Chapter 2 – Data Extraction for Resource Conservation

Introduction

❑ Data extraction – **most crucial step** for any resource conservation activity

❑ Once the data is wrongly extracted, we might end up synthesising a sub-optimum resource conservation network (RCN).

❑ **Limiting data** needed for process sinks and sources:
   ✓ Quantity aspect – flowrate
   ✓ Quality aspects:
      ❖ Mass integration-based RCN – impurity concentration
      ❖ Property integration – linearised operator for property mixing rule

Segregation for material sources

Heuristic 1

Keep material sources segregated to maximise their recovery potential.

Ex 2.1 – Water minimisation in Acrylonitrile (AN) production
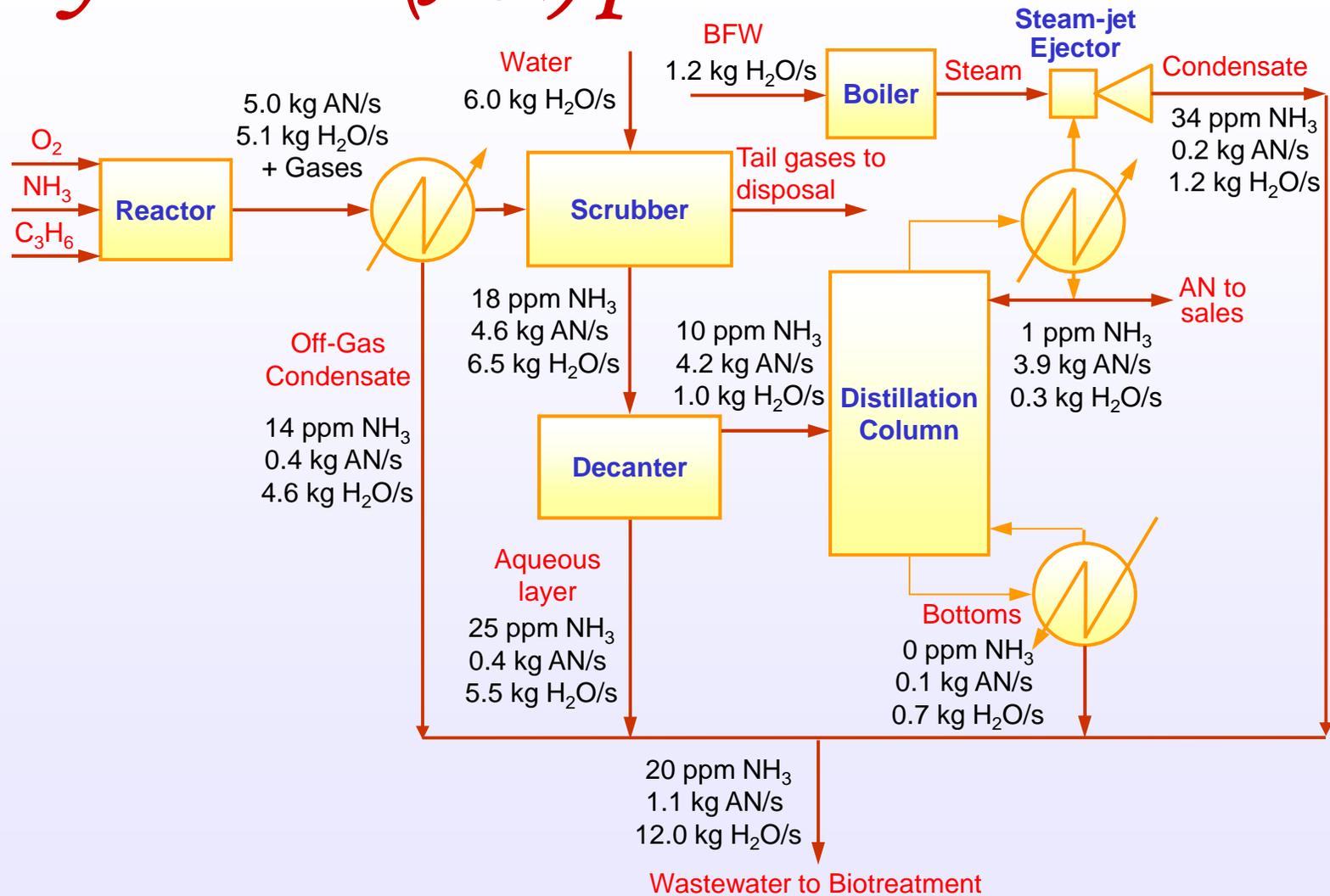
Ex 2.1 – Process description

❑ AN is produced in a fluidised-bed reactor (2 atm & 450ºC) via vapour-phase ammoxidation of propylene.

❑ The reaction is single-pass, with almost complete conversion of propylene, with following stoichiometry

$$C_3H_6 + NH_3 + 1.5O_2 \xrightarrow{\text{catalyst}} C_3H_3N + 3H_2O$$

❑ Effluent from the reactor is cooled and partially condensed. The off-gas from the condenser is sent to a scrubber for purification; while its condensate to the biotreatment facility.

Ex 2.1 – Process description

❑ Fresh water is used as the scrubbing agent in the scrubber, before the tail gas may be sent for disposal.

❑ The bottom product from the scrubber is sent to a decanter when it is separated into aqueous (sent to the biotreatment facility) & organic layers, which is fractionated in a mild vacuumed distillation column. The column is induced by a steam-jet ejector where steam condensate is produced (sent to biotreatment).

❑ Distillation column bottom also produces wastewater that is sent to the biotreatment facility.

❑ Due to increased customer demand, the plant authority is exploring opportunity to increase the plant overall AN throughput.

Ex 2.1 – Process description

❑ The stoichiometry equation reveals that water is a by-product for AN production ➔ **increased AN production leads to increased wastewater flowrate** to the biotretment facility, which is operated at full hydraulic capacity.

❑ Any increase of production capacity is only possible upon the debottlenecking of the biotreatment facility, either by:
  - ✓ reducing the total wastewater flowrate, or
  - ✓ installing another biotreatment unit (an expensive strategy).

❑ It is decided to approach the problem by reducing the total wastewater flowrate, by carrying out water recovery between its process sinks and sources.

❑ **Task: identify water sinks & sources** in order to carry out a water recovery scheme for the process.

❑ Note: **ammonia (NH_3) concentration** is the main concern for water recovery (i.e. the quality index for this case).

Ex 2.1 – Identification of sources
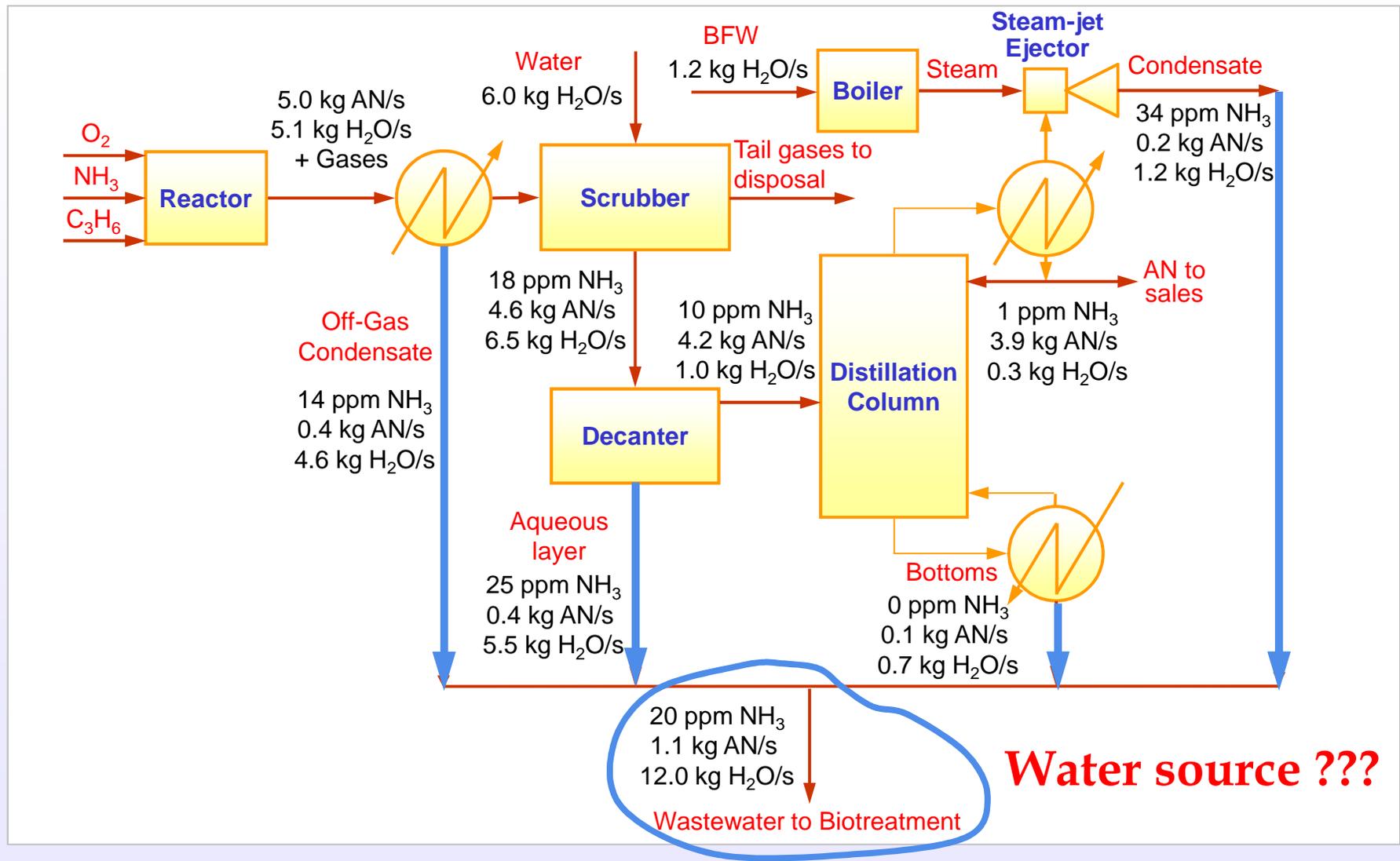
Ex 2.1 – Identification of sources

❑ Following **Heuristic 1**, the individual streams that contribute to the terminal wastewater stream are segregated as water sources for recovery:

- ✓ distillation bottom (0.1 kg/s; 0 ppm)
- ✓ off gas condensate (5.0 kg/s; 14 ppm)
- ✓ aqueous layer from the decanter (5.9 kg/s; 25 ppm)
- ✓ steam condensate from steam-jet ejector (1.4 kg/s; 34 ppm)

Heuristics 2 & 3

Minimise flowrate for a sink to reduce the overall fresh resource intake.

Maximise the inlet concentration for a sink to maximise material recovery.

Ex 2.2 – AN production
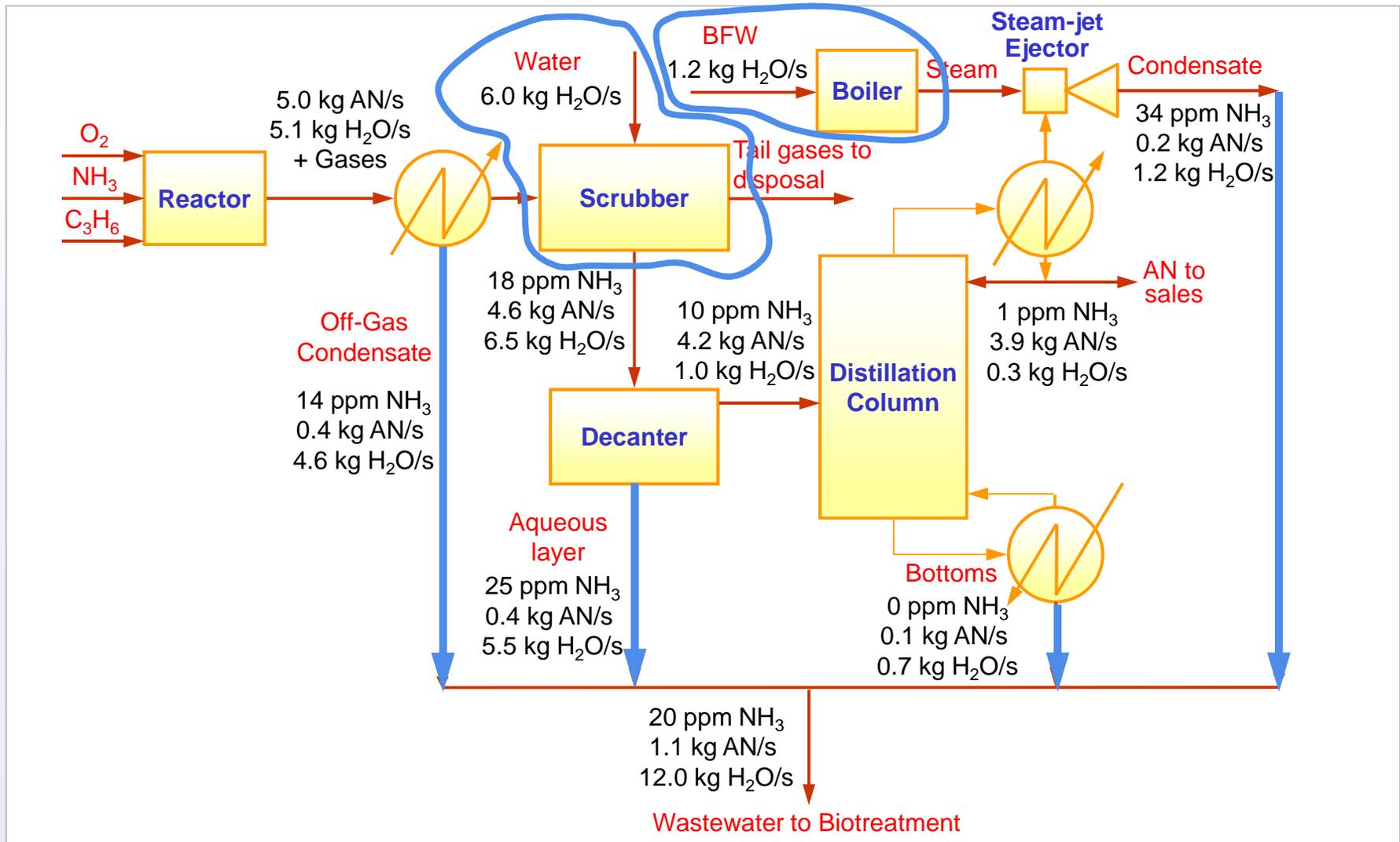
Ex 2.2 – technical constraints

i. **Scrubber**
   - ✓ **5.8 ≤ flowrate of wash feed (kg/s) ≤ 6.2**
   - ✓ **0.0 ≤ NH$_3$ content of wash feed (ppm) ≤ 10.0**

ii. Boiler feed water
   - ✓ **NH$_3$ content = 0.0 ppm**
   - ✓ AN content = 0.0 ppm

iii. Decanter
   - ✓ 10.6 ≤ feed flowrate (kg/s) ≤ 11.1

iv. Distillation column
   - ✓ 5.2 ≤ feed flowrate (kg/s) ≤ 5.7
   - ✓ 0.0 ≤ NH3 content of feed (ppm) ≤ 30.0
   - ✓ 80.0 ≤ AN content of feed (wt%) ≤ 100.0

Upper bound

Lower bound

Upper bound

Lower bound
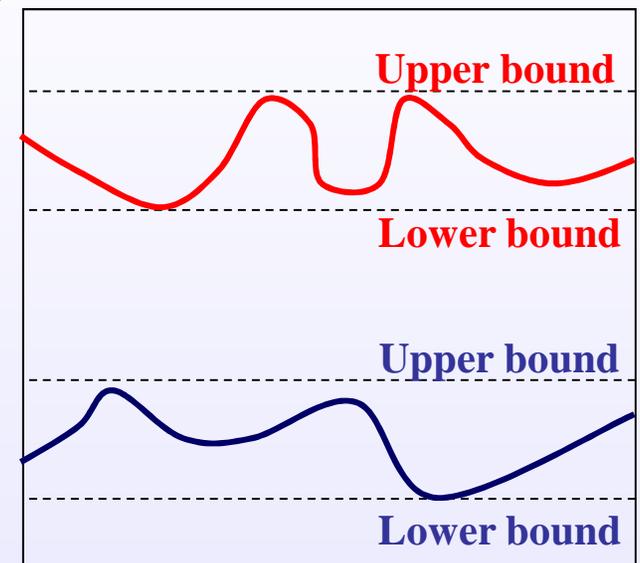
Ex 2.2 – Limiting water data

	Water sinks, SK_j	Flowrate	Concentration
j	Stream	F_{SKj} (kg/s)	C_{SKj} (ppm)
1	Boiler feed water (BFW)	1.2	0
2	Scrubber	5.8	10
	Water sources, SR_i	Flowrate	Concentration
i	Stream	F_{SRi} (kg/s)	C_{SRi} (ppm)
1	Distillation bottoms	0.8	0
2	Off-gas condensate	5.0	14
3	Aqueous layer	5.9	25
4	Ejector condensate	1.4	34

Refinery hydrogen recovery

❑ Typical hydrogen-consuming units are hydrotreating and hydrocracking processes.

Fresh H_2 makeup

Recycle

Purge

Amine unit

H_2S

Liquid hydrocarbon feed

Reactor

High pressure flash separator

Liquid product

Identification of H_2 sinks & sources

Recycle (F_R, C_R)

Fresh H_2 makeup (F_M, C_M)

Purge (F_P, C_P)

Hydrogen source (F_{SR}, C_{SR})

Hydrogen sink (F_{SK}, C_{SK})

Amine unit

H_2S

Liquid hydrocarbon feed

Reactor

High pressure flash separator

Liquid product
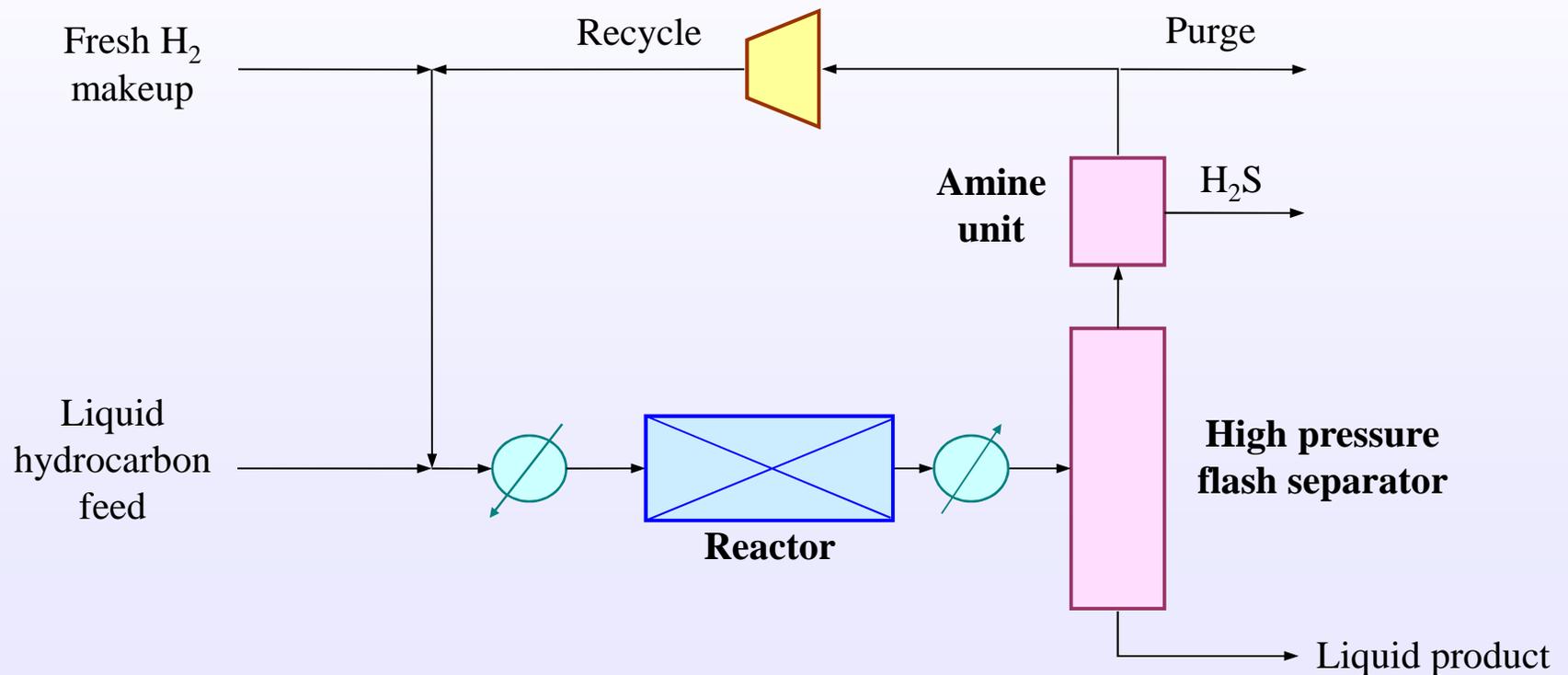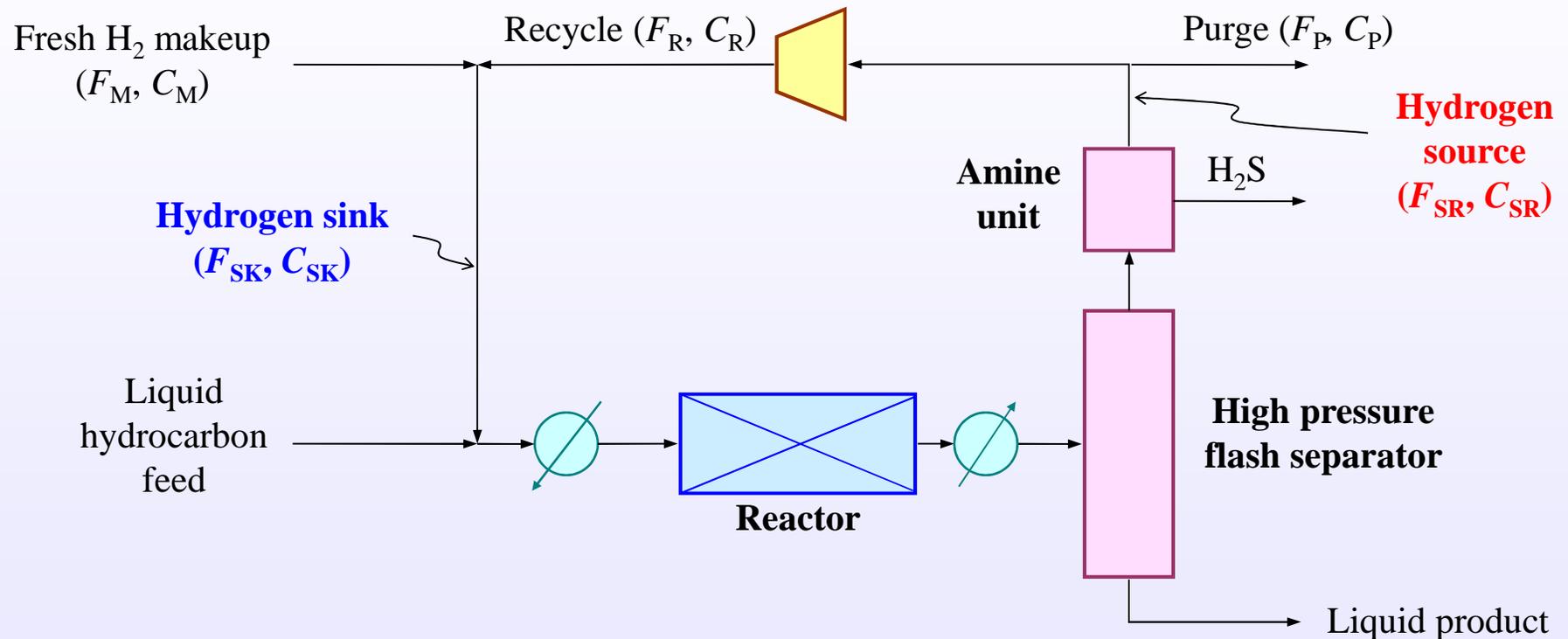
Identification of H$_2$ sinks & sources

❑ Hydrogen sink:

✓ Flowrate: $F_{SK} = F_M + F_R$

✓ impurity concentration:

$$C_{SK} = \frac{F_M C_M + F_R C_R}{F_M + F_R}$$

where F_{SK}, F_M and F_R are the respective flowrates of the hydrogen sink, make-up and recycle streams; with their respective impurity concentrations of C_{SK}, C_M and C_R.

❑ Hydrogen source:

✓ Flowrate: $F_{SK} = F_R + F_P$

✓ Concentration: $C_{SK} = F_R = F_P$

Ex 2.4 – Refinery H₂ network
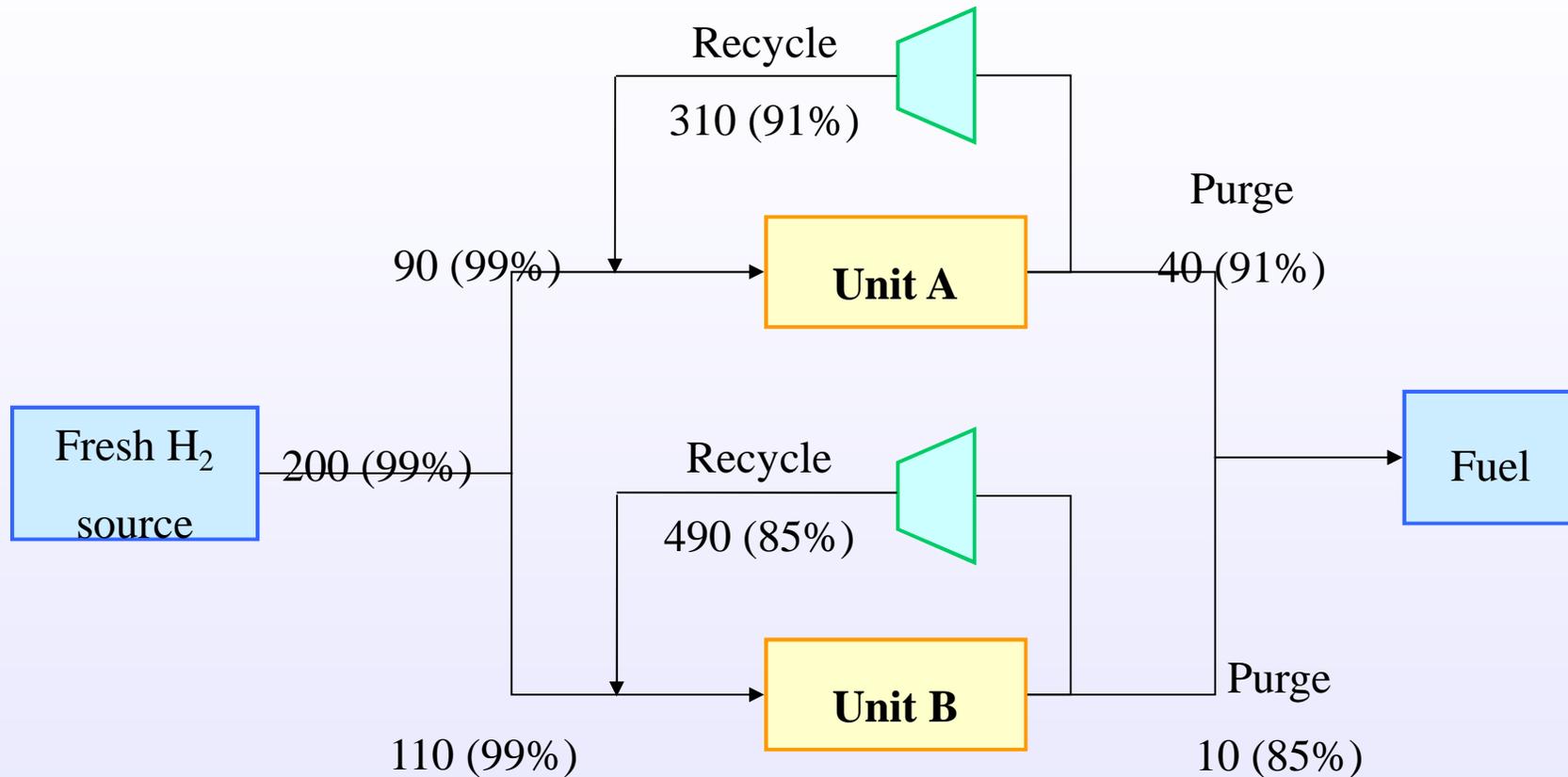
Ex 2.4 – Refinery H₂ network

	Make-up stream	Recycle stream	Purge stream	Hydrogen sink	Hydrogen source
Unit A					
Flowrate (MMscfd)	90	310	40	400	350
Concentration (%)	1	9	9	7.20	9
Unit B					
Flowrate (MMscfd)	110	490	10	600	500
Concentration (%)	1	15	15	12.43	15

Data extraction for property integration

Property integration

Solution A

(F_A, V_A, ρ_A)

Mixing
operation

Mixture

(F_M, V_M, ρ_M)

Solution B

(F_B, V_B, ρ_B)
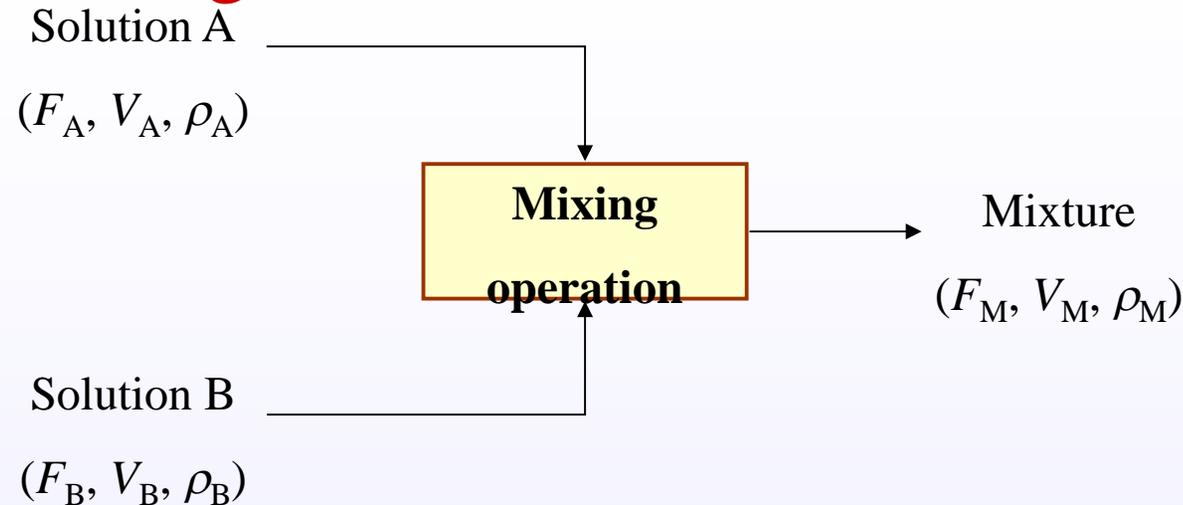
❑ Density of the mixture (ρ_M) is given by:

$$\frac{1}{\rho_M} = x_A \frac{1}{\rho_A} + x_B \frac{1}{\rho_B}$$

or the generic form

$$\frac{1}{\rho_M} = \sum_i \frac{x_i}{\rho_i}$$

❑ A generic form of the **linearised mixing rule** is given as:

$$\psi_M(P_M) = \Sigma i \; x_i \psi_i(P_i)$$

Property integration

❑ Example: Mixing of liquid of different density
- ✓ 1 kg liquid A of 1000 kg/m^3 (ρ_A)
- ✓ 1 kg liquid B of 1500 kg/m^3 (ρ_B)

❑ Mixture density (ρ_M) = 1/1000 + 1/1500 = 2/ρ_M

➜ **ρ_M = 1200 kg/m^3**

❑ If we work on the operator of density:
- ✓ Liquid A: ψ_A = 1/1000 = 0.001
- ✓ Liquid B: ψ_B = 1/1500 = 0.0067
- ✓ Density operator of mixture, **$\psi_M(P_M) = \Sigma_i \, x_i \psi_i(P_i)$**

ψ_M = 0.5(0.001) + 0.5(0.0067) = 0.000833

➜ **ρ_M = 1200 kg/m^3**

Reported linearised mixing rule

Property of mixture	Mixing rule	Operator	Reference
Density, $\overline{\rho}$	$\dfrac{1}{\overline{\rho}} = \sum_i \dfrac{x_i}{\rho_i}$	$\psi(\rho_i) = \dfrac{1}{\rho_i}$	Shelley and El-Halwagi (2000)
Reid Vapor Pressure, $\overline{RVP}$	$\overline{RVP} = \sum_i x_i RVP_i^{1.44}$	$\psi(RVP_i) = RVP_i^{1.44}$	Shelley and El-Halwagi (2000)
Material content, $\overline{M}$	$\overline{M} = \sum_i x_i M_i$	$\psi(M_i) = M_i$	Shelley and El-Halwagi (2000); El-Halwagi *et al.* (2002)
Electric resistivity, $\overline{R}$	$\dfrac{1}{\overline{R}} = \sum_i \dfrac{x_i}{R_i}$	$\psi(R_i) = \dfrac{1}{R_i}$	Kazantzi and El-Halwagi (2004)
Viscosity, μ	$\log(\overline{\mu}) = \sum_{i=1}^{N_s} x_i \log(\mu_i)$	$\psi(\mu_i) = \log(\mu_i)$	Qin *et al.* (2004)
Paper reflectivity, $\overline{R}_\infty$	$\overline{R}_\infty = \sum_i x_i R_{\infty,i}^{5.92}$	$\psi(R_{\infty,i}) = \sum_i x_i R_{\infty,i}^{5.92}$	El-Halwagi *et al.* (2002)

Heuristic 4

Choose the property operator of the sink that is
furthest from that of the fresh resource.

Ex 2.5 – Metal degreasing
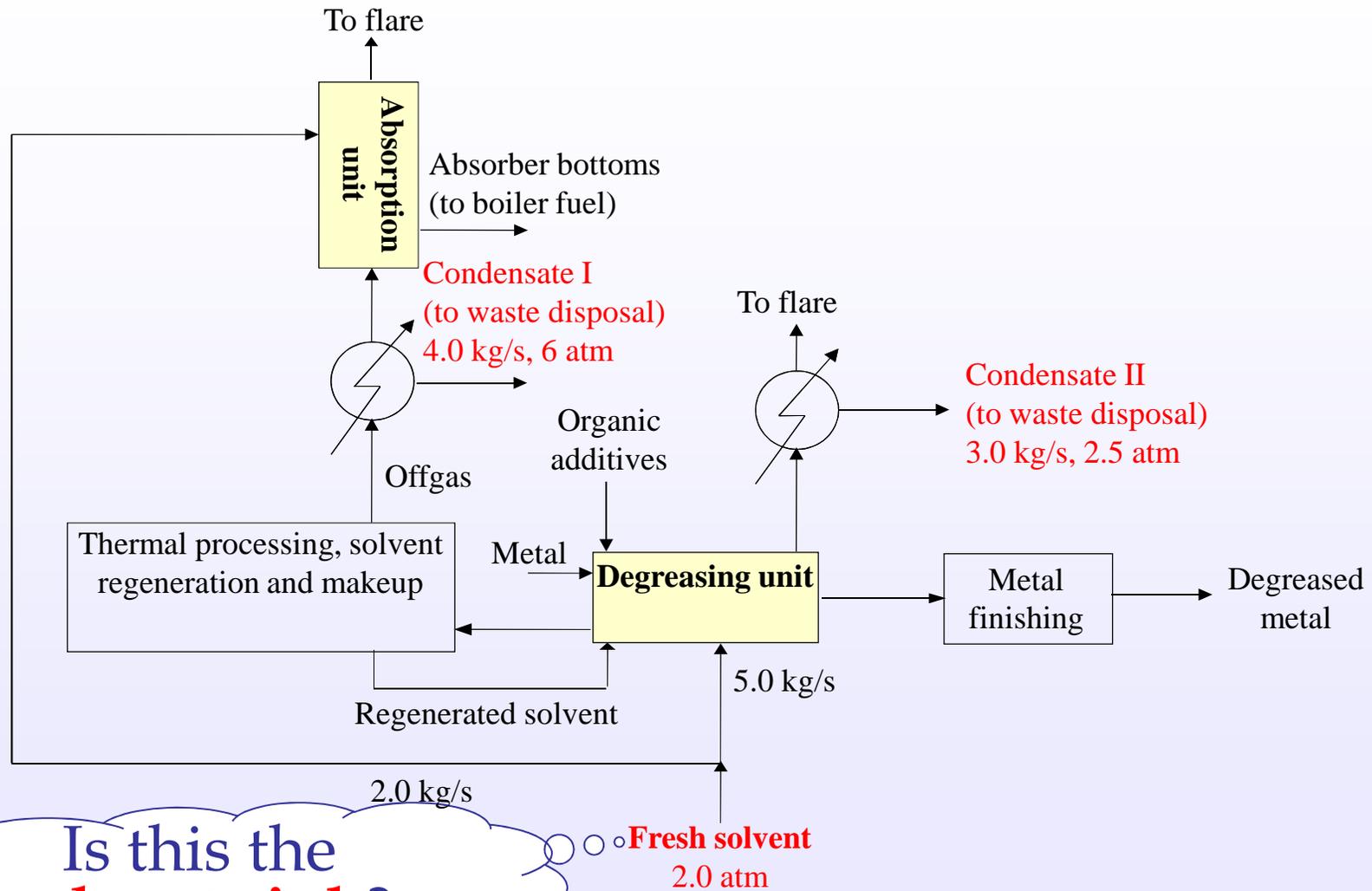
Is this the **solvent sink**?

(Shelley & El-Halwagi, 2002)

Ex 2.5 – Metal degreasing

❑ The **fresh solvent** has an RVP value of 2.0 atm.

❑ The following process constraints on flowrate and RVP values are to be complied for the process sinks, i.e.:

✓ Degreasing unit:

Flowrate of solvent = 5.0 kg/s

$2.0 \leq$ RVP of solvent (atm) ≤ 3.0

✓ Absorption unit:

Flowrate of solvent = 2.0 kg/s

$2.0 \leq$ RVP of solvent (atm) ≤ 4.0

Ex 2.5 – Metal degreasing

❑ Operator values for **sources**:

    ✓ Fresh solvent - 2.71 atm$^{1.44}$

    ✓ Condensate I - 13.20 atm$^{1.44}$

    ✓ Condensate II - 3.74 atm$^{1.44}$

❑ Operator values for **sinks**:

$$2.71 \leq \psi \text{ for degreasing unit (atm}^{1.44}) \leq 4.86$$

$$2.71 \leq \psi \text{ for absorption unit (atm}^{1.44}) \leq 7.36$$

Ex 2.5 – Metal degreasing

Sink	F_{SKj} (kg/s)	ψ_{SKj} (atm$^{1.44}$)
Degreasing unit	5	4.86
Absorption unit	2	7.36
Source	F_{SRi} (kg/s)	ψ_{SRi} (atm$^{1.44}$)
Condensate I	4	13.20
Condensate II	3	3.74
Fresh solvent	To be determined	2.71

In-class exercise(s)

P2.5 – N₂ recovery

Is this the **N₂ source**?

Decomposed organics

Gaseous emission
$F_D = 8.5$ kg/s
0.93% solvent

MEMBRANE

$F_1 = 3.0$ kg/s
$C_1 = 1.90\%$

$F_2 = 5.5$ kg/s
$C_2 = 0.40\%$

Magnetic pigments

Dispersants and lubricants

Solvent

| **RESIN PREMIXING** | → | **SLURRY PREMIXING** | → | **DISPERSION** | → | **COATING** | → | **DRYING** |

N₂

N₂

Binders

Resins   Additives

Base film

Dry tape product
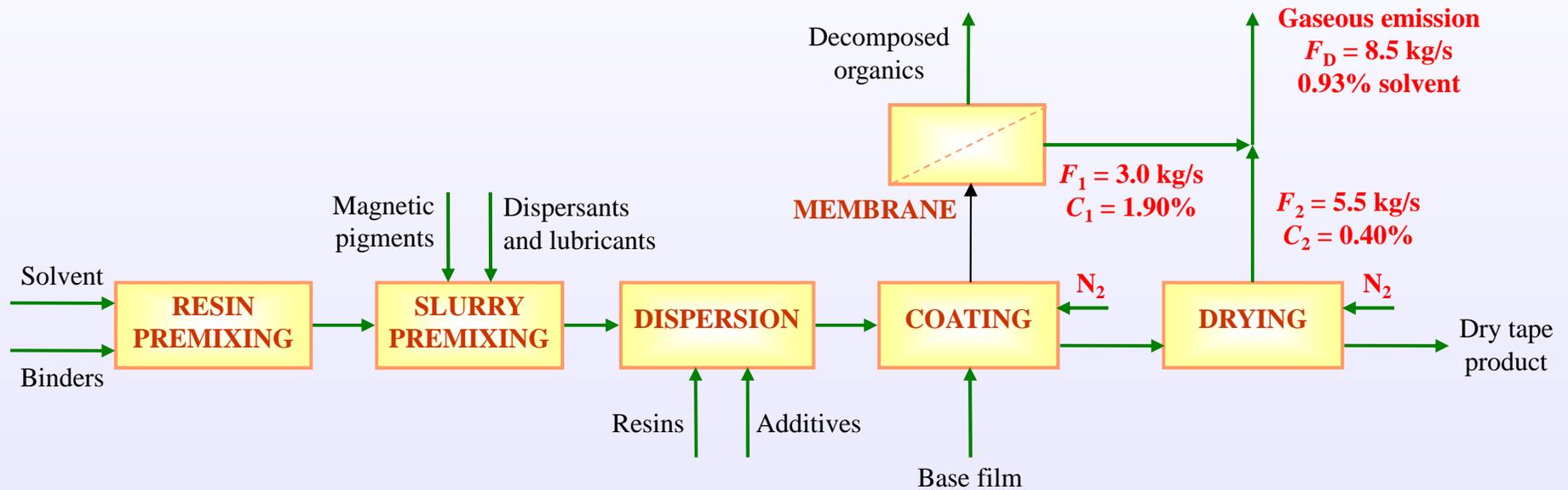
(El-Halwagi, 1997)

P2.6 – refinery H₂ network
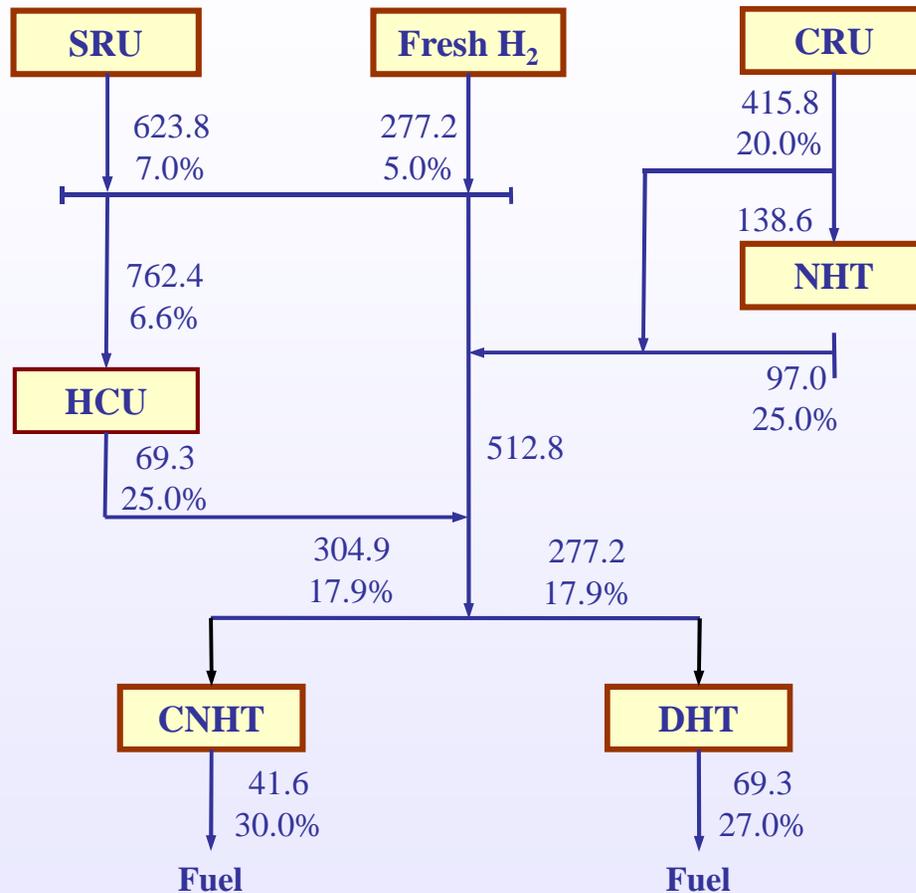
Flowrate and concentration of recycle streams in all units:

| Units	F_R (mol/s)	C_R (mol%)
HCU	1732.6	25.0
NHT	41.6	25.0
CNHT	415.8	30.0
DHT	277.2	27.0

Tasks: Identify the limiting data in order to carry out a hydrogen recovery analysis

P2.6 – solution

j	Sinks, SK$_j$	F_{SKj} (mol/s)	C_{SKi} (mol%)	i	Sources, SR$_i$	F_{SRj} (mol/s)	C_{SRi} (mol%)
1	HCU	2495.0	19. 39	1	HCU	1801.9	25.0
2	NHT	180.2	21.15	2	NHT	138.6	25.0
3	CNHT	720.7	24.86	3	CNHT	457.4	30.0
4	DHT	554.4	22.43	4	DHT	346.5	27.0
				5	SRU	623.8	7.0
				6	CRU	415.8	20.0

P2.7 – wafer fabrication process

UPW

		Wet	250 t/h (1.0 MΩm)
2000 t/h (18 MΩm)	500 t/h	(7 – 18) MΩm	200 t/h (2.0 MΩm)

	450 t/h	Lithography (8 – 15) MΩm	350 t/h (3.0 MΩm)

	700 t/h	CMP (10 – 18) MΩm	300 t/h (0.1 MΩm) / 200 t/h (2.0 MΩm)

	350 t/h	Etc (5 – 12) MΩm	280 t/h (0.5 MΩm)
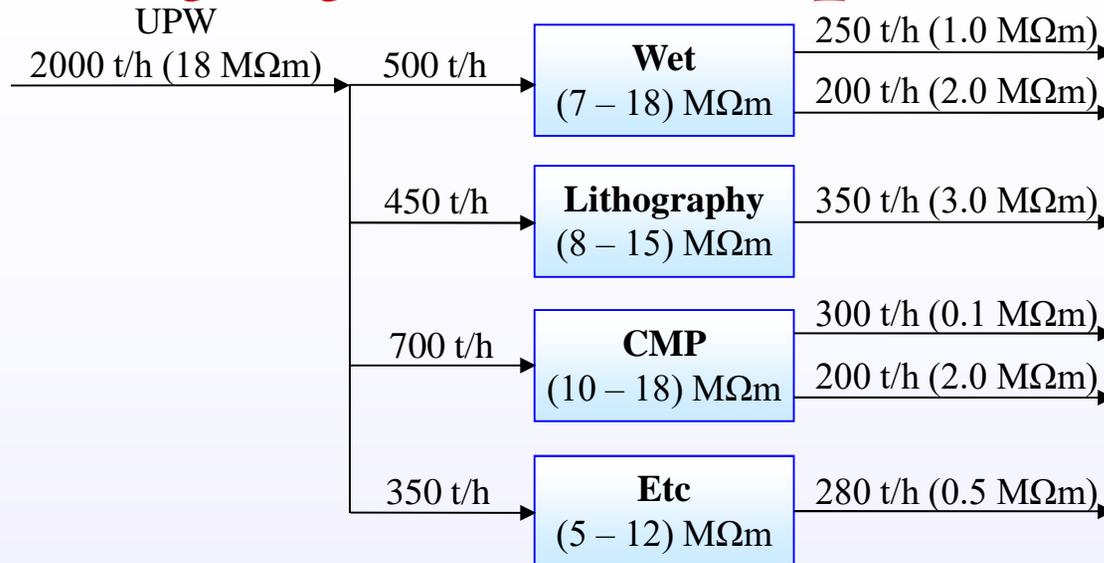
❑ Large amount of ultrapure water (UPW) is consumed in a wafer fabrication plant that consist of wet processing section (Wet), lithography, combined chemical and mechanical processing (CMP), & miscellaneous operations (Etc.).

❑ Water quality in considering water recovery is *resistivity* (R) that reflects the total ionic content in the aqueous streams, with property mixing rule:

$$\frac{1}{R_M} = \sum_i \frac{x_i}{R_i}$$

P2.7 – technical info

❑ Operator values for **UPW** = 0.0556 MΩ^{-1}.m^{-1}

❑ Operator values for **sources**:

   ✓ Wet I - 1 MΩ^{-1}.m^{-1}

   ✓ Wet II - 0.5 MΩ^{-1}.m^{-1}

   ✓ Lithography - 0.3333 MΩ^{-1}.m^{-1}

   ✓ CMP I - 10 MΩ^{-1}.m^{-1}

   ✓ CMP II – 0.5 MΩ^{-1}.m^{-1}

   ✓ Etc - 2 MΩ^{-1}.m^{-1}

Wet

R_{min} = 7 MΩ.m ➜ ψ = 0.1429 MΩ^{-1}.m^{-1}
R_{max} = 18 MΩ.m ➜ ψ = 0.0556 MΩ^{-1}.m^{-1}

$$\frac{1}{R_{M}} = \sum_{i} \frac{x_i}{R_i}$$

❑ Operator values for **sinks**:

   0.0556 ≤ ψ for Wet (MΩ^{-1}.m^{-1}) ≤ 0.1429

   0.0667 ≤ ψ for Lithography (MΩ^{-1}.m^{-1}) ≤ 0.1250

   0.0556 ≤ ψ for CMP (MΩ^{-1}.m^{-1}) ≤ 0.1000

   0.0833 ≤ ψ for Etc (MΩ^{-1}.m^{-1}) ≤ 0.2000

P2.7 – solution

Sink	F_{SKj} (kg/s)	ψ_{SKj} (MΩ^{-1}.m^{-1})
Wet (SK1)	500	0.1429
Litography (SK2)	450	0.1250
CMP (SK3)	700	0.1000
Etc (SK4)	350	0.2000
Source	F_{SRi} (kg/s)	ψ_{SRi} (MΩ^{-1}.m^{-1})
Wet I (SR3)	250	1
Wet II (SR4)	200	0.5
Litography (SR5)	350	0.3333
CMP I (SR6)	300	10
CMP II (SR7)	200	0.5
Etc (SR8)	280	2