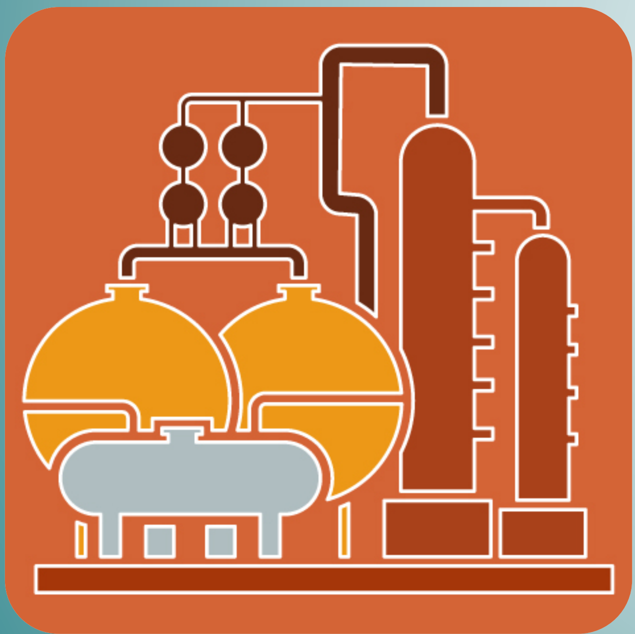
Chemical Process Design / Diseño de Procesos Químicos

Topic 4.1. to 4.3. Analysis of process. Material and heat balances

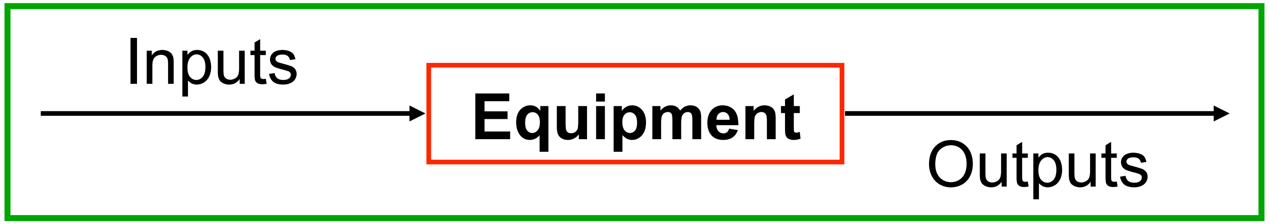


Javier R. Viguri Fuente
Eva Cifrian Bemposta

Department of Chemistry and Process & Resource Engineering
GER Green Engineering and Resources Research Group

INDEX

1.- Perspective of Sustainable Development



Two categories of relationships:

1. **Relationships independent of the equipment:**
   - **Independent of the equipment specifications.**
   - **BM / BE / Equilibrium / Kinetic.**

2. **Relationships dependent of the equipment:**
   - **Design equations with equipment specifications:**
     - **Heat transference equation (with Area value).**
     - **Frictional pressure relationships (with D, Le).**

2.- Methodology for process analysis: Material and energy balances

- **Analysis methodology to apply on the synthesized flowsheets:**
  - **Simple.**
  - **Fast.**
  - **Useful to the preliminary design.**

Due to the high number of alternatives to be analyze

- Mass balances.
- Energy balances.

→ Systematic modeling with different degree of rigorousness from low (preliminar) to high (detailed engineering).

2.- Methodology for process analysis: Material and Energy Balances

Once we synthesize flowsheet, we must do mass and energy balances to analyze its PERFORMANCE and to SIZE equipment for economic evaluation.

Equation Oriented // Sequential Modular

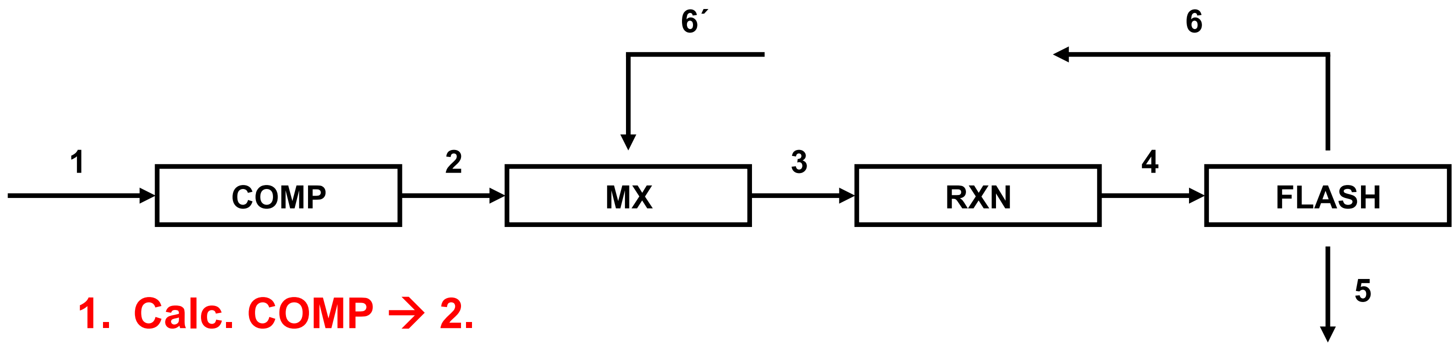
2.1.- Equation Oriented

- Write al equations that describe the process and solve them simultaneously.
- Equations:
  - Material balances.
  - Equilibrium relations.
  - Kinetic expressions.
  - Enthalpy balances, etc.
- Need solve 100´s equations with Newton´s.
- Software: gPROMS, GAMS, EXCEL, ASPEN equations.

2.- Methodology for process analysis: Material and Energy Balances

2.2.- Sequential Modular

Solve for input streams in each unit at the flowsheet following the information flow. For each module, compute outlet from given inlet (stream 1 known).



1. Calc. COMP → 2.
2. Guess stream 6'.
3. Calc. MIX → 3.
4. Cal. RXN → 4.
5. Cal. FLASH → 5, 6.
6. If stream 6 is similar 6' STOP, otherwise return to step 2.

- **More robust, but less flexible.**
- **Software: ASPENPLUS, PRO-II, HYSYS, UniSIM.**

Analysis of process diagrams in 2 Phases

Phase I. Develop LMB model and solve mass balance in each unit:

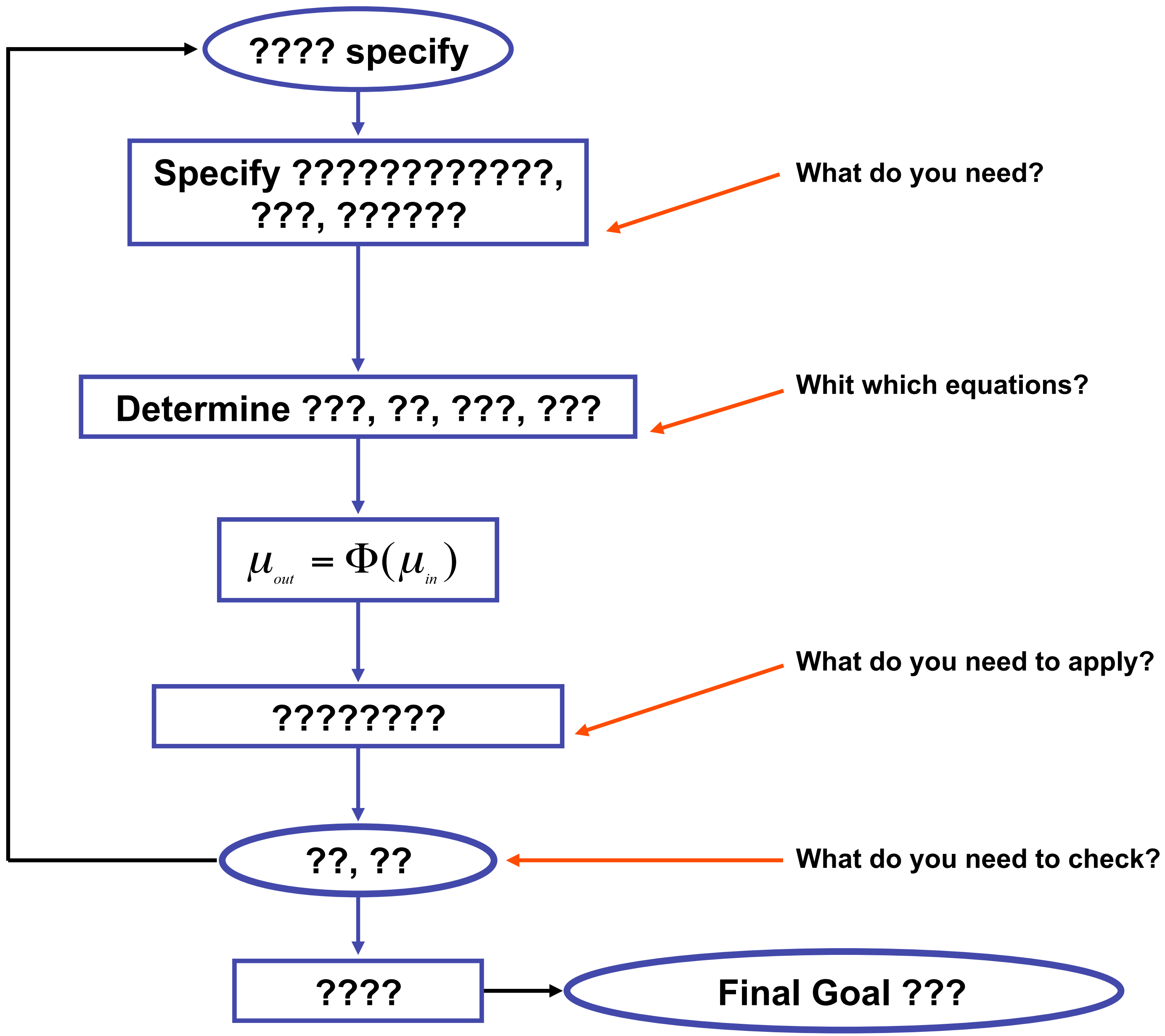
1. **Fix P and T levels in flowsheet.** Specify recoveries, split fractions, key components, conversion per pass, recycle ratios (specify Degrees of Freedom-d.f.).
2. **Determine Coefficients Linear Models** (x, in flash unit; b, g, AE in absorber) to relate linearly output molar flow with inputs.
3. **Set up linear equations and solve for molar flows** at each component.
4. **Recalculate P, T** in flowsheet with equilibrium equations:
   - If there are not big changes, go to the next Phase (Phase II).
   - If there are big changes go to step 2.
   - If process does not meet specifications (e.g. the recycle rate is to low), change recoveries or modify flowsheet structure returning to step 2 (e.g. you can need a 2º flash or distillation unit to obtain the product purity need).

Analysis of process diagrams in 2 Phases

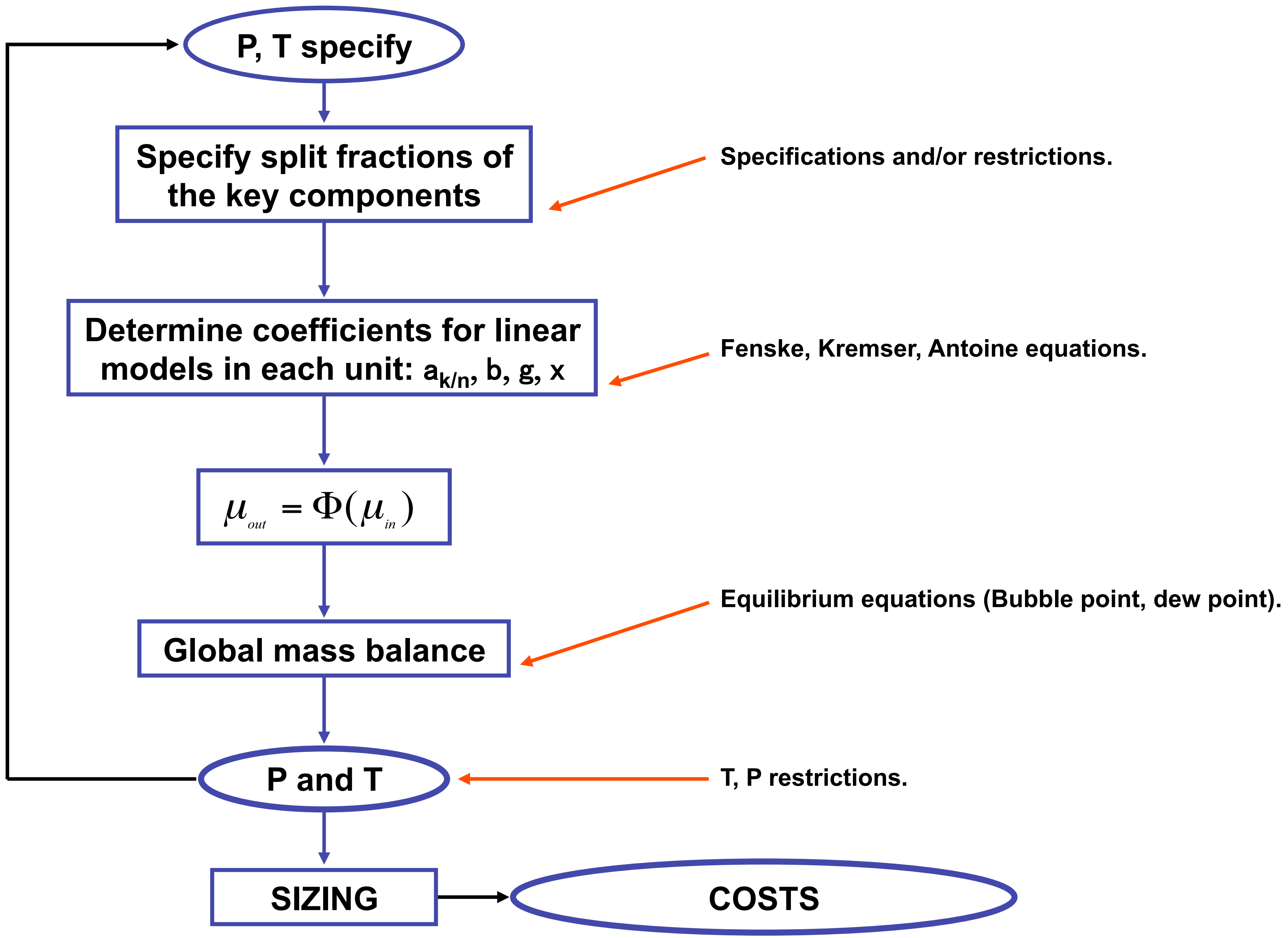
Phase II. Perform heat balances (heating – normally steam + cooling utilities – normally water):

- **Perform Heat integration at this stage.**
- **Idea → Decouple mass and heat balances.**

Build your LMB algorithm



LMB algorithm



3.- Linear Mass Balances (LMB) models

- **Assumptions:**
  - L and V streams with ideal equilibrium relationships.
  - Saturated streams.
  - Linear equations simple to solve → "tearing".
  - Convergence in few interactions (2).
  - Use basis at 100 gmol/s feed and calculate scale up factor to meet required production.

- **Approximations for following modules (See videos and screencast):**
  1. Mixer → Not real or physically equipments. Could be junctions.
  2. Splitter.
  3. Reactor.
  4. Flash → Linear in terms of split fractions.
  5. Distillation.
  6. Absorption and Stripper → Associated.

- **There are many other equipments as Adsorption, pervaporation, fermenters, etc.**

3.- Linear Mass Balances (LMB) models

- **Assumptions:**
  - L and V streams with ideal equilibrium relationships.
  - Saturated streams.
  - Linear equations simple to solve → "tearing".
  - Convergence in few interactions (2).
  - Use basis at 100 gmol/s feed and calculate scale up factor to meet required production.

- **Approximations for following modules (See videos and screencast):**
  1. Mixer → Not real or physically equipments. Could be junctions.
  2. Splitter.
  3. Reactor.
  4. Flash → Linear in terms of split fractions.
  5. Distillation.
  6. Absorption and Stripper → Associated.

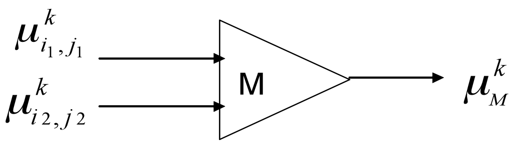
What are the diagraman of each equipment

- **There are many other equipments as Adsorption, pervaporation, fermenters, etc.**

4.- Develop of LMB models

Simplifications and approximations → Shortcut methods based on Linear equations → smaller problem.

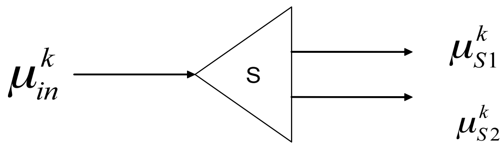
Mixer



$$\mu^k_{Mixer} = \sum_l \mu^k_{i_l, j_l}$$

Linear coefficients: ------

Splitter

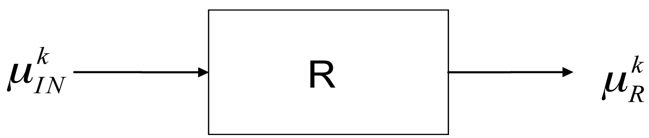


$$\mu^k_{Splitter,j} = \xi_j \mu^k_{in}$$

$$\mu^k_{Spitter,NS} = (1 - \sum_{j=1}^{NS-1} \xi_j)\mu^k_{in}$$

Split fraction

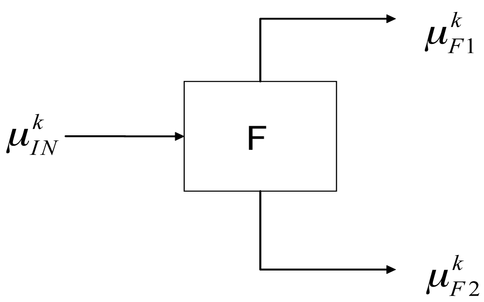
Reactor



$$\mu^k_{Reactor} = \mu^k_{in} + \sum_{r=1}^{NR} \gamma_{r,k} \eta_r \mu^{l(r)}_{in}$$

Conversion & Stoichiometric coefficients

Flash



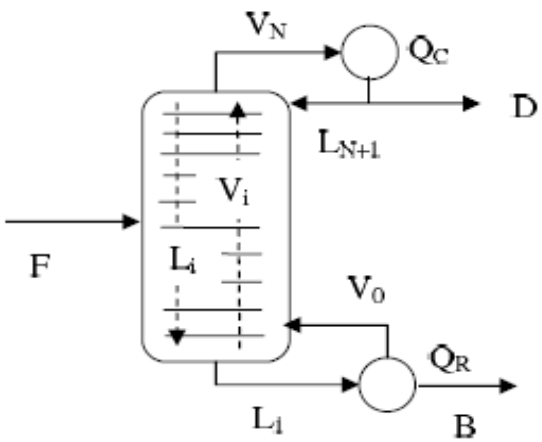
$$\mu^k_{F1} = \xi_k \mu_{in}$$

$$\mu^k_{F2} = (1 - \xi_k)\mu_{in}$$

Split fractions

4.- Develop of LMB models

Distillation



$$\mu_D^k = \xi_k \mu_{in}^k$$

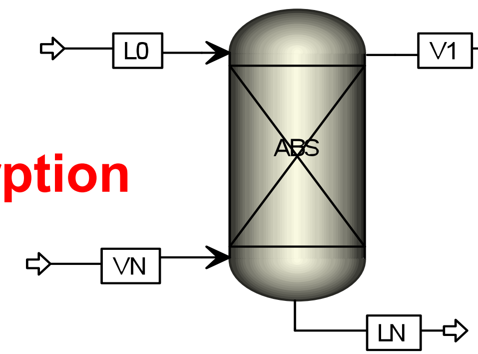
$$\mu_B^k = (1-\xi_k)\mu_{in}^k$$

$$N_m = \ln\left[\frac{\xi_{Lk}}{\xi_{Lk}}\,\frac{1-\xi_{Hk}}{\xi_{Hk}}\right] / \ln \alpha_{Lk/Hk}$$

$$\xi_k = \left[\frac{\alpha_{k/Hk}^{Nm}\,\xi_{Hk}}{1+(\alpha_{k/Hk}^{Nm}-1)\,\xi_{Hk}}\right]$$

$$T_{bub,\,c} \le T_{dew,\,c} \le T_{bub,R} \le T_{dew,R}$$

Absorption



$$v_1^k = \frac{1}{\beta_N^k}\,v_{N+1}^k + \frac{\beta_{N+1}^k}{\beta_N^k}\,l_0^k$$

$$l_N^k = v_{N+1}^k + l_0^k - v_1^k$$

$$l_N^k = \left(1-\frac{1}{\beta_N^k}\right) v_{N+1}^k + \left(1-\frac{\beta_{N+1}^k}{\beta_N^k}\right) l_0^k$$

$$N = \ln\left[\frac{l_0^n + (r^n - A_E^n)\,v_{N+1}^n}{l_0^n - A_E^n(1-r^n)v_{N+1}^n}\right] / \ln(A_E^n)$$

$$\beta_N^k = \frac{1-(A_E^k)^{N+1}}{1-(A_E^k)}$$

$$\beta_{N-1}^k = \frac{1-(A_E^k)^{N}}{1-(A_E^k)}$$

6.- Heat Balances

- **Entlaphies: H (P, T, zk) [J/gmol]:**
  - Reference state is necessary for the calculations.

    Ideal Gas; P_0 = 1 atm; T_0 = 298 K
  - Assume elemental species.
  - Assume ideal behaviour → reflect effects of P and mixing (specially in the liquid phase).

Constants for each k

C_{pk} as function of T by heat capacity coefficients Ak, Bk, Ck, Dk

$$H_v(T,y) = \sum_k y_k (\Delta H^0{}_{f_k} + \int_0^T C^0_{p_k} dT)$$

Handbook values
(Perry, 2008;
Poling *(et al.)*, 2000).

by Watson correlation in function of Tb, Tc, and DHvap (Tb)

$$H_L(T,x) = \sum_k x_k [\ \Delta H^0{}_{f_k} + \int_0^T C^0_{p_k} dT - \Delta H_v^k(T)\ ]$$

7.- Further Reading and References

- Biegler, L.; Grossmann, I. & Westerberg, A. (1997): *«Systematic methods of chemical process design»*. Prentice Hall.
- Green, D. & Perry, R. (2008): *«Perry's chemical engineers' handbook»*. 8th Ed. McGraw-Hill.
- Kent (1992): *«Riegel´s handbook of industrial chemistry»*.
- Lide, D. (Ed.) (1997): *«CRC handbook of chemistry and physics»*. CRC Press.
- McKetta, J. (Ed.) (1993): *«Chemical processing handbook»*. Marcel Dekker.
- Poling, B.; Prausnitz, J. & O'Connell, J. (2000): *«The properties of gases and liquids»*. 5th Ed. McGraw-Hill.
- Treybal, R. (1980): *«Mass transfer operations»*. 2nd Ed. McGraw Hill.
- Woods, D. (1995): *«Data for process design and engineering practice»*. Prentice-Hall.

Practical Chapter

- **Application of chemical process analysis methodology to the “case study”.**
- **Application of chemical process analysis methodology to “your process design project”.**

Relevant To Learning (I)

- To distinguish between Relationships independent of the equipment specifications and Relationships dependent of the equipment.
- Linear Mass Balances (LMB) model and Linear Mass Balances (LMB) algorithm in text and diagram.
  - To understand that is an algorithm to apply at any unit operation!!!
- To understand the main assumption in the mass balance model.
- To apply the MLB proposed to the case study and to the proposed project.

Relevant To Learning (II)

- **Given the data shown below for benzene, determine whether benzene can condense as a liquid at a pressure of 60 bar. The critical temperature is 562 K.**

Antoine coefficients for: ln P vap = A – B / (T + C) (P vap en mm Hg, T en K)			
	A	B	C
Benzene	15.9008	2788.51	–52.36

- ***Dados los datos mostrados a continuación para el benceno, determinar si el benceno puede condensar como un líquido a una presión de 60 bares. La temperatura crítica es = 562 K.***

Antoine para la expresión: ln P vap = A – B / (T + C) (P vap en mm Hg, T en K)			
	A	*B*	*C*
Benceno	*15,9008*	*2788,51*	*–52,36*

- **If you need to design an absorber, how would you select the operating pressure and temperature in order to reduce the solvent flow needed to achieve a pre-set recovery of the key component? Explain why?**
- ***Si tienes que diseñar un absorbedor, como seleccionarías la presión y temperatura de operación para reducir el flujo de disolvente necesario para conseguir una recuperación previamente fijada del componente clave? Explicar porqué?***

Relevant To Learning (II)

- **Calculate the fluxes of Air, Acetone and Water, as well as their molar fractions, in the outflows of an Absorption system in which it is intended to recover acetone from an air stream (10 mol/s of air + 1 mol/s of acetone) at r = 0.95 with AE = 1.4. Pure water is used as the process solvent. The unit operates at 300 K and 10 bar.**

$\ln P^0_{aceotone}$ (mm Hg) = 16.6513 – 2940.46 / (T (K) – 35.93)
P^0_{water} (mm Hg) = 10 exp [A – (B / (C + T (ºC)))]; A = 8.11; B = 1750.29; C = 235

- ***Calcular los flujos de Aire, Acetona y Agua, así como sus fracciones molares, en las corrientes de salida de un sistema de Absorción en el que se pretende recuperar acetona de una corriente de aire (10 mol/s de aire + 1 mol/s de acetona) a r = 0,95 con AE = 1,4. Se utiliza como disolvente del proceso agua pura. La unidad funciona a 300 k y 10 bar.***

$\ln P^0_{aceotona}$ (mm Hg) = 16,6513 – 2940,46 / (T (K) – 35,93)
P^0_{agua} (mm Hg) = 10 exp [A – (B / (C + T (ºC)))]; A = 8,11; B = 1750,29; C = 235