Lecture 4: Mass & Energy Balance

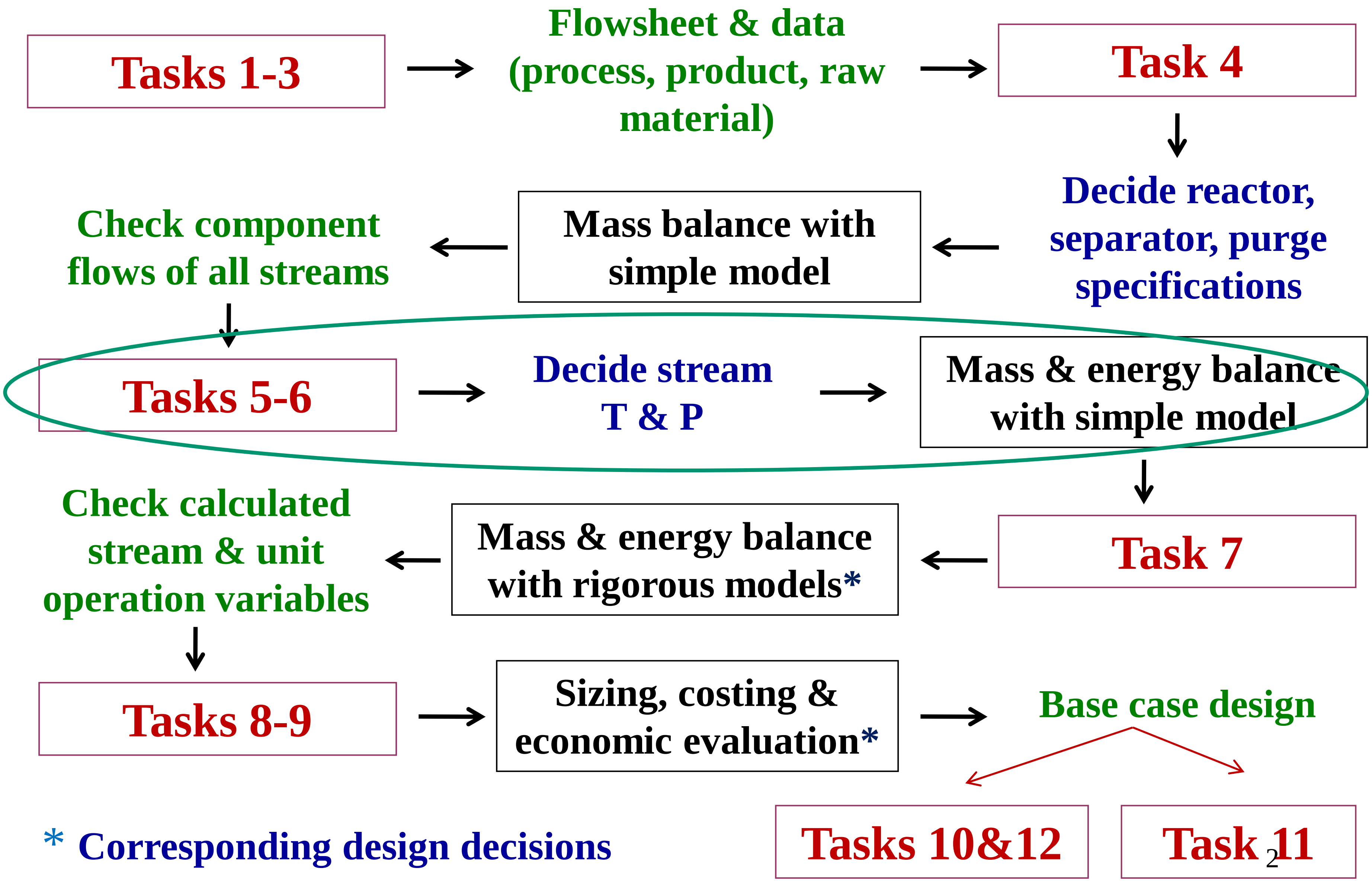
Chapters 3-4, 7-8 (Textbook) plus additional material

Part-1: Extension of the mass balance model

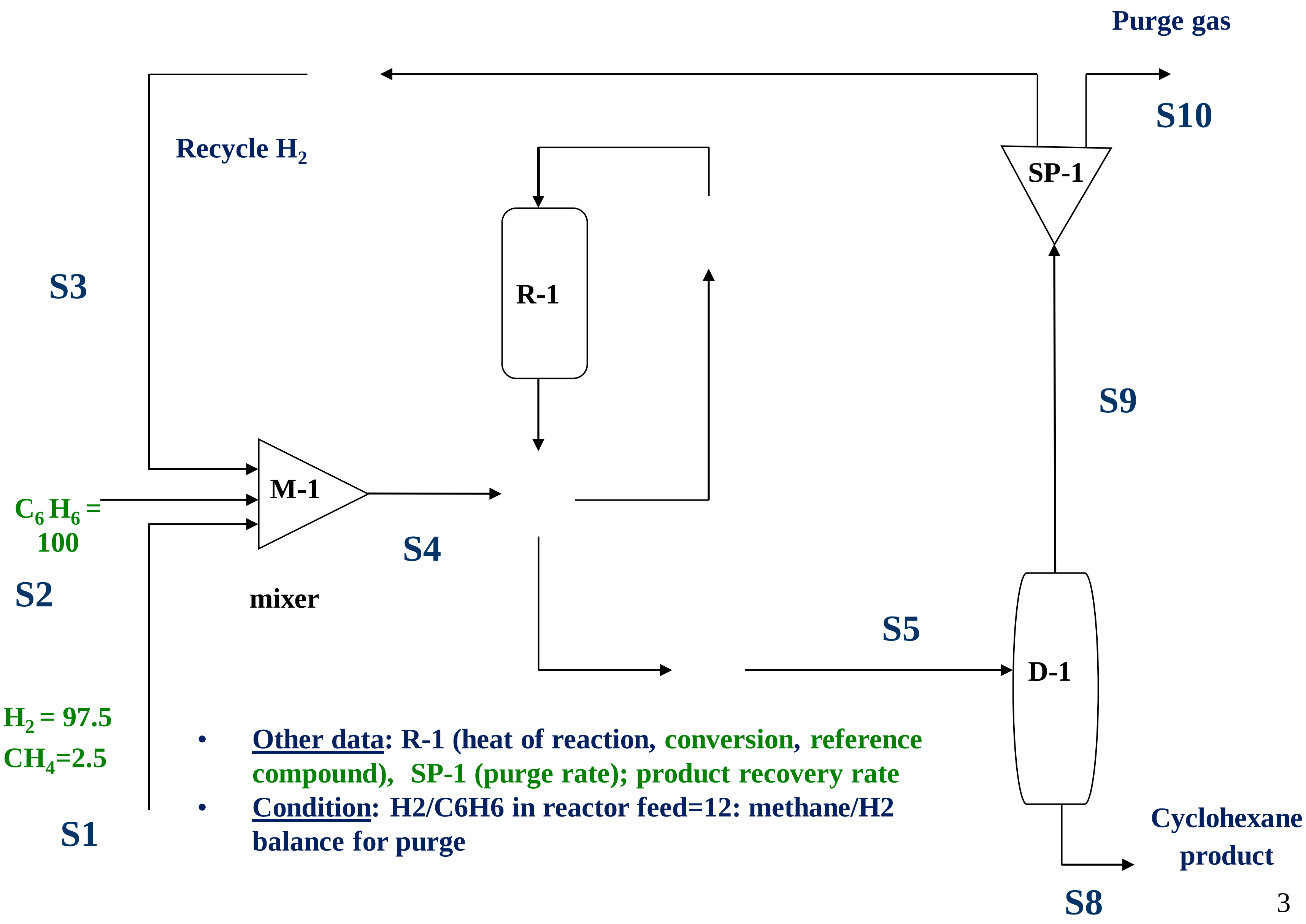
Part-II: Different types-levels of decision

Part-III: Case-study (methods for design decision making plus application of simulator for mass & energy balance with simple model)

Design decisions versus sequence of tasks



Flowsheet for cyclohexane production – Mass Balance



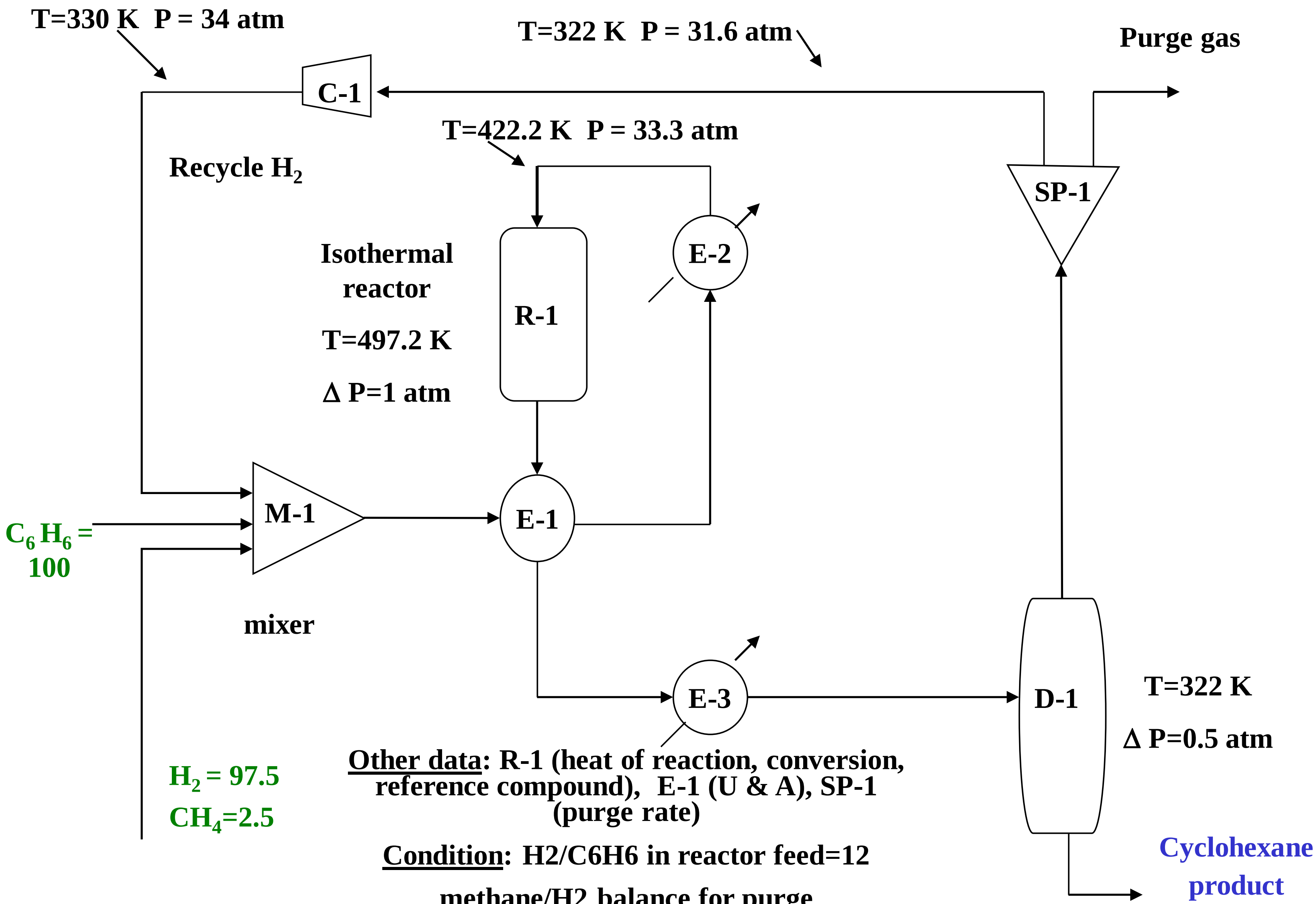
- **Other data**: R-1 (heat of reaction, conversion, reference compound), SP-1 (purge rate); product recovery rate
- **Condition**: H2/C6H6 in reactor feed=12: methane/H2 balance for purge

The objective is to fill-out the stream summary table! Which stream variables are known? x are specified variables; x are calculated mass balance model; x are obtained from x

Variables	Streams								
	S1	S2	S3	S4	S5	S8	S9	S10	
$f_{1,j}$	x	x	x	x	x	x	x	x	
$f_{2,j}$	x	x	x	x	x	x	x	x	
$f_{3,j}$	x	x	x	x	x	x	x	x	
$f_{4,j}$	x	x	x	x	x	x	x	x	
F_j	x	x	x	x	x	x	x	x	

For mass balance: Number of streams (NS) = 8; Number of independent variables = NC*NS; Number of known variables = 2*NC; Number of unknown variables = 6*NC; NC is the number of compounds; subscript j indicates any stream j

Flowsheet for cyclohexane production - What are we solving?



Other data: R-1 (heat of reaction, conversion, reference compound), E-1 (U & A), SP-1 (purge rate)

Condition: H2/C6H6 in reactor feed=12

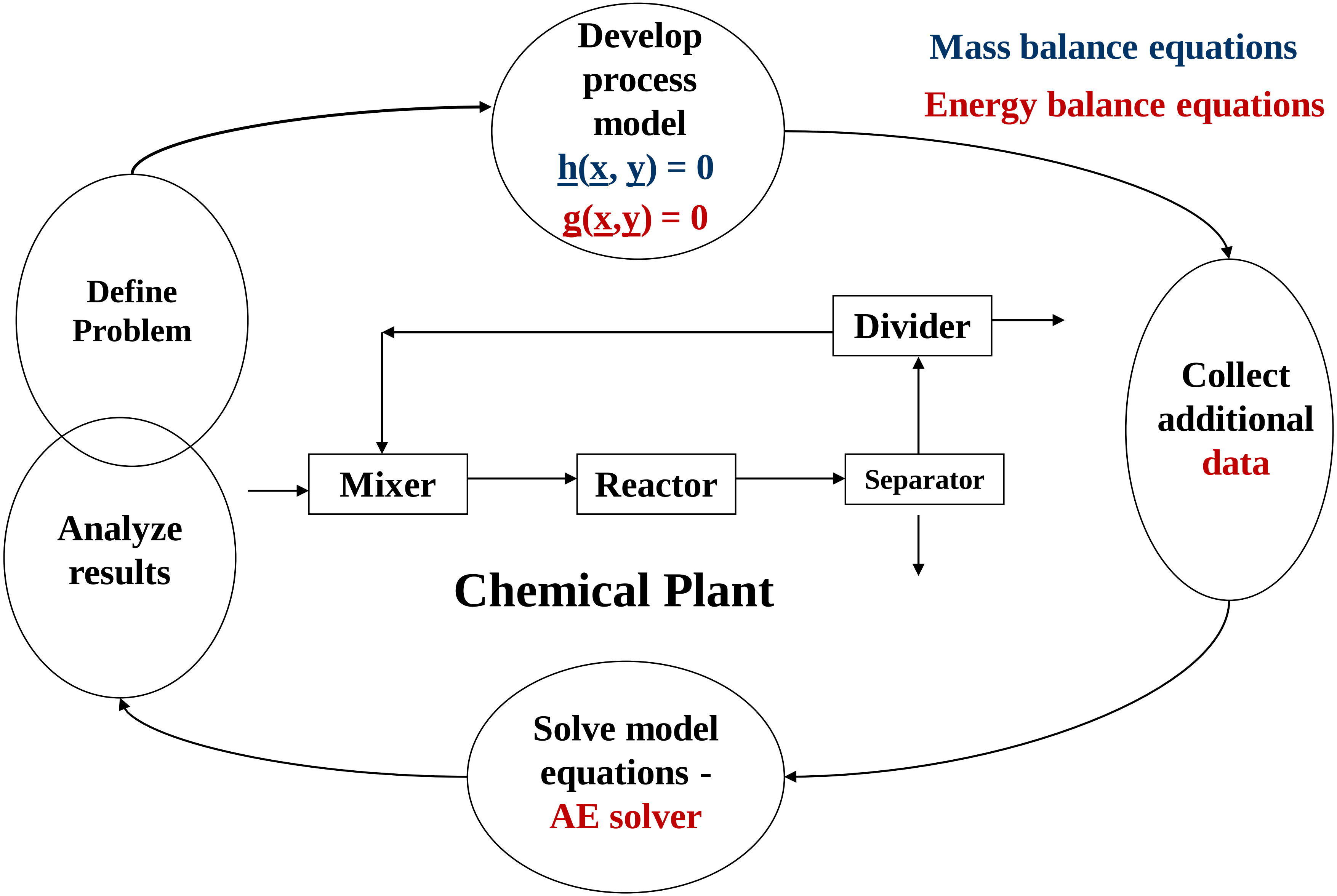
methane/H2 balance for purge

The objective is to fill-out the stream summary table! Which stream variables are known? x indicate a specified variable.

Variables	Streams					
	S1	S2	S3	S4	S5	…….	S13
f1	x	x	x	x	x	…..	x
f2	x	x	x	x	x	…..	x
f3	x	x	x	x	x	…..	x
f4	x	x	x	x	x	…..	x
T	x	x	x	x	x	…..	x
P	x	x	x	x	x	…..	x

Total number of stream variables = 13 (NC+2); Number of known stream variables = 2 (NC+2). Note: for energy balance, there will now be at least 2 more rows for enthalpy, vapor fraction of the stream

Steady state process simulation - solve algebraic equations



Two ways to perform mass & energy balance simulations

- Use a process simulator (see PROII manual)
- Build your own simulator (chapters 3, 7-8)
  - Derive the **model equations**
  - Use a suitable solver to solve the **model equations**

Both alternatives will require you to specify***** –

- The flowsheet
- Variables representing the input streams
- Parameters for all unit modules (reactor, stream calculator, divider)
- **Specify temperatures, pressures and/or phase condition**

*** By making design decisions on variables that need to be specified**

Mass & Energy Balance: Modelling Issues

Add the energy balance equations (model) to the simple mass balance model

$\underline{h}(\underline{x}, \underline{y}) = 0$ mass (component) balance; j*NC per unit

$\underline{g}(\underline{x},\underline{y}) = 0$ energy balance; 1 per unit

Mass & Energy Balance

Principle of conservation (mass)

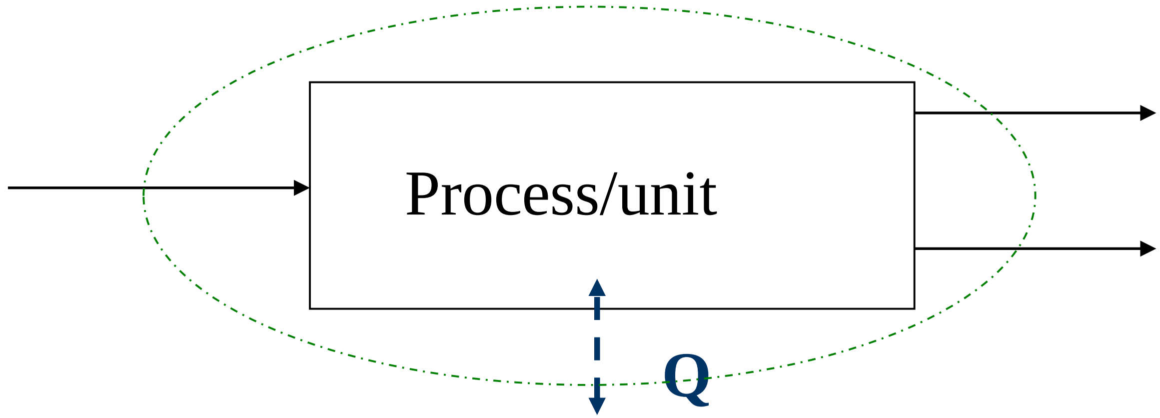
Rate of accumulation = dM/dt

$$dM/dt = Mass_{in} – Mass_{out} + Mass_{gen} = 0 \text{ (for steady state)}$$

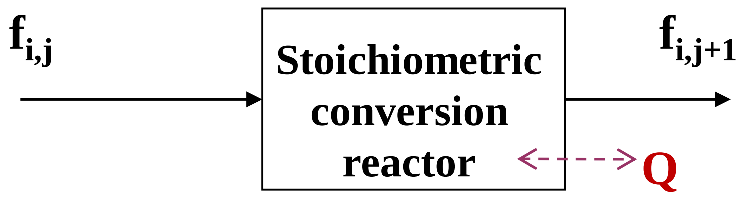
Principle of conservation (energy)

Rate of accumulation = dE/dt

$$dE/dt = Energy_{in} – Energy_{out} + \Delta H_R + Q = 0 \text{ (for steady state)}$$



Simple mass and energy balance model



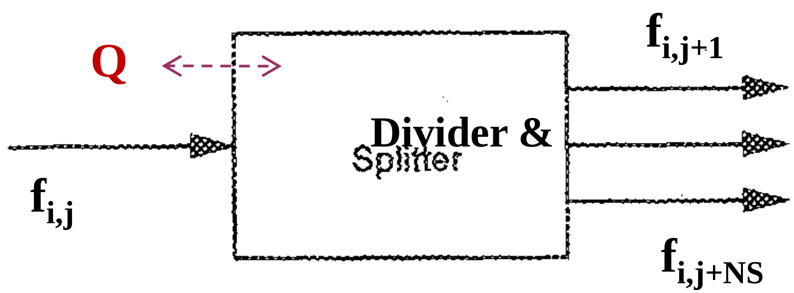
$$f_{i,j+1} = f_{i,j} + \Sigma_r \gamma_{r,i} \eta_{r,k} f_{k,j}$$

$$\gamma_{r,i} = > 0; \text{ or, } < 0; \text{ or, } = 0$$

$$F_{j+1} \Delta h_{j+1} + Q_r + F_j \Delta H_r = F_j \Delta h_j$$

$$f_{i,NM+1} = \Sigma_j f_{i,j} \qquad j=1,NM$$

$$F_{NM+1} \Delta h_{NM+1} + Q_m = \Sigma_j F_j \Delta h_j$$



$$f_{ij+1} = \xi_{i,U} f_{i,j} \qquad j=1,NS-1$$

$$f_{i,NS} = (1 - \Sigma_j \xi_{i,U}) f_{i,j}$$

$$F_{j+1} \Delta h_{j+1} + Q_s + F_{j+2} \Delta H_{j+2} = F_j \Delta h_j$$

Note: ***A flash or component splitter can use the same model as divider/splitter where ξ_{iU} (recovery of component i) is specified for each compound i***

Note: Splitter in PROII is called stream calculator

Models for Calculation of Enthalpies

Liquid Enthalpy

$$\Delta h(T) = \Delta h^0 + \sum x_i \int (C_{PL}(T))\, dT \quad \text{(from } T_0 \text{ to } T\text{)}$$

$$\Delta h(T) = \Delta H(T) - \sum x_i H_{VAPi}(T)$$

Vapour Enthalpy

$$\Delta H(T) = \Delta H^0 + \sum y_i \int (C_{PV}(T))\, dT \quad \text{(from T0 to T)}$$

$$\Delta H(T) = \Delta h(T) + \sum y_i H_{VAPi}(T)$$

Heat of Reaction

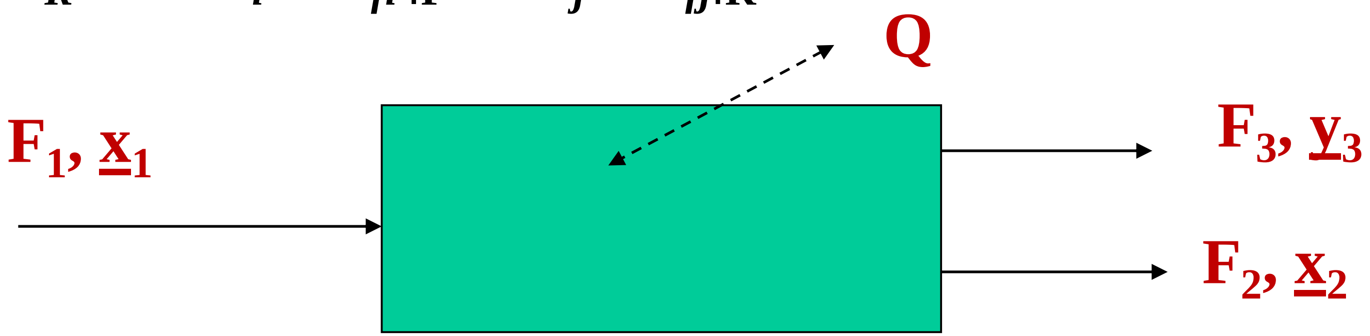
$$\Delta H_R = \sum \nu_i \Delta h_{fi}|_P - \sum \nu_j \Delta h_{fj}|_R$$

Model for Calculation of Enthalpies

$$\Delta h\,(T) = \Delta h^0 + \sum x_i \int (C_{PL}(T))\,dT \quad (\text{from } T_0 \text{ to } T)$$ **liquid**

$$\Delta H\,(T) = \Delta H^0 + \sum y_i \int (C_{PV}(T))\,dT \quad (\text{from } T_0 \text{ to } T)$$ **vapor**

$$\Delta H_R = \sum \nu_i\, \Delta h_{fi}|_P - \sum \nu_j\, \Delta h_{fj}|_R$$ **heat of reaction**



$$F_1\, \Delta h_1(T_1) + Q = F_2\, \Delta h_2(T_2) + F_3\, \Delta H_3(T_3)$$

Calculation options:

***1: Fix $T_2 = T_3$ and then calculate Q ??**

***2: Fix Q and calculate $T_2 = T_3$??**

Design of Refrigeration Cycles (Chapter-4)

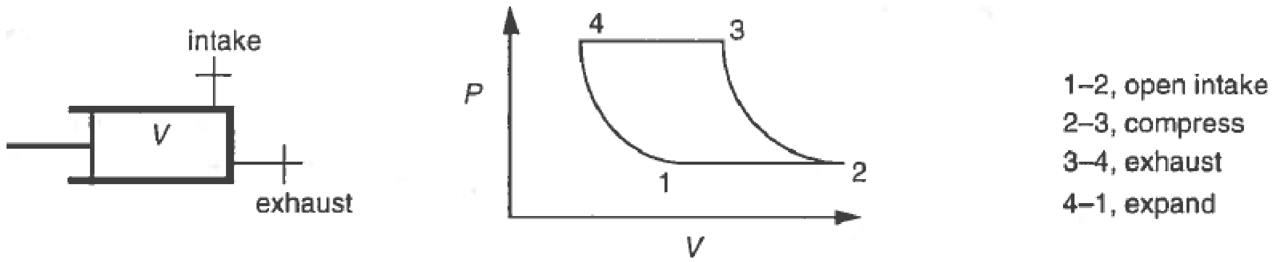


FIGURE 4.9 Compression cycle for reciprocating compressor.

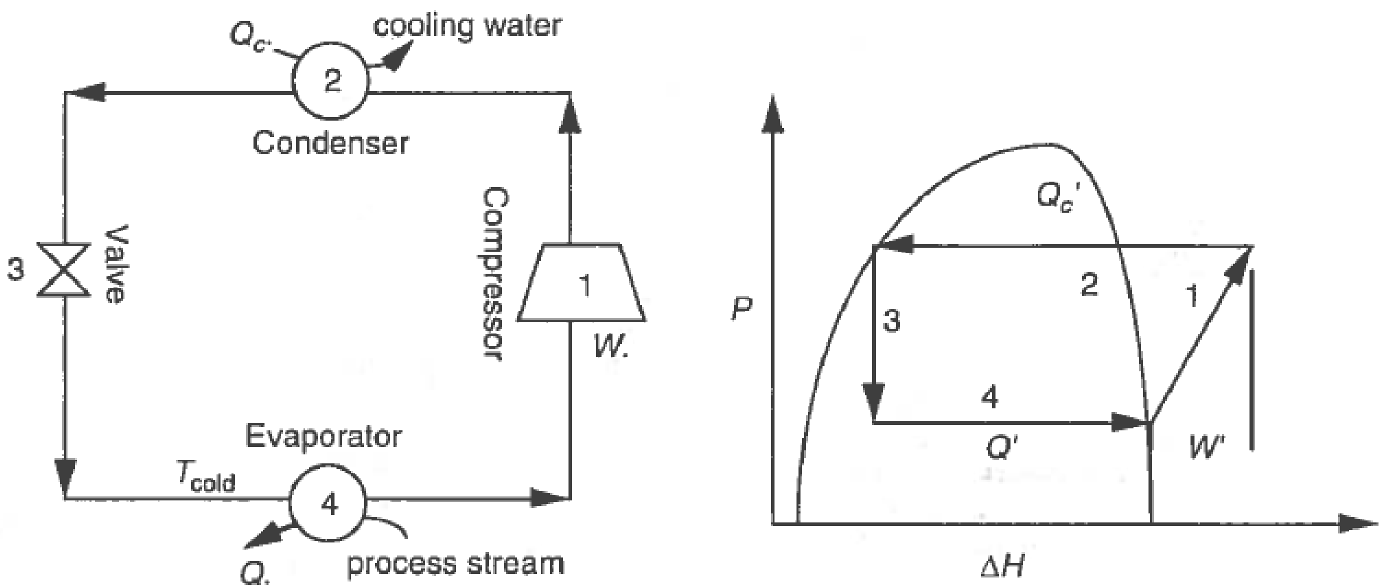


FIGURE 4.10 Refrigeration cycle and phase diagram.

Design of Refrigeration Cycles

EXAMPLE 4.3

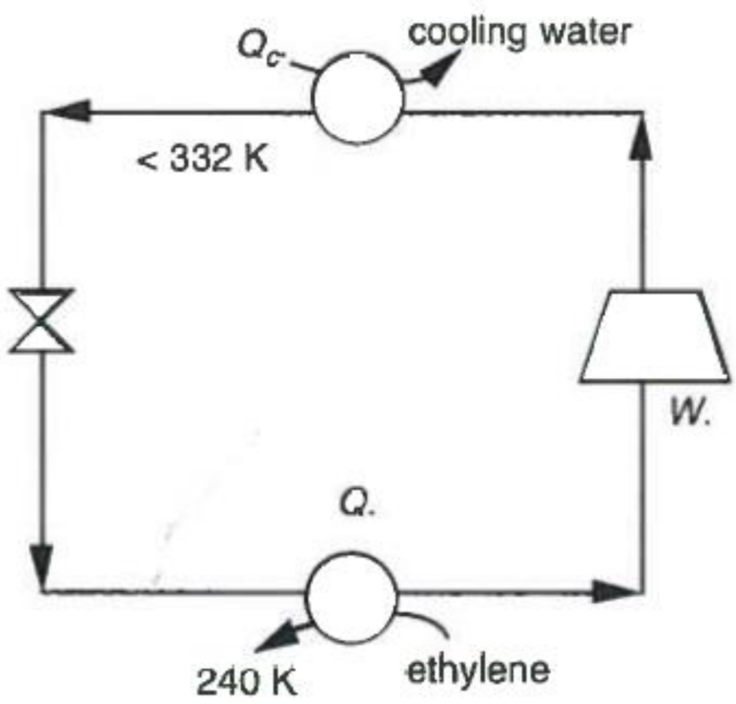
Suppose we want to cool air as a process stream to 180K. Consider the refrigerants:

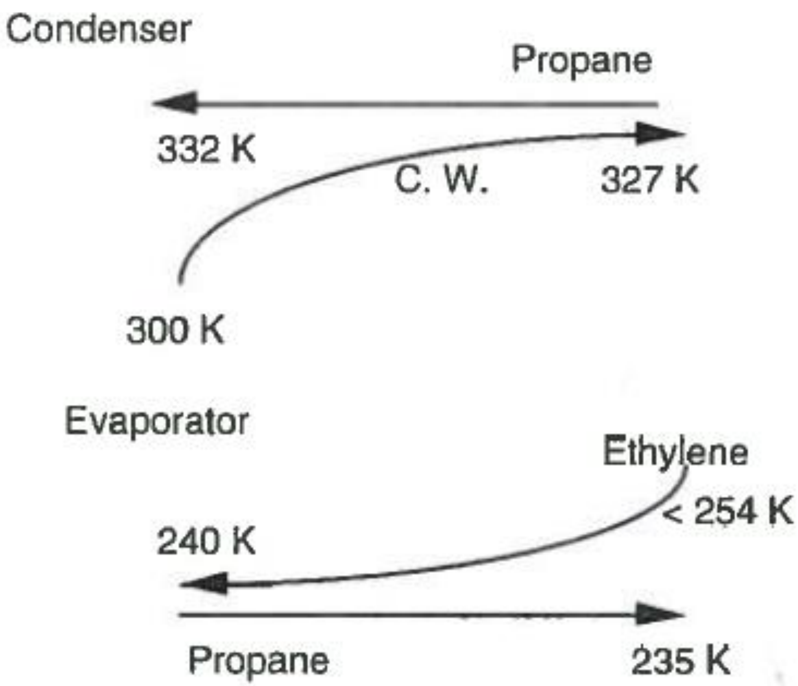
R	T_{boil}(K)	$0.9T_c$(K)
Ethylene	169	254
Propane	231	332

We know that ethylene will go down to 180 K but not up to 300 K. The opposite holds for propane. Therefore, we need at least two stages: one propane, one ethylene.

Design of Refrigeration Cycles

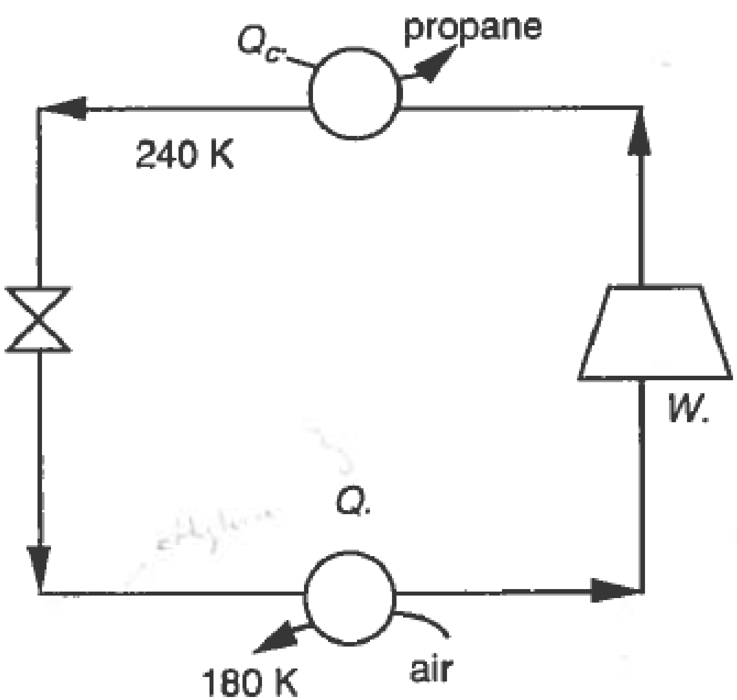
Stage 1: Consider propane as the refrigerant

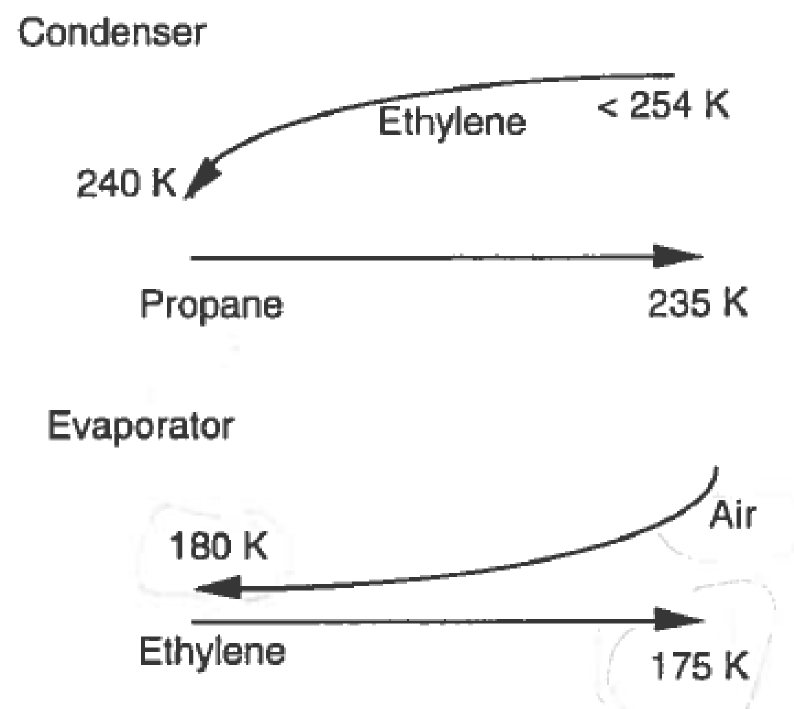




Design of Refrigeration Cycles

Stage 2: Consider ethylene as the refrigerant





Design of Refrigeration Cycles (exercise in class – Exercise 6 from Ch-4 of textbook)

A stream of n-butane needs to be cooled from 300 K to 250 K. The change in heat content for this stream is 300 KW. Possible refrigerants are:

	T_b (K)	T_C (K)
Ethane	184.5	304
Propane	231.1	370
Isobutane	261.3	408

a) How many stages of refrigerants are required? Select the refrigerants for each stage.
b) Decide the operating pressure if $\Delta T_m = 5$ K
c) For coefficient of work = 5, determine the compressor work and the cooling water duty.

Design of Refrigeration Cycles

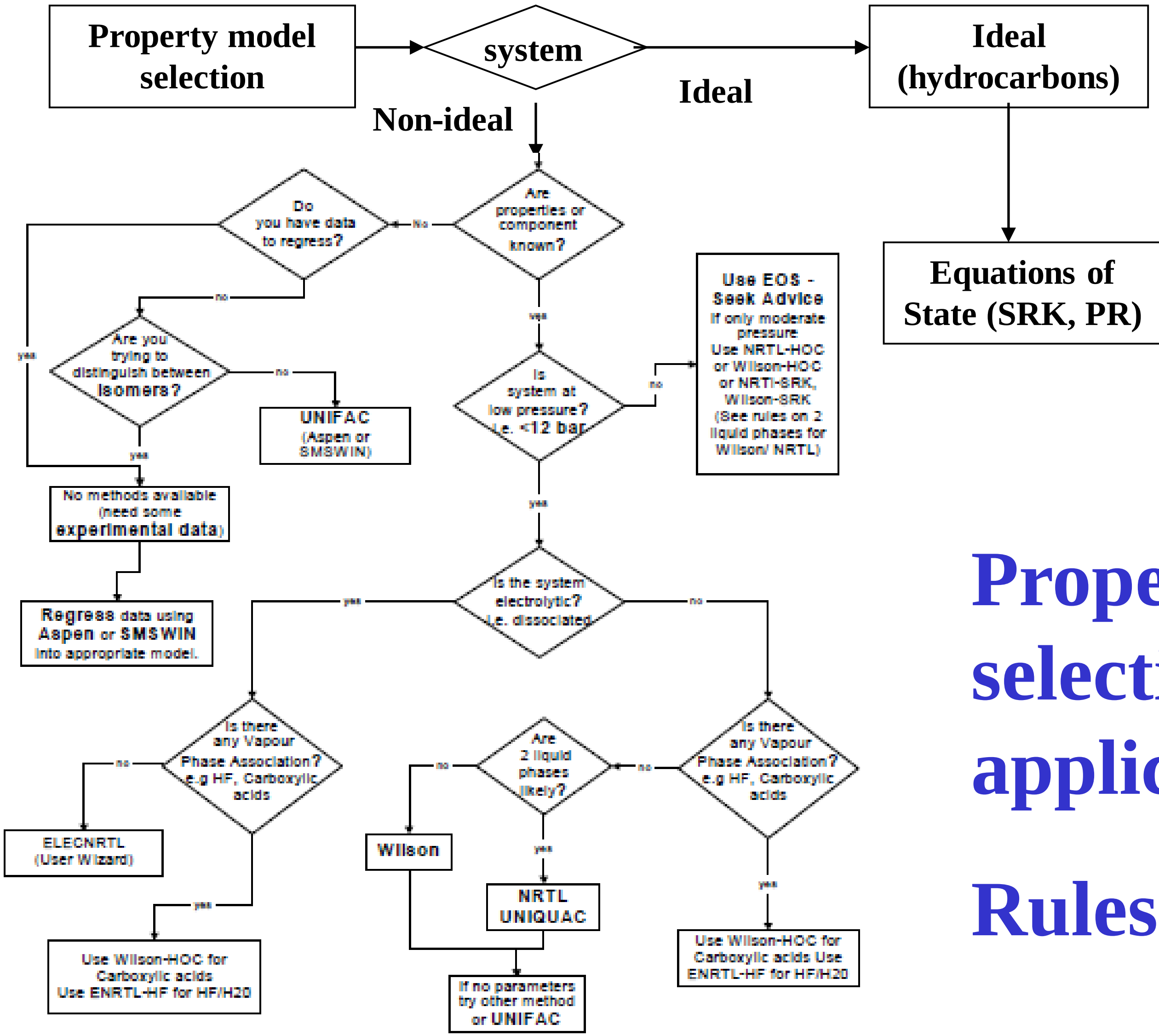
a) - Number of stages = $(T_{in} – T_{out}) /\Delta T_{cycle}$
- Check the Tb, Tc and the following rules:

$T_b \le T_{int} \le T_{cw} \le 0.9T_c$ for stage 1

$T_b \le T_{int} \le T_{cw} \le 0.9T_c$ for stage 2

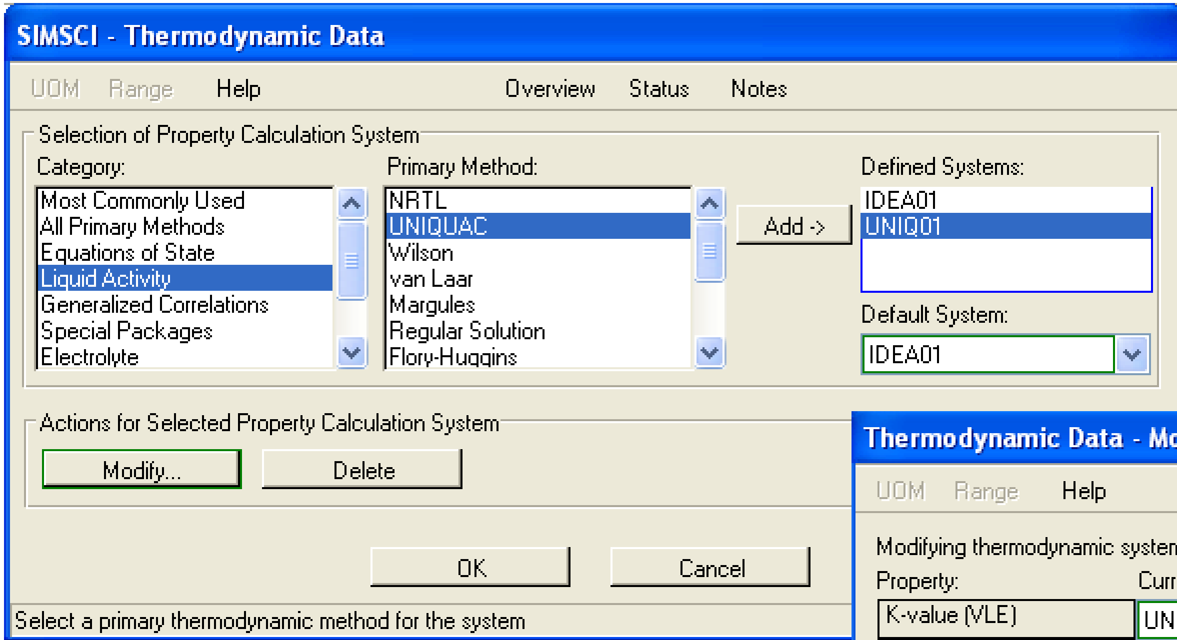
b) Decide the temperatures for the heat exchangers in the two cycles (see the refrigeration cycle diagram); use the vapor pressure model to calculate the pressures at the selected temperatures – find the Antoine constants for each compound

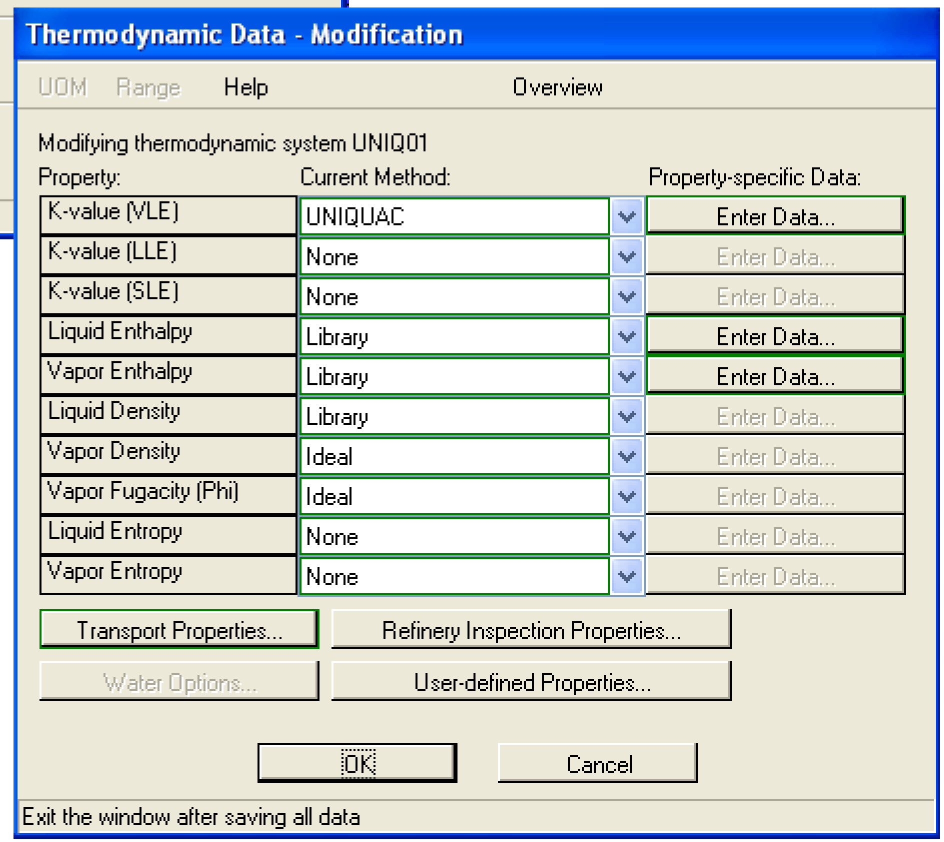
b) Use Eq. 4-40 for work; Eq. 4-41 for Q_c and W_b

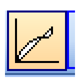


Property model selection and application:

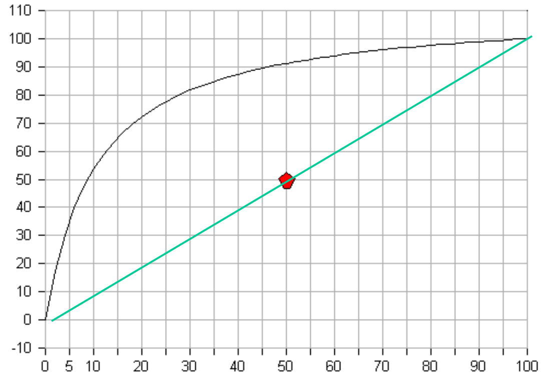
Rules for selection



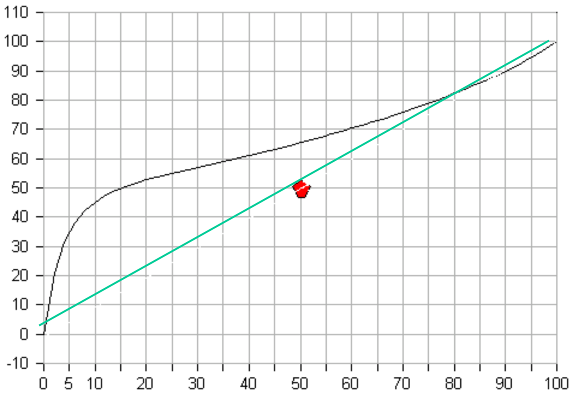


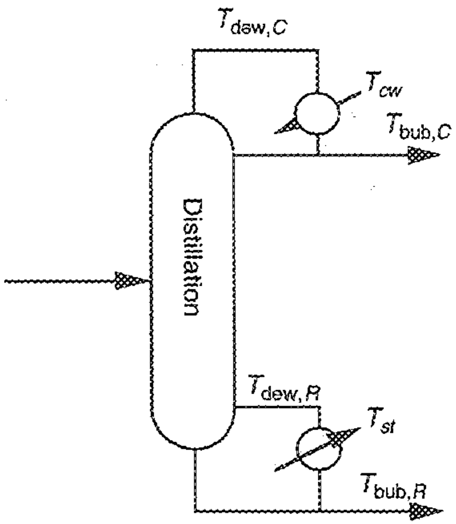
Property model selection options in PROII:  Thermodynamic data

Inconsistent choice of models: Consequences - I

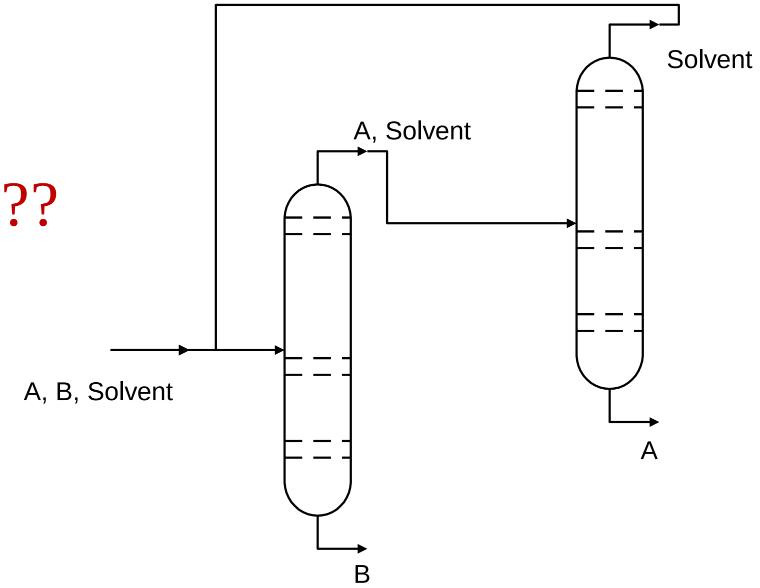


Or ??

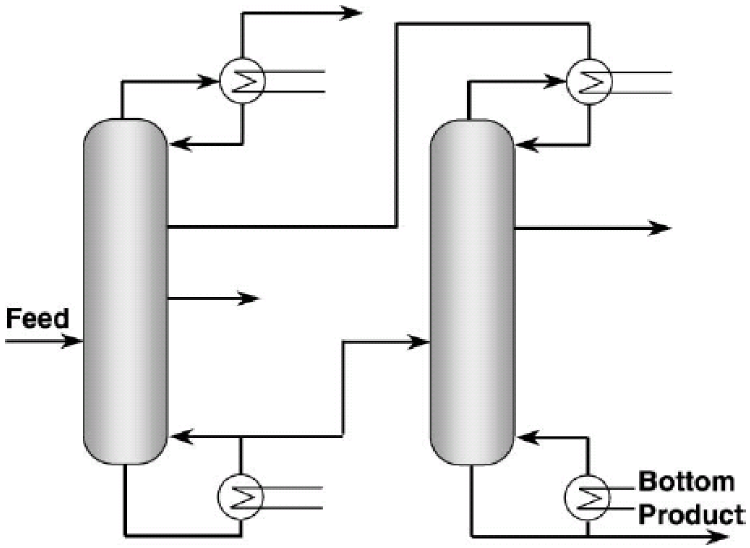




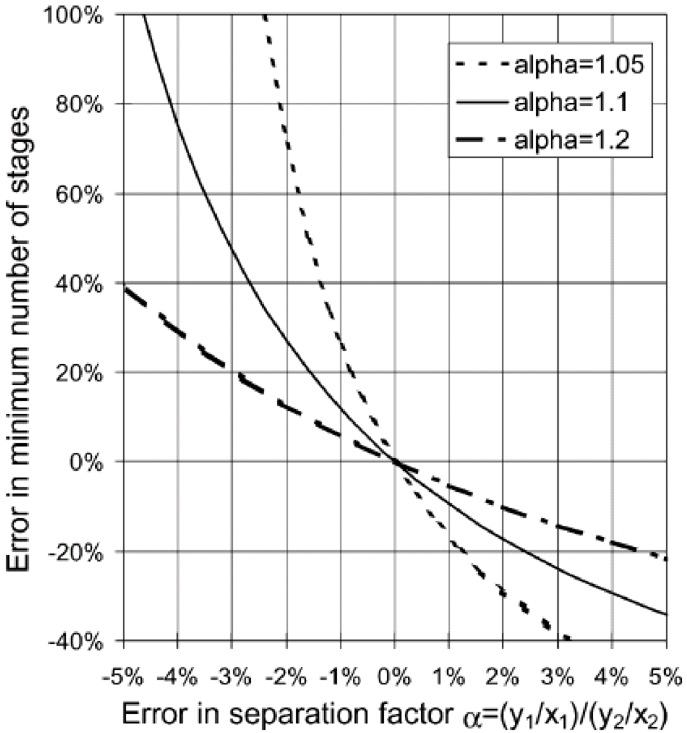
Or ??



Inconsistent choice of models: Consequences - II



Process for separation of styrene from ethylbenzene



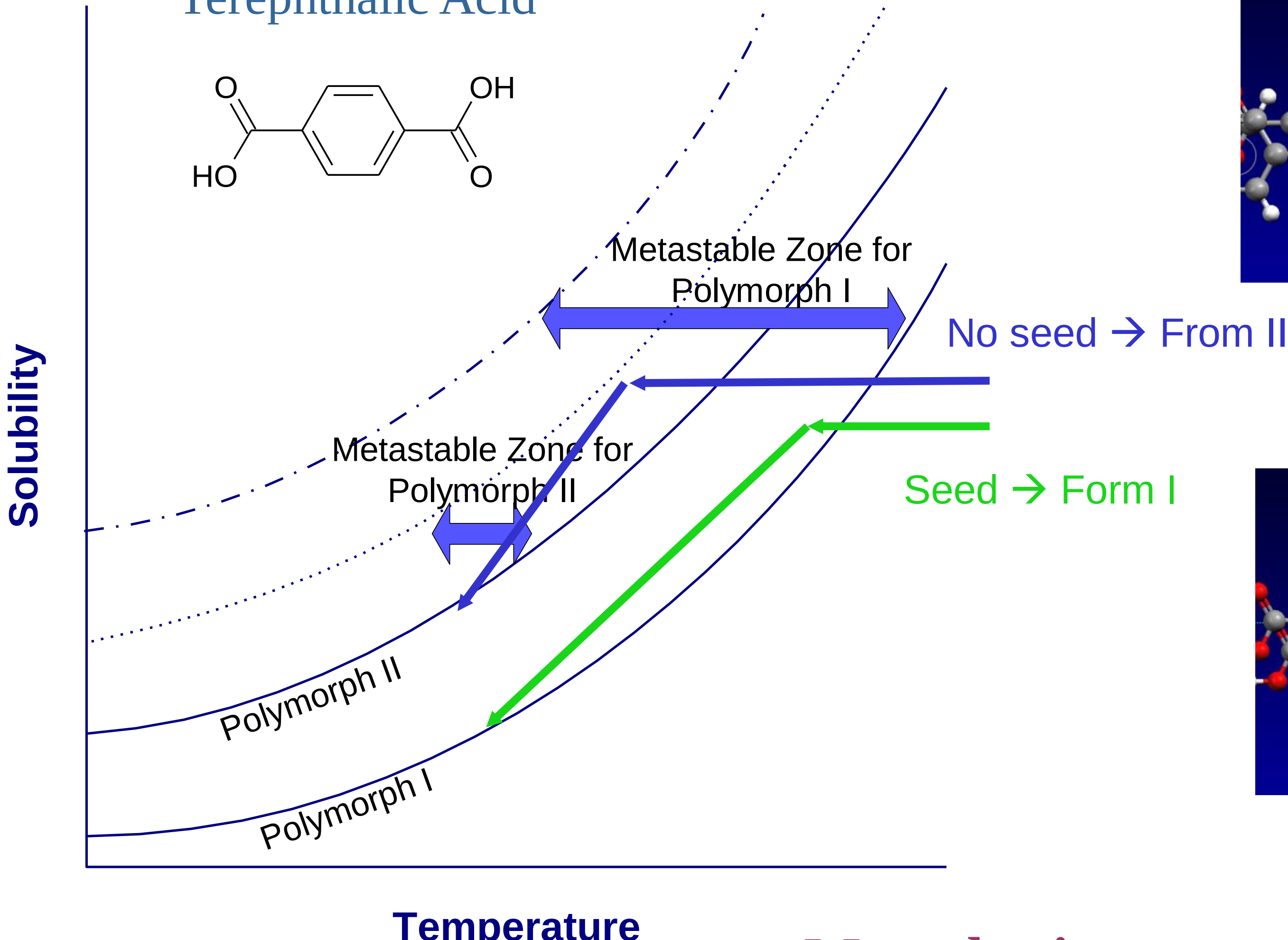
Consequence of error in calculated separation factor on number of stages

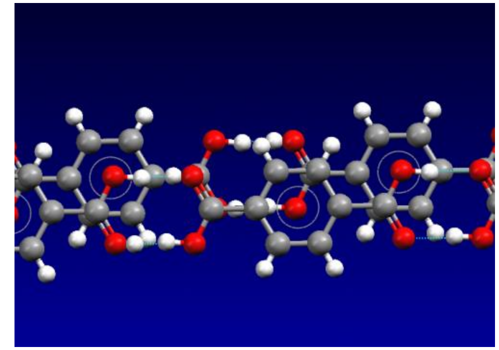
Positive error means lower cost and infeasible separation, while negative error means feasible separation at significantly higher costs

Dohrn & Pfohl, Fluid Phase Equilibira, 194-197 (2002) 15-29

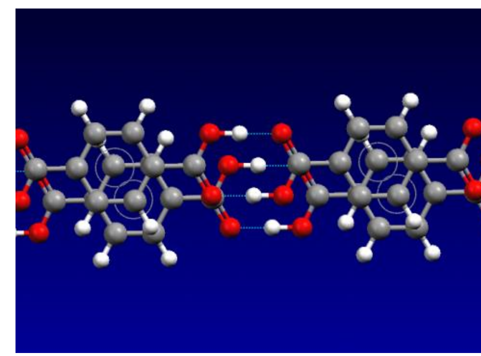
Inconsistent choice of models: Consequences - III

Terephthalic Acid





Form 2



Form 1

May obtain wrong product!

Decisions related to generation of data

Calculation decisions ??

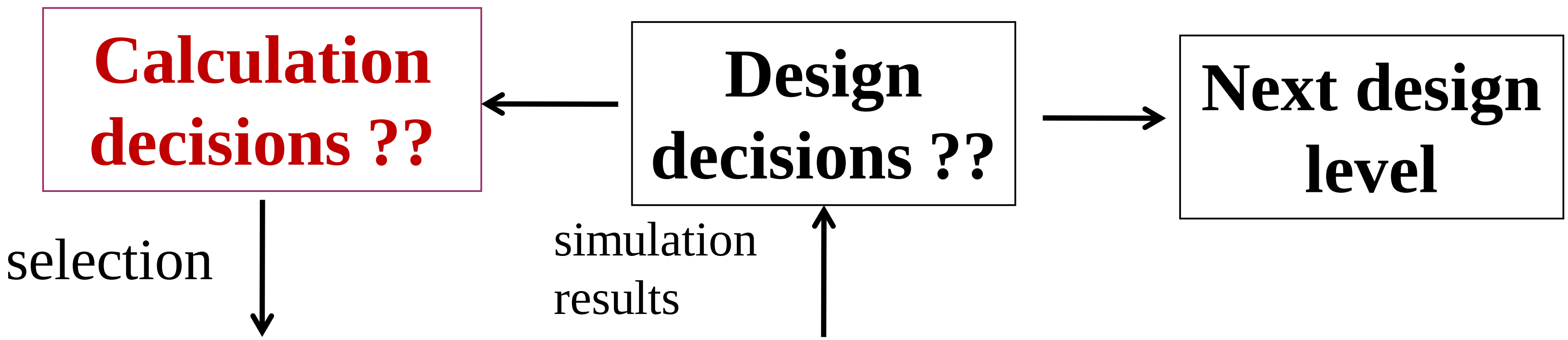
Analyze data → **Make design decisions**

selection ↓

data ↑

- **Modelling: Related to mass balance; mass & energy balance; unit operations; enthalpy; phase behaviour; ....**
  - **Operational phenomena: reaction; mass-heat transfer; phase separation; solubility; ...**
  - **Phenomena:**
  - **Properties: pure component, mixture, phase-states**
- **Calculation options: data generator (phase diagrams, saturation conditons, kinetic data, solvent data, ...)**

Decisions: Verify design



- **Modelling: Related to mass balance; mass & energy balance; unit operations; enthalpy; phase behaviour; ....**
  - **Unit operations: reactors; separators; pumps, ...**
  - **Phase behaviour: fugacity, activity coefficients, vapor pressure, ...**
  - **Energy: enthalpies; heats of reaction, heats of vaporization; ...**
- **Simulator options: models, calculation sequence, specified data, convergence criteria, ...**

Ethanol Process: Case Study (from Textbook)

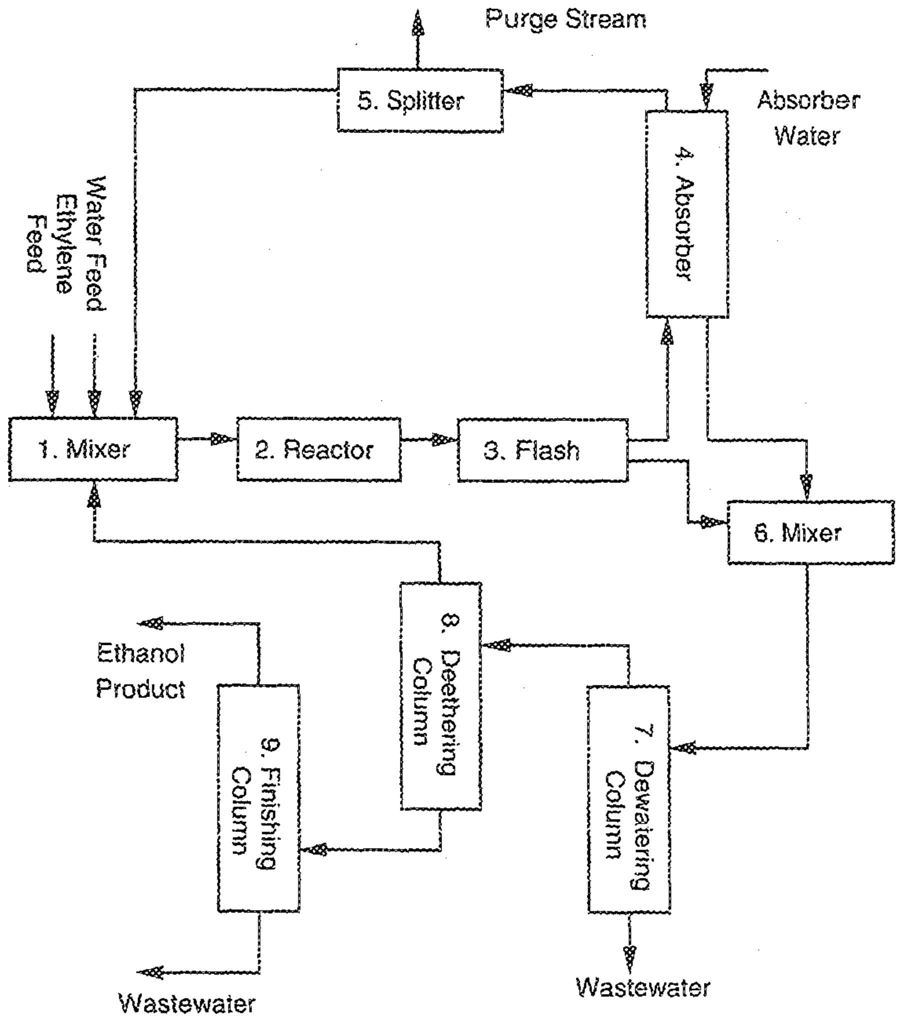


FIGURE 3.1 Ethanol flowsheet.

Mass balance has been performed & the simulation results have been verified (this completes tasks 1-4).

Start tasks 5-6 by defining the temperatures and pressures of all streams still using the simple model

With specified T & P for all streams, perform mass & energy balance and calculate heat addition/removal from each unit operation

Ethanol Process: Case Study (from Textbook)

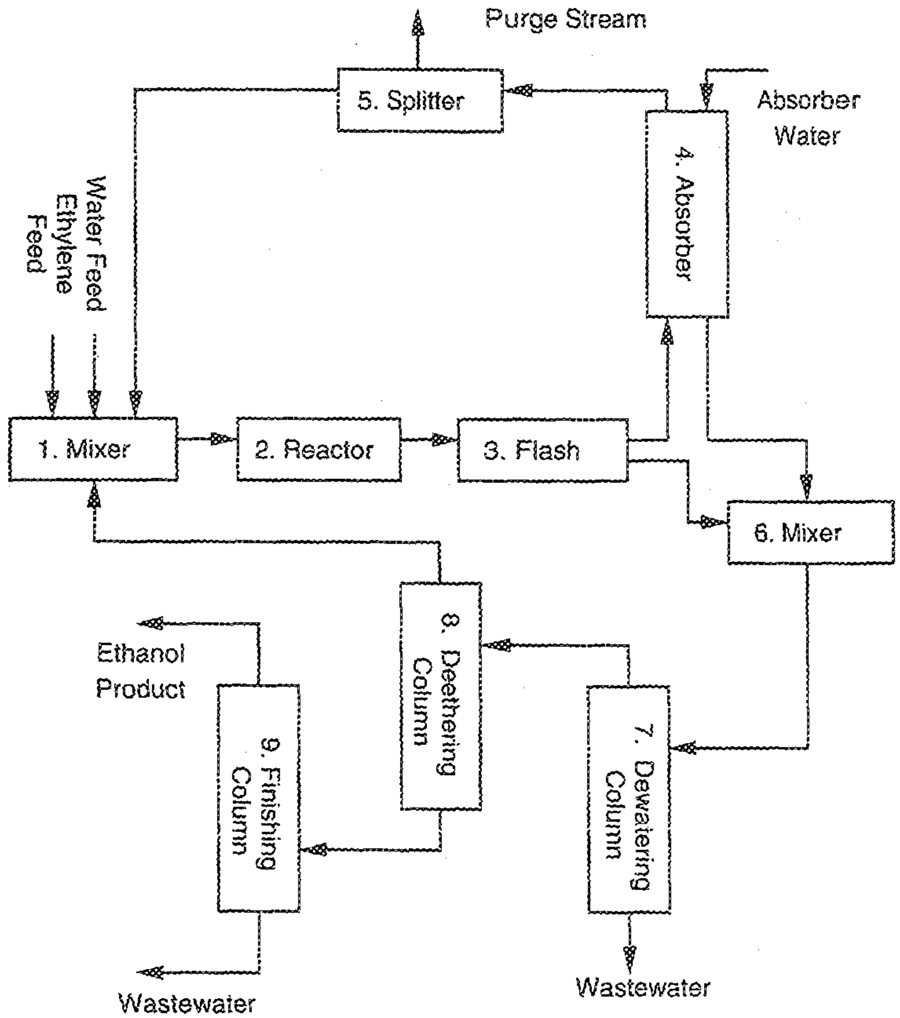
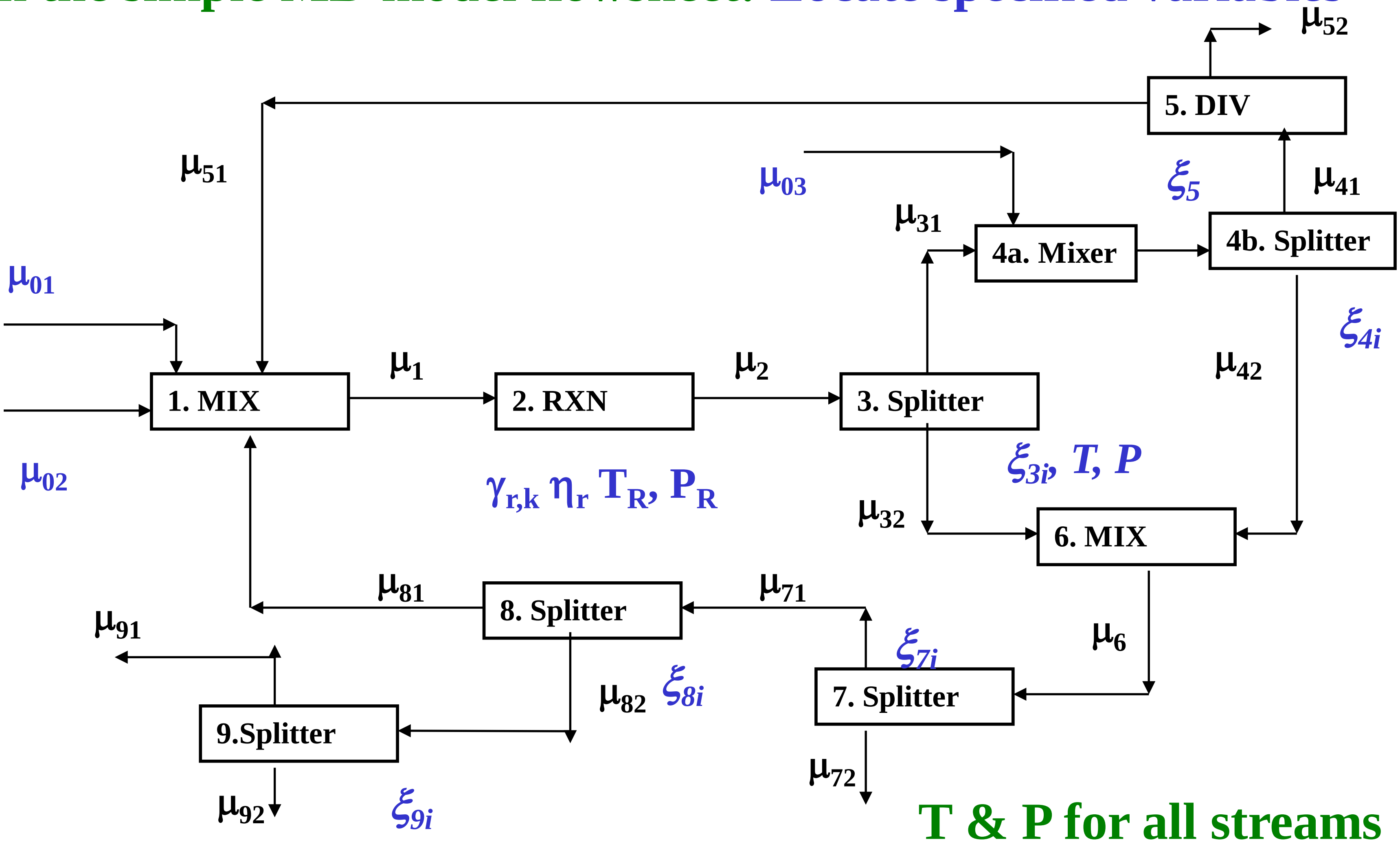


FIGURE 3.1 Ethanol flowsheet.

In order to perform mass & energy balance (simple) what do we need?

1. **Models for each unit operation?**
2. **Identify which variables need to be specified?**
3. **Use the flowsheet for MB-model!**
4. **Decide what values of P & T to specify**
5. **From the energy balance, obtain the heat duties for each unit operation**

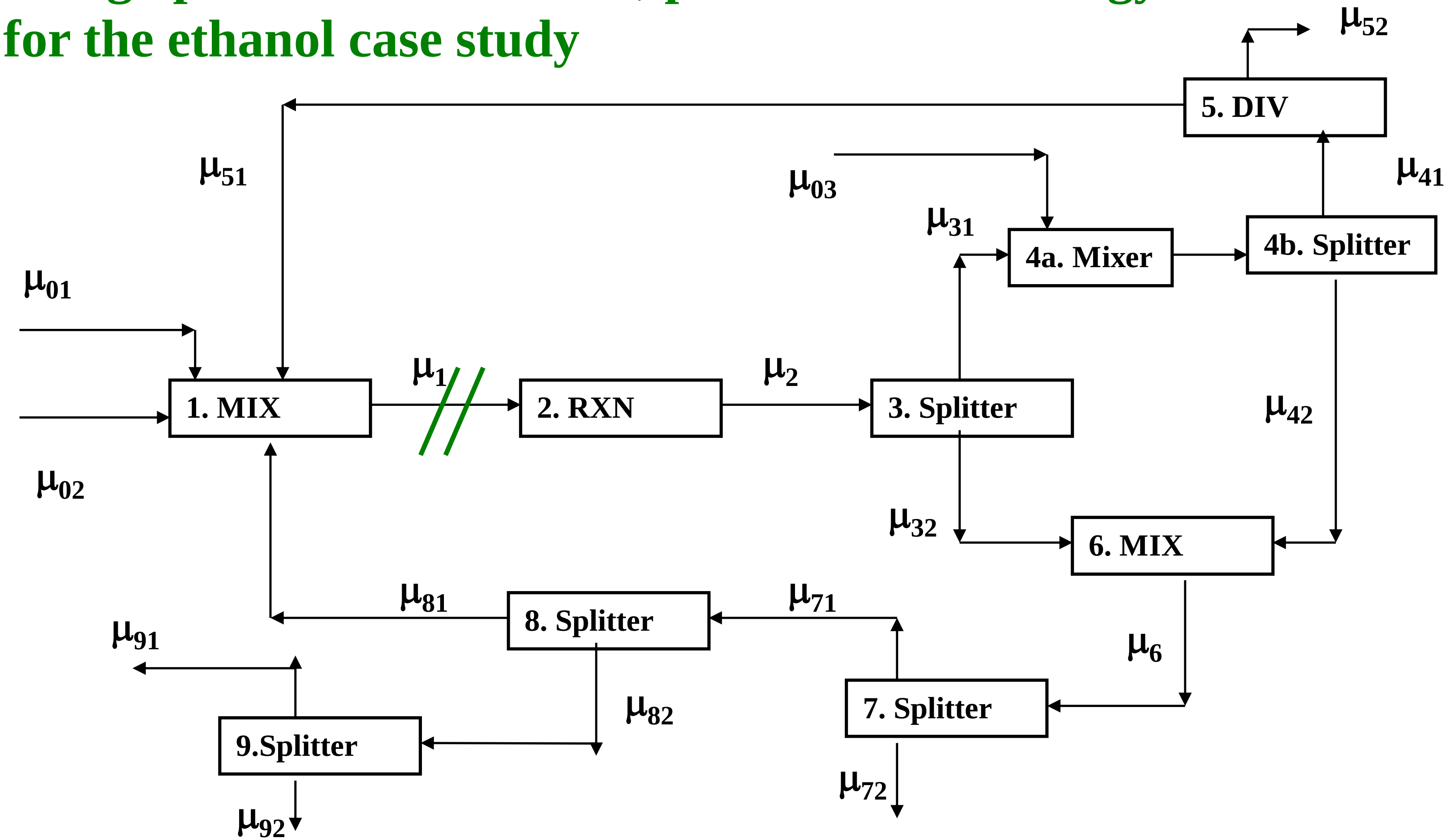
On the simple MB-model flowsheet: Locate specified variables



T & P for all streams

If all the variables marked in blue are known, then all new variables E_j (energy of stream j) & Q_U (heat duty for unit U) in the simple flowhseet can be calculated!

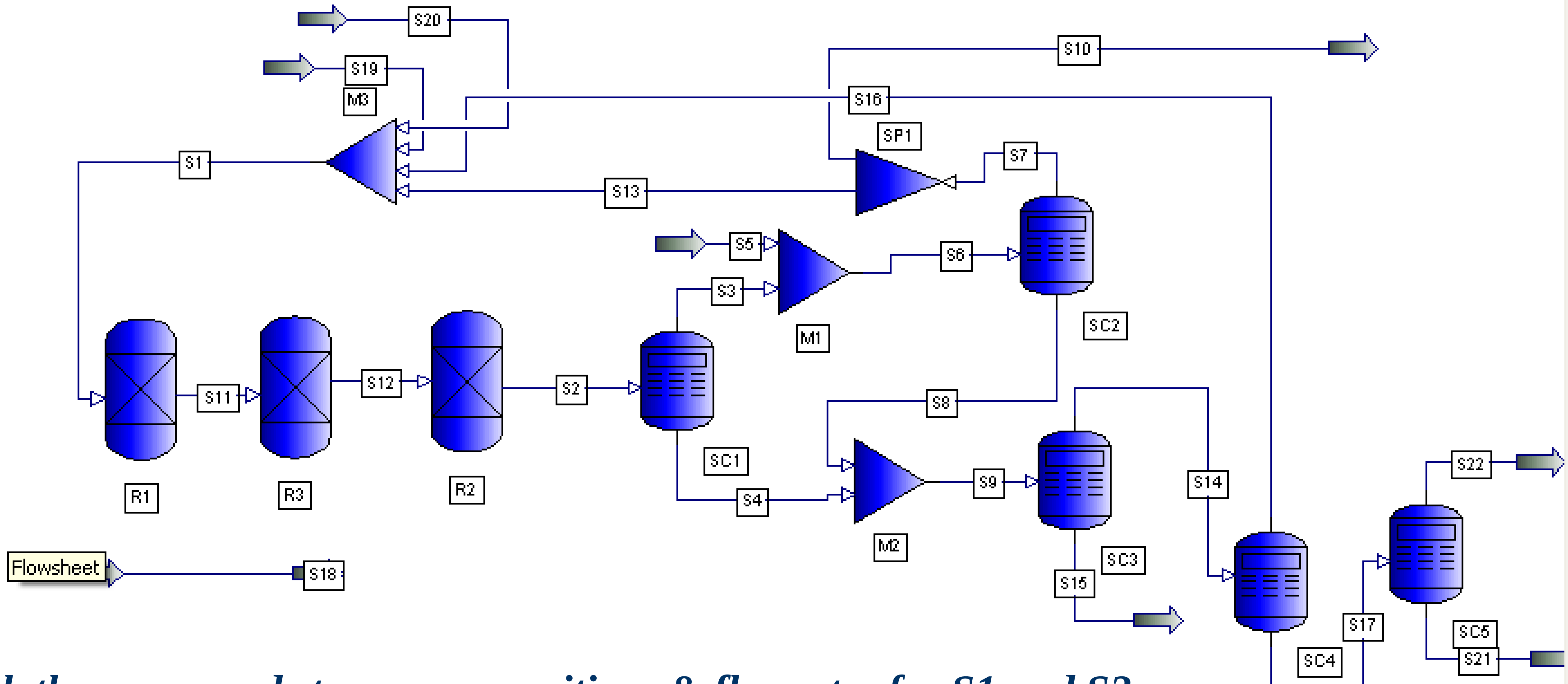
Using option 1 from slide 13, perform mass+energy balance for the ethanol case study



First identify the "tear stream", the calculation sequence & a good estimate for the tear stream; specify calc T_j & selected P_j for all streams for M+E balance

Close the recycle loop and add the last separator (end of task 4)

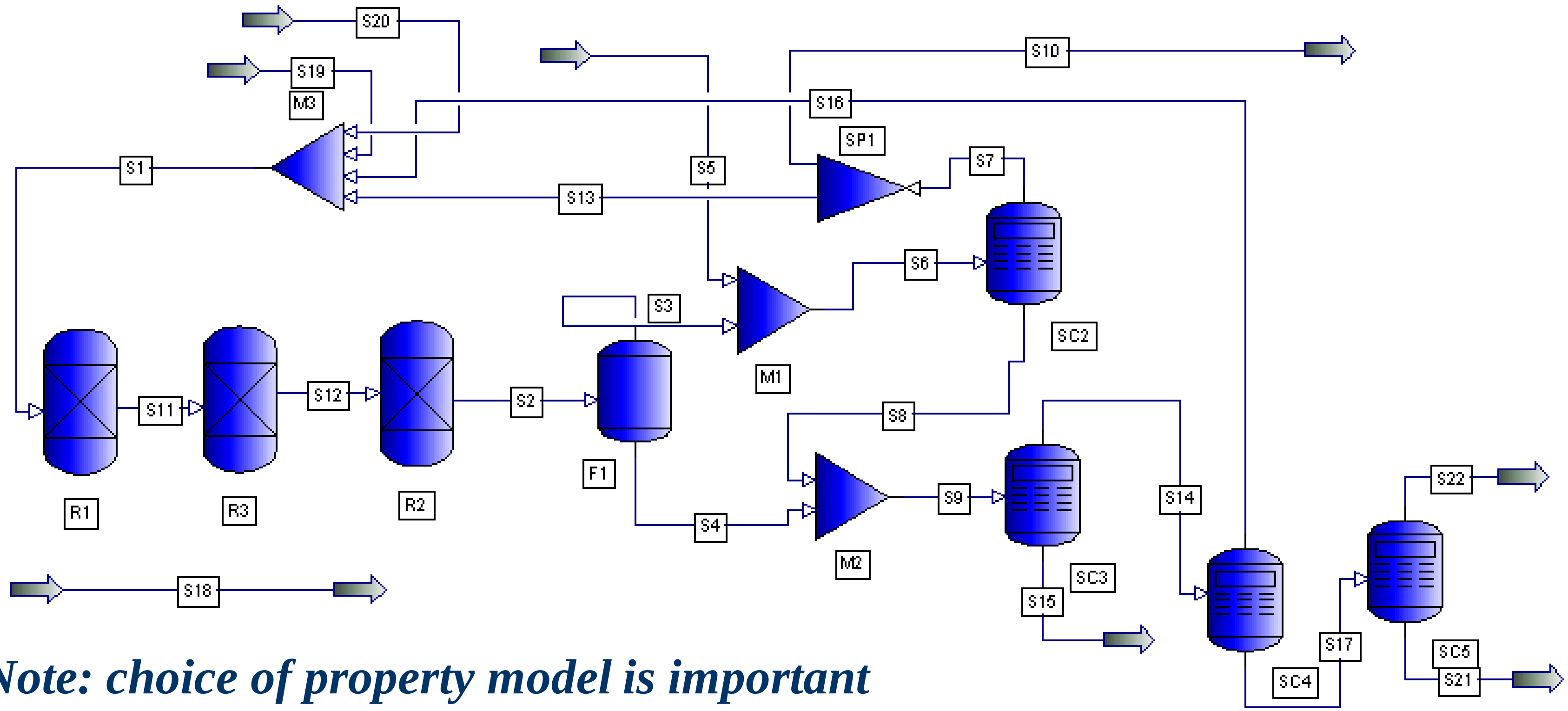
Note: recycle loop is now closed. Check the calculation sequence.



Check the converged stream compositions & flowrates for S1 and S2

S1 Mixed	S11 Vapor	S2 Vapor	S12 Vapor	S3 Vapor	S4 Mixed	S5 Liquid	S6 Mixed	S7 Vapor	S8 Mixed	S9 Mixed	S10 Vapor	S13 Vapor	S14 Mixed	S15 Liquid	S16 Vapor
292,5756	590,0000	590,0000	590,0000	310,0000	310,0000	300,0000	301,1133	300,0000	300,0000	308,9658	300,0000	300,0000	350,0000	370,0000	300,0000
1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000	1,0000
13,3936	82,6858	82,6584	82,6601	13,7204	2,5232	0,0764	13,7968	9,6881	0,8739	3,3971	0,0484	9,6396	9,6450	4,7240	1,6389
25,9916	26,9433	26,9639	26,9639	28,9286	22,6790	18,0150	28,6899	28,6080	29,5908	23,7622	28,6080	28,6080	37,3810	18,0395	42,6100
0,7010	1,0000	1,0000	1,0000	1,0000	0,0269	0,0000	0,9898	1,0000	0,3472	0,0737	1,0000	1,0000	0,9825	0,0000	1,0000

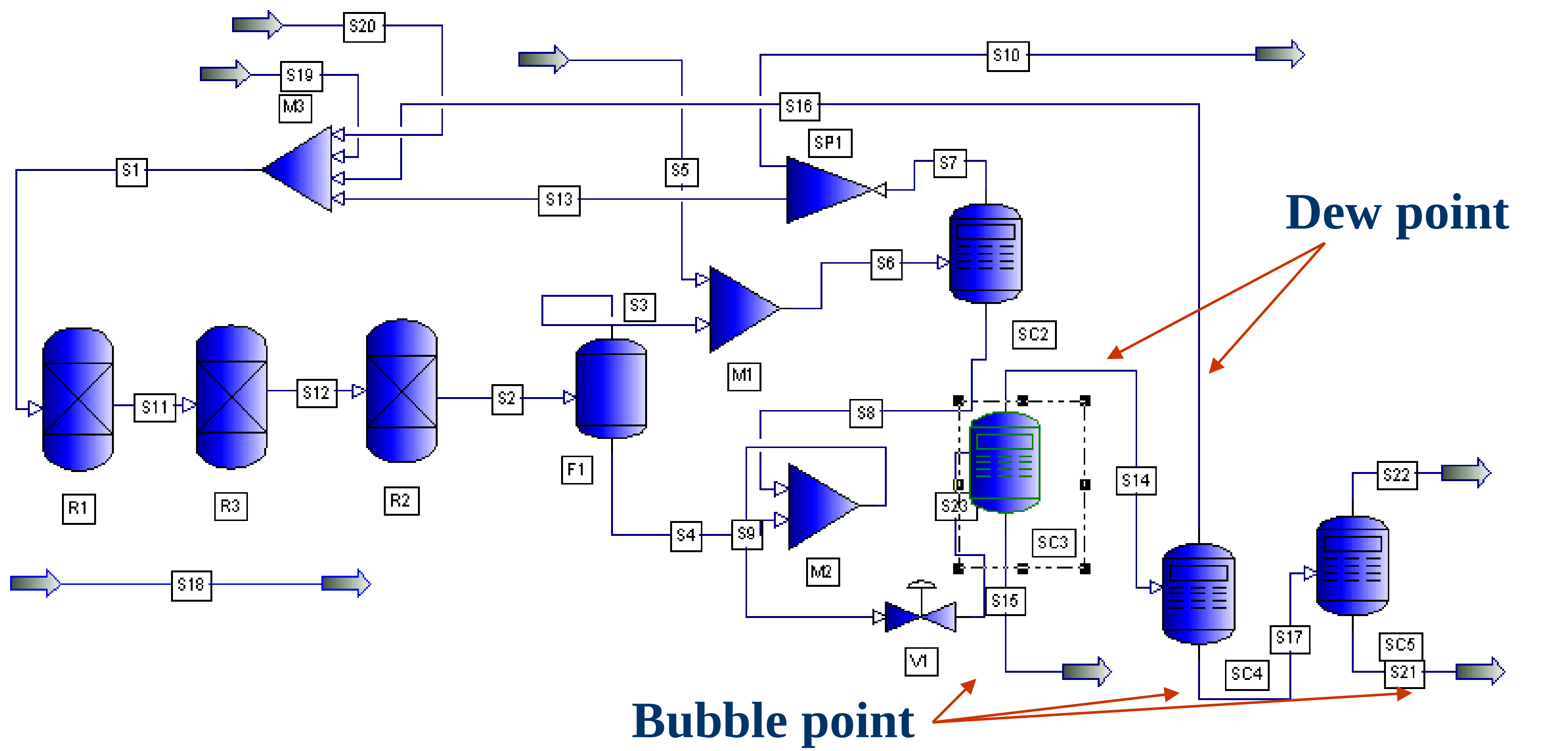
Identify P & T for the P-T Flash and replace the stream calculator with a model for the flash Unit-Op (start of tasks 5-6)



Note: choice of property model is important

	S11	S2	S12	S3	S4	S5	S6	S7	S8	S9	S10	S13	S14	S15	S16	S17
d	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid	Mixed	Vapor	Liquid	Liquid	Vapor	Vapor	Vapor	Liquid	Vapor	Liquid
7	590,0000	590,0000	590,0000	375,0000	375,0000	300,0000	376,3625	375,0000	375,0000	375,0000	375,0000	375,0000	403,0547	479,8508	319,8530	445,4099
0	69,0000	69,0000	69,0000	68,5000	68,5000	1,0000	68,5000	68,5000	68,5000	68,5000	68,5000	68,5000	17,0000	18,0000	16,0000	17,0000
0	82,7215	82,6940	82,6958	14,2225	10,6343	0,0764	14,2989	12,4808	1,0340	11,6683	0,0624	12,4184	14,6302	10,2864	4,7525	3,2939
5	26,9469	26,9675	26,9675	28,1309	25,5722	18,0150	27,8545	27,7624	29,0262	25,8569	27,7624	27,7624	34,6502	18,0395	34,9424	33,9140
7	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,9467	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	1,0000	0,0000
3	0,0000	0,0000	0,0000	0,0000	1,0000	1,0000	0,0533	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000	1,0000	0,0000	1,0000
2	2465,482	2463,597	2463,597	1343,425	1120,172	37,740	1381,165	1280,521	100,645	1220,816	6,403	1274,118	574,545	646,272	411,295	163,250

Specify T and P for distillate & bottom products in distillation columns



S1 Mixed	S11 Vapor	S2 Vapor	S12 Vapor	S3 Vapor	S4 Liquid	S5 Liquid	S6 Mixed	S7 Vapor	S8 Liquid	S9 Liquid	S10 Vapor	S13 Vapor	S14 Vapor	S15 Liquid	S16 Vapor	S17 Liquid
309,2725	590,0000	590,0000	590,0000	375,0000	375,0000	300,0000	376,4506	375,0000	375,0000	375,0000	375,0000	375,0000	404,5365	479,8643	320,4350	445,3965
1,0000	69,0000	69,0000	69,0000	68,5000	68,5000	1,0000	68,5000	68,5000	68,5000	68,5000	68,5000	68,5000	17,0000	18,0000	16,0000	17,0000
18,6212	81,5386	81,5139	81,5168	14,0961	10,2784	0,0764	14,0655	12,2509	1,0133	11,2677	0,0613	12,1896	14,2214	10,2853	4,3165	3,2950
25,7362	26,7183	26,7358	26,7358	27,9633	25,2387	18,0150	27,6791	27,5780	28,9675	25,5196	27,5780	27,5780	34,3645	18,0388	34,5620	33,9012
0,7281	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,9469	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	1,0000	0,0000
0,2719	0,0000	0,0000	0,0000	0,0000	1,0000	1,0000	0,0531	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000	1,0000	0,0000	1,0000
2512,500	2432,031	2430,438	2430,438	1335,485	1094,953	37,740	1363,141	1263,910	99,231	1192,690	6,320	1257,590	546,518	646,172	383,110	163,408
195,7569	197,6661	197,6661	197,6661	185,2389	12,4272	0,0000	183,3088	183,3088	0,0000	12,3647	0,9165	182,3923	12,3647	0,0000	12,3647	0,0000

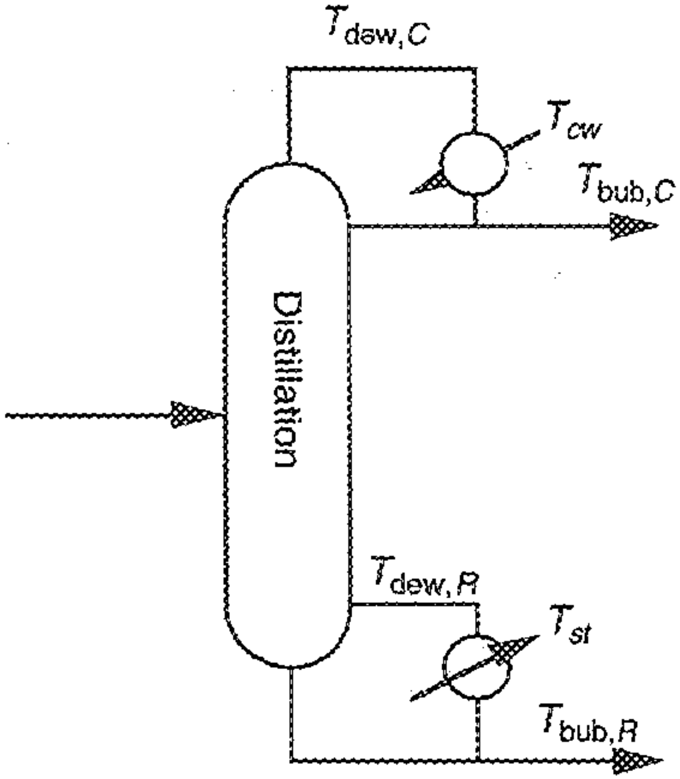


FIGURE 3.13 Setting column pressure and temperature.

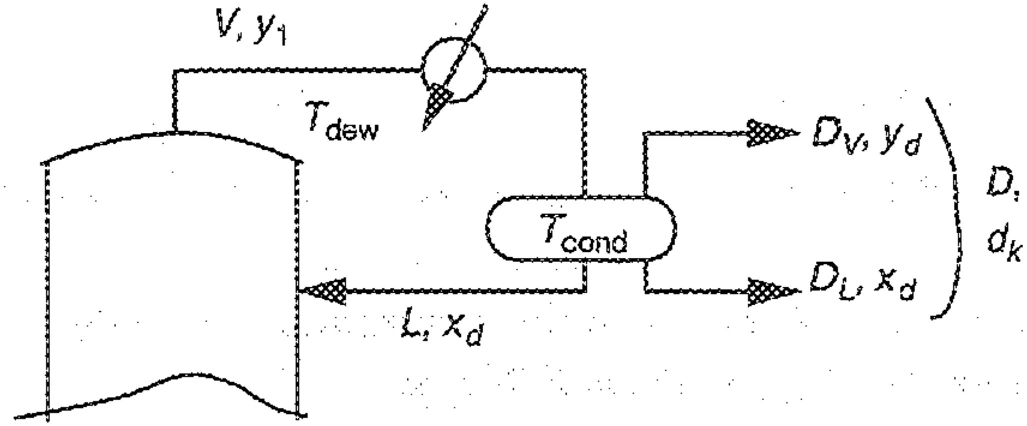


FIGURE 3.14 Partial condenser.

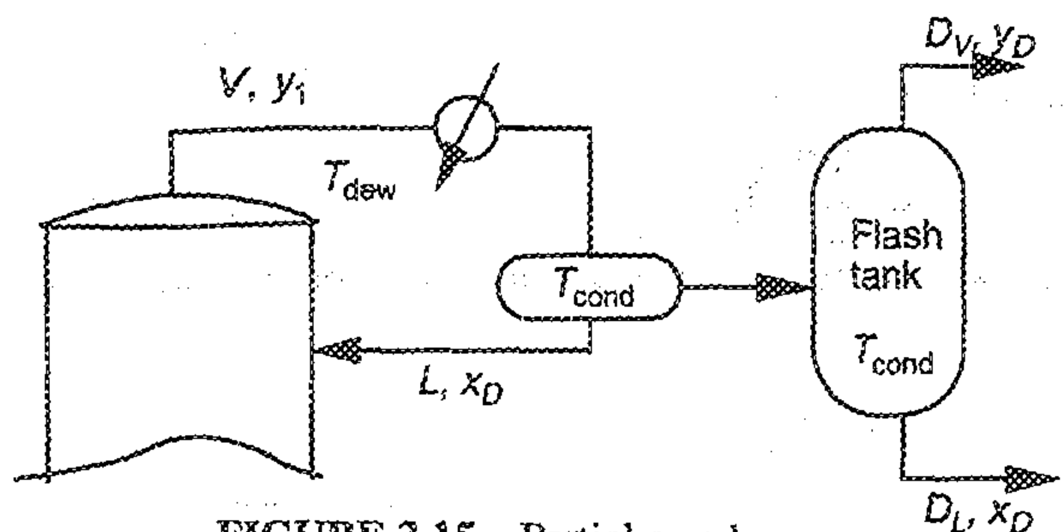


FIGURE 3.15 Partial condenser representation for calculation.

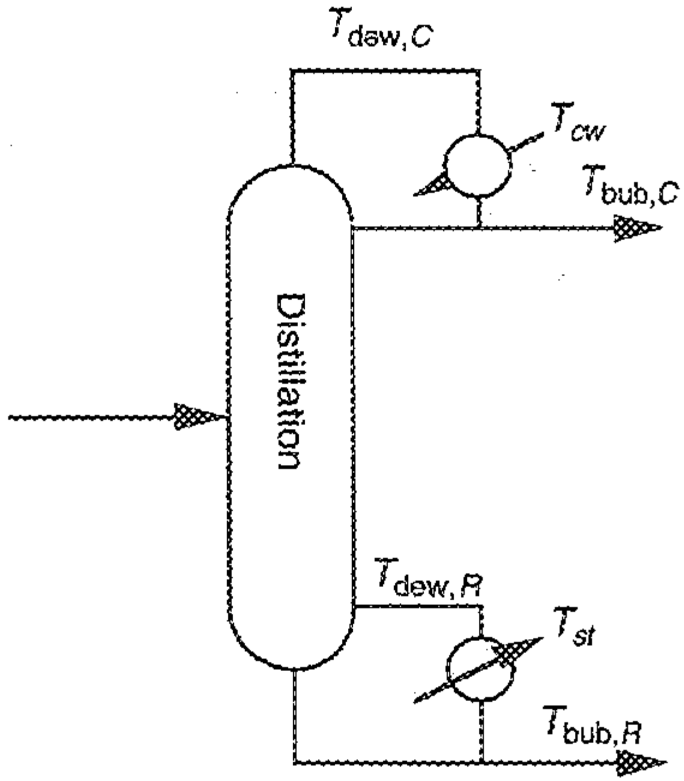
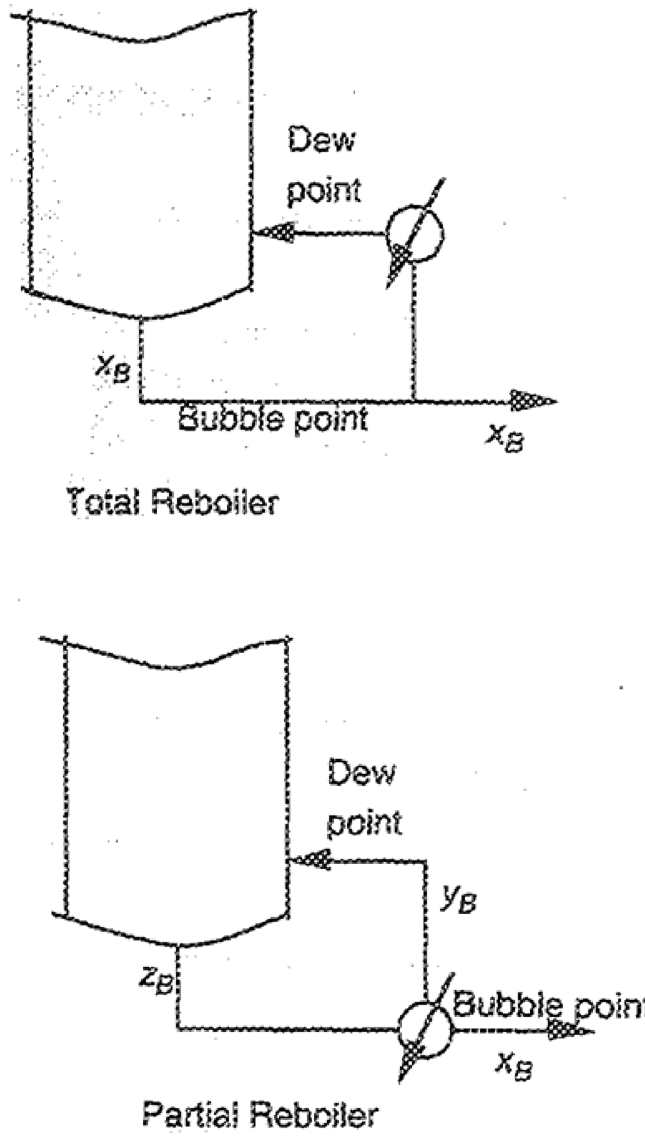
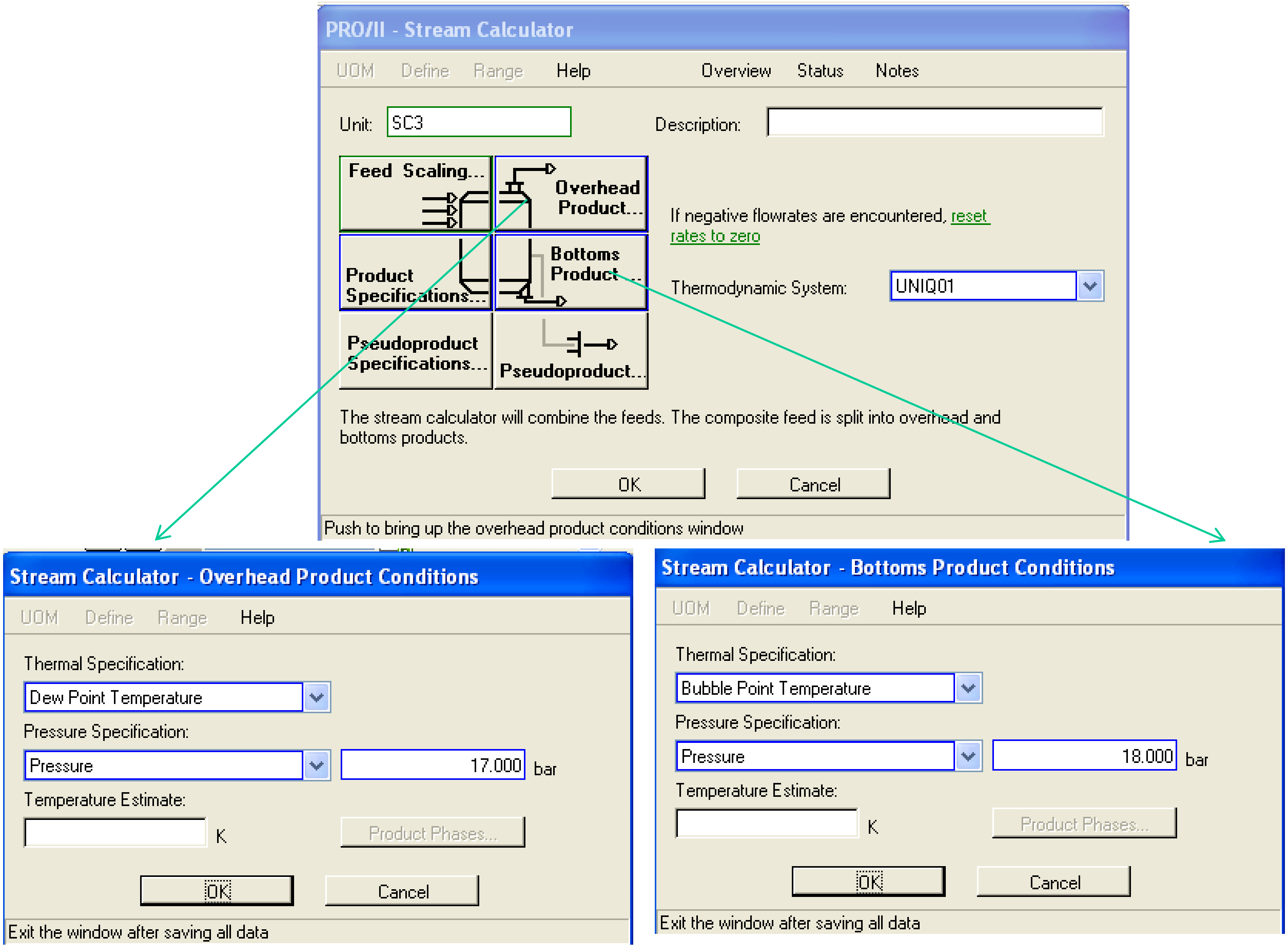


FIGURE 3.13 Setting column pressure and temperature.

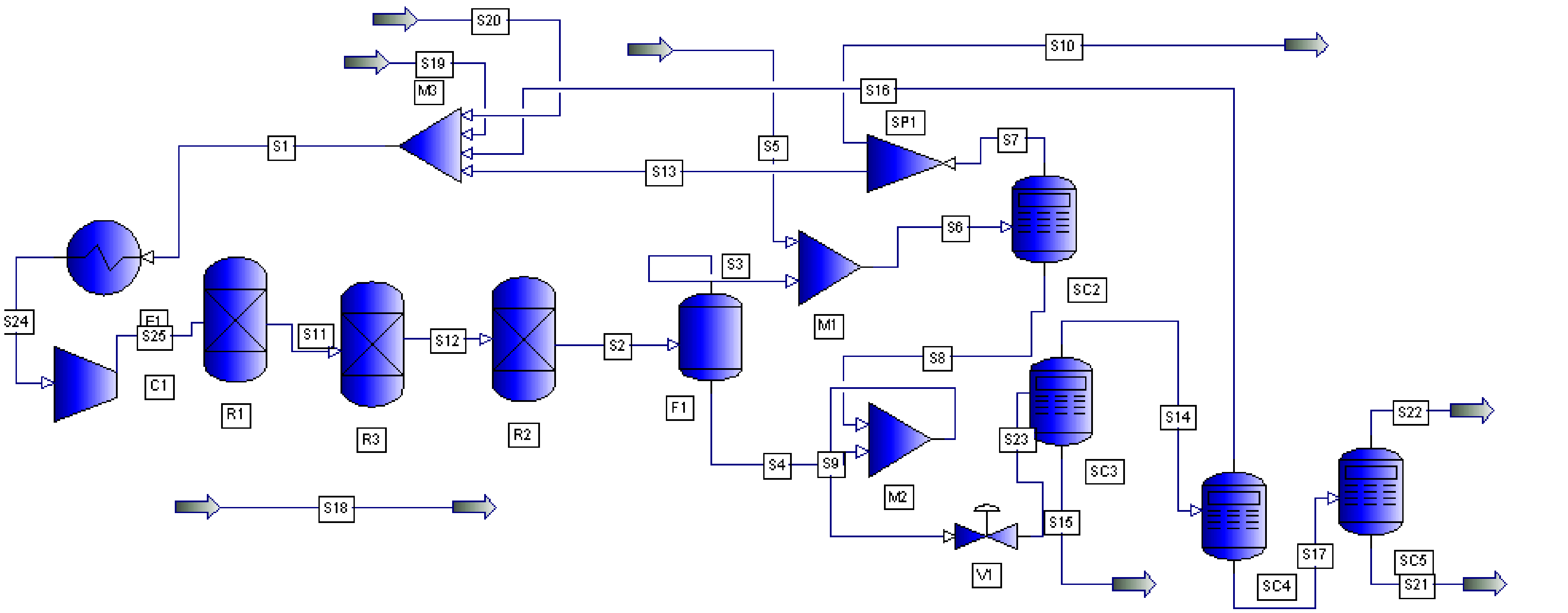
FIGURE 3.16 Reboiler configurations.



Specify T and P for distillate & bottom products in distillation columns



Add heat exchangers, pumps, compressors, expansion valves, etc., to change stream T and/or P



S1	S11	S2	S12	S3	S4	S5	S6	S7	S8	S9	S10	S13	S14	S15	S16	S17
Mixed	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid	Mixed	Vapor	Liquid	Liquid	Vapor	Vapor	Vapor	Liquid	Vapor	Liquid
309,4559	590,0000	590,0000	590,0000	375,0000	375,0000	300,0000	376,2754	375,0000	375,0000	375,0000	375,0000	375,0000	405,8932	479,9062	318,7552	445,4302
1,0000	69,0000	69,0000	69,0000	68,5000	68,5000	1,0000	68,5000	68,5000	68,5000	68,5000	68,5000	68,5000	17,0000	18,0000	16,0000	17,0000
16,2007	82,8322	82,8053	82,8071	14,3242	10,5837	0,0764	12,0275	10,5289	0,8663	10,7915	0,0526	10,4762	13,5870	10,3172	3,6094	3,2340
25,6062	26,9279	26,9480	26,9480	28,1059	25,5443	18,0150	28,3431	28,3858	27,8459	24,8758	28,3858	28,3858	33,4741	18,0365	33,3957	33,6463
0,6886	1,0000	1,0000	1,0000	1,0000	0,0000	0,0000	0,9369	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	1,0000	0,0000
0,3114	0,0000	0,0000	0,0000	0,0000	1,0000	1,0000	0,0631	0,0000	1,0000	1,0000	0,0000	0,0000	0,0000	1,0000	0,0000	1,0000
2242,405	2471,442	2469,602	2469,602	1353,274	1116,328	37,740	1109,285	1021,540	87,746	1163,607	5,108	1016,432	515,508	648,099	354,173	161,335

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

Compare the results with those obtained through PROII

Next task & next lecture