Simulación y Optimización

Simulación de plantas

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Definiciones

Modelado

- Planta: Conjunto de sectores
- Sector: Conjunto de equipos

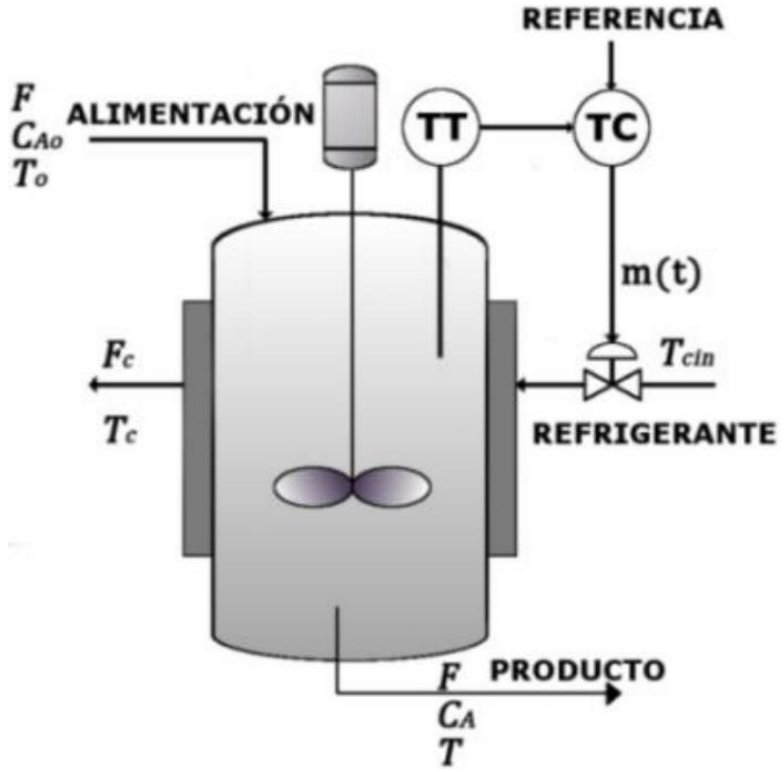
Enfoques

- Global u orientado a ecuaciones
- Modular

Enfoque global

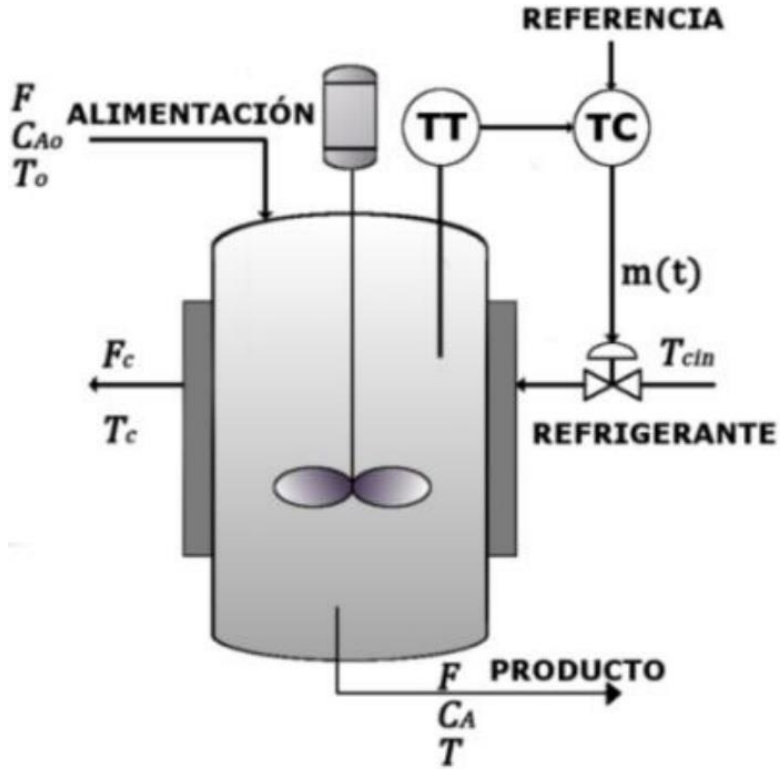
Enfoque global

- Toda la planta es un equipo.
- Modelo de espacio de estado:
  - Sistema ODEs
  - Sistema AEs
  - Datos



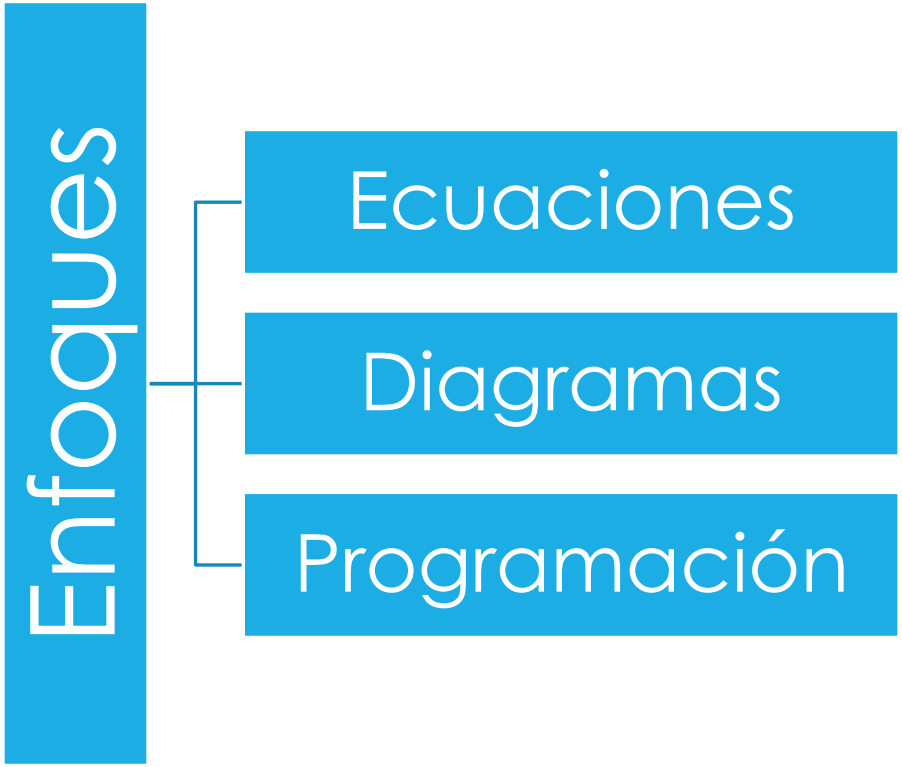
Enfoque global

- Reactor con CT:
  - Reactor
  - Serpentín
  - Válvula
  - Controlador



Alternativas para la resolución

Enfoques para la resolución de modelos



Orientado a ecuaciones

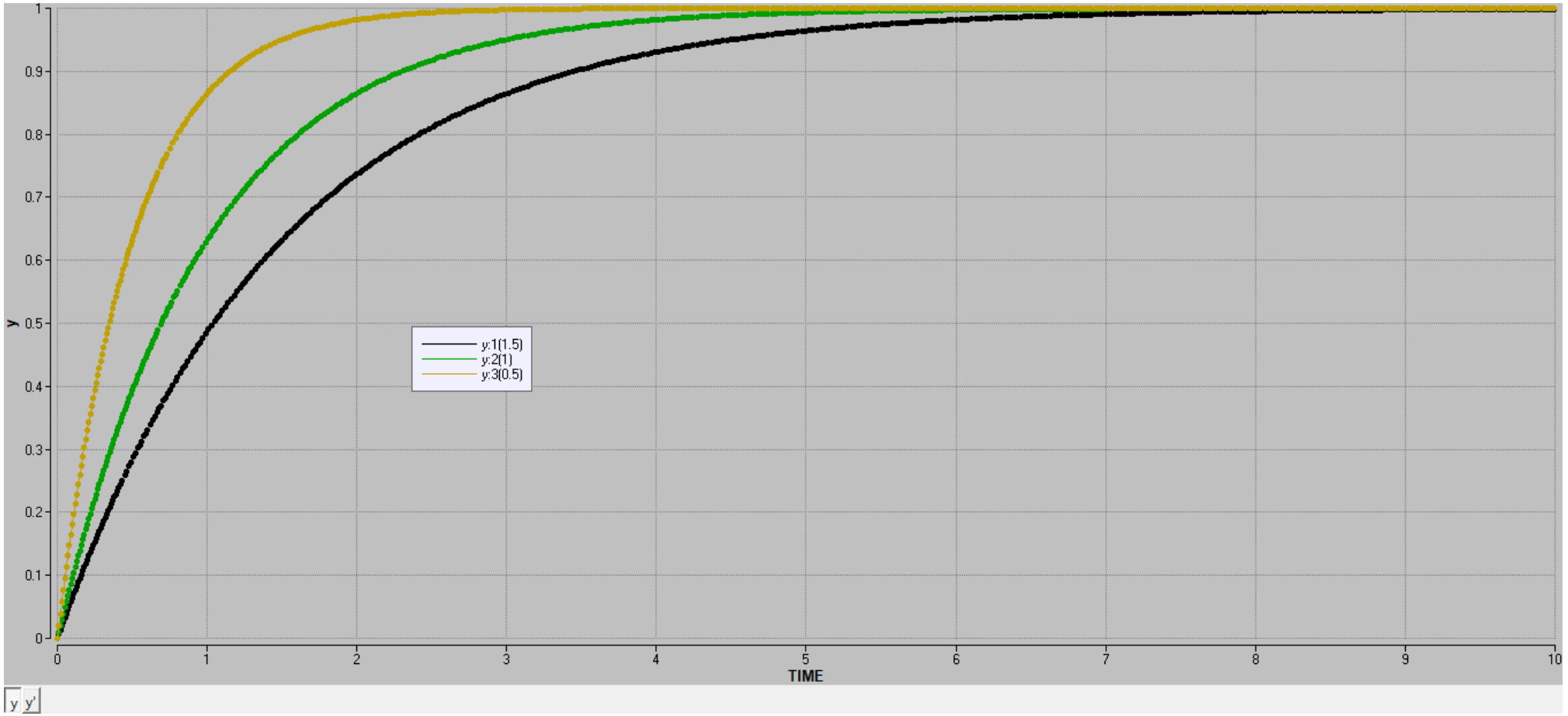
- E-Z Solve
- JSim
- EMSO
- Modelica
- gPROMS
- Berkeley Madonna

$$\frac{dy}{dt} = \frac{u_0 - y}{\tau}$$

Video de Simulación con Berkeley Madonna

```
{Sistema de primer orden.
u0: valor del escalón en la entrada.
tau: es la constante de tiempo.
y: valor de salida}

METHOD RK4

STARTTIME = 0
STOPTIME = 10
DT = 0.01

; Inicialización
INIT y = 0

; Sistema ODEs
y' = (u0-y)/tau

; Sistema AEs

; Datos
u0 = 1
tau = 1
```

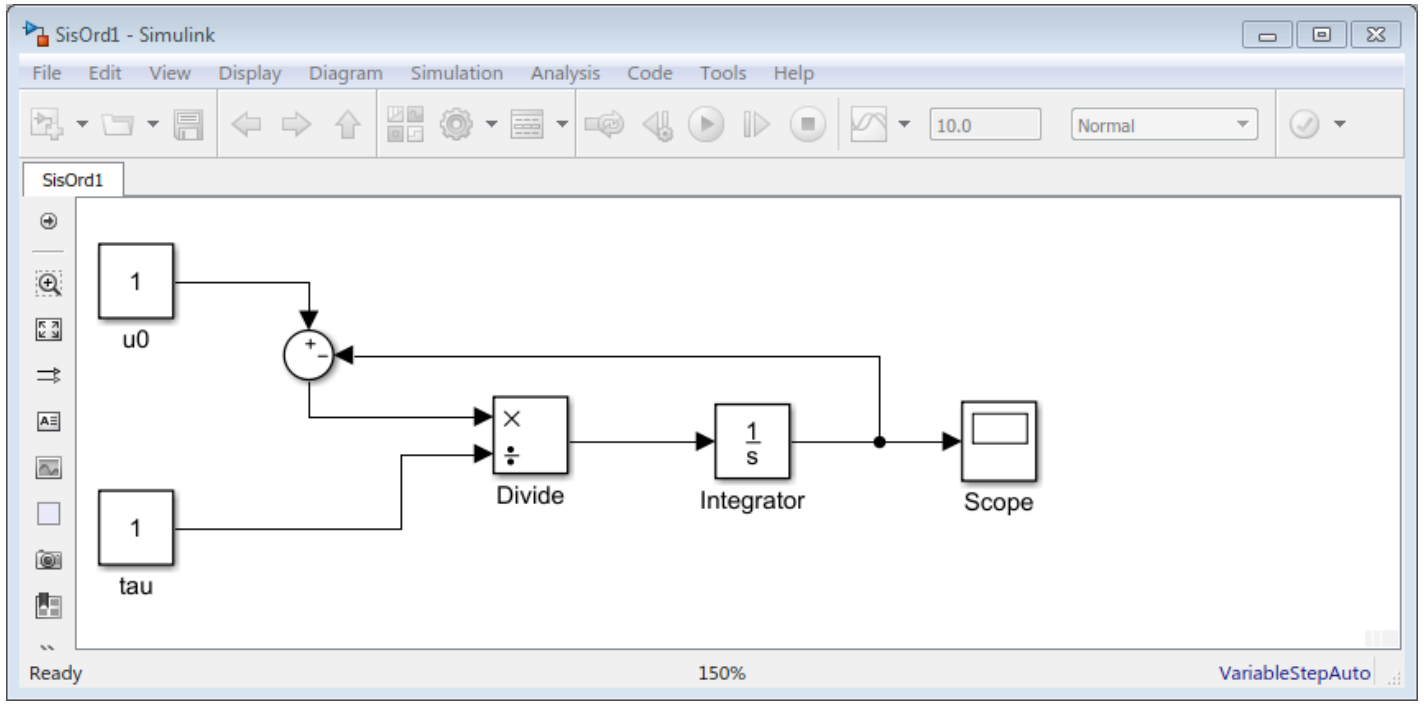
Constante de tiempo



Orientado a diagramas de bloques

- Simulink
- ViSim
- Xcos

$$\frac{dy}{dt} = \frac{u_0 - y}{\tau}$$



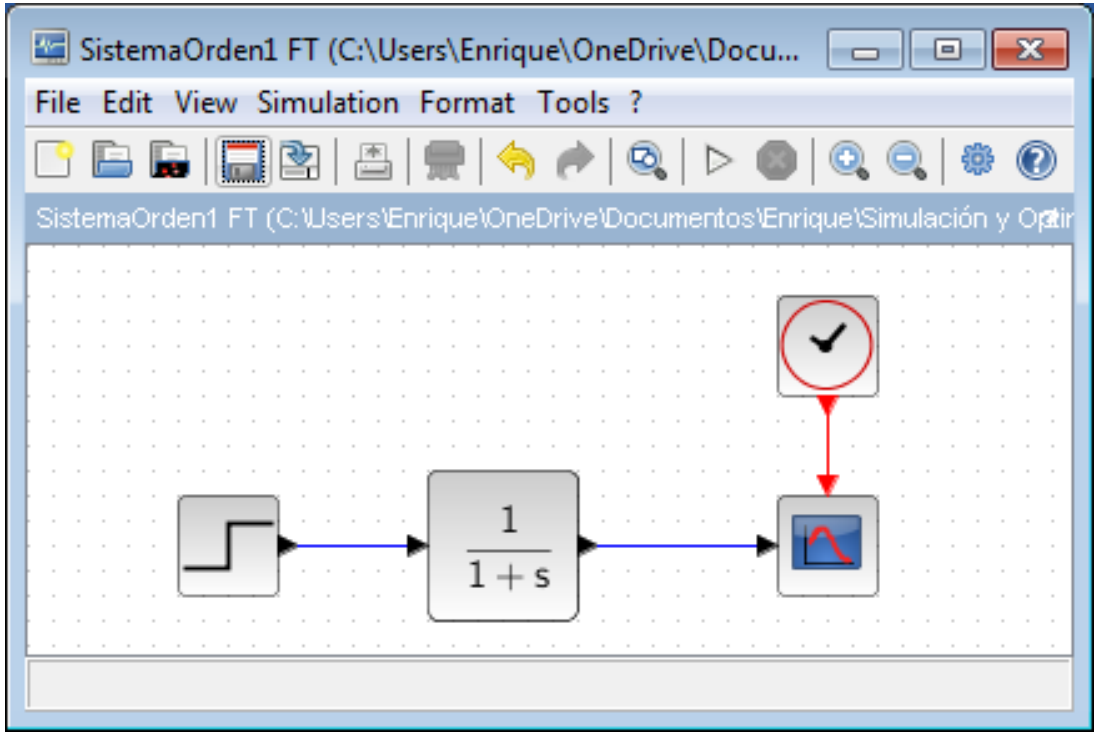
Video Simulación con Simulink

Orientado a diagramas de bloques

- Simulink
- ViSim
- Xcos

$$\frac{dy}{dt} = \frac{u_0 - y}{\tau}$$

$$G(s) = \frac{Y(s)}{U(s)} = \frac{K}{1 + \tau s}$$



Simulación con Xcos

Condiciones iniciales iguales a cero.

Orientados a programación

- Lenguajes:
  - Fortran, C, Pascal, Python, Julia
- Entornos:
  - Matlab, Octave, Scilab
  - Spyder, Visual Studio Code
  - Mathcad, SMath

$$\frac{dy}{dt} = \frac{u_0 - y}{\tau}$$

Video Simulación con Matlab

Manual de GNU Octave

```
% Sistema de primer orden

% Datos
global tau u0
tau = 1;
u0 = 1;

% ODEs
function dy = ODEs(y,t)
  global tau u0
  dy = (u0-y)/tau;
endfunction

% Parámetros de simulación
tfin = 10;
nts = 20;

% Inicialización
tpts = linspace(0, tfin, nts)';
y0 = 0;

% Resolución
y = lsode('ODEs',y0,tpts);

% Gráfica
figure(1);
plot(tpts,y)
```

Listado en Berkeley Madonna

```
{Reactor de propilenglicol con CT}

METHOD RK4
STARTTIME = 0
STOPTIME = 3
DT = 0.01

; Inicialización
INIT CA = 0.0377
INIT CB = 2.1256
INIT CC = 0.1439
INIT CM = 0.2269
INIT Tr = 138.7
INIT Ai = 0

; Sistema ODEs
CA' = F0*(CA0-CA)/V-r
CB' = F0*(CB0-CB)/V-r
CC' = F0*(CC0-CC)/V+r
CM' = F0*(CM0-CM)/V
Tr' = (F0*C0*Cp0*(T0-Tr)+V*r*(-DH)-Q)/(V*C*Cp)
Ai' = e
```

```
; Sistema AEs
r = alpha*exp(-Ea/(Rg*(Tr+460)))*CA

Ts = Ts0+(Tr-Ts0)*(1-exp(-UA/(Ns0*Cps0)))
Q = Ns0*Cps0*(Tr-Ts0)*(1-exp(-UA/(Ns0*Cps0)))

C = CA+CB+CC+CM
Cp = (CA*CpA0+CB*CpB0+CC*CpC0+CM*CpM0)/C
C0 = CA0+CB0+CC0+CM0
Cp0 = (CA0*CpA0+CB0*CpB0+CC0*CpC0+CM0*CpM0)/C0

e = Tsp-Tr
Ac = Ab+Kp*(e+Ai/taui)
xs = 1-Ac
LIMIT xs >= 0
LIMIT xs <= 1
Fs0 = Cvs*xs*sqrt(DPs)
Ns0 = Fs0*rhos/PMs
```

```
; Datos
V = 66.84

F0 = 440.63
T0 = 70
CA0 = 0.1816
CB0 = 2.2695
CC0 = 0
CM0 = 0.2269

CpA0 = 35
CpB0 = 18
CpC0 = 46
CpM0 = 19.5

Ts0 = 60
Cps0 = 18
UA = 16000

DH = -36000
alpha = 16.96E12
Ea = 32400
Rg = 1.987

Tsp = 138.7
Ab = 0.5
Kp = 4.25E-3
taui = 0.152

rhos = 62.43
PMs = 18
DPs = 4.383E11
Cvs = 8.71E-4
```

Ver Reactor con CT.mmd

Enfoque global

Ventajas

- Más fácil de programar.
- Hecho a medida para el sistema.
- Puede funcionar en cualquier modo de simulación.
- Resolución eficiente.

Desventajas

- Difícil de depurar.
- Difícil de adaptar a cambios en el sistema.
- Requiere la solución de sistemas grandes de ecuaciones no lineales.
- No amigable con el usuario.

Aplicaciones

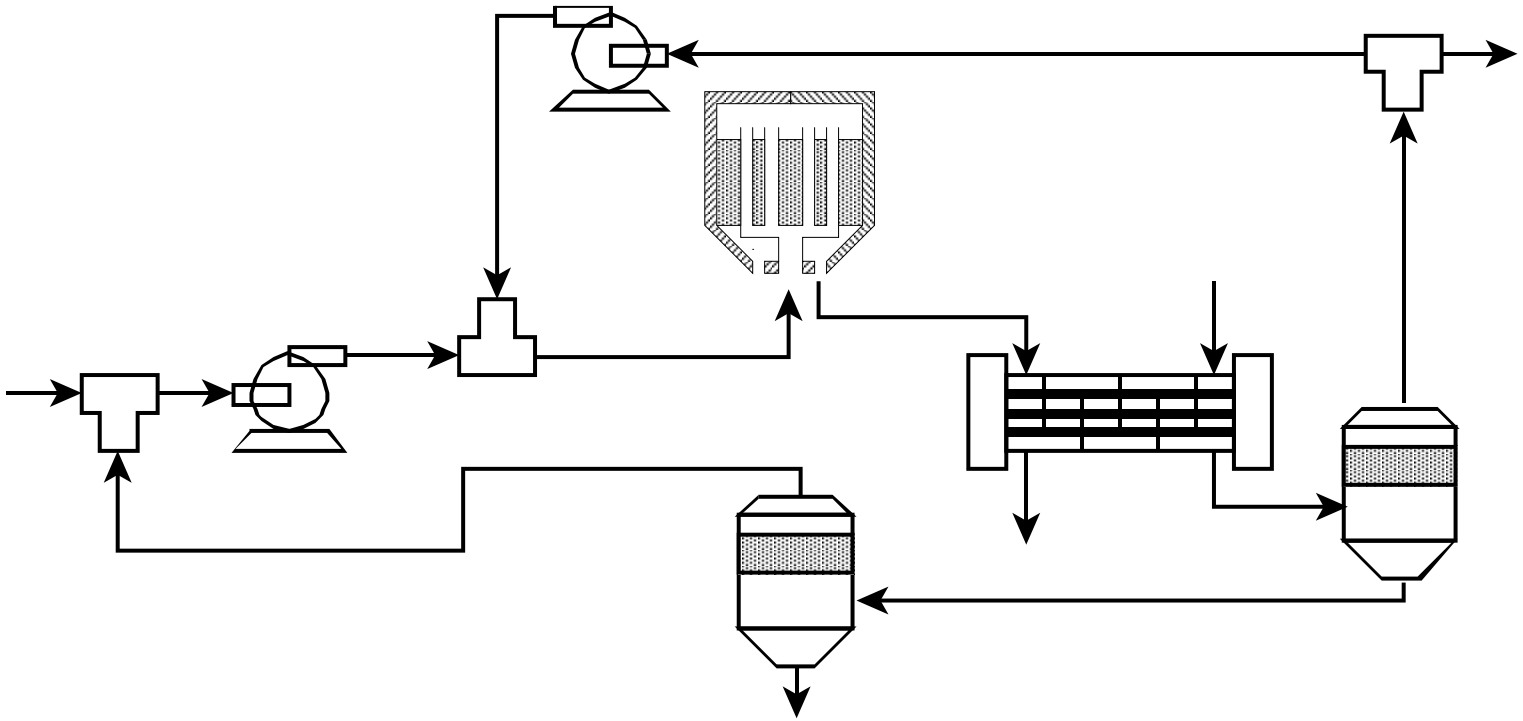
- Investigación
- Equipos especiales

Enfoques

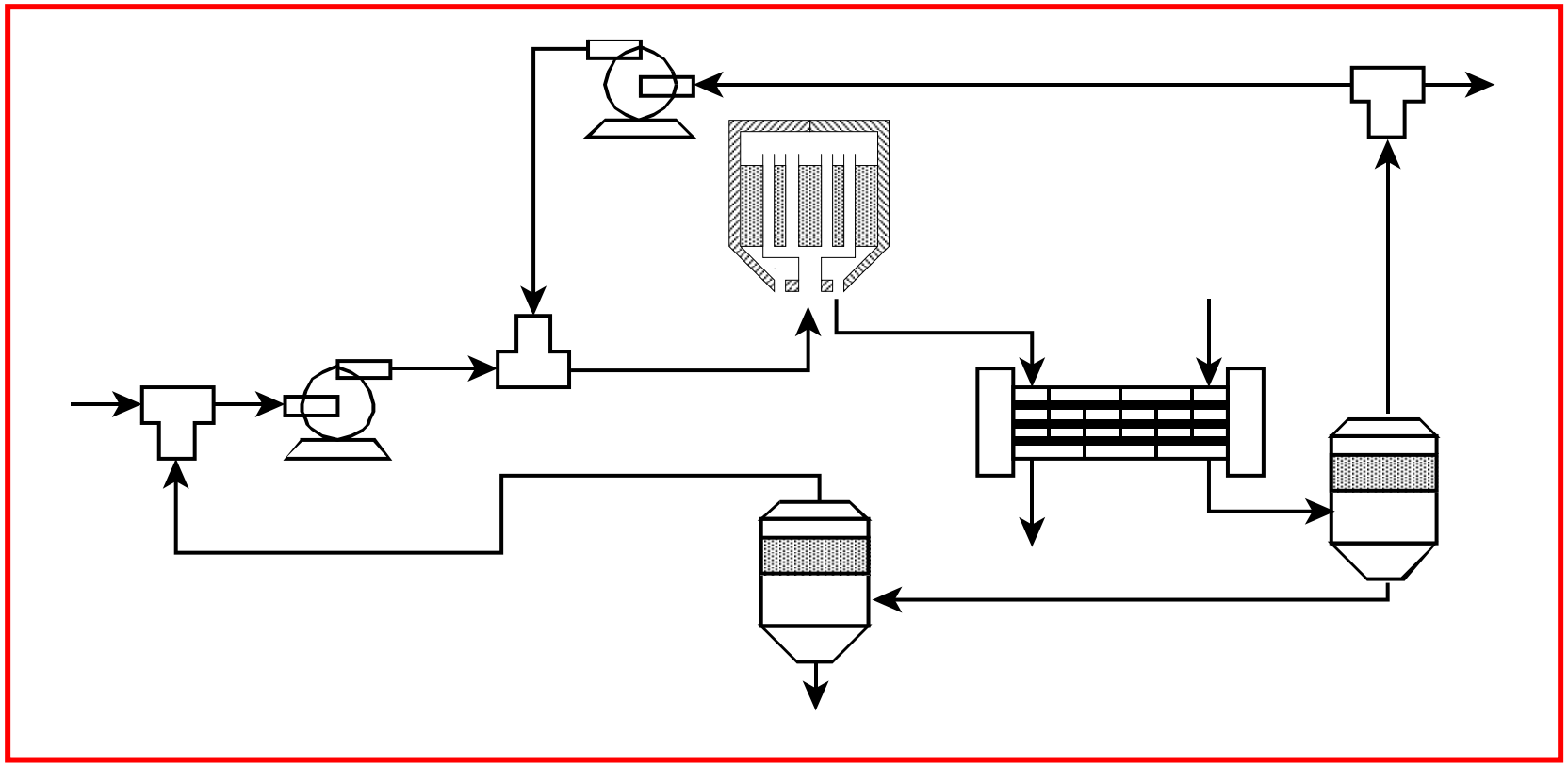
- Global u orientado a ecuaciones
- Modular

Enfoque modular

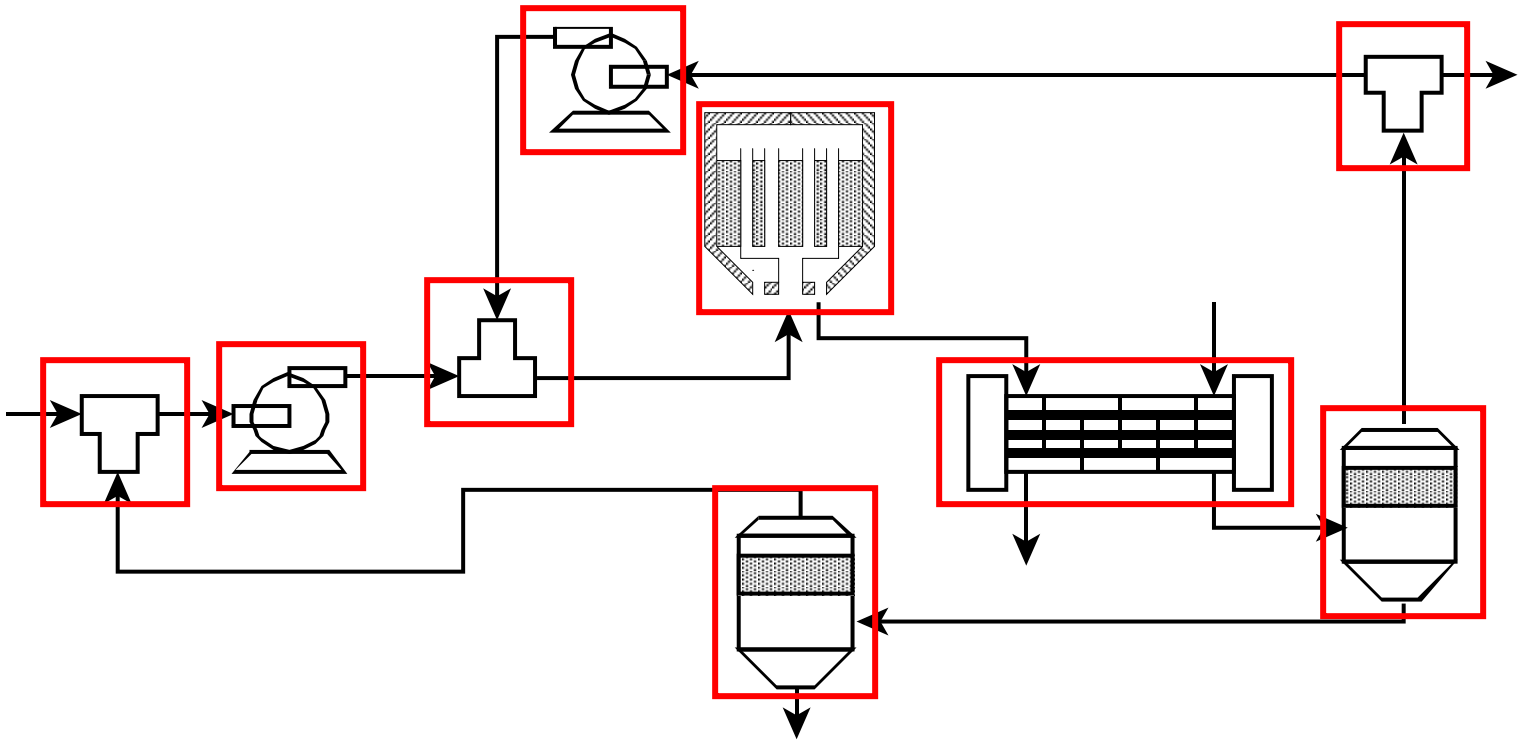
Planta de NH_3



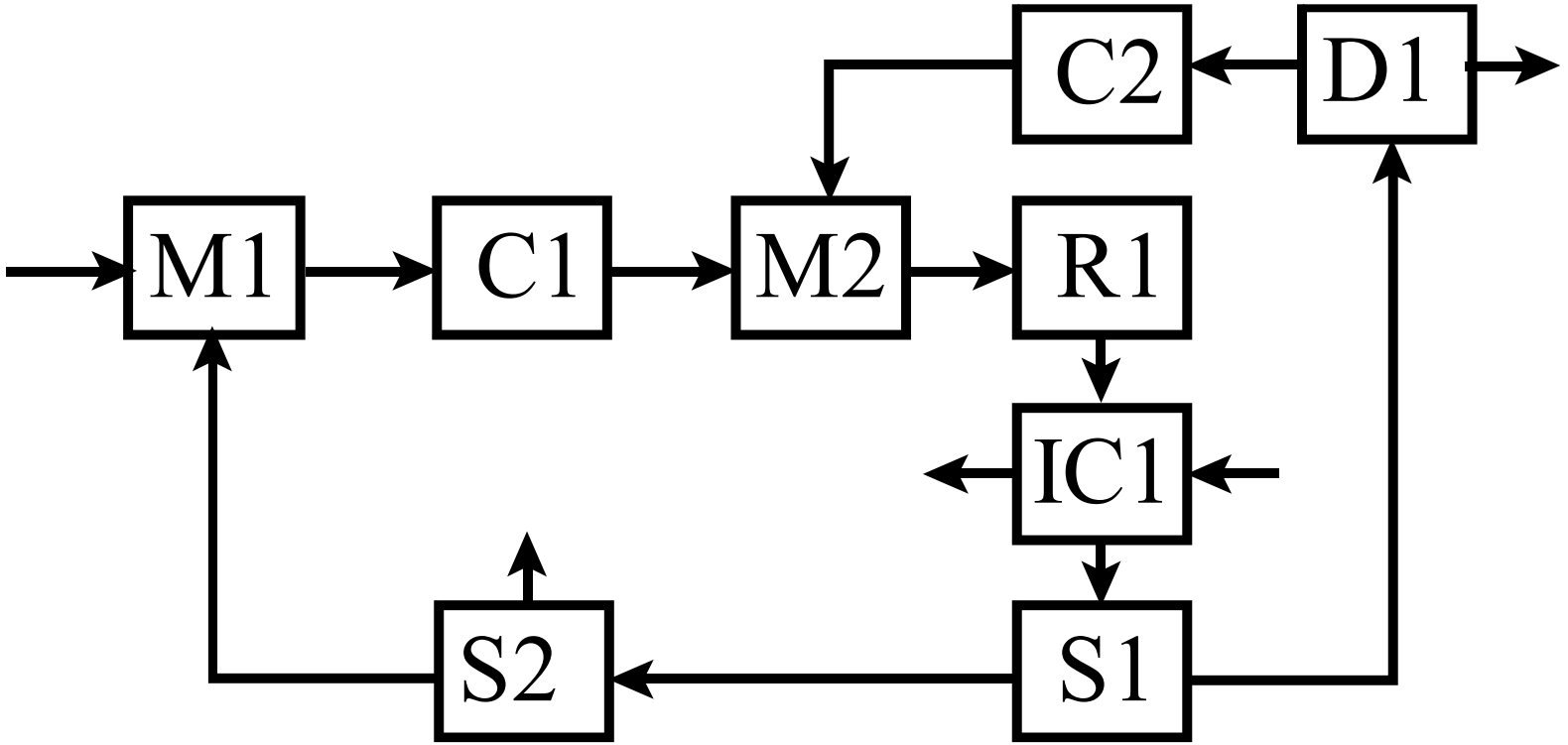
Enfoque global

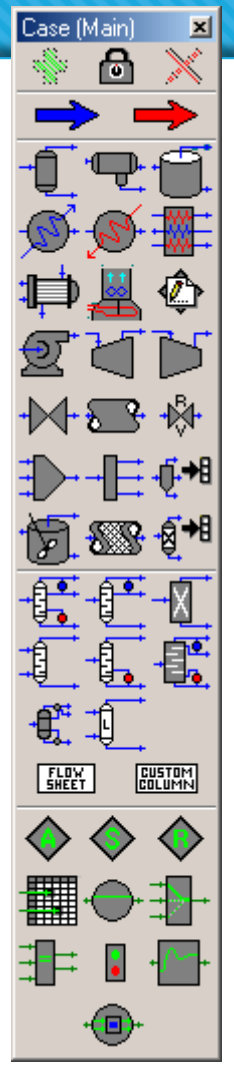


Enfoque modular



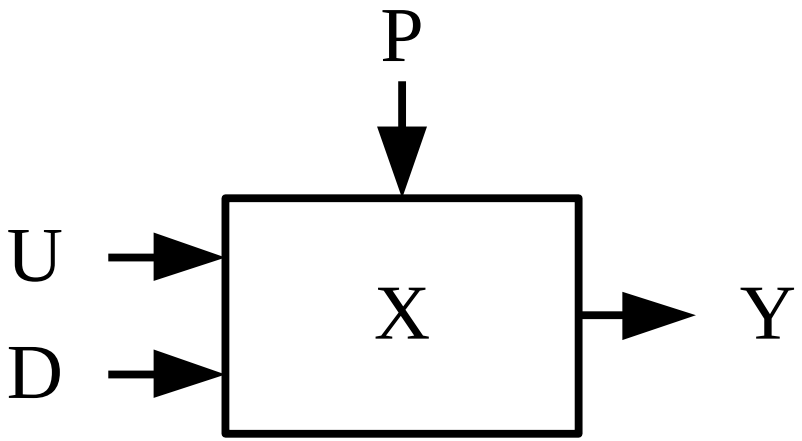
Enfoque modular





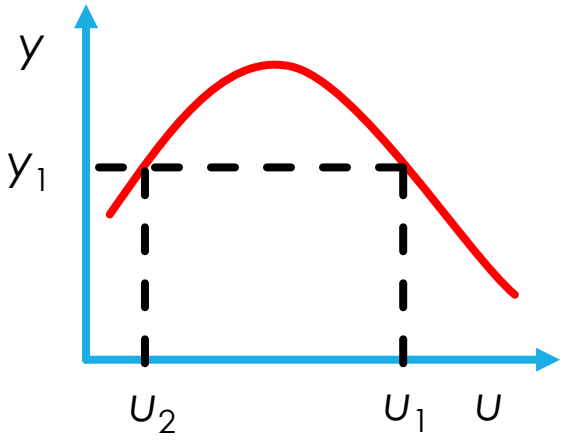
Módulo en modo análisis

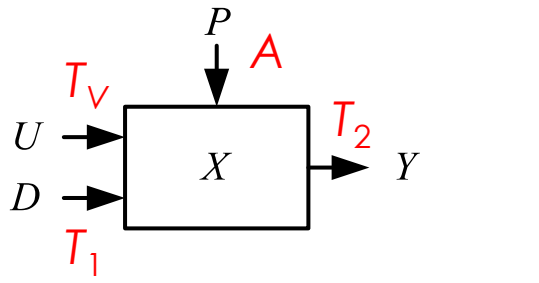
- Entrada (*U* y *D*)
- Parámetros (*P*)
- Estado (X)
- Salida (*Y*)

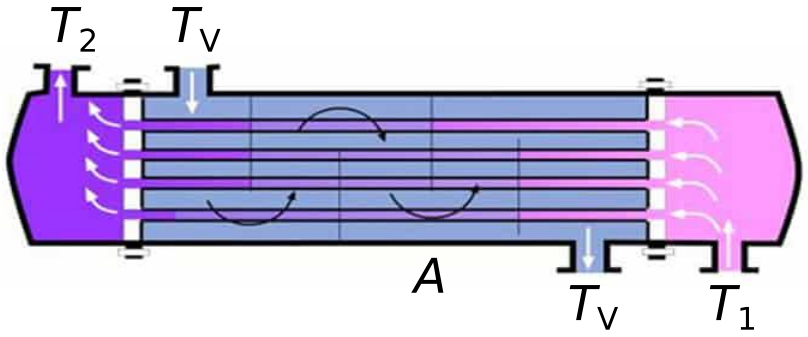


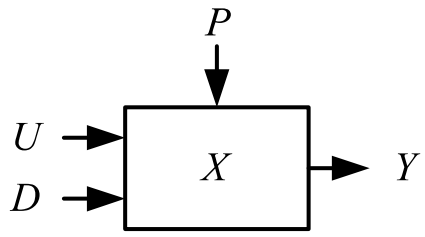
Intercambiador de calor

Modos de simulación

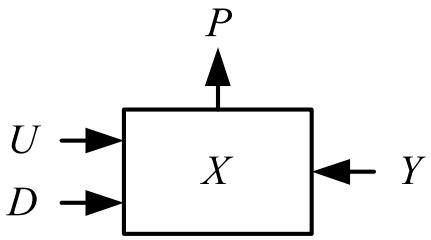




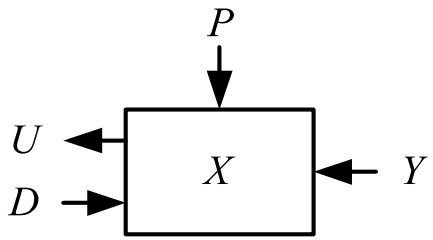




Modo Análisis

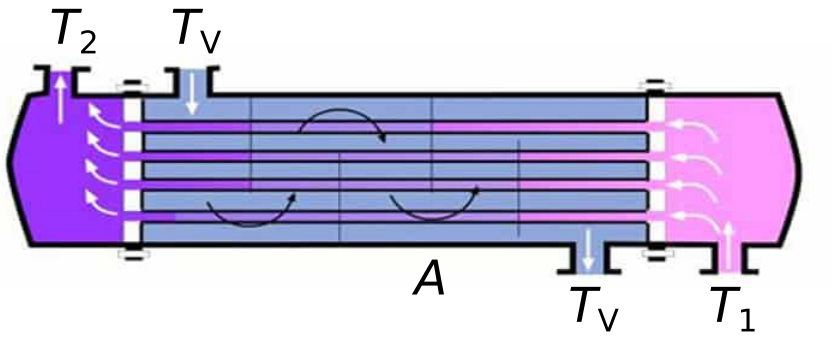


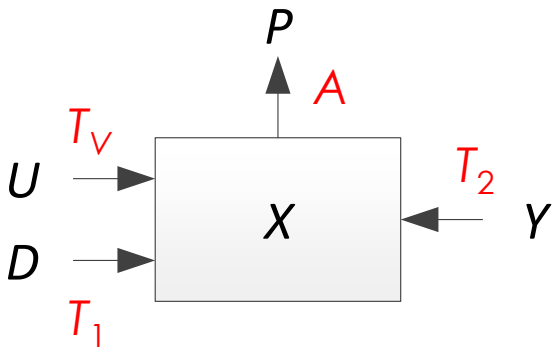
Modo Diseño



Modo Control

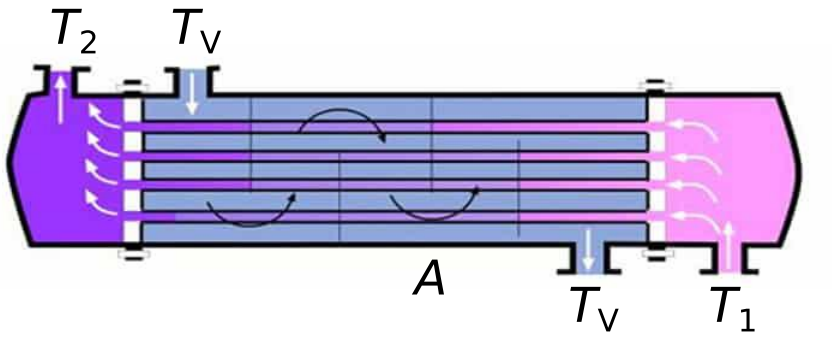
Emulación de modo diseño

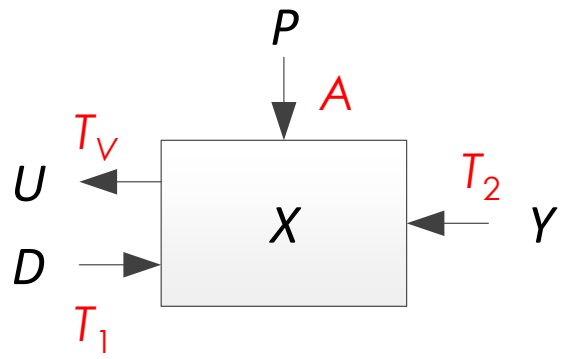




Modo Diseño

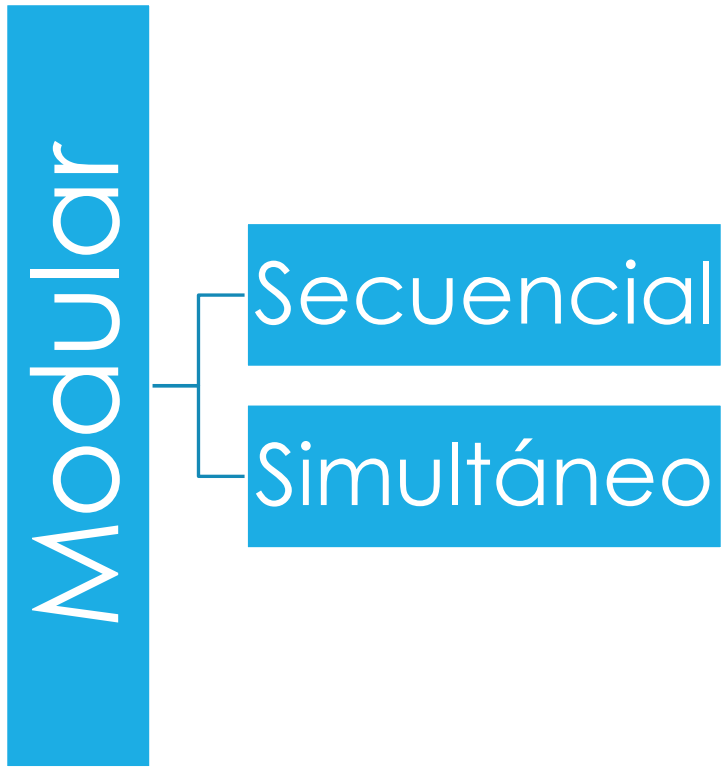
Emulación de modo control



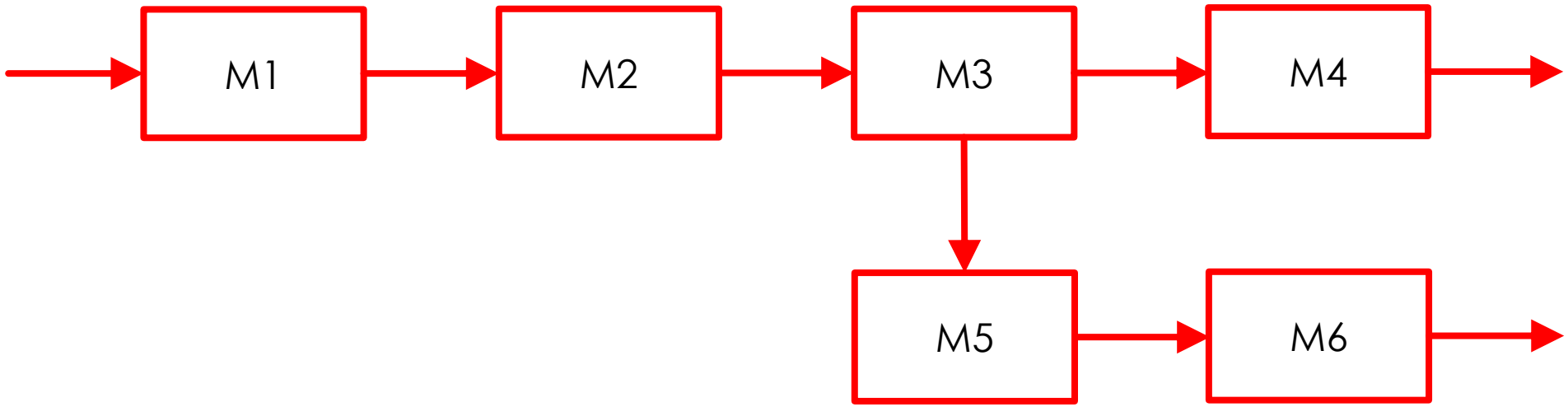


Modo Control

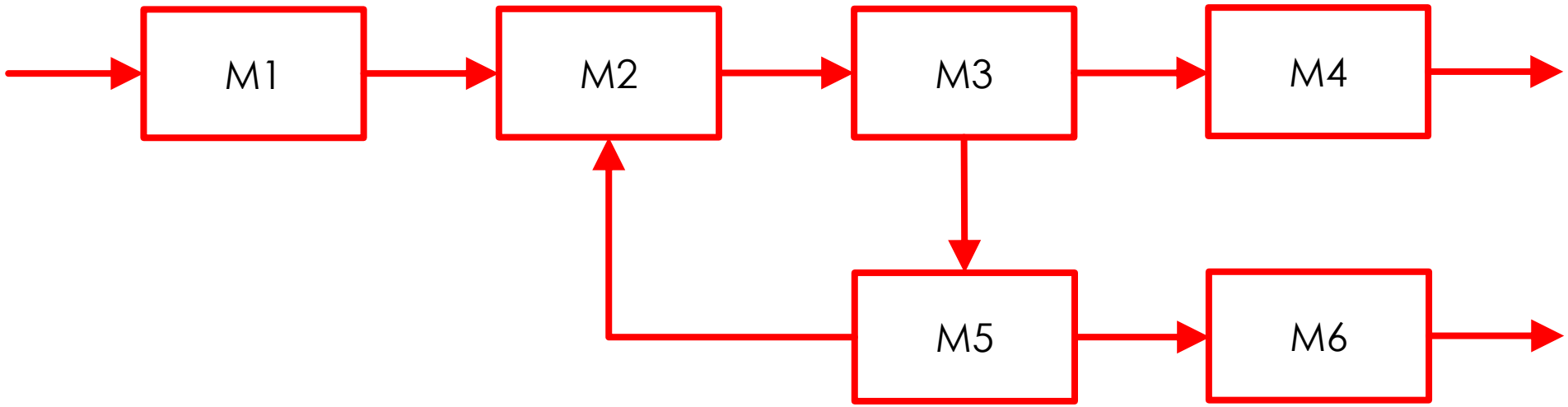
Enfoque modular



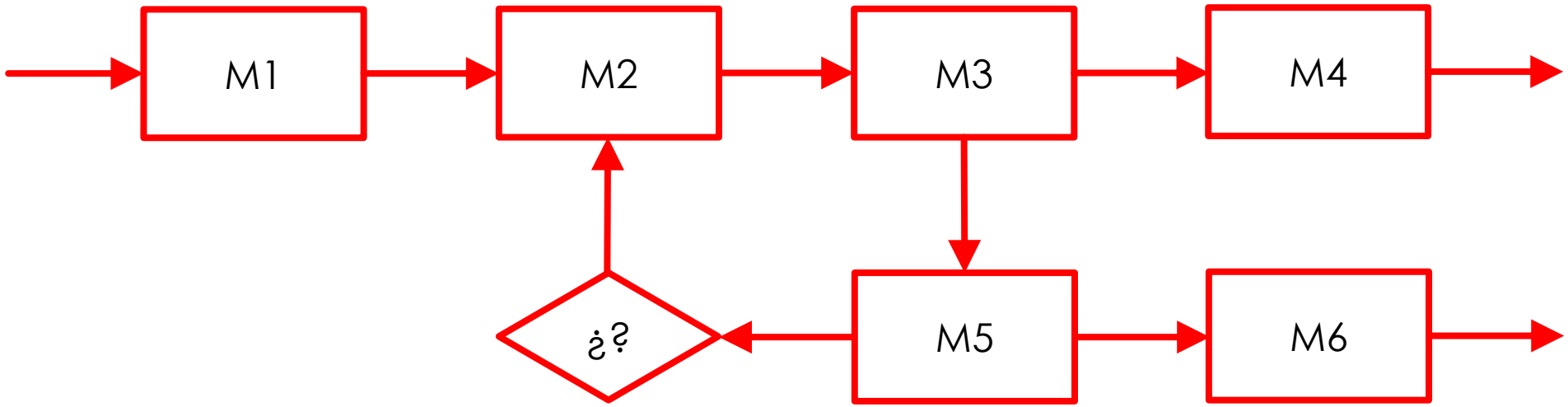
Modular secuencial



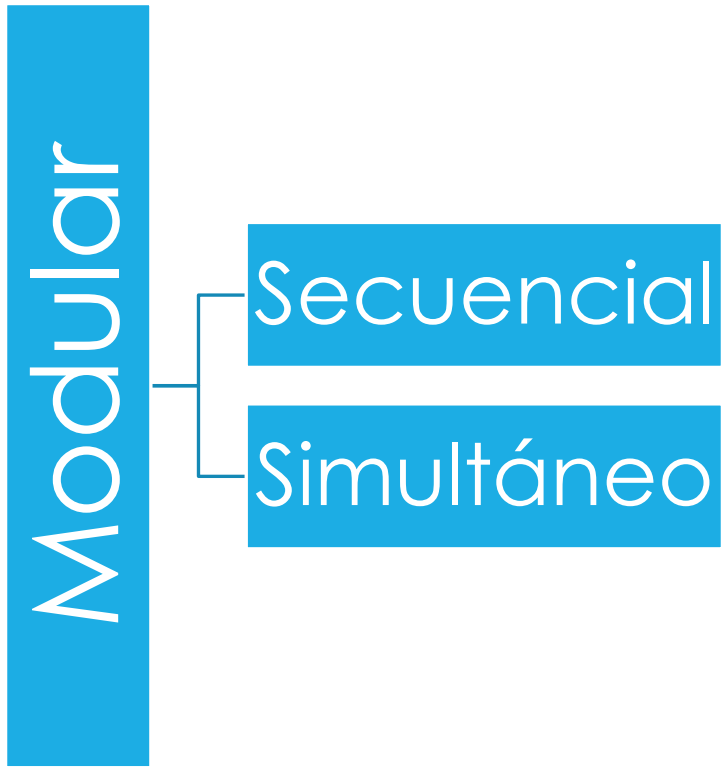
Modular secuencial



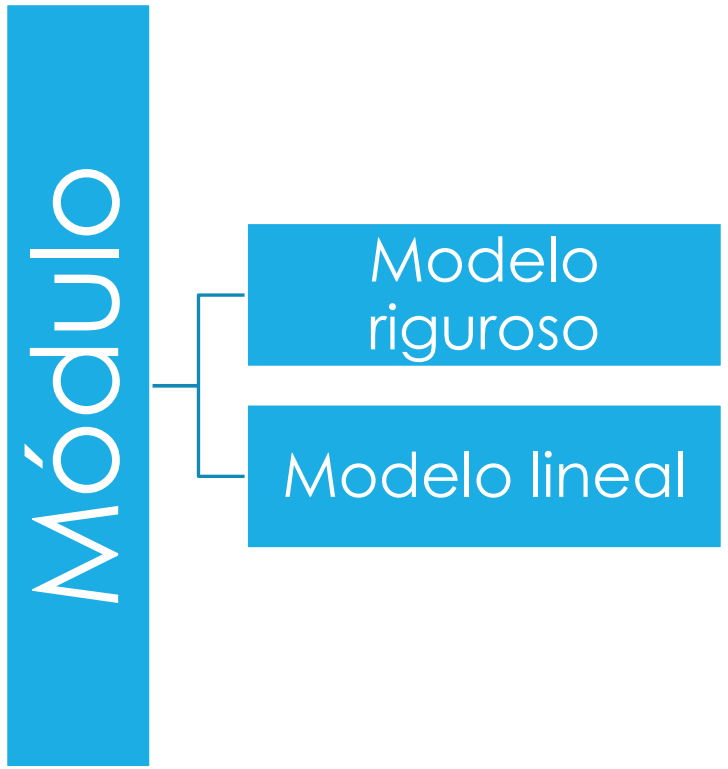
Modular secuencial



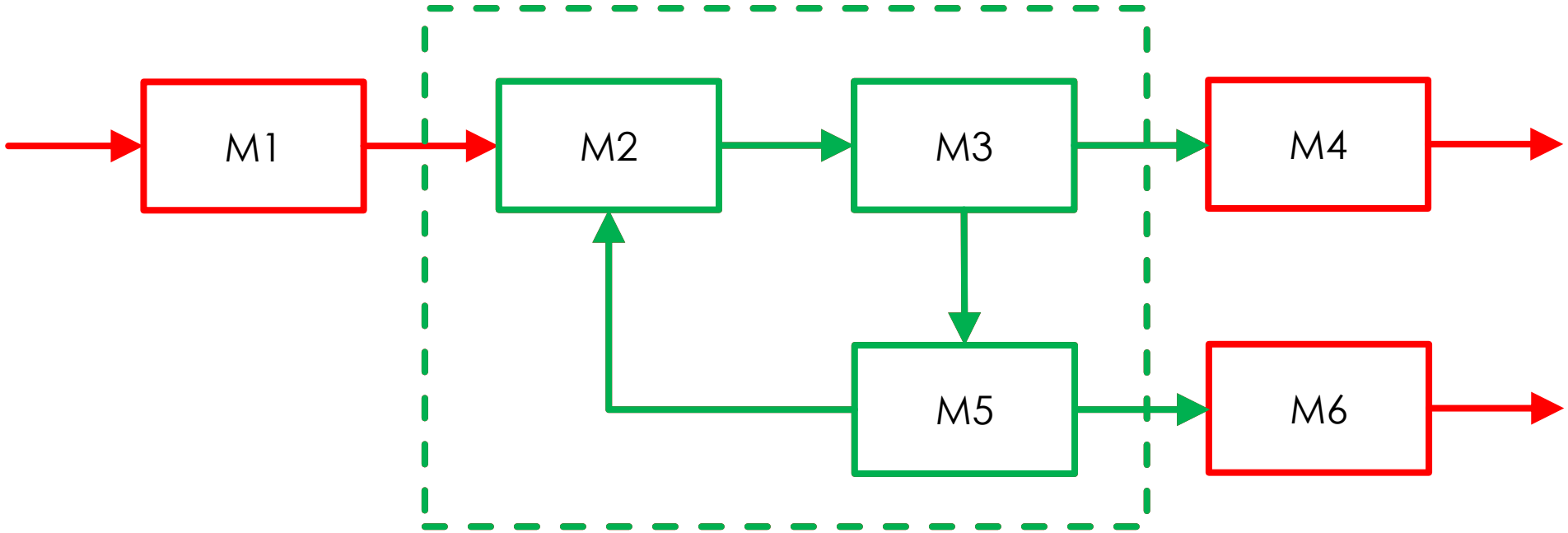
Enfoque modular



Modular simultáneo



Modular simultáneo



Modelo lineal

$$\begin{cases} a_{11}x_1 & +a_{12}x_2 & +\ldots & +a_{1n}x_n & = b_1 \\ a_{21}x_1 & +a_{22}x_2 & +\ldots & +a_{2n}x_n & = b_2 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ a_{m1}x_1 & +a_{m2}x_2 & +\ldots & +a_{mn}x_n & = b_m \end{cases}$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}$$

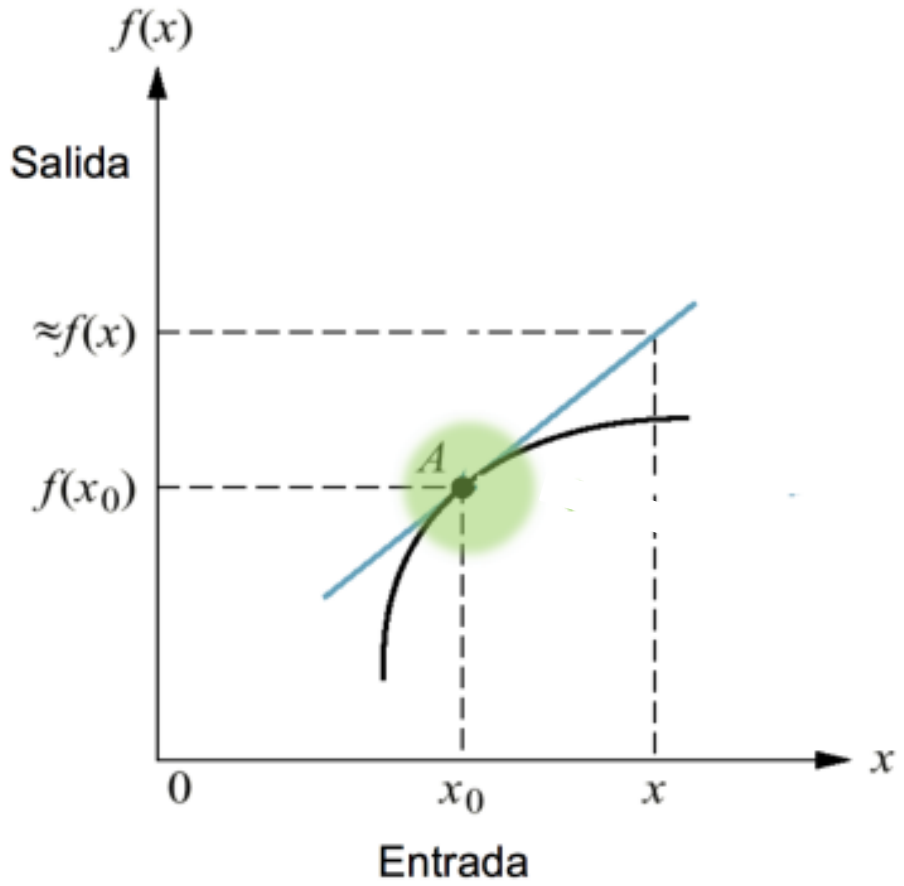
$\Rightarrow Ax = b \Rightarrow x = A^{-1}b$

Sistema de ecuaciones lineales

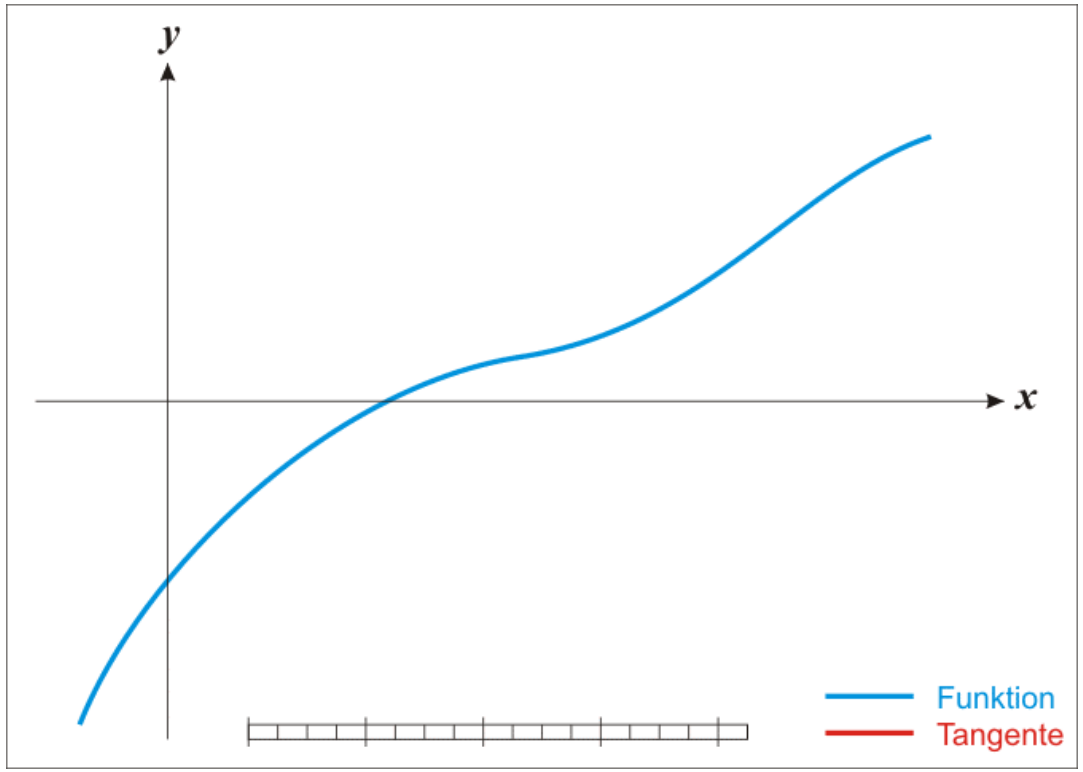
Modular simultáneo

1. Proponer A para el sistema lineal $Ax = b$.
2. Resolver el sistema $x = A^{-1}b$.
3. Usar x y los modelos rigurosos para determinar la nueva A_{n}.
4. Si $|A - A_{\mathrm{n}}| < tol$, fin; si no, $A \leftarrow A_{\mathrm{n}}$, ir a 2.

Linealización



Método de Newton



$$
\begin{aligned}
x_1 &= x_0 - \frac{f(x_0)}{f'(x_0)} &&= 0,5 - \frac{\cos(0,5) - 0,5^3}{-\sin(0,5) - 3 \times 0,5^2} &&= 1,112141637097 \\
x_2 &= x_1 - \frac{f(x_1)}{f'(x_1)} && \vdots && = \underline{0},909672693736 \\
x_3 & \vdots && \vdots && = \underline{0,867263818209} \\
x_4 & \vdots && \vdots && = \underline{0,865477135298} \\
x_5 & \vdots && \vdots && = \underline{0,865474033111} \\
x_6 & \vdots && \vdots && = \underline{0,865474033102}
\end{aligned}
$$

Enfoque modular

Ventajas

- Flexible a cambios en el sistema.
- Grupos especializados en cada módulo.
- Físico-química separada.
- Consume menos memoria.
- Amigable con el usuario.
- Generales.

Desventajas

- Difícil de programar.
- No está disponible para algunos sistemas.
- Funciona solo en modo análisis.
- Resolución ineficiente.

Aplicaciones

- Simuladores comerciales
- Plantas refinadoras

Simuladores de planta

Estructura del simulador

Fluid Package

- Propiedades de compuestos puros:
  - Termodinámicas: *H*, *S*.
  - Físicas y de transporte: ρ, μ, k_T, σ.
- Propiedades de mezclas:
  - Termodinámicas
  - Físicas y de transporte
- Compuestos y propiedades del usuario

- EOSs:
  - Base teórica
  - Sistemas ideales: Petróleo, gas y petroquímica.
  - PR, PRSV
- *Activity Models*:
  - Empíricos
  - Sistemas no ideales: Substancias líquidas polares.
  - NRTL, Margules, UNIQUAC

Modelos físicos-químicos

- Chao Seader Models:
  - H_2, hidrocarburos pesados
- *Vapour Pressure Models*:
  - Mezclas ideales a baja presión
  - Antoine
- *Micellaneous*:
  - Amine, ASME Steam, NBS Steam

- Opciones:
  - Estimación de entalpía
  - Estimación de fase vapor
  - Estimación de múltiples fases líquidas

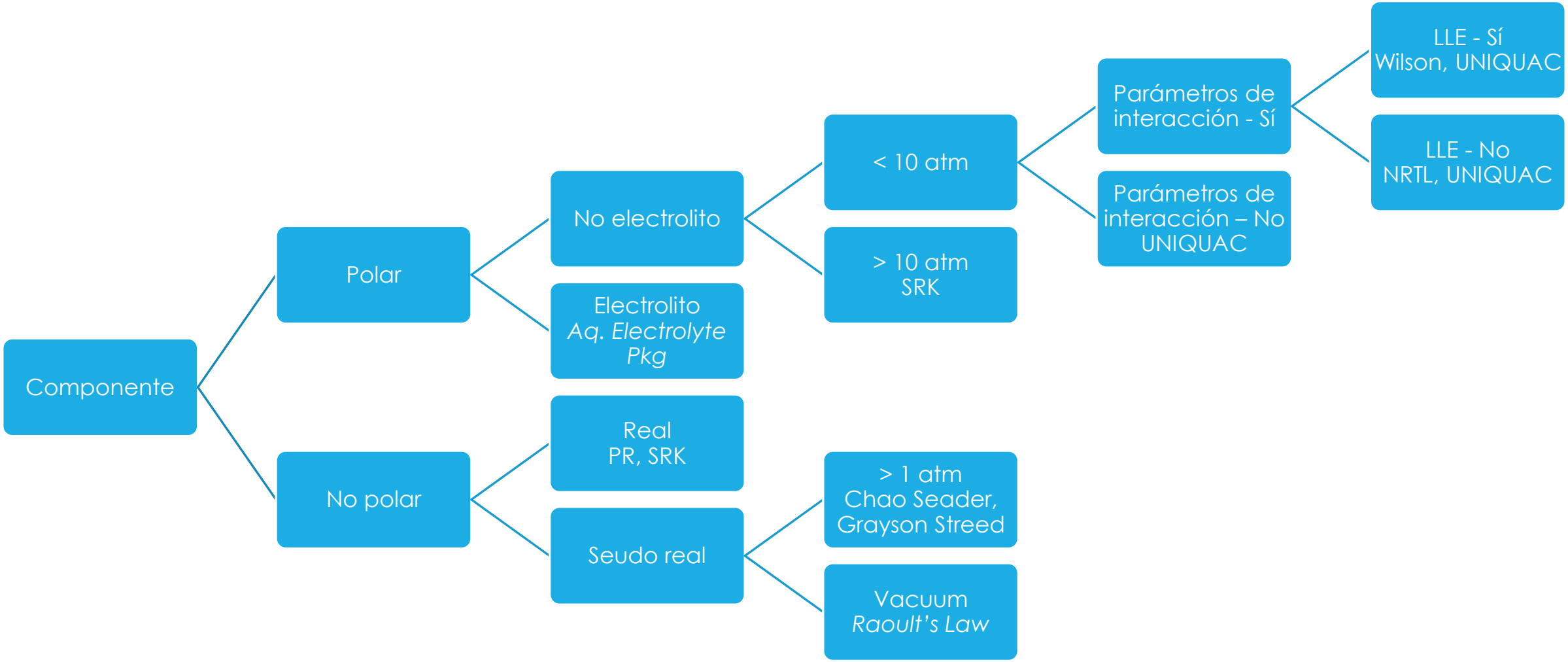
Selección del *fluid package*

Guía general

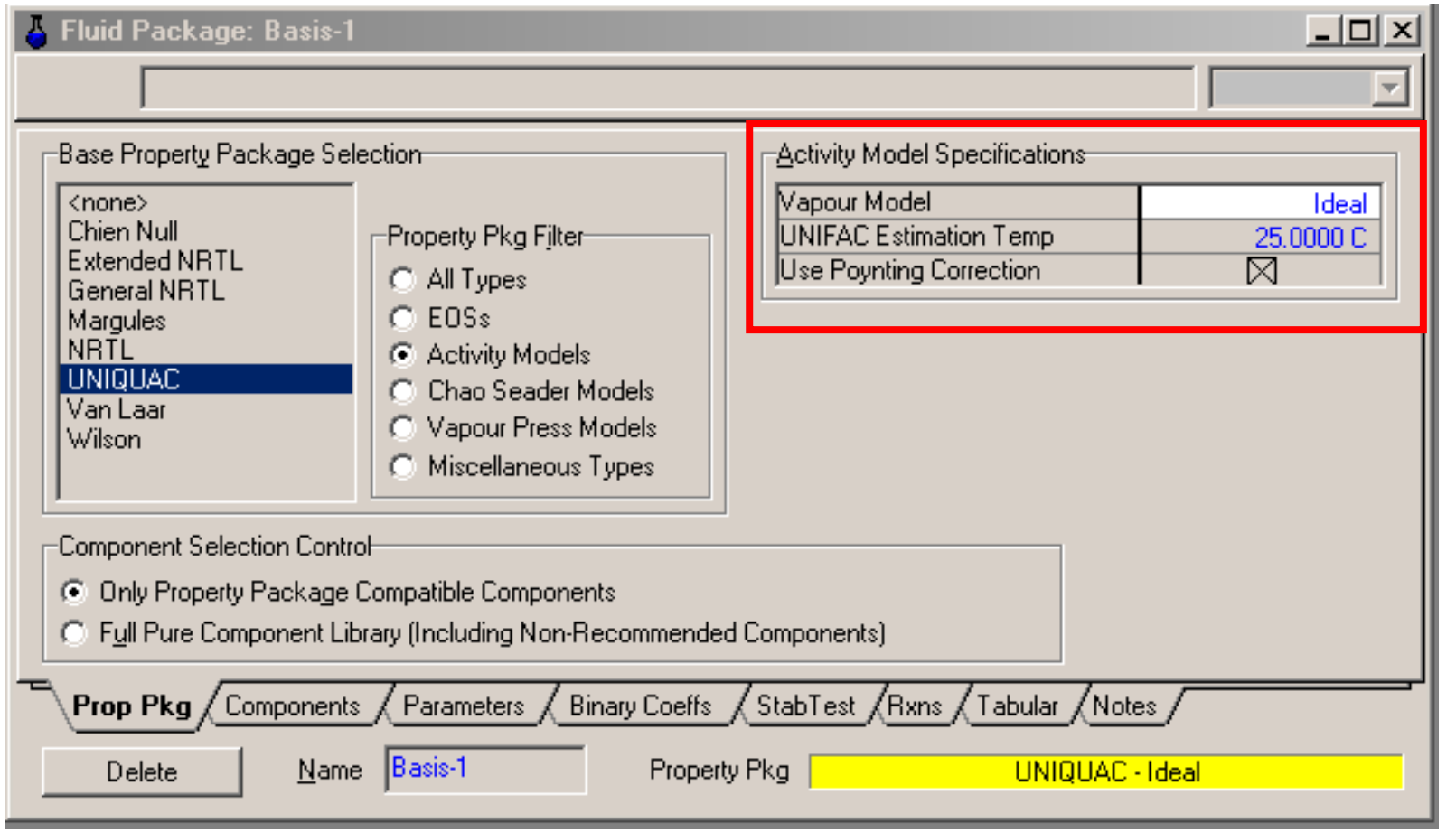
- EOSs: Componentes no polares. Amplio rango de *P* y *T*.
- *Activity Models*: Líquidos no ideales.
- Comparar los diagramas de fase con los experimentales.

Casos

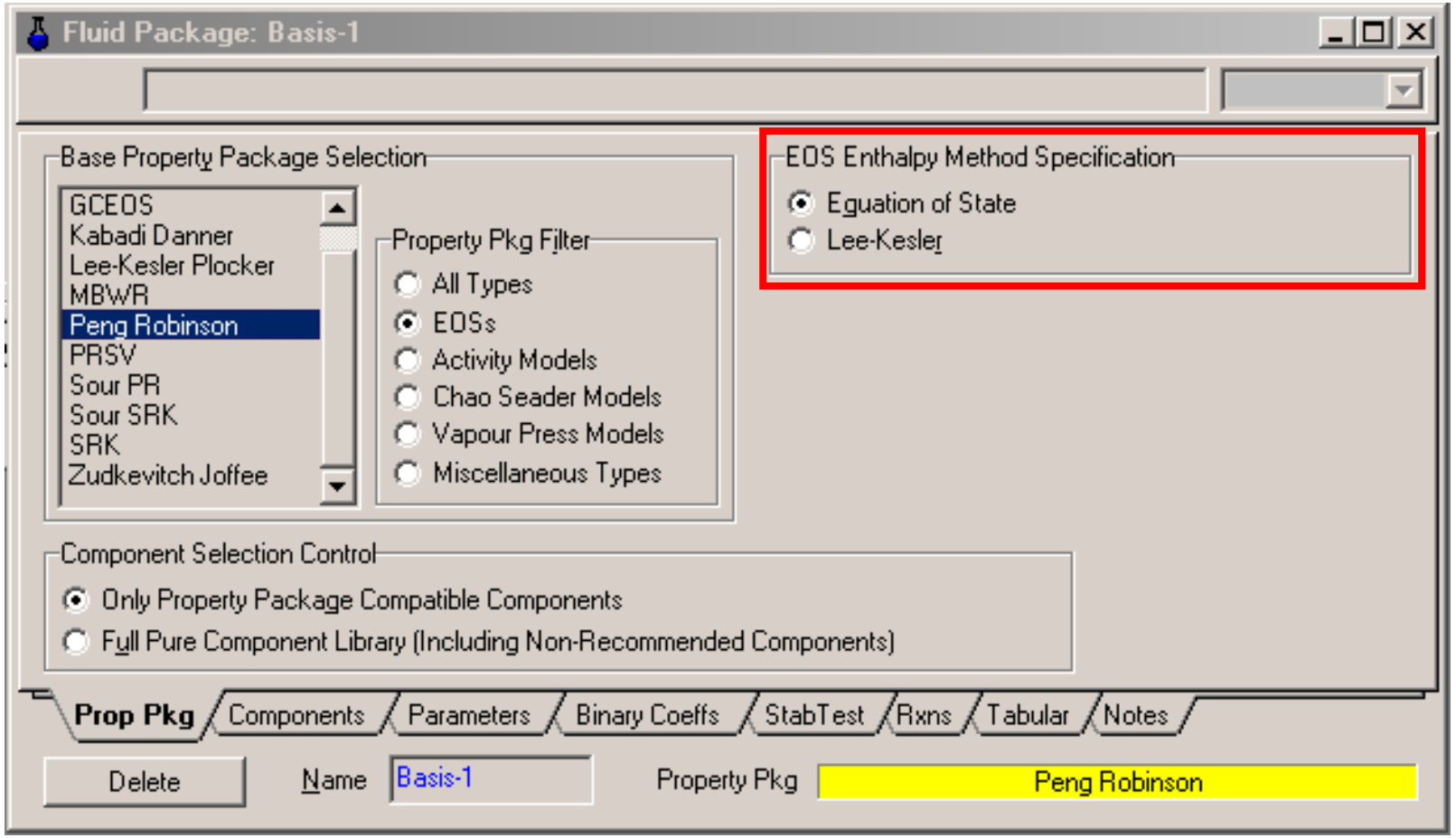
- Hidrocarburos: Peng Robinson.
- Agua y varpor: *Steam Package*.
- H_2S, CO_2 y NH_3: *Sour wáter*.
- Hidrocarburos, 0-500 °C, menos de 10000 kPa: Chao Seader.


Componente
Polar
No polar
No electrolito
Electrolito
Aq. Electrolyte
Pkg
Real
PR, SRK
Seudo real
< 10 atm
> 10 atm
SRK
> 1 atm
Chao Seader,
Grayson Streed
Vacuum
Raoult's Law
Parámetros de interacción - Sí
Parámetros de interacción – No
UNIQUAC
LLE - Sí
Wilson, UNIQUAC
LLE - No
NRTL, UNIQUAC

Modelos físicos-químicos



Modelos físicos-químicos



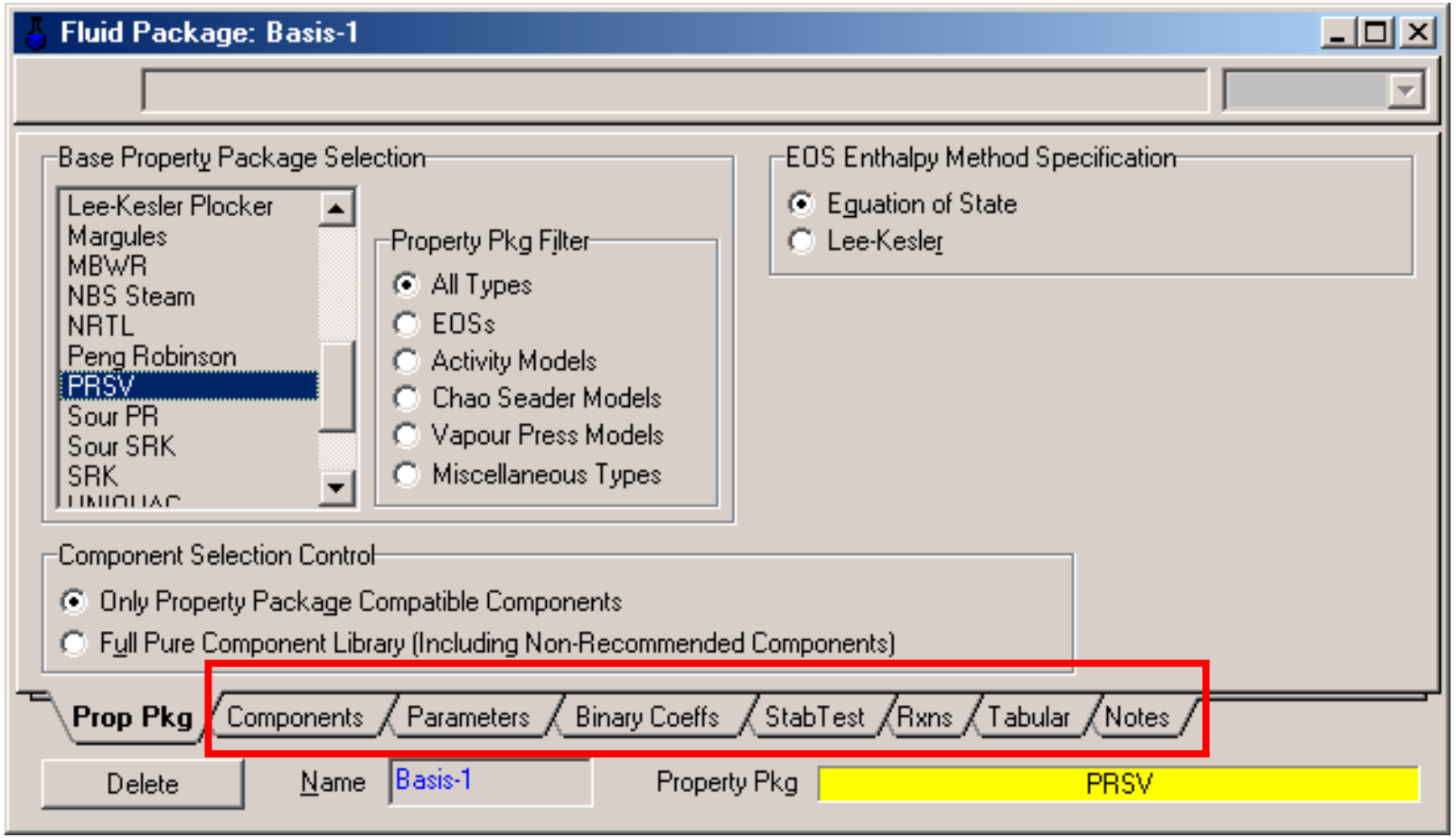
Modelos físicos-químicos

- Rango de aplicación:
  - Compuestos recomendados
  - Condiciones del proceso (*P*, *T*, x)

Modelos físicos-químicos

- Personalización:
  - Parámetros;
  - Tabular (regresión);
  - Hypothetical;
  - Oil Manager;
  - User Property.

Modelos físicos-químicos

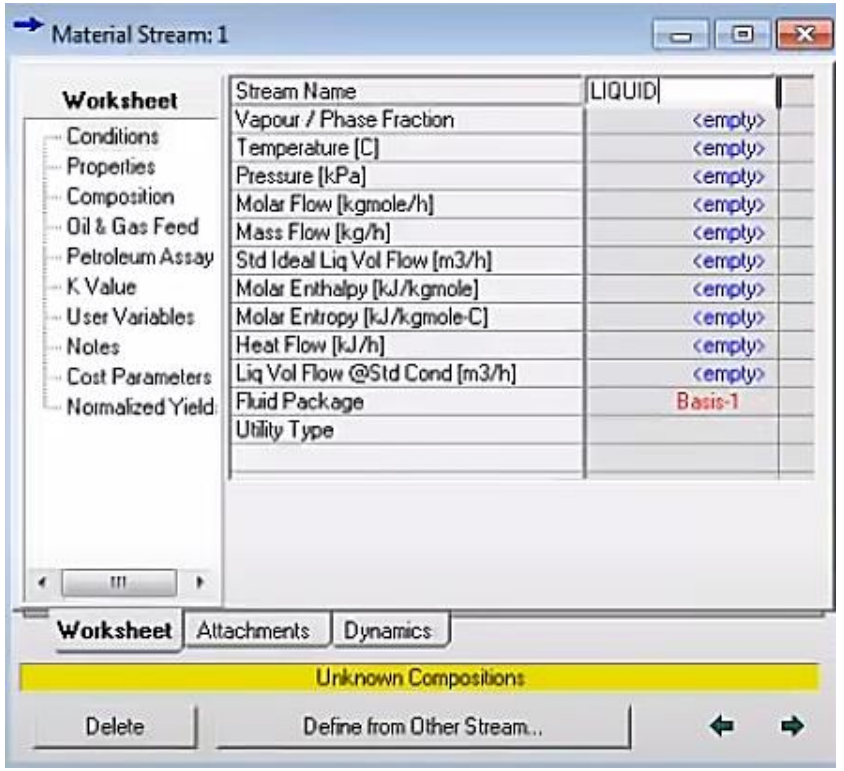


Cálculo de flash

Corriente material

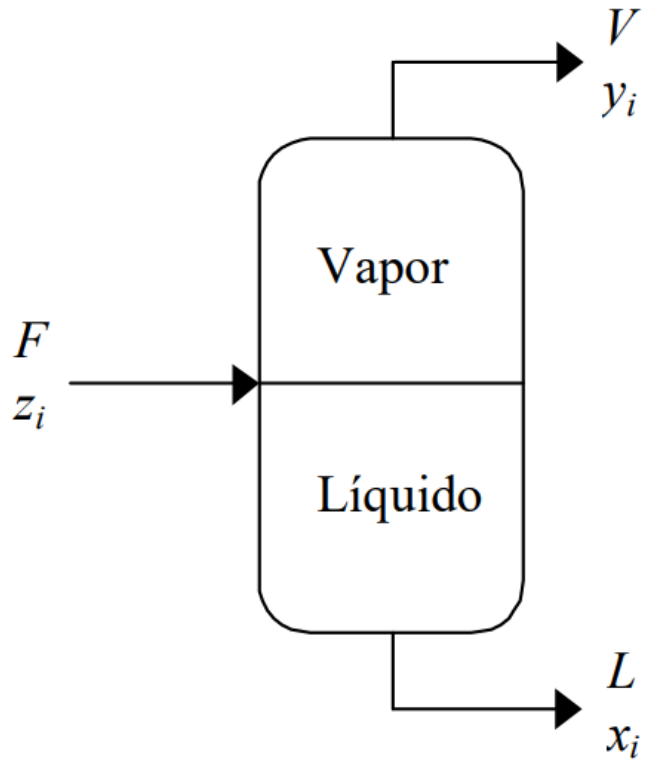
Corriente material

- Composición
- Flujo
- Presión
- Temperatura
- →Cálculo flash isotérmico



Cálculo flash

- BM: $F = L + V$
- BC: $z_i F = x_i L + y_i V$
- Equilibrio: $y_i = K_i x_i$
- Fracción vapor: $\theta = \frac{V}{F}$
- $\sum_i x_i = 1 , \sum_i y_i = 1$
- Incógnitas: x_i, y_i, L, V, θ

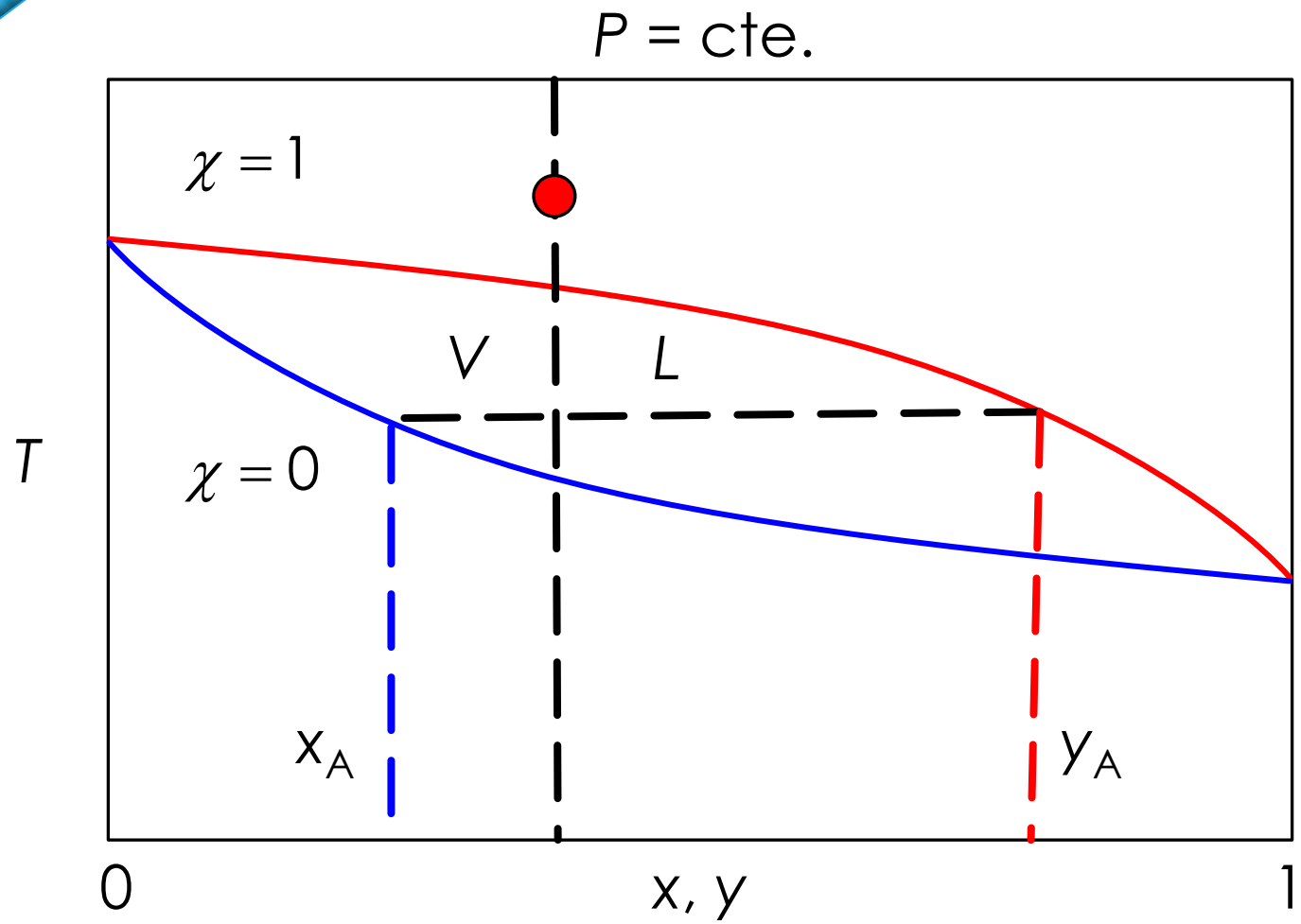


Video de cálculo flash

MATLAB

Apunte de flash

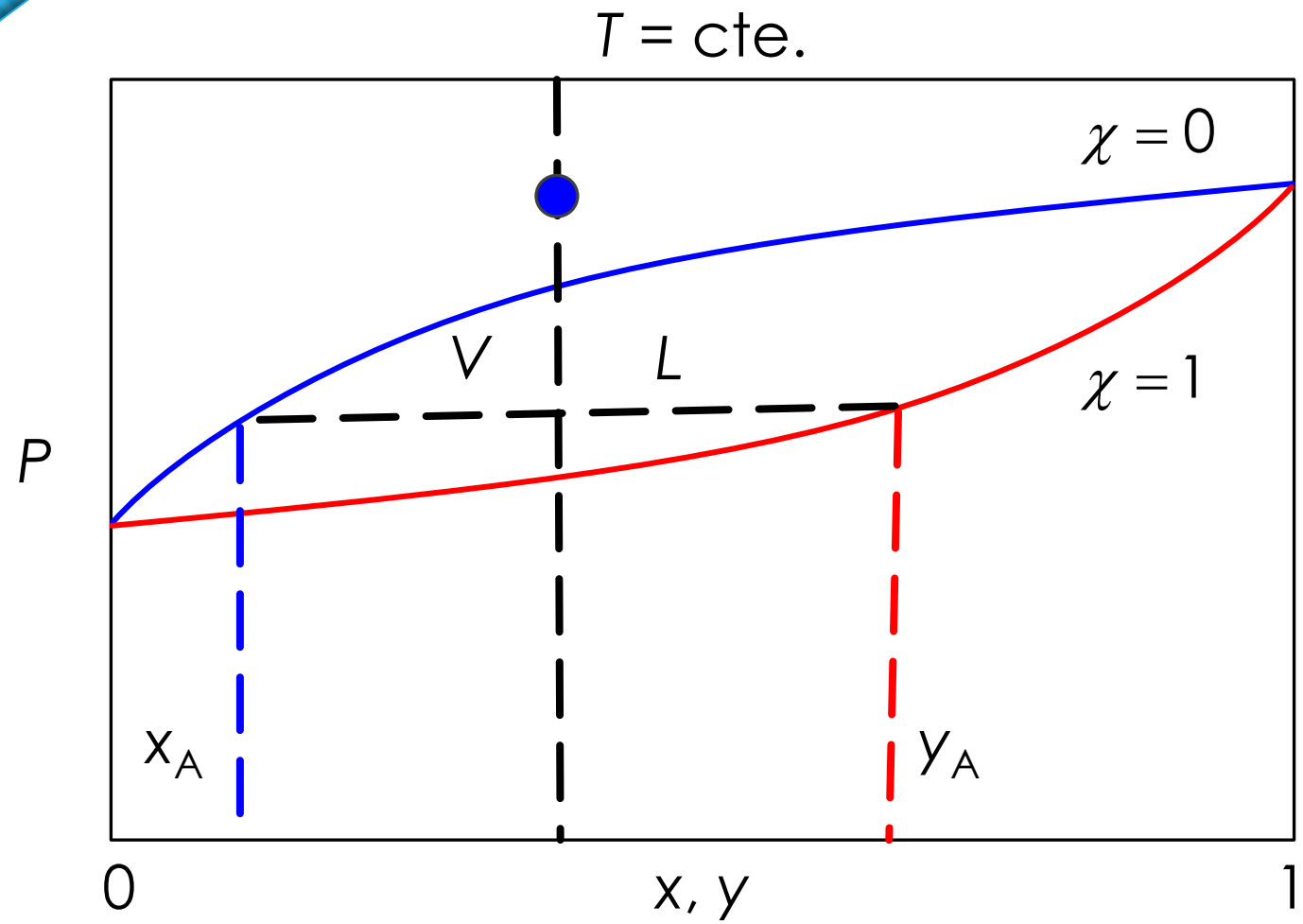
Bubble point y dew point



$$\chi = \frac{m_V}{m_V + m_L}$$

Curva de burbuja
Curva de rocío

Bubble point y dew point



$$\chi = \frac{m_V}{m_V + m_L}$$

Curva de burbuja
Curva de rocío

Cálculo de flash

Título como resultado

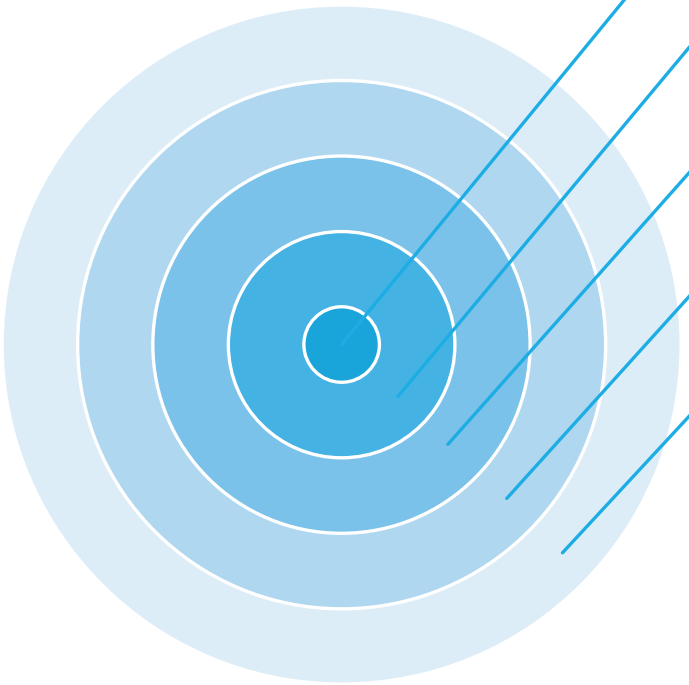
- Datos: x, *P*, *T*
  - Resultado: χ
    - Si $\chi = 0$, líquido.
    - Si $\chi = 1$, vapor.
    - Si $0 < \chi < 1$, líquido y vapor.

Título como dato

- Datos: x, *P*, χ
  - Resultado: *T*
    - Si $\chi = 0$, *T bubble point*.
    - Si $\chi = 1$, *T dew point*.
- Datos: x, *T*, χ
  - Resultado: *P*
    - Si $\chi = 0$, *P bubble point*.
    - Si $\chi = 1$, *P dew point*.

Síntesis de procesos

Síntesis de procesos



Reacciones

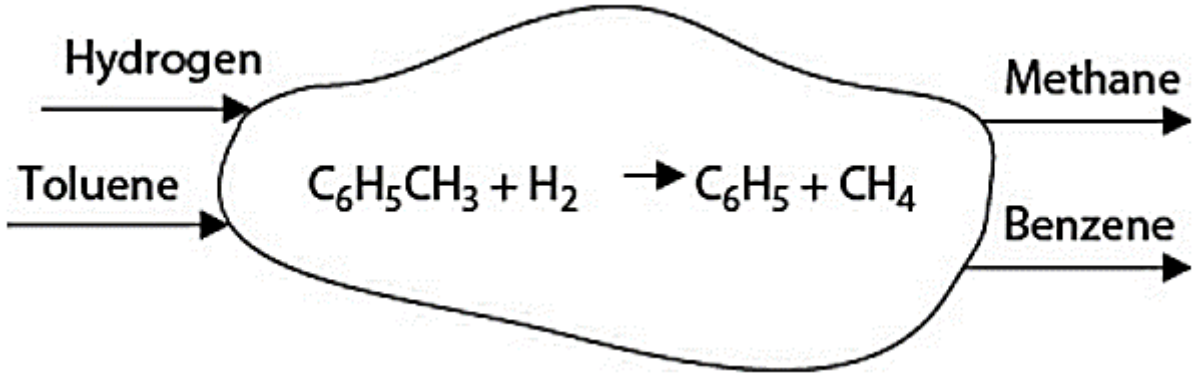
Reactores

Separadores

Intercambiadores

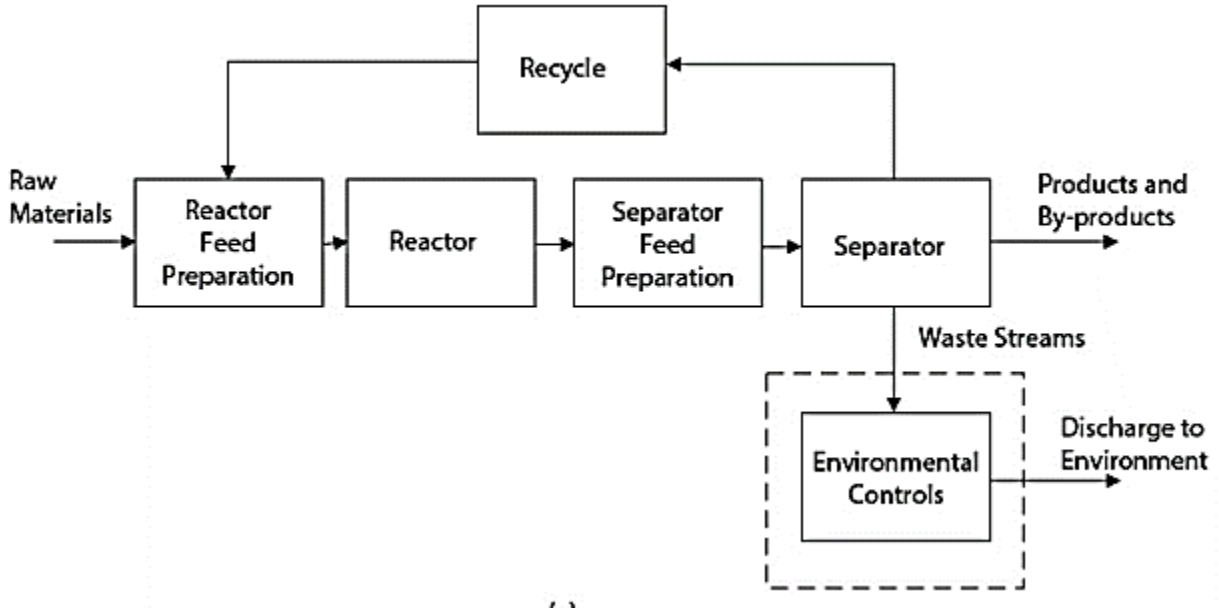
Servicios y controladores

Hidrodesalquilación de tolueno



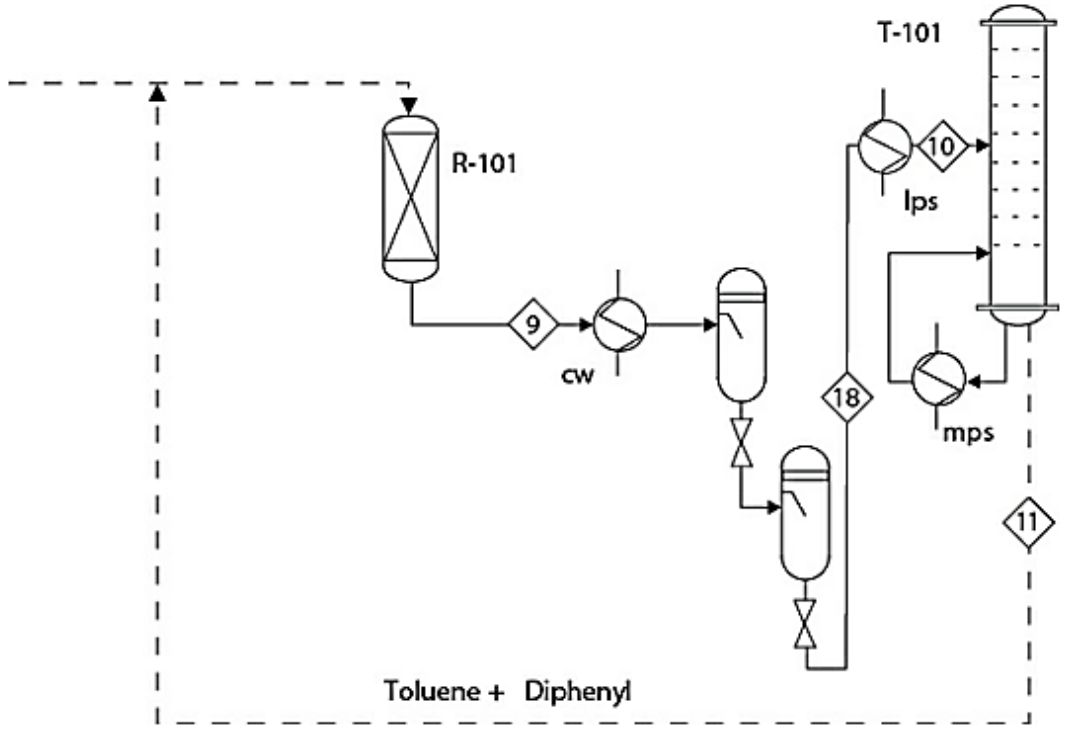
Estructura de entrada-salida

Hidrodesalquilación de tolueno



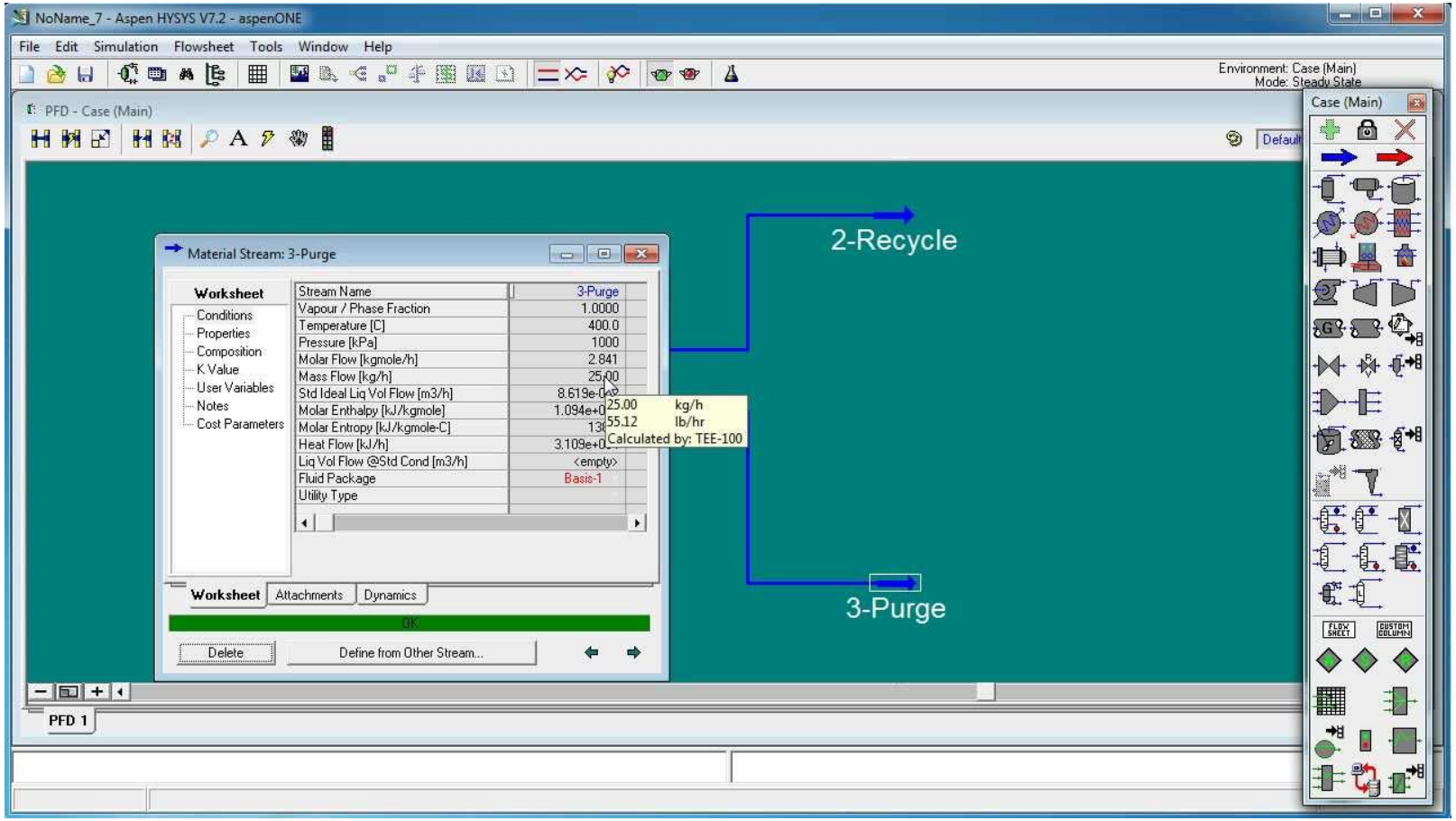
Block Flow Process diagram (BFD)

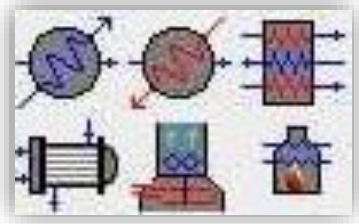
Hidrodesalquilación de tolueno

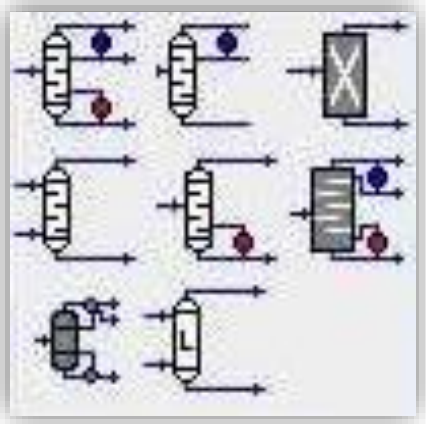


Process Flow diagram (PFD)

Niveles de modelado





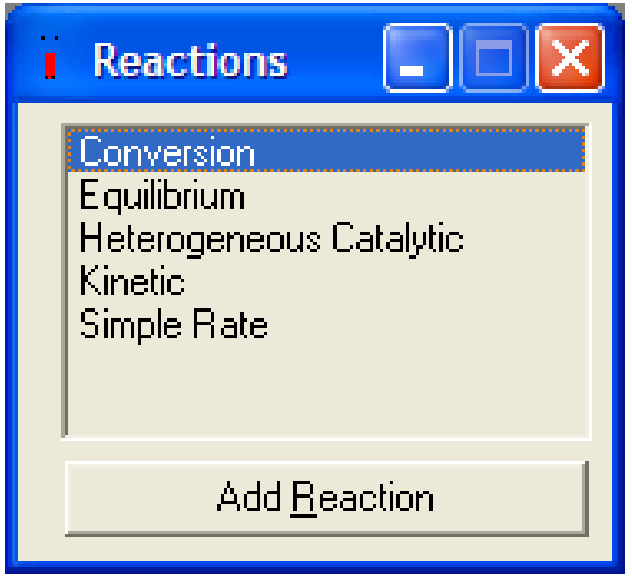


Reacciones

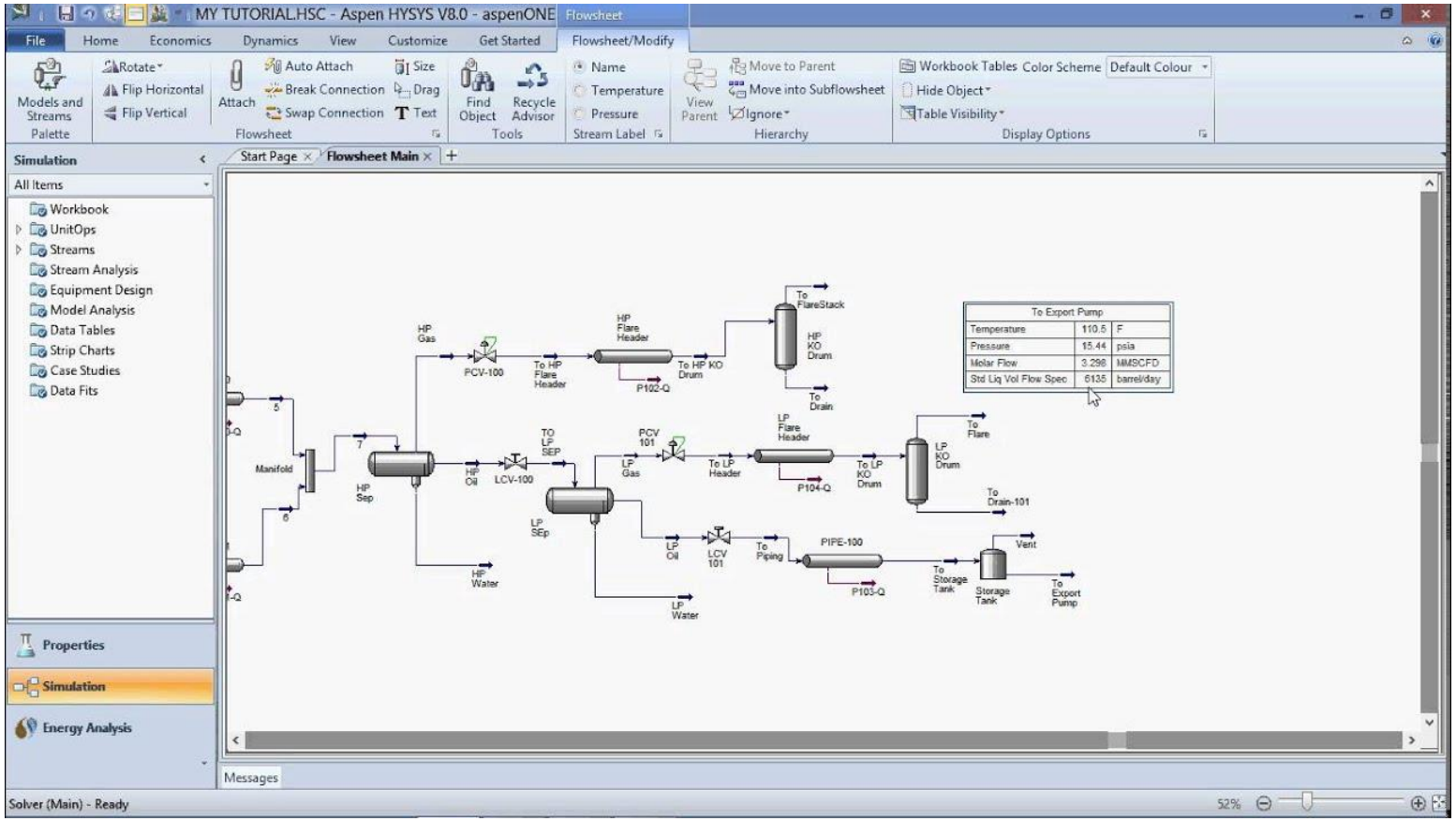
- De conversión;
- De equilibrio;
- Cinéticas;
- Cinéticas-equilibrio reverso.

$$r = k_d C_A - k_i C_B$$

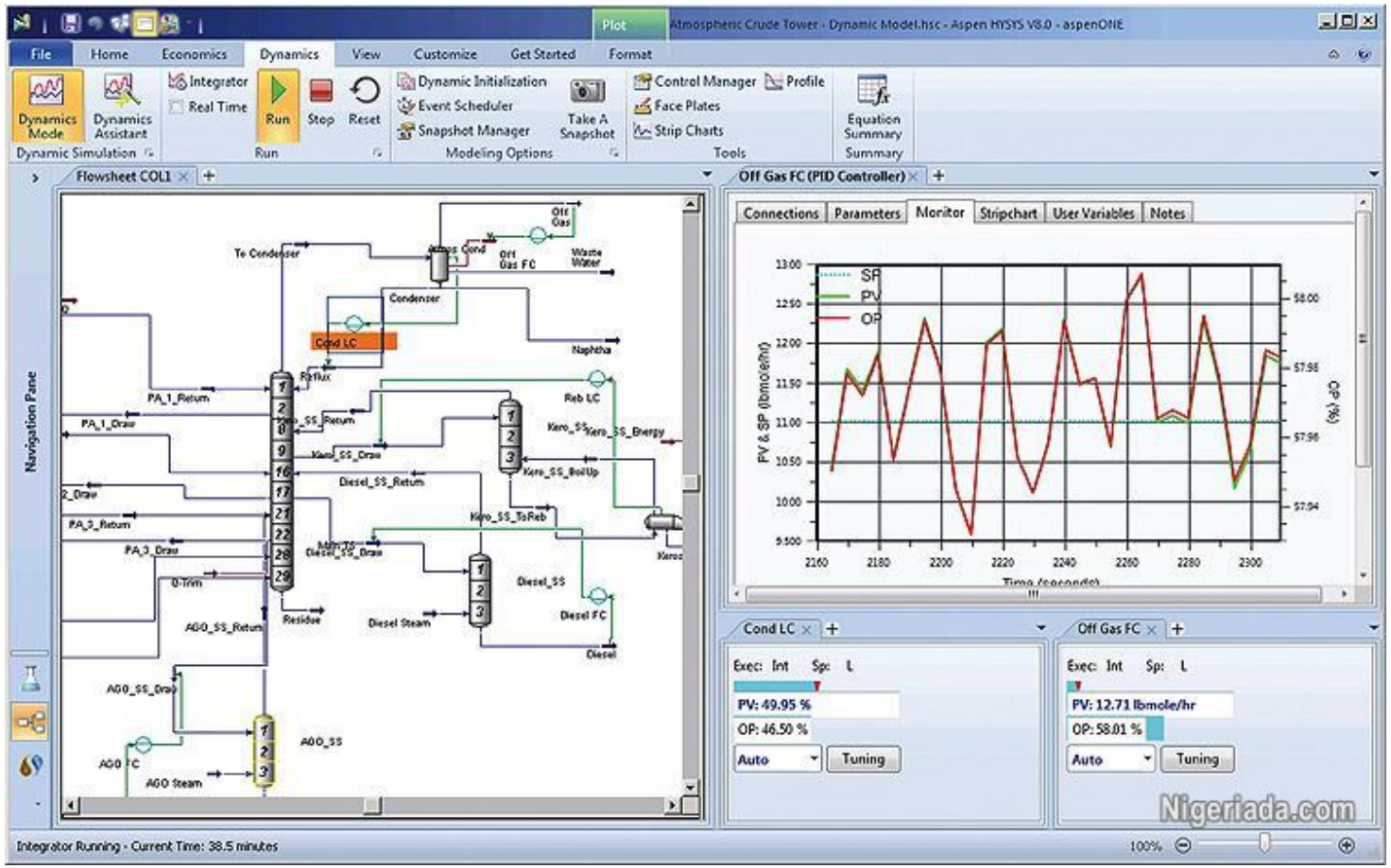
$$k = \frac{k_d}{k_i}$$



Simulación estacionaria

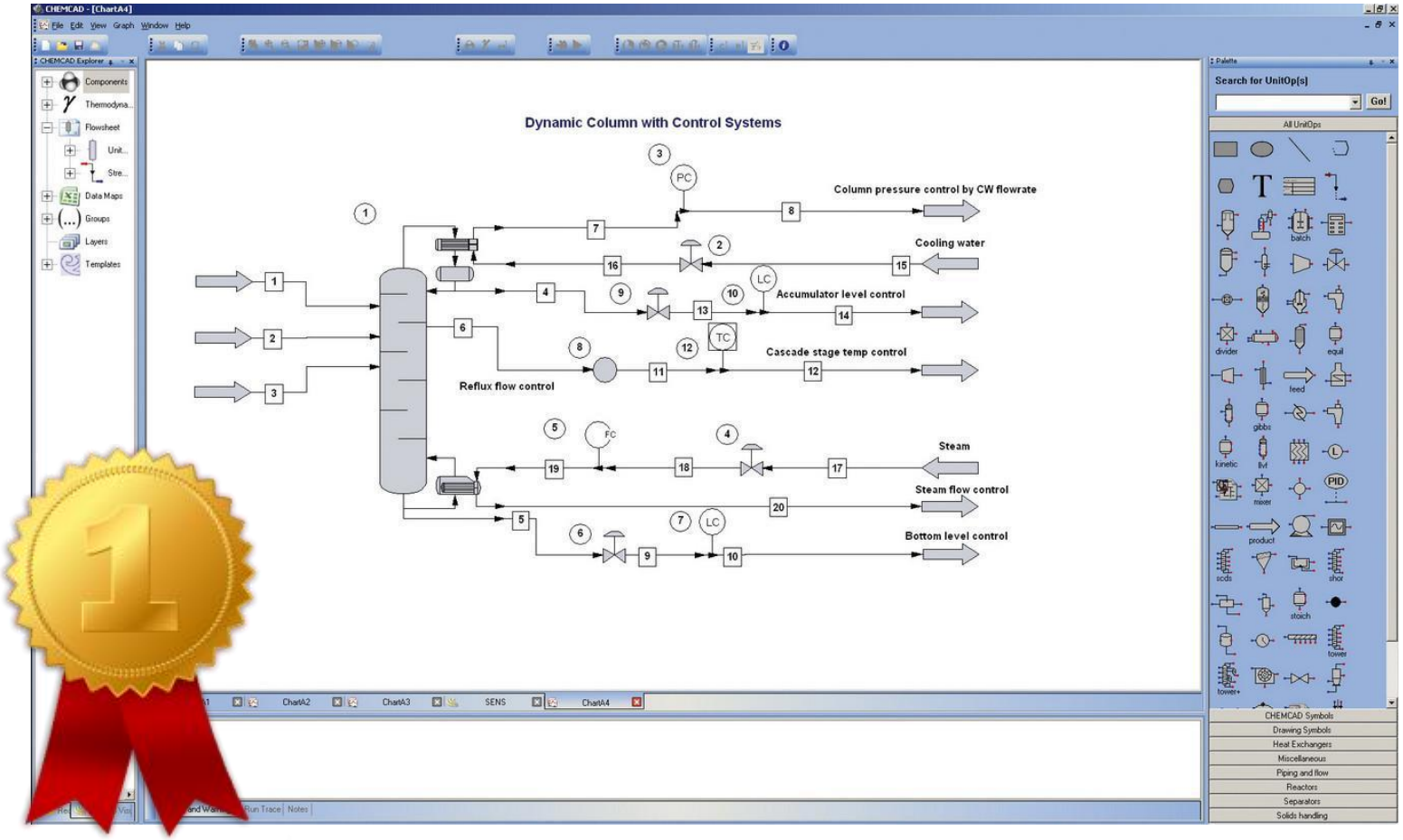


Simulación dinámica

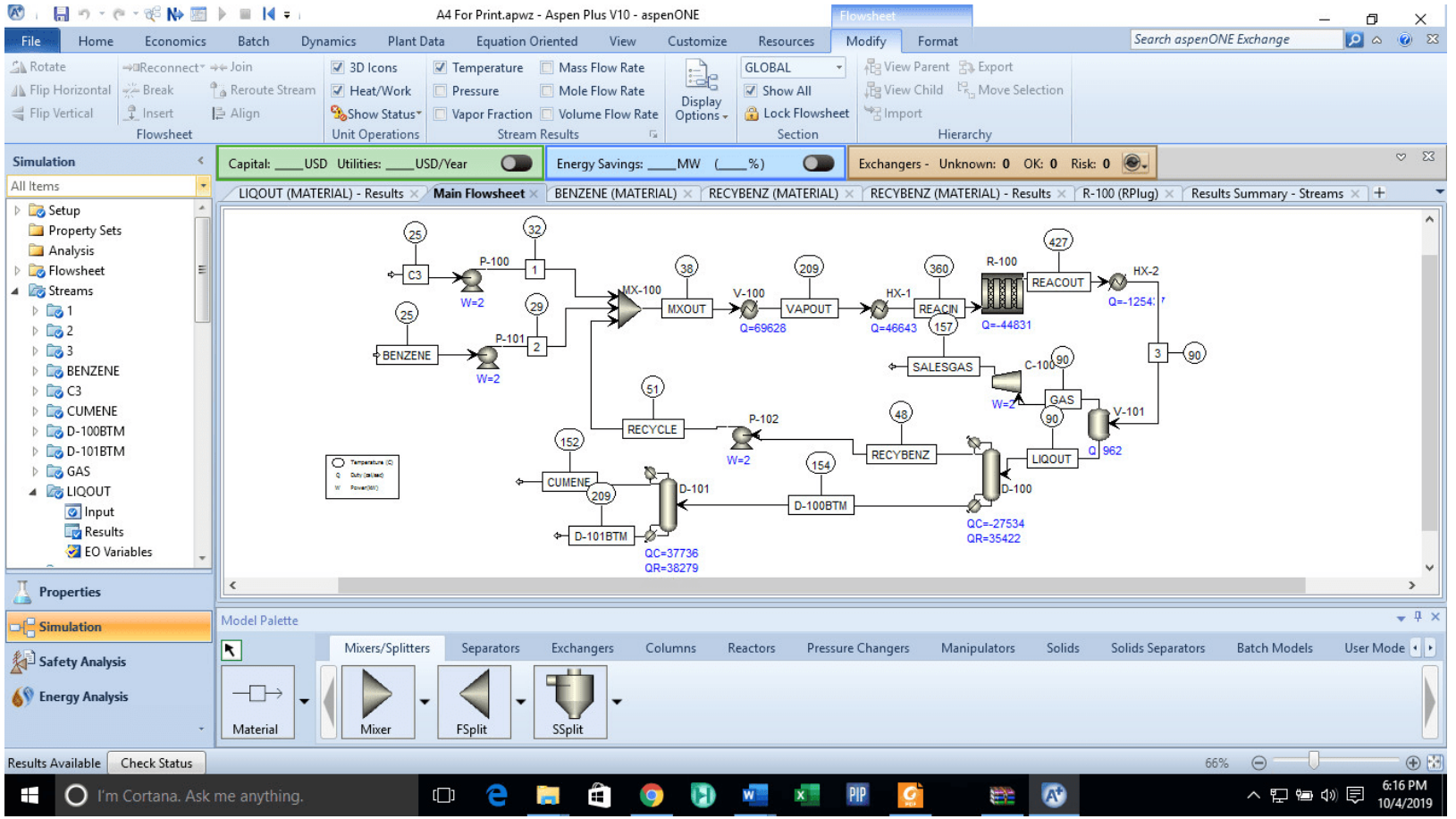


Simuladores comerciales

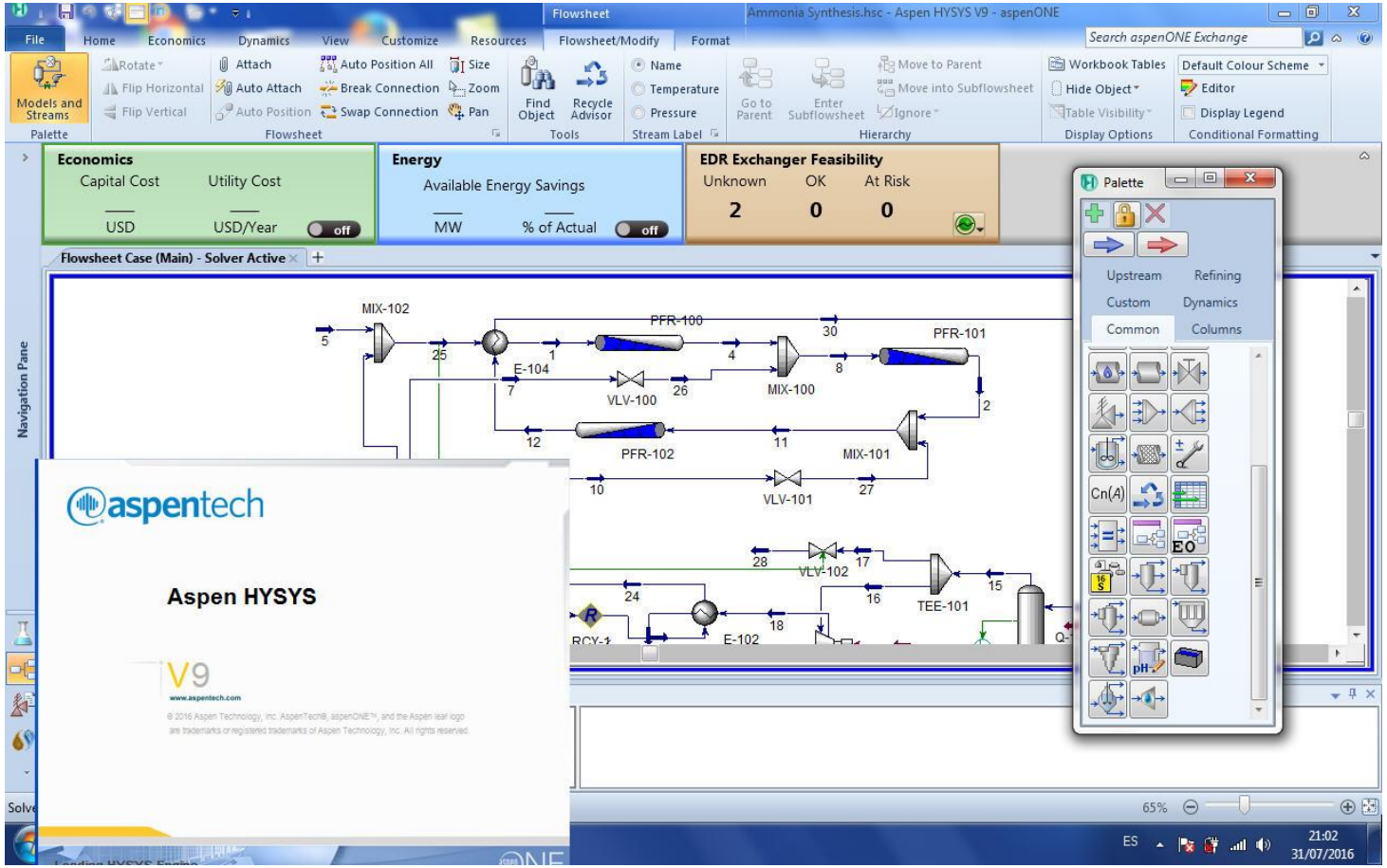
Chemcad


CHEMCAD - [ChartA4]
Dynamic Column with Control Systems
Column pressure control by CW flowrate
Cooling water
Accumulator level control
Cascade stage temp control
Reflux flow control
Steam
Steam flow control
Bottom level control
Search for UnitOp(s)
Go!
All UnitOps
CHEMCAD Symbols
Drawing Symbols
Heat Exchangers
Miscellaneous
Piping and flow
Reactors
Separators
Solids handling

Aspen plus

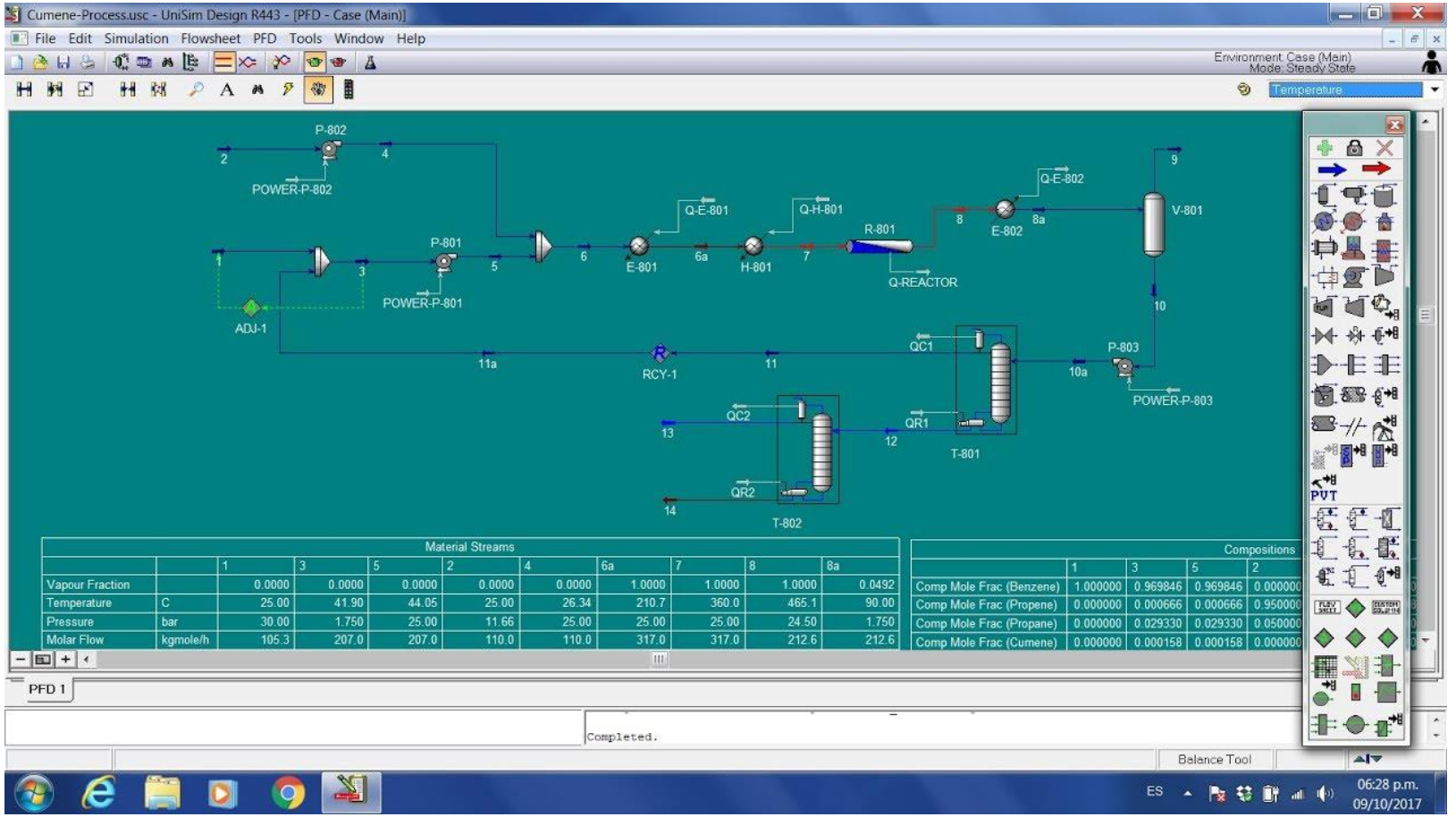

A4 For Print.apwz - Aspen Plus V10 - aspenONE
Flowsheet
File
Home
Economics
Batch
Dynamics
Plant Data
Equation Oriented
View
Customize
Resources
Modify
Format
Search aspenONE Exchange
Rotate
Flip Horizontal
Flip Vertical
Reconnect
Break
Insert
Join
Reroute Stream
Align
Flowsheet
3D Icons
Heat/Work
Show Status
Unit Operations
Temperature
Pressure
Vapor Fraction
Mass Flow Rate
Mole Flow Rate
Volume Flow Rate
Stream Results
Display Options
GLOBAL
Show All
Lock Flowsheet
Section
View Parent
View Child
Import
Export
Move Selection
Hierarchy
Simulation
All Items
Setup
Property Sets
Analysis
Flowsheet
Streams
1
2
3
BENZENE
C3
CUMENE
D-100BTM
D-101BTM
GAS
LIQOUT
Input
Results
EO Variables
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Exchangers - Unknown: 0 OK: 0 Risk: 0
LIQOUT (MATERIAL) - Results
Main Flowsheet
BENZENE (MATERIAL)
RECYBENZ (MATERIAL)
RECYBENZ (MATERIAL) - Results
R-100 (RPlug)
Results Summary - Streams
C3
P-100
W=2
BENZENE
P-101
W=2
MX-100
MXOUT
V-100
Q=69628
VAPOUT
HX-1
Q=46643
REACIN
R-100
Q=-44831
REACOUT
HX-2
Q=-1254:
SALESGAS
C-100
W=2
GAS
V-101
Q 962
LIQOUT
RECYCLE
P-102
W=2
RECYBENZ
D-100
QC=-27534
QR=35422
D-100BTM
D-101
CUMENE
D-101BTM
QC=37736
QR=38279
Properties
Simulation
Safety Analysis
Energy Analysis
Model Palette
Mixers/Splitters
Separators
Exchangers
Columns
Reactors
Pressure Changers
Manipulators
Solids
Solids Separators
Batch Models
User Mode
Material
Mixer
FSplit
SSplit
Results Available
Check Status
66%
I'm Cortana. Ask me anything.
6:16 PM
10/4/2019

Aspen HYSYS


Ammonia Synthesis.hsc - Aspen HYSYS V9 - aspenONE
Economics
Capital Cost
Utility Cost
USD
USD/Year
Energy
Available Energy Savings
MW
% of Actual
EDR Exchanger Feasibility
Unknown
OK
At Risk
Flowsheet Case (Main) - Solver Active
MIX-102
PFR-100
PFR-101
E-104
VLV-100
MIX-100
PFR-102
MIX-101
VLV-101
VLV-102
TEE-101
E-102
Palette
Upstream
Refining
Custom
Dynamics
Common
Columns
aspentech
Aspen HYSYS
V9

UNISIM

Honeywell



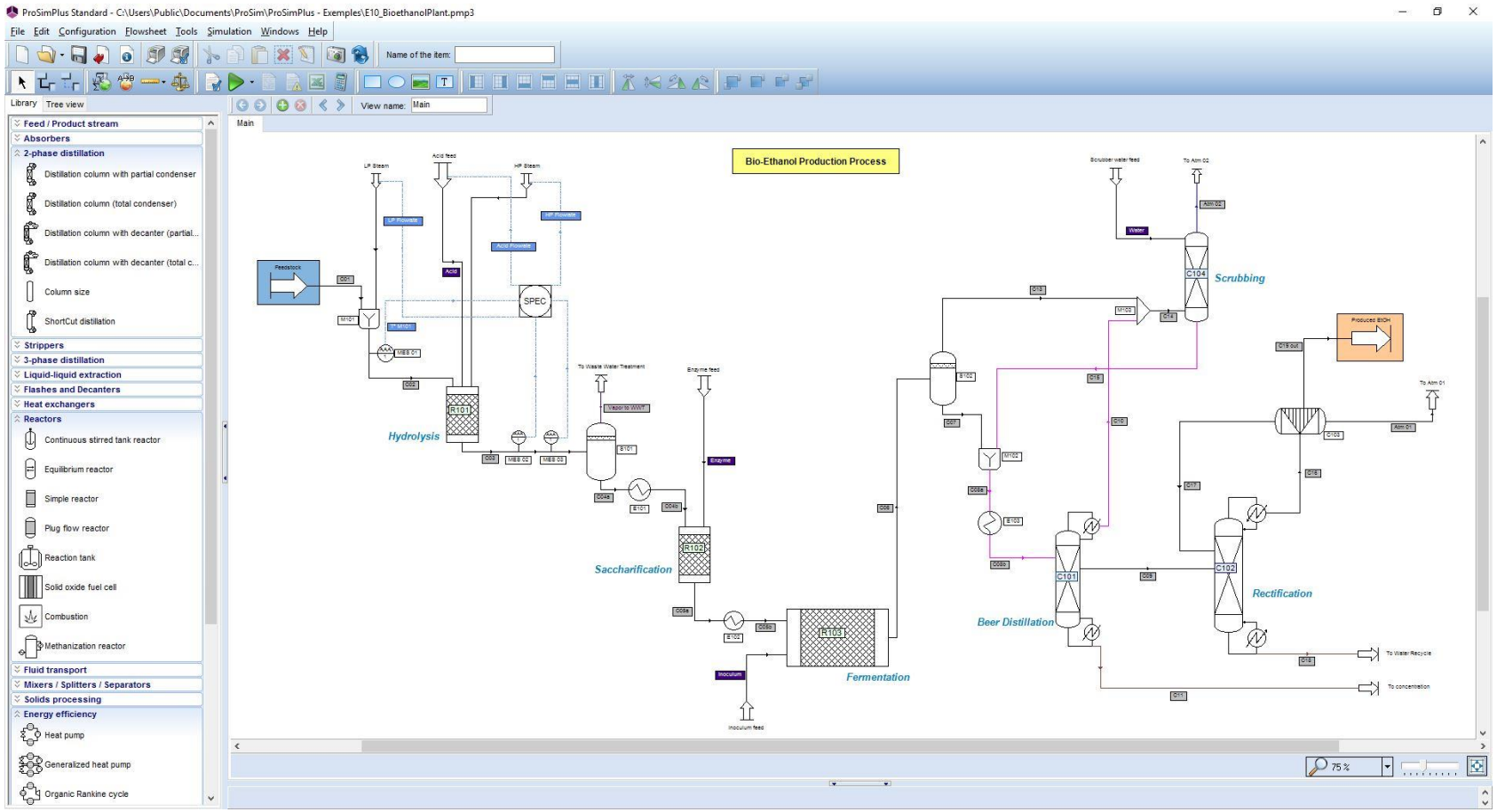
Material Streams

		1	3	5	2	4	6a	7	8	8a
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0492
Temperature	C	25.00	41.90	44.05	25.00	26.34	210.7	360.0	465.1	90.00
Pressure	bar	30.00	1.750	25.00	11.66	25.00	25.00	25.00	24.50	1.750
Molar Flow	kgmole/h	105.3	207.0	207.0	110.0	110.0	317.0	317.0	212.6	212.6

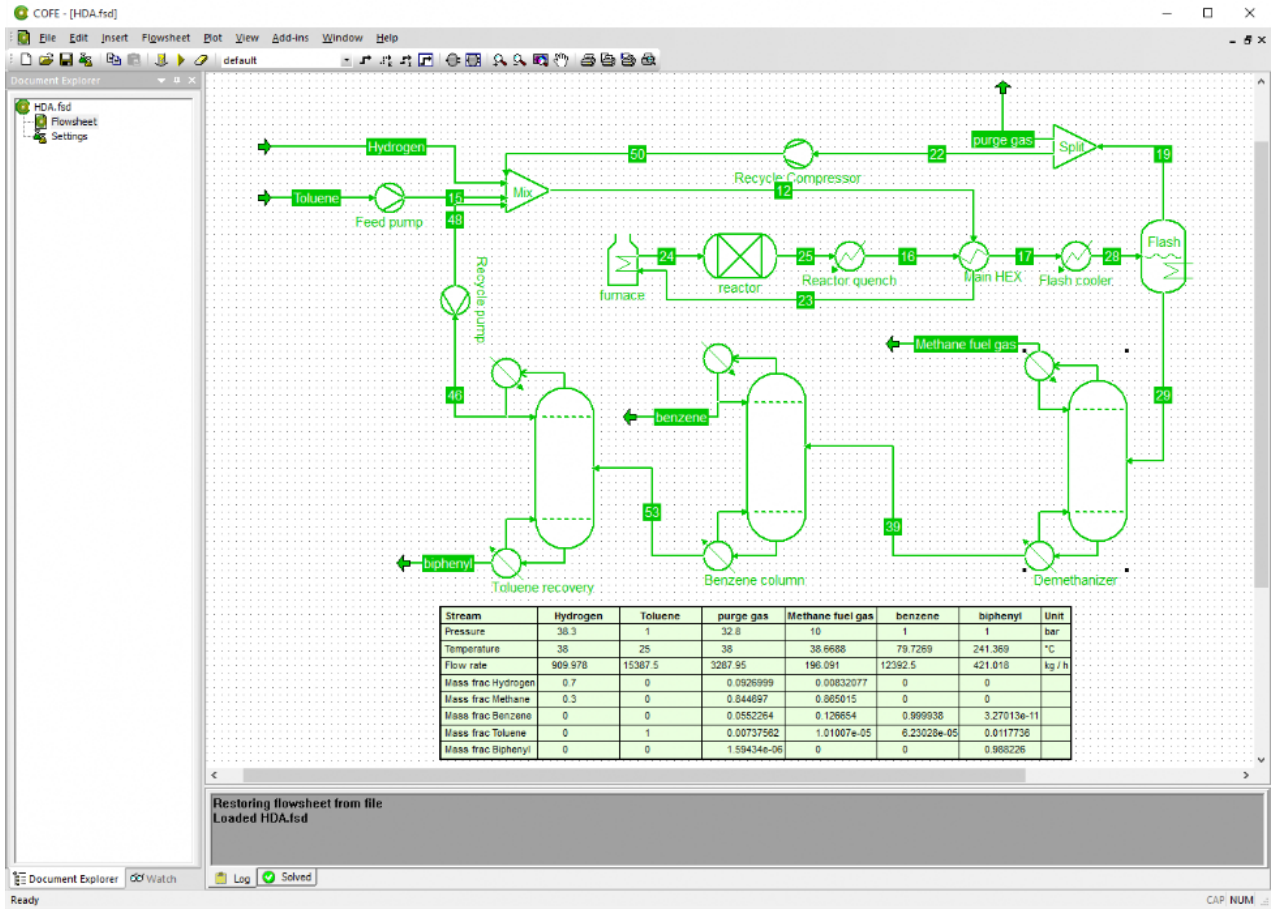
Compositions

	1	3	5	2
Comp Mole Frac (Benzene)	1.000000	0.969846	0.969846	0.000000
Comp Mole Frac (Propene)	0.000000	0.000666	0.000666	0.950000
Comp Mole Frac (Propane)	0.000000	0.029330	0.029330	0.050000
Comp Mole Frac (Cumene)	0.000000	0.000158	0.000158	0.000000

ProSimPlus

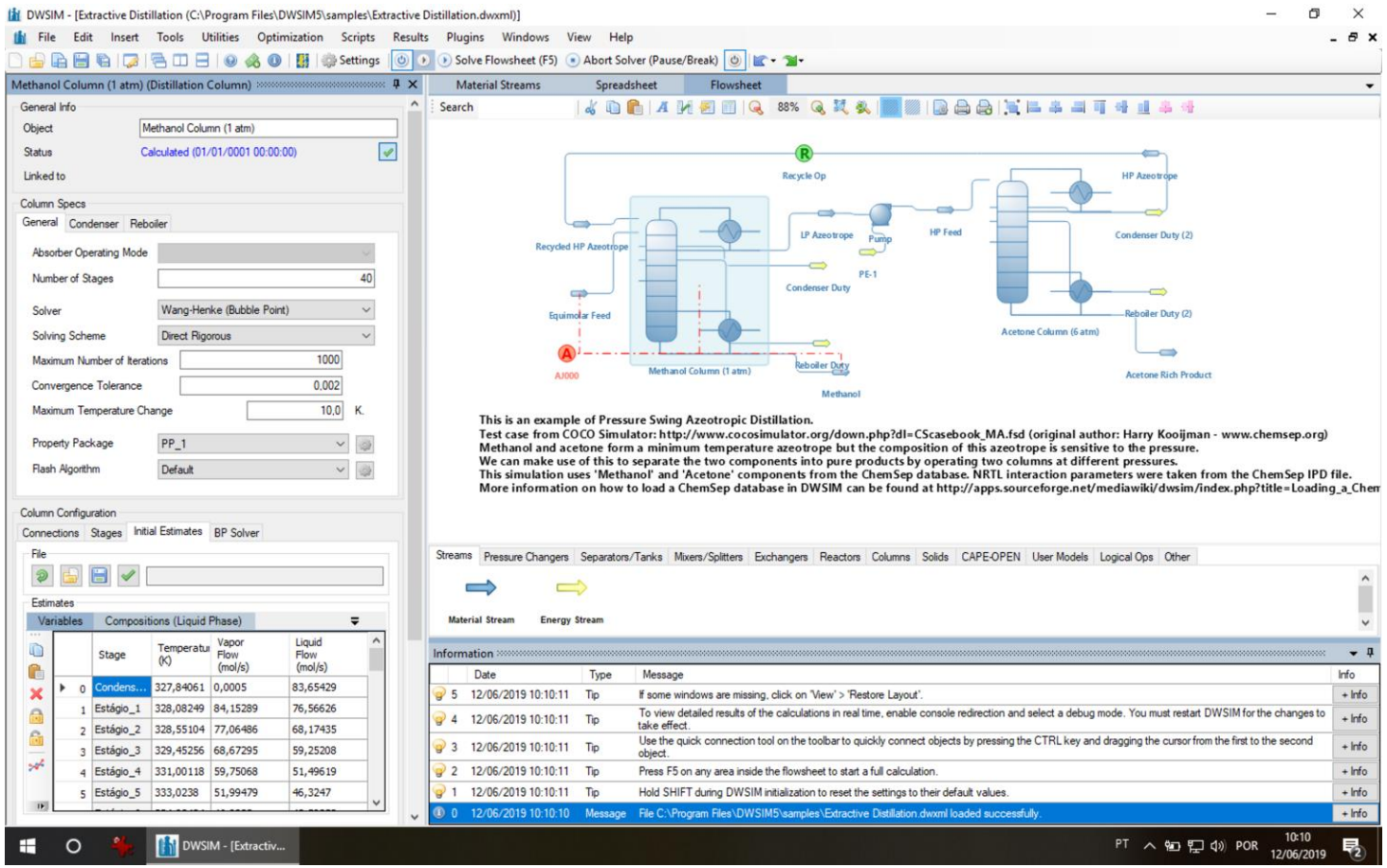

ProSimPlus Standard - C:\Users\Public\Documents\ProSim\ProSimPlus - Exemples\E10_BioethanolPlant.pmp3
File Edit Configuration Flowsheet Tools Simulation Windows Help
Library Tree view
Feed / Product stream
Absorbers
2-phase distillation
Distillation column with partial condenser
Distillation column (total condenser)
Distillation column with decanter (partial...
Distillation column with decanter (total c...
Column size
ShortCut distillation
Strippers
3-phase distillation
Liquid-liquid extraction
Flashes and Decanters
Heat exchangers
Reactors
Continuous stirred tank reactor
Equilibrium reactor
Simple reactor
Plug flow reactor
Reaction tank
Solid oxide fuel cell
Combustion
Methanization reactor
Fluid transport
Mixers / Splitters / Separators
Solids processing
Energy efficiency
Heat pump
Generalized heat pump
Organic Rankine cycle
Main
Bio-Ethanol Production Process
Hydrolysis
Saccharification
Fermentation
Beer Distillation
Rectification
Scrubbing
SPEC
R101
R102
R103
C101
C102
C104
75 %

COCO



Stream	Hydrogen	Toluene	purge gas	Methane fuel gas	benzene	biphenyl	Unit
Pressure	38.3	1	32.8	10	1	1	bar
Temperature	38	25	38	38.6688	79.7269	241.369	°C
Flow rate	909.978	15387.5	3287.95	196.091	12392.5	421.018	kg / h
Mass frac Hydrogen	0.7	0	0.0926999	0.00832077	0	0	
Mass frac Methane	0.3	0	0.844697	0.865015	0	0	
Mass frac Benzene	0	0	0.0552264	0.126654	0.999938	3.27013e-11	
Mass frac Toluene	0	1	0.00737562	1.01007e-05	6.23028e-05	0.0117736	
Mass frac Biphenyl	0	0	1.59434e-06	0	0	0.988226	

DWSIM


DWSIM - [Extractive Distillation (C:\Program Files\DWSIM5\samples\Extractive Distillation.dwxml)]
File Edit Insert Tools Utilities Optimization Scripts Results Plugins Windows View Help
Settings Solve Flowsheet (F5) Abort Solver (Pause/Break)
Methanol Column (1 atm) (Distillation Column)
General Info
Object Methanol Column (1 atm)
Status Calculated (01/01/0001 00:00:00)
Linked to
Column Specs
General Condenser Reboiler
Absorber Operating Mode
Number of Stages 40
Solver Wang-Henke (Bubble Point)
Solving Scheme Direct Rigorous
Maximum Number of Iterations 1000
Convergence Tolerance 0,002
Maximum Temperature Change 10,0 K
Property Package PP_1
Flash Algorithm Default
Column Configuration
Connections Stages Initial Estimates BP Solver
File
Estimates
Variables Compositions (Liquid Phase)
Stage Temperatu (K) Vapor Flow (mol/s) Liquid Flow (mol/s)
0 Condens... 327,84061 0,0005 83,65429
1 Estágio_1 328,08249 84,15289 76,56626
2 Estágio_2 328,55104 77,06486 68,17435
3 Estágio_3 329,45256 68,67295 59,25208
4 Estágio_4 331,00118 59,75068 51,49619
5 Estágio_5 333,0238 51,99479 46,3247
Material Streams Spreadsheet Flowsheet
Search 88%
Recycle Op
HP Azeotrope
Condenser Duty (2)
Recycled HP Azeotrope
LP Azeotrope
Pump
HP Feed
PE-1
Condenser Duty
Equimolar Feed
Reboiler Duty (2)
Acetone Column (6 atm)
AJ000
Methanol Column (1 atm)
Reboiler Duty
Acetone Rich Product
Methanol
This is an example of Pressure Swing Azeotropic Distillation.
Test case from COCO Simulator: http://www.cocosimulator.org/down.php?dl=CScasebook_MA.fsd (original author: Harry Kooijman - www.chemsep.org)
Methanol and acetone form a minimum temperature azeotrope but the composition of this azeotrope is sensitive to the pressure.
We can make use of this to separate the two components into pure products by operating two columns at different pressures.
This simulation uses 'Methanol' and 'Acetone' components from the ChemSep database. NRTL interaction parameters were taken from the ChemSep IPD file.
More information on how to load a ChemSep database in DWSIM can be found at http://apps.sourceforge.net/mediawiki/dwsim/index.php?title=Loading_a_Chem
Streams Pressure Changers Separators/Tanks Mixers/Splitters Exchangers Reactors Columns Solids CAPE-OPEN User Models Logical Ops Other
Material Stream
Energy Stream
Information
Date Type Message Info
5 12/06/2019 10:10:11 Tip If some windows are missing, click on 'View' > 'Restore Layout'. + Info
4 12/06/2019 10:10:11 Tip To view detailed results of the calculations in real time, enable console redirection and select a debug mode. You must restart DWSIM for the changes to take effect. + Info
3 12/06/2019 10:10:11 Tip Use the quick connection tool on the toolbar to quickly connect objects by pressing the CTRL key and dragging the cursor from the first to the second object. + Info
2 12/06/2019 10:10:11 Tip Press F5 on any area inside the flowsheet to start a full calculation. + Info
1 12/06/2019 10:10:11 Tip Hold SHIFT during DWSIM initialization to reset the settings to their default values. + Info
0 12/06/2019 10:10:10 Message File C:\Program Files\DWSIM5\samples\Extractive Distillation.dwxml loaded successfully. + Info
DWSIM - [Extractiv...
PT POR 10:10 12/06/2019

DWSIM