OPTIMIZATION PROBLEM FORMULATION

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PROBLEM

To produce 100 $kmol/h$ of n-buthyl acetate (AcBu), through the reaction:

$$\underset{Buthanol}{BuOH} + \underset{Acetic\ acid}{AcAc} \underset{H^+}{\leftrightharpoons} \underset{Buthyl\ acetate}{BuAc} + \underset{Water}{H_2O}$$

The kinetics is defined by the Langmuir-Hinshelwood-Hougen-Watson equation (M-LHHW). Sources (Gangadwala, Mankar, & Mahajani, 2003) (The Dow Chemical Company®)

$$r_i = v_i\ M_{cat} K_f K_{s,AcH} K_{s,BuOH} \frac{a_{AcH}\ a_{BuOH} - \frac{1}{K_a} a_{BuAc}\ a_{H2O}^{\alpha}}{\left(1 + K_{s,AcH} a_{AcH} + K_{s,BuOH} a_{BuOH} + K_{s,BuAc} a_{BuAc} + K_{s,H2O} a_{H2O}^{\alpha}\right)^2}$$

$\boldsymbol{K_f^0}$	$14.0093\times10^6 kmol/kg/s$
$\boldsymbol{E_f}$	$72.896\times10^3\ kJ/kmol$
$\boldsymbol{K_a^0}$	3.8207
$\boldsymbol{E_a}$	$-3.5817\times10^3\ kJ/kmol$
$\boldsymbol{K_{s,AcH}}$	4.4521
$\boldsymbol{K_{s,BuOH}}$	6.9211
$\boldsymbol{K_{s,BuAc}}$	3.5995
$\boldsymbol{K_{s,H2O}}$	9.0304
$\boldsymbol{\alpha}$	2.00

A reactor for this process will be designed and it must accomplish with the lowest fixed costs and the lowest operating costs.

REACTOR CONDITIONS

Variable		**Ranges**
F_{BuOH}	Reactor's butanol feed flow	$100 - 500\ kmol/h$
F_{AcAc}	Reactor's acetic acid feed flow	$100 - 500\ kmol/h$
T	Operating temperature	$50 - 120$ ℃
P	Operating pressure	$1 - 10\ bar$

- Inlet temperature
    - 25 °C
- Pressure
    - 1-10 bar

      1 – to avoid vacuum

      10 - larger costs

- Optimal relationship between reactives flows (AcAc : BuOH)

  1 : 5

RESTRICTIONS

- Steam fraction = 0
- Outlet temperature bounds: 25 – 120 °C
- BuAc = spec

Nombre de la restricción	Definición
Outlet temperature limit T_{out}. Amberlyst 15 catalyst works up to 120 °C, keep temperature below of it avoids the formation of DBE	$T_{out} \leq 120°C$
No formation of steam inside the reactor. Outlet steam fraction X_{vap} cero	$X_{vap} = 0$
Established prodution accomplishment	$F_{BuAc} = 120\ kmol/h$

COSTS

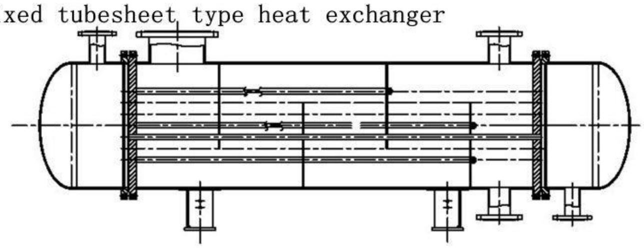
Fixed costs

$$C_{fijos} = reactor\ cost = W \times \$_{catalyst} + C_{shell}$$

C_{fijos}	Fixed costs
W_{cat}	Catalyst weight
$\$_{catalizador}$	Catalyst cost per kilogram
C_{shell}	Reactor's shell costs

Reactor costs:

Fixed tubesheet type heat exchanger



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$$Cp \ = \ F_P F_M F_L C_B$$

Fixed head

$$c_B = \exp(11.0545 - 0.9228 * \ln(A) + 0.09861 * \ln(A)^2)$$

$$F_M = a + \left(\frac{A}{100}\right)^b$$

$$a = 0$$

$$b = 0$$

$$F_M = 1$$

$$F_L = 1.05$$

$$F_P = 1$$

All for CE index of 394, now is 556.8

Operating costs

Corresponding to the annual costs of the currents of power

$$C_{operación} = \frac{costo\ de}{las\ corrientes} = F_0 \cdot x_{BuOH_0} \cdot \$_{BuOH} + F_0 \cdot x_{AcAc_0} \cdot \$_{AcAc}$$

$C_{operación}$	Operating costs per year
F_0	Reactor feed flow rate
x_{BuOH_0}	Inlet butanol composition
$\$_{BuOH}$	Cost of butanol per kilogram
x_{AcAc_0}	Inlet acetic acid composition
$\$_{AcAc}$	Cost of acetic acid per kilogram

- The plant operates 330 days a year

Optimization variables

The variables chosen for optimization are the following:

F_{BuOH}	Inlet butanol flow rate
F_{AcAc}	Inlet acetic acid flow rate
T	Reactor operating temperature
P	Reactor operating pressure
x_{BuOH_0}	Inlet butanol composition
x_{AcAc_0}	Inlet acetic composition

References

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