Concept of Design Process

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Outline

- Steps in Design
- Process Creation
- Heuristics in Process Design

Steps in Design

Engineering Design

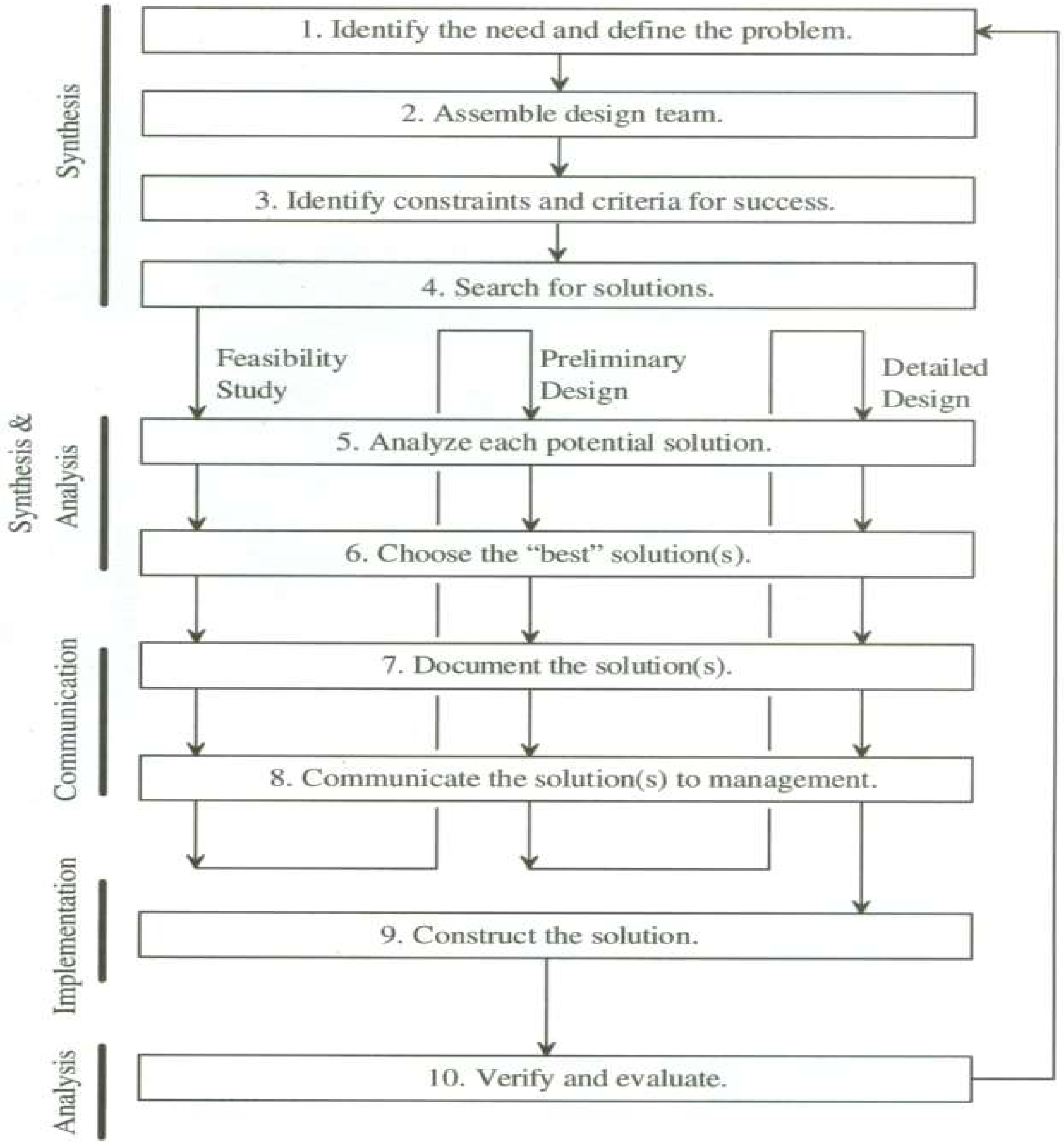
Problem-solving methodology

- Definition of the problem
- Generating of information
- Generation of alternative solutions
- Evaluation of alternatives
- Solution to the problems
- Communication of the results

Design Requirements

- The identification and establishment of Design Requirements are critical for a Good Design
- Acceptable performance is essential
- Performance requirements include
  - Products
    - Functional
    - Complementary
  - Process
    - key lifecycle functions, such as process stability, quality of the products, etc
    - key process activities to be undertaken across the lifecycle functions such as handling capacity, production rate, conversion ratio, etc
    - procedures that may be required to manage the processes, such as automation, failure control, employee training etc.

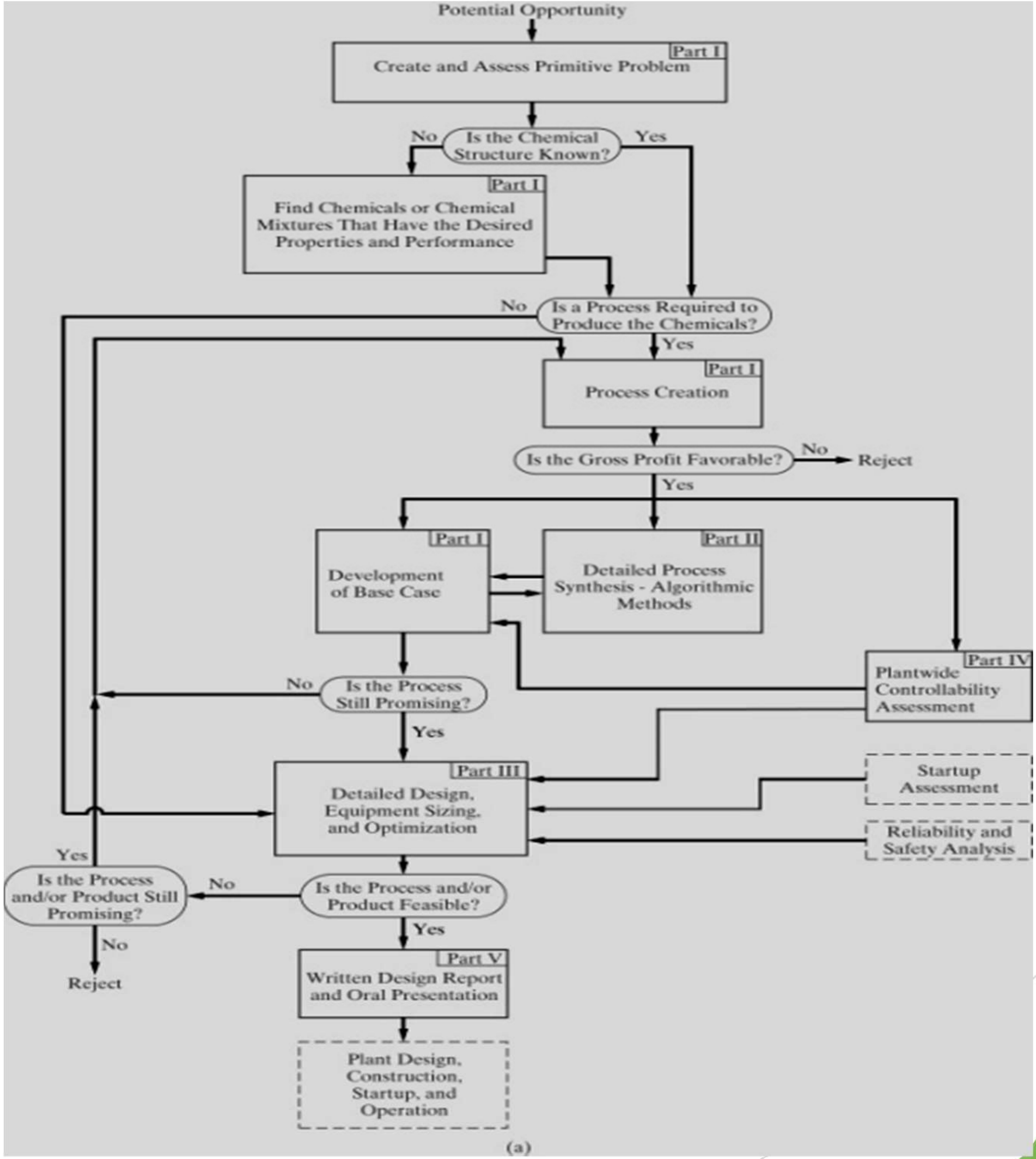
Design Step

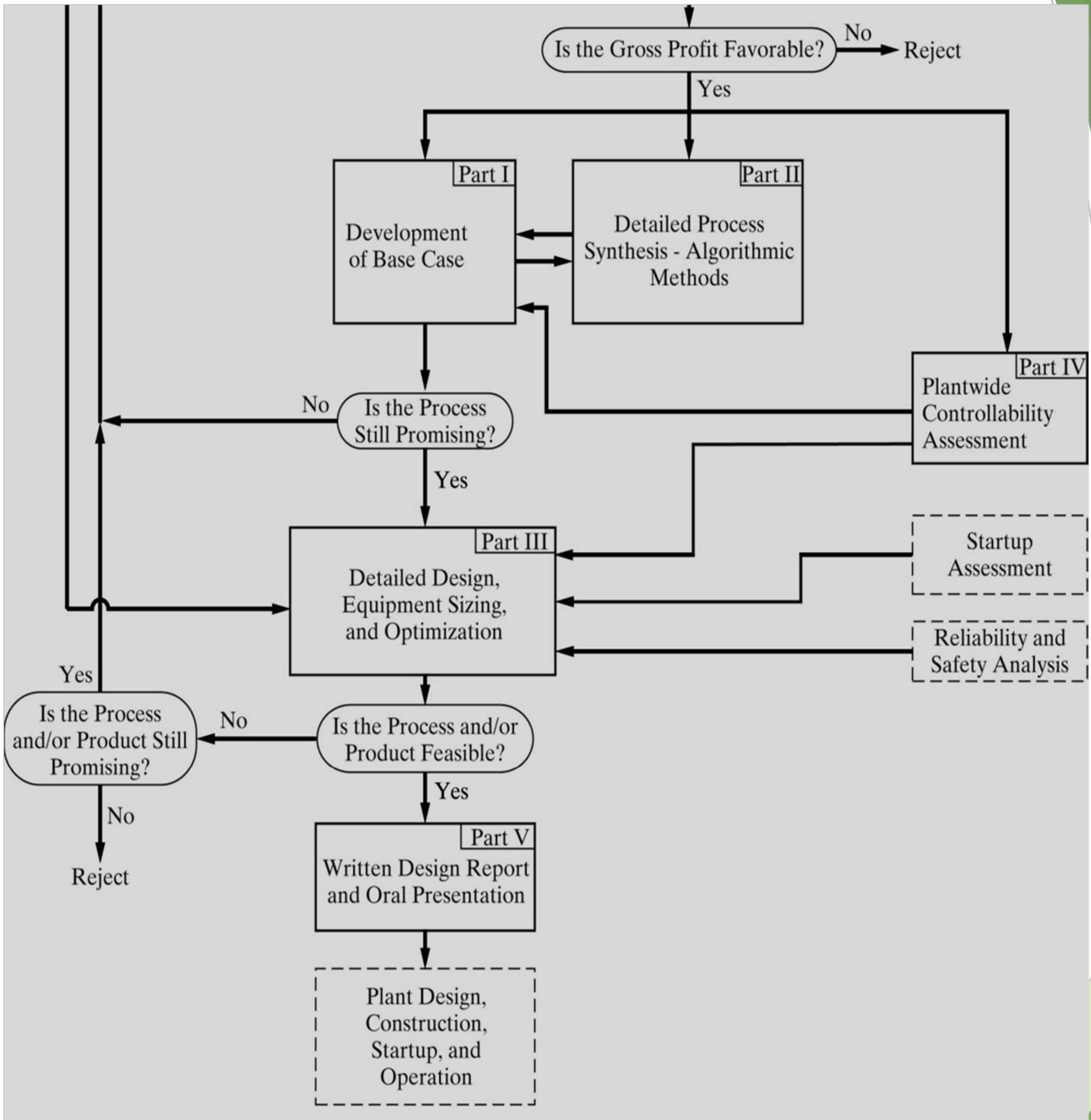


Synthesis
1. Identify the need and define the problem.
2. Assemble design team.
3. Identify constraints and criteria for success.
4. Search for solutions.
Feasibility Study
Preliminary Design
Detailed Design
Synthesis & Analysis
5. Analyze each potential solution.
6. Choose the "best" solution(s).
Communication
7. Document the solution(s).
8. Communicate the solution(s) to management.
Implementation
9. Construct the solution.
Analysis
10. Verify and evaluate.

Process Of Chemical Engineering Design

Map




Is the Gross Profit Favorable?
No
Reject
Yes
Part I
Development of Base Case
Part II
Detailed Process Synthesis - Algorithmic Methods
Part IV
Plantwide Controllability Assessment
No
Is the Process Still Promising?
Yes
Part III
Detailed Design, Equipment Sizing, and Optimization
Startup Assessment
Reliability and Safety Analysis
Yes
Is the Process and/or Product Still Promising?
No
Is the Process and/or Product Feasible?
Yes
No
Reject
Part V
Written Design Report and Oral Presentation
Plant Design, Construction, Startup, and Operation
(a)

Steps in Process/Product Design

1. Design problems - assume they are open ended with many solutions that are attractive and near optimal.
2. Steps to design are not the same generally between different designers.
3. Product and process development ← experiments to uncover and explain reaction mechanisms.
4. Product/process design ← composition of mixtures, complex flow sheets, select operating conditions, optimization, creating configured industrial/commercial products.
5. Engineers frequently obtain patents.
6. Basic steps → Detailed description
7. Potential opportunity → Design team creates a primitive problem.
8. Primitive problem : Seeking chemicals/mixtures w/ desired properties.
9. When a process is required → implement process creation.
10. If profitable → Base case is developed.

Issues In Design

- ❖Utility and cost
- ❖Single and multi-functionality
- ❖Batch or mass production
- ❖Patents
- ❖Aesthetics
- ❖Integrity of product (wholeness)
- ❖Whole life-cycle planning
- ❖Health effects and safety
- ❖Recycling and disposal
- ❖End of product life and replacement issues
- ❖Failure modes
- ❖Effects on society

Economic Analysis

- What is the relevance of economic analysis to design?
- Economic assumption : Measure of value is “monetary”
- Process cost in context of the company
- Reporting costs, financial status, and transactions.
- Value today, value tomorrow.
- Material cost, labor cost, indirect cost
- Manufacturing cost, storage cost, transport cost
- Product cost scaling and correction factors

Statistical analysis

- What relevance is statistics to design?
- Statistical focus : “The one and the many”
- Measures of central tendency
- Measures of variation
- Probability
- Uncertainty analysis
- Linear regression
- Six sigma quality concept
- Optimization and development of designs
- Statistics in process control for quality

Aspentech HYSYS Modeling Code

- Menu driven, Mouse driven.
- Flow sheets, Modular units.
  - Mixers, Reactors, Flash separators, Distillation units, Heat exchangers.
- Reaction databases.
- Chemical property calculations.
- Species, Mass, Momentum, Heat Balances.
- Equipment Sizing.
- Economic calculations.
- Optimization.

CAD, MAP Window

- CAD – develop engineering drawings
- MAP Window– work with mapping systems for various geographical analyses

Process Creation

Process Creation

- **Preliminary Database Creation**
  - to assemble data to support the design.
- **Experiments**
  - often necessary to supply missing database items or verify crucial data.
- **Preliminary Process Synthesis**
  - top-down approach.
  - to generate a “synthesis tree” of design alternatives.
  - illustrated by the synthesis of processes for the manufacture of VCM.
- **Development of Base-case Design**
  - focusing on the most promising alternative(s) from the synthesis tree.

Preliminary Database Creation

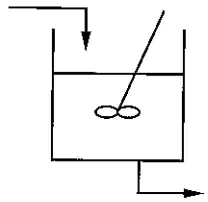
- Thermo physical property data
  - physical properties
  - phase equilibrium (VLE data)
  - Property prediction methods
- Environmental and safety data
  - toxicity data
  - flammability data
- Chemical Prices
  - e.g. as published in the *Chemical Marketing Reporter*
- Experiments
  - to check on crucial items above

Preliminary Process Synthesis

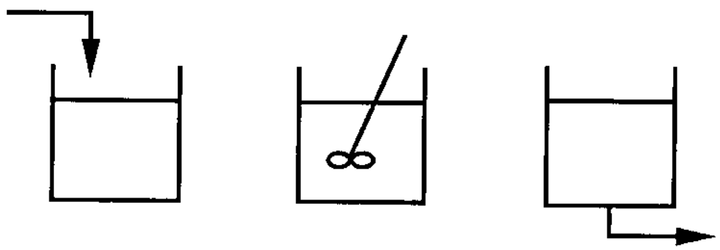
Synthesis of chemical processes involves:

- Selection of processing mode: continuous or batch
- Fixing the chemical state of raw materials, products, and by-products, noting the differences between them.
- Process operations (unit operations) - flow sheet building blocks
- Synthesis steps -
  1. Eliminate differences in molecular types
  2. Distribute chemicals by matching *sources* and *sinks*
  3. Eliminate differences in composition
  4. Eliminate differences in temperature, pressure and phase
  5. Integrate tasks (combine *tasks* into *unit operations*)

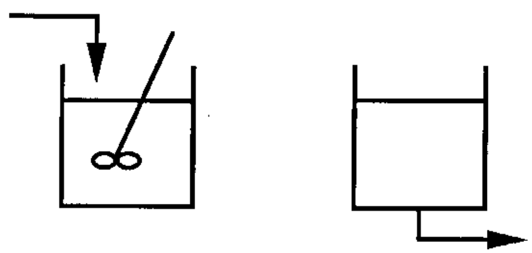
Continuous or batch processing?



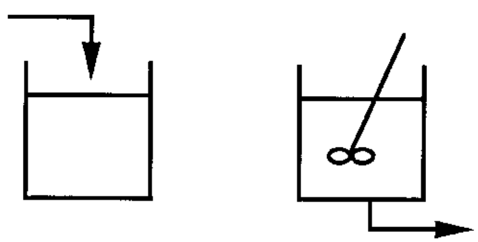
Continuous



Batch



Fed-batch



Batch-product removal

The Chemical State

- Decide on the raw material and product specifications (*states*):
  - Mass (flow rate)
  - Composition (mole or mass fraction of each chemical species having a unique molecular type)
  - Phase (solid, liquid, or gas)
  - Form (e.g., particle-size distribution and particle shape)
  - Temperature
  - Pressure

Process Operations

- Chemical reaction
  - Positioning in the flow sheet involves many considerations (conversion, rates, etc.), related to T and P at which the reaction are carried out.
- Separation of chemicals
  - needed to resolve difference between the desired composition of a product stream and that of its source. Selection of the appropriate method depends on the differences of the physical properties of the chemical species involved.
- Phase separation
- Change of temperature
- Change of pressure
- Change of phase
- Mixing and splitting of streams and branches

Process Creation

Example 1:

Vinyl Chloride Manufacture

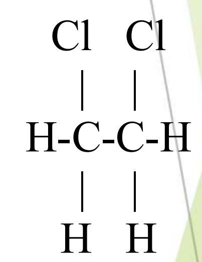
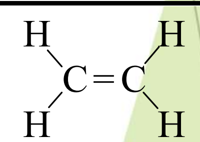
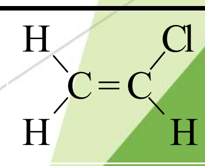
(VCM)

Assess Primitive Problem

- Process design begins with a primitive design problem that expresses the ***current situation*** and provides an ***opportunity to satisfy*** a societal need.
- Normally, the primitive problem is examined by a small design team, who begins to assess its possibilities, to refine the problem statement, and to generate more specific problems:
  - Raw materials - available in-house, can be purchased or need to be manufactured?
  - Scale of the process (based upon a preliminary assessment of the current production, projected market demand, and current and projected selling prices)
  - Location for the plant
- Refined through meetings with engineering technical management, business and marketing.
- *Brainstorming* to generate alternatives

❶ Eliminate differences in molecular types

Chemicals participating in VC Manufacture:

Chemical	Molecular weight	Chemical formula	Chemical structure
Acetylene	26.04	C_2H_2	H - C ≡ C - H
Chlorine	70.91	Cl_2	Cl-Cl
1,2-Dichloroethane	98.96	$C_2H_4Cl_2$	
Ethylene	28.05	C_2H_4	
Hydrogen chloride	36.46	HCl	H-Cl
Vinyl chloride	62.50	C_2H_3Cl	

Selection of pathway to VCM (1)

- Direct chlorination of ethylene:

$$C_2H_4 + Cl_2 \rightarrow C_2H_3Cl + HCl \qquad (2.1)$$

Advantages:

- Attractive solution to the specific problem denoted as Alternative 2 in analysis of primitive problem.
- Occurs spontaneously at a few hundred ^oC.

Disadvantages:

- Does not give a high yield of VC without simultaneously producing large amounts of by-products such as dichloroethylene
- Half of the expensive chlorine is consumed to produce HCl by-product, which may not be sold easily.

Selection of pathway to VCM (2)

- Hydro chlorination of acetylene:

$$C_2H_2 + HCl \rightarrow C_2H_3Cl \qquad (2.2)$$

Advantages:

- This exothermic reaction is a potential solution for the specific problem denoted as Alternative 3. It provides a good conversion (98%) of C_2H_2 VC in the presence of $HgCl_2$ catalyst impregnated in activated carbon at atmospheric pressure.
- These are fairly moderate reaction conditions, and hence, this reaction deserves further study.

Disadvantages:

- Flammability limits of C_2H_2 (2.5 $\rightarrow$100%)

Selection of pathway to VCM (3)

❸ Thermal cracking of $C_2H_4Cl_2$ from chlorination of C_2H_4:

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2 \qquad (2.3)$$

$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl \qquad (2.4)$$

$$C_2H_4 + Cl_2 \rightarrow C_2H_3Cl + HCl \qquad (2.1)$$

Advantages:

- Conversion of ethylene to 1,2-dichloroethane in exothermic reaction (2.3) is ≈98% at 90 ^oC and 1 atm with a Friedel-Crafts catalyst such as $FeCl_3$. This intermediate is converted to vinyl chloride by thermal cracking according to the endothermic reaction (2.4), which occurs spontaneously at 500 ^oC with conversions as high as 65% (Alternative 2).

Disadvantage:

- Half of the expensive chlorine is consumed to produce HCl by-product, which may not be sold easily.

Selection of pathway to VCM (4)

❹ Thermal Cracking of $C_2H_4Cl_2$ from Oxychlorination of C_2H_4:

$$C_2H_4 + 2HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O \quad (2.5)$$

$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl \quad (2.4)$$

$$C_2H_4 + HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_3Cl + H_2O \quad (2.6)$$

Advantages:

- Highly exothermic reaction (2.5) achieves a 95% conversion to $C_2H_4Cl_2$ in the presence of $CuCl_2$ catalyst, followed by pyrolysis step (2.4) as Reaction Path 3.
- Excellent candidate when cost of HCl is low
- Solution for specific problem denoted as Alternative 3.

Disadvantages:

- Economics dependent on cost of HCl

Selection of pathway to VCM (5)

- Balanced Process for Chlorination of Ethylene:

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2 \qquad (2.3)$$

$$C_2H_4 + 2HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O \qquad (2.5)$$

$$2C_2H_4Cl_2 \rightarrow 2C_2H_3Cl + 2HCl \qquad (2.4)$$

$$2C_2H_4 + Cl_2 + \tfrac{1}{2}O_2 \rightarrow 2C_2H_3Cl + H_2O \qquad (2.7)$$

Advantages:

- Combination of Reaction Paths 3 and 4 - addresses Alternative 2.
- All Cl_2 converted to VC
- No by-products!

Evaluation of Alternative Pathways

- Reaction Path ❶ is eliminated due its low selectivity.
- This leaves four alternative paths, to be compared first in terms of Gross Profit.

Chemical Bulk Prices

Chemical	Cost (cents/lb)
Ethylene	18
Acetylene	50
Chlorine	11
Vinyl chloride	22
Hydrogen chloride	18
Water	0
Oxygen (air)	0

Computing Gross Profit

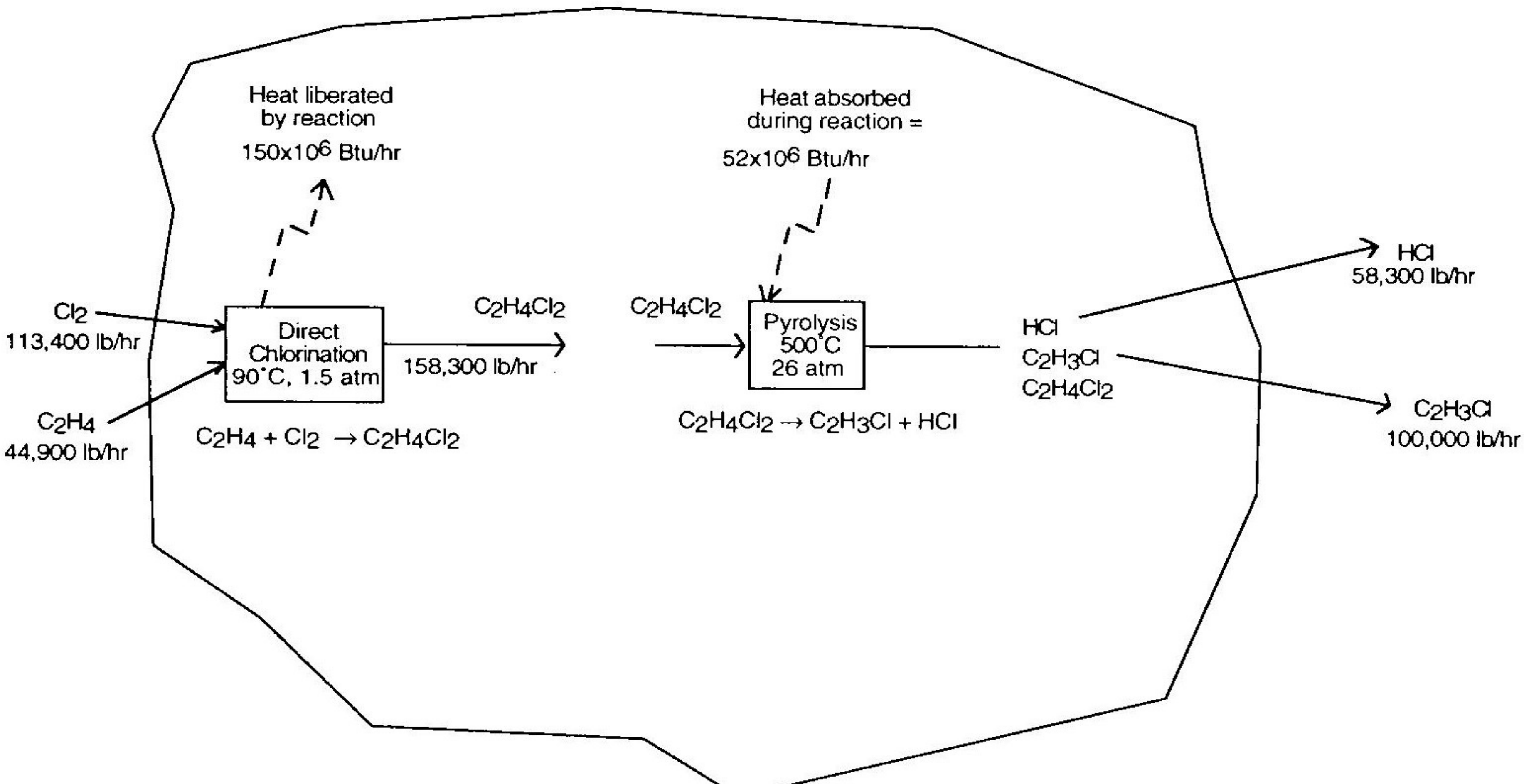
Reaction path ❸	C_2H_4	+	Cl_2	=	C_2H_3Cl	+	HCl
lb-mole	1		1		1		1
Molecular weight	28.05		70.91		62.50		36.46
lb	28.05		70.91		62.50		36.46
lb/lb of vinyl chloride	0.449		1.134		1		0.583
cents/lb	18		11		22		18

Gross profit = 22(1) + 18(0.583) - 18(0.449) - 11(1.134) = 11.94 cents/lb VC

Reaction Path	Overall Reaction	Gross Profit (cents/lb of VC)
❷	$C_2H_2 + HCl = C_2H_3Cl$	-9.33
❸	$C_2H_4 + Cl_2 = C_2H_3Cl + HCl$	11.94
❹	$C_2H_4 + HCl + \frac{1}{2}O_2 = C_2H_3Cl + H_2O$	3.42
❺	$2C_2H_4 + Cl_2 + \frac{1}{2}O_2 = 2C_2H_3Cl + H_2O$	7.68

❷ Distribute the chemicals

- A conversion of 100% of the C_2H_4 is assumed in the chlorination reaction.



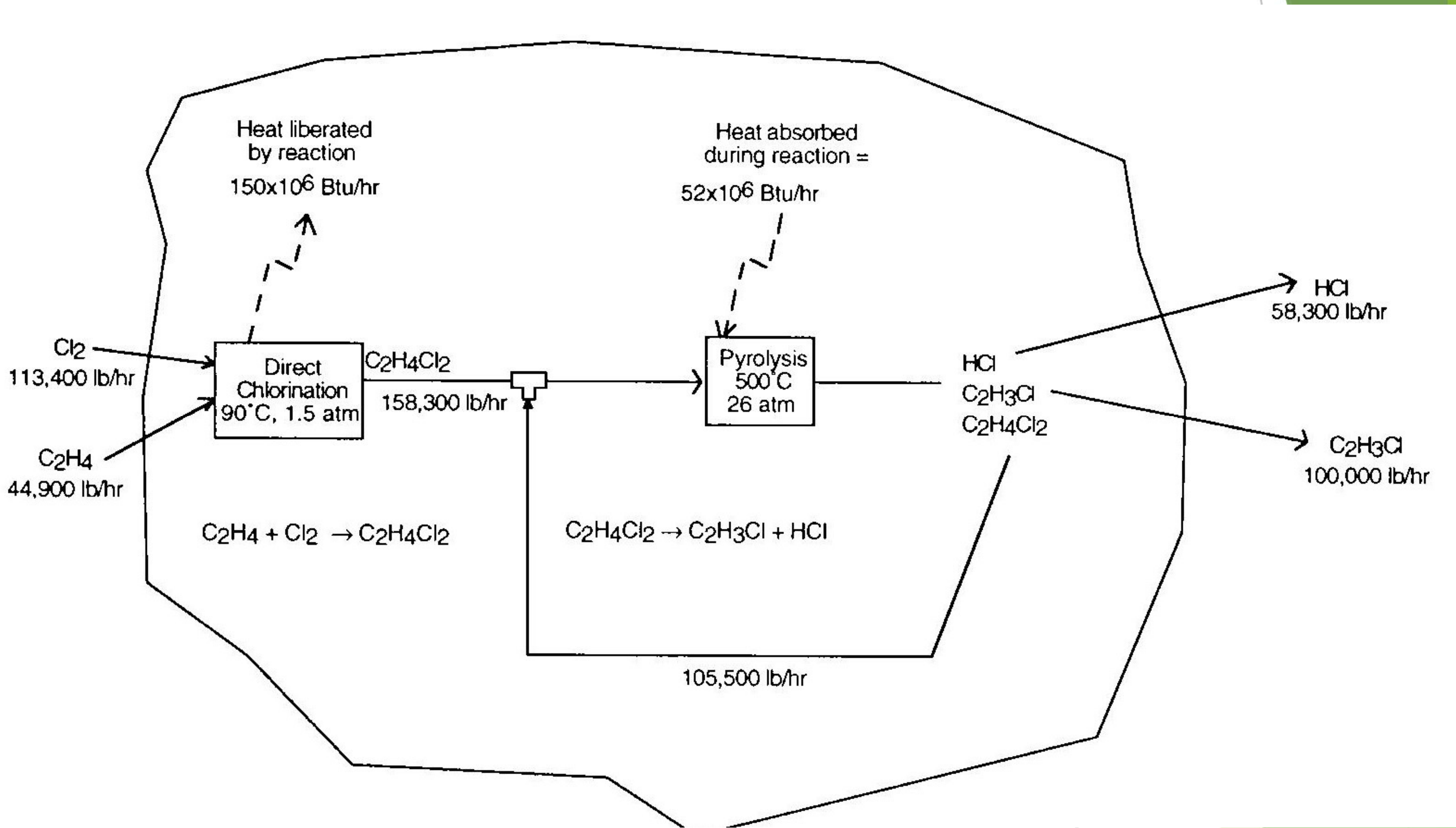
❷ Distribute the chemicals

- Only 60% of the $C_2H_4Cl_2$ is converted to C_2H_3Cl with a byproduct of HCl, according to Eqn. (2.4).
- To satisfy the overall material balance, 158,300 lb/h of C_2H_4Cl must produce 100,000 lb/h of C_2H_3Cl and 58,300 lb/h of HCl.
- But a 60% conversion only produces 60,000 lb/h of VC.
- The additional $C_2H_4Cl_2$ needed is computed by mass balance to equal:

  [(1 - 0.6)/0.6] x 158,300 or 105,500 lb/h.
- Its source is a recycle stream from the separation of C_2H_3Cl from unreacted $C_2H_4Cl_2$, from a mixing operation, inserted to combine the two sources, to give a total 263,800 lb/h.

❷ Distribute the chemicals

- The effluent stream from the pyrolysis operation is the source for the C_2H_3Cl product, the HCl by-product, and the $C_2H_4Cl_2$ recycle.



❷ Distribute the chemicals

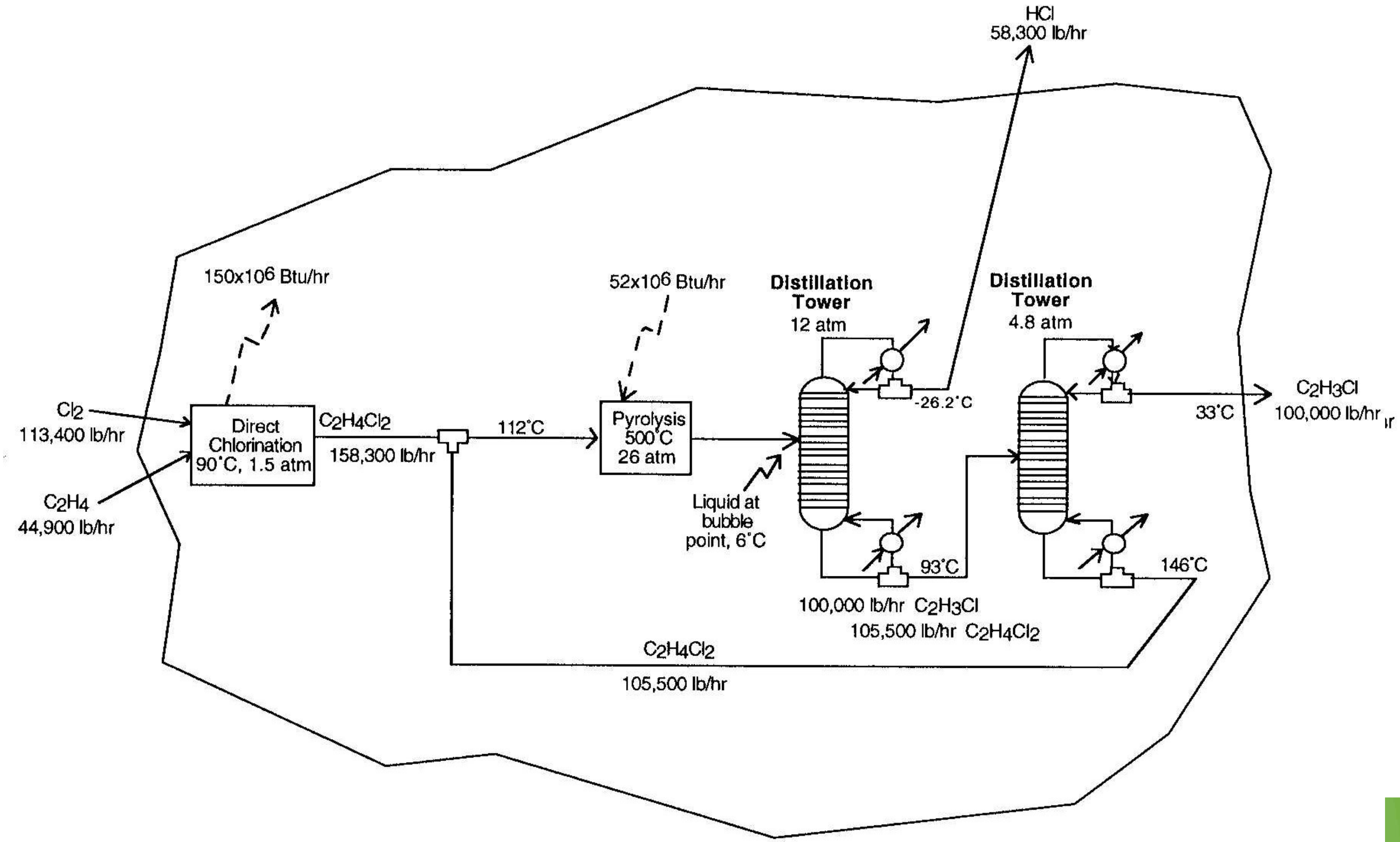
- **Reactor pressure levels:**
  - Chlorination reaction: 1.5 atm is recommended, to eliminate the possibility of an air leak into the reactor containing ethylene.
  - Pyrolysis reaction: 26 atm is recommended by the B.F. Goodrich patent (1963) without any justification. Since the reaction is irreversible, the elevated pressure does not adversely affect the conversion. Most likely, the patent recommends this pressure to reduce the size of the pyrolysis furnace, although the tube walls must be considerably thicker and many precautions are necessary for operation at elevated pressures.
  - The pressure level is also an important consideration in selecting the separation operations, as will be discussed in the next synthesis step.

❸ Eliminate Differences in Composition

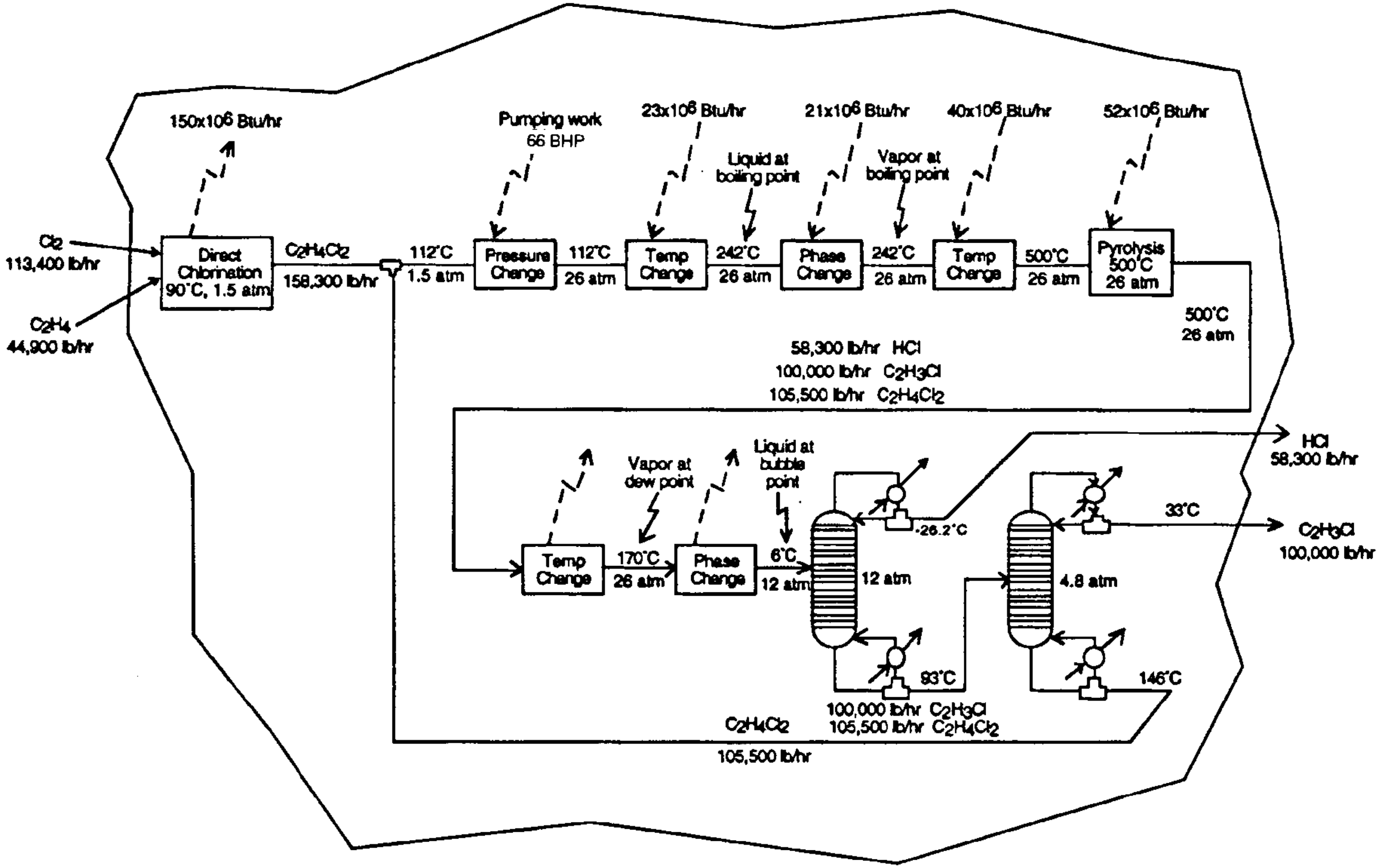
- The product of the chlorination reaction is nearly pure $C_2H_4Cl_2$, and requires no purification.
- In contrast, the pyrolysis reactor conversion is only 60%, and one or more separation operations are required to match the required purities in the C_2H_3Cl and HCl sinks.
- One possible arrangement is given in the next slide. The data below explains the design decisions made.

	Boiling point (°C)				Critical constants	
Chemical	1 atm	4.8 atm	12 atm	26 atm	T_c, °C	P_c, atm
HCl	-84.8	-51.7	-26.2	0	51.4	82.1
C_2H_3Cl	-13.8	33.1	70.5	110	159	56
$C_2H_4Cl_2$	83.7	146	193	242	250	50

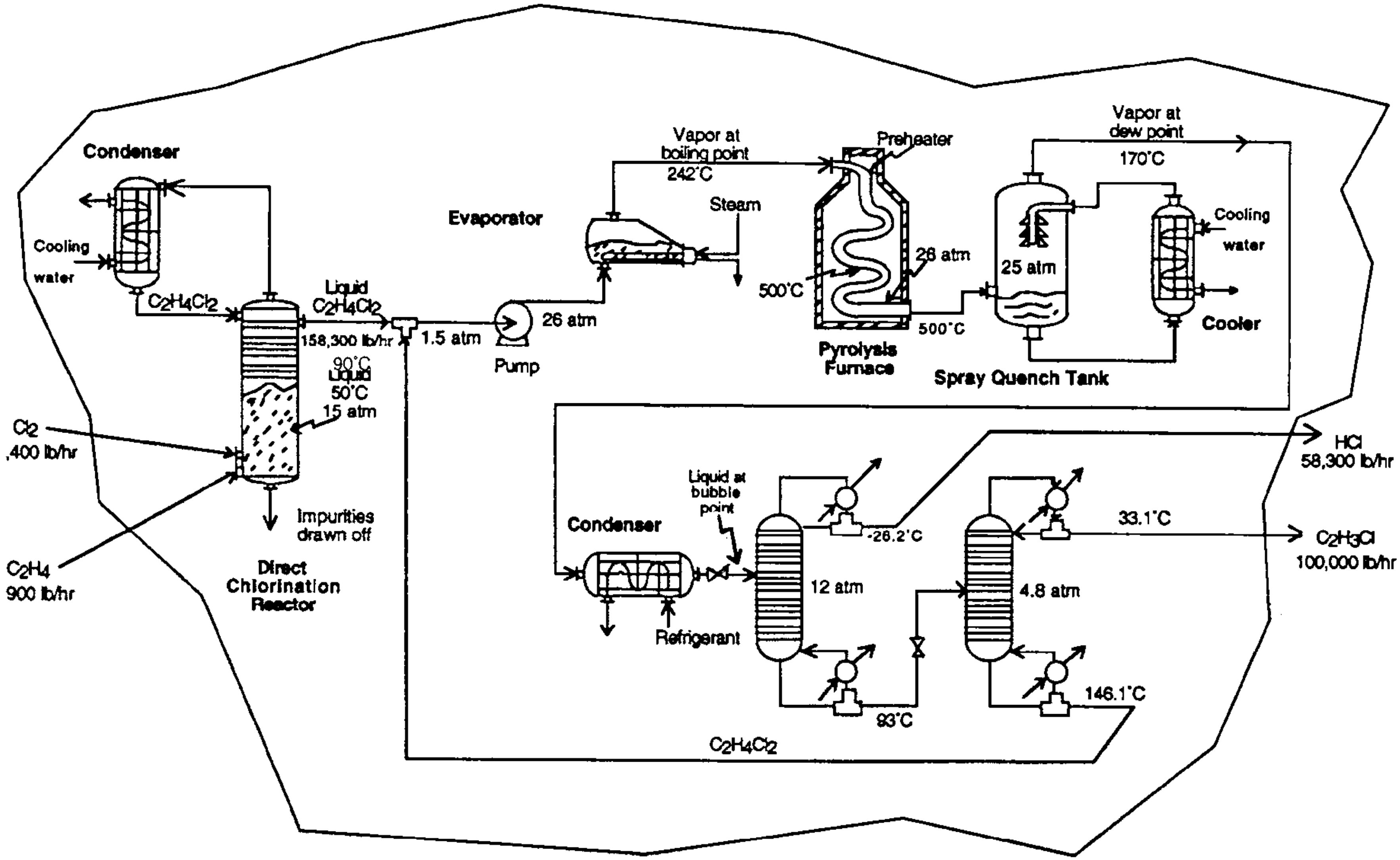
❸ Eliminate Differences in Composition



❹ Eliminate differences in T, P and phase



❺ Integrate tasks (*tasks* ⇒ *unit operations*)



Development of Base-case Design

Develop one or two of the more promising flow sheets from the synthesis tree for more detailed consideration.