

Plant Design CHEN 451

Engineering design of new chemical and petrochemical plants and the expansion or revision of existing ones require the use of engineering principles and theories combined with a practical realization of the limits imposed by industrial conditions. A successful engineer needs more than a knowledge and understanding of the fundamental sciences and the related engineering subjects such as thermodynamics, reaction kinetics, and computer technology. The engineer must also have the ability to apply this knowledge to practical situations for the purpose of accomplishing something that will be beneficial to society. There are three parameters that must be defined namely:

1-Design: design is a creative activity and is defined as the synthesis, the putting together of ideas to achieve a desired purpose. Also it can be defined as the creation of manufacturing process to fulfill a particular need. The need may be public need or commercial opportunity.

2-Process Design: process design establishes the sequence of chemical and physical operations; operating conditions; the duties, major specifications, and materials of construction (where critical) of all process equipment (as distinguished from utilities and building auxiliaries); the general arrangement of equipment needed to ensure proper functioning of the plant; line sizes; and principal instrumentation. The process design is summarized by a process flowsheet.

Process design is intended to include:

1. Flowsheet development.
2. Process material and heat balances.
3. Auxiliary services material and heat balances (utilities requirements).
4. Chemical engineering performance design for specific items of equipments required for a flowsheet.
5. Instrumentation as related to process performance.
6. Preparation of specifications (specification sheets) in proper form for use by the project team as well as for the purchasing function.
7. Evaluation of bids and recommendation of qualified vendor.

3-Plant Design: includes items related directly to the complete plant, such as plant layout, general service facilities, and plant location.

Design Development Stages:

The stages in the development of a design, from the initial identification of the objectives to the final design are shown in Fig.(1).

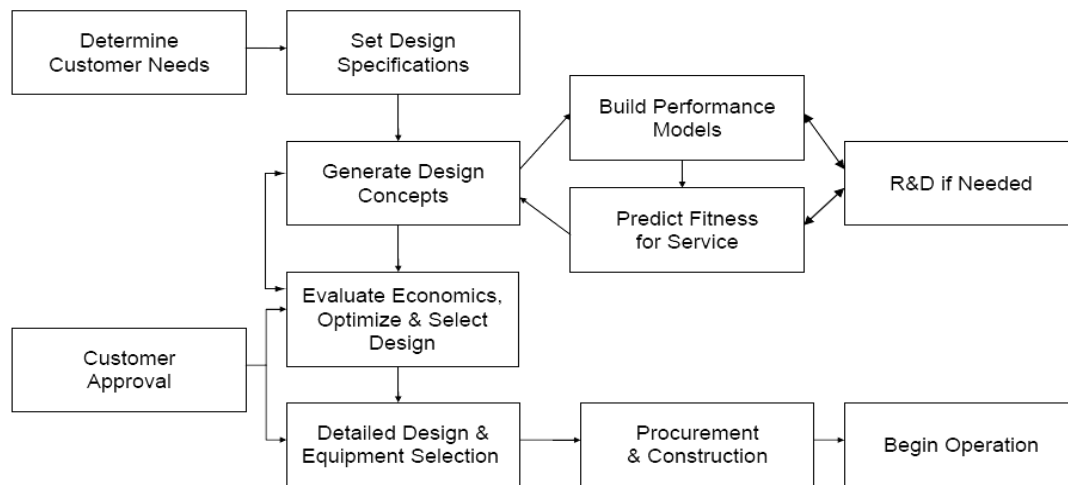


Fig.(1) The design process.

(I) The Design Objectives (The Need)

Engineering projects can be divided into three types:

- A. New process development.
- B. New production capacity to meet growing sales.
- C. Modification and addition to existing plant.

In the design of a chemical process the need is the public need for the product, the commercial opportunity as foreseen by the sales and marketing organization.

(II) Setting The Design Basis (Data Collection)

The most important step in starting a process design is translating the customer need into a design basis. The design basis is a more precise statement of the problem that is to be solved. It will normally include the production rate and purity specifications of the main product, together with information on constraints that will influence the design, such as:

1. Information on possible processes and the system of units to be used.
2. The national, local or company design codes that must be followed.
3. Details of raw materials that are available.
4. Information on potential sites where the plant might be located, including climate data, seismic conditions, and infrastructure availability.
5. Information on the conditions, availability, and price of utility services such as fuel (gas), steam, cooling water, process air, process water, and electricity, that will be needed to run the process.

(III) Generation of Possible Design Concepts (Solutions)

It is the creative part of the design process. This part is concerned with the generation of possible solutions for analysis, evaluation, and selection (ways of meeting objective problems).

Source of solutions:

- a- Past experiences.
- b- Tried and tested methods.

(IV) Build Performance Model and Fitness Testing

When design alternatives are suggested, they must be tested for fitness of purpose. In other words, the design engineer must determine how well each design concept meets the identified need. In the field of chemical engineering, it is usually prohibitively expensive to build several designs to find out which one works best (a practice known as “**prototyping**” which is common in other engineering disciplines). Instead, the design engineer builds a mathematical model of the process, usually in the form of computer simulations of the process, reactors, and other key equipment. In some cases, the performance model may include a pilot plant or other facility for predicting plant performance and collecting the necessary design data.

The design engineer must assemble all of the information needed to model the process so as to predict its performance against the identified objectives. For process design this will include information on possible processes, equipment performance, and physical property data

If the necessary design data or models do not exist, then research and development work is needed to collect the data and build new models. Once the data has been collected and a working model of the process has been established, then the design engineer can begin to determine equipment sizes and costs. At this stage it will become obvious that some designs are uneconomical and they can be rejected without further analysis. From this step a few candidate designs that meet the customer objective are identified.

(V) Economic Evaluation, Optimization, and Selection

Once the designer has identified a few candidate designs that meet the customer objective, then the process of design selection can begin. The primary criterion for design selection is usually economic performance, although factors such as safety and environmental impact may also play a strong role. The economic evaluation usually entails analyzing the capital and operating costs of the process to determine the return on investment (R.O.I).

The economic analysis of the product or process can also be used to **optimize the design**. Every design will have several possible variants that make economic sense under certain conditions. For example, the extent of process heat recovery is a tradeoff between the cost of energy and the cost of heat exchangers (usually expressed as a cost of heat exchange area). In regions where energy costs

are high, designs that use a lot of heat exchange surface to maximize recovery of waste heat for reuse in the process will be attractive. In regions where energy costs are low, it may be more economical to burn more fuel and reduce the capital cost of the plant.

When all of the candidate designs have been optimized, the best design can be selected. Very often, the design engineer will find that several designs have very close economic performance, in which case the **safest design** or that which has the best commercial track record will be chosen. At the selection stage an experienced engineer will also look carefully at the candidate designs to make sure that they are safe, operable, and reliable, and to ensure that no significant costs have been overlooked.

(VI) Detailed Design and Equipment Selection

Here the detailed specifications of equipment such as vessels, exchangers, pumps, and instruments are determined. During the detailed design stage there may still be some changes to the design, and there will certainly be ongoing optimization as a better idea of the project cost structure is developed. The detailed design decisions tend to focus mainly on equipment selection though, rather than on changes to the flowsheet. For example, the design engineer may need to decide whether to use a U-tube or a floating-head exchanger, or whether to use trays or packing for a distillation column.

(VII) Procurement, Construction, and Operation

When the details of the design have been finalized, the equipment can be purchased and the plant can be built. Procurement and construction are usually carried out by an EPC firm (Engineering, Procurement, and Construction) unless the project is very small. Because they work on many different projects each year, the EPC firms are able to place bulk orders for items such as piping, wire, valves, etc., and can use their purchasing power to get discounts on most equipment. The EPC companies also have a great deal of experience in field construction, inspection, testing, and equipment installation. They can therefore normally contract to build a plant for a client cheaper (and usually also quicker) than the client could build it on its own. Finally, once the plant is built and readied for **startup**, it can begin operation. The design engineer will often then be called upon to help resolve any startup issues and teething problems with the new plant.

Design Constraints

When considering possible ways of achieving the objective the designer will be constrained by many factors which are called the design constraints.

Design constraints are divided into two types Fig.(2):

- A. Internal constraints: over which the designer has some control.
- B. External constraints: fixed, invariable.

What is meant by design constraints? What are the different types? Give examples?

What are the main items that should be included in the process design?

Draw a block diagram showing the main steps involved in the development of a design process?

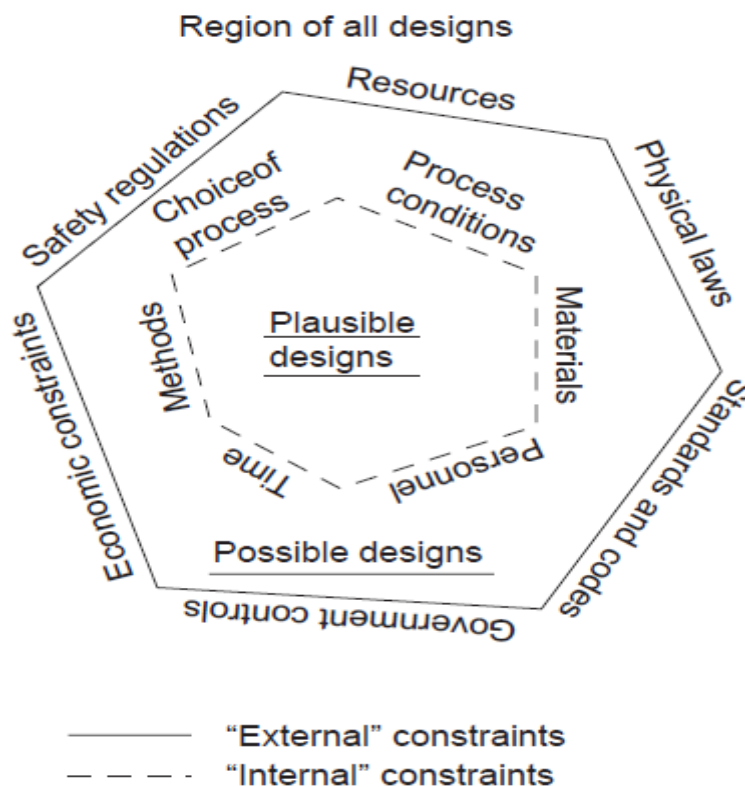


Fig.(2) Design constraints.

Flow-sheeting (special language conveying information)

Process design normally starts with a process scheme (flowsheet). The flowsheet is the key document or road map in process design. It's a diagrammatic model of the process describe the process steps in a proper sequence using symbols to represent the various components (equipment, lines, and control instrumentation) that make up the unit.

The Flow-sheet Importance

- Shows the arrangement of the equipment selected to carry out the process.
- Shows the streams concentrations, flow rates & compositions.
- Shows the operating conditions.
- During plant start up and subsequent operation, the flow sheet from a basis for comparison of operating performance with design. It's also used by operating personnel for the preparation of operating manual and operator training.

Flowsheet Presentation

1- Block diagram

- Represent the process in a simplified form.
- No details involved.
- Don't describe how a given step will be achieved.

When is it used?

- In survey studies.
- Process proposal for packaged steps.
- Talk out a processing idea.

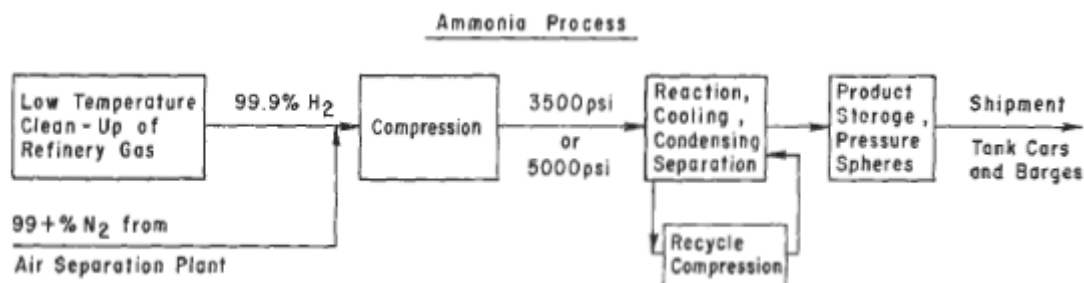


Fig.(3) Block diagram.

2- Pictorial Flow Sheet

The equipments are normally drawn in a stylized pictorial form. For tender documents or company brochures actual scale drawing of the equipment are sometimes used.

Types of pictorial flow-sheets

a) Process Flow Diagram (PFD)

A PFD is a simplified flow diagram of a single process unit, a utility unit, a complete process module. The purpose of a PFD is to provide a preliminary understanding of the process system indicating only the main items of equipment, the main pipelines and the essential instruments, switches and control valves.

A PFD also indicates operating variables, such as mass flow, temperatures and pressures, which are tabulated at various points in the system.

The PFD is a document containing information on:

- Process conditions and physical data of the main process streams.
- Main process equipment with design data.
- Main Process lines.
- Mass (material) balance.
- Heat balance (if applicable).

NOTE: If the PFD doesn't contain any data about the flow rates, it is called a **qualitative flowsheet**, while if the flow rates are involved the PFD is called a **combined flowsheet** in which qualitative information and quantitative data are combined on the basis of one flowsheet.

b) Piping and Instrumentation Diagram (P & ID) (mechanical flow diagram)

A P&ID diagram shows the arrangement of the process equipment, piping, pumps, instruments, valves and other fittings. It should include:

- All process equipment identified by an equipment number.
- All pipes identified by a line size, material code and line number.
- All valves with an identified size and number.
- Fittings.
- All pumps identified by a suitable code number.
- All control loops and instruments.

c) Utility Flowsheet (Process Engineering Utility Flow Diagram (PEUFD))

Used to summarize and detail the interrelationship of utilities such as air, water (various types), steam (various types), heat transfer mediums, process vents and purges, safety relief blow-down,

etc., to the basic process. The amount of detail is often too great to combine on other sheets, so separate sheets are prepared.

The PEUFD is a document containing information on:

- Main distribution or arrangement of each individual utility system, except electrical systems.

PEUFD Function:

A typical process uses utilities such as water, air and electric power. Water may be used either in the process, or for cooling and/or production of steam. Air may also be used in the process or for instrument applications. Electric power of course is typically used at various points in the process and throughout the site.

It is always useful to develop diagrams that show the flow and utilization of each utility. An example of a water balance/utility diagram is shown below.

The PEUFD shall state characteristics and consumption figures of the particular utility concerned, cooling water, fire water, drinking water, steam, plant air, instrument air, fuel oil/gas, inert gas and similar utilities.

d) Process Safeguarding Flow Diagram (PSFD)

The PSFD is a document highlighting information on:

- Types and levels of protection offered by the devices installed and their inter relation to demonstrate the plant's safety.

The P&ID contains all information required for a PSFD; however, the PSFD highlights protection in case of extreme conditions and measures to be taken to safeguard personnel and environment.

Note: In general these schemes will only be made for complex installations like offshore process platforms. For simple applications the information shown on the P&ID is usually sufficient to highlight safety devices and aspects.

- ✓ **What is meant by the following identifications? PFD, P&ID, PEUFD and PSFD**
- ✓ **State the information you can get from the following schemes: PFD, P&ID, PEUFD and PSFD?**

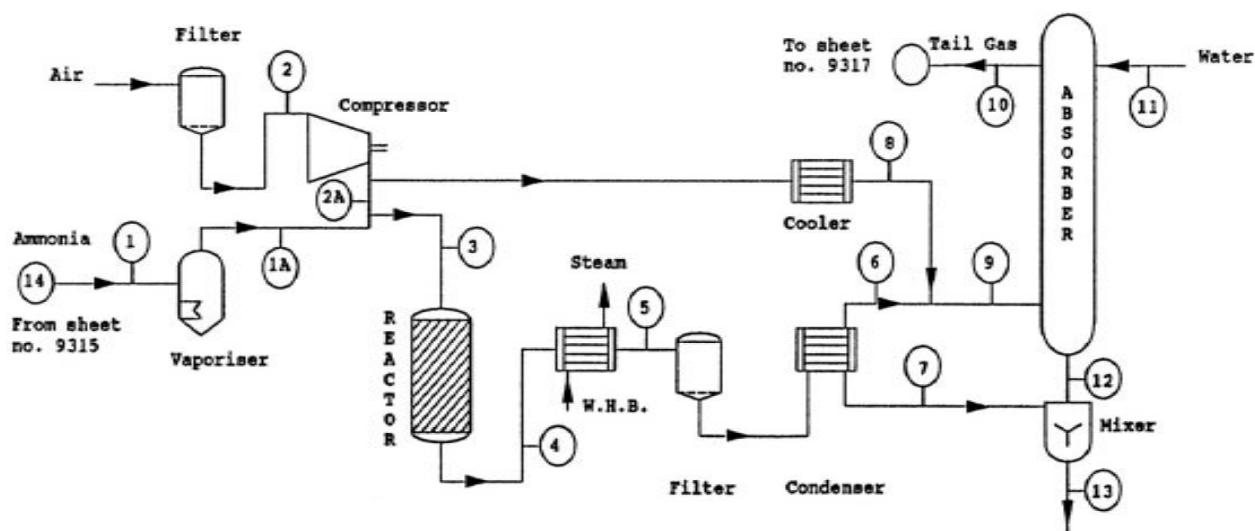


Fig.(4) PFD [Qualitative flow diagram for the manufacture of nitric acid by the ammonia-oxidation process].

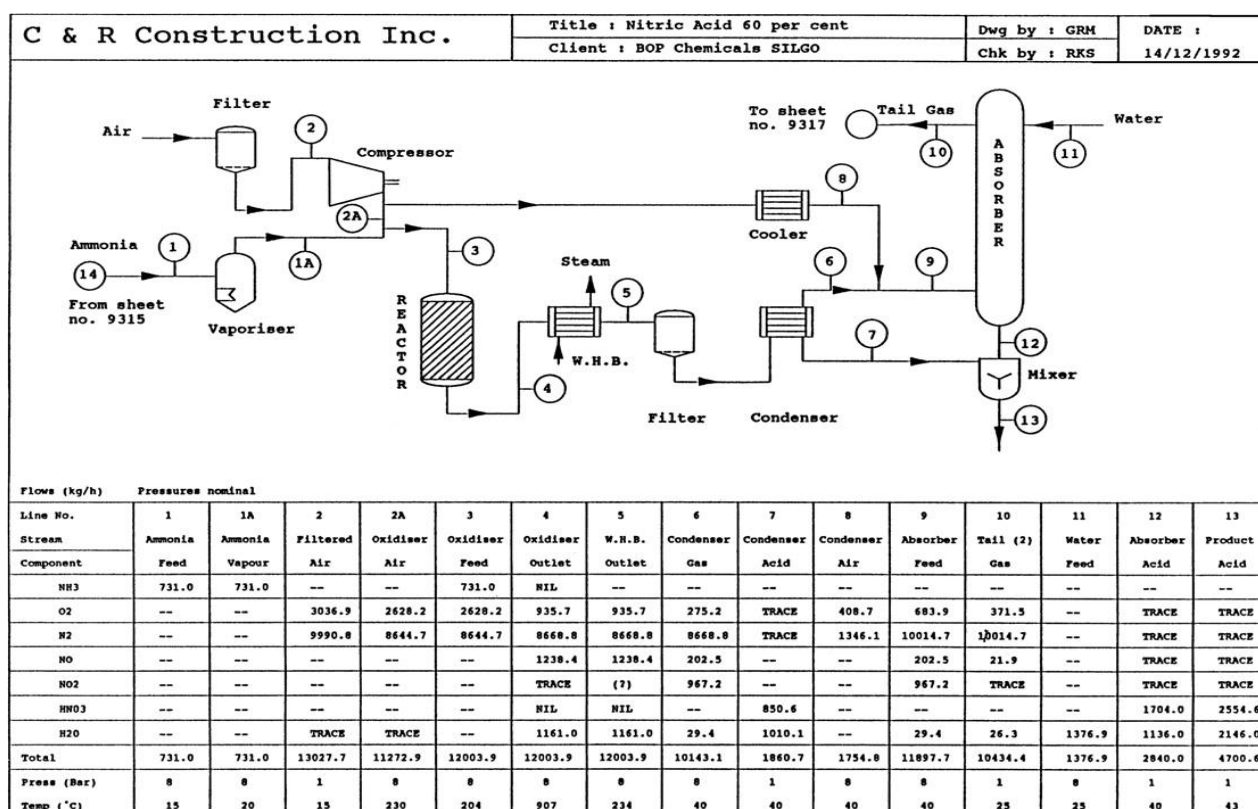


Fig.(5) PFD [Combined flow diagram for the manufacture of nitric acid by the ammonia-oxidation process].

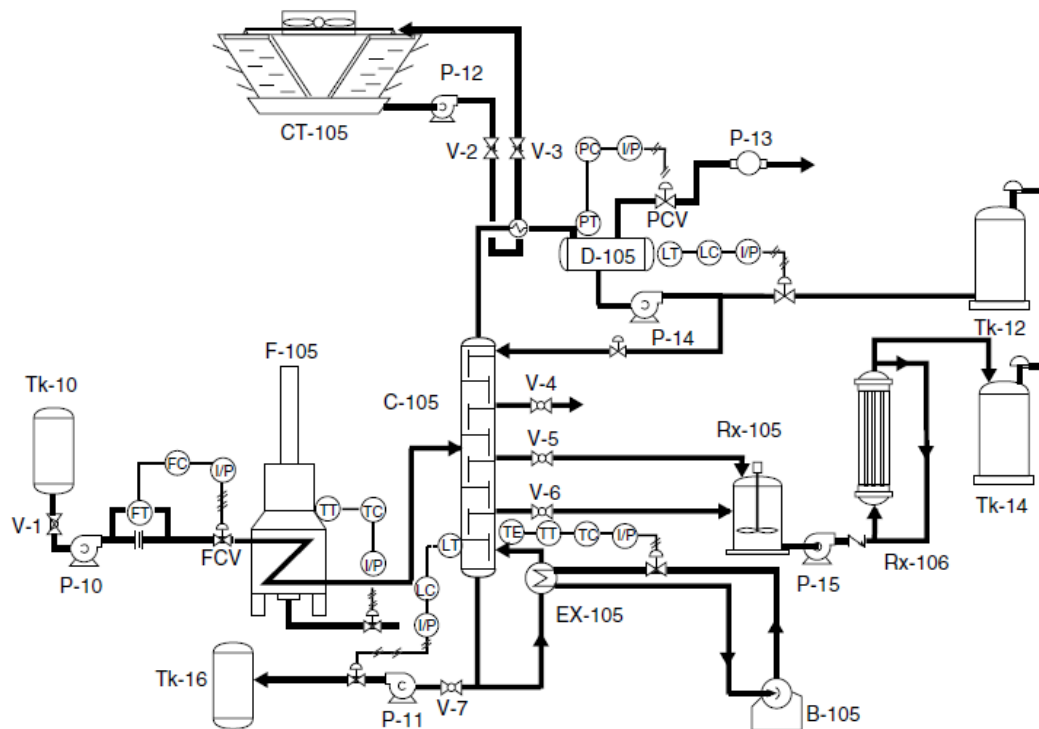


Fig.(6) Process and Instrument Diagram (P&ID)

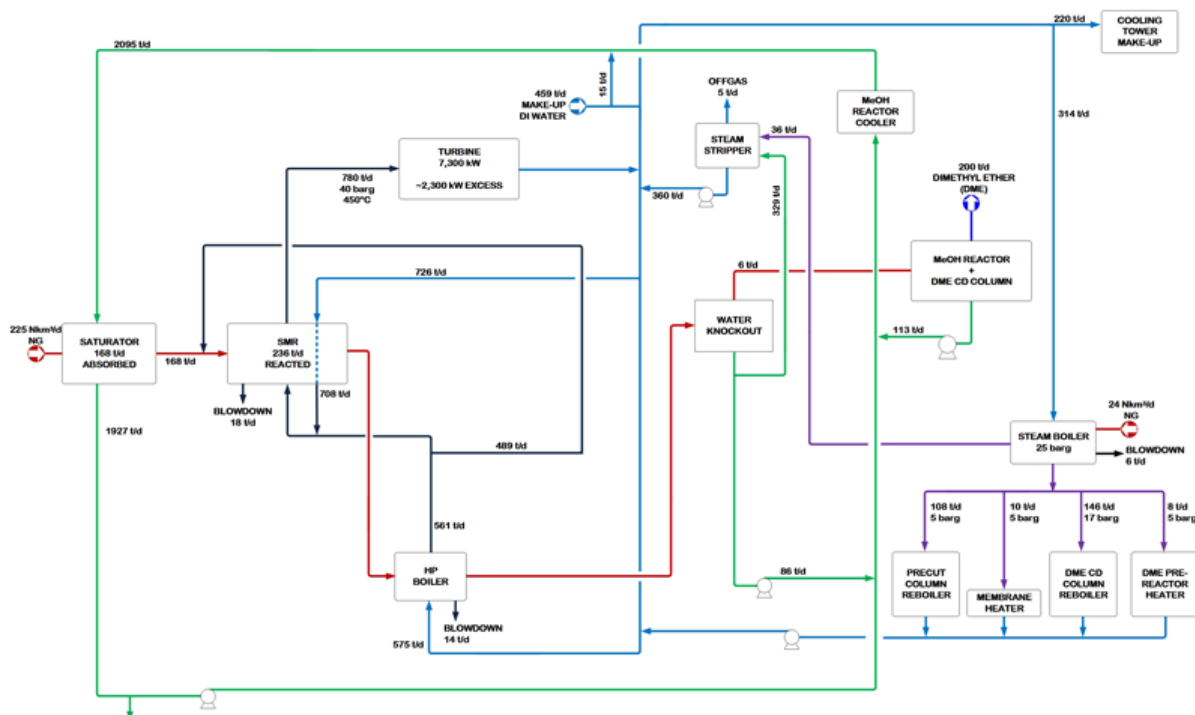


Fig.(7) Typical utility flow diagram.

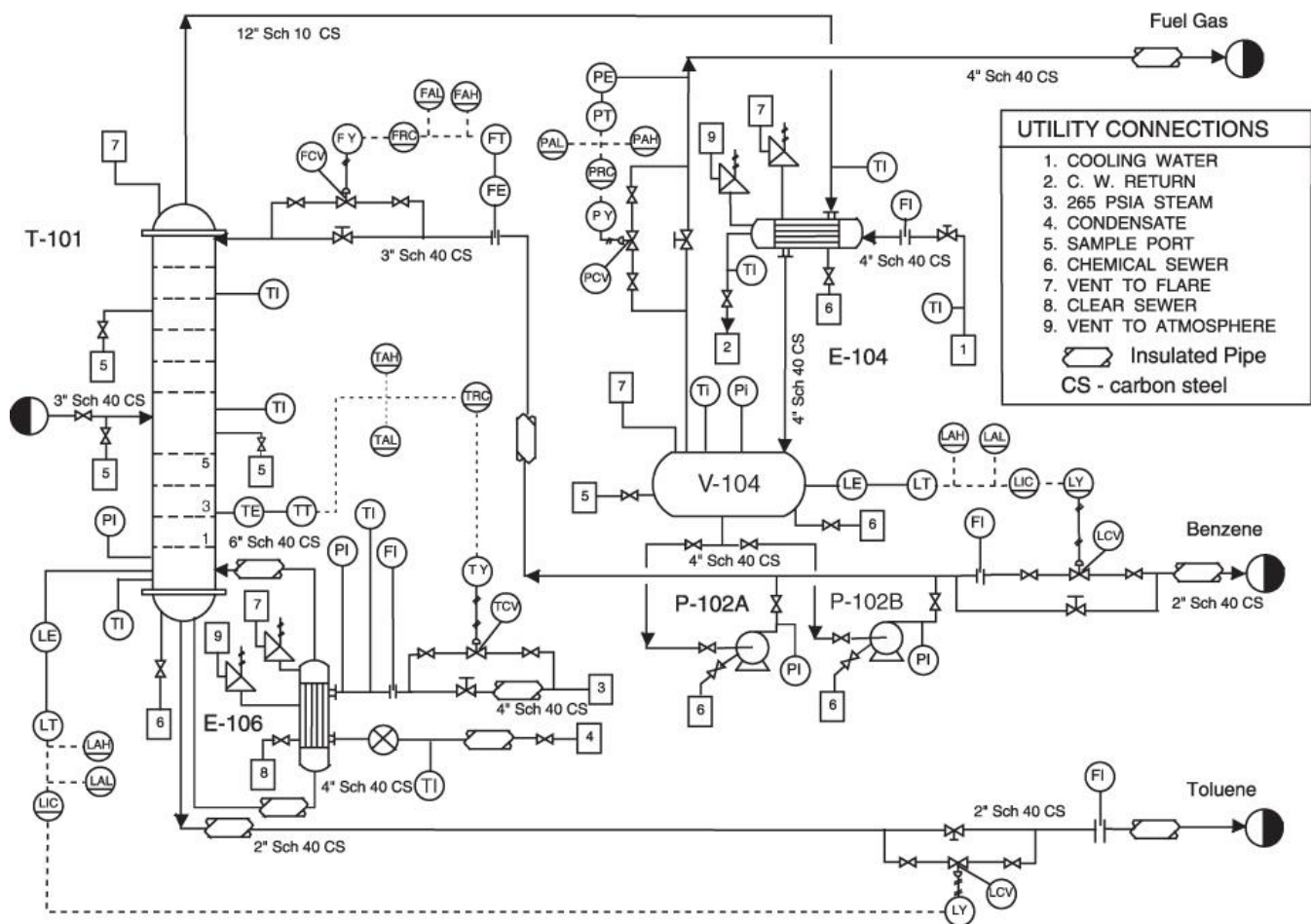


Fig.(8) Engineering P&ID flowsheet

Flowsheet Symbols

To reduce detailed written descriptions on flowsheets, it is usual practice to develop or adopt a set of symbols and codes which suit the purpose. Many symbols are pictorial which is helpful in representing process as well as control and mechanical operations. See Fig.(9)

Line Symbols and Designation

The two types of lines on a flowsheet are (1) those representing outlines and details of equipment, instruments, etc., and (2) those representing pipe carrying process or utility liquids, solids, or vapors and electrical or instrument connections. The latter must be distinguished among themselves as suggested by Figure (10).

The usual complete line designation contains the following: (1) line size (nominal); (2) material cod; (3) sequence number; and (4) materials of construction.

Examples: 2"-CL6-CS40

3"-CL6a-CS40

Equipment Designation

Equipment code designations can be developed to suit the particular process, or as is customary a master coding can be established and followed for all projects. A suggested designation list (not all inclusive for all processes) for the usual process plant equipment is given in Table (1). The various items are usually numbered by type and in process flow order as set forth on the flowsheets. For example:

Item code	Designation
S-1	First separator in a process
S-2	Second separator in a process
C-1	First compressor in a process

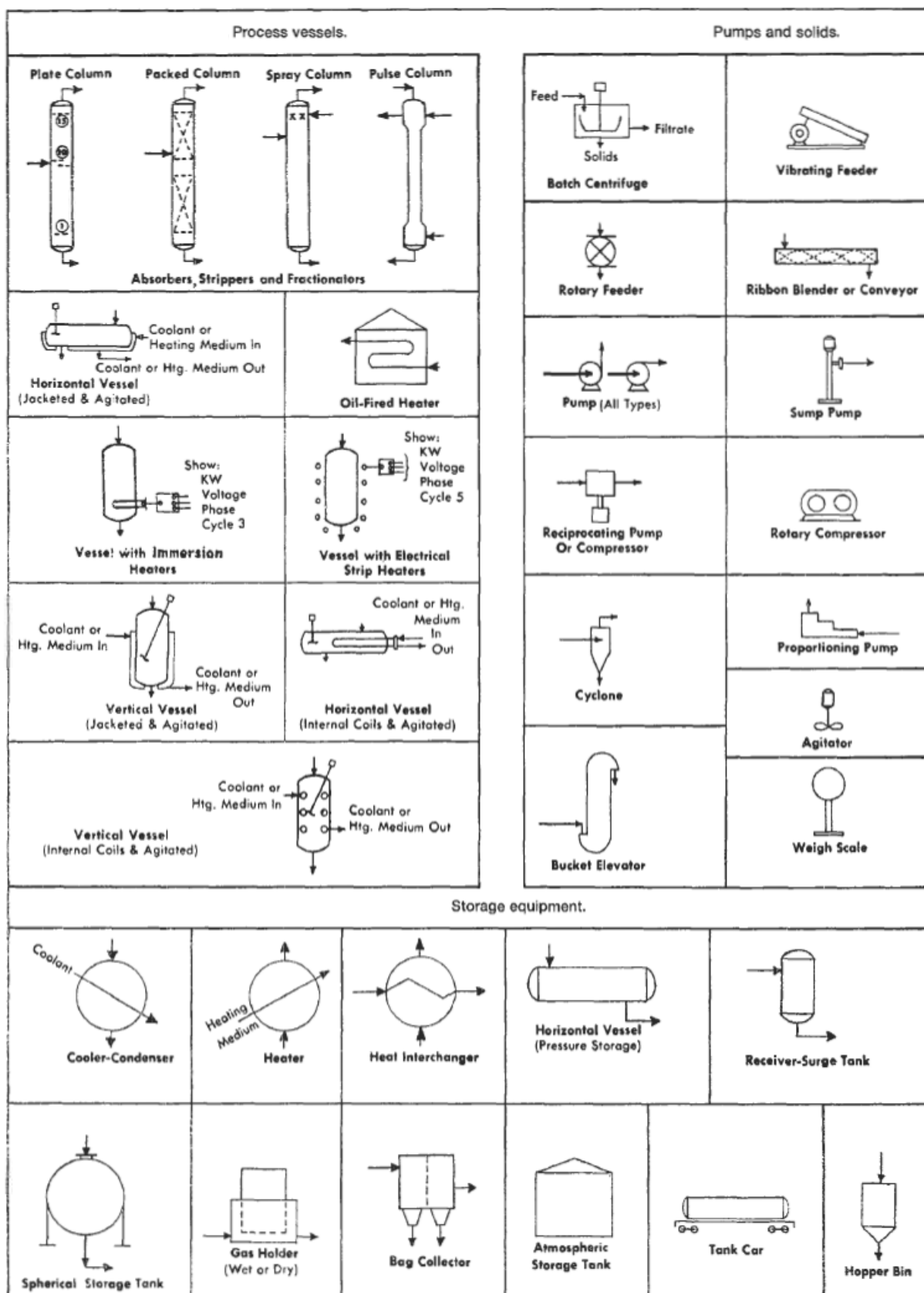


Fig. (9.a) Flowsheet symbols.

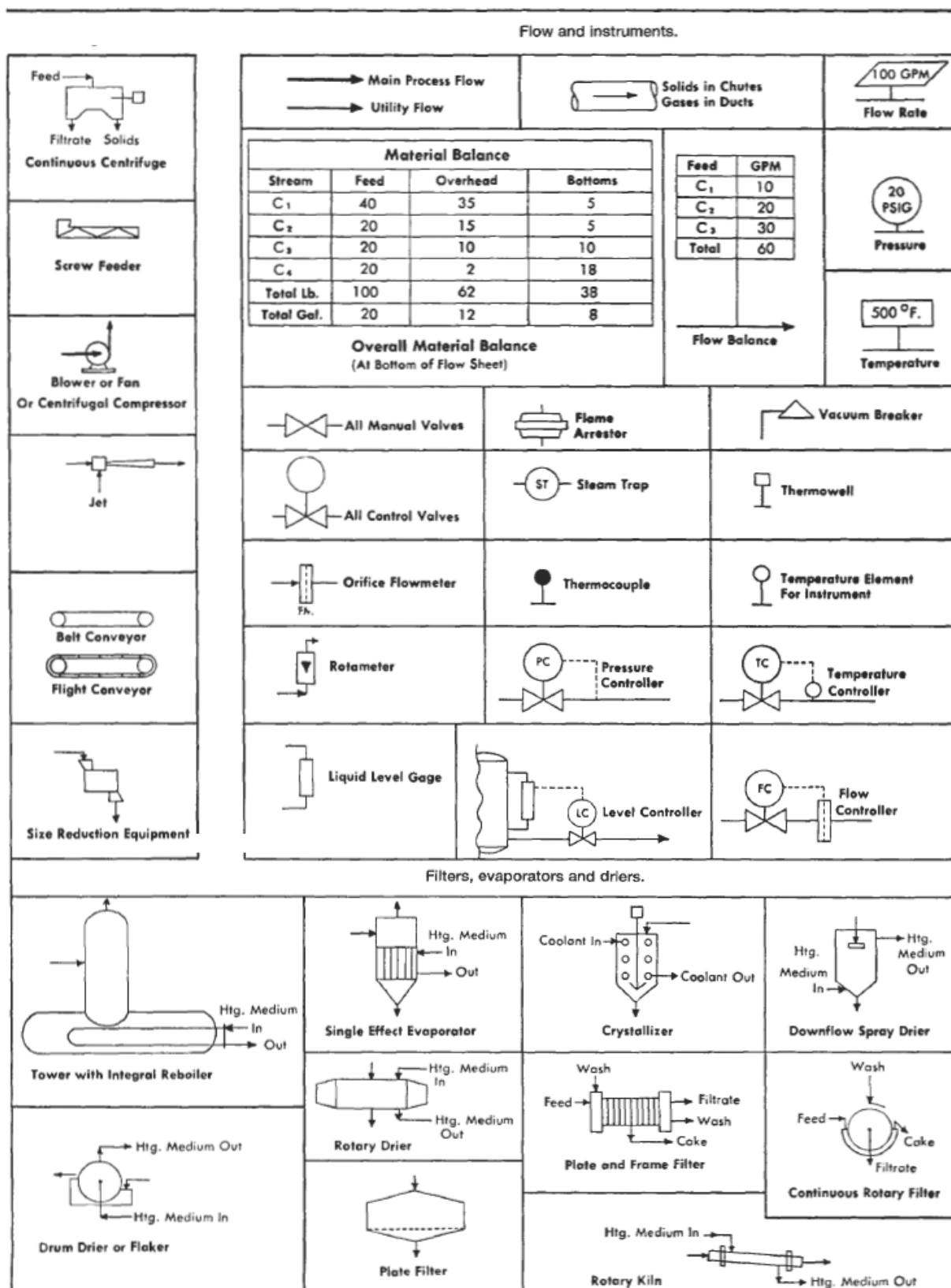


Fig. (9.b) Flowsheet symbols contd.

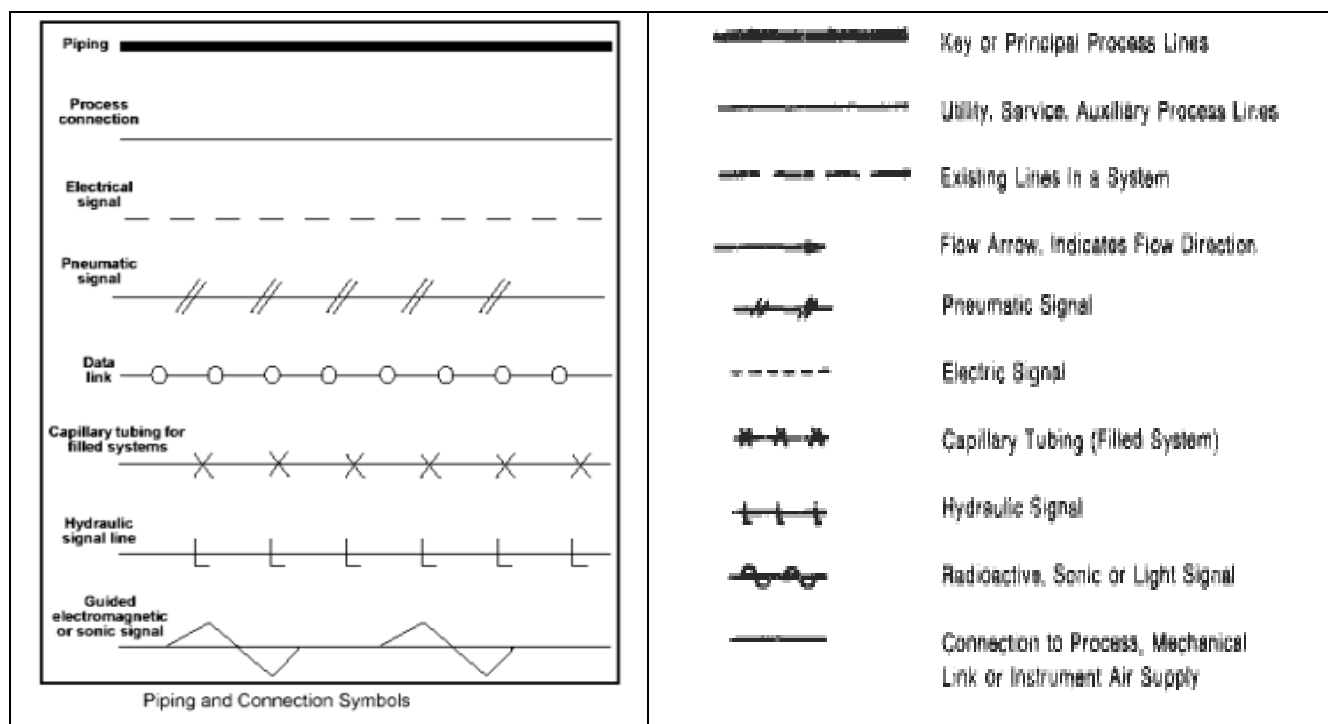


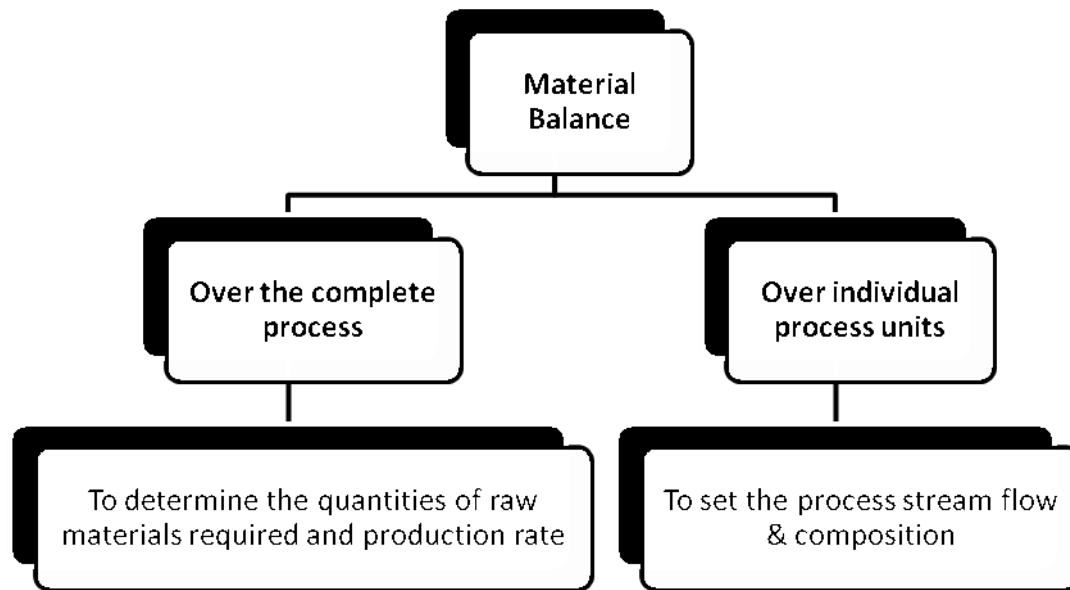
Fig.(10) piping and connection symbols from different sources(Line symbols)

Table 1

A System of Equipment Designations	
AD	— Air Drier
AF	— Air Filter
Ag	— Agitator
B	— Blower
BR	— Barometric Refrigeration Unit
C	— Compressor
CP	— Car Puller
CT	— Cooling Tower
CV	— Conveyor
D	— Drum or tank
DS	— Desuperheater
E	— Heat Exchanger, condenser, reboiler, etc.
Ej	— Jet Ejector
Ex	— Expansion Joint
F	— Fan
FA	— Flame Arrestor
Fi	— Filter (line type, tank, centrifugal)
GT	— Gas Turbine
MB	— Motor for Blower
MC	— Motor for Compressor
MF	— Motor for Fan
MP	— Motor for Pump
P	— Pump
PH	— Process Heater or Furnace
R	— Reactor
S	— Separator
St	— Strainer
ST	— Steam Turbine
Str	— Steam trap
SV	— Safety Valve
Tr	— Trap
V	— Valve
VRV	— Vacuum Relief Valve

Fundamentals of Material Balance

Material balances are the basis of process design



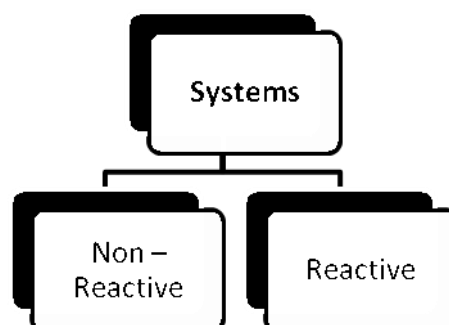
Material balance is also useful tool for the following:

1. The study of the plant operation & troubleshooting.
2. Check performance against design.
3. Check the instrument calibration.

Conservation of Mass:

The general mass balance equation:

Input – output + generation – consumption = Accumulation



For steady-state non reactive system: Input = Output

[Number of equations = Number of components]

For steady-state reactive system: Input – output + generation – consumption = 0.0

Some Important Parameters for Reactive System:

Limiting Reactant:

It's the reactant that would be completely consumed if the reaction proceeded to completion. As it disappears the reaction stops. It's also called the rate determining component since its concentration determines the reaction rate. All other reactants must either be fed in stoichiometric proportion to the limiting reactant (the feed rates are in the ratio of the stoichiometric coefficients) or in excess of the limiting reactant (in greater than stoichiometric proportion to it).

Stoichiometry:

It's used to balance chemical reaction equations. The stoichiometric equation for a chemical reaction states the number of molecules of the reactants and products that take part, from which the quantities can be calculated.

For simple reactions → can be done by inspection. بمجرد النظر

For complex reactions → take a base of 1 mole of one component and make an atomic balance on each element (It's better to choose one with many atoms as possible).

Fractional Conversion:

It's the ratio of amount reacted to amount fed. The fractional conversions of different reactants are generally different unless the reactants are fed in stoichiometric proportion.

$$\begin{aligned}\text{Fractional Conversion} &= \frac{\text{Amount reacted from the limiting reactant}}{\text{Amount fed from the limiting reactant}} \\ &= \frac{\text{Input of the limiting reactant} - \text{Output of the limiting reactant}}{\text{Input of the limiting reactant}}\end{aligned}$$

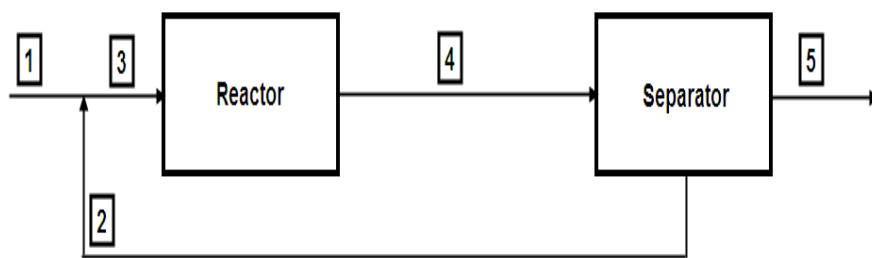
Note: In case of reaction process with recycling of unreacted reactants, there are 2 types of conversion:

a- Single pass conversion

$$= \frac{\text{Input to the reactor} - \text{Output from the reactor}}{\text{Input to the reactor}} = \frac{3-4}{3}$$

b- Overall conversion

$$= \frac{\text{Input to the process} - \text{Output from the process}}{\text{Input to the process}} = \frac{1-5}{1}$$



The overall conversion should be >>> single pass conversion [one of the recycle functions is to maximize conversion]

Selectivity:

It's a measure of the efficiency of the reactor in converting reagent to the desired product. It is the fraction of the reacted material that was converted into the desired product. If no byproducts are formed, then the selectivity is 100%.

$$\text{Selectivity} = \frac{\text{moles of desired product actually formed}}{\text{moles of desired product theoretically could be formed}}$$

$$\text{Selectivity} = \frac{\text{moles of desired product actually formed}}{\text{moles of reagent consumed} \times \text{stoichiometric factor}}$$

Yield:

It's a measure of the performance of a reactor or a plant.

There are 2 types of yield:

a- Reaction yield (Chemical yield)

Reaction yield = Conversion $\times$ Selectivity

$$= \frac{\text{Moles product produced}}{\text{Moles reagent converted}} \times \text{Stoichiometric factor}$$

Where moles reagent converted includes that consumed in both main & side reactions.

Note: Reaction yield = conversion when there is no side reactions take place.

b- Plant Yield

Plant yield is a measure of the overall performance of the plant and includes all chemical & physical losses (during separation process).

$$\text{Plant Yield} = \frac{\text{Moles product produced}}{\text{Moles reagent supplied to the process}} \times \text{Stoichiometric factor}$$

Stoichiometric factor = theoretical moles of reagent required per moles of product produced in the reaction balanced equation.

Excess:

A reagent may be supplied in excess to promote the desired reaction to:

- 1- Maximize the use of an expensive reagent.
- 2- Ensure complete reaction of a reagent, as in combustion.

$$\begin{aligned}\% \text{ Excess} &= \frac{\text{Actual Feed} - \text{Theoretical Feed}}{\text{Theoretical Feed}} \times 100 \\ &= \frac{\text{Actual Feed} - \text{Stoichiometric Feed}}{\text{Stoichiometric Feed}} \times 100\end{aligned}$$

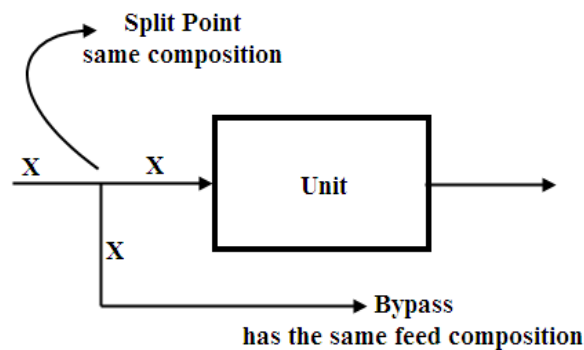
Note: Excess component actual feed = Theoretical feed $\times (1 + \text{fraction excess})$

Tie Component:

If one component passes unchanged through a process unit (inert component), it can be used to tie the inlet & outlet compositions. Since its amount is the same in input & output so the total amount of input & output can be calculated if their compositions are known. Example: Nitrogen in combustion reactions.

Bypass:

A flow stream may be divided and some part diverted (bypassed) around some units. This procedure is often used to control stream composition or temperature.

**Recycle:**

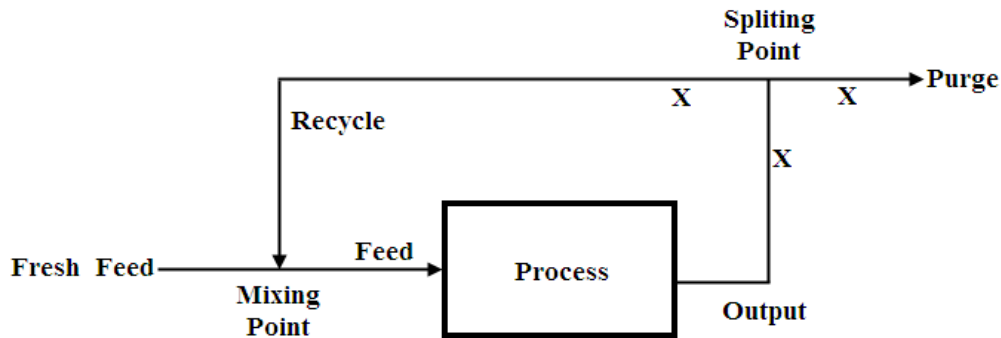
It's used to send unused raw materials emerging from a process unit back to the unit. Overall system balances are usually (but not always) convenient starting points for analyzing process with recycle.

Purge:

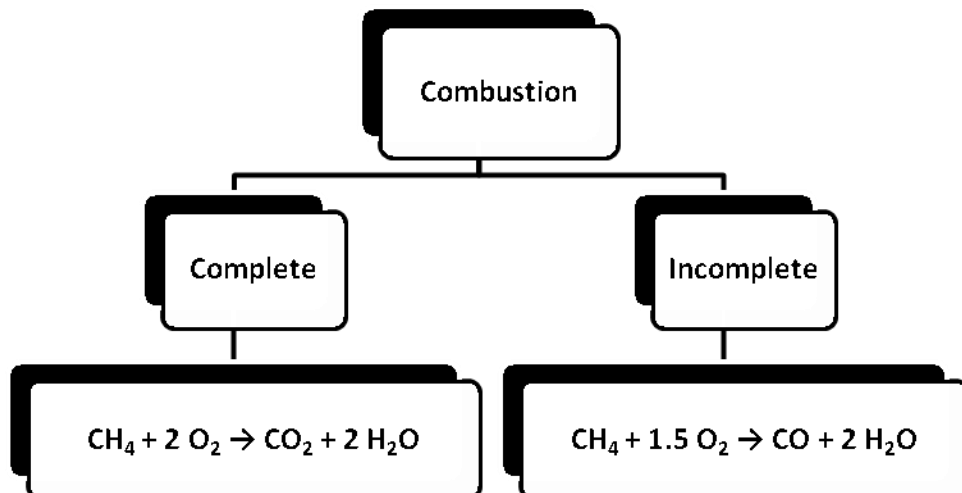
A stream that's withdrawn from a process when a species enters in the process feed and is completely recycled. If this species weren't removed in the purge, it would keep accumulating in the process system and eventually lead to shutdown.

Purge stream used to:

- Maintain the steady state conditions in the system
- Prevent the accumulation of inert or undesired materials [To rid the process of the undesired material]



Combustion Reactions:



Excess air is used in combustion to:

- 1- Ensure complete combustion.
- 2- Minimize Co & smoke formation.

Note: % excess air = % excess oxygen

Air = 79% N_2 + 21% O_2 by moles

Air = 77% N_2 + 23% O_2 by mass

The calculated amount of excess air doesn't depend on how much material is actually burned but what can be burned. Excess O_2 (air) is calculated from the complete combustion equation, i.e. based on conversion of all $\text{C} \rightarrow \text{CO}_2$, $\text{S} \rightarrow \text{SO}_2$ & $\text{H} \rightarrow \text{H}_2\text{O}$.

Important Note: Using too much excess air means that more air will be heated (i.e. high energy losses). While if %excess air is less than 3, **flame impingement** to the furnace tubes.

Expressing the Composition of a Material Stream:

- Mass fraction = component mass / total stream mass
- Mole fraction = component moles / total stream moles
- Volume fraction = component volume / total stream volume

Note: volume fraction = mole fraction for gases up to 25 bar.

For trace quantities:

ppm ► part per million

ppb ► part per billion

Note: UK billion = 10^{12} while USA billion = 10^9

Choice of a basis for Calculations:

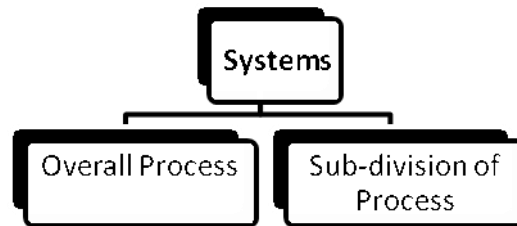
A basis of calculation for a process is an amount or flow rate of one of the process streams, preferably that stream with known composition. The basis may be a period of time for example, hours, or a given mass of material.

- 1- For continuous process (production or feed rate is given as kg/hr, ton/day, etc) ► Basis is 1 hr or 1 operating day (unit of Time)
- 2- For batch process (production or feed rate is given as kg/batch, ton/batch, ... etc) ► Basis is 1 batch.
- 3- If the flow rates are not given ►
 - For composition given as mass fraction (in case of liquids or solids), basis is often 1 or 100 lb_m or kg.
 - For composition given as mole fraction (in case of gases), basis is often 1 or 100 lb_{mol} or kmol.

Note: It's important that your basis be indicated near the beginning of the problem.

Choice of the system boundary

System boundary: The part of the process being considered.



The system chosen must have a degree of freedom = 0.0 in order to be able to be solved (i.e. No. of equations = No. of unknowns).

Note: For any reactive system, the following parameters should be defined:

- 1- Yield or conversion.
- 2- % Excess if present.
- 3- Concentrations (strength) of reactants & products streams.
- 4- Recovery.

$$\text{Recover} = \frac{\text{Amount of product finally out from the plant}}{\text{Amount of product produced from the reactor}}$$

General Procedures for Material Balance Problems:

- 1- Draw a block diagram of the process.
- 2- List all the available data.
- 3- List all the information required from the balance.
- 4- Write out all the chemical reactions involved.
- 5- Decide the basis of your calculations.
- 6- Decide the system boundary.

Fundamentals of Heat Balance

Heat balance is a special case of energy balance. Target of heat balance depends on the type of the system.

1. Reactive System:

Heat balance is important to:

- 1- Calculate the rate of heat addition or removal from the system to maintain the reaction mixture at the desired temperature to ensure certain degree of conversion.
- 2- Calculate the flow rates of heating or cooling utilities required.
- 3- Calculate the heat transfer area required for heating or cooling.

a- Calculation of rate of heat removal / addition:

i- For continuous system:

$$Q = \frac{n^\circ}{\gamma} \Delta \bar{H}$$

n° : Molar reaction rate of the limiting reactant (mol/ hr)

$= n^\circ_{\text{feed}} \times \text{single pass conversion}$

$\Delta \bar{H}$: Standard specific heat of reaction at 298K (kJ/mol)

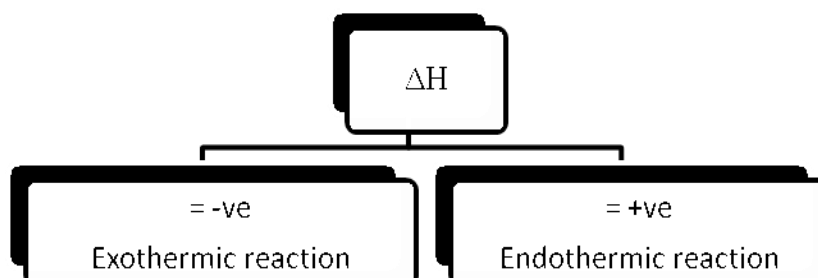
$$= \sum \gamma_i \Delta \bar{H}_f (\text{products}) - \sum \gamma_i \Delta \bar{H}_f (\text{reactants})$$

γ_i : Component stoichiometric coefficient in the balanced equation.

$\Delta \bar{H}_f$: Component standard heat of formation (kJ/mol).

Note: For a reaction $A + 2 B \rightarrow C$ $\Delta \bar{H} = -240$ kJ/mol

That means that the heat released from the reaction of 1 mole of A with 2 mole of B to produce 1 mole of C = 240 kJ. If 100 mole of B reacts with 50 mole of A the heat produced = $100/2 \times 240$ or = $50/1 \times 240 = 1200$ kJ.



For exothermic reaction:

∴ Cooling is must

Calculate flow rate of cooling water:

$$Q = m^{\circ} C_p \Delta T$$

m° : cooling water mass flow rate

C_p $\begin{cases} \nearrow 4.2 \text{ kJ/kg.K} \\ \searrow 1 \text{ Btu/lb}_m.\text{°F} \end{cases}$

ΔT : $T_{\text{out}} - T_{\text{in}} = 10 \rightarrow 15 \text{ °C}$ (if not given)

Cooling water pump capacity (pump volumetric flow rate) can be calculated:

Capacity of the cooling water pump = $\frac{m^{\circ}}{\rho}$ (m^3/hr , Gpm or Lpm)

For endothermic reaction:

∴ Heating is must

Calculate the steam consumption:

- If steam enters as saturated vapor & exit as saturated liquid

$$Q = m_s^{\circ} \lambda_s$$

m_s° : Steam mass flow rate (kg/hr)

λ_s : Latent heat of vaporization (kJ/kg) (from steam tables)

- If steam enters as super heated vapor & exit as sub-cooled liquid:

$$Q = m_s^{\circ} C_{p_v} \Delta T_1 + m_s^{\circ} \lambda_s + m_s^{\circ} C_{p_L} \Delta T_2$$

$\Delta T_1 = T_{\text{steam}} - T_{\text{boiling}}$ C_{p_v} : Steam specific heat (kJ/kg.K)

$\Delta T_2 = T_{\text{boiling}} - T_{\text{out}}$ C_{p_L} : water specific heat (kJ/kg.K)

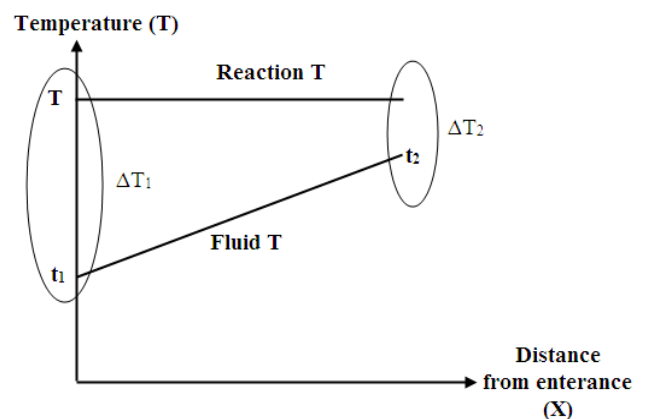
Note: you can calculate steam consumption regardless type of phase change:

$$Q = m_s [\bar{H}_{\text{in}} - \bar{H}_{\text{out}}]$$

- If heating is done by using oil: Mass flow rate of the heating oil:

$$Q = m^{\circ} C_p \Delta T_{\text{oil}}$$

m° : oil mass flow rate.



$$\Delta T_{oil} = T_{in} - T_{out}$$

ii- For batch system:

$$Q = \frac{n \Delta \hat{H}_r / \gamma}{\text{Reaction time}}$$

Reaction time = cycle time (if not given)

$\Delta \hat{H}_r$: Specific heat of reaction

n: no of moles reacted form the limiting reactant per cycle

n = n fed per cycle $\times$ conversion

$$n \text{ fed per cycle} = \frac{\text{No. of moles fed/day}}{\text{No. of cycles}}$$

$$\text{No. of cycles} = \frac{24 \text{ hr}}{\text{cycle time}}$$

Important note:

To calculate $\Delta \hat{H}_r$ at any temperature:

$$\Delta \hat{H}_r = \Delta \hat{H}_r^\circ + R \int_{T_0=298 \text{ K}}^T \frac{\Delta C_p}{R} dT$$

$$\int_{T_0}^T \frac{\Delta C_p}{R} dT = \Delta A T_0 [\tau - 1] + \frac{\Delta B}{2} T_0^2 [\tau^2 - 1] + \frac{\Delta C}{3} T_0^3 [\tau^3 - 1] + \frac{\Delta D}{T_0} \left[\frac{\tau - 1}{\tau} \right]$$

$\tau = \frac{T}{T_0}$, A, B, C & D are constants (from thermodynamic tables)

$\Delta A = \sum \gamma_i A_i (\text{products}) - \sum \gamma_i A_i (\text{reactants})$ & so for ΔB , ΔC & ΔD

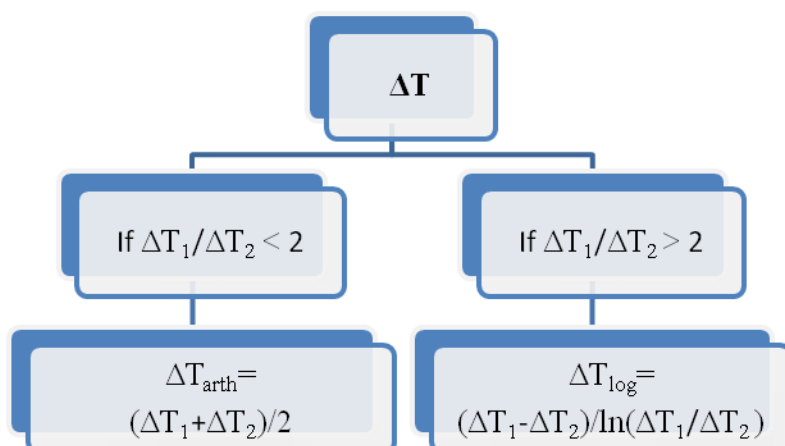
b- Calculation of Heat Transfer Area Required for Heating or Cooling:

$$Q = U A \Delta T_{lm}$$

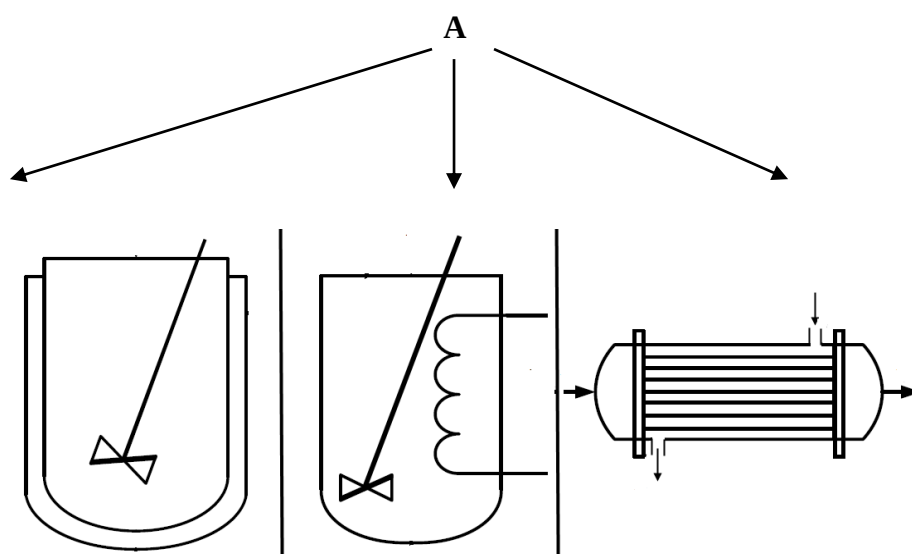
U: Overall heat transfer coefficient (W/m².K).

A: Heat transfer area (m²).

ΔT_{lm} : Temperature difference (K or °C).



Note: ΔT is calculated based on counter current flow unless otherwise is given.



Reactor with jacket

A = Jacket area

Reactor with coil

A = coil area

$$= \pi d_0 L$$

Coil length (L) can be calculated if d_0 is known

Heat Exchanger

A = tubes area

$$= N \pi d_0 L$$

Number of tubes (N) can be calculated if the tube dims. are known (L & d_0)

2. Non-Reactive System:

This includes all the systems in which heat transfer takes place without chemical reaction. Q in this case depends on the system.

a. For Heaters/Coolers:

$$Q = m^\circ C_p \Delta T \quad \text{Only sensible heat (no phase change)}$$

b. For Vaporizers:

General heat load equation:

$$Q = m^\circ C_{pL} (T_{\text{boiling}} - T_{\text{feed}}) + m^\circ \lambda + m^\circ C_{pV} (T_{\text{out}} - T_{\text{boiling}})$$

If the outlet is saturated vapor:

$$Q = m^\circ C_{pL} (T_{\text{boiling}} - T_{\text{feed}}) + m^\circ \lambda$$

If the feed is saturated liquid:

$$Q = m^\circ \lambda + m^\circ C_{pV} (T_{\text{out}} - T_{\text{boiling}})$$

If the feed is saturated liquid & the outlet is saturated vapor:

$$Q = m^{\circ} \lambda$$

c. For Condenser:

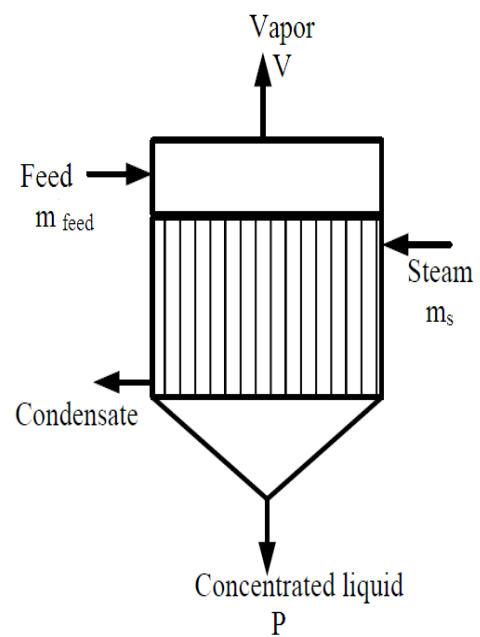
$$Q = m^{\circ} \lambda$$

d. For Cooler-Condenser:

$$Q = m^{\circ} C_p \Delta T + m^{\circ} \lambda$$

e. For Evaporators:

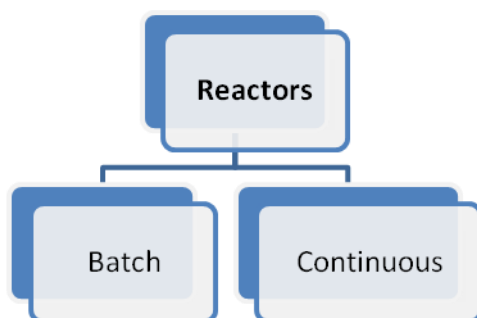
$$Q = m^{\circ}_{\text{feed}} C_{p \text{ feed}} (T_{\text{boiling}} - T_{\text{feed}}) + V \lambda$$



Equipment Sizing

i.e. Calculation of reactors volume & dimensions.

Calculation of storage (holding) tank volumes.



1- Batch Reactor:

$$= [V_{\text{reactants fed/cycle}} + V_{\text{catalyst (if exist)}}] * \frac{100}{\% \text{ Full}}$$

% Full = 75 if not given

$$V_{\text{reactants fed/cycle}} = \frac{V_{\text{reactants fed/cycle}}}{\text{No. of cycles}}$$

$$\text{No of cycles} = \frac{24}{t_{\text{cycle}} \text{ (hr)}}$$

After calculation of the reactor volume, its dimensions can be calculated:

$$V_{\text{reactor}} = \frac{\pi}{4} D^2 H$$

H/D : Aspect ratio (If not given it can be assumed = 5)

2- Continuous Reactor:

$$\text{Space time } \tau = \frac{V_{\text{reactor}}}{V^{\circ}_{\text{reactants}}}$$

$$\text{Space velocity } v = \tau^{-1} = \frac{V^{\circ}_{\text{reactants}}}{V_{\text{reactor}}}$$

For gas phase:

$$P V^{\circ}_{\text{reactants}} = n^{\circ} R T \text{ (assuming ideal gas behavior } P < 15 \text{ bar)}$$

$V^{\circ}_{\text{reactants}}$: Feed reactants volumetric flow rate.

n° : Feed reactants molar flow rate.

For liquid phase:

$$V^{\circ}_{\text{reactants}} = m^{\circ} / \rho$$

Note: For mixed phase reaction the volume is calculated based on the gas volume.

General Procedure for Reactor Design:

- 1) Collect together all the kinetic & thermodynamic data on the desired reaction and the possible side reactions (these data are obtained from literature or laboratory & pilot plant test).
- 2) Collect the physical properties required for the design 9 from literature, estimation by laboratory measurements).
- 3) Identify the controlling step [Kinetic or mass] and choose the suitable reactor type based on the experience with similar reactions or from the laboratory or pilot plant work.
- 4) Make initial selection of the reactor conditions to give the desired conversion & yield.
- 5) Size the reactor.
- 6) Select a suitable material of construction.
- 7) Make a preliminary mechanical design for the reactor.
- 8) Cost the proposed design (repeat steps 4→8 to optimize the design).

Storage (Holding) Tank:

Storage tank is used for raw materials & final products.

Holding tanks is used in case of batch process.

$$V_{\text{Storage tank for a reactant}} = V_{\text{consumed per day}} \times \text{storage period in days}$$

$$V_{\text{Storage tank for a product}} = V_{\text{produced per day}} \times \text{storage period in days}$$

$$\text{Note: \% Tank full} = \frac{\text{Liquid height inside the tank}}{\text{Total tank height}}$$

Types of Designs

The methods for carrying out a design project may be divided into the following classifications, depending on the accuracy and detail required:

1. Preliminary or quick-estimate designs

Used as a basis for determining whether further work should be done on the proposed process. This type of design is based on approximate process methods, and rough cost estimates are prepared. Few details are included, and the time spent on calculations is kept at a minimum.

2. Detailed-estimate designs

In this type of design, the cost and profit potential of an established process is determined by detailed analysis and calculations. However, exact specifications are not given for the equipment, and drafting-room work is minimized. The following factors should be established within narrow limits before a detailed-estimate design is developed:

- Manufacturing process
- Material and energy balances
- Temperature and pressure ranges
- Raw-material and product specifications
- Yields, reaction rates, and time cycles
- Materials of construction
- Utilities requirements
- Plant site

i.e the above factors should be determined after a preliminary design.

3. Firm process designs or detailed designs

When the detailed-estimate design indicates that the proposed project should be a commercial success, the final step before developing construction plans for the plant is the preparation of a firm process design. In this type complete specifications are presented for all components of the plant, without any change in the process flowsheet and accurate costs based on quoted prices are obtained. The firm process design includes blueprints and sufficient information to permit immediate development of the final plans for constructing the plant.

Design Information (literature survey)

General information and specific data required to the development of a design project can be obtained from many different sources such as:

A. Textbooks

A large number of textbooks covering the various aspects of chemical engineering principles and design are available. In addition, many handbooks have been published giving physical properties and other basic data which are very useful to the design engineer. A primary source of information on all aspects of chemical engineering principles, design, costs, and applications is “The Chemical Engineers’ Handbook” published by McGraw-Hill Book Company with R. H. Perry and D. W. Green as editors and Encyclopedia of Chemical Technology by Kirk Othmer.

B. Technical journals

Regular features on design-related aspects of equipment, costs, materials of construction, and unit processes are published in Chemical Engineering. In addition to this publication, there are many other periodicals that publish articles of direct interest to the design engineer. The following periodicals are suggested as valuable sources of information for the chemical engineer who wishes to keep abreast of the latest developments in the field:

- American Institute of Chemical Engineers journal (AIChE)
- Chemical Engineering Progress
- Chemical and Engineering News
- Chemical Engineering Science
- Industrial and Engineering Chemistry Fundamentals
- Industrial and Engineering Chemistry Process Design and Development
- Journal of the American Chemical Society, Journal of Physical Chemistry
- Journal of the American Chemical Society
- Hydrocarbon Processing
- Oil and Gas Journal
- Engineering News-Record
- Canadian Journal of Chemical Engineering

C. Trade bulletins

Trade bulletins are published regularly by most manufacturing concerns, and these bulletins give much information of direct interest to the chemical engineer preparing a design. Some of the trade-bulletin information is condensed in an excellent reference book on chemical engineering equipment, products, and manufacturers. This book is known as the “Chemical Engineering Catalog,” and contains a large amount of valuable descriptive material. New information is constantly becoming available through publication in periodicals, books, trade bulletins, government reports, university bulletins, and many other sources. Many of the publications are devoted to shortcut methods for

estimating physical properties or making design calculations, while others present compilations of essential data in the form of nomographs or tables. The effective design engineer must make every attempt to keep an up-to-date knowledge of the advances in the field.

D. Patents

A patent is essentially a contract between an inventor and the public. In consideration of full disclosure of the invention to the public, the patentee is given exclusive rights to control the use and practice of the invention. A patent gives the holder the power to prevent others from using or practicing the invention for a period of 17 years from the date of granting. In contrast, trade-secrets and certain types of confidential disclosures can receive protection under common-law rights only as long as the secret information is not public knowledge. A new design should be examined to make certain no patent infringements are involved. If the investigation can uncover even one legally expired patent covering the details of the proposed process, the method can be used with no fear of patent difficulties.

THE PRELIMINARY DESIGN

In order to amplify the remarks made earlier concerning the design-project procedure, it is appropriate at this time to look more closely at a specific preliminary design. Only a brief presentation of the design will be attempted at this point. However, sufficient detail will be given to outline the important steps which are necessary to prepare such a preliminary design. The problem presented is a practical one of a type frequently encountered in the chemical industry; it involves both process design and economic considerations.

Problem Statement

A conservative petroleum company has recently been reorganized and the new management has decided that the company must diversify its operations into the petrochemical field if it wishes to remain competitive. The research division of the company has suggested that a very promising area in the petrochemical field would be in the development and manufacture of biodegradable synthetic detergents using some of the hydrocarbon intermediates presently available in the refinery. A survey by the market division has indicated that the company could hope to attain 2.5 percent of the detergent market if a plant with an annual production of 15 million pounds were to be built. To provide management with an investment comparison, the design group has been instructed to proceed first with a preliminary design and an updated cost estimate for a non biodegradable detergent producing facility similar to ones supplanted by recent biodegradable facilities.

Literature Survey

A survey of the literature reveals that the majority of the non biodegradable detergents are alkyl benzene sulfonates (ABS). Theoretically, there are over 80,000 isomeric alkyl benzenes in the range of C₁₀ to C₁₅ for the alkyl side chain. Costs, however, generally favor the use of dodecene (propylene tetramer) as the starting material for ABS.

There are many different schemes in the manufacture of ABS. Most of the schemes are variations of the one shown in Fig. (11) for the production of sodium dodecylbenzene sulfonate. A brief description of the process is as follows:

This process involves:

- i. Reaction of dodecene with benzene in the presence of aluminum chloride catalyst (alkylation)
- ii. Fractionation of the resulting crude mixture to recover the desired boiling range of dodecylbenzene.
- iii. Sulfonation of the dodecylbenzene.
- iv. Neutralization of the sulfonic acid with caustic soda.
- v. Blending the resulting slurry with chemical “builders”; and drying.

Process Description

Dodecene is charged into a reaction vessel containing benzene and aluminum chloride. The reaction mixture is agitated and cooled to maintain the reaction temperature of about **115°F** maximum. An excess of benzene is used to suppress the formation of by-products. Aluminum chloride requirement is **5 to 10 wt%** of dodecene. After removal of aluminum chloride sludge, the reaction mixture is fractionated to recover excess benzene (which is recycled to the reaction vessel), a light alkylaryl hydrocarbon, dodecylbenzene, and a heavy alkylaryl hydrocarbon.

Sulfonation of the dodecylbenzene may be carried out continuously or batch-wise under a variety of operating conditions using sulfuric acid (100 percent), oleum (usually 20 percent SO₃), or anhydrous sulfur trioxide. The optimum sulfonation temperature is usually in the range of **100 to 140°F** depending on the strength of acid employed, mechanical design of the equipment, etc. Removal of the spent sulfuric acid from the sulfonic acid is facilitated by adding water to reduce the sulfuric acid strength to about **78 percent**. This dilution prior to neutralization results in a final neutralized slurry having approximately **85 percent** active agent based on the solids. The inert material in the final product is essentially Na₂SO₄.

The sulfonic acid is neutralized with **20 to 50 percent** caustic soda solution to a pH of 8 at a temperature of about **125°F**. Chemical “builders” such as trisodium phosphate, tetrasodium pyrophosphate, sodium silicate, sodium chloride, sodium sulfate, carboxymethyl cellulose, etc., are added to enhance the deterative, wetting, or other desired properties in the finished product. A flaked,

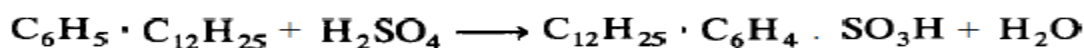
dried product is obtained by drum drying or a bead product is obtained by spray drying.

The basic reactions which occur in the process are the following.

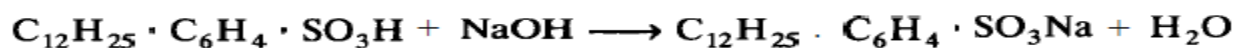
Alkylation:



Sulfonation:



Neutralization:



A literature search indicates that yields of **85 to 95 percent** have been obtained in the alkylation step, while yields for the sulfonation process are substantially **100 percent**, and yields for the neutralization step are always **95 percent** or greater. All three steps are exothermic and require some form of jacketed cooling around the stirred reactor to maintain isothermal reaction temperatures.

Laboratory data for the sulfonation of dodecylbenzene, described in the literature, provide additional information useful for a rapid material balance.

This is summarized as follows:

1. Sulfonation is essentially complete if the ratio of 20 percent oleum to dodecylbenzene is maintained at 1.25.
2. Spent sulfuric acid removal is optimized with the addition of 0.244 lb of water to the settler for each 1.25 lb of 20 percent oleum added in the sulfonation step.
3. A 25 percent excess of 20 percent NaOH is suggested for the neutralization step.

Operating conditions for this process, as reported in the literature, vary somewhat depending upon the particular processing procedure chosen.

Required:

- 1- Making material and energy balances.
- 2- Equipment sizing and selection.

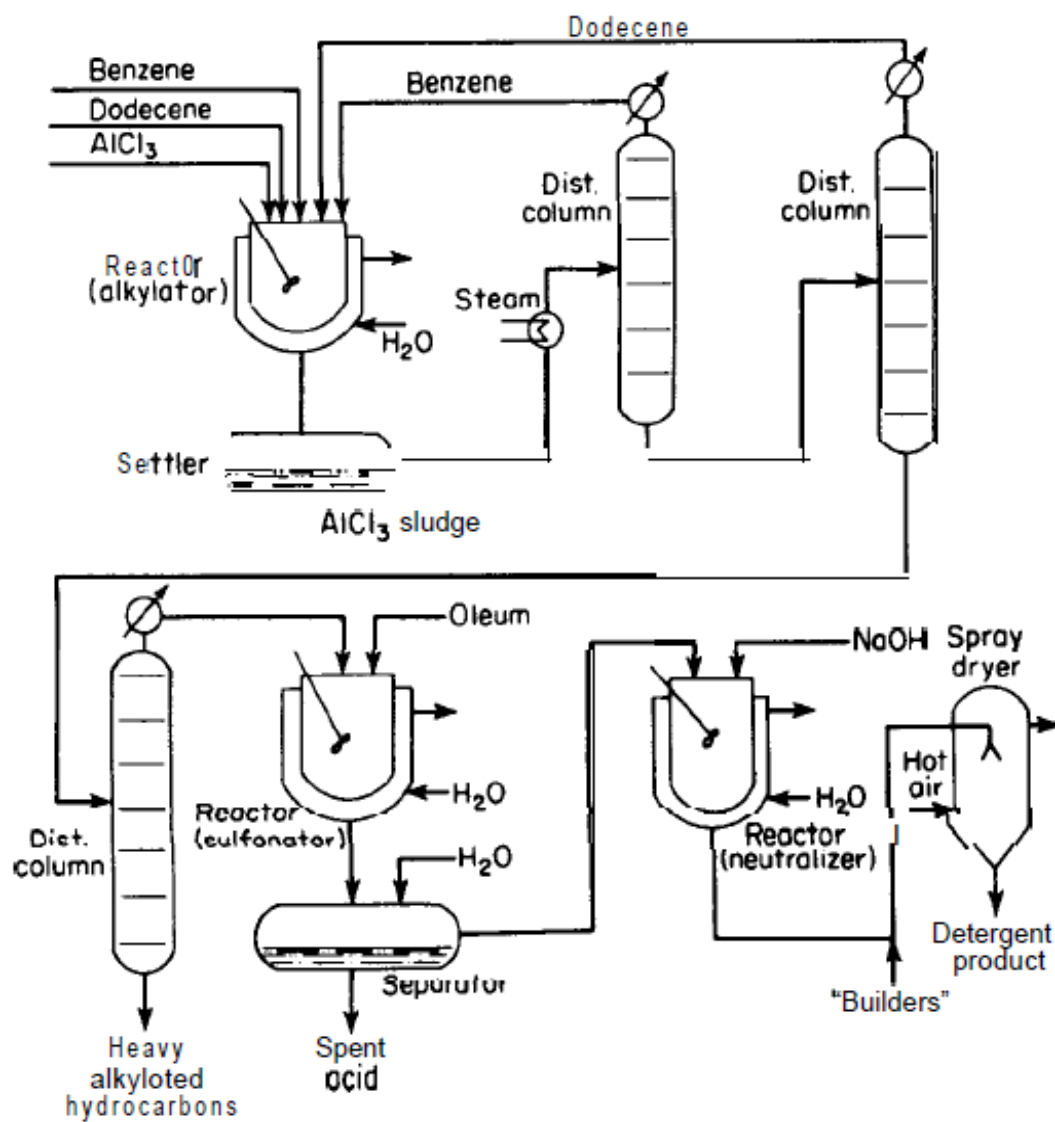


Fig. (11) Qualitative flow diagram for the manufacture of sodium dodecylbenzene sulfonate.

Economic Evaluation

The design project can be economically evaluated through the following steps:

1. Estimation of the total capital investment.

Total capital investment = fixed capital + working capital

2. Estimation of the total annual product cost.

Total product cost = direct cost + indirect cost

3. Estimation of the expected annual profit.

Annual net profit = (total annual sales – total product cost) (1 – income taxes rate)

4. Using profitability estimation methods such as R.O.I to evaluate the attractiveness of the proposed projet.

Safety Factors (Design Margins)

Definition: These factors represent the amount of overdesign that would be used to account for the changes in the operating performance with time (fouling in H.X) and potential increases in capacity requirements.

Experienced designers include a degree of over-design known as a “design factor,” “design margin,” or “safety factor,” to ensure that the design that is built meets product specifications and operates safely.

Design factors are applied in process design to give some tolerance in the design. For example, the process stream average flows calculated from material balances are usually increased by a factor, typically 10%, to give some flexibility in process operation. This factor will set the maximum flows for equipment, instrumentation, and piping design. Where design factors are introduced to give some contingency in a process design, they should be agreed upon within the project organization and clearly stated in the project documents (drawings, calculation sheets, and manuals). If this is not done, there is a danger that each of the specialist design groups will add its own “factor of safety,” resulting in gross and unnecessary over-design. Companies often specify design factors in their design manuals. When selecting the design factor, a balance has to be made between the desire to make sure the design is adequate and the need to design to tight margins to remain competitive (economic consideration). Greater uncertainty in the design methods and data requires the use of bigger design factors.

In general design work, the magnitudes of safety factors are dictated by:

- Economic or market considerations,
- Accuracy of the design data and calculations,
- Potential changes in the operating performance,
- Background information available on the overall process.

Each safety factor must be chosen on basis of the existing conditions, and the chemical engineer should not hesitate to use a safety factor of zero if the situation warrants it. Some examples of recommended safety factors for equipment design are shown in Table (2).

What is meant by design margins and what are the factors that control its values?

Specification Sheets

Standard specification sheets are normally used to transmit the information required for the detailed design, or purchase, of equipment items, such as heat exchangers, pumps, columns, pressure vessels, etc. As well as ensuring that the information is clearly and unambiguously presented, standard specification sheets serve as check lists to ensure that all the information required is included. A generalization for equipment design is that standard equipment should be selected whenever possible. If the equipment is standard, the manufacturer may have the desired size in stock. In any case, the manufacturer can usually quote a lower price and give better guarantees for standard equipment than for special equipment.

Before a manufacturer is contacted, the engineer should evaluate the design needs and prepare a preliminary specification sheet for the equipment. This preliminary specification sheet can be used by the engineer as a basis for the preparation of the final specifications, or it can be sent to a manufacturer with a request for suggestions and fabrication information. Preliminary specifications for equipment should show the following:

- 1) Identification 2) Function 3) Operation 4) Materials handled 5) Basic design data
 - 6) Essential controls 7) Insulation requirements 8) Allowable tolerances
 - 9) Special information and details pertinent to the particular equipment, such as materials of construction including gaskets, installation, necessary delivery date, supports, and special design details or comments.
- Figures 12 and 13 show typical types of specification sheets for equipment. These sheets apply for the normal type of equipment encountered by a chemical engineer in design work. The details of mechanical design, such as shell or head thicknesses, are not included, since they do not have a direct effect on the performance of the equipment. However, for certain types of equipment involving unusual or extreme operating conditions, the engineer may need to extend the specifications to include additional details of the mechanical design.

Table (2)

Factors in equipment scale-up and design

Type of equipment	Is pilot plant usually necessary?	Major variables for operational design (other than flow rate)	Major variables characterizing size or capacity	Maximum scale-up ratio based on indicated characterizing variable	Approximate recommended safety or over-design factor, %
Agitated batch crystallizers	Yes	Solubility-temperature relationship	Flow rate Heat transfer area	>100:1	20
Batch reactors	Yes	Reaction rate Equilibrium state	Volume Residence time	>100:1	20
Centrifugal pumps	No	Discharge head	Flow rate Power input Impeller diameter	>100:1 >100:1 10:1	10
Continuous reactors	Yes	Reaction rate Equilibrium state	Flow rate Residence time	>100:1	20
Cooling towers	No	Air humidity Temperature decrease	Flow rate Volume	>100:1 10:1	15
Cyclones	No	Particle size	Flow rate Diameter of body	10:1 3:1	10
Evaporators	No	Latent heat of vaporization Temperatures	Flow rate Heat-transfer area	>100:1 >100:1	15
Hammer mills	Yes	Size reduction	Flow rate Power input	60:1 60:1	20
Mixers	No	Mechanism of operation System geometry	Flow rate Power input	>100:1 20:1	20
Nozzle-discharge centrifuges	Yes	Discharge method	Flow rate Power input	10:1 10:1	20 20

Factors in equipment scale-up and design (Continued)

Type of equipment	Is pilot plant usually necessary?	Major variables for operational design (other than flow rate)	Major variables characterizing size or capacity	Maximum scale-up ratio based on indicated characterizing variable	Approximate recommended safety or over-design factor, %
Packed columns	No	Equilibrium data Superficial vapor velocity	Flow rate Diameter Height to diameter ratio	>100:1 10:1	15
Plate columns	No	Equilibrium data Superficial vapor velocity	Flow rate Diameter	>100:1 10:1	15
Plate-and-frame filters	Yes	Cake resistance or permeability	Flow rate Filtration area	>100:1 >100:1	20
Reboilers	No	Temperatures Viscosities	Flow rate Heat-transfer area	>100:1 >100:1	15
Reciprocating compressors	No	Compression ratio	Flow rate Power input Piston displacement	>100:1 >100:1 >100:1	10
Rotary filters	Yes	Cake resistance or permeability	Flow rate Filtration area	>100:1 25:1	20
Screw conveyors	No	Bulk density	Flow rate Diameter Drive horsepower	90:1 8:1	20
Screw extruders	No	Shear rate	Flow rate Power input	100:1 100:1	20 10
Sedimentation centrifuges	No	Discharge method	Flow rate Power input	10:1 10:1	20 20
Settlers	No	Settling velocity	Volume Residence time	>100:1	15
Spray columns	No	Gas solubilities	Flow rate Power input	10:1	20

HEAT EXCHANGER	
Identification: Item Condenser Item No. <i>H-S</i> No. required <i>I</i>	Date <i>I-I-90</i> By <i>JRL</i>
Function: Condense overhead <i>vapors from methanol fractionation column</i>	
Operation: <i>Continuous</i>	
Type: <i>Horizontal</i> Fixed tube sheet Expansion ring in shell Duty <i>3,400,000 Btu/h</i> Outside area <i>470 sq ft</i>	
Tube side: Fluid handled <i>Cooling water</i> Flow rate <i>380 gpm</i> Pressure <i>20 psig</i> Temperature <i>15°C to 25°C</i> Head material <i>Carbon steel</i>	Tubes: <i>1 in. diam. 14 BWG</i> <i>1.25" Centers A Pattern</i> <i>225 Tubes each 8 ft long</i> <i>2 Passes</i> Tube material <i>Carbon steel</i>
Shell side: Fluid handled <i>Methanol vapor</i> Flow rate <i>7000 lb/h</i> Pressure <i>0 psig</i> Temperature <i>65°C to (constant temp.)</i>	Shell: <i>22 in. diam. I Passes</i> <i>(Transverse baffles Tube support Req'd)</i> <i>(Longitudinal baffles 0 Req'd)</i> Shell material <i>Carbon steel</i>
Utilities: <i>Untreated cooling water</i> Controls: <i>Cooling-water rare controlled by vapor temperature in vent line</i> Insulation: <i>2-in. rock cork or equivalent; weatherproofed</i> Tolerances: <i>Tubular Exchangers Manufacturers Association (TEMA) standards</i> Comments and drawings: <i>Location and sizes of inlets and outlets are shown on drawing</i>	

Fig. (12) Specification sheet for heat exchangers using U.S. customary units.

SIEVE-TRAY COLUMN				
Identification:	Item _____ Item No. _____ No. required _____	Date _____ By _____		
Function:				
Operation:				
Materials handled:	<i>Feed</i>	<i>Overhead</i>	<i>Reflux</i>	<i>Bottoms</i>
Quantity	_____	_____	_____	_____
Composition	_____	_____	_____	_____
Temperature	_____	_____	_____	_____
Design data:				
No. of trays		Reflux ratio		
Pressure		Tray spacing		
Functional height		Skirt height		
Material of construction _____				
Diameter: Liquid density _____ lb/ft ³ (- k g / m ³)				
Vapor density _____ lb/ft ³ (- k g / m ³)				
Maximum allowable vapor velocity (superficial) _____ ft/s (_____ m/s)				
Maximum vapor flow rate _____ ft ³ /s (_____ m ³ /s)				
Recommended inside diameter _____				
Hole size and arrangement _____				
Tray thickness _____				
Utilities:				
Controls:				
Insulation:				
Tolerances:				
Comments and drawings:				

Fig. (13) Specification sheet for sieve-tray distillation column.

