Chapter 1

Problem 1.1

There are many possible correct answers to this question and it can be answered in varying levels of detail. The key steps that should be included for each process with typical required times are listed below. The project plan can be sketched using a spreadsheet or drawn up using a project planning tool such as MS Project (as in Problem 1.2).

i) A petrochemical process using established technology, to be built on an existing site. Since the technology is established, there will be no need to generate design concepts and carry out R&D. The steps are then:
    Set design basis (1 week)
    Evaluate economics, optimize and select design (typically 10-30 weeks, depending on project scope)
    Detailed design and equipment selection (typically six months to one year)
    Procurement and construction (typically one year)
    Shakedown and start-up (typically one month)
   These steps are usually more or less sequential, although some procurement of long lead-time items may be started during detailed design.

ii) A process for full-scale manufacture of a new drug, based on a process currently undergoing pilot plant trials. Since the pilot plant is already operating the designer already has a good idea of the process flowsheet and the goal is to be prepared to ramp up production to full scale once the drug is approved. The steps are:

Set design basis (1 week)
Confirm performance/scale-up of pilot plant operations (2-20 weeks, depending on how smoothly pilot plant runs)
Optimize and select design (10-20 weeks)
Detailed design and equipment selection (about six months)

In parallel to these process design activities there will be activities related to getting approval for the new drug:

Conduct clinical trials (6 months to 2 years)
Review clinical trial results (typically 3 to 6 months)
Obtain FDA approval

Some of the procurement and construction activities will be started as soon as the first clinical results look promising, but final construction and shakedown will not occur until the review of clinical trials is completed.

iii) A novel process to convert cellulosic waste to fuel. The technology and flowsheet will need considerable development, so a schedule might be:

Set design basis (1 week)
Generate design concepts & carry out R&D (one to five years)
Evaluate economics, optimize and select design (six months, but could run parallel to generating design concepts for up to five years)
Detailed design and equipment selection (six months to one year)
Procurement and construction (about one year)
Shakedown and start-up (one month to one year, as there may be start-up hiccups with a new technology)

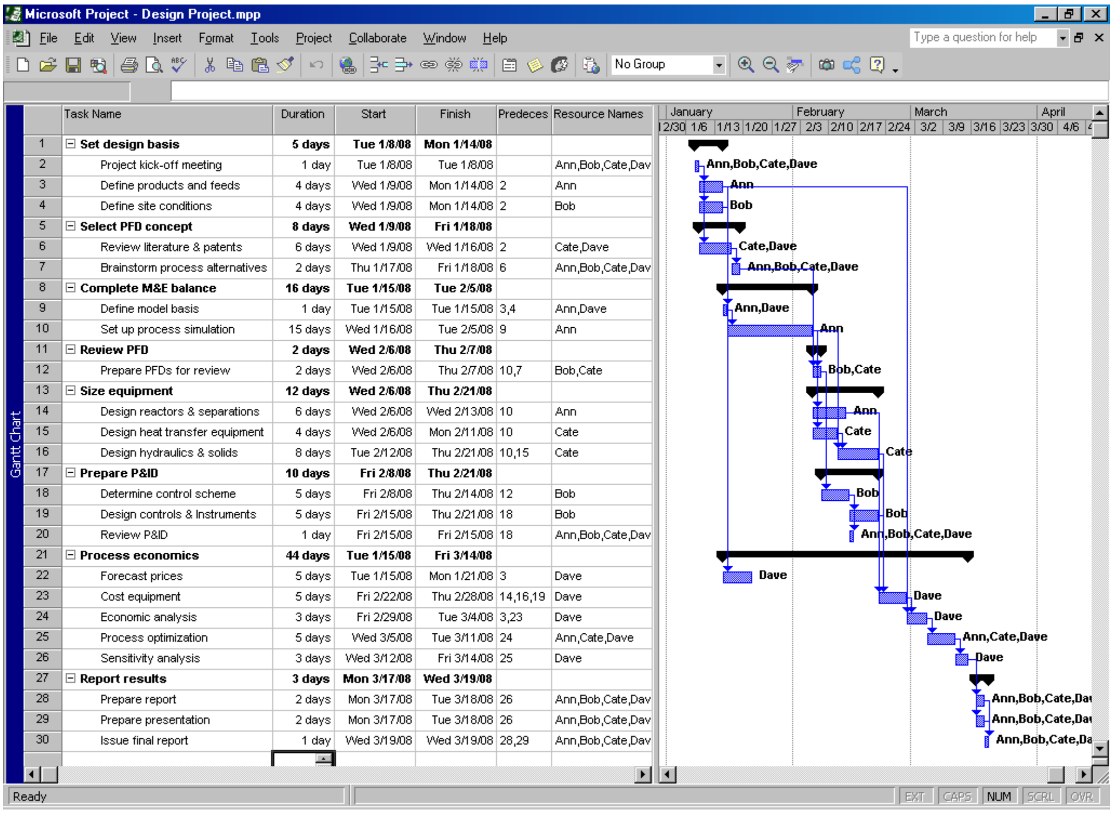
iv) A spent nuclear fuel reprocessing facility. There is established technology for nuclear fuel reprocessing, but new processes are always possible. For an established technology the schedule would look much like problem (i) and for new technology it would look like problem (iv). All of the steps would probably take longer because of the scale of the plant and additional steps would be needed for obtaining local, state and federal permits and revising them after setting the design basis, selecting the design, and completing detailed design. The time taken to obtain permits could be several years and the total time to operation would probably exceed ten years.

v) A solvent recovery system for electronics production. This is a relatively small project, so the steps would be:

Set design basis (1 – 2 days)
Generate design concepts (1 to 2 months)
Evaluate economics, optimize and select design (ten weeks or less)
Detailed design and equipment selection (2 to 3 months)
Procurement and construction (3 to 6 months)
Shakedown and start-up (one month)

Problem 1.2

This requires a more detailed breakdown than problem 1.1. A sample project plan is given in the lecture slides and shown below (in MS Project format):



	Task Name	Duration	Start	Finish	Predeces	Resource Names
1	**Set design basis**	**5 days**	**Tue 1/8/08**	**Mon 1/14/08**		
2	Project kick-off meeting	1 day	Tue 1/8/08	Tue 1/8/08		Ann,Bob,Cate,Dav
3	Define products and feeds	4 days	Wed 1/9/08	Mon 1/14/08	2	Ann
4	Define site conditions	4 days	Wed 1/9/08	Mon 1/14/08	2	Bob
5	**Select PFD concept**	**8 days**	**Wed 1/9/08**	**Fri 1/18/08**		
6	Review literature & patents	6 days	Wed 1/9/08	Wed 1/16/08	2	Cate,Dave
7	Brainstorm process alternatives	2 days	Thu 1/17/08	Fri 1/18/08	6	Ann,Bob,Cate,Dav
8	**Complete M&E balance**	**16 days**	**Tue 1/15/08**	**Tue 2/5/08**		
9	Define model basis	1 day	Tue 1/15/08	Tue 1/15/08	3,4	Ann,Dave
10	Set up process simulation	15 days	Wed 1/16/08	Tue 2/5/08	9	Ann
11	**Review PFD**	**2 days**	**Wed 2/6/08**	**Thu 2/7/08**		
12	Prepare PFDs for review	2 days	Wed 2/6/08	Thu 2/7/08	10,7	Bob,Cate
13	**Size equipment**	**12 days**	**Wed 2/6/08**	**Thu 2/21/08**		
14	Design reactors & separations	6 days	Wed 2/6/08	Wed 2/13/08	10	Ann
15	Design heat transfer equipment	4 days	Wed 2/6/08	Mon 2/11/08	10	Cate
16	Design hydraulics & solids	8 days	Tue 2/12/08	Thu 2/21/08	10,15	Cate
17	**Prepare P&ID**	**10 days**	**Fri 2/8/08**	**Thu 2/21/08**		
18	Determine control scheme	5 days	Fri 2/8/08	Thu 2/14/08	12	Bob
19	Design controls & Instruments	5 days	Fri 2/15/08	Thu 2/21/08	18	Bob
20	Review P&ID	1 day	Fri 2/15/08	Fri 2/15/08	18	Ann,Bob,Cate,Dav
21	**Process economics**	**44 days**	**Tue 1/15/08**	**Fri 3/14/08**		
22	Forecast prices	5 days	Tue 1/15/08	Mon 1/21/08	3	Dave
23	Cost equipment	5 days	Fri 2/22/08	Thu 2/28/08	14,16,19	Dave
24	Economic analysis	3 days	Fri 2/29/08	Tue 3/4/08	3,23	Dave
25	Process optimization	5 days	Wed 3/5/08	Tue 3/11/08	24	Ann,Cate,Dave
26	Sensitivity analysis	3 days	Wed 3/12/08	Fri 3/14/08	25	Dave
27	**Report results**	**3 days**	**Mon 3/17/08**	**Wed 3/19/08**		
28	Prepare report	2 days	Mon 3/17/08	Tue 3/18/08	26	Ann,Bob,Cate,Dav
29	Prepare presentation	2 days	Mon 3/17/08	Tue 3/18/08	26	Ann,Bob,Cate,Dav
30	Issue final report	1 day	Wed 3/19/08	Wed 3/19/08	28,29	Ann,Bob,Cate,Dav

Suitable intermediate deliverables could include:

The design basis
A completed PFD (or PFD review)
A completed process simulation
A completed PID (or review)

Problem 1.3

Number of components, $C = 3$

Degrees of freedom for a process stream = $C + 2$ (molar flowrates of C components plus temperature and pressure)

Variables:

Streams	$4(C + 2)$
Separator pressure	1
Separator temperature	1
Total	$4C + 10$

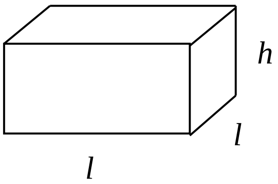
Relationships:

Material balances	C
v-l-e relationships	C
l-l-e relationships	C
Equality of temperature, pressure	6
Total	$3C + 6$

Degrees of freedom = $(4C + 10) - (3C + 6) = C + 4$

For $C = 3$, degrees of freedom = 7
The feed stream conditions are fixed which fixes $C + 2$ variables and so the design variables to be decided = 7 – 5 = 2.
Choose separator temperature and pressure.
Note: temperature and pressure taken as the same for all streams.

Problem 1.4



Volume = $l^2 \times h = 8\ \text{m}^3$

(i) *Closed Top*

The minimum area will obviusly be given by a cube, $l = h$

Proof:

Area of plate $= 2l^2 + 4lh$

Objective function $= 2l^2 + 32l^{-1}$

Differentiate and equate to zero:

$$0 = 4l - 32l^{-2}$$

$$l = \sqrt[3]{8} = 2\ \text{m}$$

$$h = \frac{8}{2^2} = 2\ \text{m}$$

(ii) *Open Top*

Area of plate $= l^2 + 4lh$

$= l^2 + 4l \times 8l^{-2}$

Objective function $= l^2 + 32l^{-1}$

Differentiate and equate to zero:

$$0 = 2l - 32l^{-2}$$

$$l = \sqrt[3]{16} = 2.52\ \text{m} \qquad h = 1.26\ \text{m} \quad (= l/2)$$

Problem 1.5

Insulation problem easily solved using a spreadsheet, given below and in the spreadsheet file.

All calculations are peformed per m^2 area

Heat loss (or gain) = (U)(temp. diff.)(time) = (U)(heating or cooling degree days)(sec/day)
Savings = (heat or cooling saved)(cost of fuel or cooling)
Insulation Costs = (thickness)(cost per cu. m)(capital charge ratio)

Data: cost of fuel \$8/GJ
cost of cooling \$5/GJ
cost of insulation \$120/m^3
capital charges 20% per year

Number of heating degree days and cooling degree days can be calculated from climate data by multiplying number of days by temperature difference between internal and external temperature. Values for the U.S.A. can also be found on-line from the National Climatic Data Center, but these are based on internal temperature of 65F.

Month	No of days		Average temp difference		Degree days	
	> 80F	< 70F	> 80 F	< 70 F	Cooling	Heating
January	0	31	0	50	0	1550
February	0	28	0	55	0	1540
March	0	25	0	40	0	1000
April	0	20	0	28	0	560
May	5	15	2	10	10	150
June	10	5	5	4	50	20
July	20	0	8	0	160	0
August	20	0	7	0	140	0
September	10	5	4	5	40	25
October	2	20	2	15	4	300
November	0	30	0	25	0	750
December	0	31	0	45	0	1395
				total	404	7290

(Average heating and cooling days can also be found from National Climatic Data Center)

Thickness (mm)	U (W/m^{2}K)	Heating load (GJ/m^{2}y)	Cooling load (GJ/m^{2}y)	Heating cost (\$/m^{2}y)	Cooling cost (\$/m^{2}y)	Capital cost (\$/m^{2}y)	Total cost (\$/m^{2}y)	
0	20	12.59712	0.698112	100.77696	3.49056	0	104.2675	
25	0.9	0.5668704	0.03141504	4.5349632	0.1570752	0.6	5.292038	
50	0.7	0.4408992	0.02443392	3.5271936	0.1221696	1.2	4.849363	
100	0.3	0.1889568	0.01047168	1.5116544	0.0523584	2.4	3.964013	optimum
150	0.25	0.157464	0.0087264	1.259712	0.043632	3.6	4.903344	
200	0.2	0.1259712	0.00698112	1.0077696	0.0349056	4.8	5.842675	
250	0.15	0.0944784	0.00523584	0.7558272	0.0261792	6	6.782006	

A sensitivity analysis could be used to look at the effect of changing the inside temperature.

Problem 1.6

Optimum shape would have minimum surface to volume, i.e. a hemisphere.

Used in many societies where building resources are scarce (e.g., huts, igloos, etc.)

Seldom used in richer societies because hemispherical shape is hard to subdivide into internal rooms.

Problem 1.7

The reactions are:

$CH_4 + H_2O = CO + 3H_2$
and
$CH_4 + ½ O_2 = CO + 2H_2$ (which is actually mildly exothermic, but is usually carried out in the presence of some steam).
The endothermic steam reforming reaction would need to be run at high temperature. The partial oxidation reaction, if carried out alone could be run at low temperature, but in combination with steam reforming would also need high temperature.
Both reactions lead to an increase in the total number of moles in the gas phase and so would be favored by low pressure.
The temperature and pressure used in practice are determined by some of the constraints:

- Materials constraint: If very high temperatures are used, the materials of construction become too expensive (or simply are not available). This limits the process temperature to less than about 850ºC. As temperature is reduced there is less conversion of methane and product yields decrease. The optimum temperature is usually between 800 and 850 ºC.
- Downstream processing constraint: The gas product must be treated to separate hydrogen from carbon oxides. This separation is usually carried out by either pressure-swing adsorption or amine scrubbing. Both of these separation processes require high pressure to operate. The minimum pressure at which these processes are effective is about 14 bar, which sets a lower bound on the pressure. The optimum pressure is usually in the range 30 to 50 bar, as it is cheaper to compress the feed (i.e., pump water to raise steam and compress one mole of methane) than the gaseous product (4 moles of product gas per mole methane).
- Corrosion constraint: Methane can undergo thermal decomposition if heated in the absence of steam or oxygen, leading to coking and metal dusting corrosion. This constraint limits the use of preheat in partial oxidation unless the methane is mixed with steam.
- Catalyst constraint: The catalysts for methane reforming are not particularly active below 450ºC, and even the partial oxidation catalysts are not active below 100ºC. These constraints do not limit the temperature as the process is usually operated at much higher temperatures.

Problem 1.8

Objective function:

Minimize total cost of production per lb of ethylene

= {(annual cost of feed compression) + (annual cost of refrigeration) + (annual cost of reboiler heat) + (annualized capital cost of column, reboiler, condenser, feed compressor, refrigeration plant and associated equipment) + (fixed costs)}/(annual production of ethylene)

Key constraints:

- Column must meet product ethylene purity specifications
- (possibly) column height less than 180 ft (to avoid needing an expensive crane)
- (possibly) column diameter less than 13.5 ft (to avoid site fabrication)

- (possibly) try to keep to a single column shell

These last three "constraints" are often violated by C2 splitter columns in world-scale ethylene plants, which are among the largest distillation columns ever designed.

The main trade-offs are between feed compression vs. refrigeration compression and between ethylene recovery and total cost of production.

Problem 1.9

Constraints on a milk-pasteurizing plant:

- Metal surface temperature must not exceed temperature known to cause severe fouling by milk (about 100 ºC? – milk fouls a saucepan before it boils).
- Residence time at temperature must be greater than minimum required for pasteurization
- Liquid velocity must be greater than value determined to be necessary to prevent fouling.
- Equipment must be designed for cleaning-in-place.
- Storage must be designed to allow sterile filling and emptying so that reinfection does not occur.
- Plant must meet FDA/USDA guidelines for food handling, cleaning, etc.

Problem 1.10

There is an error in the typesetting of the question. The last term in the formula for WHSV should read exp ($-8.0 \times 10^{-5} \times t \times T$).

The goal of this problem is to find the optimum temperature profile, i.e. $T(t)$ subject to a set of constraints.

The design case produces 150 te/y when the reactor is operated at 500ºF, so the design WHSV is:

$$\text{WHSV} = 4.0 \times 10^6 \exp(-8000/500) \exp(0) = 0.45 \text{ lb/hr.lb catalyst}$$

(note use of temperature in ºF, as the equation is empirical)

150 te/y = 150 × 2200 /12 = 27500 lb/month = 38.2 lb/hr
So one catalyst load = 38.2/0.45 = 84.89 lb of catalyst
Cost of reloading catalyst = $849

The maximum production rate is constrained by the downstream equipment to 120% of the design case = 1.2 × 38.2 = 45.8 lb/hr
The maximum temperature is constrained by the safety limit to 620ºF.

The maximum revenue when the plant is running corresponds to maximum production. When the plant operates at maximum capacity, WHSV = 1.2 × 0.45 = 0.54, so

$$0.54 = 4 \times 10^6 \exp\{(-8000/T) - 8 \times 10^{-5}\, t\, T\}$$

Hence:

$$15.818 = (8000/T) + 8 \times 10^{-5}\, t\, T$$

$$8 \times 10^{-5}\, t\, T^2 - 15.818\, T + 8000 = 0$$

So when $t = 0$, $T = 8000/15.818 = 505.7$ºF
And when $T = 620$ (upper constraint), $8 \times 10^{-5}\, t\, (620)^2 - 15.818\,(620) + 8000 = 0$

Which solves to $t = 58.8$ months.

The general solution for temperature as a function of time is:

$$T = \frac{988864}{t} - \sqrt{\left(\frac{98864}{t}\right)^2 - \frac{10^8}{t}}$$

So the maximum production schedule would be to start at 505.7ºF and increase the temperature in accordance with the above equation for 58 months, then change out the catalyst for two months and start again. This gives a total 60 months (5 years) operational cycle. The average annual profit produced by the plant is

Profit = 27500 × 1.2 × 12 × 0.25 ×(58/60) – 849/5

(since the catalyst is replaced every five years)

= $95,530

It could be argued that it might be better to operate the catalyst at a lower temperature for longer. This is easily evaluated. If the plant ran at 110% of capacity, the equation between t and T would be:

$$8 \times 10^{-5}\, t\, T^2 - 15.905\, T + 8000 = 0$$

In which case, the time to reach 620ºF becomes 60.5 months. The annual profit is then:

Profit = 27500 × 1.1 × 12 × 0.25 ×(60.5/62.5) – 849/5.21

= $87,683

So clearly the temperature profile that maximizes production is optimal.

(Note also, the problem would be more realistic if the production rate was 150 thousand metric tons per year, but this would not change the optimum temperature profile).

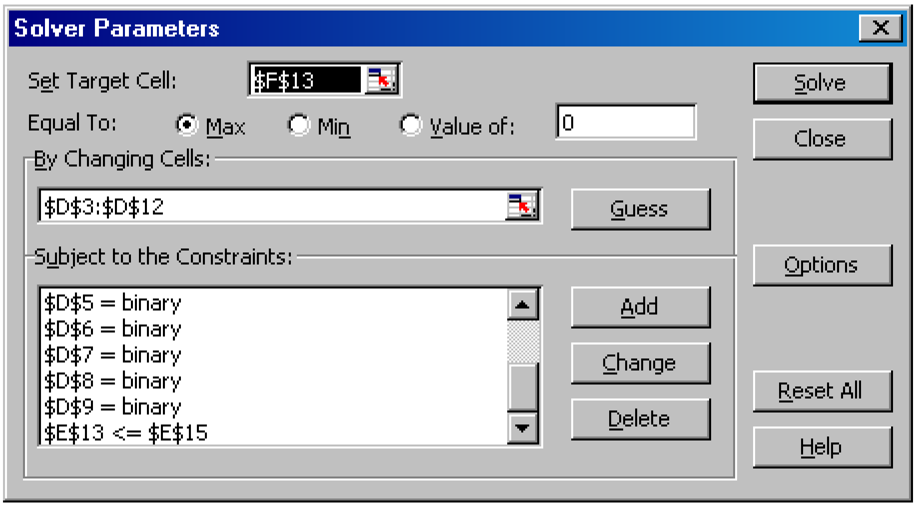
Problem 1.11

Set up as a spreadsheet then solve the MILP using solver to maximize sum of NPV subject to sum of cost ≤ constraint and selection parameter (Project Present) constrained to be binary:

Project	NPV (MM$)	Cost (MM$)	Project Present	Cost*	NPV*
A	100	61	0	0	0
B	60	28	0	0	0
C	70	33	0	0	0
D	65	30	0	0	0
E	50	25	1	25	50
F	50	17	1	17	50
G	45	25	0	0	0
H	40	12	1	12	40
I	40	16	1	16	40
J	30	10	1	10	30
			sum	80	210
			constraint	80	

Use solver to maximize sum of NPV s.t. sum of cost ≤ constraint, & D3:D12 binary

i)	BCFHJ	NPV = 250
ii)	DEFHIJ	NPV = 275
iii)	EFHIJ	NPV = 210
iv)	FHJ	
v)	Always tends to pick small projects, because they help match the constraint Could use an alternative measure such as NPV/cost or IRR and see if maximizing that gave the same set	



Set Target Cell: $F$13

Equal To: ● Max ○ Min ○ Value of: 0

By Changing Cells: $D$3:$D$12

Subject to the Constraints:

$D$5 = binary
$D$6 = binary
$D$7 = binary
$D$8 = binary
$D$9 = binary
$E$13 <= $E$15