Coourse:

Process Design Principles & Methods

2017

Lecture 1: Introduction

Professor Rafiqul Gani

Course Information

Schedule: see the course document

Exam & Grading: Design project report; oral presentation; 3 take-home exam problems.

Design project: Work in groups of 2 members; details will be given later today.

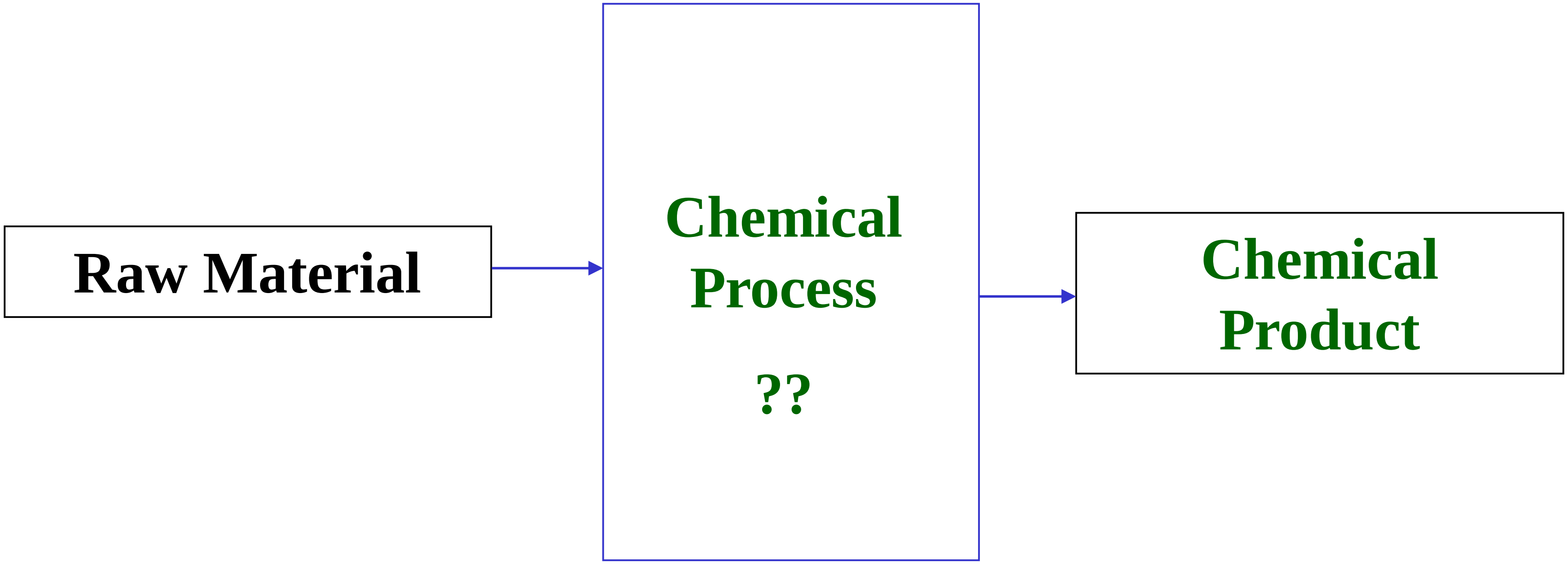
Consulting: During the tutorials groups can consult the teacher for questions on the process design project

Textbook

Textbook-1: LT Biegler, IE Grossmann and AW Westerberg, *Systematic Methods of Chemical Process Design*, Prentice Hall, 1997.

Textbook-2:
PRODUCT AND PROCESS DESIGN PRINCIPLES: Synthesis, Analysis and Evaluation (Seider, Lewin, Seader, Widgado, Gani, Ng), John Wiley & sons, New York, USA, Spring 2016 (**4th Edition**)

Chemical Process Design & Green Engineering



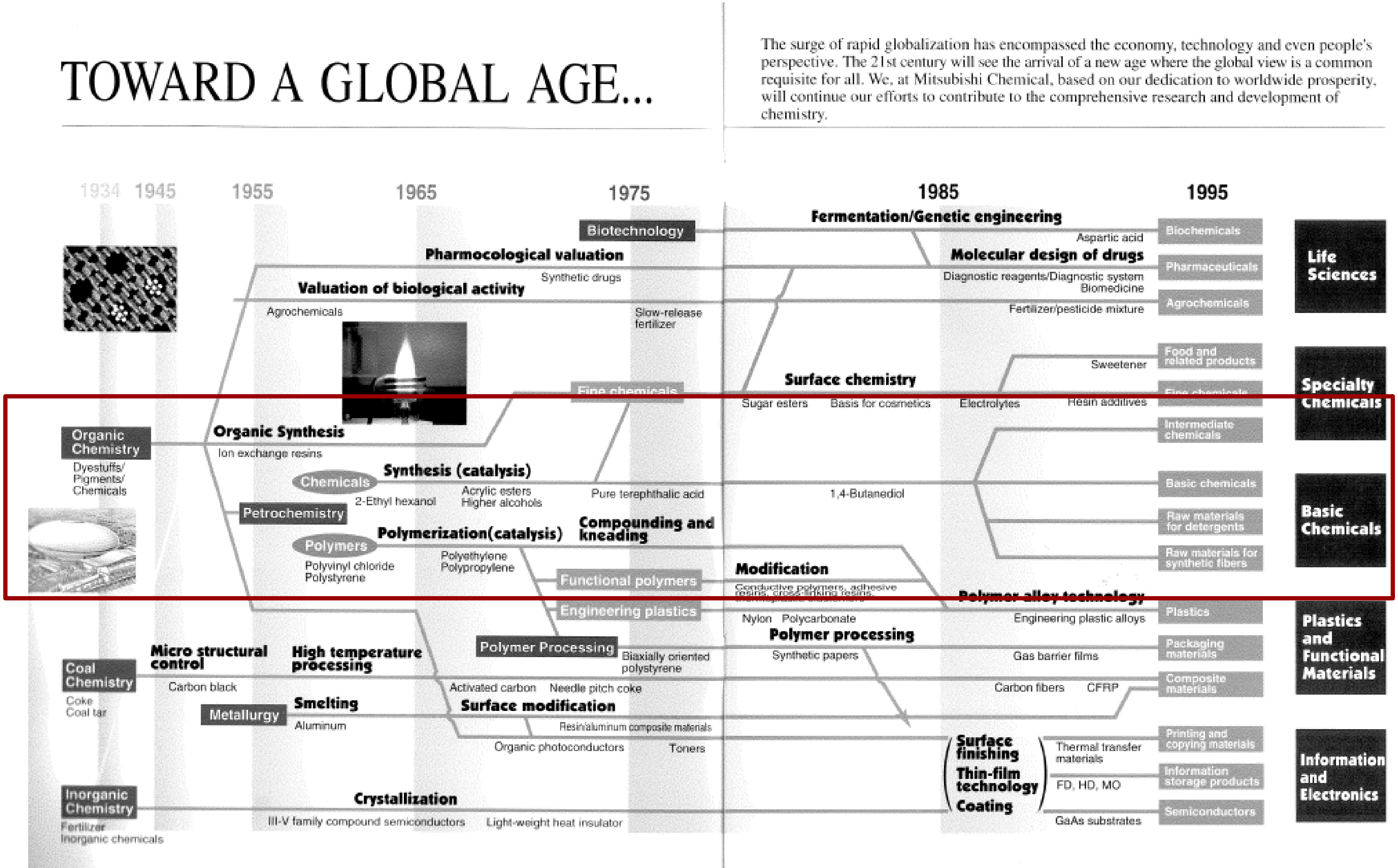
Chemical process design is about finding a sustainable process that can convert the raw materials to the desired chemical products

Sustainable: Economic, low environmental impact, low waste, efficient operation, correct raw material, …..

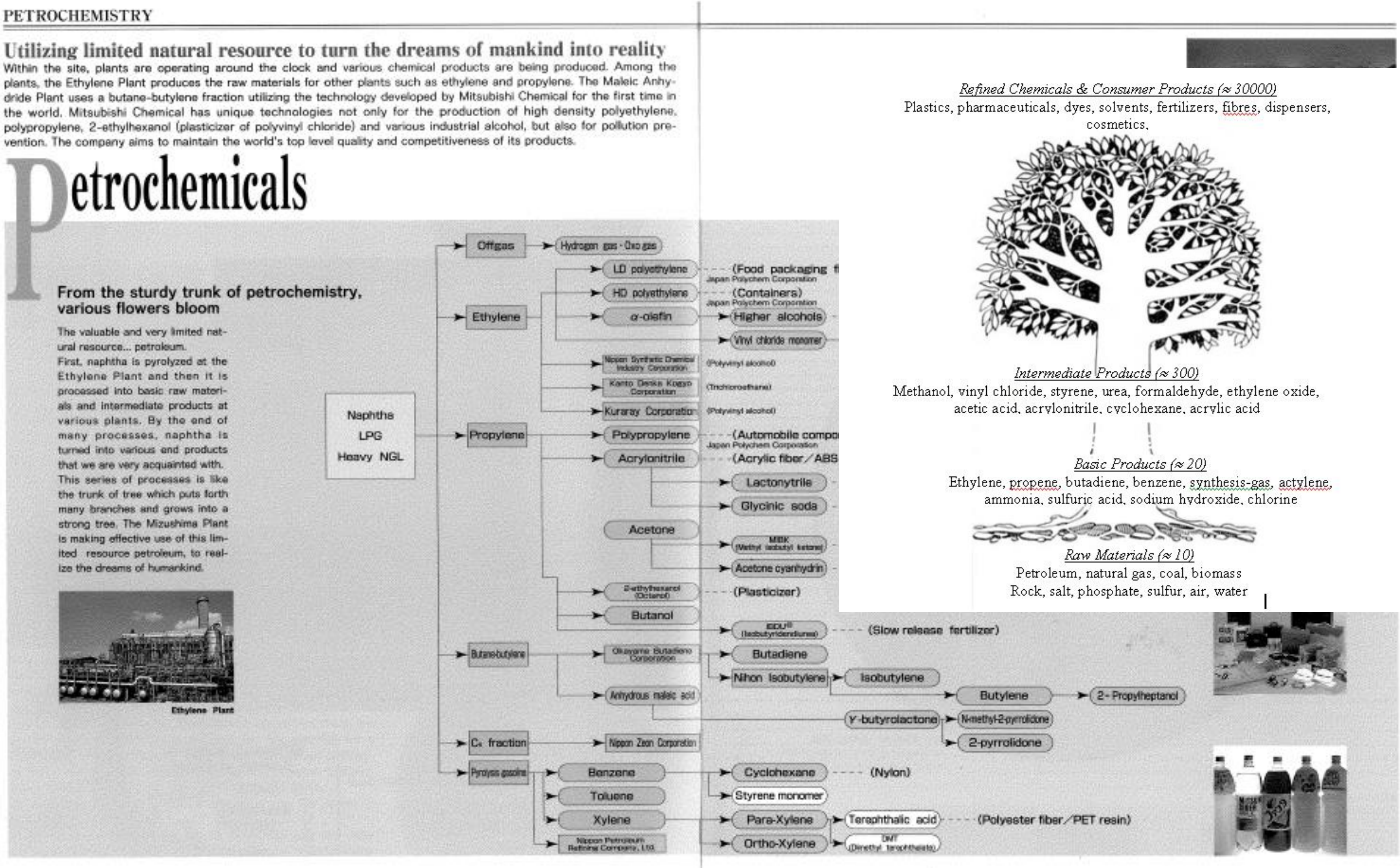
The Product Tree

It is important to choose the right product and the corresponding raw material from which the product can be made. This also defines the path (process route)

Development of the chemical product tree



Product-Raw Material Paths


PETROCHEMISTRY

Utilizing limited natural resource to turn the dreams of mankind into reality

Within the site, plants are operating around the clock and various chemical products are being produced. Among the plants, the Ethylene Plant produces the raw materials for other plants such as ethylene and propylene. The Maleic Anhydride Plant uses a butane-butylene fraction utilizing the technology developed by Mitsubishi Chemical for the first time in the world. Mitsubishi Chemical has unique technologies not only for the production of high density polyethylene, polypropylene, 2-ethylhexanol (plasticizer of polyvinyl chloride) and various industrial alcohol, but also for pollution prevention. The company aims to maintain the world's top level quality and competitiveness of its products.

Petrochemicals

From the sturdy trunk of petrochemistry, various flowers bloom

The valuable and very limited natural resource... petroleum. First, naphtha is pyrolyzed at the Ethylene Plant and then it is processed into basic raw materials and intermediate products at various plants. By the end of many processes, naphtha is turned into various end products that we are very acquainted with. This series of processes is like the trunk of tree which puts forth many branches and grows into a strong tree. The Mizushima Plant is making effective use of this limited resource petroleum, to realize the dreams of humankind.

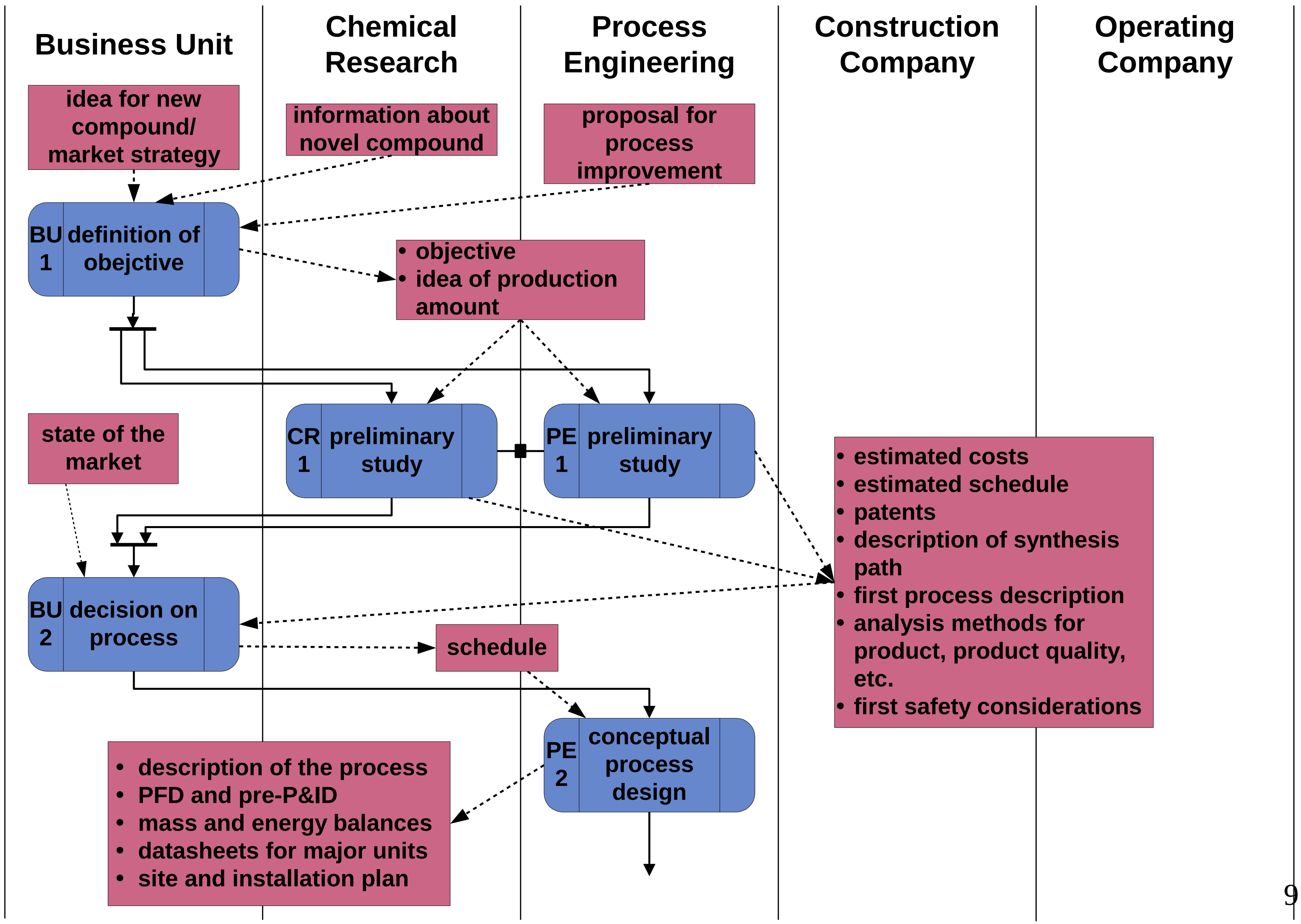
Ethylene Plant

A Scenario for Chemical Process Design

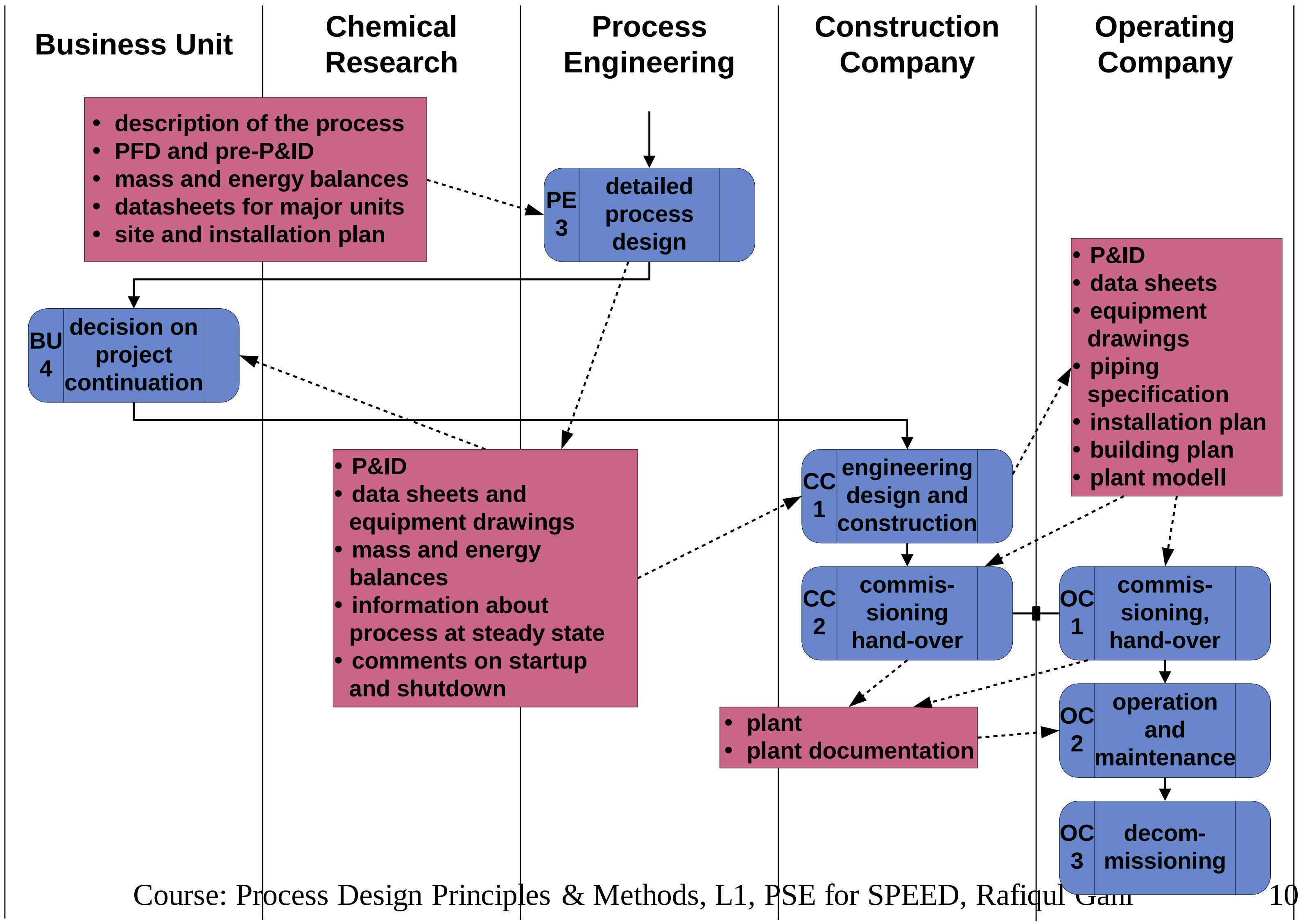
1. **Board of Directors' Design Problem**
2. **Discovery of possible new projects**
3. **Feedback & customer reaction**
4. **Planning & organizational design**
5. **Preliminary (conceptual) process design**
6. **Layout & three dimensional modelling**
7. **Construction**
8. **Startup & commissioning**
9. **Plant Operation**
10. **Debottelnecking**
11. **Decommissioning**

Stages in the life of a process !

Roles of different groups of people in the different stages of the life of a process - I



Roles of different groups of people in the different stages of the life of a process - II



The Synthesis Step

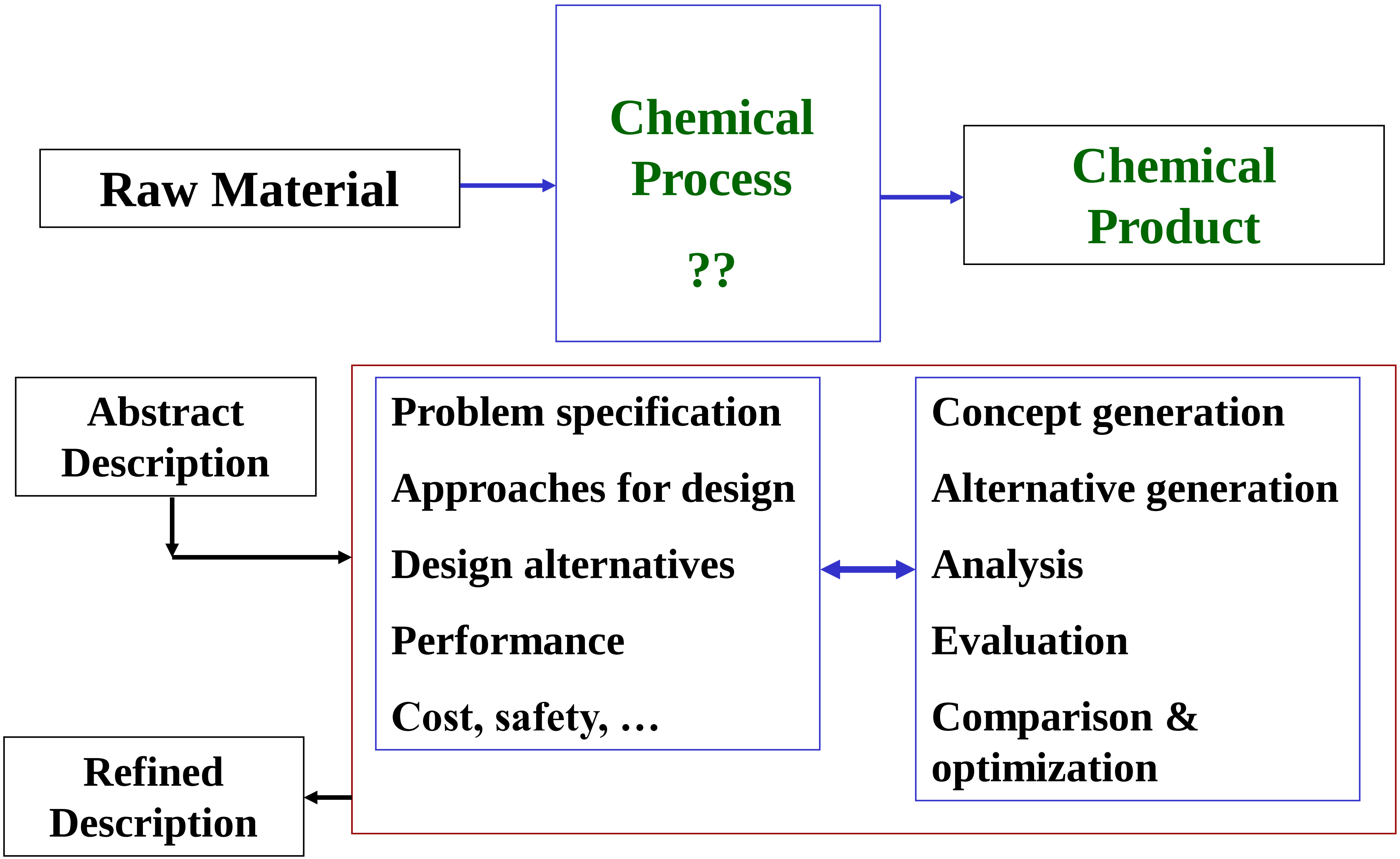
Raw Material → **Chemical Process ??** → **Chemical Product**

Abstract description of design problem

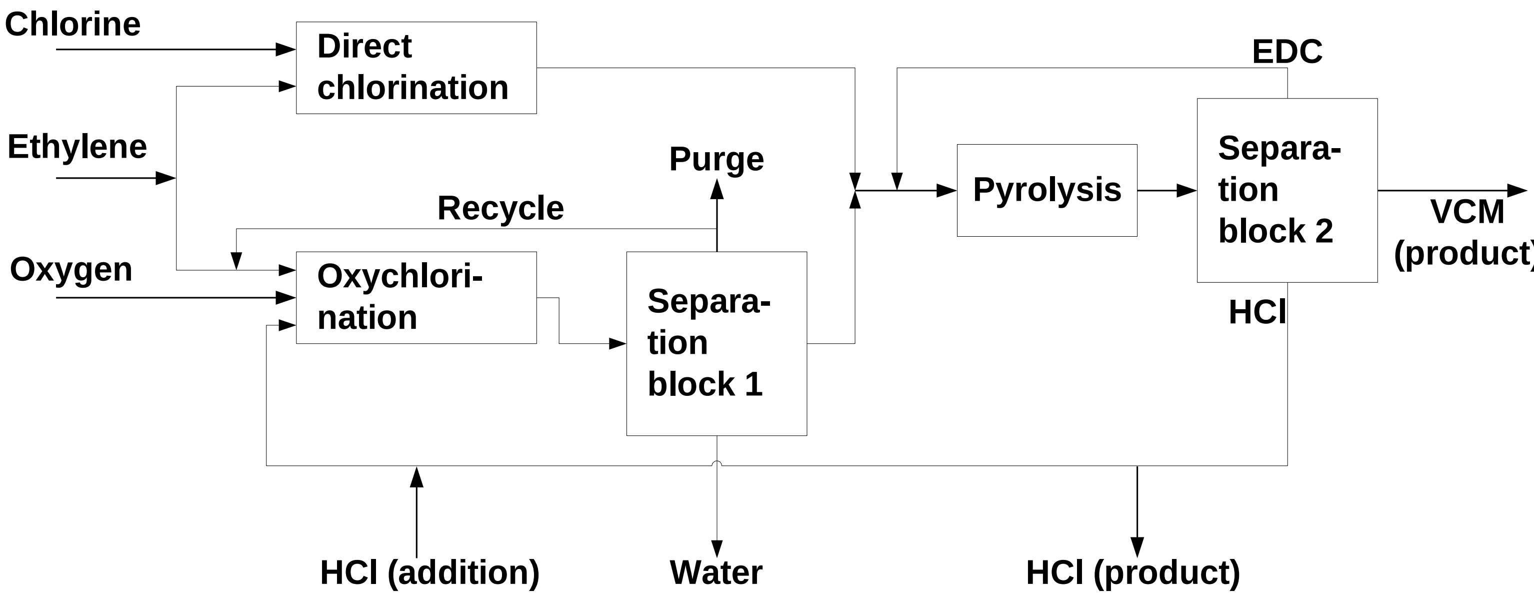
Concept Generation
Generation of Alternatives
Analysis of Alternatives
Evaluation of Alternatives
Comparison & Optimization

Refined description of design problem

The Synthesis Step



Example of a Chemical Process & Product



The production of VCM is usually done from ethylene. In this case the process is carried out in two steps, first reaction with either chlorine or hydrogen chloride in order to produce ethylene dichloride (EDC) and next pyrolysis (cracking) to form VCM. The compounds in the system are Ethylene, EDC, VCM, HCl, O_2, Cl_2 and H_2O. The reactions involved is the process are:

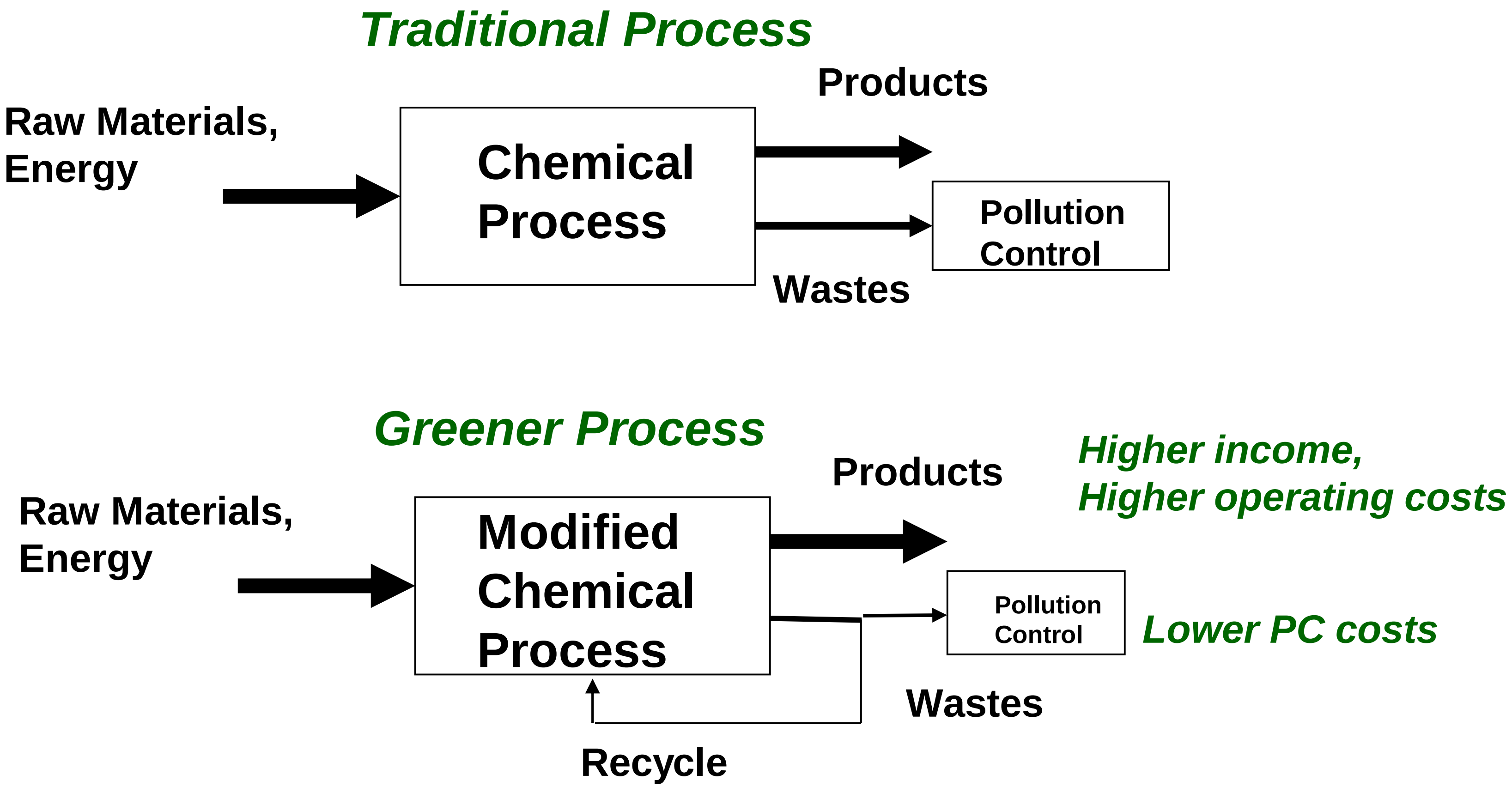
Direct chlorination: $C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$

Oxychlorination: $C_2H_4 + 2HCl + ½O_2 \rightarrow C_2H_4Cl_2 + H_2O$

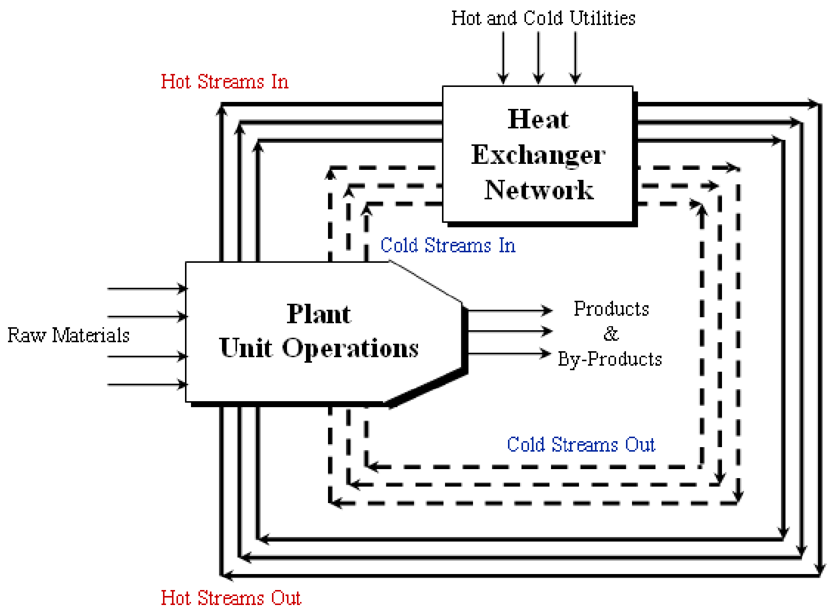
Pyrolysis (cracking): $C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$

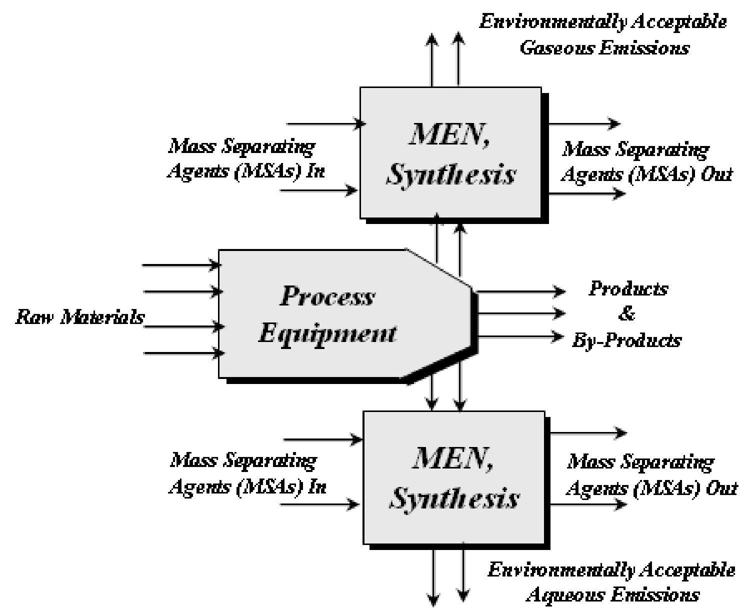
The two step process also requires two separation blocks. In the first step (formation of EDC) two different reactions are considered (Direct chlorination and oxychlorination). Oxychlorination produces water in addition to EDC and it also requires a recycle.

Aspects of Green Engineering



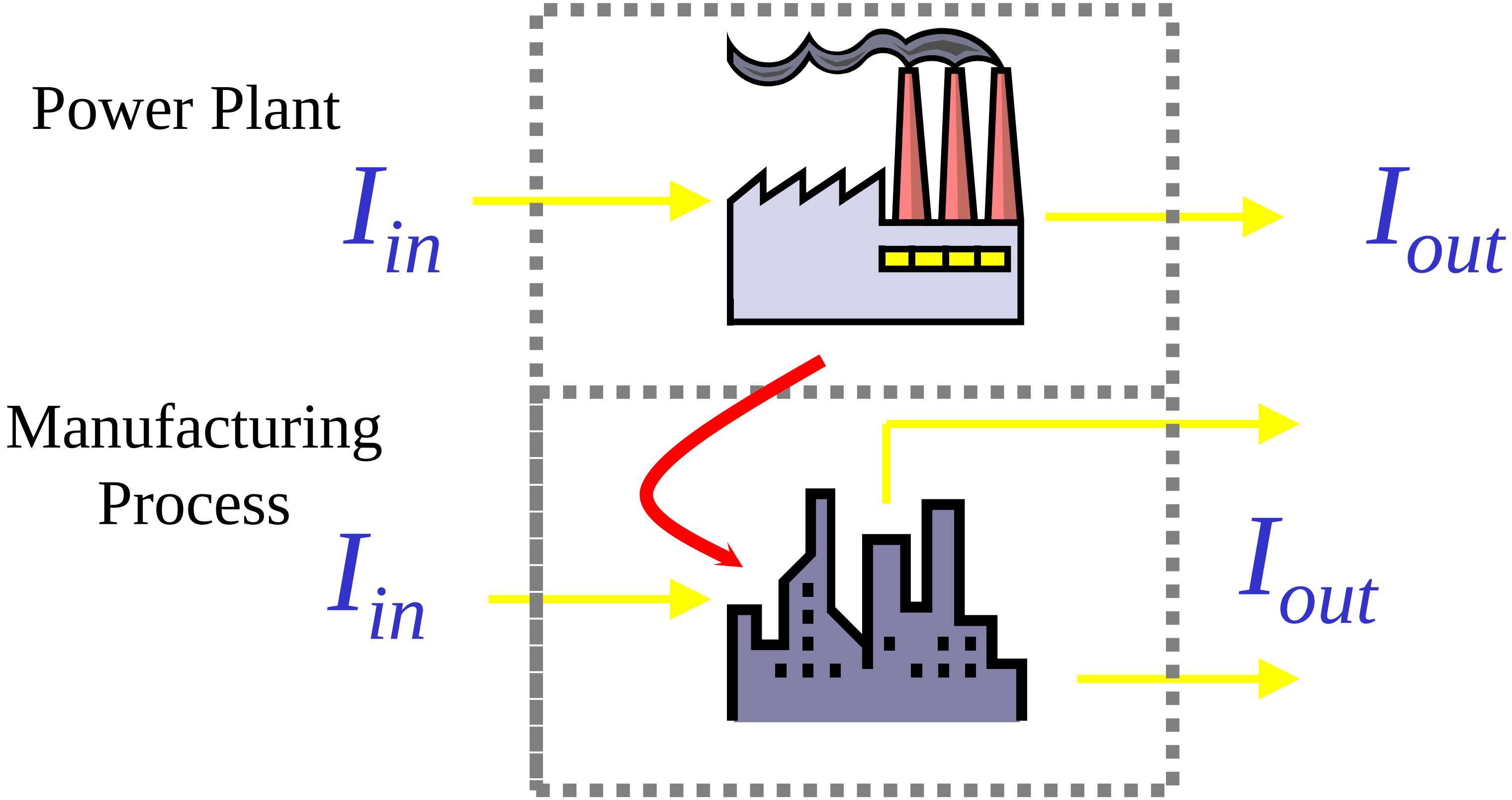
The Total Picture: Process plus utilities





Heat Integration & Utilities **Mass Integration & Utilities**

The Total Picture: Process plus utilities plus environmental impact & sustainability



How to convert ill-posed (abstract definition) problems to well-posed (refined definition) ones?

Establish goals

Propose tests to verify if goals are satisfied

Identify starting points

Identify the space of design alternatives

Note: these are open-ended problems having many solutions! The specific solution obtained by one depends on the specific decisions made by the designers.

How to convert ill-posed (abstract definition) problems to well-posed (refined definition) ones?

Establish goals

> **Make profit, maximize profit, minimize cost, ensure safety, ensure low environmental impact, easy to control, flexible , ……**

Propose tests to verify if goals are satisfied

Identify starting points

Identify the space of design alternatives

How to convert ill-posed (abstract definition) problems to well-posed (refined definition) ones?

Establish goals

Propose tests to verify if goals are satisfied

- **Criteria for success – profit model [net present value (economic evaluation) based on a cost estimation method]; safety test; environment impact test; ……**

Identify starting points

Identify the space of design alternatives

How to convert ill-posed (abstract definition) problems to well-posed (refined definition) ones?

Establish goals

Propose tests to verify if goals are satisfied

Identify starting points

- **What is the starting point (information) – do we already have a process flowsheet plus mass & energy balance completed or only a flowsheet or nothing except that X-amount of product is to be made from Y-amount of raw material**

Identify the space of design alternatives

How to convert ill-posed (abstract definition) problems to well-posed (refined definition) ones?

Establish goals

Propose tests to verify if goals are satisfied

Identify starting points

Identify the space of design alternatives

- **Design related decisions**
  - **Identify them**
  - **Identify alternatives**
  - **Consider base case design**

How much product must be produced?

- **Market demand**
- **Raw material availability**
- **Cost of size of equipments**
  - **Batch process (residence time versus equipment size versus production rate)**
  - **Continuous process (residence time versus equipment size versus production rate)**

How to solve the process design problem (refined definition)?

- **Many ways to solve the problem**
- **We will teach you to do this systematically by performing a predefined set of tasks (work-flow)**
- **The tasks are arranged in a specific sequence**
  - **Within each task, a set of decisions need to be made**
  - **Calculations are made to verify the decisions**
  - **Data generated in one task is used in the subsequent tasks**

Design Tasks 1-6

- **Task 1**: Collect information on the product
- **Task 2**: Collect information on the process; alternative paths to convert other raw materials to the desired product
- **Task 3**: Generate (and/or select) preliminary process flowsheet
- **Task 4**: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a simple mass balance on the selected flowsheet
- **Task 5**: Based on the results from above, set temperatures and pressures on the process flowsheet
- **Task 6**: Based on the results from above, perform a simple mass & energy balance

Design Tasks 6-12

- **Task 7**: Perform detailed process simulation – convert each of the simple models with the more rigorous option, one at a time, until all simple models have been converted.

- **Task 8**: Based on the simulation results from task 7, perform equipment sizing and costing calculations

- **Task 9**: Based on the results from tasks 1-8, perform an economic evaluation, using the current design as the "base case"

- **Task 10**: Investigate if opportunities for heat and mass transfer exist. If yes, apply them and check by how much the cost of operation can be further reduced? (or Task 11)

- **Task 11**: Perform environmental impact analysis (or Task 12)

- **Task 12**: Investigate how the current design can be further improved; formulate process optimization problems (or Task 10)

Case Study: Utilize 75 million kg/y of excess ethylene

What can we produce from Ethylene that can be sold profitably?

Task 1: Identify the product & collect product information (*see also chapter 1 of textbook*)

Case Study: Utilize 75 million kg/y of excess ethylene

What can we produce from Ethylene that can be sold profitably?

Task 1: a) One alternative product – Ethanol

b) Collect information about ethanol –

Formula: C_2H_5OH;

Properties: Tb = 351.44 K; Tm = 159.05 K; Miscible with water; used as solvent; …….

Case Study: Utilize 75 million kg/y of excess ethylene

What can we produce from Ethylene that can be sold profitably?

Task 2: Collect information on process to convert raw material (ethanol) to product (ethanol) – *see also chapters 1-2 of textbook*

Questions

How pure is ethylene source?
What are the consequences of impurities?
How much ethanol to make and at what purity?
What information on the reaction is available?
Any known process flowsheets?

Case Study: Utilize 75 million kg/y of excess ethylene

What can we produce from Ethylene that can be sold profitably?

One alternative – Ethanol

Questions (task 2)

How pure is ethylene source? **96%EL, 3%PL, 1%M**

What are the consequences of impurities?

By-products (DEE, IPA, W, CA) & purge?

How much ethanol to make and at what purity?

Ethanol at 190 proof (85.44% mole)

What is the next step? **Find out about reactions**

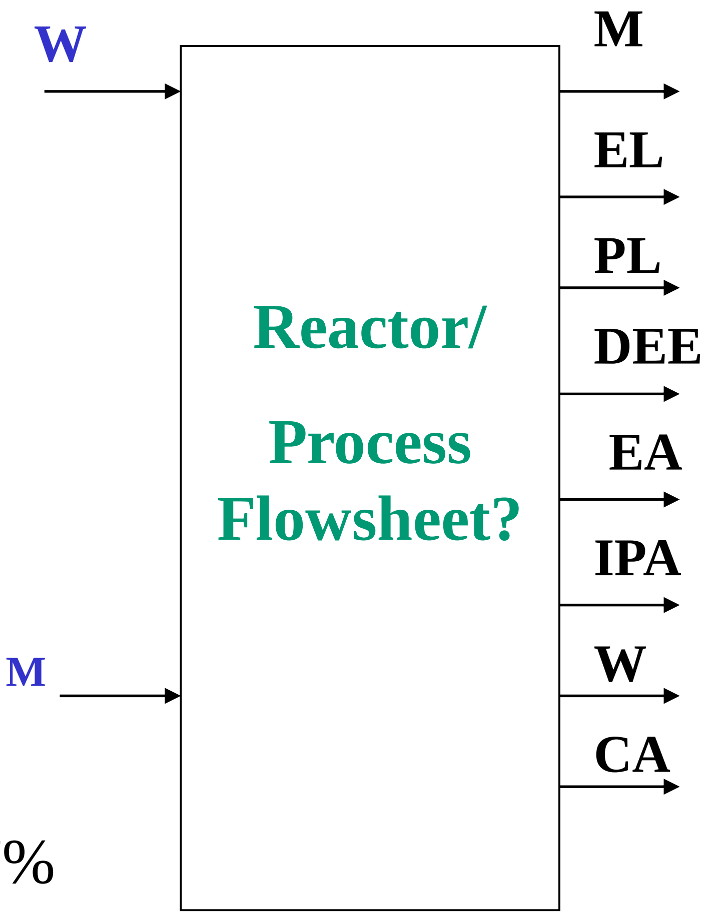
Case Study: Utilize 75 million kg/y of excess ethylene

Task2: Collect process information

$CH2{=}CH2 + H2O \rightarrow CH3CH2OH$

535 K < T < 575; P approx 68 atm; homogeneous noncatalytic reactor; low conversion 5-7% of ethylene to ethanol

$2CH3CH2OH \rightarrow C2H5OC2H5 + H2O$



Keep concentration of methane < 10%

Conversion of propylene approx 0.5-0.7%

Properties: M_w, density, T_m, T_b, H_{vap}, $P_{vap}(T)$, T_c, P_c

Case Study: Utilize 75 million kg/y of excess ethylene

What can we produce from Ethylene that can be sold profitably?

One alternative – Ethanol

Questions

How pure is ethylene source? **96%EL, 3%PL, 1%M**

What are the consequences of impurities?

By-products (DEE, IPA, W, CA) & purge?

How much ethanol to make and at what purity?

150000m3/y at 190 proof (85.44% mole) of ethanol

What is the next step?

Make a quick cost evaluation & establish the flowsheet requirements (see section 2.4.1 of textbook) - $72 - $82 million/y (profit), but operating cost/y and annualized capital cost/y needs to be subtracted.

Case Study: Utilize 75 million kg/y of excess ethylene to produce 150000 m3/y at 85.44%mole purity ethanol

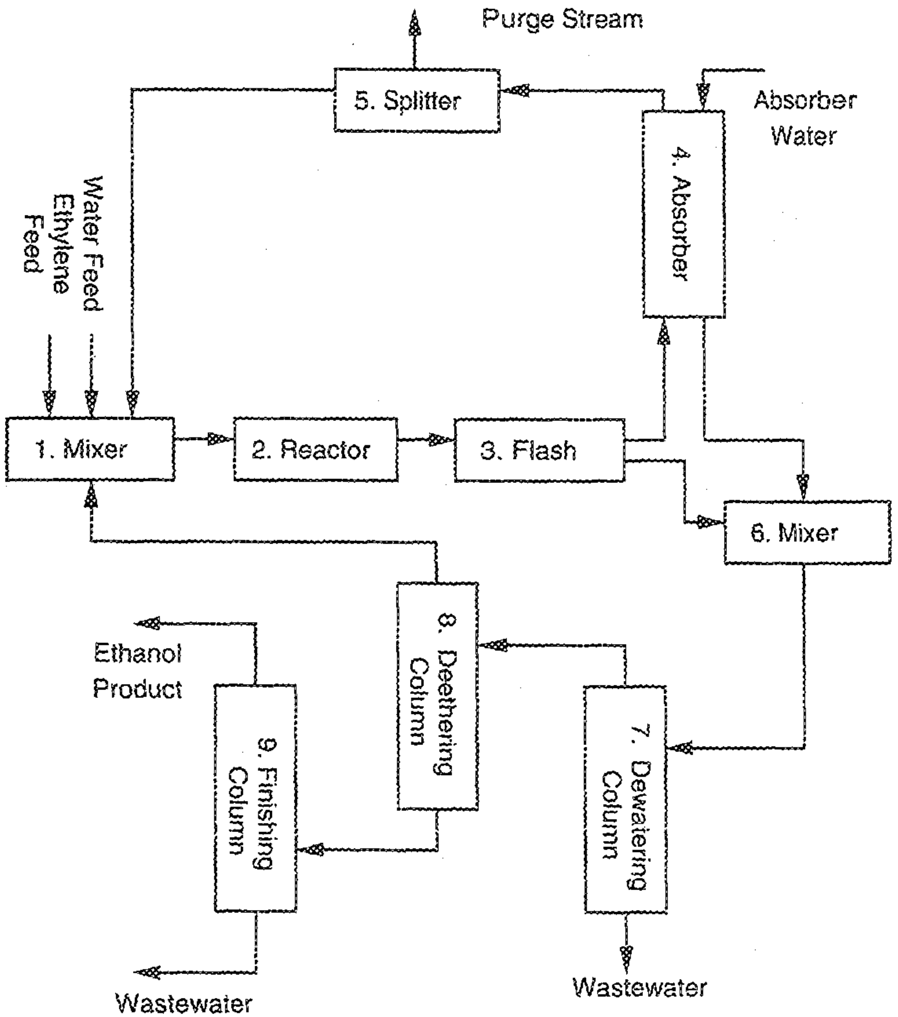
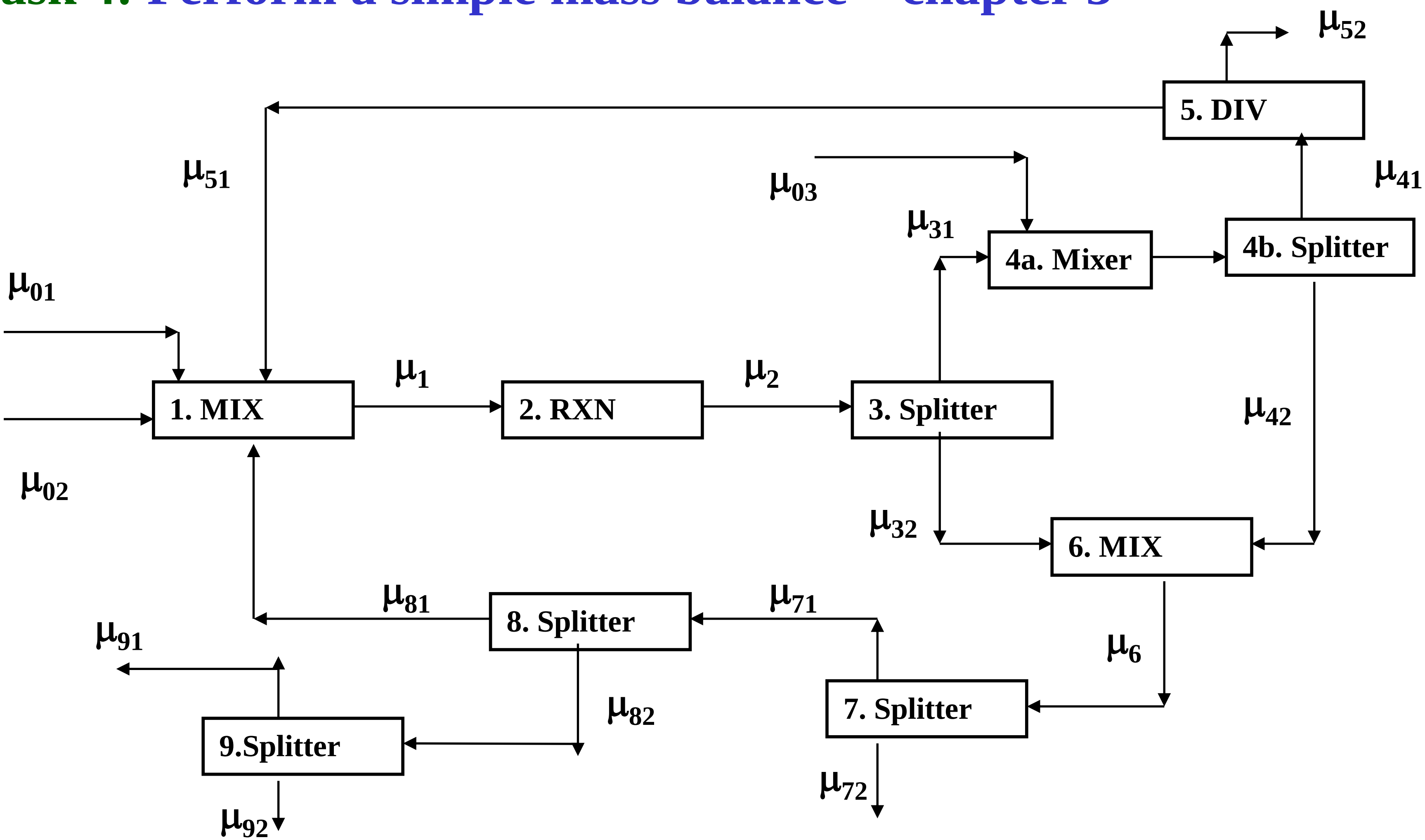


FIGURE 3.1 Ethanol flowsheet.

Task 3: Generate a process flowsheet (chapter 2)

Next: Task 4 (perform a simple mass balance)

Task 4: Perform a simple mass balance – chapter 3

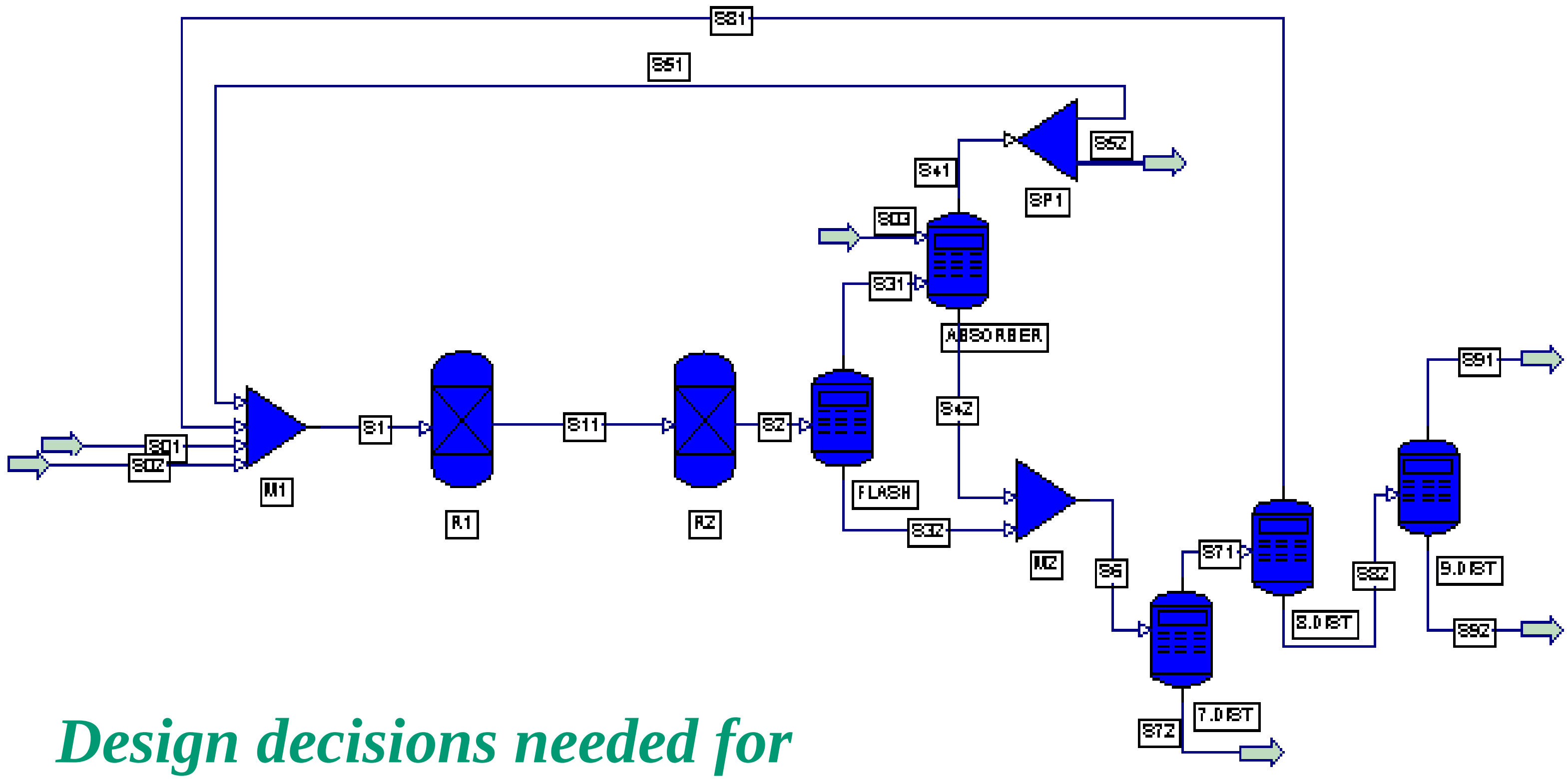


Redraw flowsheet for MB-model: Redrawn flowsheet

Use only mixers, reactors, dividers and splitters (component)!

Task 4: **Perform a simple mass balance - chapter 3 plus notes**

Use PROII or generate your own mass balance model



Design decisions needed for reactors, separators, dividers

Task 4: Perform a simple mass balance – chapter 3 plus notes

Use PROII or generate your own mass balance model

Stream Name		S01	S02	S1	S11	S2	S31	S32	S41	S03	S42
Stream Description											
Phase		Vapor	Liquid	Mixed	Vapor	Mixed	Vapor	Liquid	Vapor	Liquid	Liquid
Temperature	K	300.0000	300.0000	296.0452	590.0000	300.0000	300.0000	100.0000	310.0000	300.0000	1.0000
Pressure	BAR	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Enthalpy	M*KJ/HR	0.9523	1.9528	13.7051	81.2619	15.1154	12.3960	-10.4588	10.5934	0.0764	-2.9907
Molecular Weight		28.3547	18.0150	25.5778	26.5429	26.5429	28.6348	21.9402	28.5307	18.0150	26.8922
Mole Fraction Vapor		1.0000	0.0000	0.7055	1.0000	0.7049	1.0000	0.0000	1.0000	0.0000	0.0000
Mole Fraction Liquid		0.0000	1.0000	0.2945	0.0000	0.2951	0.0000	1.0000	0.0000	1.0000	1.0000
Rate	KG-MOL/HR	100.000	771.200	2533.177	2441.076	2441.076	1678.305	762.771	1580.383	37.747	135.668
Fluid Rates	KG-MOL/HR										
METHANE		1.0000	0.0000	200.8031	200.8031	200.8031	199.9998	0.8032	199.9998	0.0000	0.0000
ETHYLENE		96.0000	0.0000	1238.2995	1198.6458	1198.6458	1180.6960	17.9797	1195.8721	0.0000	24.7940
PROPENE		3.0000	0.0000	268.5943	266.7141	266.7141	248.5775	18.1366	223.9684	0.0000	24.6092
EETHER		0.0000	0.0000	2.4110	2.4110	2.4231	1.2116	1.2116	0.2908	0.0000	0.9208
H2O		0.0000	771.2000	771.9409	679.8400	679.8521	36.7120	643.1401	0.1415	37.7470	74.3175
ETHANOL		0.0000	0.0000	0.9502	90.7809	90.7957	10.9816	79.7751	0.1098	0.0000	10.8717
IPROPNOL		0.0000	0.0000	0.0010	1.8812	1.8812	0.1961	1.7290	0.0010	0.0000	0.1951

Stream Name		S51	S52	S6	S71	S72	S81	S82	S91	S92
Stream Description										
Phase		Vapor	Vapor	Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Mixed
Temperature	K	310.0000	310.0000	84.2671	310.0000	1.0000	310.0000	328.2792	100.0000	372.3232
Pressure	BAR	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Enthalpy	M*KJ/HR	10.5166	0.0528	-13.4495	1.9995	-13.4911	1.0734	0.8821	-1.6983	2.5804
Molecular Weight		28.5307	28.5307	22.6880	34.9992	18.0396	35.8814	33.9012	42.0014	19.2366
Mole Fraction Vapor		1.0000	1.0000	0.0000	0.3637	0.0000	1.0000	0.0000	0.0000	0.8981
Mole Fraction Liquid		0.0000	0.0000	1.0000	0.6363	1.0000	0.0000	1.0000	1.0000	0.1019
Rate	KG-MOL/HR	1572.481	7.902	898.440	252.199	645.240	88.295	163.304	105.089	58.235
Fluid Rates	KG-MOL/HR									
METHANE		198.9998	1.0000	0.8032	0.8032	0.0000	0.8032	0.0000	0.0000	0.0000
ETHYLENE		1150.0927	5.7794	42.7737	42.7737	0.0000	42.7737	0.0000	0.0000	0.0000
PROPENE		222.8485	1.1198	42.7457	42.7457	0.0000	42.7457	0.0000	0.0000	0.0000
EETHER		0.2893	0.0015	2.1323	2.1323	0.0000	2.1217	0.0107	0.0106	0.0001
H2O		0.1408	0.0007	717.4576	71.7458	645.7119	0.0000	71.7458	15.3005	56.4453
ETHANOL		0.1093	0.0005	90.6458	90.1936	0.4532	0.4510	89.7426	89.6529	0.0897
IPROPNOL		0.0010	0.0000	1.8802	1.8049	0.0752	0.0000	1.8049	0.1051	1.6998

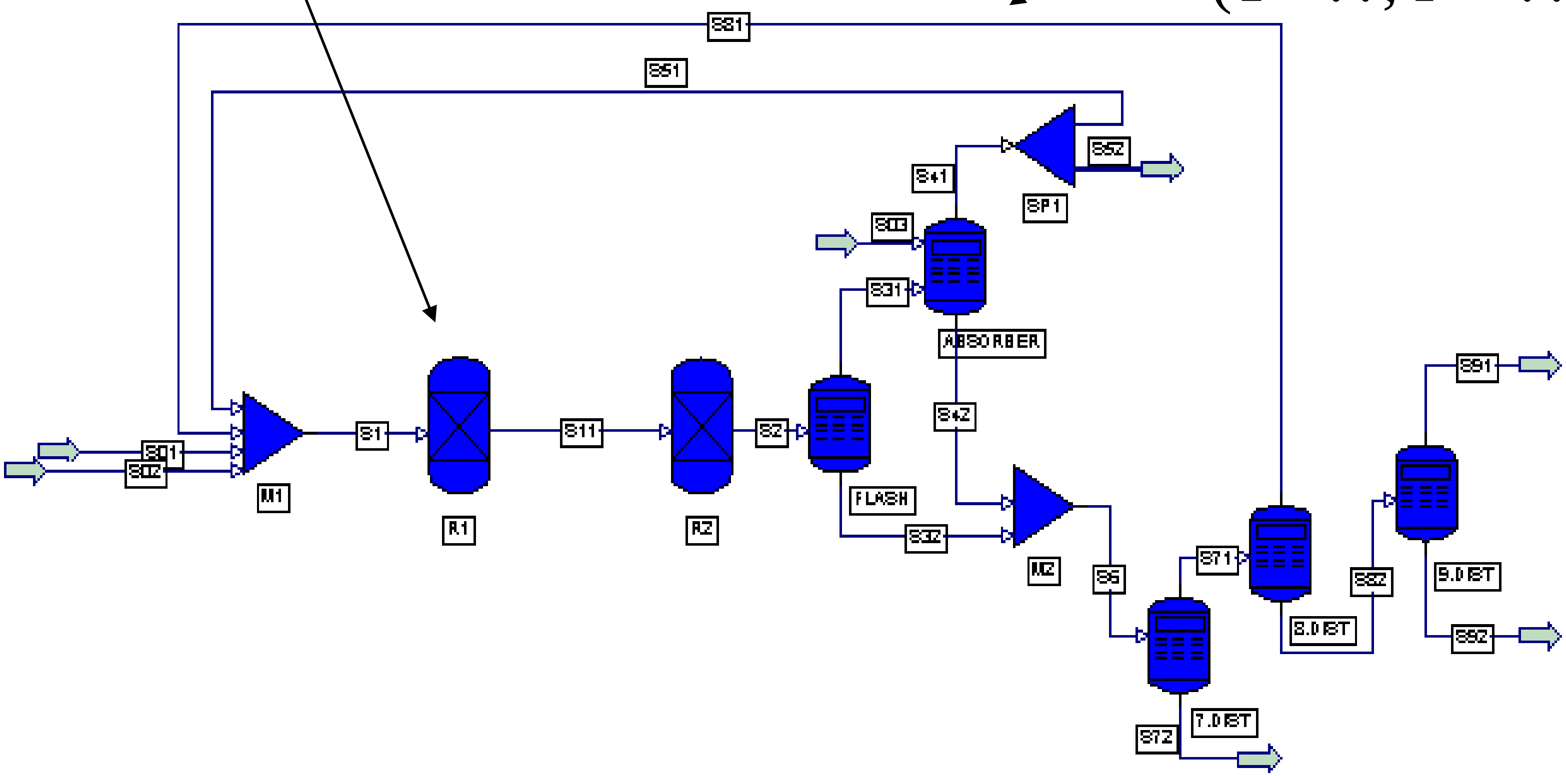
Note: Simulation (simulator) is used mainly to verify design decisons. It does not do process design!

Task 5: **Set temperatures and pressures on streams and unit operations (see also chapter 3 of textbook)**

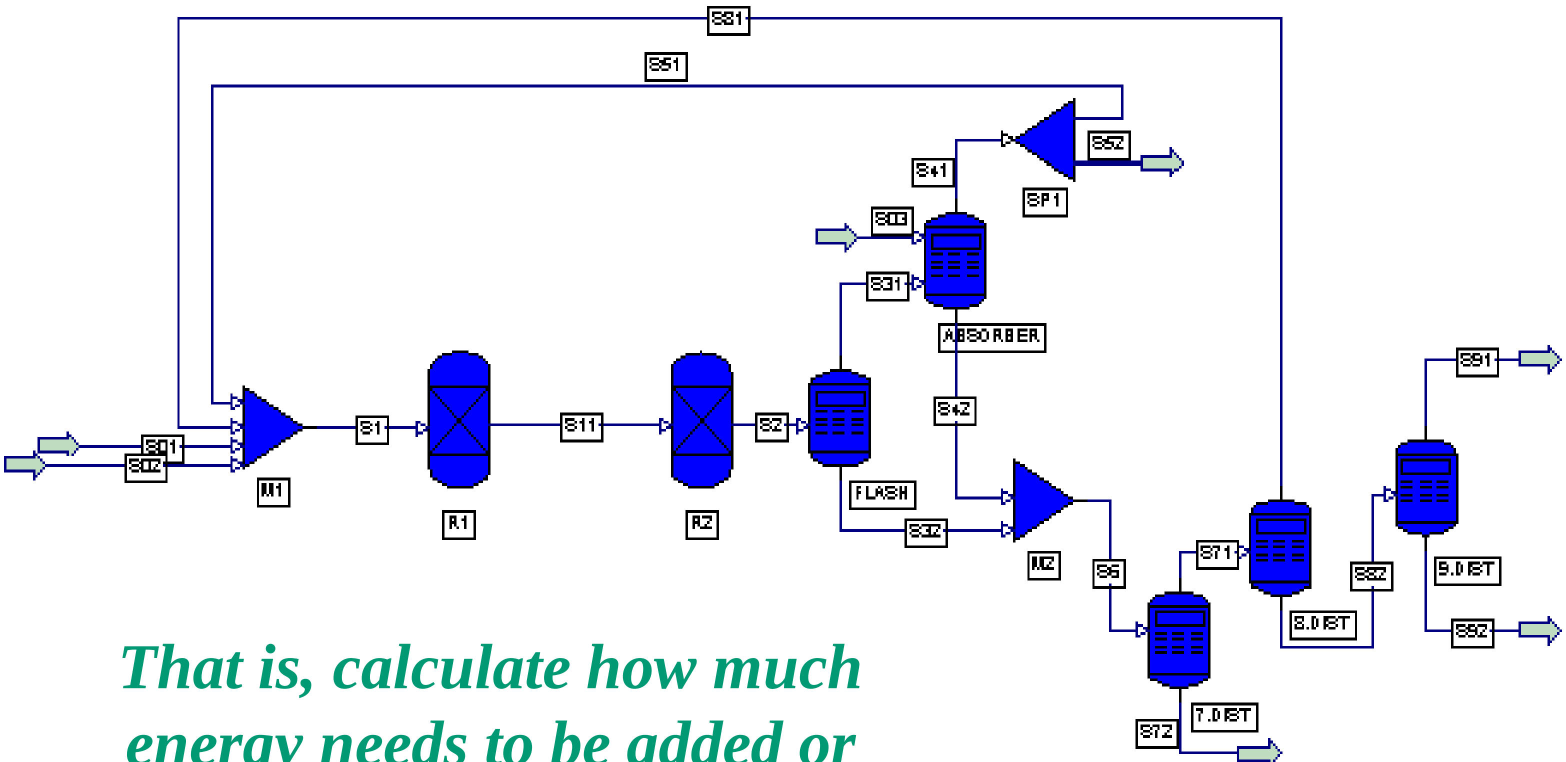
example

example

(T= ??; P = ??)



Task 6: **With all temperatures and pressures known, perform mass and energy balance for the simple flowsheet (see also chapter 3 of textbook)**



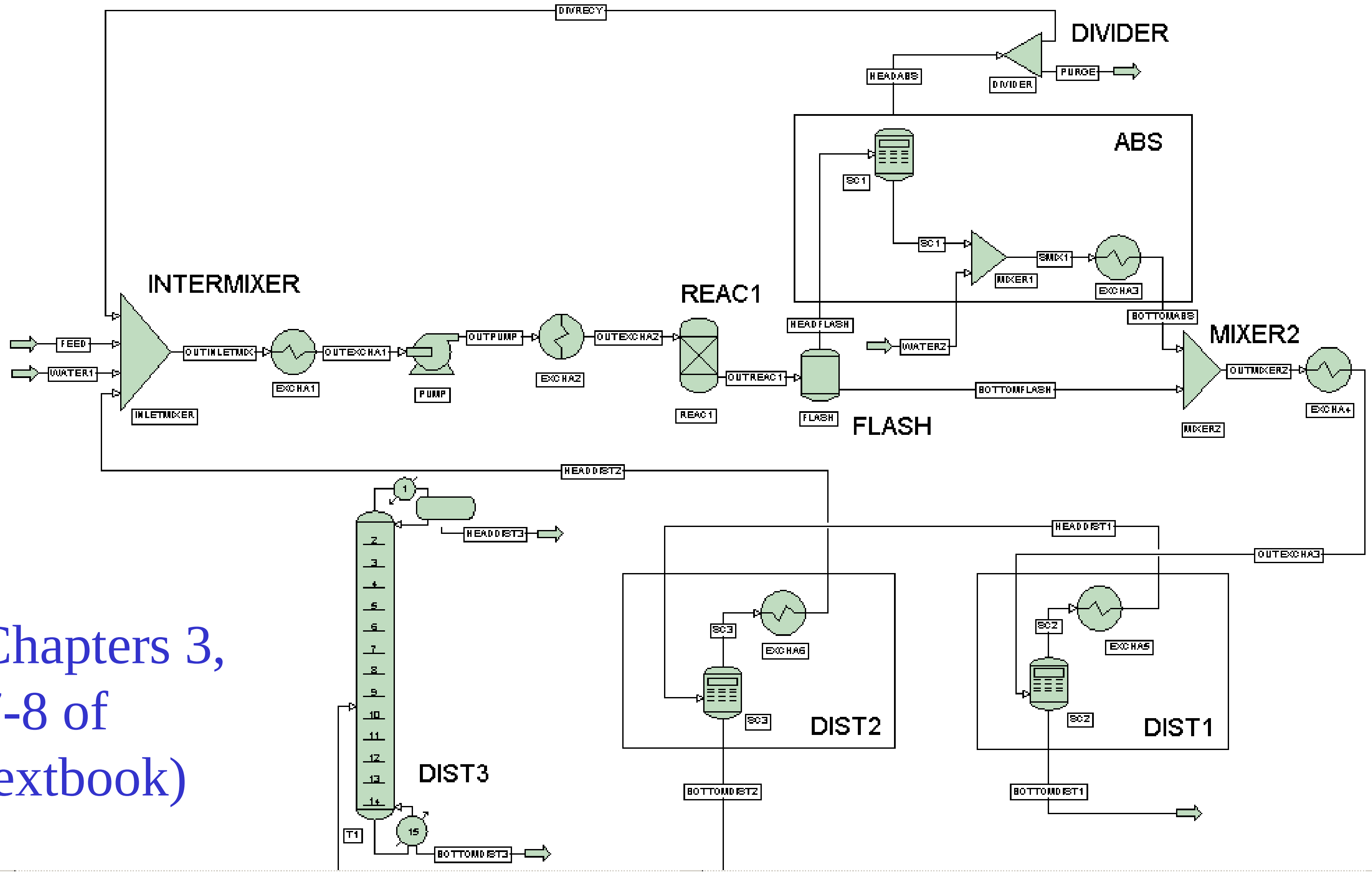
That is, calculate how much energy needs to be added or removed for each unit operation?

Mass and Energy balances for Ethanol Process Flowsheet

	μ_{01}	μ_{02}	μ_{1}	μ_{2}	μ_{31}	μ_{32}	μ_{41}	μ_{42}	μ_{03}
Methane (gmol/s)	1	0	200	200	199.2	0.8	199.2	0	0
Ethylene	96	0	1289	1198.77	1180.78	17.98	1155.99	24.796	0
Propylene	3	0	268.6	266.71	248.58	18.136	223.97	24.609	0
Diethyl Ether	0	0	0	2.421	1.210	1.2108	0.2906	0.9202	0
Ethanol	0	0	0.56	90.79	10.98	79.80	0.1098	10.87	0
Isopropanol	0	0	0	1.8802	0.156	1.724	0.001018	0.1550	0
Water	0	771.797	773.4	680.72	36.75	643.97	1.610	72.896	37.747
Total	100	771.797	2531.56	2441.31	1677.68	763.62	1581.177	134.25	37.747
Temperature, K	300	300	590	590	393	393	381.57	338.7	310
Pressure, bar	1	1	69	69	68.5	68.5	68	68	68
Vap. Frac	1	0	1	1	1	0	1	0	0
Enthalpy, kcal/s	1198.85	−52097.04	−21683.63	−22689.24	11515.18	−47920.28	13439.75	−5324.42	−2544.97

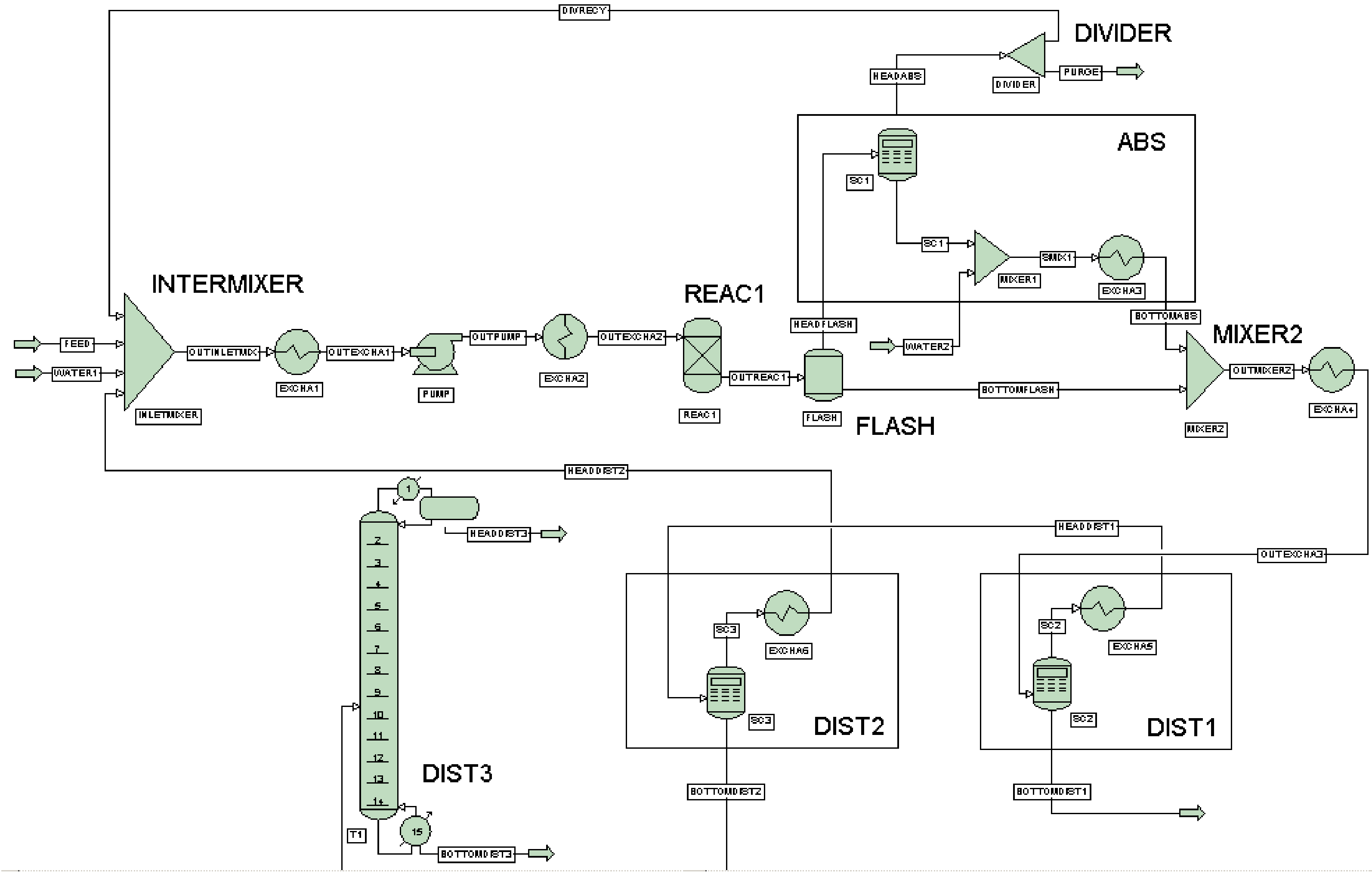
	μ_{51}	μ_{52}	μ_{6}	μ_{71}	μ_{72}	μ_{81}	μ_{82}	μ_{91}	μ_{92}
Methane (gmol/s)	198.204	0.996	0.8	0.8	0	0.8	0	0	0
Ethylene	1150.21	5.780	42.778	42.778	0	42.7781	0	0	0
Propylene	222.85	1.1198	42.746	42.746	0	42.7466	0	0	0
Diethyl Ether	0.2891	0.00145	2.131	2.131	0	2.1205	0.01065	0.01065	0
Ethanol	0.1093	0.000549	90.680	90.226	0.4534	0.451	89.775	89.3267	0.4489
Isopropanol	0.001013	5.09323E-06	1.879	1.804	0.075	0	1.804	0.1046	1.6994
Water	1.6024	0.00805	716.867	71.68	645.18	0	71.686	15.1490	56.537
Total	1573.27	7.9058	897.882	252.173	645.70	88.896	163.277	104.591	58.686
Temperature, K	381.57	381.57	372	310	480	310	418	350	383
Pressure, bar	67.5	67.5	68	17.56	18.06	10.7	11.2	1	1.5
Vap. Frac	1	1	0	0	0	1	0	0	0
Enthalpy, kcal/s	13372.55	67.197	−53244.70	−10436.14	−42629.37	590.10	−10576.78	−6787.79	−3930.30

Task 7: Replace each of the component stream calculators (splitters) with their corresponding rigorous models (one at a time) and perform the mass and energy balance for the total flowsheet

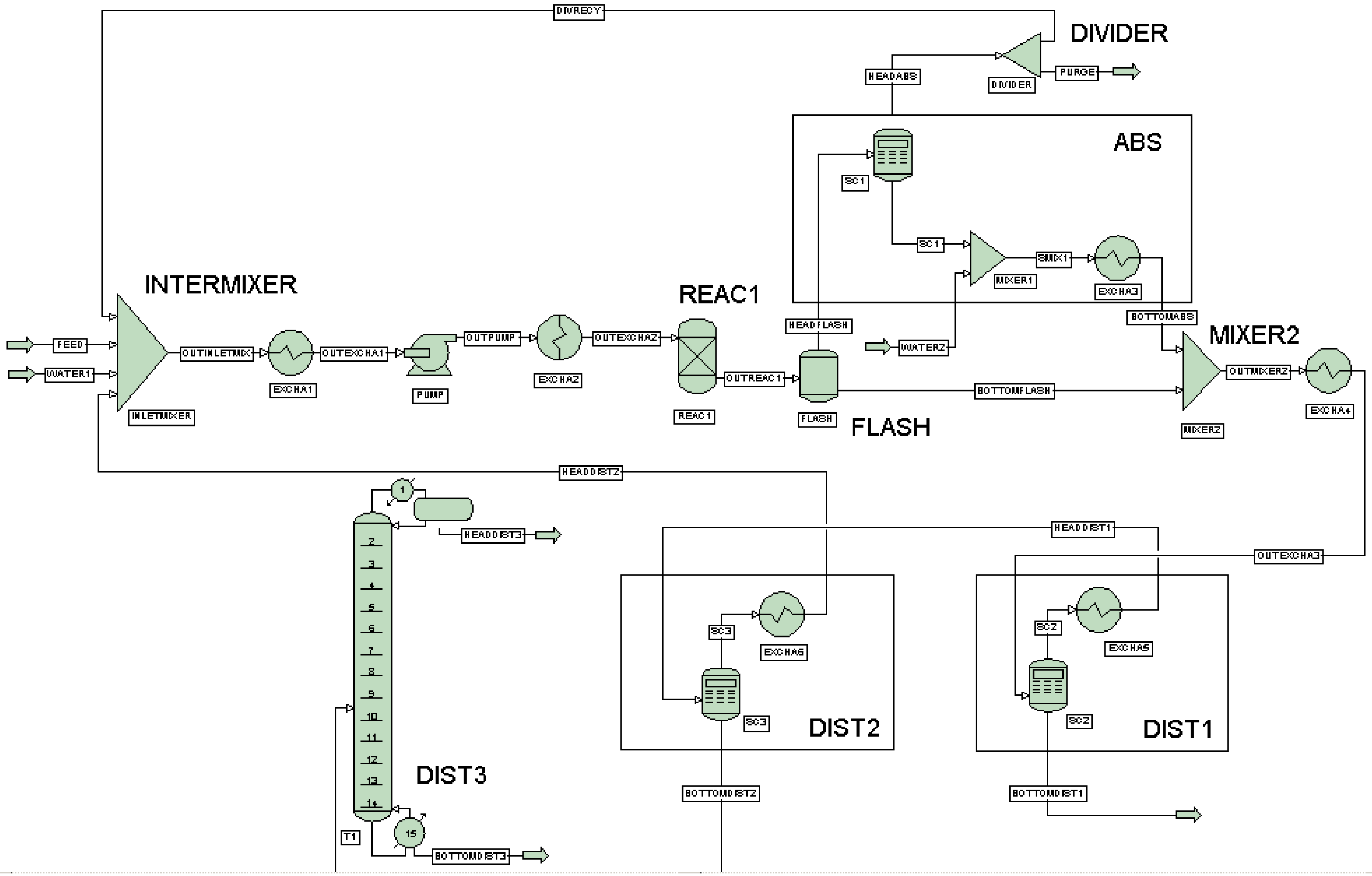


Chapters 3, 7-8 of textbook)

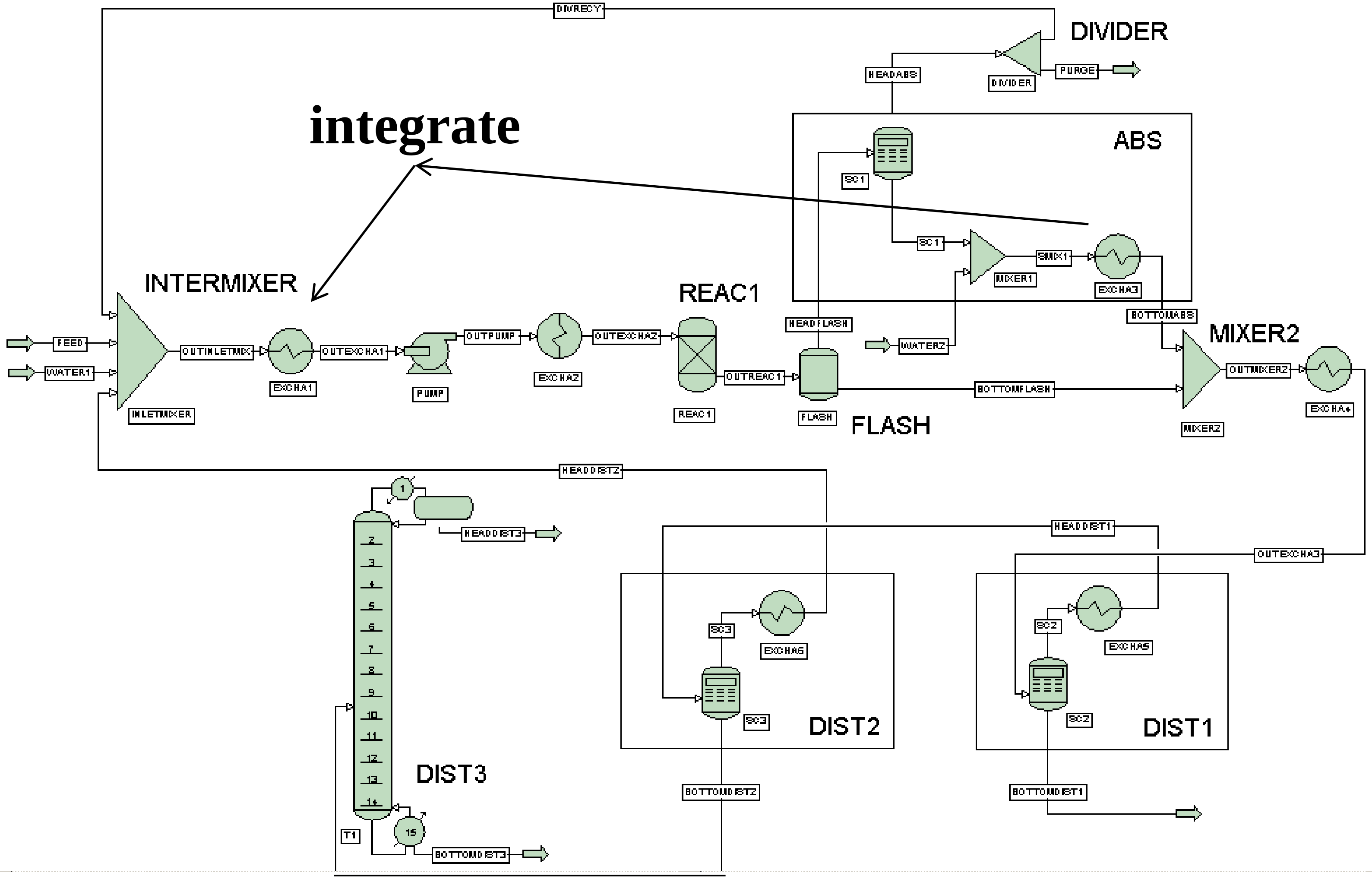
Task 8: Perform equipment sizing and costing calculations for all equipments in the process flowsheet (Chapter 4)



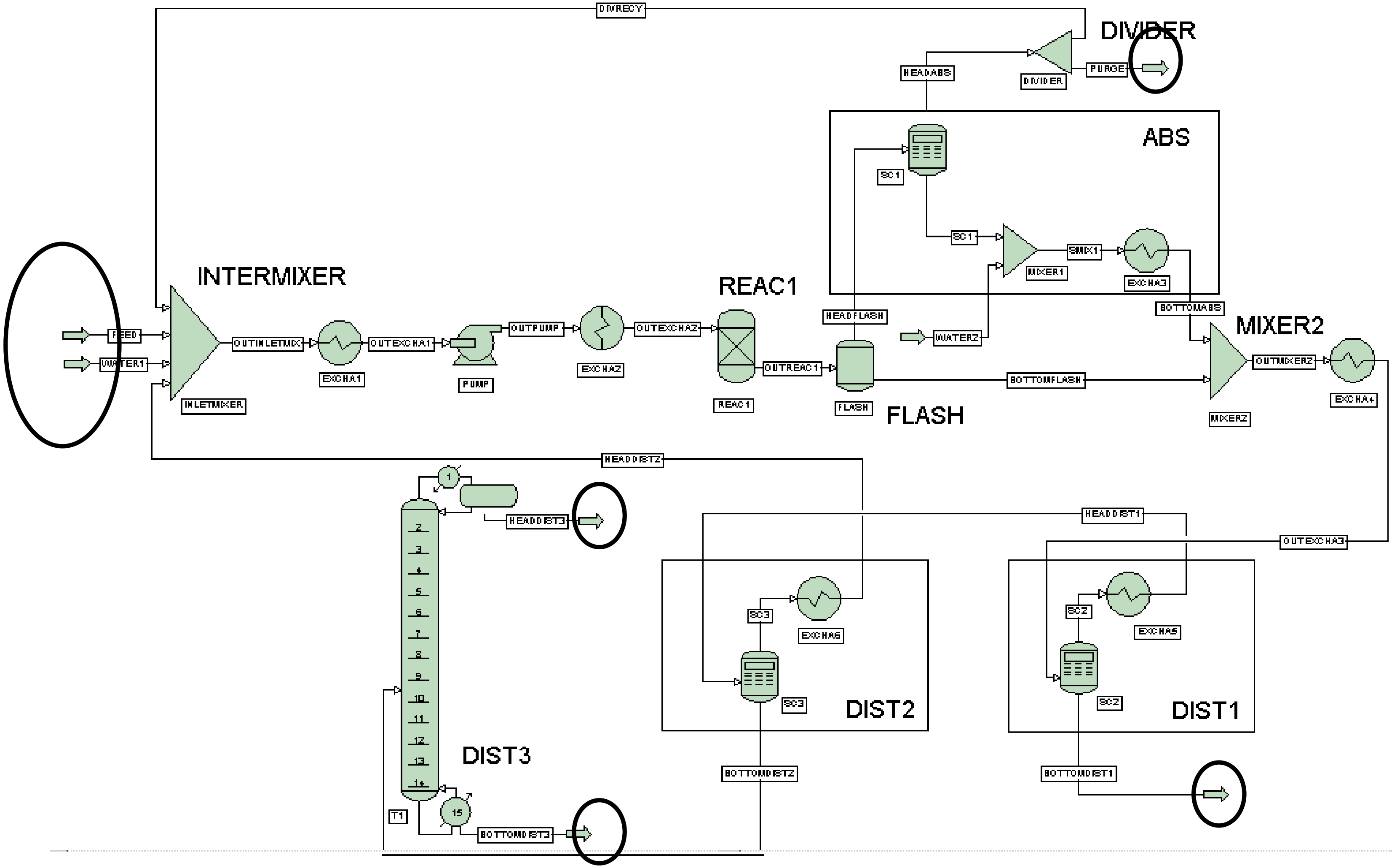
Task 9: Perform economic evaluation for designed process (Chapters 4-5 plus notes) – this will be the base case design



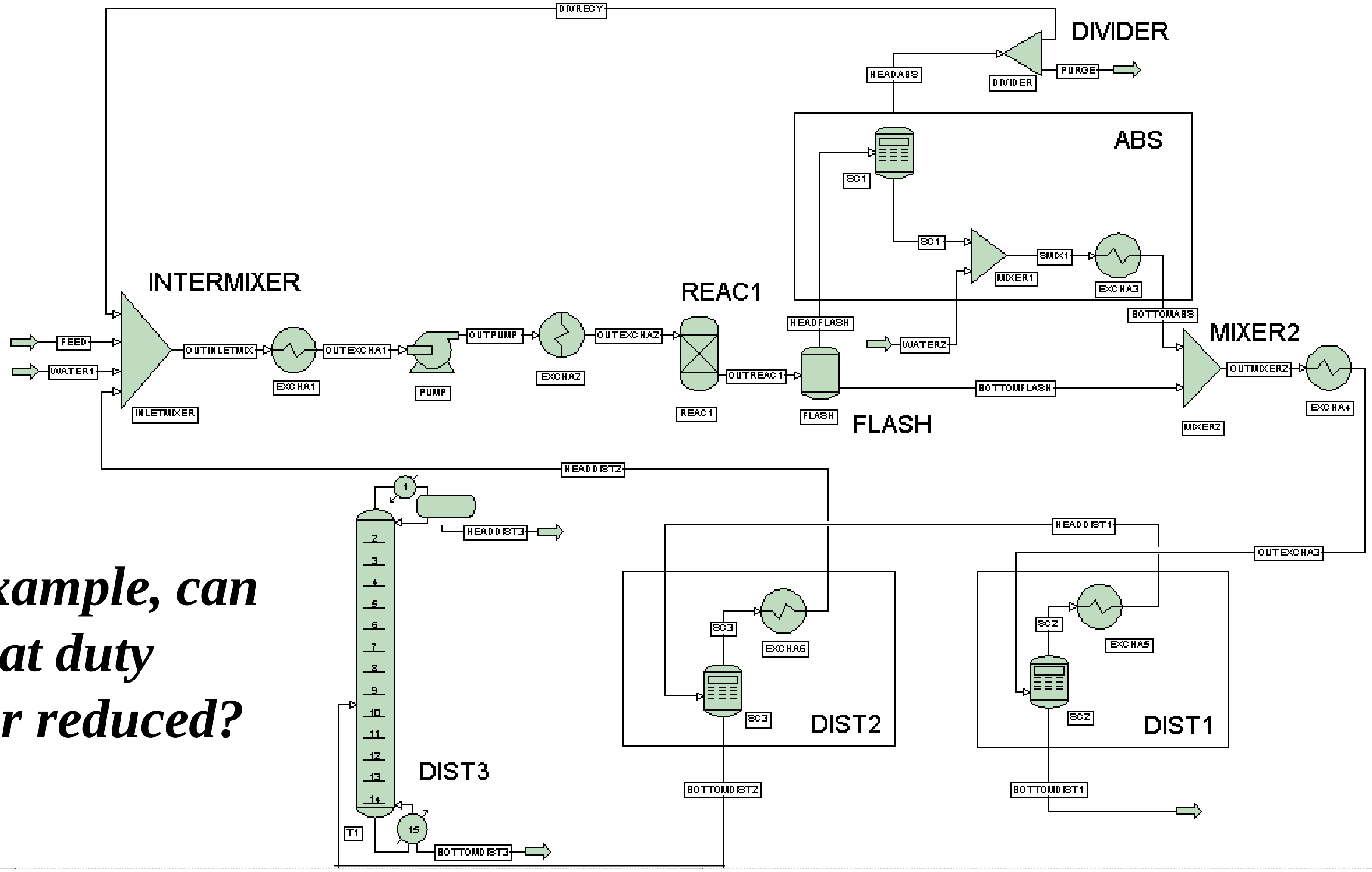
Task 10: Investigate opportunities for heat and mass integration (chapters 10 & 16 plus notes)



Task 11: Perform environmental impact analysis (supplied notes)



Task 12: **Investigate how to improve the base case design – formulate process optimization problems (chapter 9 plus notes)**



For example, can the heat duty further reduced?

Important Issues to Note in Chemical Process Design

1. **Process design is about making design decisions (which decisions, when & how) & verifying if they are acceptable.**
2. **Process simulators should not be used for blind trial and error but for fast evaluation of design decisions**
3. **Process design is iterative by nature but if a systematic procedure is followed, better results can be obtained faster**
4. **Use everything (knowledge) that you have learned from other courses**

Course: Tutorials

1. **First week**
   – **get familiar with software (Process simulator: PROII) & (ICAS: Database & utility calculations)**
   – **start with process design project (tasks 1-2); Friday, 10 February finish task-3**
2. **Design project report needs to be submitted in terms of tasks at different stages of the course (only for checking the design not for grading)**
3. **Work on design projects can be done in groups of 3 with one report per group but for the 3 extra exam problems, the reports must be individually submitted**