Introduction to process design

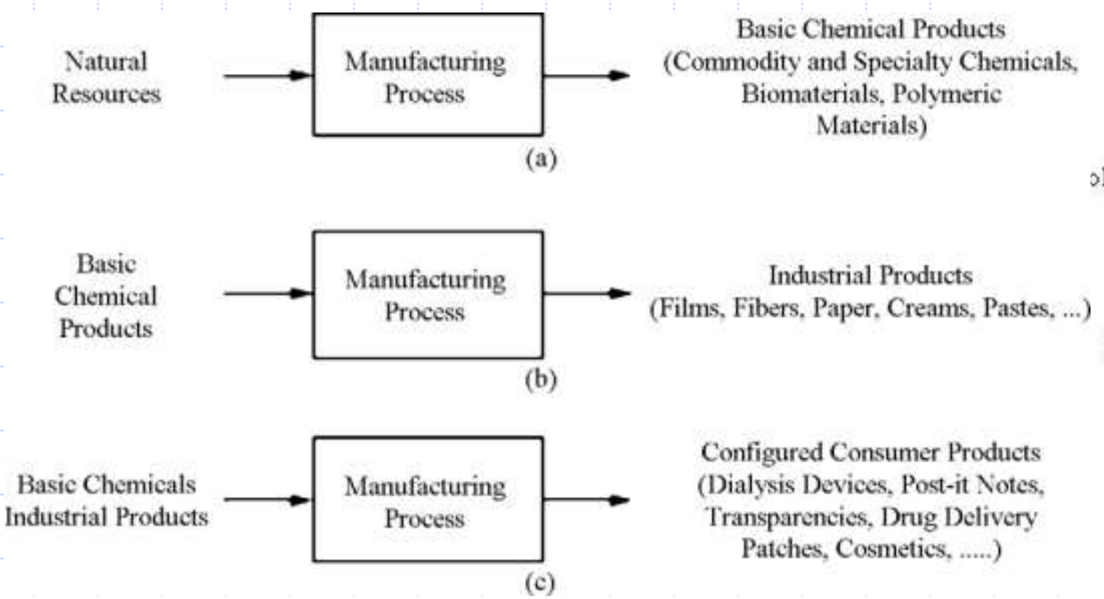
Maurizio Fermeglia
Maurizio.fermeglia@units.it
Department of Engineering & Architecture
University of Trieste

Agenda

- Steps in Designing/Retrofitting Chemical Processes
  - Assess Primitive Problem
  - Process Creation
  - Development of Base Case
  - Detailed Process Synthesis - Algorithmic Methods
  - Process Controllability Assessment
  - Detailed Design, Sizing, Cost Estimation, Optimization
  - Construction, Start-up and Operation
- Environmental Issues
- Safety Issues
- Process schemes

Manufacture of chemical products

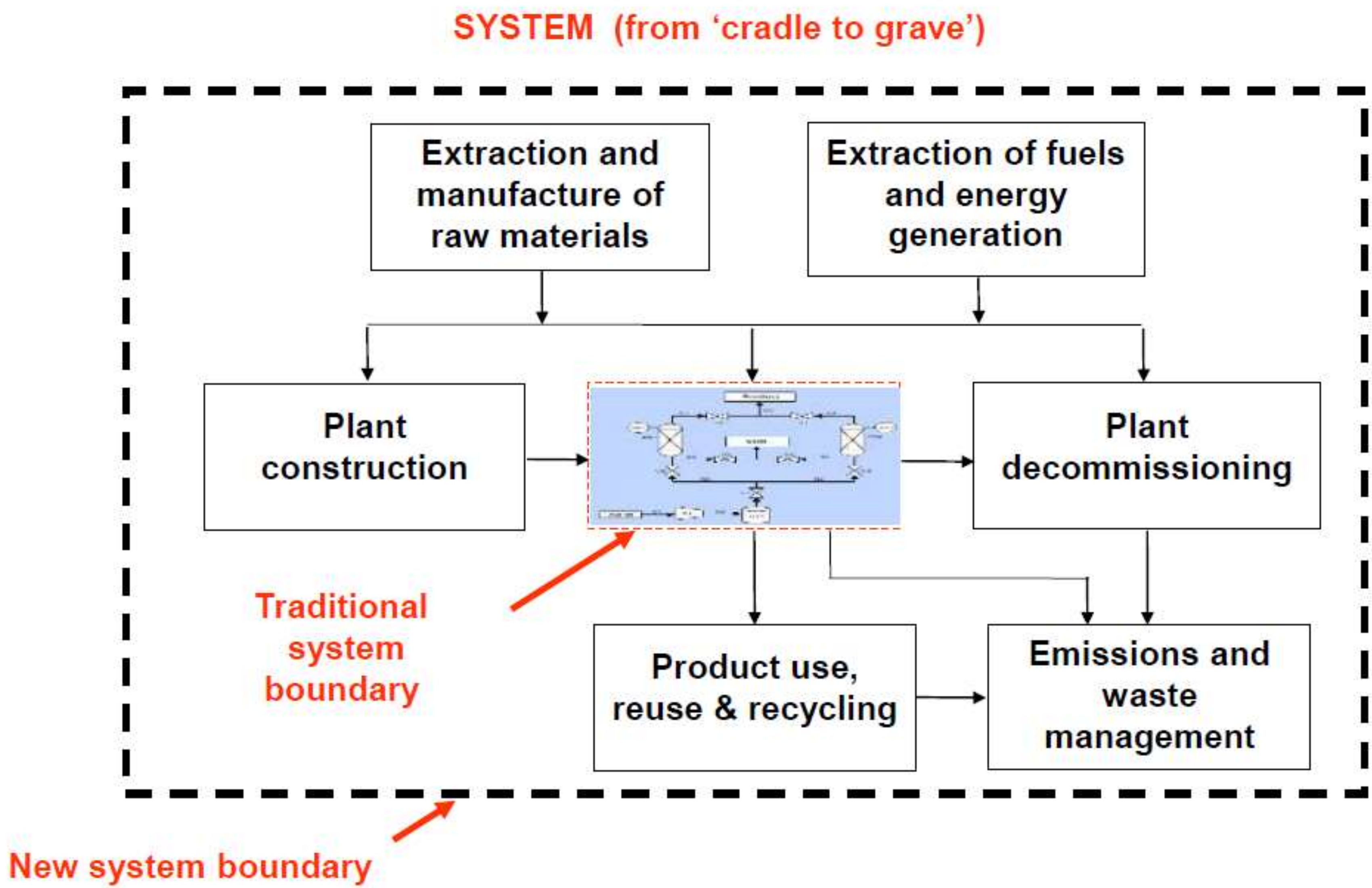
- The design or retrofit of chemical processes begins with a desire to produce profitable chemicals that satisfy societal needs
- Partly due to the growing awareness of the public, many design projects involve the redesign, or *retrofitting*, of existing chemical processes to solve environmental problems and to adhere to stricter standards of safety



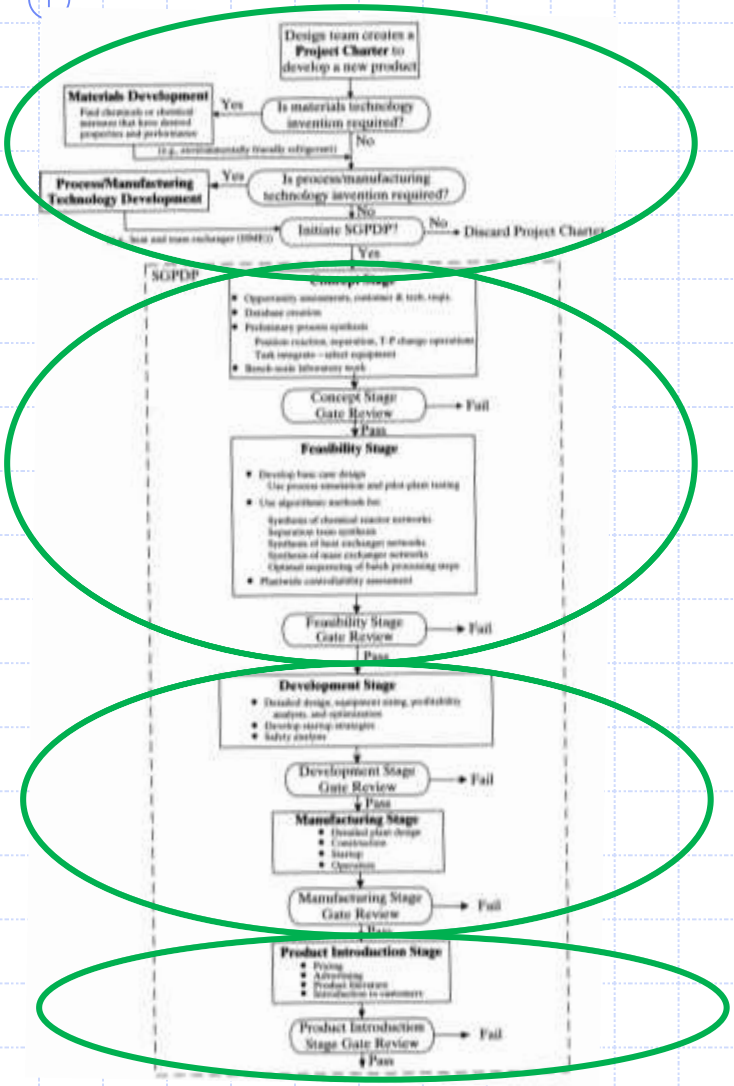
Origin of Design Problems

- Explorations of chemists, biochemists, and engineers in research labs
  - to satisfy the desires of customers
  - to obtain chemicals with improved properties for applications.
- … several well-known products, like Teflon (poly-tetrafluoroethylene), were discovered by accident.
- … an inexpensive source of a raw material(s) becomes available.
- … the engineer himself,
  - inclination that a new chemical or route to produce an existing chemical can be very profitable.

New system boundary definition



Steps in Product/Process Design



Initial Decision

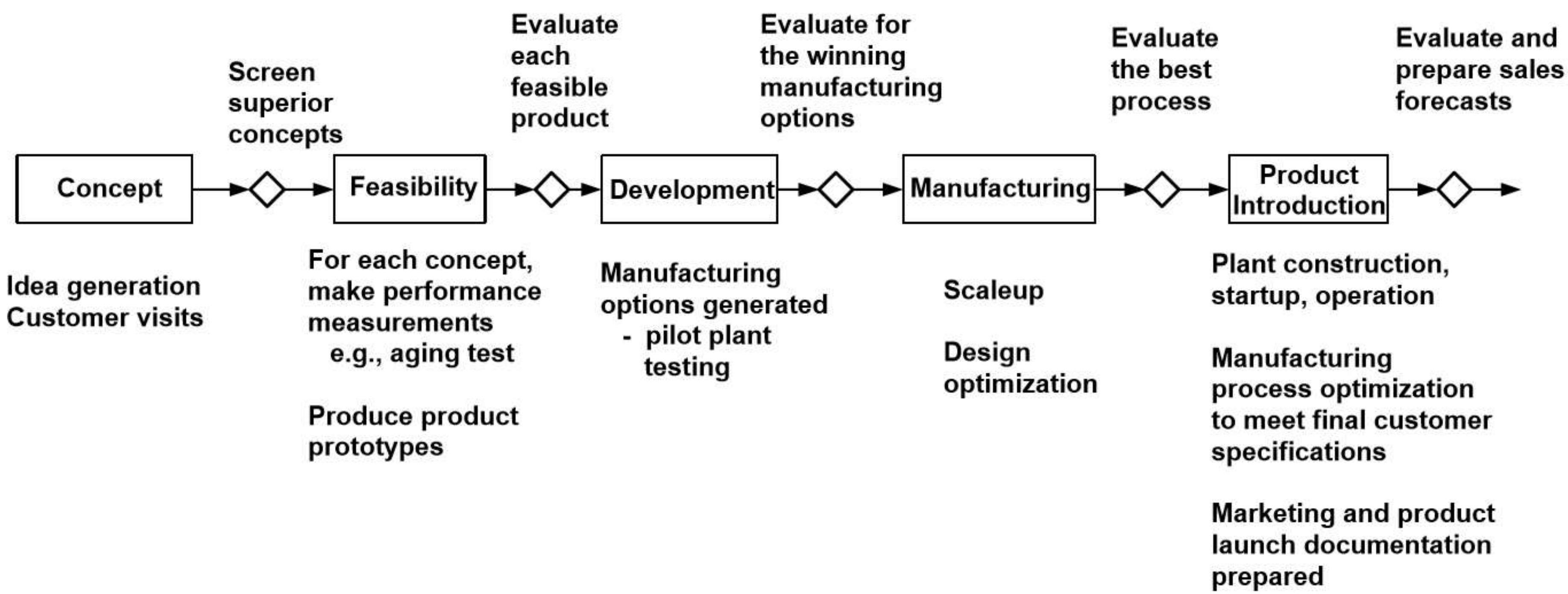
Concept & Feasibility

Development & Manufacturing

Product Introduction

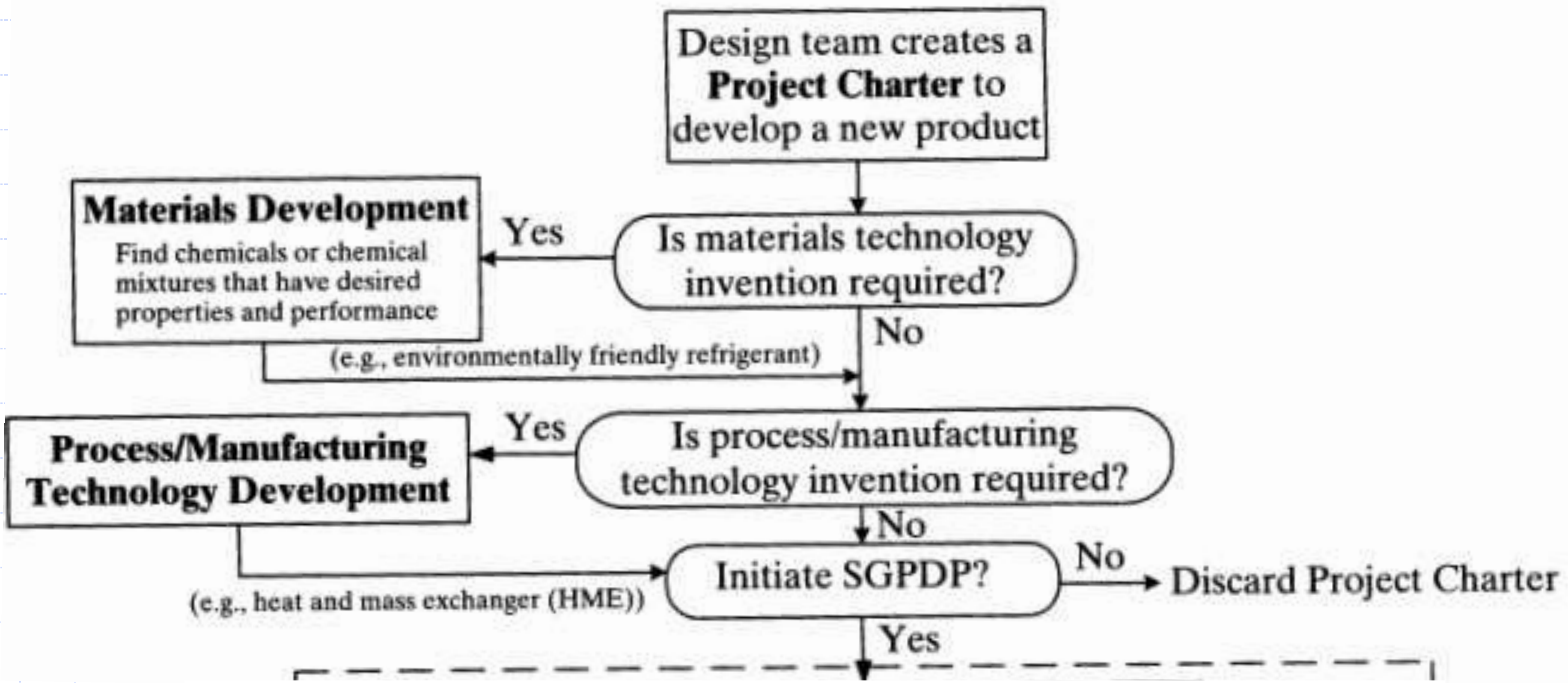
Stage-Gate Product Development Process

- SGPDP – Developed by Robert Cooper (2001, 2002, 2005)
- Roadmap for transforming new ideas into products that satisfy customer needs - ready to be launched



Steps in Product/Process Design

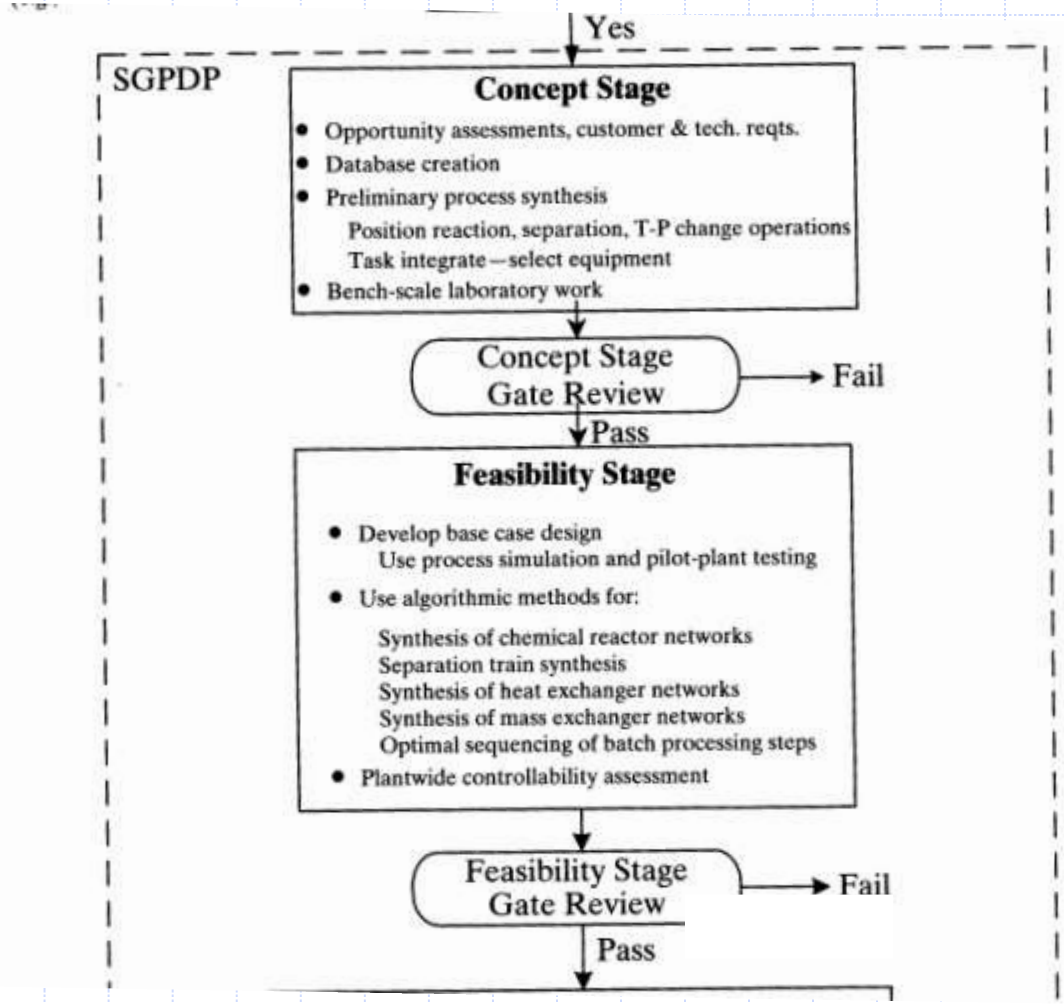
- Initial Decision



Stage-Gate™ product-development process (SGPDP)

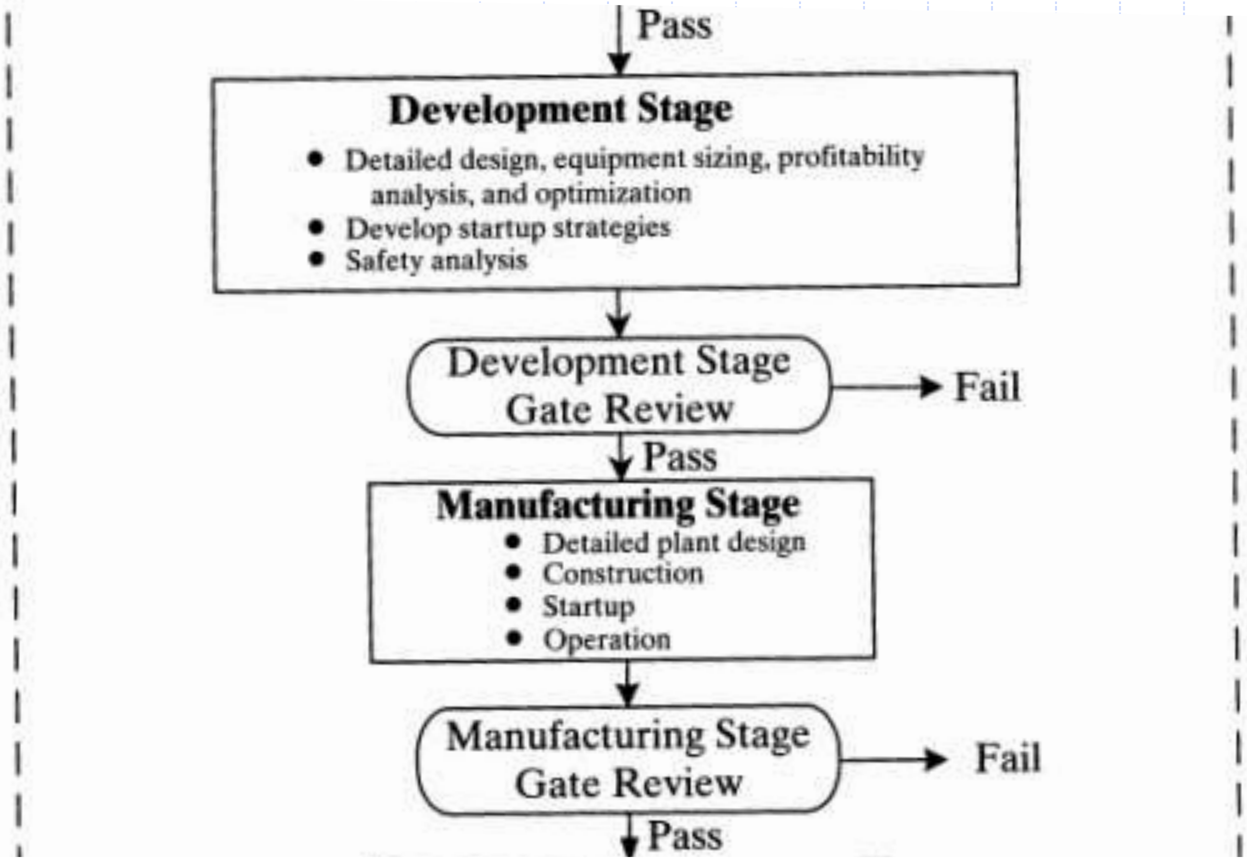
Steps in Product/Process Design

- Concept & Feasibility



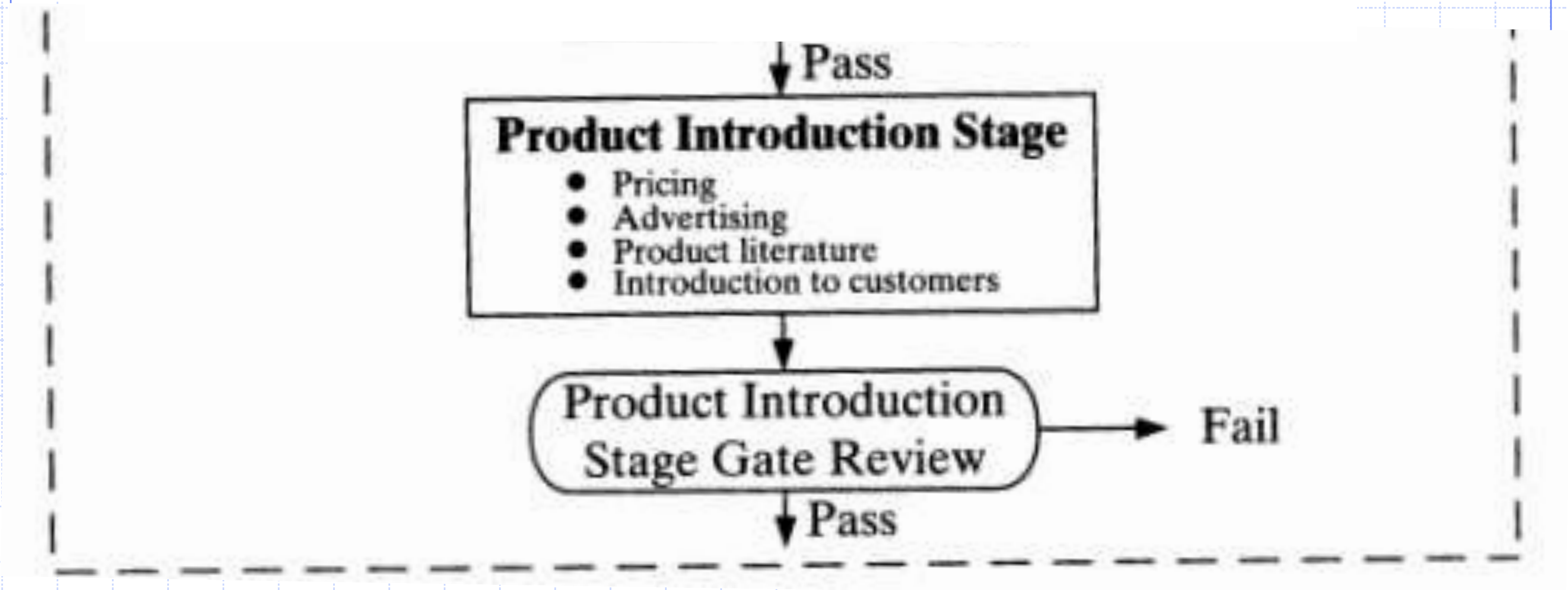
Steps in Product/Process Design

- Development & Manufacturing

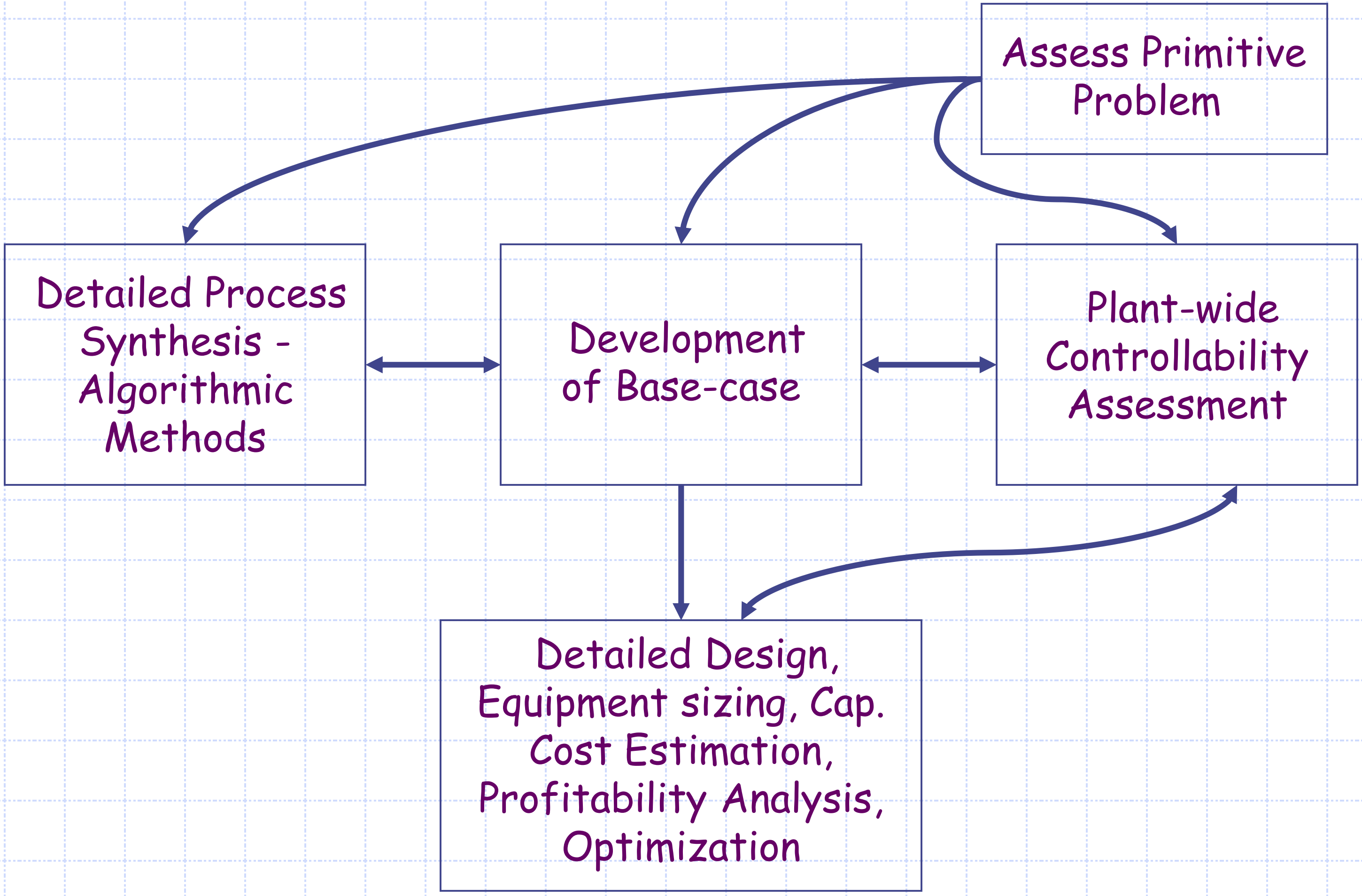


Steps in Product/Process Design

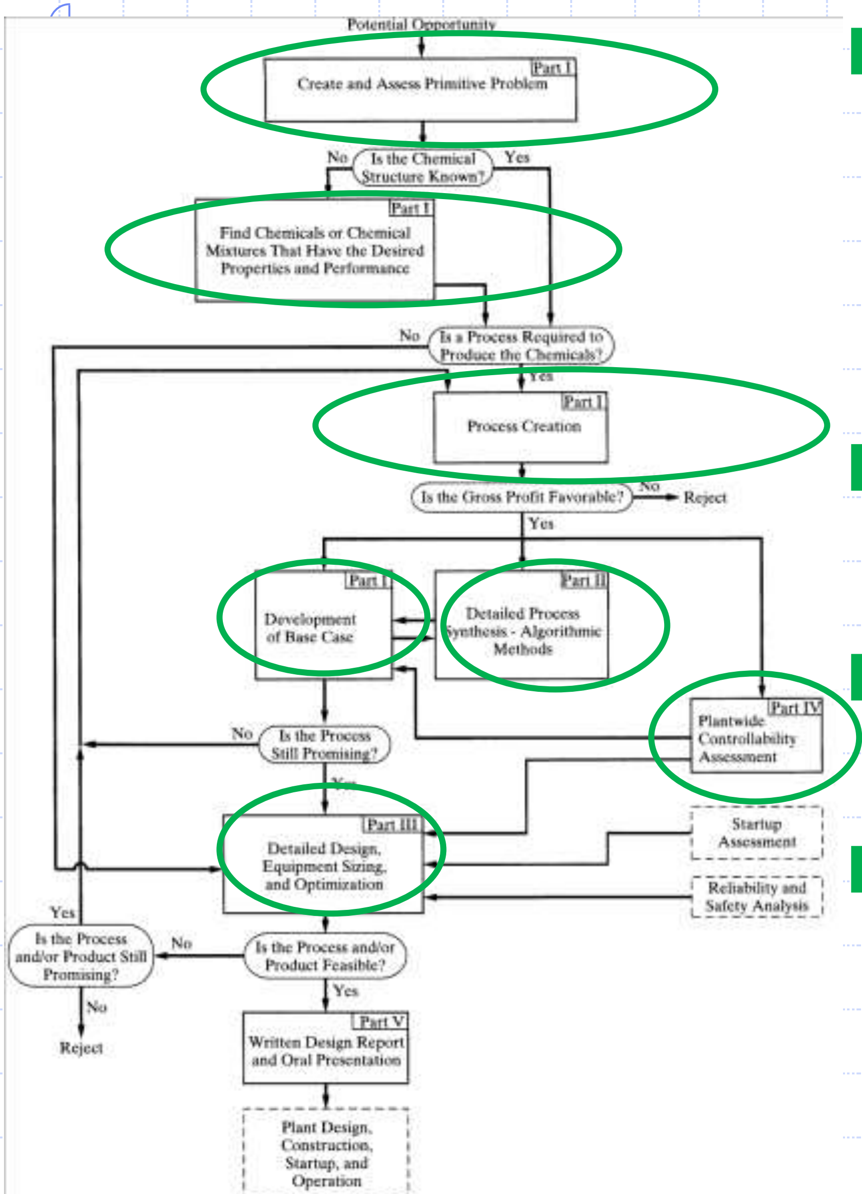
- Product Introduction



Steps in Process Design



Steps in Process Design



Part I

- Assess Primitive Problem
- Find Suitable Chemicals
- Process Creation
- Development of Base Case

Part II

- Detailed Process Synthesis

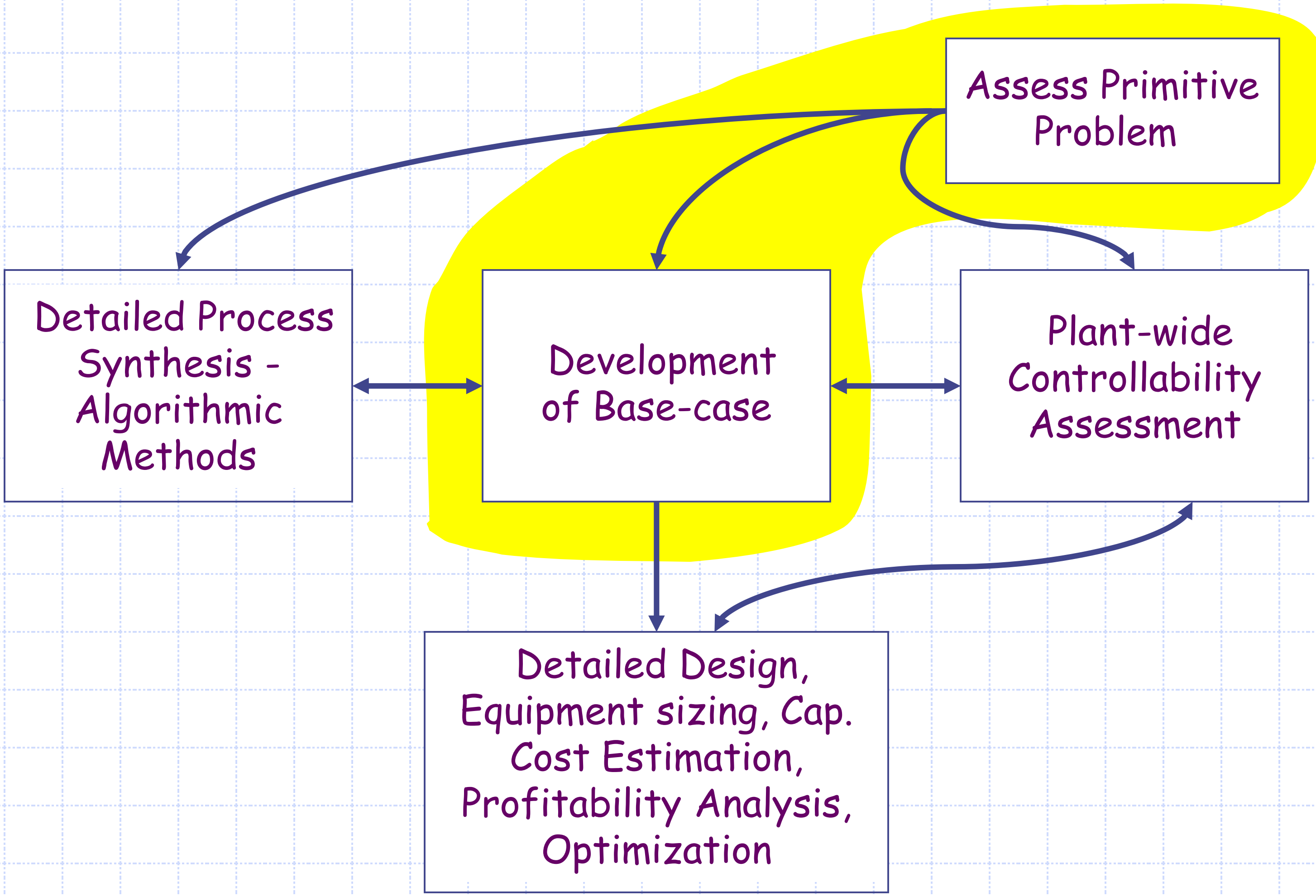
Part III

- Detailed Design & Optimization

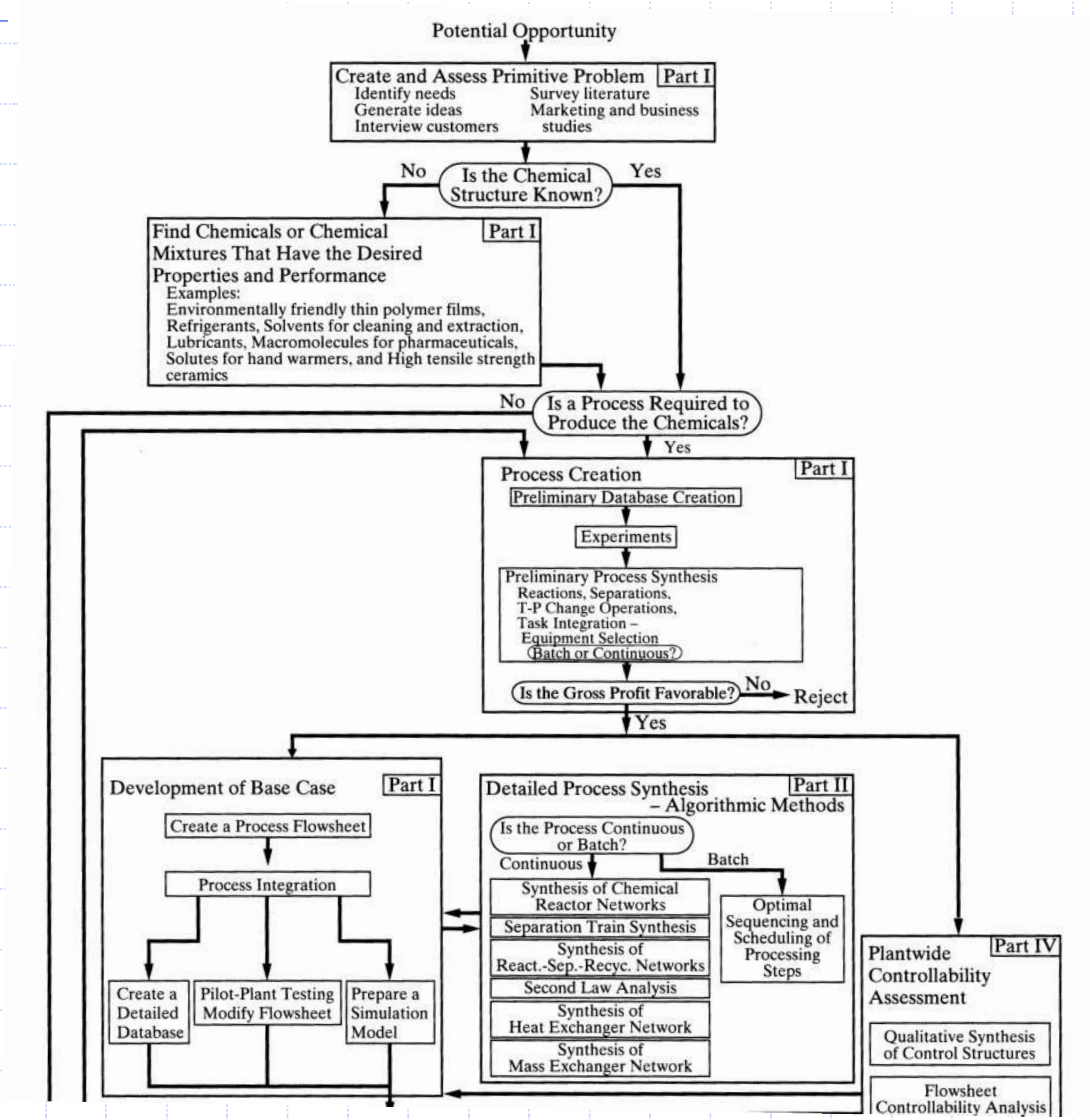
Part IV

- Plantwide Controllability

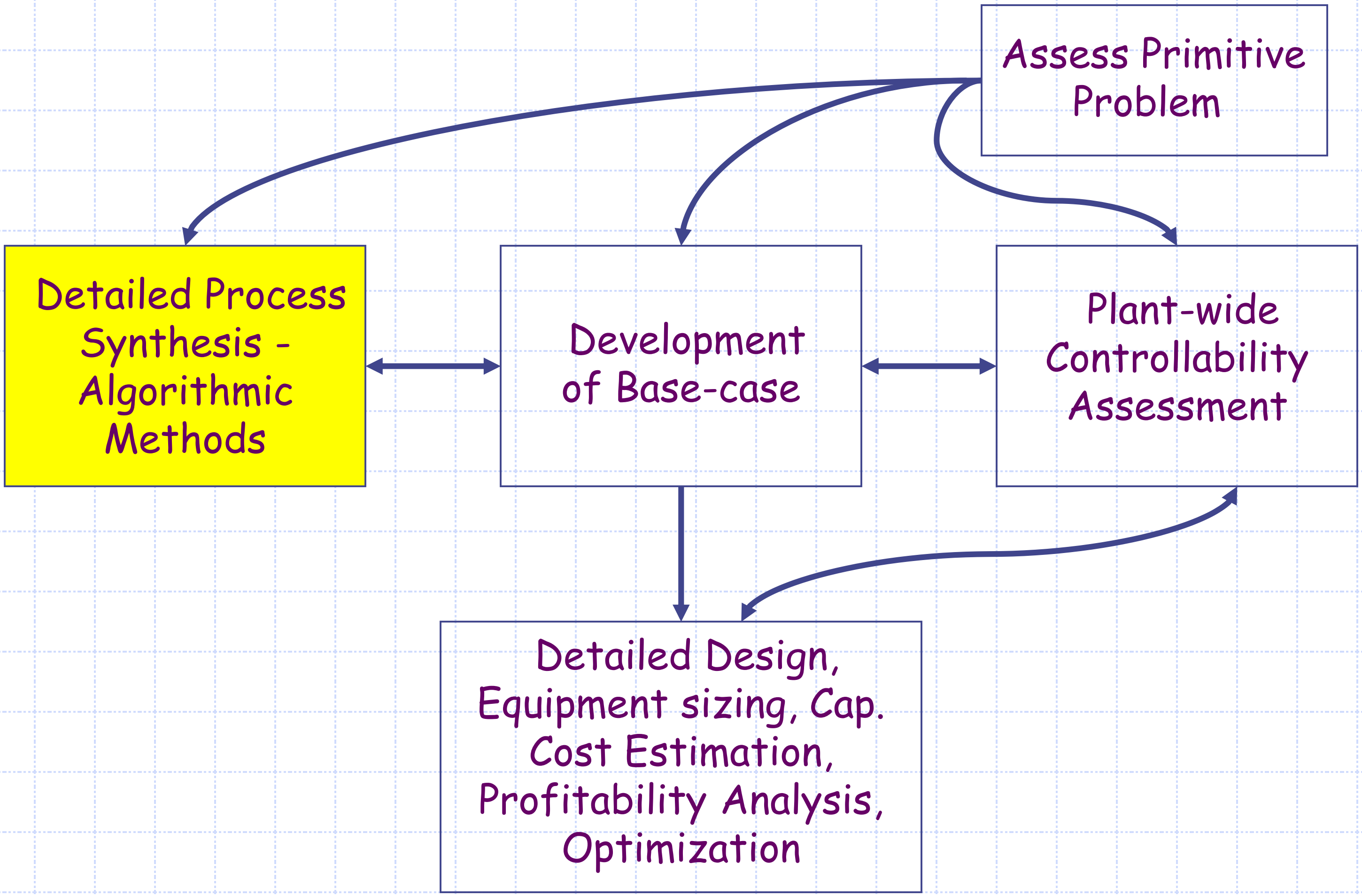
Steps in Process Design



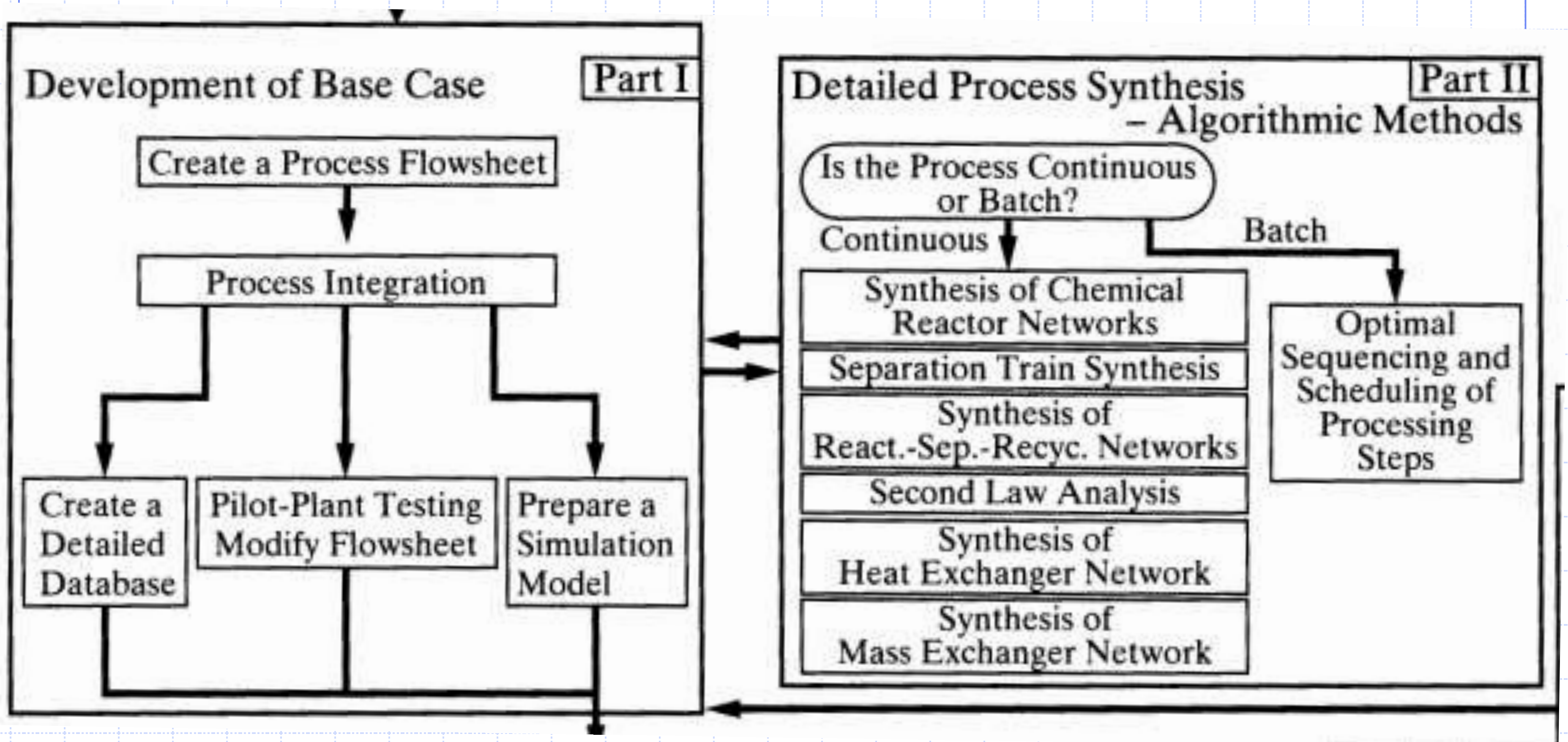
Steps in Process Design



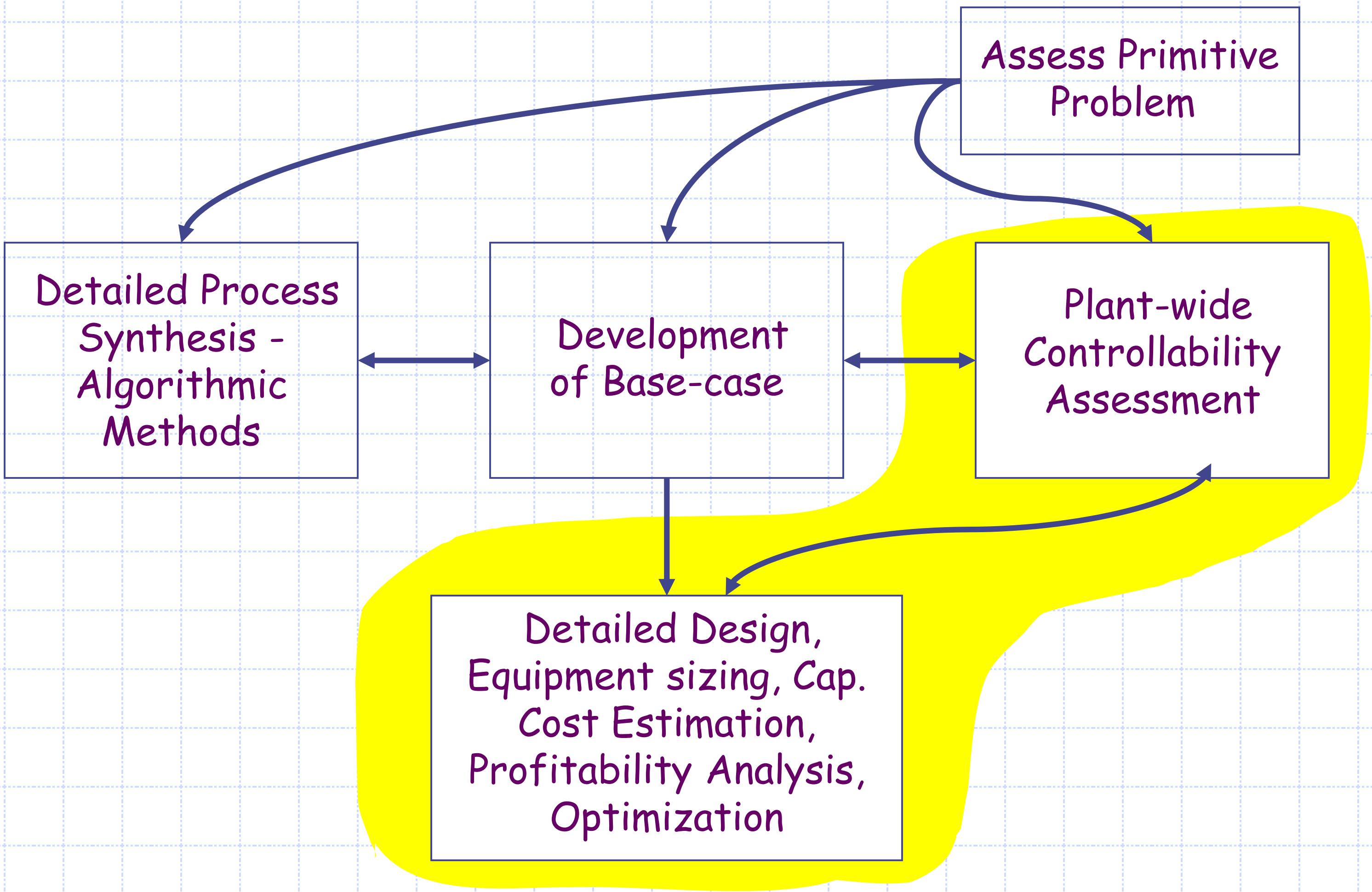
Steps in Process Design



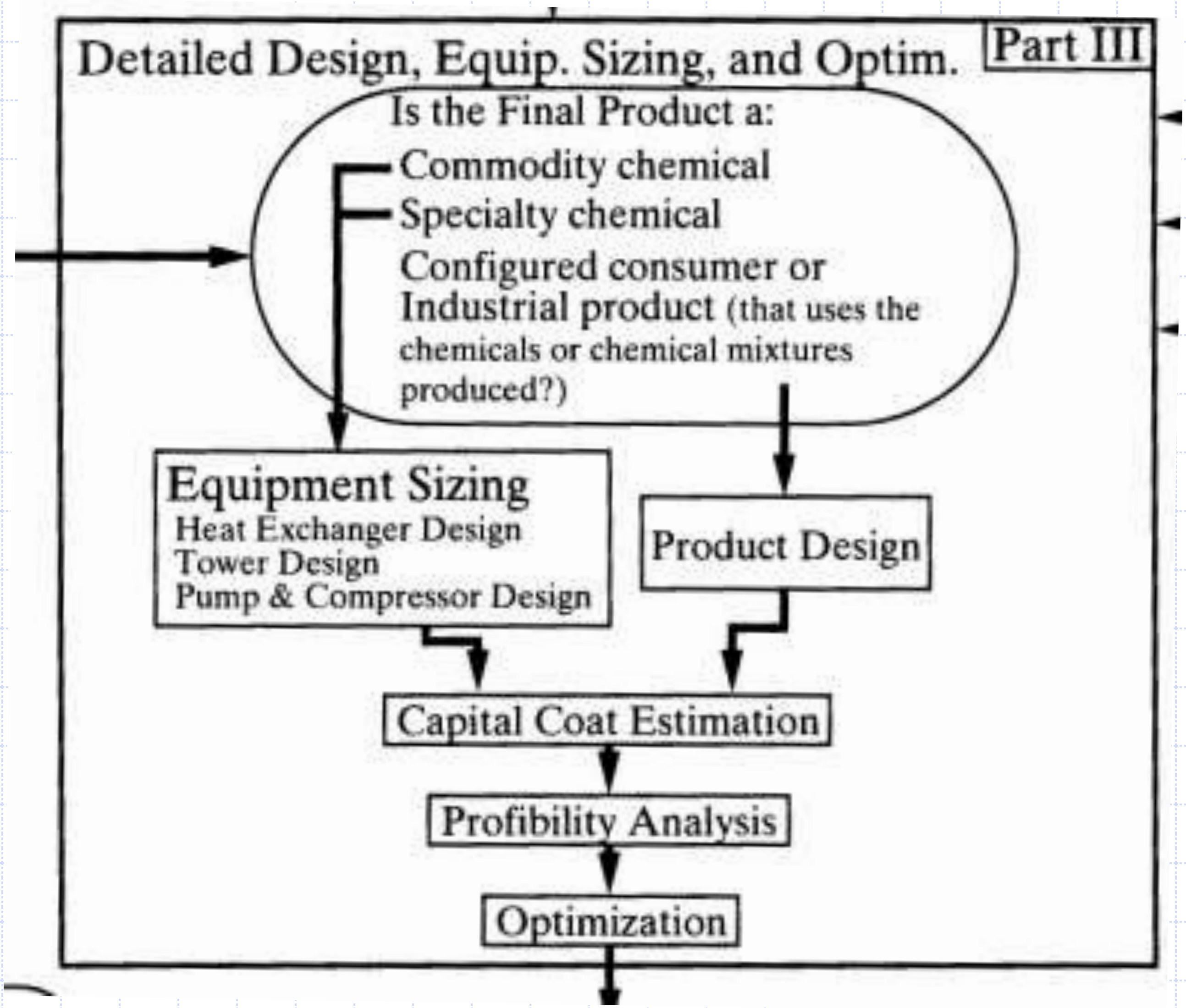
Steps in Process Design



Steps in Process Design



Steps in Process Design



Environmental Issues …

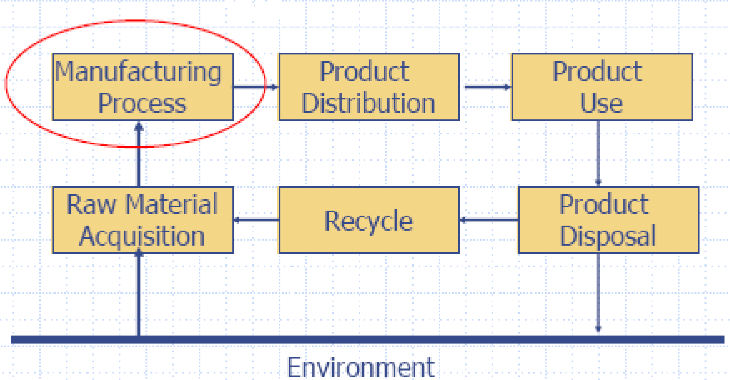
- Handling of toxic wastes
  - 97% of hazardous waste generation by the chemicals and nuclear industry is wastewater.
  - In process design, it is essential that facilities be included to remove pollutants from waste-water streams.
- Reaction pathways to reduce by-product toxicity
  - As the reaction operations are determined, the toxicity of all of the chemicals, especially those recovered as byproducts, needs to be evaluated.
  - Pathways involving large quantities of toxic chemicals should be replaced by alternatives, except under unusual circumstances.
- Reducing and reusing wastes
  - Environmental concerns place even greater emphasis on recycling, not only for unreacted chemicals, but for product and by-product chemicals, as well. (i.e., production of segregated wastes - e.g., production of composite materials and polymers).

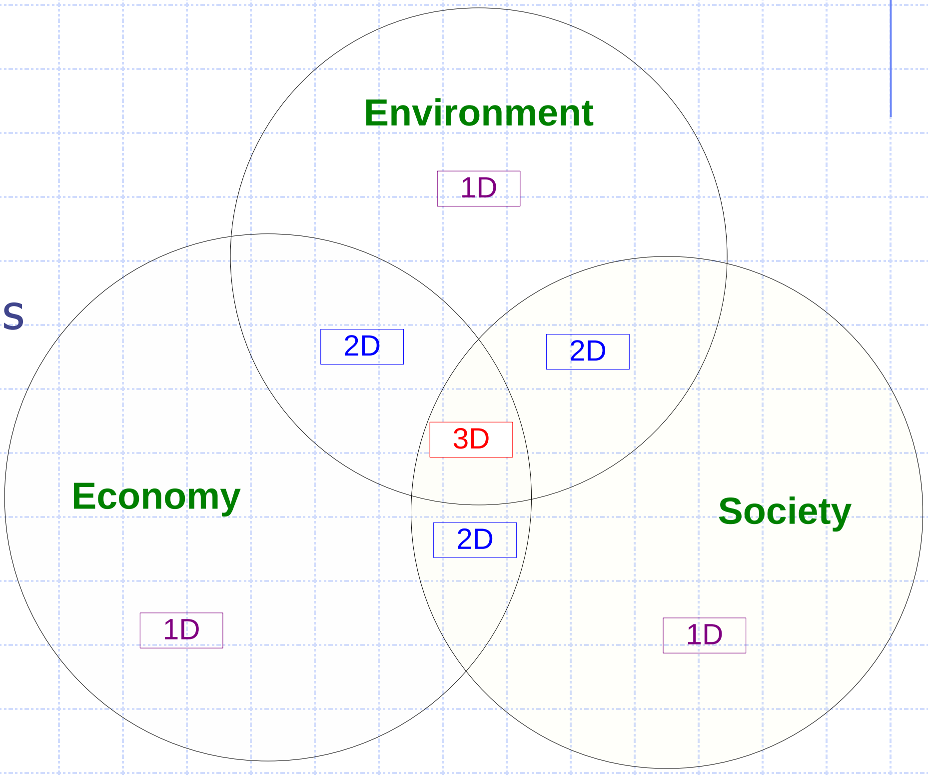
Environmental Issues

- Avoiding non-routine events
  - Reduce the likelihood of accidents and spills through the reduction of transient phenomena, relying on operation at the nominal steady-state, with reliable controllers and fault-detection systems.
- Design objectives, constraints and optimization
  - Environmental goals often not well defined because economic objective functions involve profitability measures, whereas the value of reduced pollution is often not easily quantified economically.
  - Solutions: mixed objective function ("price of reduced pollution"), or express environmental goal as "soft" or "hard" constraints.
  - Environmental regulations = constraints
  - Example: PSP (see next slides)

Sustainability evaluation (of a process)…

- The question of Indicators
  - 1D indicators: economical, ecological, or social;
  - 2D indicators: socio-ecological, socio-economical, or economic-ecological;
  - 3D indicators: all three dimensions of sustainability
- Indicators in this study:
  - Four 3D
  - Four 1D (environment)



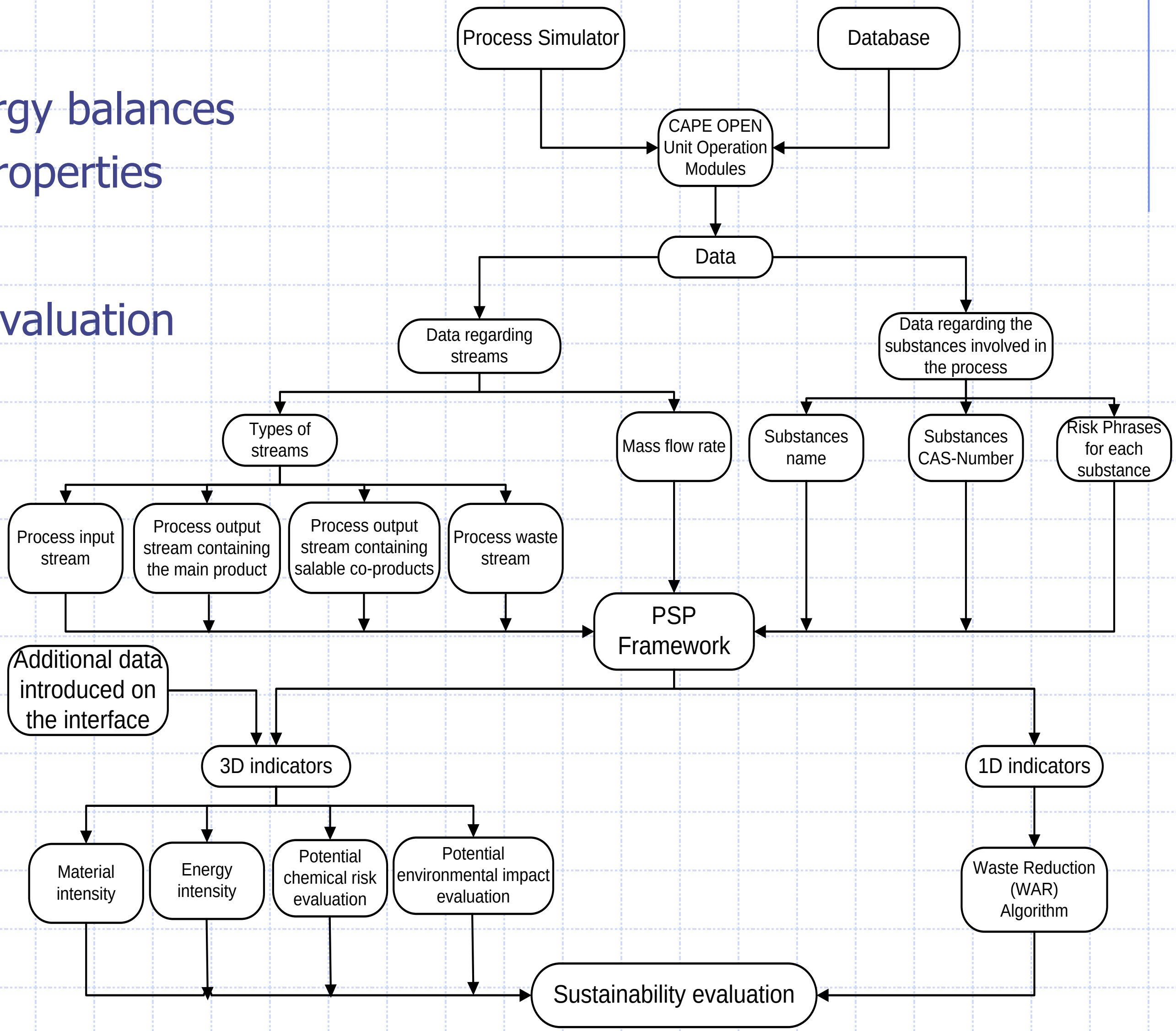


From Martins, 2006

Fermeglia M., Longo G., Toma L., AIChE J, 2009

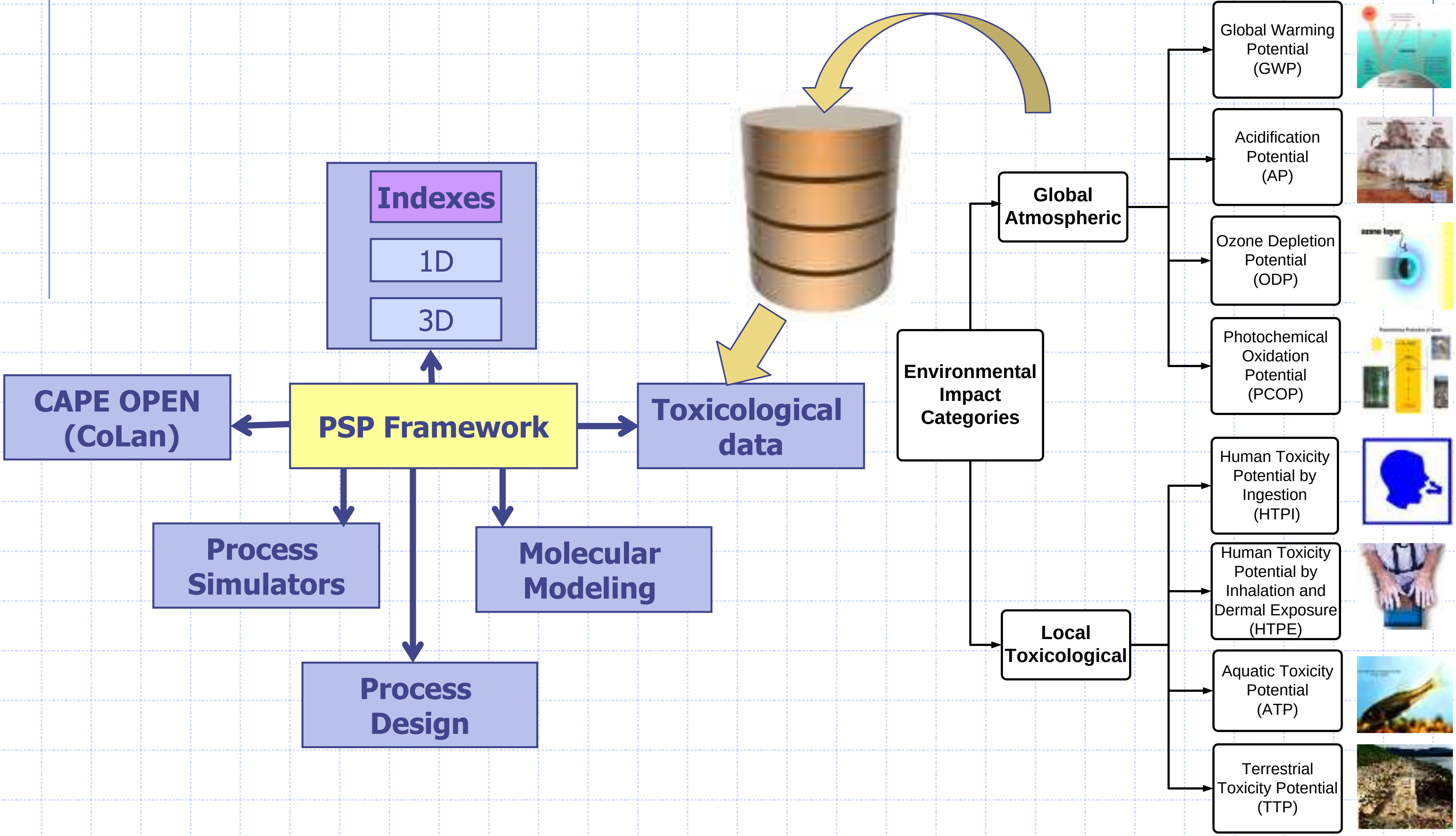
PSP framework

- Input data
  - Material & Energy balances
  - Toxicological properties
- Output
  - Sustainability evaluation

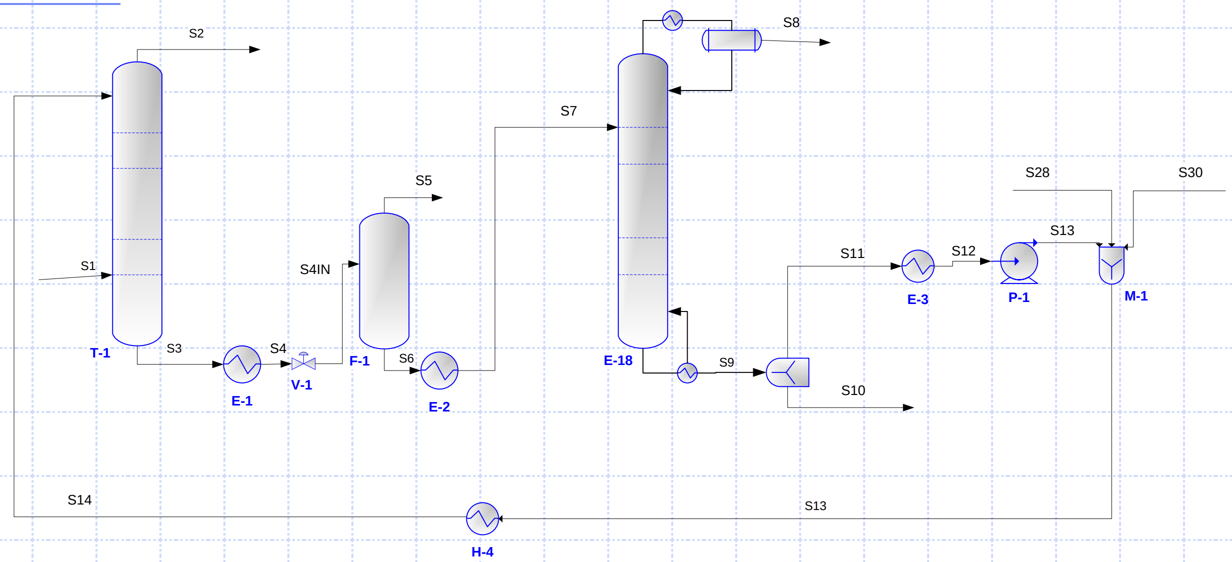


Fermeglia M., Longo G., Toma L., AIChE J, 2009

PSP framework & Indexes

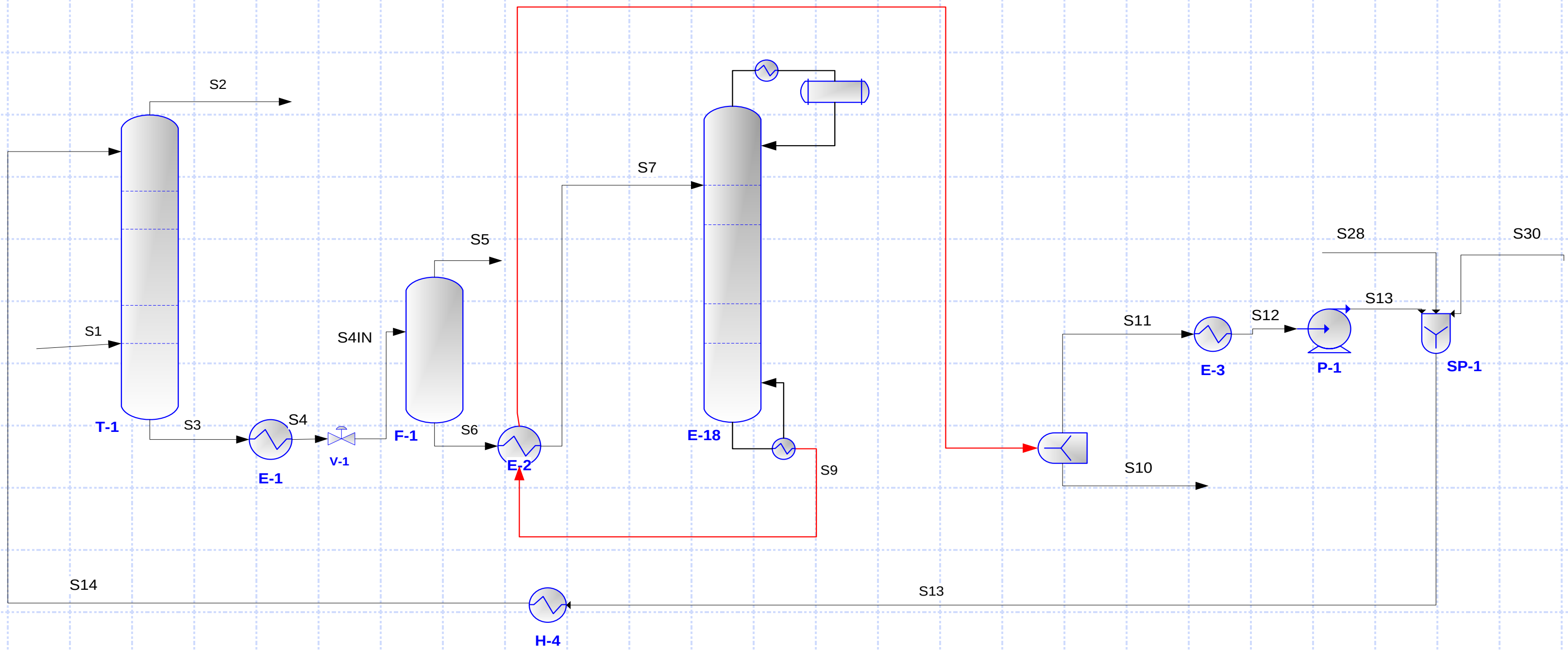


Sweetening natural gas by DGA absorption - base case



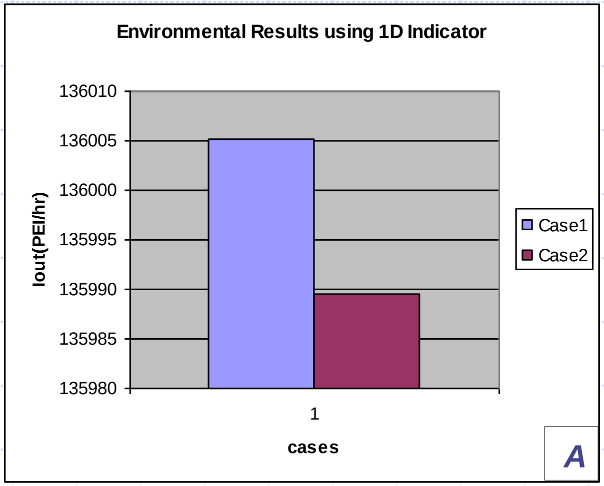
- Natural gas, S1(CH4, CO2 and H2S) and the stream S14 (DGA solution), are sent to T-1.
- The goal of this absorption column is to separate the CH4. The products of the column are: stream S2, containing the removed CH4, and stream S3 containing water, DGA, CO2, H2S and small amounts of CH4.
- S3 is heated in E-1 and sent to the second separation device, F-1. The top stream of F-1, S5 contains the remained CH4 traces.
- The bottom stream, S6, is sent to the second distillation column, T-2. The top stream of the second column, S8, contains removed gases. The bottom stream, S9, is made of DGA and water.
- The losses of DGA and water are supplied with S28 and S30 streams. These are mixed with S13 in M-1 and recycled back to the absorber, T-1.
- From an environmental point of view, it is desired to reduce the gaseous streams, S2, S5 and S8, released in the atmosphere.

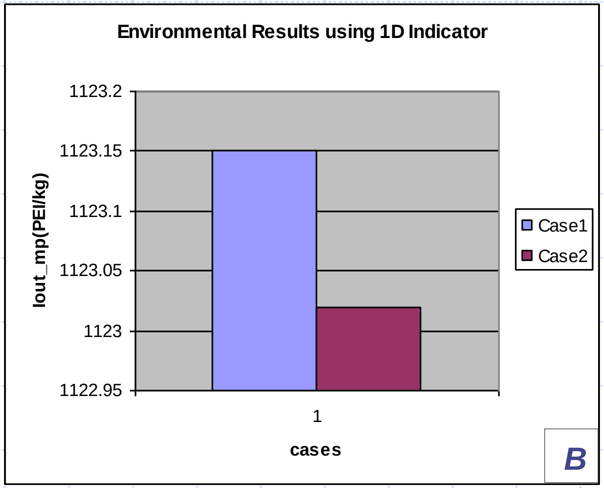
Sweetening natural gas by DGA absorption - alternative

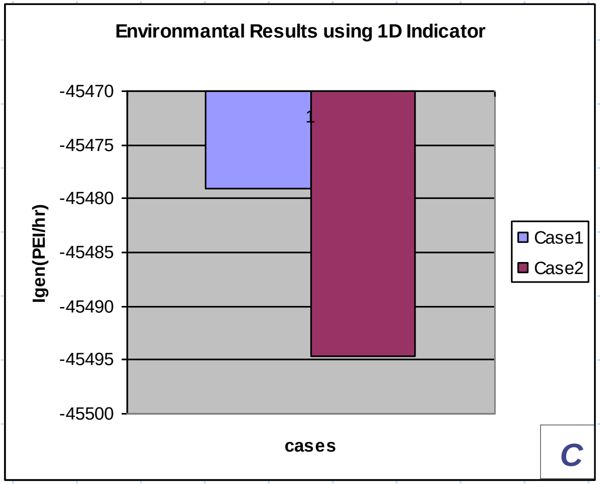


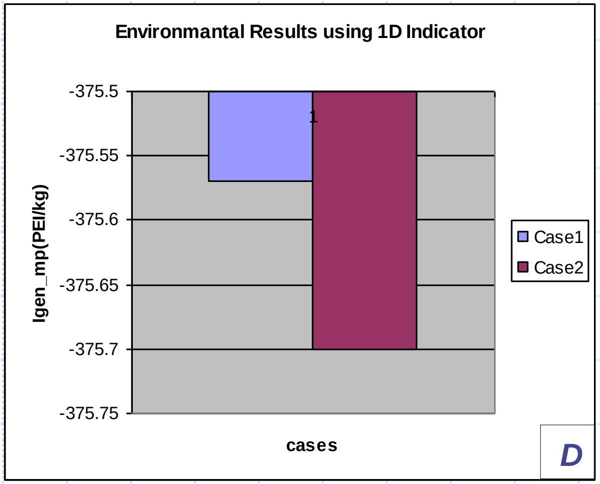
- One modification has been made, starting from the base case.
- The stream, S9, coming from the bottom of the second column, T-2, was used to heat S7. In this way the heat for E-2 is supplied using some internal stream of the process

1D: Results









1 D Indicator

A) Iout

B) Iout_mp

C) Igen

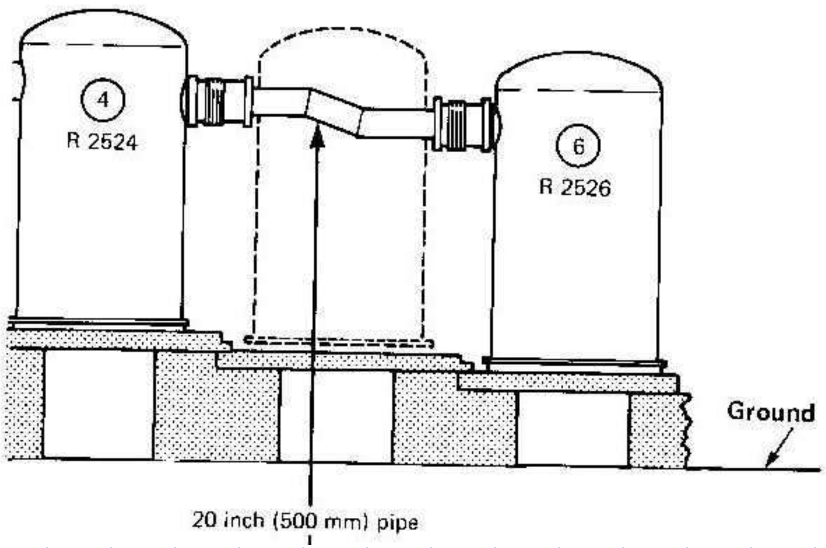
D) Igen_mp

Safety Considerations

- Example Disaster 1 – Flixborough: 1st June 1974
  http://www.hse.gov.uk/hid/land/comah/level3/5a591f6.htm
  - 50 tons of cyclohexane were released from Nypro's KA plant (oxidation of cyclohexane) leading to release of vapor cloud and its detonation. Total loss of plant and death of 28 plant personnel.
  - Highly reactive system - conversions low, with large inventory in plant. Process involved six, 20 ton stirred-tank reactors.

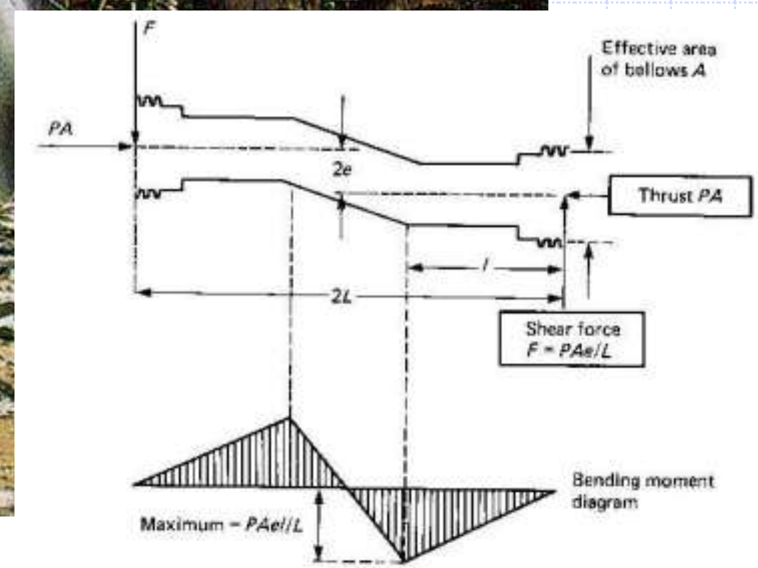
– Discharge caused by failure of temporary pipe installed to replace cracked reactor.

– The so-called "dog-leg" was not able to contain the operating conditions of the process (10 bar, 150 ^oC)



Safety Considerations

- Flixboro... What can we learn?
  - Develo... fluids ("what you do...
  - Before... possible cause
  - Carry...
  - Const...
  - Use bl...



Safety Considerations (Cont'd)

- Example Disaster 2 – Bhopal: 3rd December 1984
  http://www.bhopal.com/chrono.htm
  - Water leakage into MIC (Methyl isocyanate) storage tank leading to boiling and release of 25 tons of toxic MIC vapor, killing more than 3,800 civilians, and injuring tens of thousands more.
  - MIC vapor released because the refrigeration system intended to cool the storage tank holding 100 tons of MIC had been shut down, the scrubber was not immediately available, and the flare was not in operation.

- Bhopal - What can we learn?
  - Avoid use of hazardous materials. Minimize stocks of hazardous materials ("what you don't have, can't leak").
  - Carry out HAZOP analysis.
  - Train operators not to ignore unusual readings.
  - Keep protective equipment in working order.
  - Control building near major hazards.

Safety Considerations (Cont'd)

- Example Disaster 3 – Challenger: 28th January 1986
- http://www.onlineethics.com/moral/boisjoly/RB-intro.html
  - An O-ring seal in one of the solid booster rockets failed. A high-pressure flame plume was deflected onto the external fuel tank, leading to a massive explosion at 73 sec from lift-off, claiming the Challenger with its crew.
  - The O-ring problem was known several months before the disaster, but down-played by management, who over-rode concerns by engineers.
- Challenger - What can we learn?
  - Design for safety.
  - Prevent 'management' over-ride of 'engineering' safety concerns.
  - Carry out HAZOP analysis.

Safety Issues

- Flammability Limits of Liquids and Gases
  - LFL and UFL (vol %) in Air at 25 oC and 1 Atm

Compound	LFL (%)	UFL (%)
Acetylene	2.5	100
Cyclohexane	1.3	8
Ethylene	2.7	36
Gasoline	1.4	7.6
Hydrogen	4.0	75

- These limits can be extended for mixtures, and for elevated temperatures and pressures.
- With this kind of information, the process designer makes sure that flammable mixtures do not exist in the process during startup, steady-state operation, or shut-down.

Design for Safety

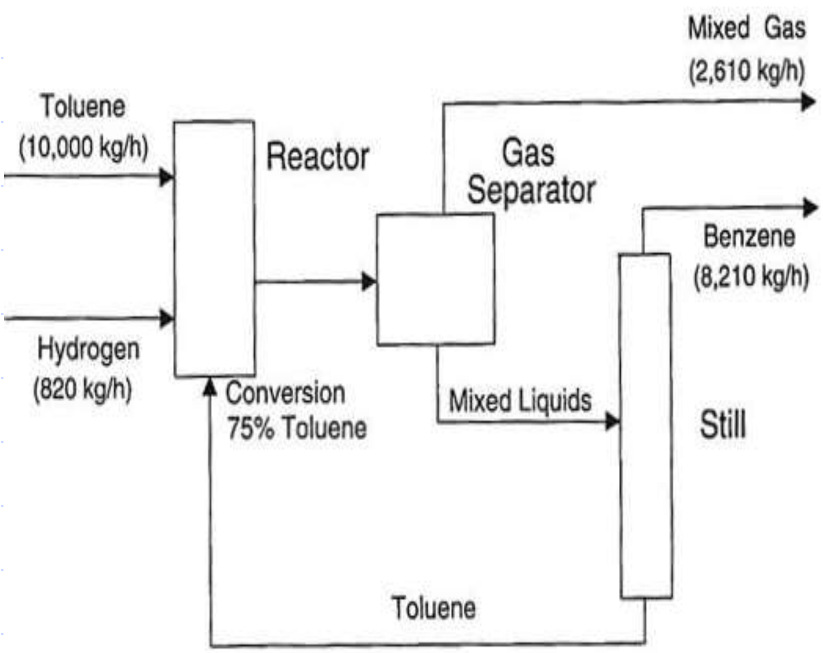
- Techniques to Prevent Fires and Explosions
  - Inerting - addition of inert dilutant to reduce the fuel concentration below the LFL
  - Installation of grounding devices and anti-static devices to avoid the buildup of static electricity
  - Use of explosion proof equipment
  - Ensure ventilation - install sprinkler systems
- Relief Devices
- Hazard Identification and Risk Assessment
  - The plant is scrutinized to identify sources of accidents or hazards.
  - Hazard and Operability (HAZOP) study is carried out, in which all of the possible paths to an accident are identified.
  - When sufficient probability data are available, a fault tree is created and the probability of the occurrence for each potential accident computed.

Process schemes

- Block Flow Diagram (BFD): **illustrative, very general**
- Process Flow Diagram (PFD): technical, they allow design
  - **Simplified**: reports unit operations and necessary equipment
  - **Quantified**: add to the simplified flow diagram material and energy balances
  - **Instrumental**: add the quantified flow diagram the control systme
- Piping and Instrumentational Diagram (P&I)
  - **Main document** of the design, the PFD is enhanced and quantified:
  - **Instrumentation** and **control** system is added
  - Is a '**technical photo**' of the process
  - Allows to identify and **recognize all units and piping** of the plant

Block Flow Diagram BFD

- Series of boxes labeled with the **name of the operation**
- **Streams** indicated as continuum lines with arrows
  - At least two **sections**: reaction and separation
  - At least 2 **streams**: feed and product
- Usually at least **one recycle** and **one purge**

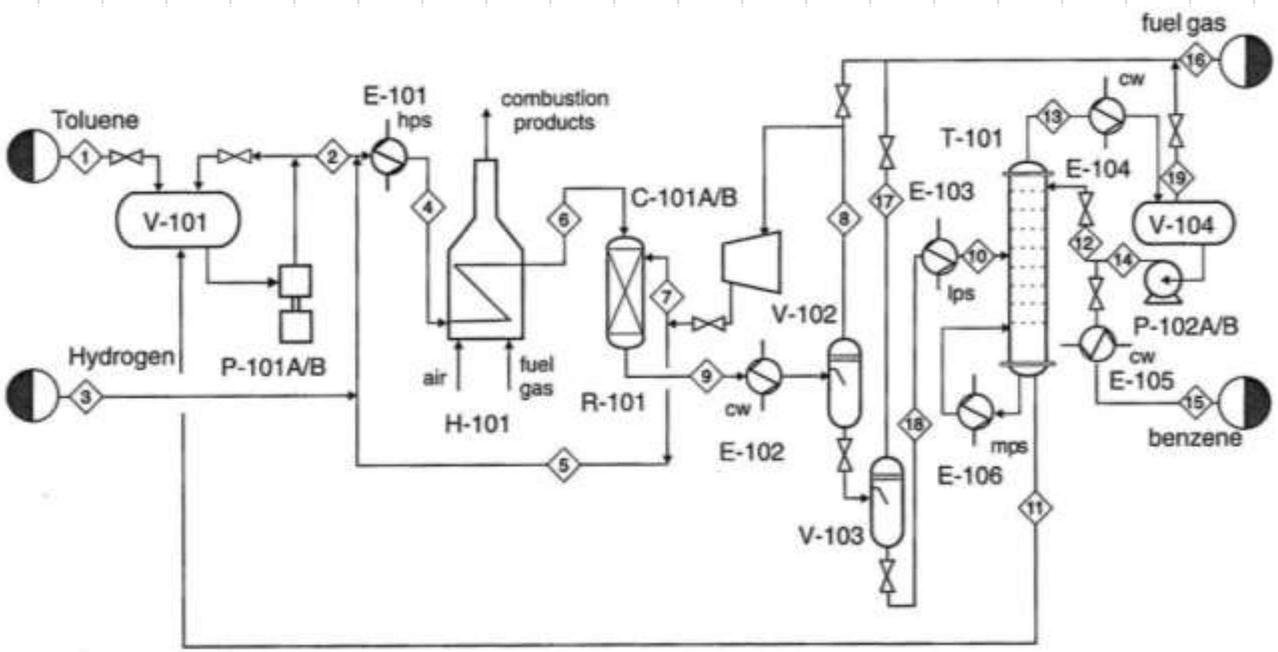


- More BFD could be generated from one patent or know-how
  - The optimal one will be selected based on **economical considerations**

Process Flow Diagram PFD

- Complete flow diagram in which **all units and streams** involved are represented.
- Units are shown schematically and **conventionally labeled**
  - (in Italy UNICHIM - Tab. 1)

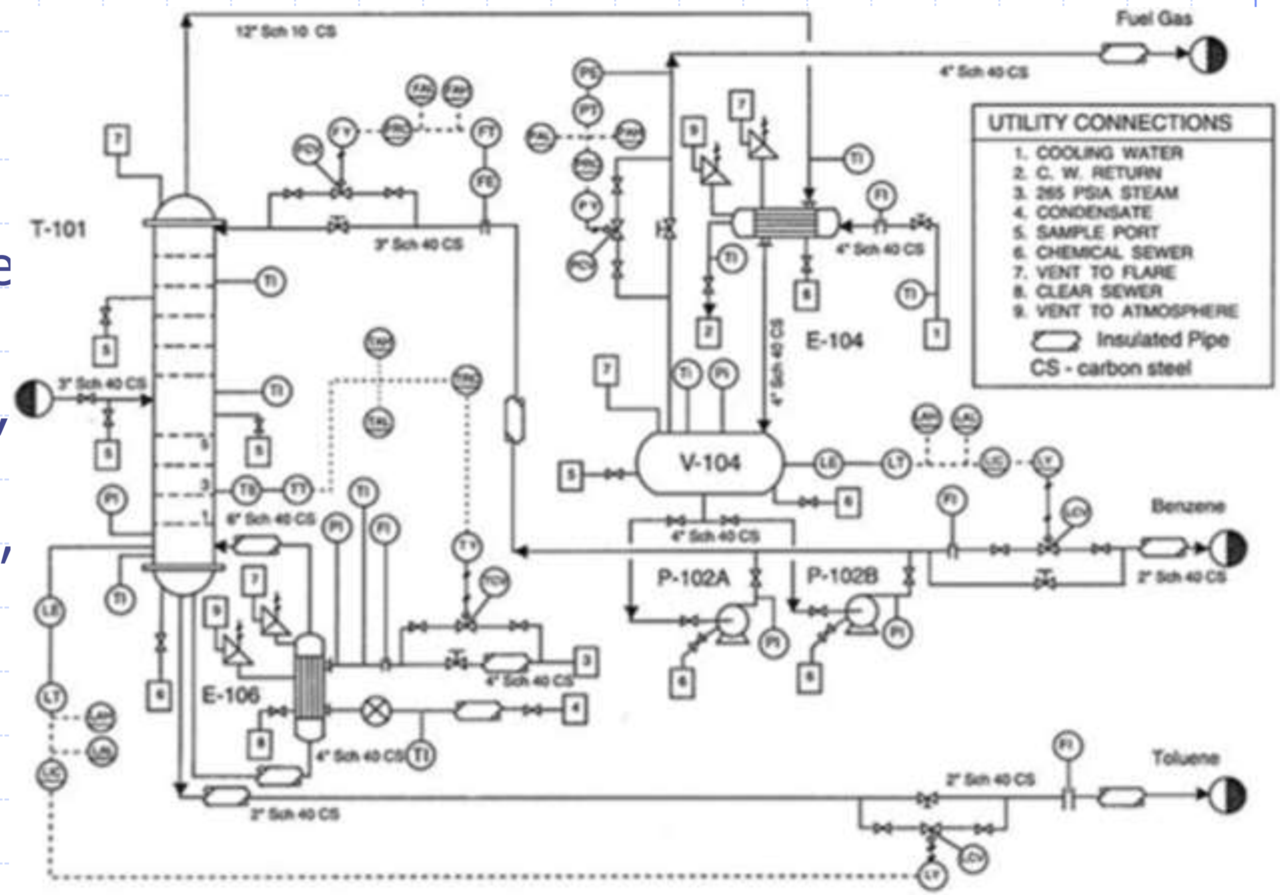
APPARECCHI	SIGLA
Agitatori	AG
Centrifughe	CE
Compressori alternativi	CA
" centrifughi	CC
" rotativi	CR
Recipienti e separatori	D
Essiccatori	DE
Scambiatori di calore	E
Eiettori	EJ
Evaporatori	EV
Forni	F
Filtri	FI
Pompe dosatrici	PA
" centrifughe	PC
" volumetriche	PV
Reattori	R
Serbatoi stoccaggio	S
Trasportatori di solidi	TS
Ventilatori	V



PFD of toluene de-alchilation process

Piping and Instrumentational Diagram P&I

- Service lines are indicated connecting the units that need the specific service
- Indication of: by-pass, pipes slopes, insulations, condensate drains, …
- Complex schema: clarity, sufficient spacing, no winding paths



P&I of a distillation column for toluene de-alchilation process