Lecture 3: Mass Balance & Flowsheet Decomposition

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

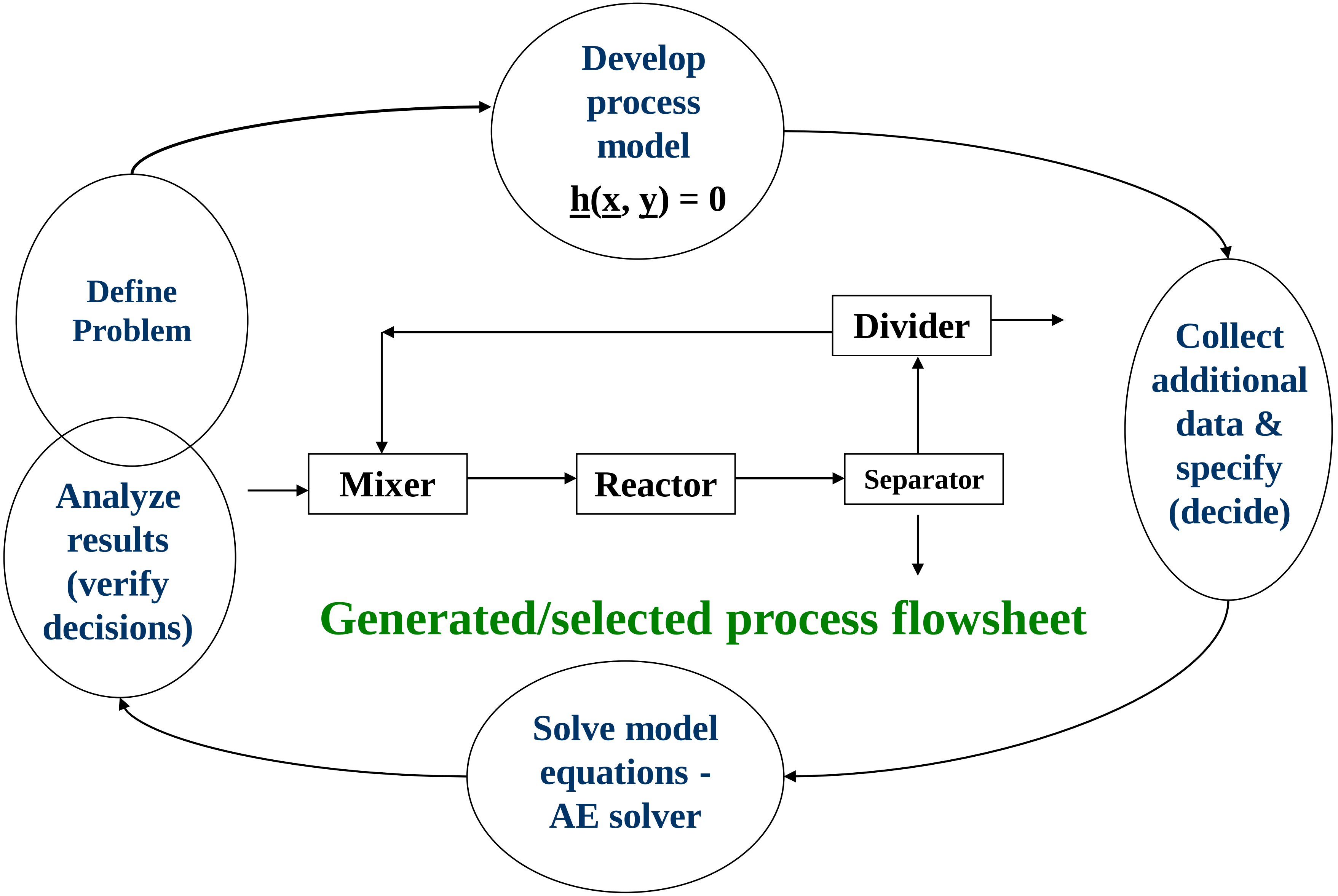
Part-1: Main concepts & mass balance

Part-II: Method for flowsheet decomposition

Part-III: Case-study (methods for design decision making plus application of simulator for mass balance)

Course 28350 (Spring 2017)

Steady state process simulation - solve algebraic equations



Two ways to perform mass balance simulations

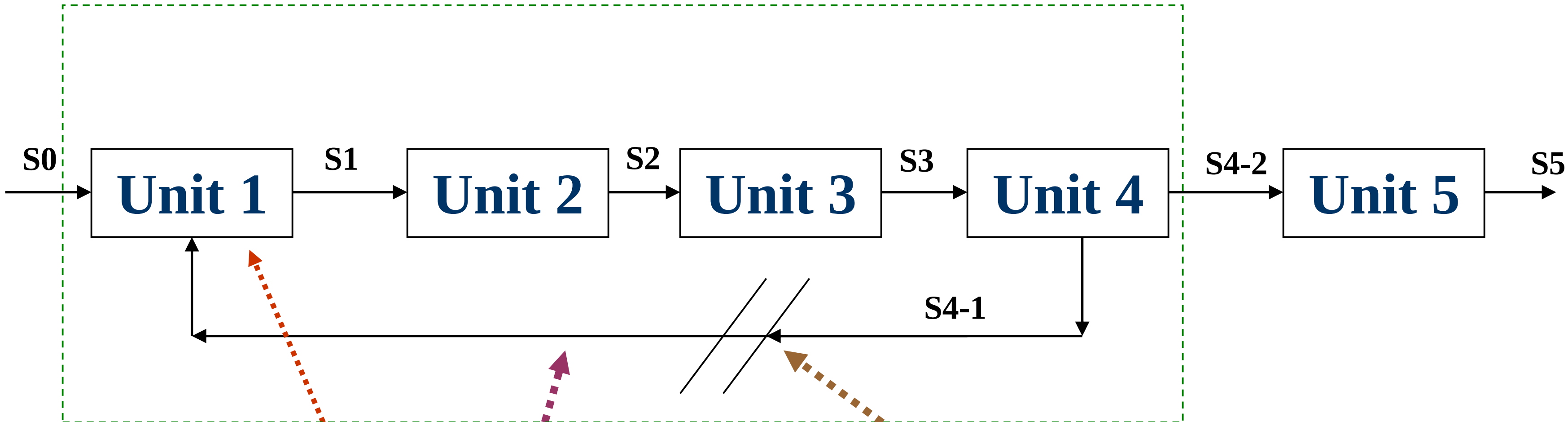
- Use a process simulator (see PROII manual)
- Build your own simulator (chapters 3, 7-8) plus new chapter (supplied)
  - Derive the model equations
  - Use a suitable solver to solve the model equations

Both alternatives will require you to specify* –

- The flowsheet
- Variables representing the input streams
- Parameters for all unit modules (reactor, stream calculator, divider)

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

Some Definitions & Concepts



Module; Stream; Flowsheet decomposition; Partitions;Recycle loop; *Tear* stream; Calculation sequence; Simulation approach; Convergence technique

Solve Unit1 - Unit2 - Unit3 - Unit4; repeat until convergence of recycle loop; solve Unit5 (modular approach - solve one unit at a time)

<u>Flowsheet Decomposition</u>

**** Identify <u>partitions</u>***

**** Identify <u>recycle-loops</u>***

**** Determine <u>tear-streams</u>***

**** Determine <u>calculation order</u>***

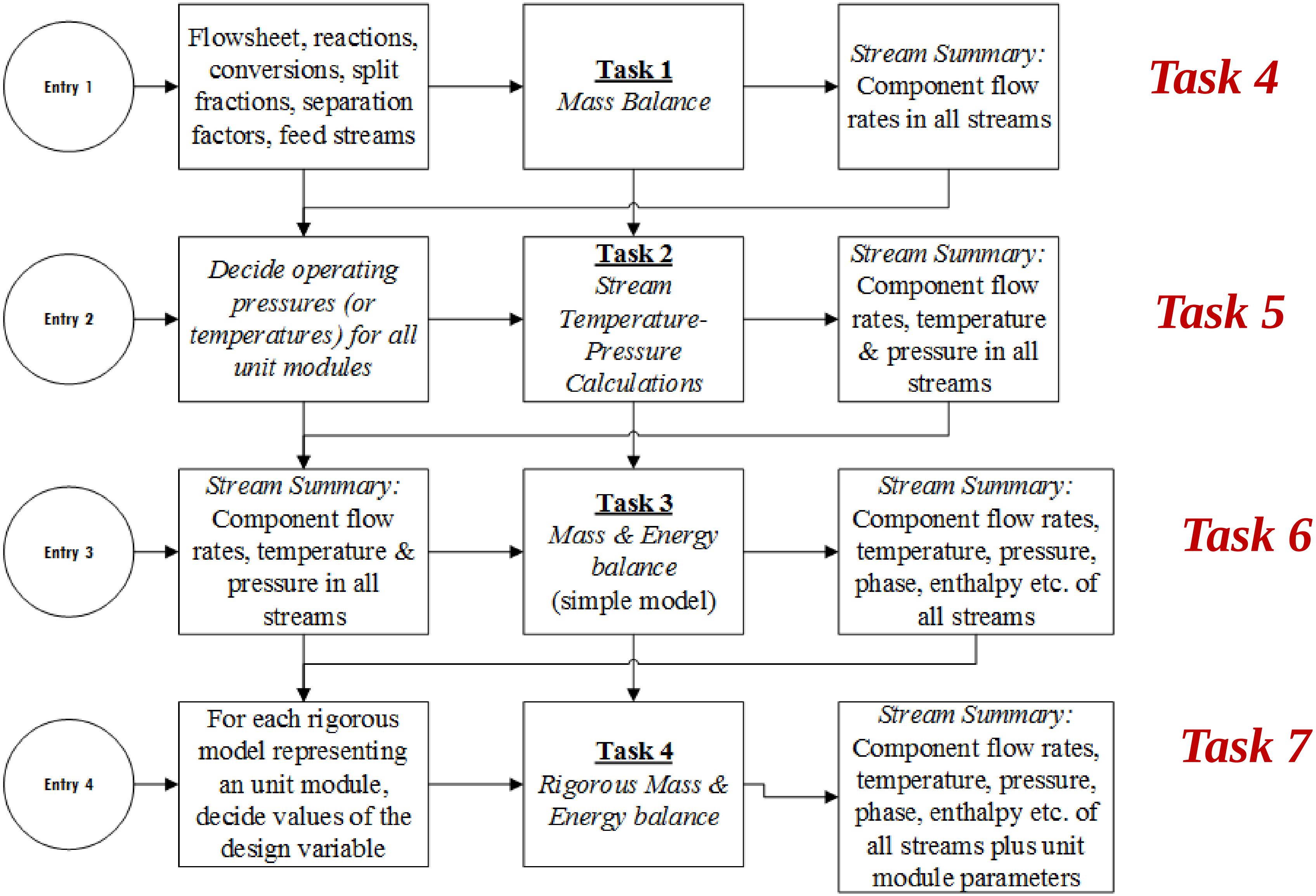
<u>Equation Ordering</u>

**** Rearrange model equations***

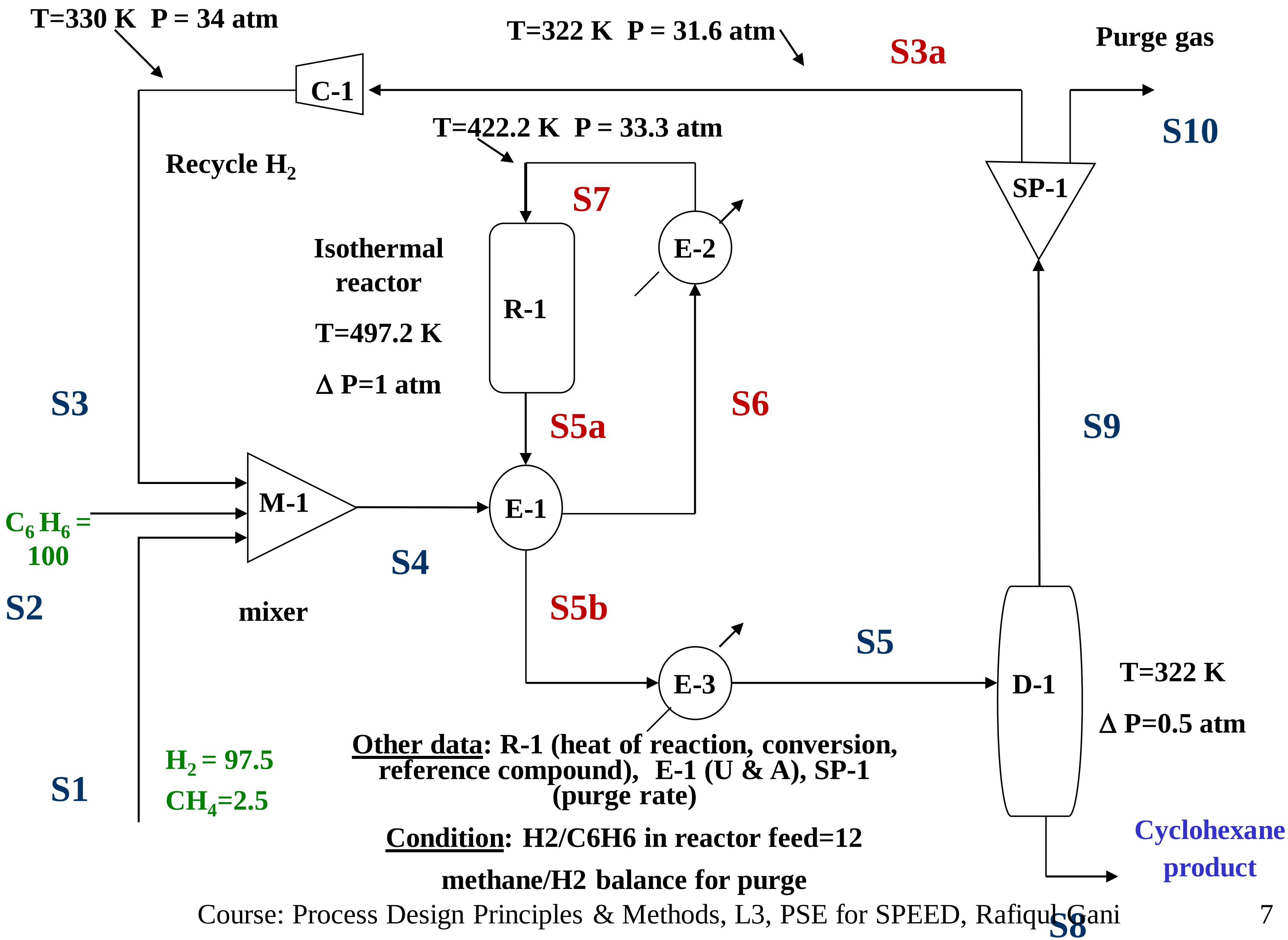
**** Identify <u>partitions</u>***

**** Determine <u>sparse pattern</u>***

Decomposition of process simulation problem into sub-tasks



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

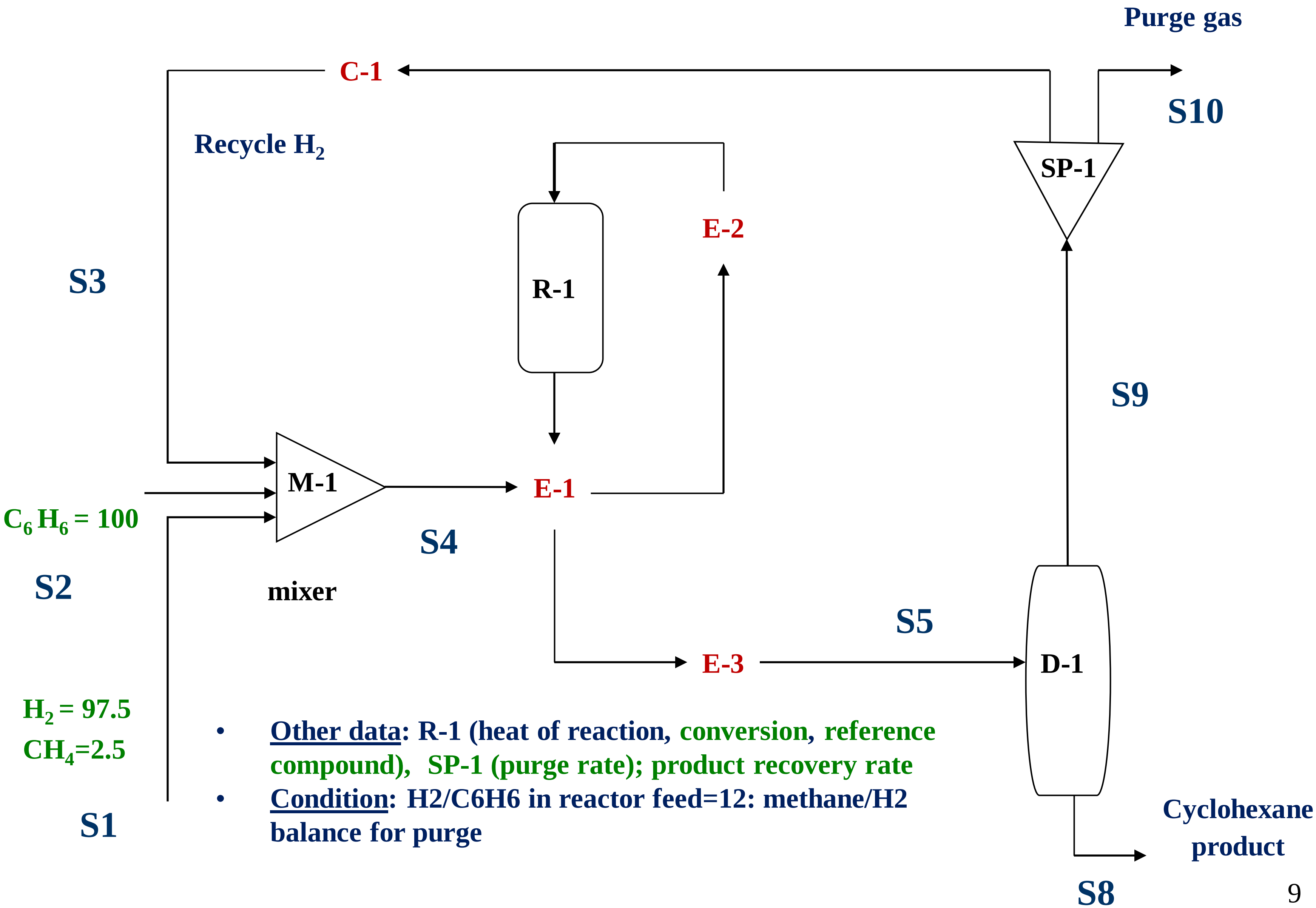
The objective is to fill-out all the stream summary table through mass and then mass-energy balance!

Variables	**Streams**						
	S1	**S2**	**S3**	**S4**	**S5**	**…….**	**S10**
$\mathbf{f_{1,j}}$							
$\mathbf{f_{2,j}}$							
$\mathbf{f_{3,j}}$							
$\mathbf{f_{4,j}}$							
$\mathbf{T_j}$							
$\mathbf{P_j}$							

All streams are defined by NC+2 variables (component flows, T & P)

NC=4 (H2, CH4, C6H6, Cyclohexane)

Flowsheet for cyclohexane production – Mass Balance



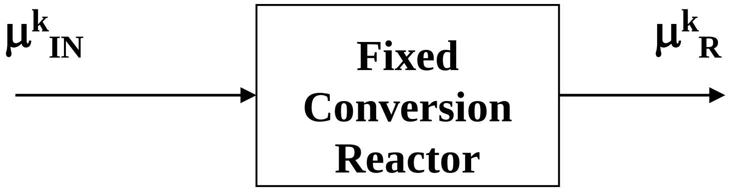
- **Other data: R-1 (heat of reaction, conversion, reference compound), SP-1 (purge rate); product recovery rate**
- **Condition: H2/C6H6 in reactor feed=12: methane/H2 balance for purge**

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

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

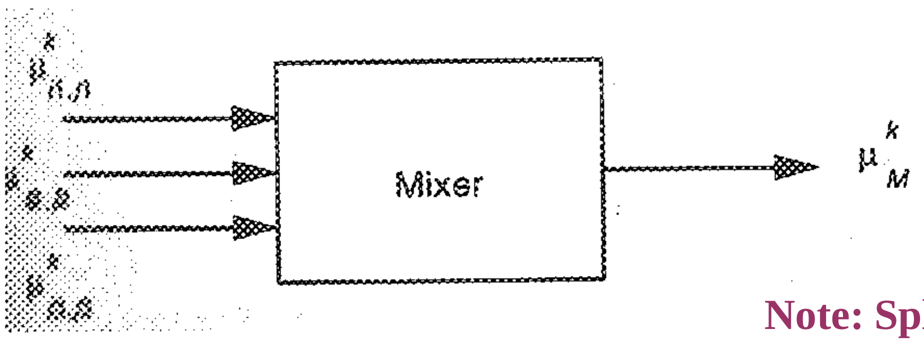
For mass balance: Number of streams (NS) = 8; Number of independent variables = NC*NS; Number of known variables = 2*NC; Number of unknown variables = 6*NC; NC is the number of compounds; subscript j indicates any stream j

1. MB-model: Simple Models for Mass Balance (based on text-book chapter 3)



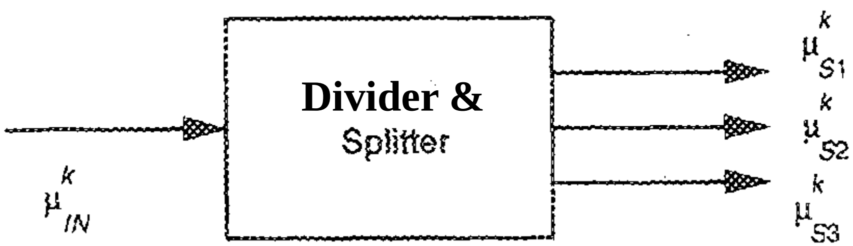
$$\mu^k_R = \mu^k_{IN} + \Sigma_r \gamma_{r,k}\, \eta_r\, \mu^{l(r)}_{IN}$$

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



$$\mu^k_M = \Sigma_i\, \mu^k_i \qquad i=1,NM$$

Note: Splitter in PROII is called stream calculator

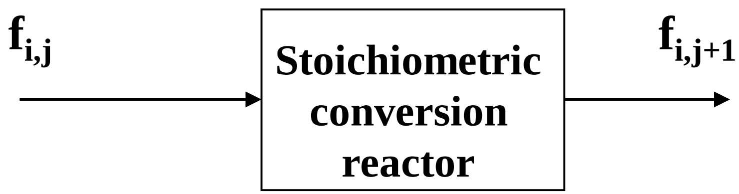


$$\mu^k_{Sj} = \xi_{jk}\, \mu^k_{IN} \qquad j=1,NS-1$$

$$\mu^k_{S,NS} = (1 - \Sigma_j\, \xi_j)\mu^k_{IN}$$

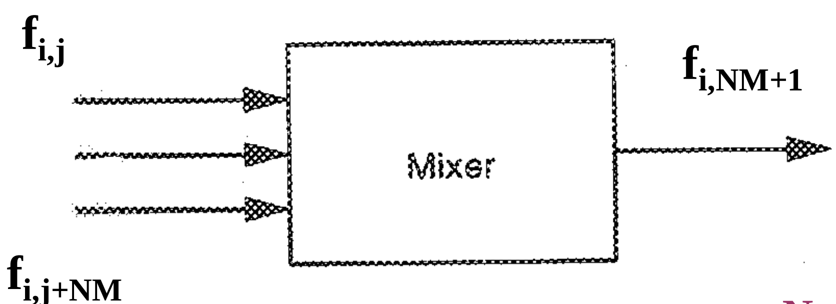
Note: *A flash or component splitter can use the same model as divider/splitter where ξ_{jk} (recovery of component k) is specified for each compound k*

1. MB-model: Simple Models for Mass Balance (for each component i): General derivation



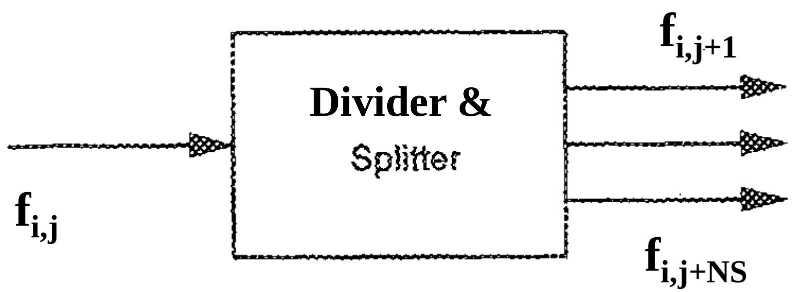
$$f_{i,j+1} = f_{i,j} + \Sigma_r \gamma_{r,i} \, \eta_{r,k} \, f_{k,j}$$

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



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

Note: Splitter in PROII is called stream calculator

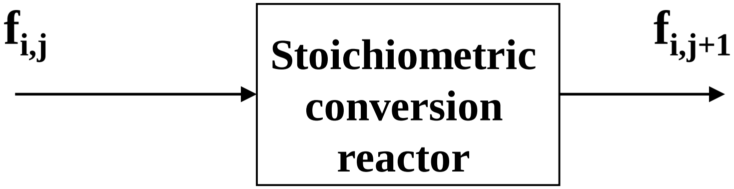


$$f_{ij+1} = \xi_{i,j} \, f_{i,j} \qquad j=1,NS-1$$

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

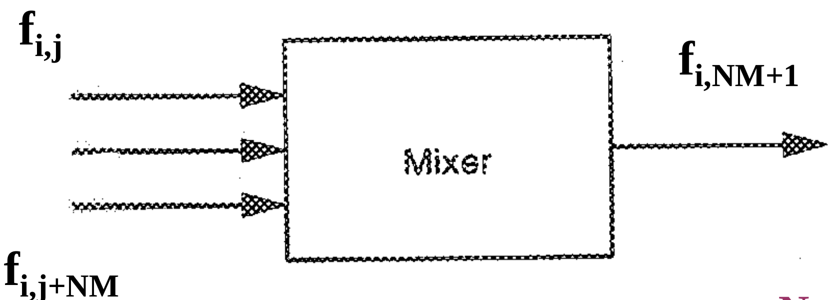
***Note:** A flash or component splitter can use the same model as divider/splitter where ξ_{ji} (recovery of component i) is specified for each compound i*

2. Which variables to specify? That is, all decision variables (module parameters).



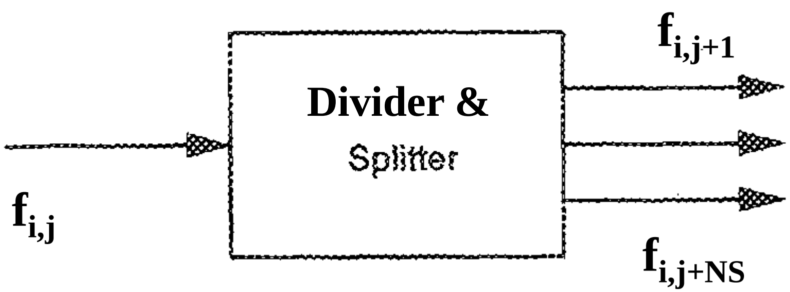
$$f_{i,j} = f_{i,j} + \Sigma_r \gamma_{r,i}\, \eta_{r,k}\, f_{k,j}$$

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



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

Note: Splitter in PROII is called stream calculator



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

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

***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*

3. Solve the model equations. Derive a solution strategy

The full-model (for mass balance only)

Mixer:

$f_{i,NM+1} = \Sigma_j f_{ij}$ for i=1,NC; j=1,3; NM = 3 (1)

Reactor:

$f_{i5} = f_{i4} + \gamma_i \eta_k f_{k4}$ for i=1,NC; k=C6H6 (2)

Stream calculator:

$$\left.\begin{aligned} f_{i8} &= \xi_{iS} f_{i5} \\ f_{i9} &= (1 - \xi_{iS}) f_{i5} \end{aligned}\right\}$$

for i=1, NC (3), (4)

Dvider:

$f_{i10} = \xi_{iD} f_{i9}$ for i=1, NC (5)

$f_{i3} = (1 - \xi_{iD}) f_{i9}$ for i=1, NC; $\xi_{1D} = \xi_{iD} = \xi_{NCD}$ (6)

3a. Collect all the model equations

3b. Analyze the model

3c. Analyze the incidence matrix

3d. Derive the solution strategy

3. Solve the model equations. 3b - Analyze the model

Equations:	**Number**
Eq. 1	NC
Eq. 2	NC
Eq. 3	NC
Eq. 4	NC
Eq. 5	NC
Eq. 6	NC
Total: NE	6*NC
Number of Variables:	
Component flow-rates: $\underline{f}_1$, $\underline{f}_2$, $\underline{f}_3$, $\underline{f}_4$, $\underline{f}_5$, $\underline{f}_8$, $\underline{f}_9$, $\underline{f}_{10}$	8*NC
Reactor parameters: γ, η_k	NC+1
Stream calculator parameters: $\underline{\xi}_S$	NC
Divider parameters: $\underline{\xi}_D$	NC
Total: NV	11*NC+1
Degrees of freedom: NV - NE	5*NC +1
Variables to specify (decisions): $\underline{f}_1$, $\underline{f}_2$ (2NC process variables); γ, η_k, $\underline{\xi}_S$, $\underline{\xi}_D$ (3NC+1 equipment parameters)	
Unknown variables: $\underline{f}_3$, $\underline{f}_4$, $\underline{f}_5$, $\underline{f}_8$, $\underline{f}_9$, $\underline{f}_{10}$ (6NC process variables)	

Known Data for Cyclohexane Process*

Unit/Stream	Specifications	Specified value
Reactor	Reaction, stoichiometric coefficients ($\underline{v}$), conversion (X_k), key component (k)	$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$ $\underline{v}$ (-3, 0, -1, 1); X_k (0.97, k=3)
Separation	Component split-fractions in overhead product ($\underline{\xi}_S$)	$\underline{\xi}_S$ (1.0, 1.0, 0.0, 0.0)
Purge	Stream-divider split fraction (β_D)	β_D (0.025)
Feed stream 1	Component flow rates (f_1, kmol/hr)	f_1 (0, 0, 45.36, 0)
Feed stream 2	Component flow rates (f_2, kmol/hr)	f_2 (146.25, 3.75, 0, 0)

* See variable definitions in ~~Eqs. (7.1)-(7.6)~~

(Eqs. 1-6)

3. Solve the model equations. 3c - Analyze the incidence matrix

	f_1	f_2	γ	η_k	ξ_S	ξ_D	f_5	f_8	f_9	f_{10}	f_3	f_4
Eq. 2			*	*			(*)					*
Eq. 3					*		*	(*)				
Eq. 4					*		*		(*)			
Eq. 5						*			*	(*)		
Eq. 6						*			*		(*)	
Eq. 1	*	*									*	(*)

3. Solve the model equations. 3d – Derive solution strategy

Solve all the equations simultaneously, or, solve them sequentially

Solve Eq.2 → Solve Eq.3 → Solve Eq.4 → Solve Eq.5 → Solve Eq.6 → Solve Eq.1

guess f_4

new f_4

3. Solve the model equations. 3c - Analyze the incidence matrix

	$\underline{f}_1$	$\underline{f}_2$	$\underline{\gamma}$	η_k	$\underline{\xi}_S$	$\underline{\xi}_D$	$\underline{f}_5$	$\underline{f}_8$	$\underline{f}_9$	$\underline{f}_{10}$	$\underline{f}_3$	$\underline{f}_4$
Reactor			*	*			(*)					*
SC					*		*	(*)				
SC					*		*		(*)			
Divider						*			*	(*)		
Divider						*			*		(*)	
Mixer	*	*									*	(*)

3. Solve the model equations. 3d – Derive solution strategy

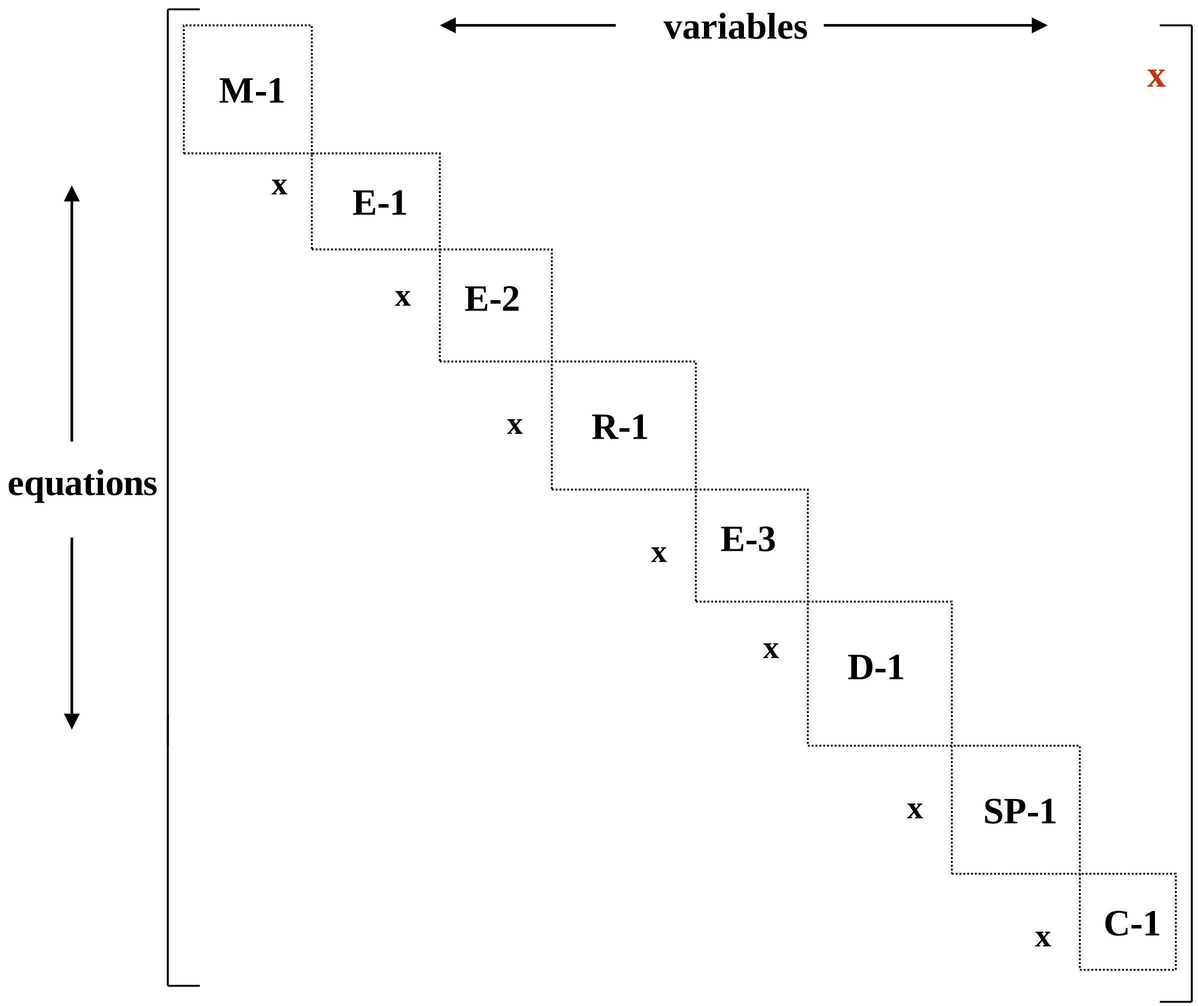
Solve all the equations simultaneously, or, solve them sequentially

Solve reactor (Eq. 2) → Solve SC (Eqs. 3-4) → Solve divider (Eqs- 5-6) → Solve mixer (Eq.1)

guess $\underline{f}_4$

new $\underline{f}_4$

Summary of solution strategies: modular versus simultaneous



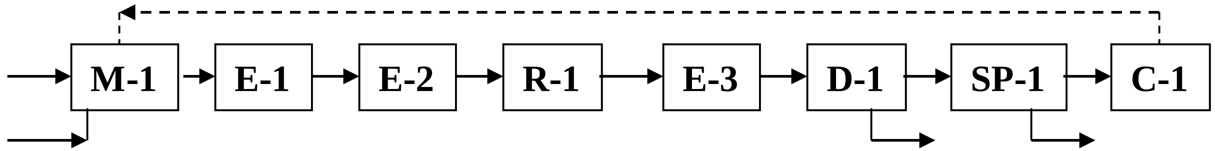
Solve

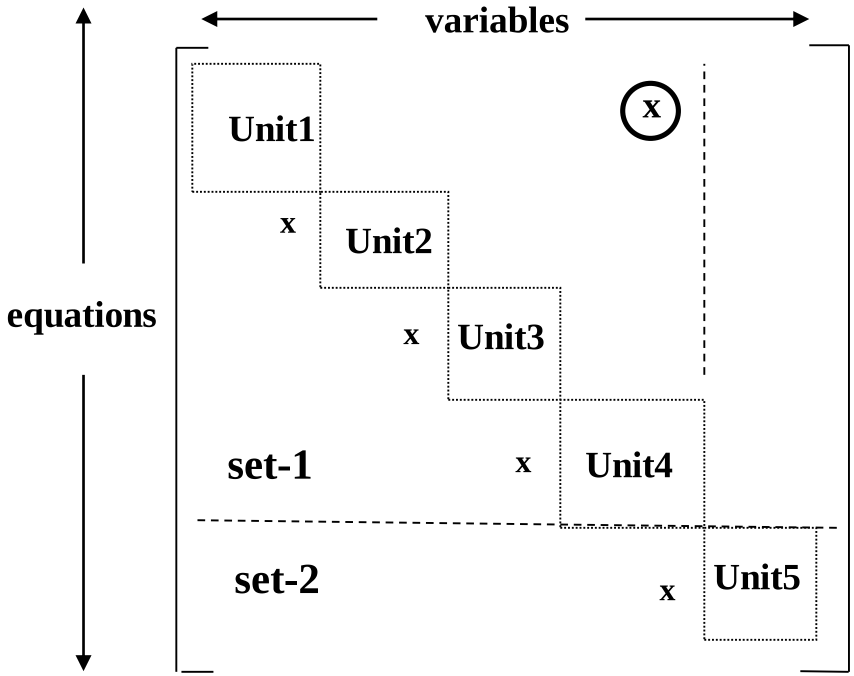
$$\underline{A}\ \underline{x} = \underline{b}$$

Equation Oriented

x represents variables of the connecting streams

Sequential Modular





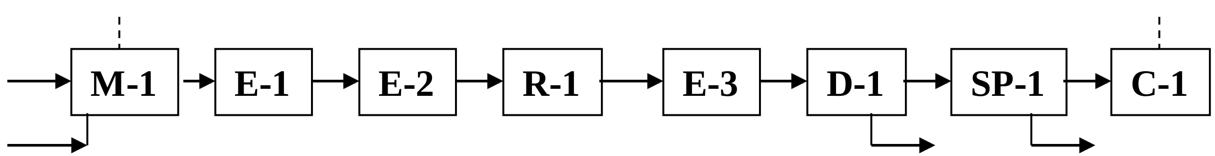
Solve

$$\underline{\mathbf{A}}\,\underline{\mathbf{x}} = \underline{\mathbf{b}}$$

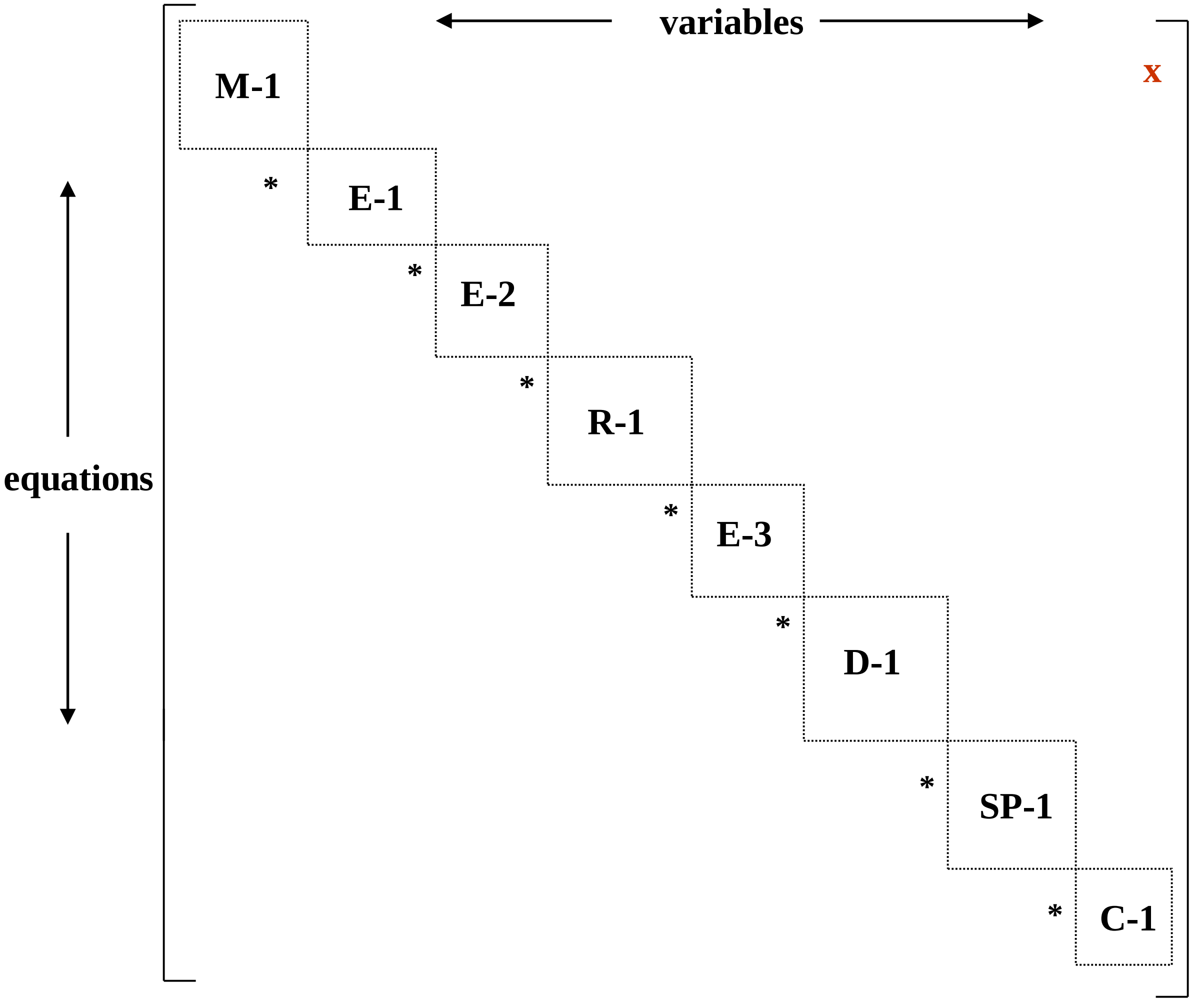
Equation Oriented

x represents variables of the connecting streams

Sequential Modular



Concepts: flowsheet decomposition & equation ordering



Convergence procedure

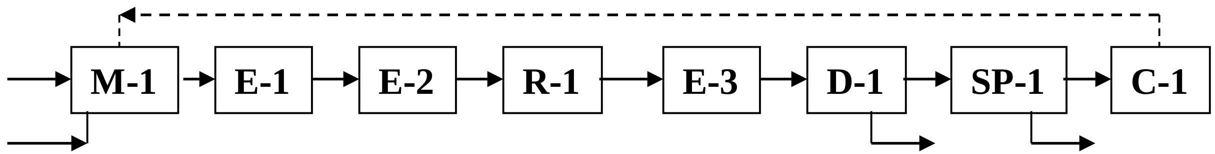
$$\underline{x}^{k+1} = \underline{x}^{k} - \underline{F} / \underline{J}$$

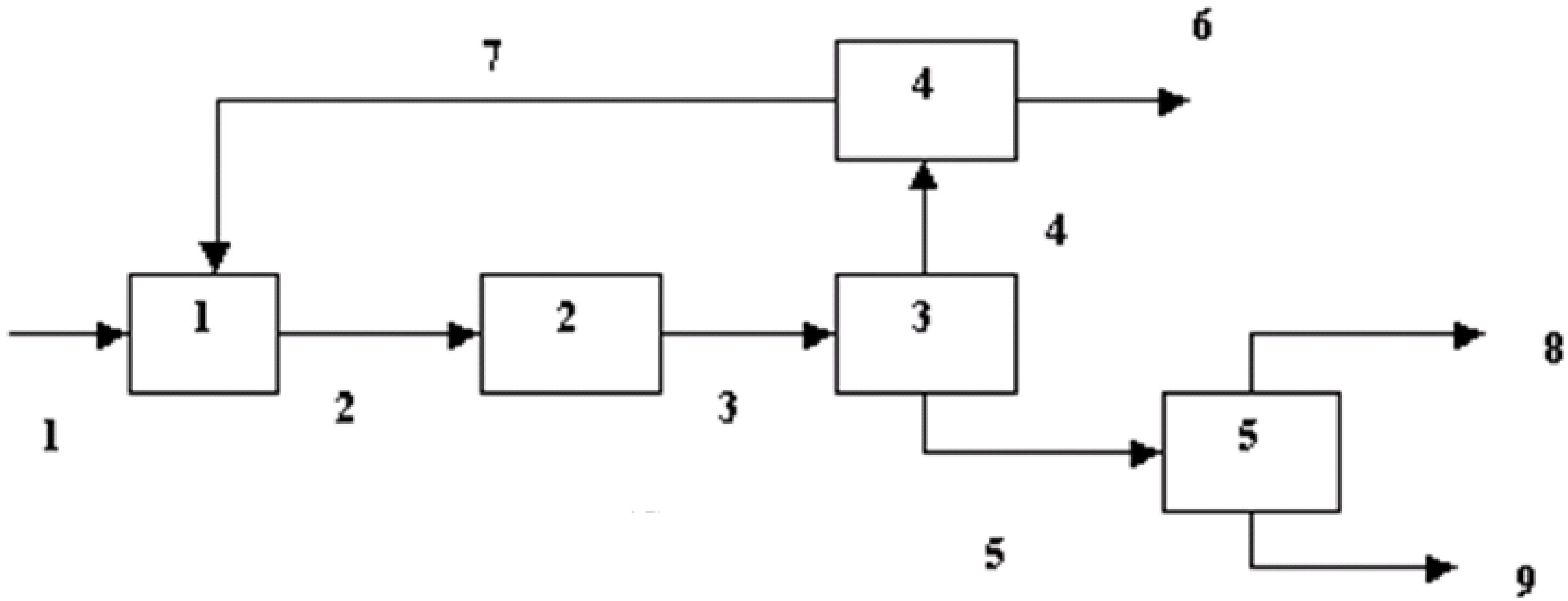
$$\underline{F} \equiv \underline{A}\,\underline{x} - \underline{b} = 0$$

Mathematical model

*** represents variables of the connecting streams**

Calculation order





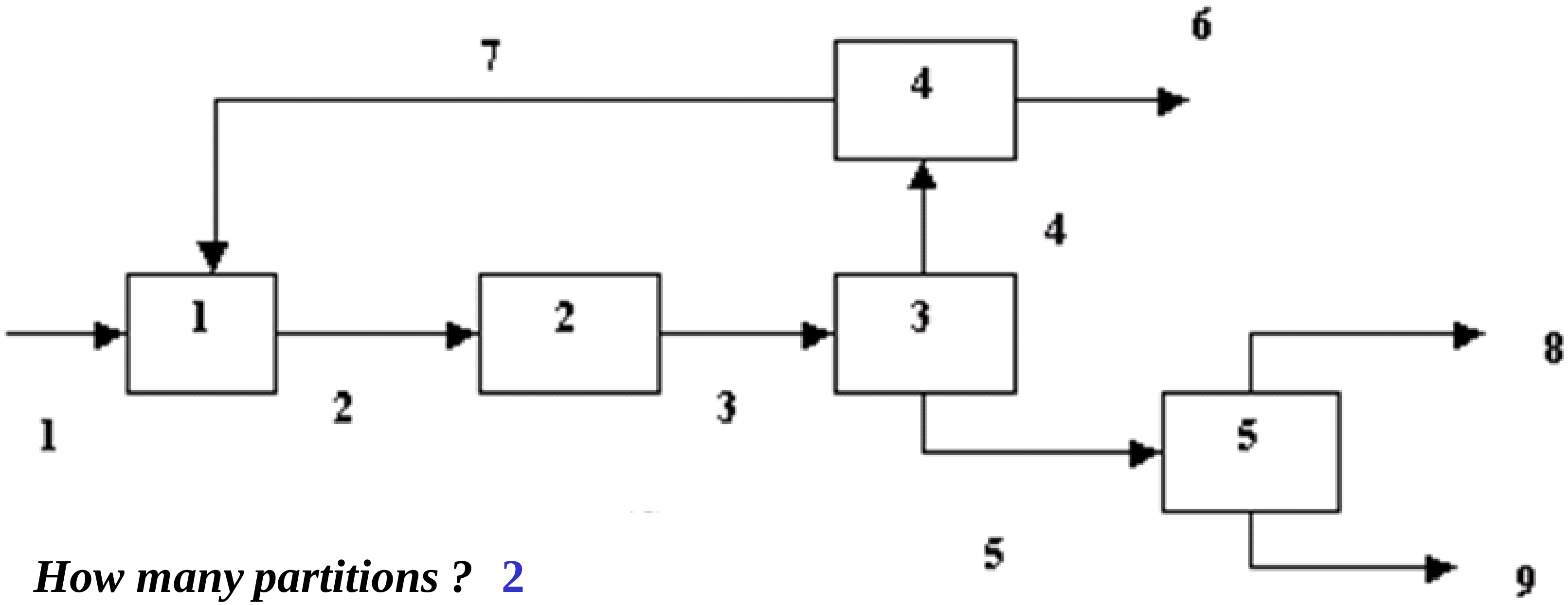
How many partitions ?

How many recycle loops ?

How many tear streams and which are they ?

Flowsheet Decomposition

Flowsheet Decomposition



How many partitions ? **2**

How many recycle loops ? **1**

How many tear streams and which are they ? **1 ; any stream from 2,3,4,7**

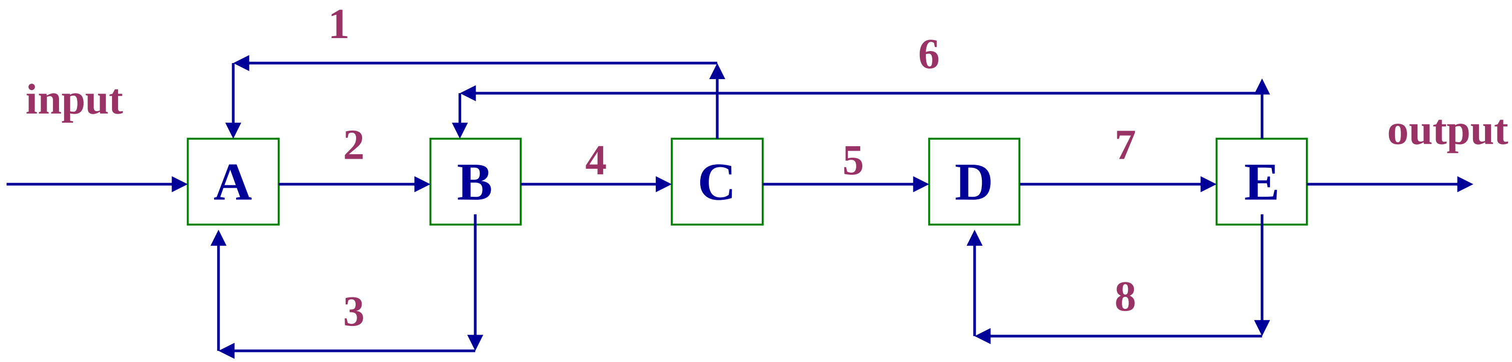
Solve (for tear-stream = 2) unit 2, unit 3, unit 4, unit 1; after convergence, solve unit 5

Method for flowsheet decomposition & deriving a calculation sequence

- **Convert** flowsheet into **signal flowgraph** (digraph)
- **Create** a table of **nodes** and **precursers**
- Follow the reduction rules
  - **Eliminate nodes** with single precursers
  - **Replace eliminated nodes** in all their occurances in the list of precursers, by their precursers
  - **Identify self-loops** (node appears in its precurser list) or two-way loops
  - **Cut nodes** (cut a node from the self-loop and eliminate them from the list)
  - **Create another list** of precursers and continue until all nodes have been eliminated

Flowsheet decomposition & Calculation sequence

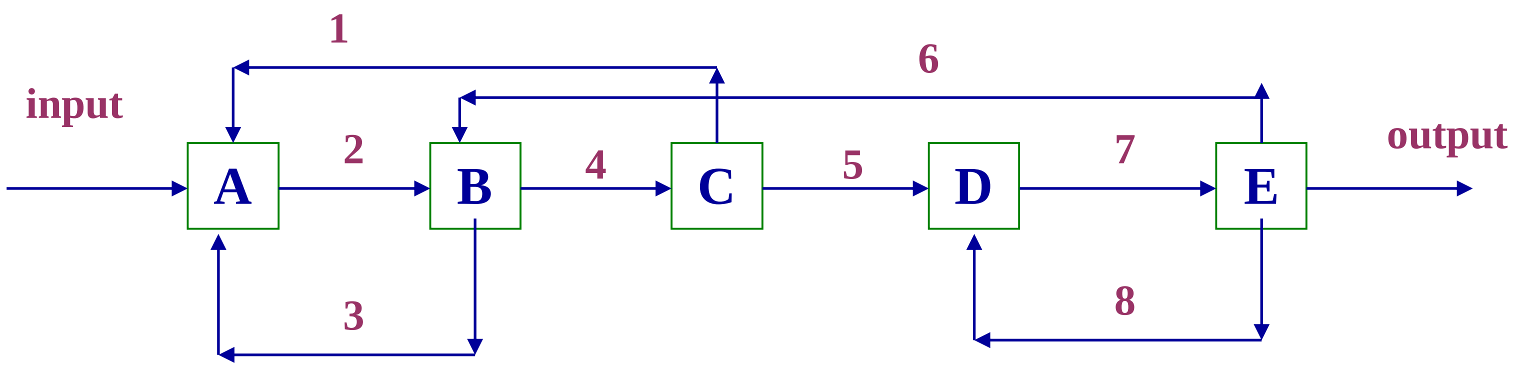
Signal flowgraph based technique (simple example)



Nodes	Precursers (1)
1	4
2	3, 1
3	2, 6
4	2, 6
5	4
6	7
7	5, 8
8	7

Flowsheet decomposition & Calculation sequence

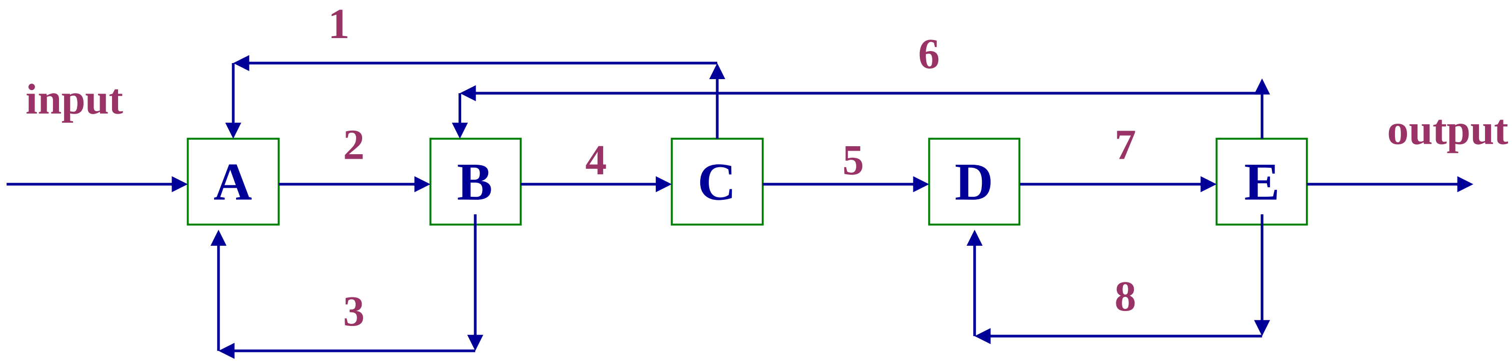
Signal flowgraph based technique (simple example)



Nodes	Precursers (1)	Precur. (2)	
1	4		
2	3, 1	3, 4	
3	2, 6	2, 7	
4	2, 6	2, 7	
5	4		
6	7		
7	5, 8	4, 7	cut
8	7		

Flowsheet decomposition & Calculation sequence

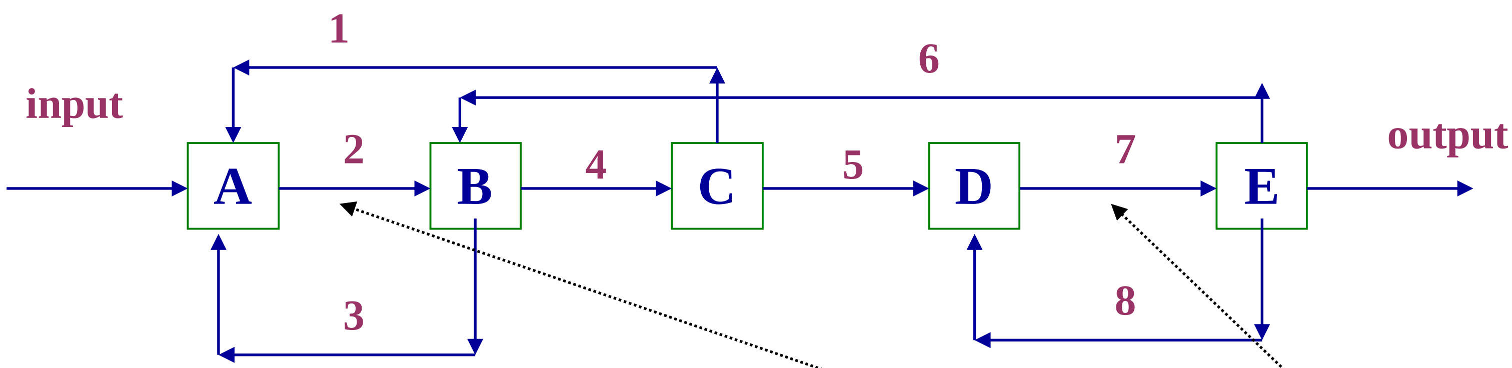
Signal flowgraph based technique (simple example)



Nodes	Precursers (1)	Precur. (2)	Precur. (3)
1	4		
2	3, 1	3, 4	2, 2
3	2, 6	2, 7	2
4	2, 6	2, 7	2
5	4		
6	7		
7	5, 8	4, 7 cut	
8	7		

Flowsheet decomposition & Calculation sequence

Signal flowgraph based technique (simple example)



Nodes	Precursers (1)	Precur. (2)	Precur. (3)
1	4		
2	3, 1	3, 4	2, 2 cut
3	2, 6	2, 7	2
4	2, 6	2, 7	2
5	4		
6	7		
7	5, 8	4, 7 cut	
8	7		

Tear streams: 2 & 7

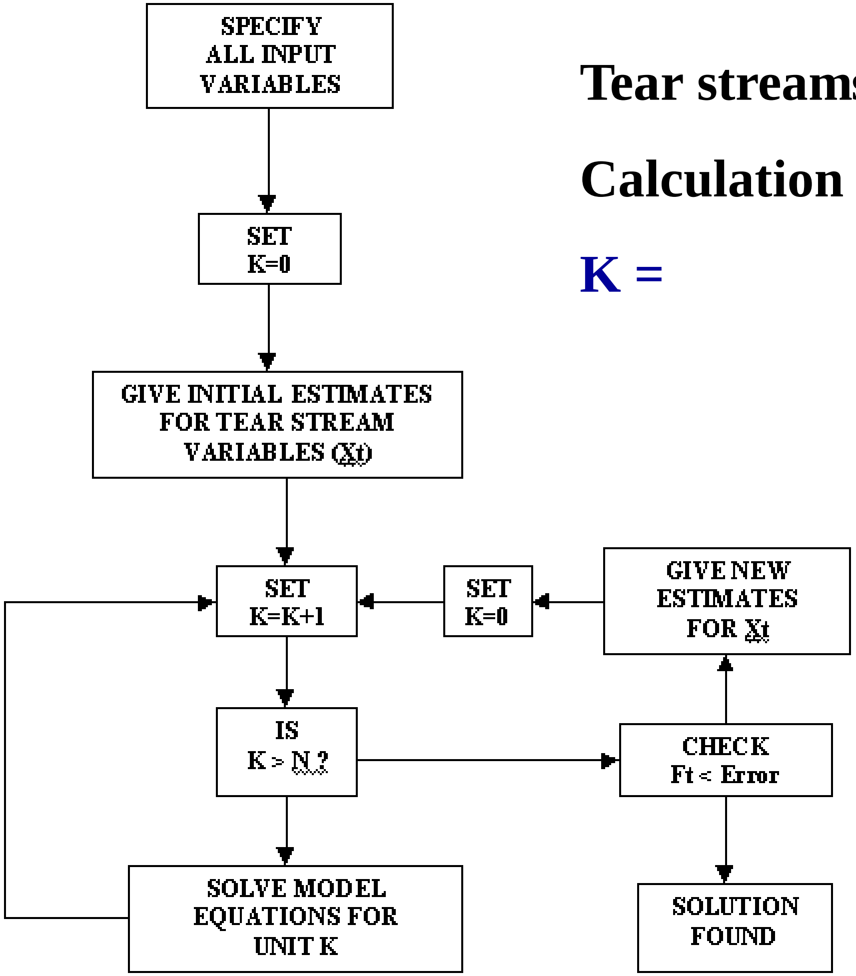
Calculation sequence:

E → B → C → D → A

Or

E → B → C → A → D

Flow-diagram for Sequential Modular Approach



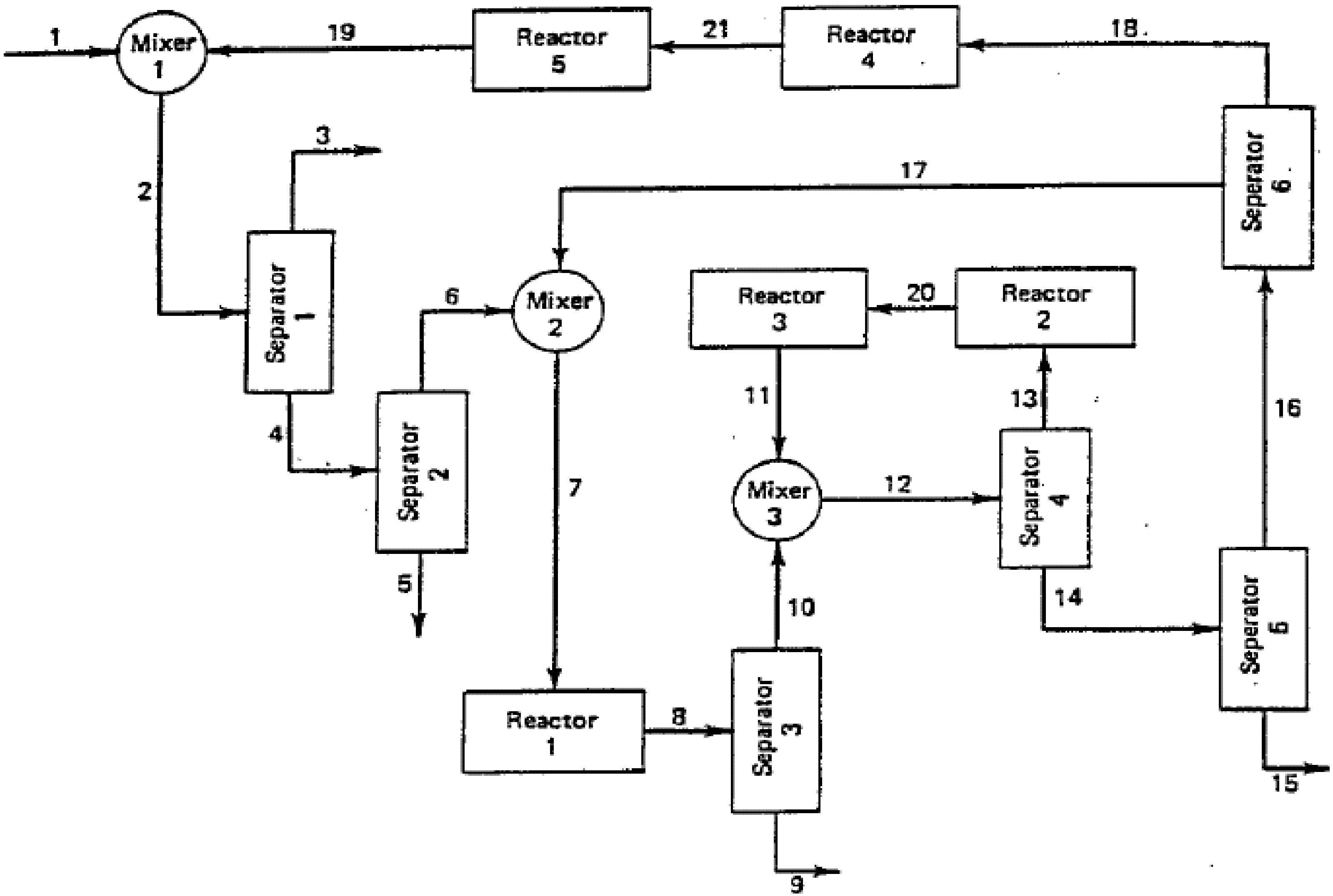
Tear streams: 2 & 7 (give initial estimates)

Calculation sequence: E → B → C → D → A

K = 1 2 3 4 5

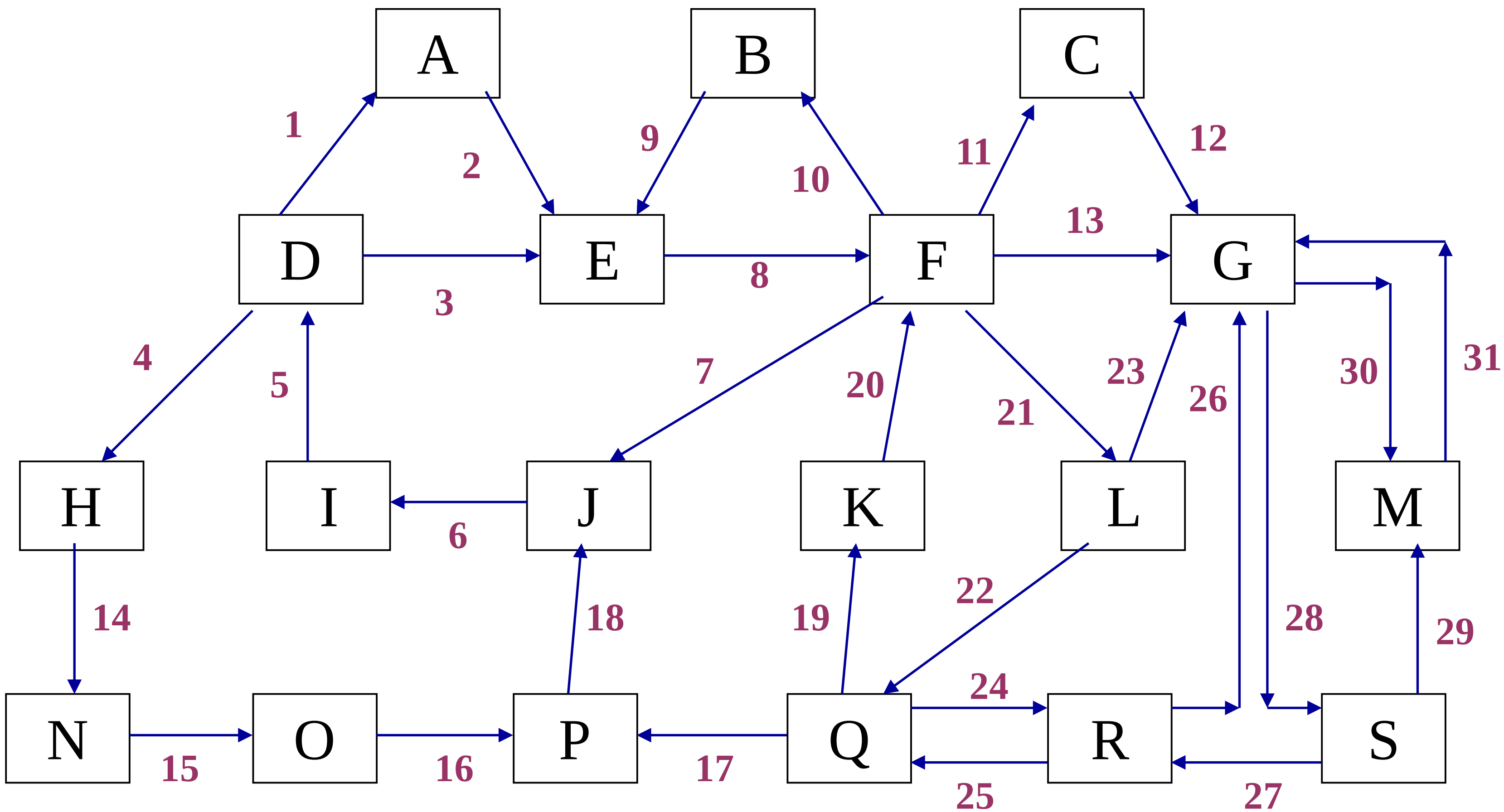
Flowsheet decomposition & Calculation sequence

Tutorial Exercise in Class (find the minimum number of tear streams)



Flowsheet decomposition & Calculation sequence

Signal flowgraph based technique (another example)



Flowsheet decomposition & Calculation sequence

Signal flowgraph based technique (another example)

Nodes	Precursers
1	5
2	1
3	5
4	5
5	6
6	7, 18
7	8, 20
8	2, 3,9
9	10
10	8, 20
11	8, 20
12	11
13	8, 20
14	4
15	14
16	15
17	22, 25
18	16, 17
19	22, 25
20	19
21	8, 20
22	21
23	21
24	22, 25
25	24, 27
26	24, 27
27	28
28	12, 13, 23, 26, 31
29	28
30	12, 13, 23, 26, 31
31	29, 30

1. Eliminate nodes with single precursers and create a new list of precursers

2. Locate self-loops; cut (or two-way loops) & eliminate node ; for more than one self-loop (two-way loops), cut the one with the largest number of precursers

Nodes	Precursers	Precursers (1)
1	5	
2	1	
3	5	
4	5	
5	6	
6	7, 18	7, 18
7	8, 20	8, 19
8	2, 3,9	6, 10
9	10	
10	8, 20	8, 19
11	8, 20	8, 19
12	11	
13	8, 20	8, 19
14	4	
15	14	
16	15	
17	22, 25	21, 25
18	16, 17	6, 17
19	22, 25	21, 25
20	19	
21	8, 20	8, 19
22	21	
23	21	
24	22, 25	21, 25
25	24, 27	24, 28
26	24, 27	24, 28
27	28	
28	12, 13, 23, 26, 31	11, 13, 21, 26, 31
29	28	
30	12, 13, 23, 26, 31	11, 13, 21, 26, 31
31	29, 30	28, 30

Flowsheet decomposition & Calculation sequence

Signal flowgraph based technique (another example)

Nodes	Precursers	Precursers (1)
1	5	
2	1	
3	5	
4	5	
5	6	
6	7, 18	7, 18
7	8, 20	8, 19
8	2, 3,9	6, 10
9	10	
10	8, 20	8, 19
11	8, 20	8, 19
12	11	
13	8, 20	8, 19
14	4	
15	14	
16	15	
17	22, 25	21, 25
18	16, 17	6, 17
19	22, 25	21, 25
20	19	
21	8, 20	8, 19
22	21	
23	21	
24	22, 25	21, 25
25	24, 27	24, 28
26	24, 27	24, 28
27	28	
28	12, 13, 23, 26, 31	11, 13, 21, 26, 31
29	28	
30	12, 13, 23, 26, 31	11, 13, 21, 26, 31
31	29, 30	28, 30

→

Nodes	Precursers	Precursers (1)	Self-loop pairs	Precursers (2)
1	5			
2	1			
3	5			
4	5			
5	6			
6	7, 18	7, 18	(1)	7, 18
7	8, 20	8, 19		8, 19
8	2, 3,9	6, 10	(2)	6, 10
9	10			
10	8, 20	8, 19	(2)	8, 19
11	8, 20	8, 19		8, 19
12	11			
13	8, 20	8, 19		8, 19
14	4			
15	14			
16	15			
17	22, 25	21, 25		21, 25
18	16, 17	6, 17	(1)	6, 17
19	22, 25	21, 25	(3)	21, 25
20	19			
21	8, 20	8, 19		8, 19
22	21			
23	21			
24	22, 25	21, 25	(4)	21, 25
25	24, 27	24, 28	(4)	24
26	24, 27	24, 28	(5)	24
27	28			
28	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(5), (6) **cut 28**	C
29	28			
30	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(6), (7)	11, 13, 21, 26, 30
31	29, 30	28, 30	(6)	30

Flowsheet decomposition & Calculation sequence

Nodes	Precursers	Precursers (1)	Self-loop pairs	Precursers (2)	Precursers (3)
1	5				
2	1				
3	5				
4	5				
5	6				
6	7, 18	7, 18	(1)	7, 18	7, 18
7	8, 20	8, 19		8, 19	8, 21
8	2, 3, 9	6, 10	(2)	6, 10	6, 10
9	10				
10	8, 20	8, 19	(2)	8, 19	8, 21
11	8, 20	8, 19		8, 19	8, 21
12	11				
13	8, 20	8, 19		8, 19	8, 21
14	4				
15	14				
16	15				
17	22, 25	21, 25		21, 25	21
18	16, 17	6, 17	(1)	6, 17	6, 21
19	22, 25	21, 25	(3)	21, 25	21
20	19				
21	8, 20	8, 19		8, 19	8, 21
22	21				
23	21				
24	22, 25	21, 25	(4)	21, 25	21, 24 **Cut3**
25	24, 27	24, 28	(4)	24	
26	24, 27	24, 28	(5)	24	
27	28				
28	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(5), (6) **cut 1**	C	C
29	28				
30	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(6), (7)	11, 13, 21, 26, 30	11, 13, 21, 30 **Cut2**
31	29, 30	28, 30	(6)	30	

Cut1: 28

Cut2: 30

Cut3: 24

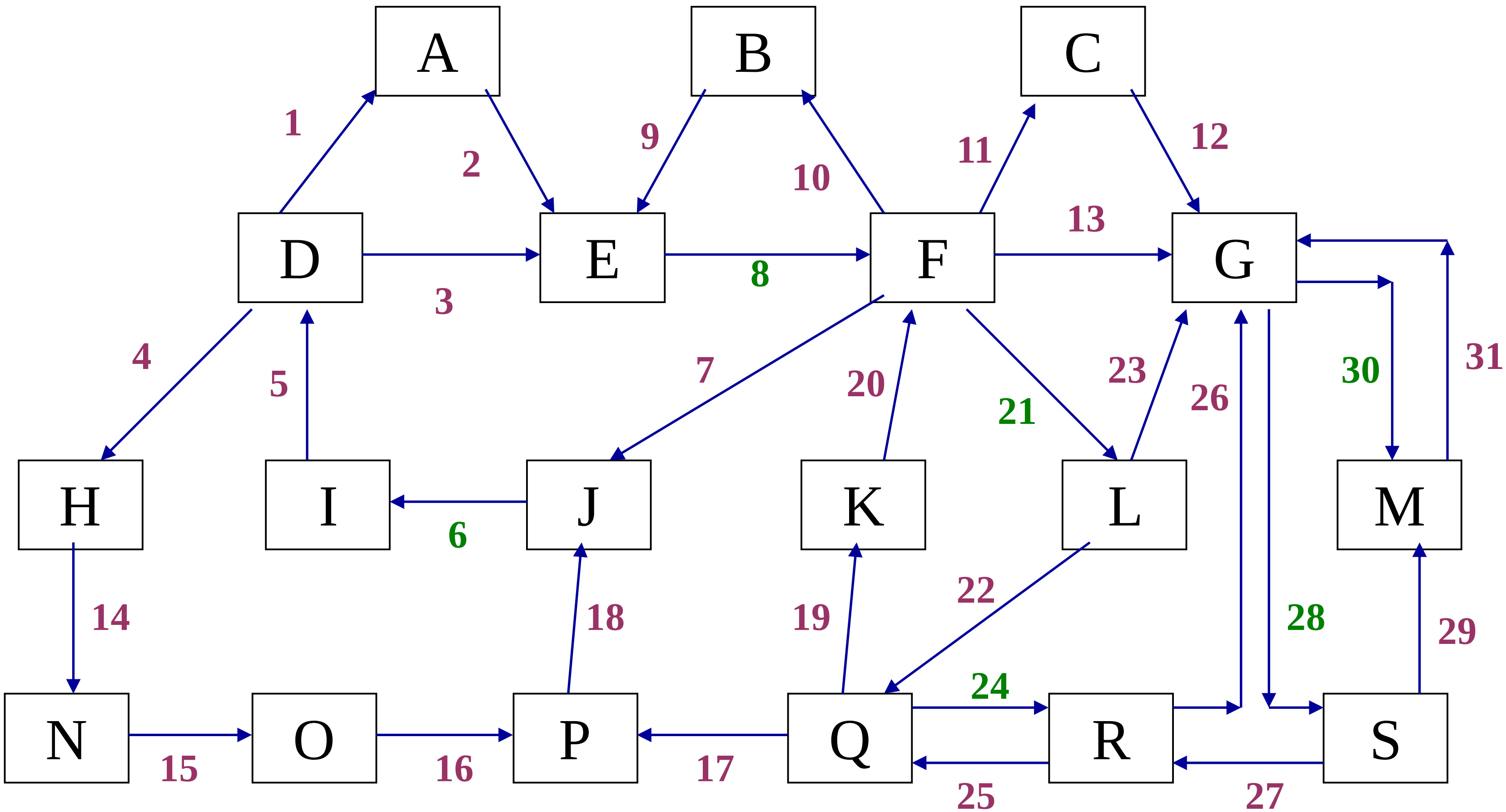
Flowsheet decomposition & Calculation sequence

Nodes	Precursers	Precursers (1)	Self-loop pairs	Precursers (2)	Precursers (3)	Precursers (4)	Precursers (5&6)
1	5						
2	1						
3	5						
4	5						
5	6						
6	7, 18	7, 18	(1)	7, 18	7, 18	7, 18	8, 6 **Cut 5**
7	8, 20	8, 19		8, 19	8, 21	8, 21	8
8	2, 3,9	6, 10	(2)	6, 10	6, 10	6, 10	6, 8 **Cut 6**
9	10						
10	8, 20	8, 19	(2)	8, 19	8, 21	8, 21	8
11	8, 20	8, 19		8, 19	8, 21	8, 21	8
12	11						
13	8, 20	8, 19		8, 19	8, 21	8, 21	8
14	4						
15	14						
16	15						
17	22, 25	21, 25		21, 25	21		
18	16, 17	6, 17	(1)	6, 17	6, 21	6, 21	6
19	22, 25	21, 25	(3)	21, 25	21		
20	19						
21	8, 20	8, 19		8, 19	8, 21	8, 21 **Cut4**	C
22	21						
23	21						
24	22, 25	21, 25	(4)	21, 25	21, 24 **Cut3**	C	C
25	24, 27	24, 28	(4)	24			
26	24, 27	24, 28	(5)	24			
27	28						
28	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(5), (6) **cut 1**	C	C	C	C
29	28						
30	12, 13, 23, 26, 31	11, 13, 21, 26, 31	(6), (7)	11, 13, 21, 26, 30	11, 13, 21, 30**Cut2**	C	C
31	29, 30	28, 30	(6)	30			

Cut 4: 21; Cuts 5 & 6: 6 & 8; List of tear streams: 6, 8, 21, 24, 28, 30

Flowsheet decomposition & Calculation sequence

Signal flowgraph based technique (another example)



List of tear streams: 6, 8, 21, 24, 28, 30

Ethanol Process: Case Study (from Textbook)

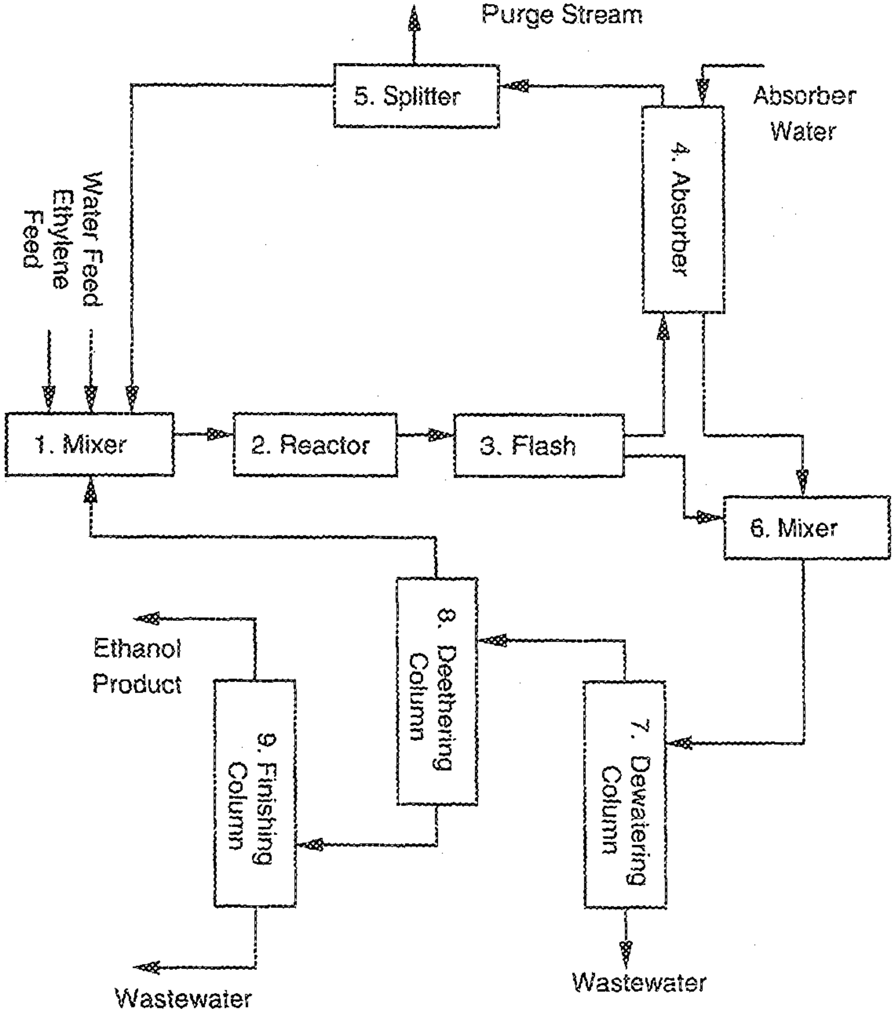
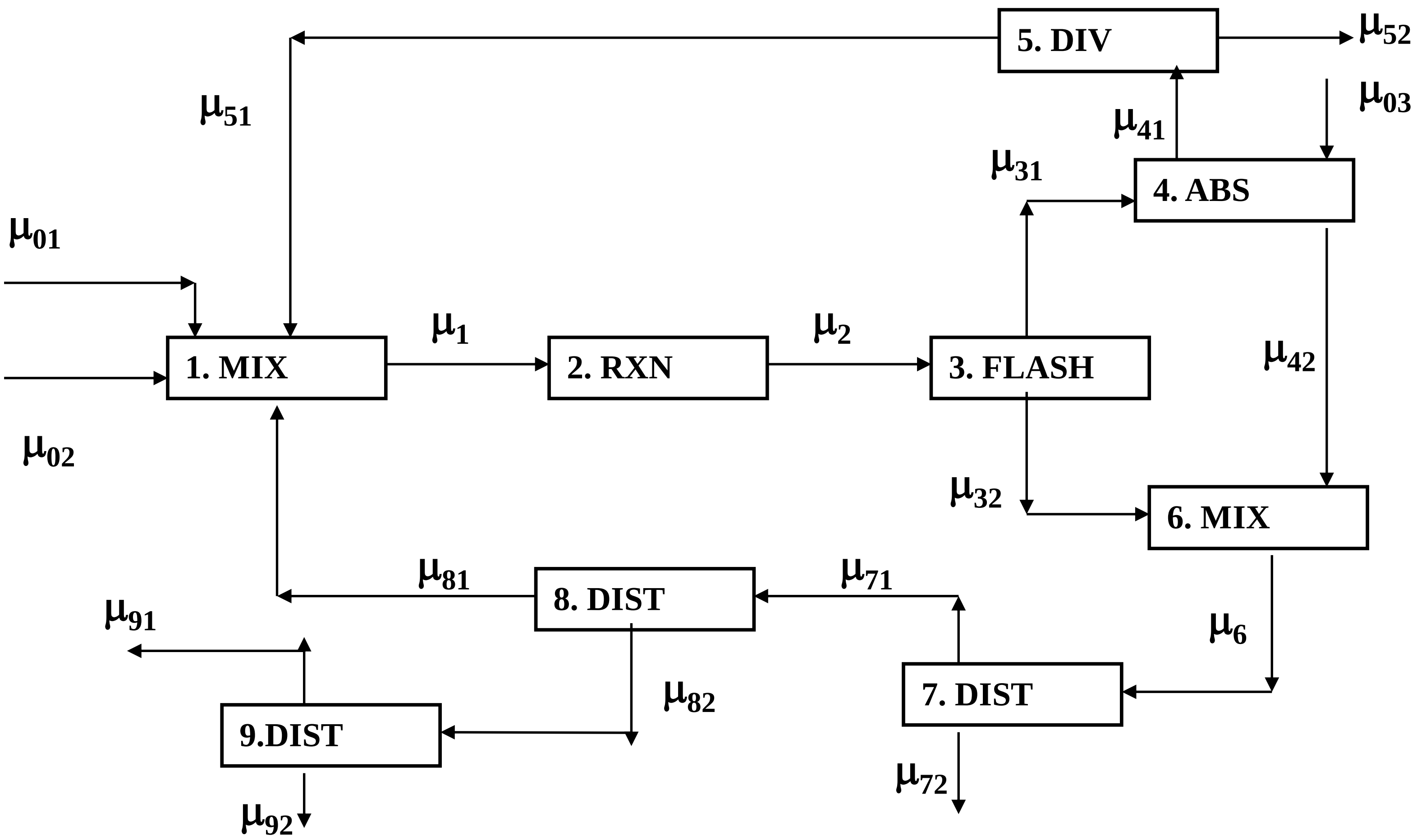


FIGURE 3.1 Ethanol flowsheet.

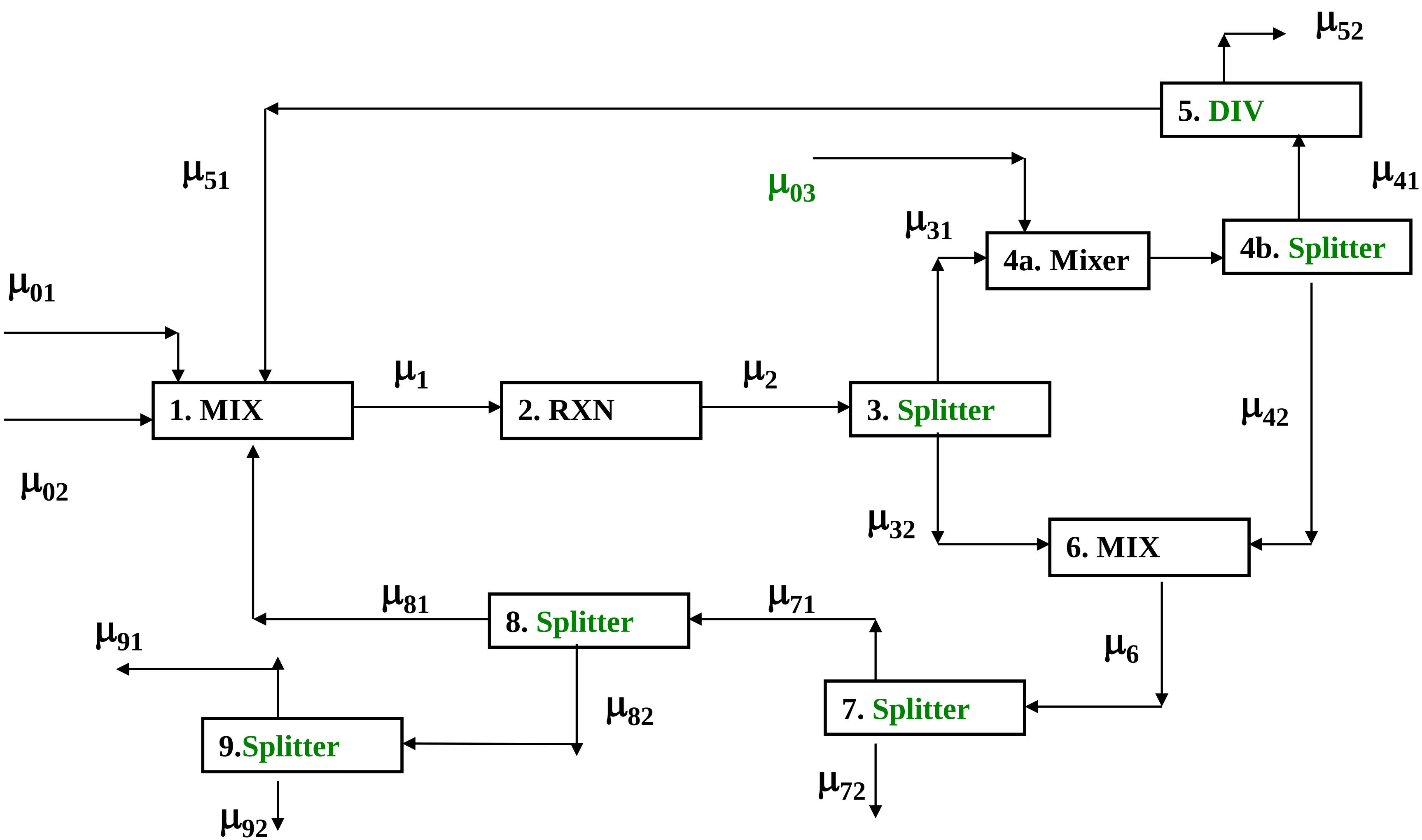
In order to perform mass balance (MB) what do we need?

1. Models for each unit operation?
2. Identify which variables need to be specified?
3. Derive solution strategy
4. Solve model equations (simulation) – 4.1 specify variables; 4.2 solve equationa
5. Verify if design objectives are satisfied

Start: Redraw flowsheet for MB-model - original flowsheet

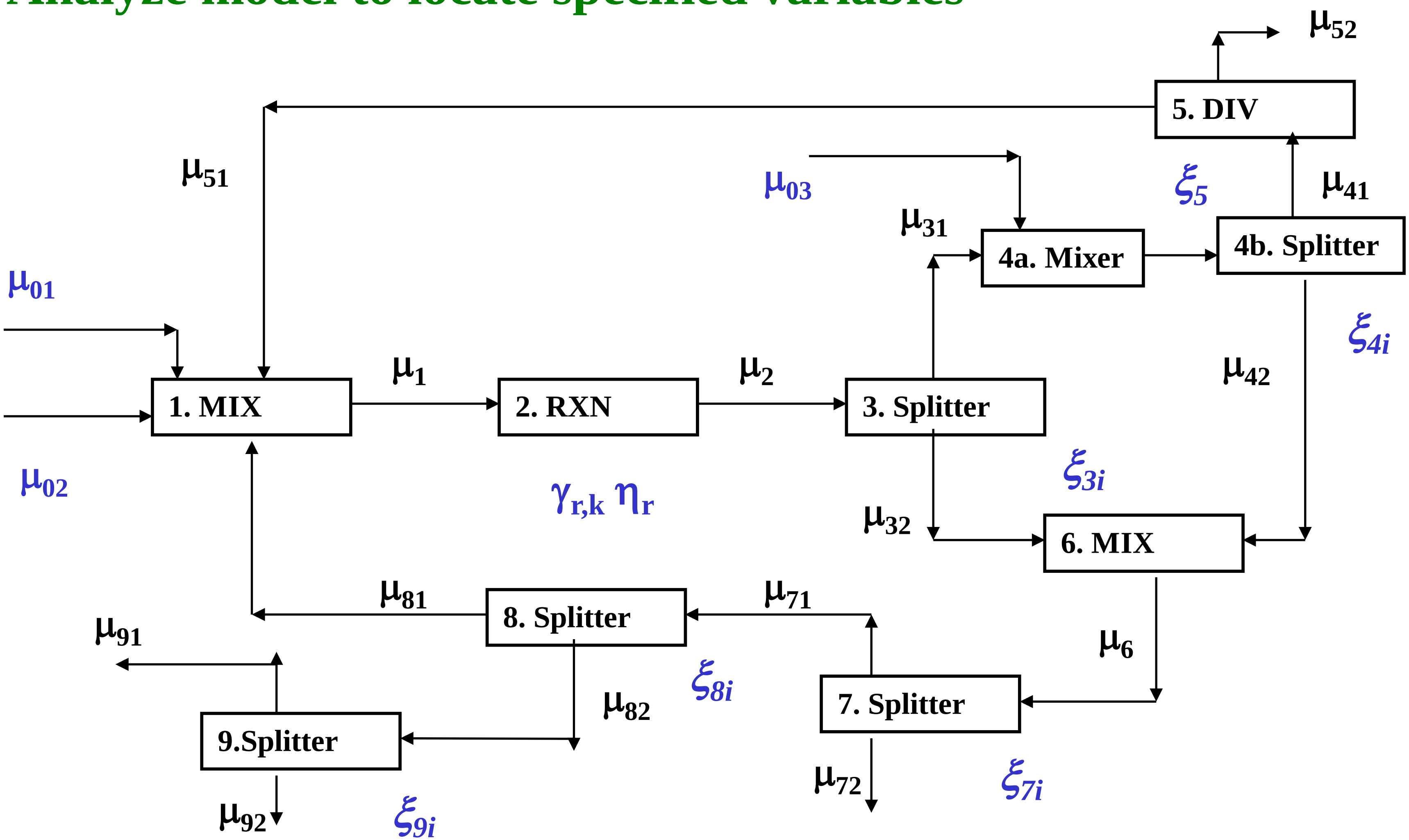


Start: Redraw flowsheet for MB-model: Redrawn flowsheet



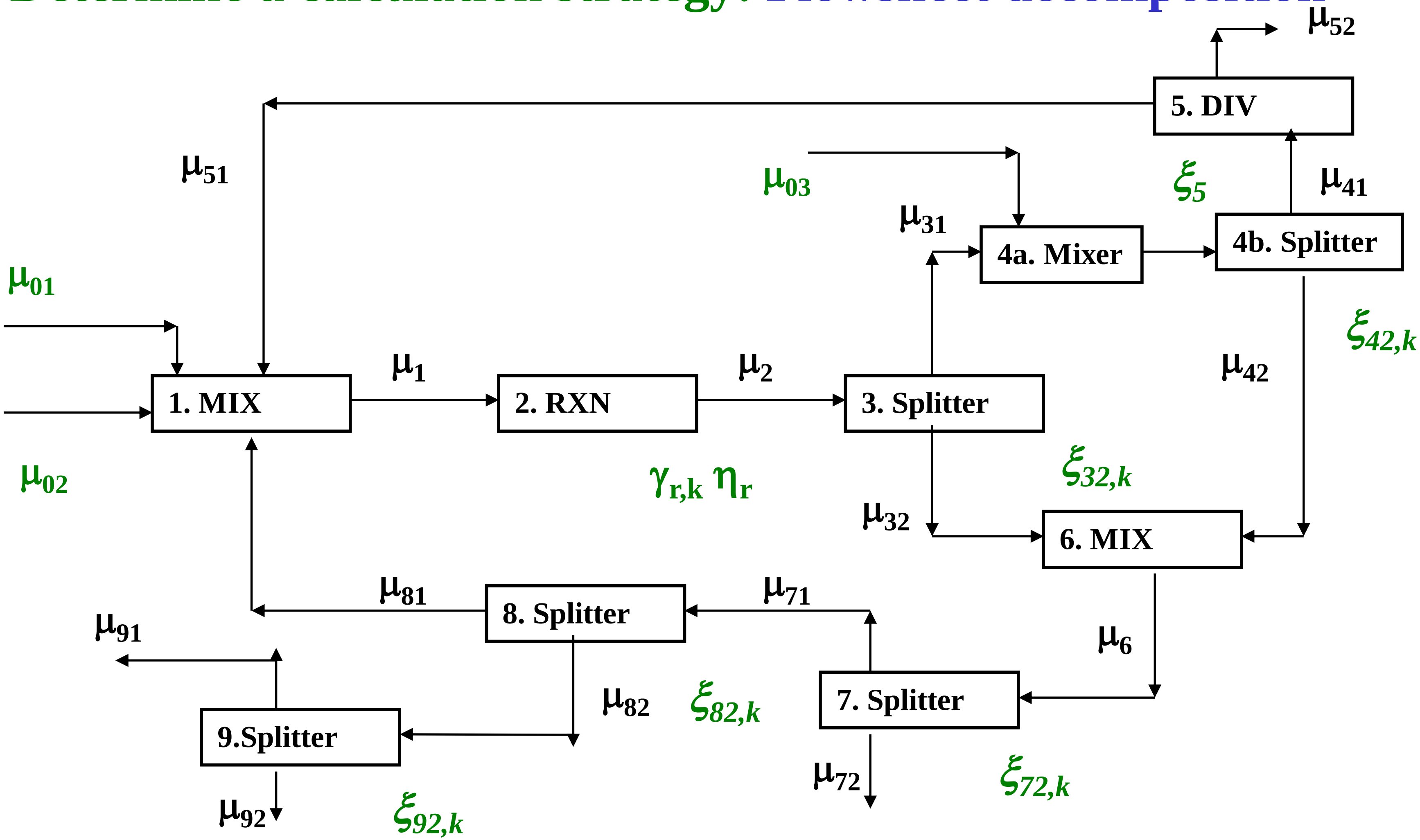
Use only mixers, reactors (conversion reactor), dividers (splitters) and splitters (stream calculators)!

2. Analyze model to locate specified variables



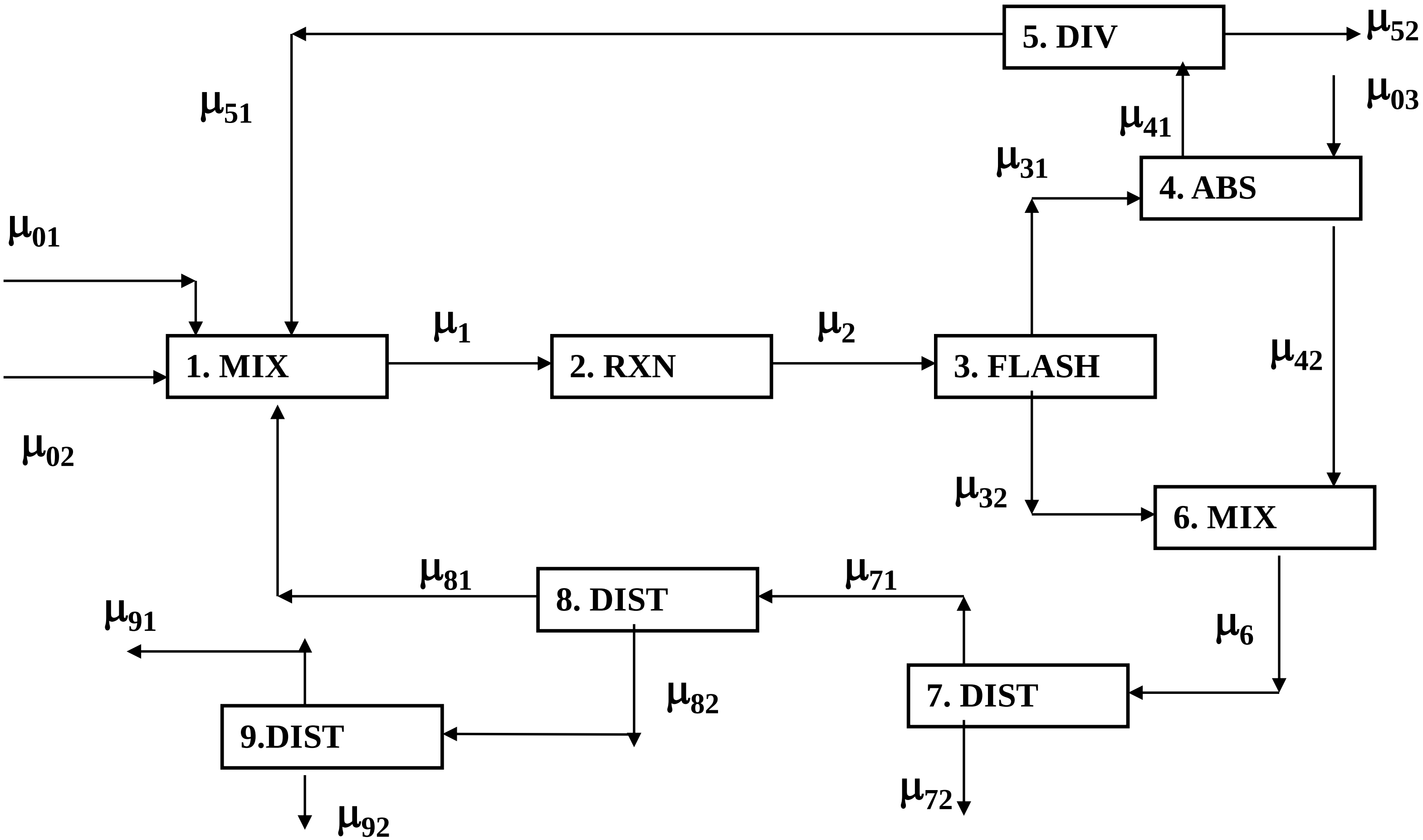
If all the variables marked in blue are known (decisions), then all other variables representing the flowhseet (MB-model) can be calculated!

3. Determine a calculation strategy: Flowsheet decomposition

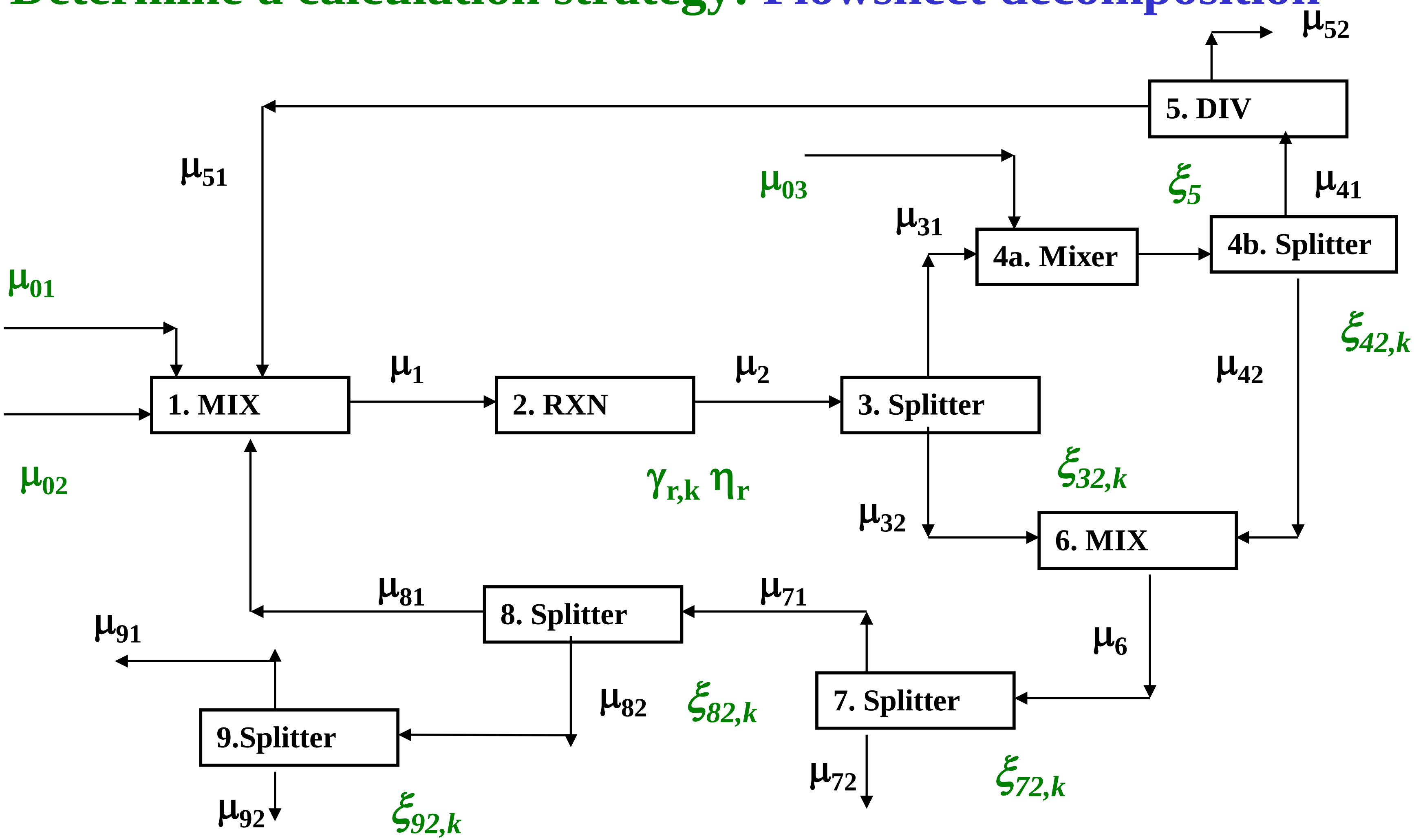


How should we solve the MB-model equations? How should we set-up the simulation problem for the simulator? Given, all variables marked in green, calculate all other variables

3. Process Flowsheet Decomposition & Tearing



3. Determine a calculation strategy: Flowsheet decomposition

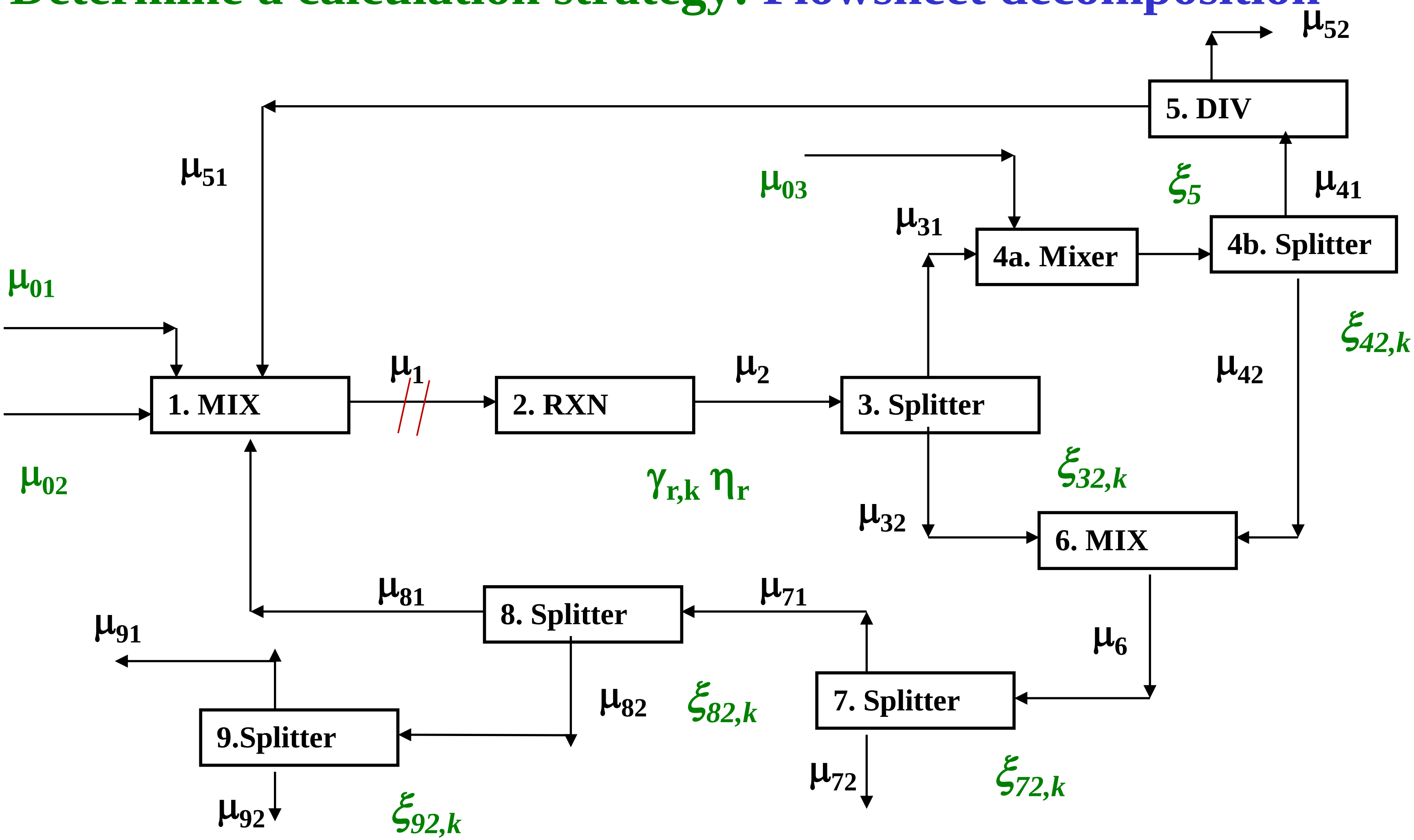


How many recyle loops?

How many tear streams?

Calculation order?

3. Determine a calculation strategy: Flowsheet decomposition



How many recyle loops? 3

How many tear streams? Stream 1

Calculation order? Guess μ_1, then solve units 2,3,4a,4b,5; 6,7,8,9,1, then check calculated μ_1

4.1 How to make the design decisions (mass balance)?

Process

Feed streams: raw material, solvents, process fluids

Equipment

Equipment parameters

- Reactor (conversion, reaction stoichiometry)
- Stream calculators (compound recoveries)
- Divider-purge (divide factor)

Others

Absorber, solvent-based distillation, ...

- Solvent, solubility

Membrane based operation

- membrane (permeability)

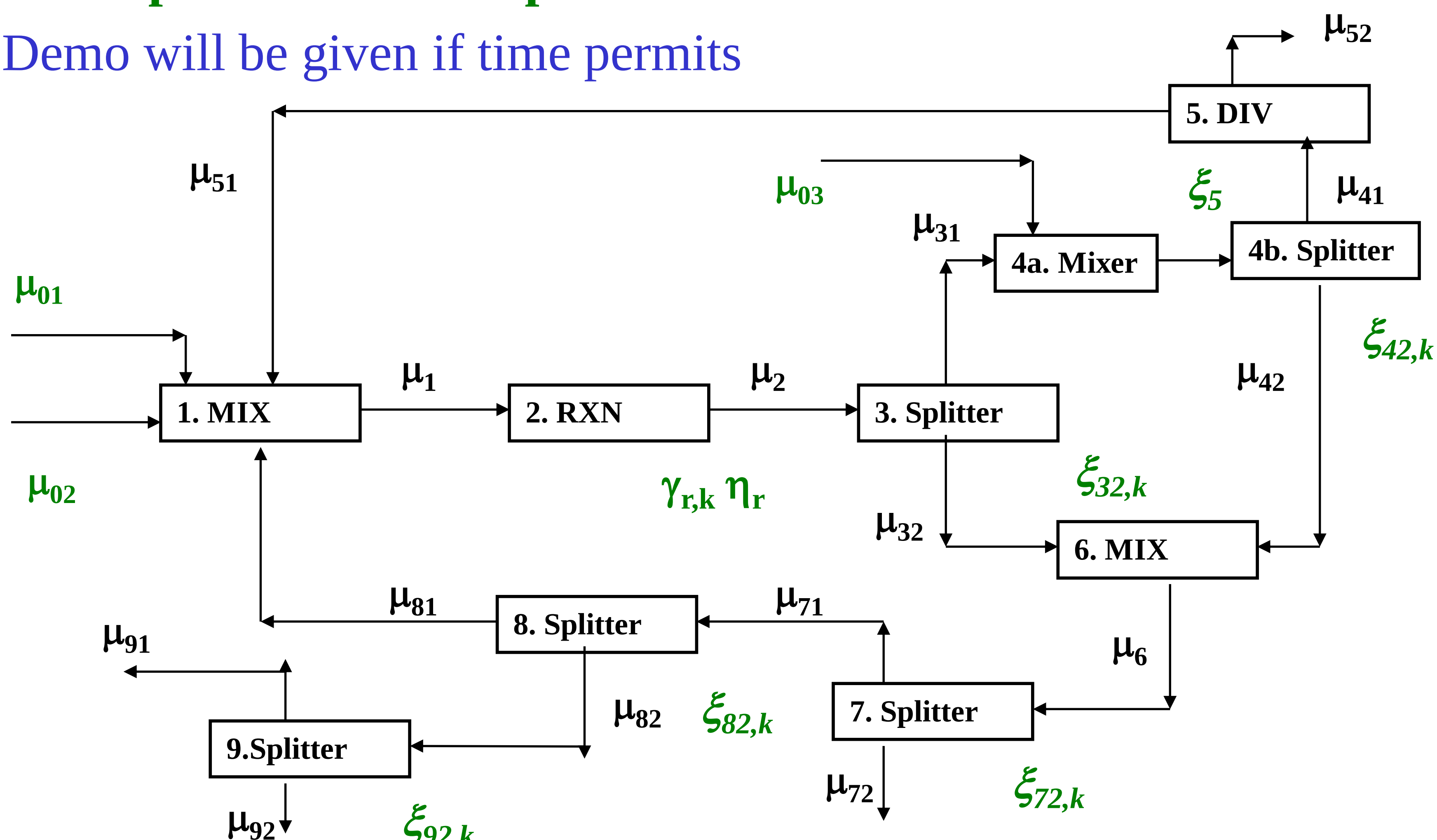
4.1 Specified Variables for Ethylene to Ethanol Process Mass Balance

	ξ_{Flash}	ξ_{Abs}	$\xi_{Split} = \beta_D$	$\xi_{Dist\text{-}1}$	$\xi_{Dist\text{-}2}$	$\xi_{Dist\text{-}3}$	$\xi_{Dist\text{-}4}$	$\xi_{Dist\text{-}5}$
Ethylene	0.95	1	0.995	1	1	1	-	-
Propylene	0.9	1	0.995	1	1	1	-	-
Methane	1.0	1	0.995	1	1	1	-	-
Ethanol	0.15	0.01	0.995	1	0	1	0.99	1
Isopropanol (IPA)	0.0	0.0	0.995	1	0	0	-	-
Water	0.0	0.0	0.995	0.1	0	0.33	0	1
Diethyl-ether (DEE)	0.5	0.01	0.995	1	1	1	-	-
Ethylene Glycol (EG)	0.0	0	0.995	0	0	0	0	0

Note: Same values of $\xi_{Split} = \beta_D$ for all components indicate a stream-divider (splitter)

4.2 Set-up the simulation problem in Pro-II or ICAS or EXCEL

Demo will be given if time permits

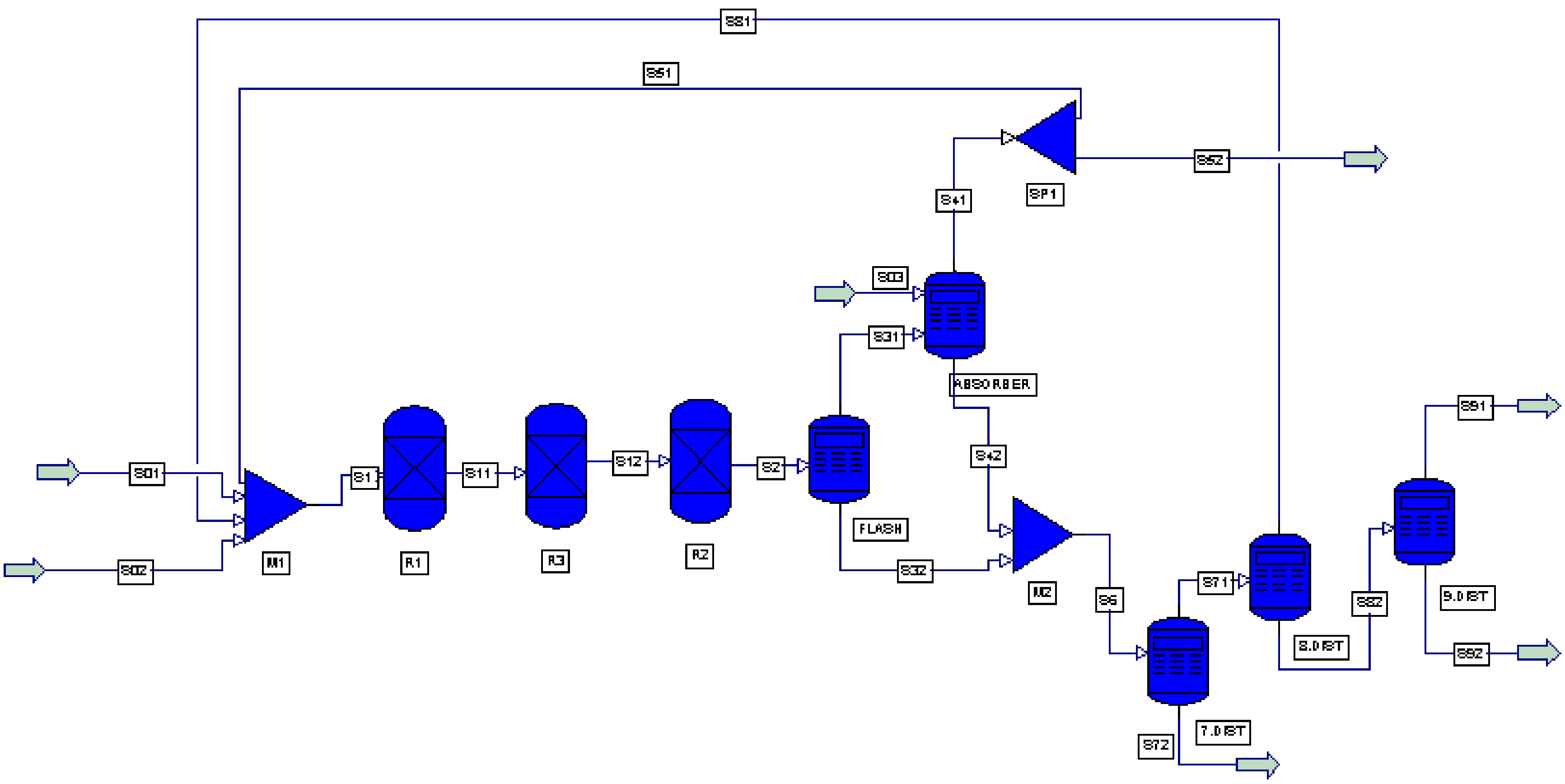


How many recyle loops? 3

How many tear streams? Stream 1

Calculation order? Guess μ_1, then solve units 2,3,4a,4b,5; 6,7,8,9,1, then check calculated μ_1

4.2 Mass balances for Ethanol Process Flowsheet - PROII



4.2 Mass balances for Ethanol Process Flowsheet - EXCEL

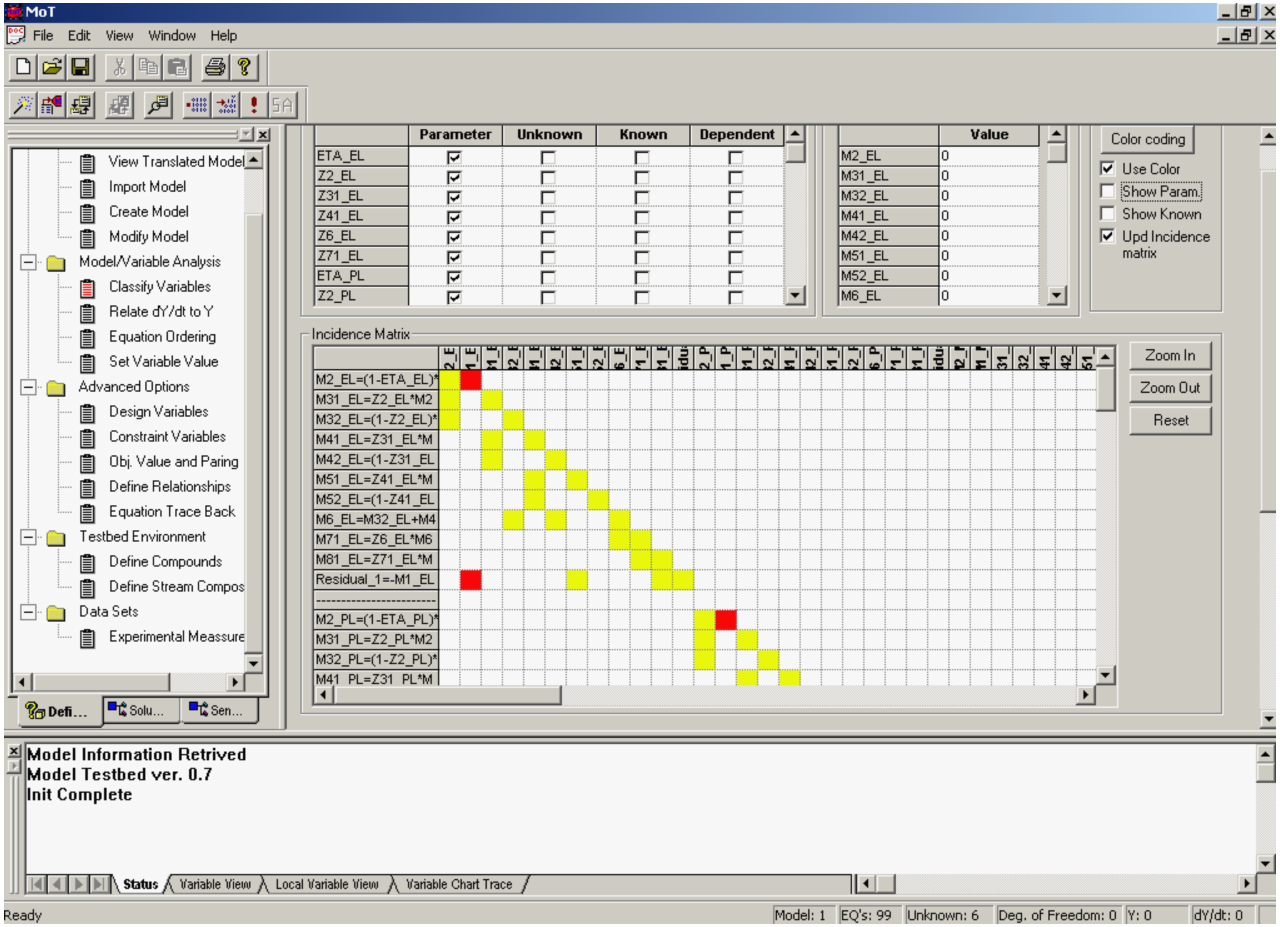
Microsoft Excel - exmple3.xls

	A	C	D	E	F	H	J	K	L	M	N	O	P	Q	
1		splitfactor of unit													
2	Componen	1	2	3	4	5	6	7	8	9	of azeotrope				
3	M	1		0.996	1	0.995	1	1	1	1	0.995	EA =	0.854		
4	EL	1		0.985	0.979	0.995	1	1	1	1		W =	0.146		
5	PL	1		0.932	0.901	0.995	1	1	1	1			1		
6	DEE	1		0.5	0.24	0.995	1	1	0.995	1					DE
7	EA	1		0.121	0.01	0.995	1	0.995	0.005	0.999					E
8	IPA	1		0.083	6.50E-03	0.995	1	0.96	0	0.058236					IP
9	W	1		0.054	1.90E-03	0.995	1	0.1	0	0.21326					W
10															
11		Stream													
12	Componen	m01	m02	m03	m1	m2	m31	m32	m41	m42	m51	m52	m6	m71	m7
13	M	1	0	0	200.8032129	200.8032129	200	0.803213	200	0	199	1	0.803213	0.803213	
14	EL	96	0	0	1288.866287	1198.645647	1180.666	17.97968	1155.871977	24.79399	1150.093	5.77936	42.77367	42.77367	
15	PL	3	0	0	268.5941128	266.713954	248.5774	18.13655	223.968242	24.60916	222.8484	1.119841	42.74571	42.74571	
16	DEE	0	0	0	2.407445728	2.419543445	1.209772	1.209772	0.290345213	0.919427	0.288893	0.001452	2.129198	2.129198	
17	EA	0	0	0	0.560384936	90.78102505	10.9845	79.79652	0.10984504	10.87466	0.109296	0.000549	90.67118	90.21782	0
18	IPA	0	0	0	0.001009816	1.881168606	0.156137	1.725032	0.00101489	0.155122	0.00101	5.07E-06	1.880154	1.804948	0
19	W	0	771.797	37.747	773.3197724	681.2189735	36.78582	644.4331	0.069893067	74.46293	0.069544	0.000349	718.8961	71.88961	6
20	Total	100	771.797	37.747	2534.552226	2442.463525	1678.38	764.0839	1580.311318	135.8153	1572.41	7.901557	899.8992	252.3642	
21															
22															
23		Reactor													
24	CONVERS	1EL+1W=EA		γ1 =	0.07										
25	CONVERS	PL+W=IPA		γ2 =	0.007										
26	EQUILIBRI	2EA==DEE+W		K =	0.2	0.2									

reaction1

4.2 Mass balances for Ethanol Process Flowsheet - MoT

```
# Linear Mass Balance Algorithm:

# balance for Ethylene (EL)

# Across 2.RXN
M2_EL = (1-ETA_EL)*M1_EL

# Across 3.FLASH
M31_EL = Z2_EL*M2_EL
M32_EL = (1-Z2_EL)*M2_EL

# Across 4.ABS
M41_EL = Z31_EL*M31_EL
M42_EL = (1-Z31_EL)*M31_EL

# Across 5.SPL
M51_EL = Z41_EL*M41_EL
M52_EL = (1-Z41_EL)*M41_EL

# Across 6.MIX
M6_EL = M32_EL + M42_EL

# Across 7.DIST
M71_EL = Z6_EL*M6_EL

# Across 8.DIST
M81_EL = Z71_EL*M71_EL
```



....

6. Verify if flowsheet design is OK

Check if conservation of mass is satsified? If yes, check the following:

The component flow-rates of outlet streams – do they satisfy the specifications?

Check the solvent loss (if solvents are used)

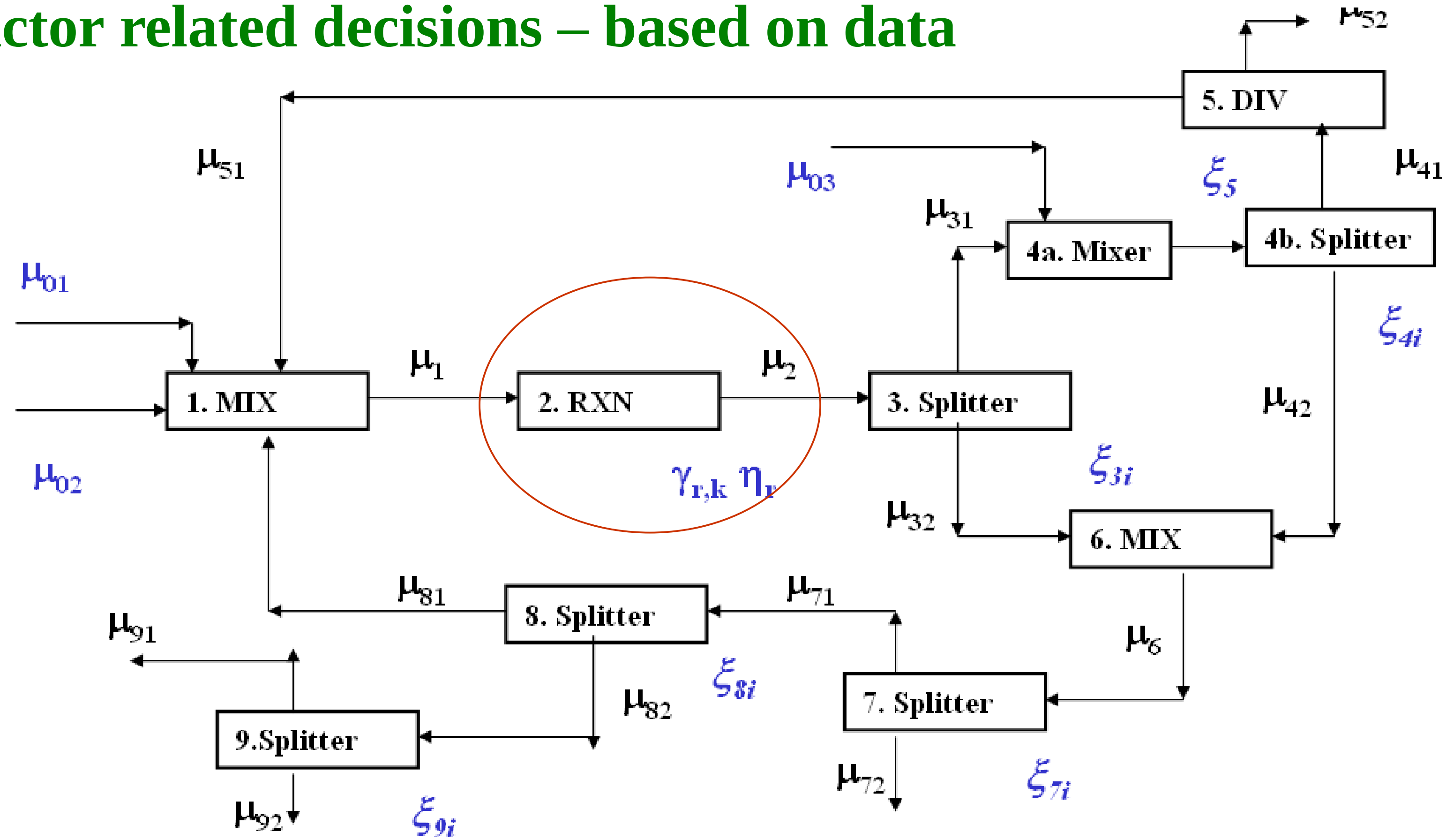
Check the emission for non-product outlet streams – are they likely to cause enviornmental problems?

....

If no, check the model and/or model specifications (simulator specifications)

Additional material on finding values (design decisions) for specified variables

Reactor related decisions – based on data

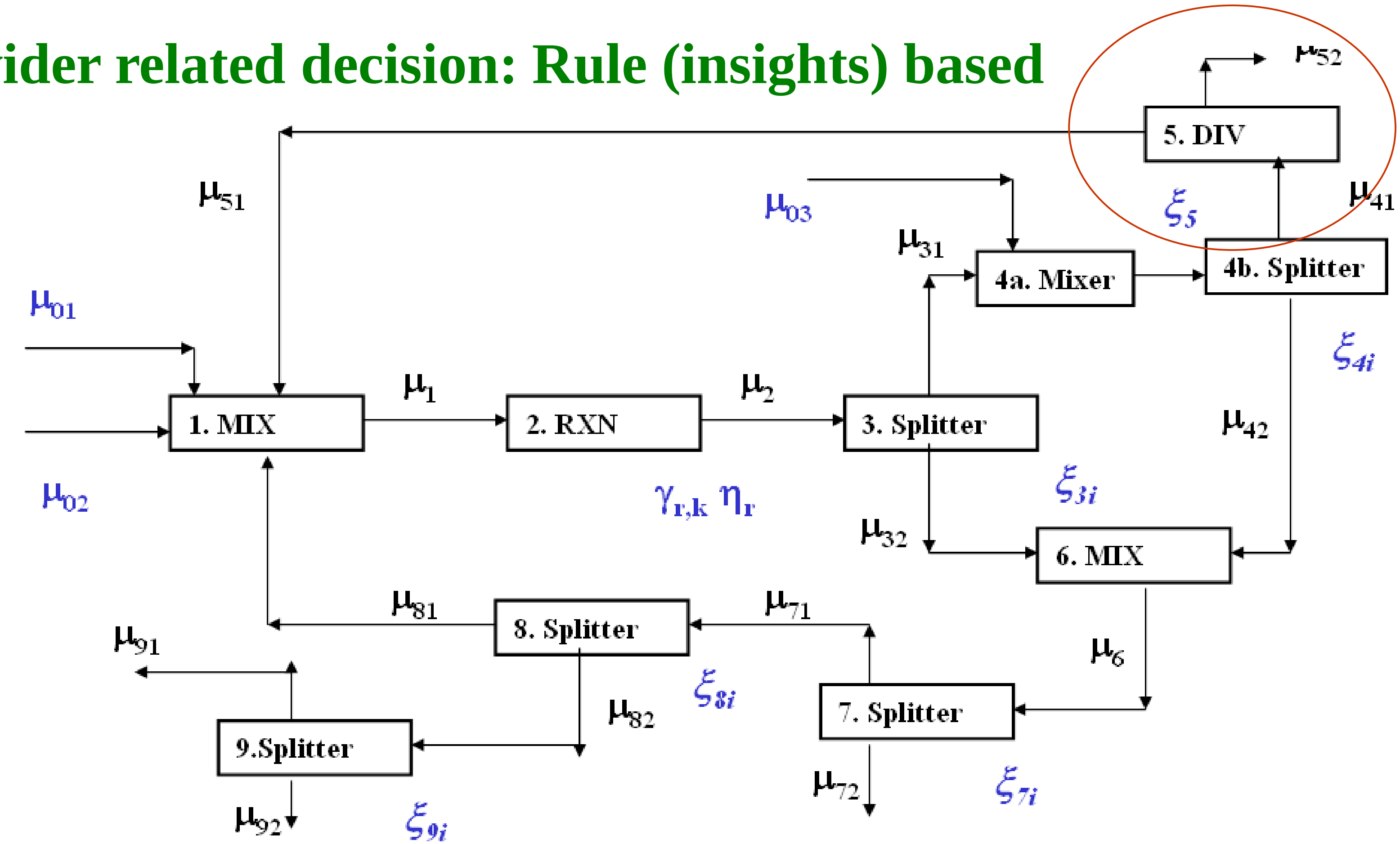


$EL + W \rightarrow EA$ 7% conversion/pass EL to EA (η_1)

$PL + W \rightarrow EA$ 0.7% conversion/pass PL to IPA (η_2)

$2EA \leftrightarrow DEE + W$ Equilibrium controlled, K(T, P) = 0.2

Divider related decision: Rule (insights) based



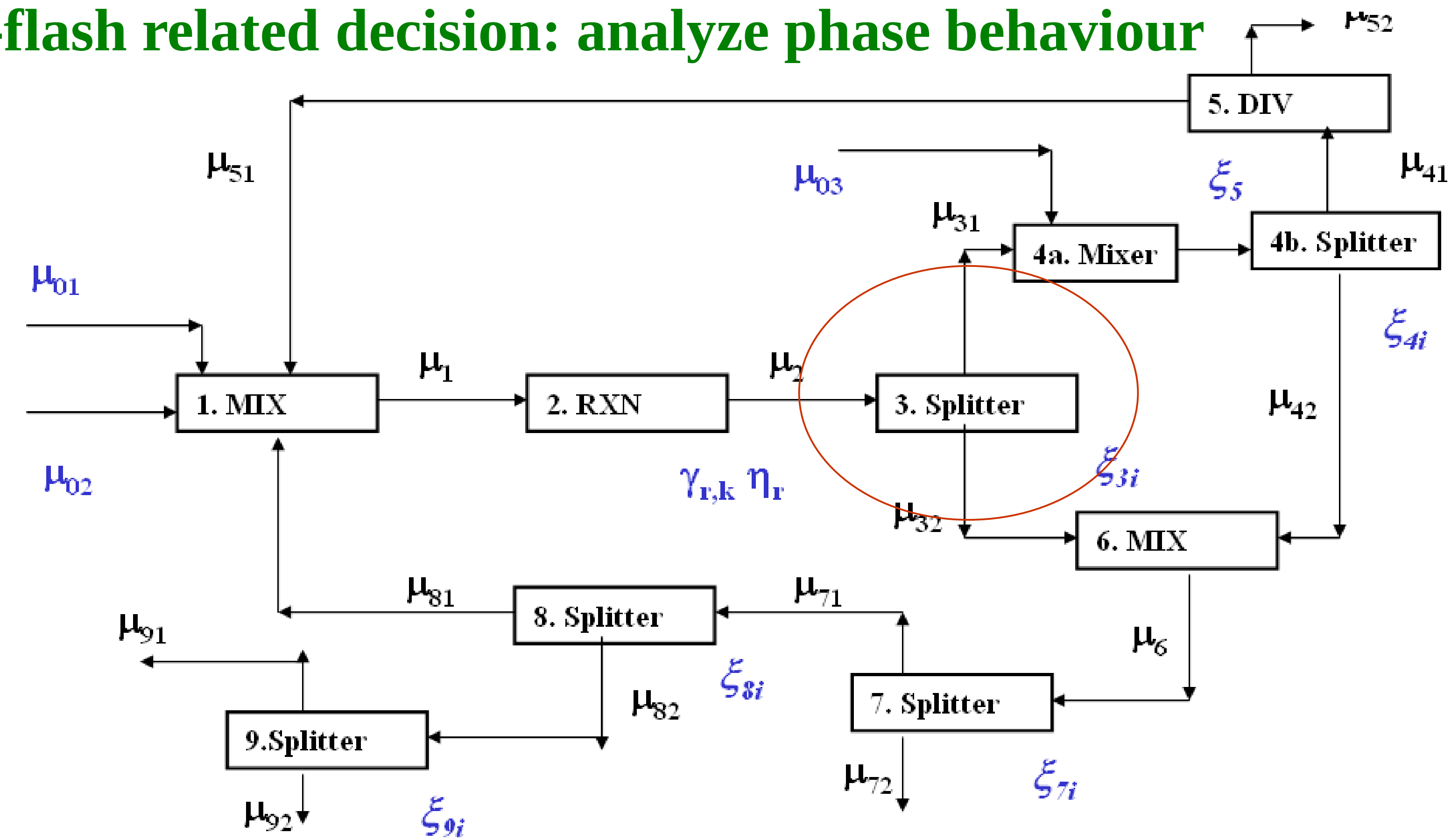
Divider Model

$\mu_{51} = (1 - \xi_5)\ \mu_{41}$

$\mu_{52} = \xi_5\ \mu_{41}$

- **Value of ξ_5 effects the recycle flow μ_{51}**
- **Select a value between 0 – 0.1 (as an initial estimate**

PT-flash related decision: analyze phase behaviour



Component Splitter model (for component k)

$\mu^k_{31} = \xi_{3k}\, \mu^k_2$; vapor (or light product)

$\mu^k_{32} = (1 - \xi_{3k})\mu^k_2$; liquid (or heavy product)

- **Use the method given in the book**
- **Perform a quick (single –stage) flash simulation**

Case 1: ξ_n and P (or T) Fixed Hand calculation

a. For a specified ξ_n and P (or T), guess T (or P).

b. Calculate K_k, $\alpha_{k/n}$ at specified T.

c. Evaluate $\xi_k = \alpha_{k/n}\,\xi_n/(1 + (\alpha_{k/n} - 1)\xi_n)$ for each component k.

d. Reconstruct a mass balance and calculate mole fractions.

$$v_k = \xi_k f_k \qquad y_k = v_k/\sum v_i$$
$$l_k = (1 - \xi_k) f_k \qquad x_k = l_k/\sum l_i$$

e. For T fixed, $P = \dfrac{\bar{\alpha}}{\alpha_{k/n}} P_k^0(T)$.

For P fixed, solve for T from $P_k^0(T) = \alpha_{k/n} P/\alpha$.

Case 2: T and P Fixed Using software

a. For a specified T and P, pick a key component n and guess ξ_n.
Follow steps b, c, and d of algorithm for Case 1.

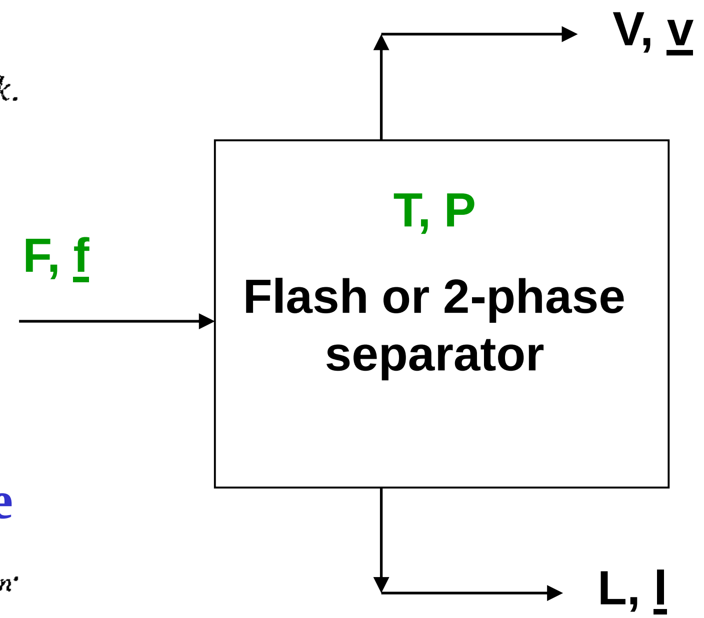
e. If the bubble point equation is satisfied: $\alpha = P\alpha_{k/n}/P_k^0$, stop. Otherwise, reguess ξ_n, and go to step c. (Simple iterative methods, such as the secant algorithm in Chapter 8, can be used to obtain convergence for ξ_n.)

Case 3: ϕ and P (or T) Fixed

a. For a specified $\phi = V/F$ and P (or T)

b. Guess T (or P), calculate $\alpha_{k/n}$, K_k and define $\theta = K_n\,\phi/(1 - \phi) = v_n/l_n$
Define $\xi_n = \theta/(1 + \theta)$.
Then follow steps c and d of the previous algorithm.

e. If the bubble point equation is satisfied: $\alpha = P\alpha_{k/n}/P_k^0$, stop. Otherwise, reguess T (or P), and go to step b. (Simple iterative methods, such as the secant algorithm can be used to obtain convergence for ξ_n.)



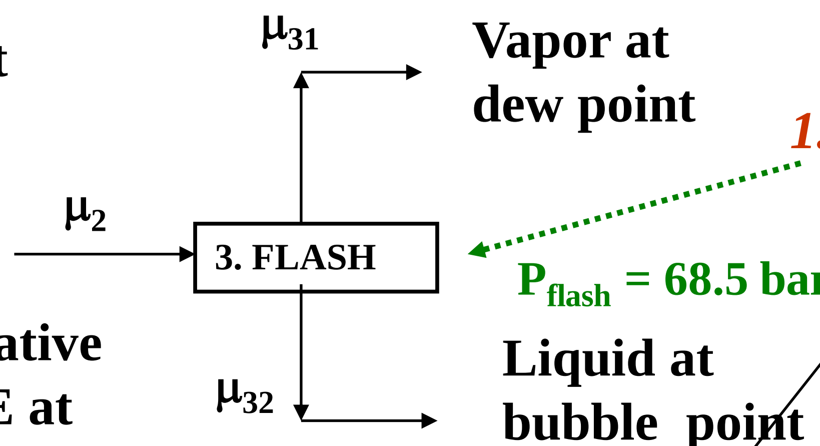
Specify F, f and any two of T, P, V/F, v_k/f_k

See example 3.2

PT-flash related decisions: short-cut calculations

2. **Calculate by using a vapor pressure model at specified T**

1. Assume/decide

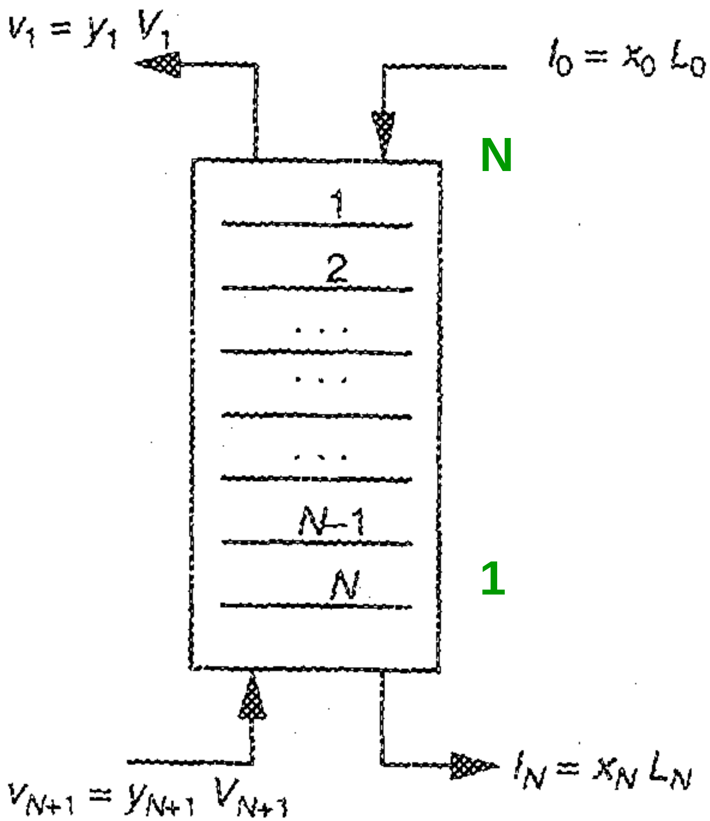


3. **Calculate by relative volatility w.r.t DEE at specified T = P^0_k/P^0_{DEE}**

	M	*EL*	*PL*	*DEE*	*EA*	*IPA*	*W*
$P^0(T=310\ K)$	*2.1×10^5*	*5.5×10^4*	*11360*	*824*	*114.5*	*75.1*	*47.1*
$\alpha_{k/DEE}$	*256.1*	*67.3*	*13.8*	*1.0*	*0.138*	*0.091*	*0.057*
ξ_{3K}	*0.996*	*0.985*	*0.932*	*0.5*	*0.121*	*0.083*	*0.054*

4. **Calculate ξ_{3K} using the formula given in the book** ***(see Eq. on slide 44)***

Absorber related decisions: short-cut calculations



Absorber and Stripper Preliminary Calculations

Mass balance model for absorber/stripper has 4 degrees of freedom: P, T, key component recovery and liquid rate

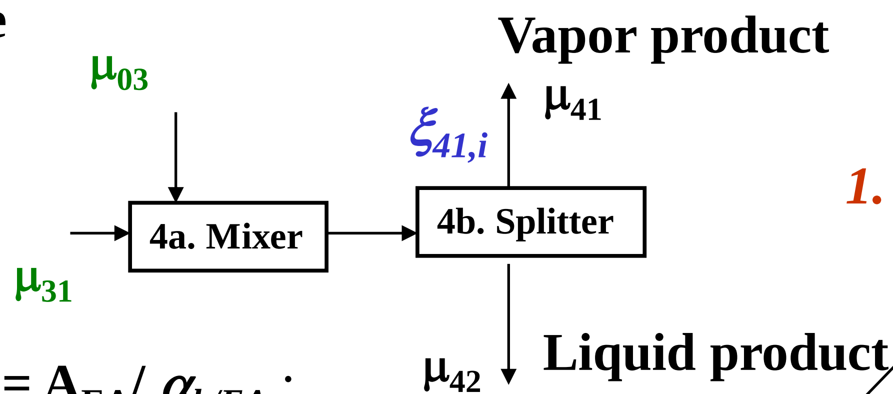
That is, the designer needs to select values for the 4 variables and values of all other variables can be calculated if the component separation (split) factors are known

$\xi_{A1,k} = v_{1,k}/v_{N+1,k} = 1/\beta_{N-1,k} = 1 - \xi_{A2,k}$ **; top product**

$\xi_{A2,k} = l_{N,k}/v_{N+1,k} = 1 - (1/\beta_{N,k}) = 1 - \xi_{A1,k}$ **; bottom product**

Absorber related decisions: short-cut calculations

2. Calculate by relative volatility w.r.t EA at specified T = P^0_k/P^0_{DEE}



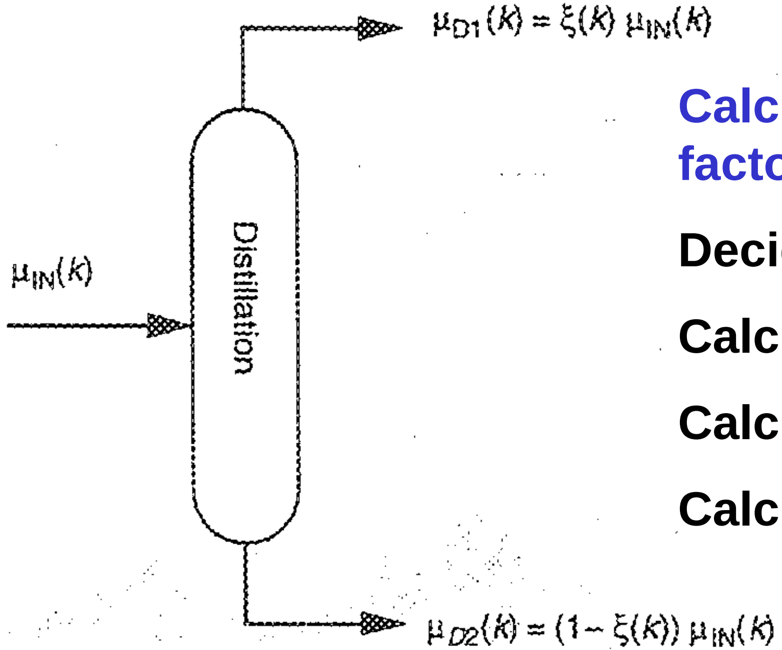
1. Assume/decide

3. Calculate $A_k = A_{EA}/\ \alpha_{k/EA}$;
then $\beta_{N,k}$ & $\beta_{N-1,k}$ (see page 88)

	M	EL	PL	DEE	EA	IPA	W
$\alpha_{k/EA}$	1854	486.3	99.5	7.24	1.0	0.79	0.41
A_k	0.0054	0.021	0.101	1.38	10	12.66	24.4
$\beta_{N,k}$	1	1.021	1.11	4.17	98.92	153.2	529.1
$\beta_{N-1,k}$	1	1.021	1.10	2.30	9.79	12.02	21.6
$\xi_{42,k}$	0	0.021	0.099	0.760	0.99	0.993	0.998

4. Calculate $\xi_{42,k}$ using the formula given in the book (see slide 44)

Distillation related decisions: short-cut calculations



Calculation of component separation factors for distillation columns

Decide on values for $\zeta_k = d_k/f_k$

Calculate $\alpha_{lk/hk}$

Calculate N_m by Fenske Equation

Calculate $\xi_k = (\alpha_k)^{Nm}\,\zeta_{hk} / [1+(\alpha_k)^{Nm}]\zeta_{hk}$

Set N_m = 1 for flash

Component type	ξ_k
1. Lighter than light key	1, ($\alpha_{k/hk} > 1$, as $N_m \to \infty$, $\xi_k = 1$)
2. Light key	ξ_{lk} fixed (e.g., 0.99)
3. Distributed component	from equation for ξ_k
4. Heavy key	ξ_{hk} fixed (e.g., 0.01)
5. Heavier than heavy key	0, ($\alpha_{k/hk} < 1$, as $N_m \to \infty$, $\xi_k = 0$)

Distillation related decisions: rule (insights) based decisions

	M	EL	PL	DEE	EA	IPA	W	
ξ_k	1.0	1.0	1.0	1.0	0.995	0.96	0.1	7.dist

Recover 99.5% ethanol and remove 90% water

	M	EL	PL	DEE	EA	IPA	W	
ξ_k	1.0	1.0	1.0	0.995	0.005	0.00	0.00	8.dist

Recover 99.5% DEE plus gases at the top and recycle and 99.5% Ethanol at the bottom

---

Ethanol-water azeotrope at 85.4% EA & 14.6% W (mole percent)

Recover 99.5 % azeotrope, that is, $\xi_{az} = 0.995$ 9.dist

IPA in distillate is 0.1%