineering
  - engineering work performed in the development stage of a project prior to capital funds being committed (through Scope Estimate).
- capitalized engineering
  - engineering work performed on a project after capital funds are committed to implement the project (Definitive and Detailed Estimates).

Stages of the Design Process

1. Ratio Estimate (feasibility survey)
2. Factored Estimate (conceptual design)
3. Preliminary/Definitive/Detailed Designs
4. Construction
5. Start-up & operations

Cost consequences for design changes increase as the process moves from phases 1 thru 4.

Step 1 - Feasibility Survey

- Gathering of data for quick-estimate, including:
  - availability of suppliers, specifications and cost of raw materials
  - thermodynamic/kinetic data for reactions (including by-product reactions)
  - existing facilities & equipment available
  - facilities & equipment needed
  - corrosion data
  - safety requirements
  - chemical and physical properties of all reactants, products & intermediates
  - shipping (DOT regulations)
  - patent & licensing restrictions

Step 2 - Conceptual Design

- *process development*
- flowsheet definition
- cost estimate
- technology package
  - simulation
  - PFD
  - spec sheets
  - line lists
  - equipment lists
- environmental & safety review

Process Development

- The collection of additional reaction and physical property data (after preliminary design) to increase the accuracy of the quick-estimate generated from the feasibility survey.
- May include lab research and/or pilot operations as necessary to obtain missing information.
- Semi-works data is collected to obtain design data, including accurate material and energy balances, an understanding of the effects of various process conditions and corrosion data.

Step 3 – Process Design

- equipment design
- piping layout
- plot plan
- instrument loop diagrams
- safety review
- environmental permitting
- Stages
  - preliminary, detailed, firm

Preliminary Design

- Rough design, calculations kept at a minimum
- Costs likely based on *factored estimates* and design is based on approximate methods.
- Used as a tool to determine whether continued development is justified.
- Preliminary design is a *workable* process for the production of desired product.
- Includes simplified flow diagram, rough material balance from which direct raw materials costs are calculated, specs for each process unit, utility estimates & labor requirements.

Preliminary Design

- From this design, capital investment & product cost can be determined.
- These documents are continually modified as piloting reveals new information about the process, often suggesting changes to the design.

Preliminary Design

- Once development is complete, preliminary designs used to prepare technology package, from which detailed-estimates & designs are prepared. Package includes:
  - manufacturing process
  - material & energy balances
  - temperature & pressure ranges
  - materials of construction
  - raw material and product specs
  - utilities requirements
  - rates, yields, cycle times
  - plant site and plot plan

Definitive/Detailed Designs

- Definitive Design
  - Includes more details than the quick-estimate, though not detailed equipment designs & specs are, nor detailed P&IDs.
  - Transition from Preliminary to Detailed Designs tied to a financial commitment to proceed.
- Detailed Design
  - Includes detailed P&IDs, plot plans, pipe layouts & wire diagrams, design specifications for each component, costs for equipment and raw materials based on quoted prices from vendors.

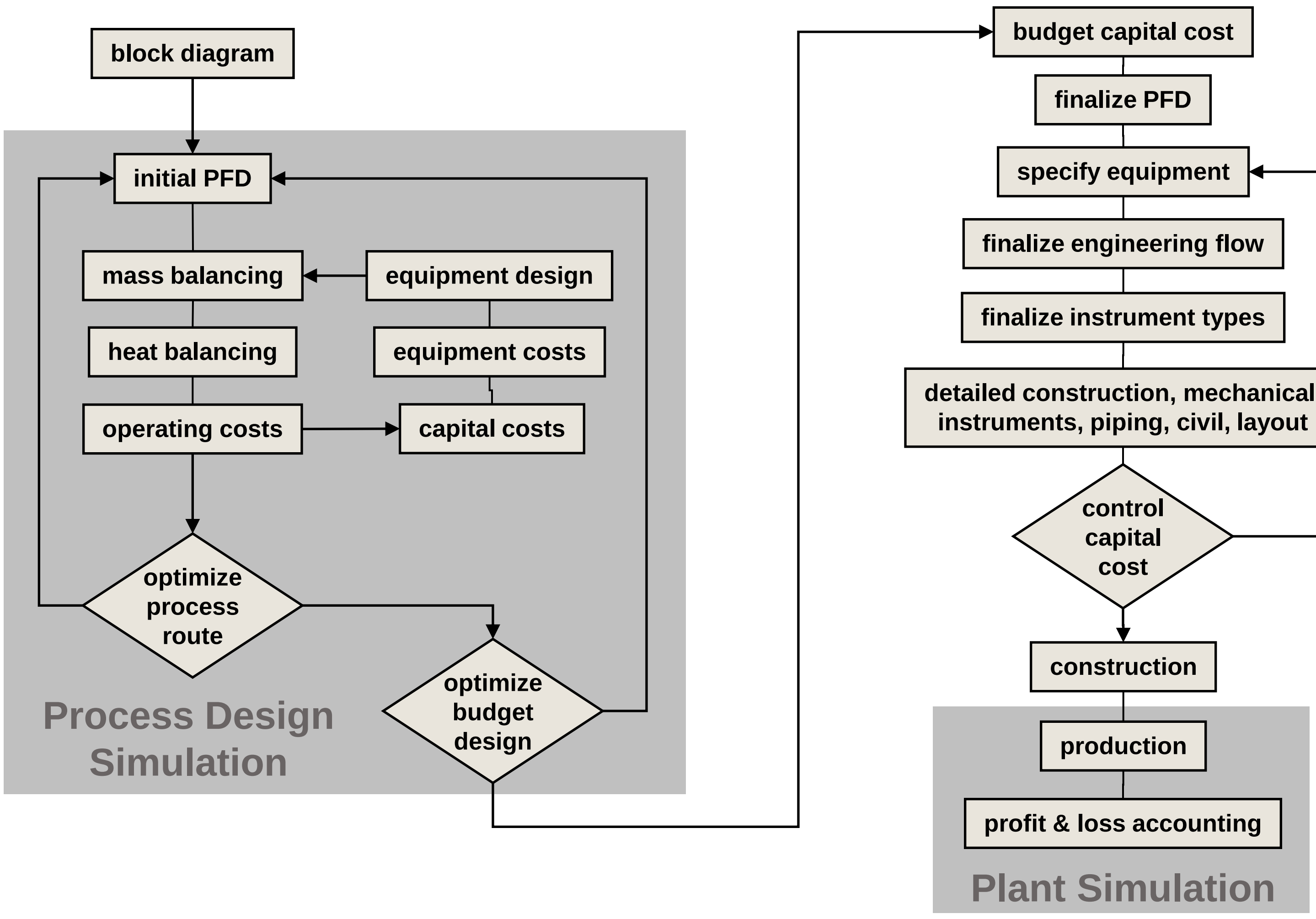
Step 4 - Construction

- site prep
- vessel fabrication
- facilities erection
- piping & conduit/wiring
- control loop checkout
- safety review
- operator training

Step 5 – Start-up & Operations

- pressure testing
- flow testing / instrument calibration
- closed loop operation
- startup safety review
- startup
- operation
- environmental monitoring

Use of Computer Simulation in the Process Design Process



Decision Hierarchy

- Input data and Batch vs. continuous process
- Input-output structure of flowsheet
  - Raw materials typically account for 33-85% of product cost; thus, overall material balances are a dominant design factor.
- Recycle structure of the flowsheet
  - Allows evaluation of separation needs
- Separation System structure
  - Vapor recovery, liquid recovery
- Heat integration