

# DSOySP

## Módulos de DWSIM (II) Torres de destilación Shortcut, Rigurosa y ChemSep

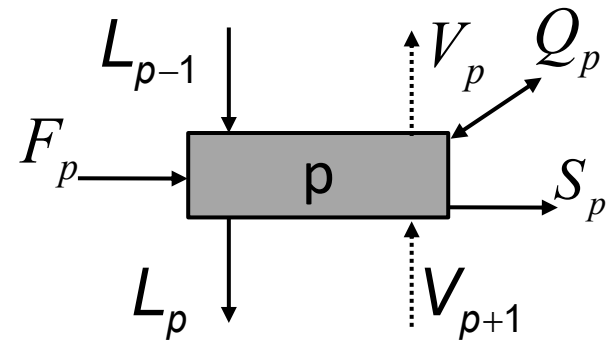
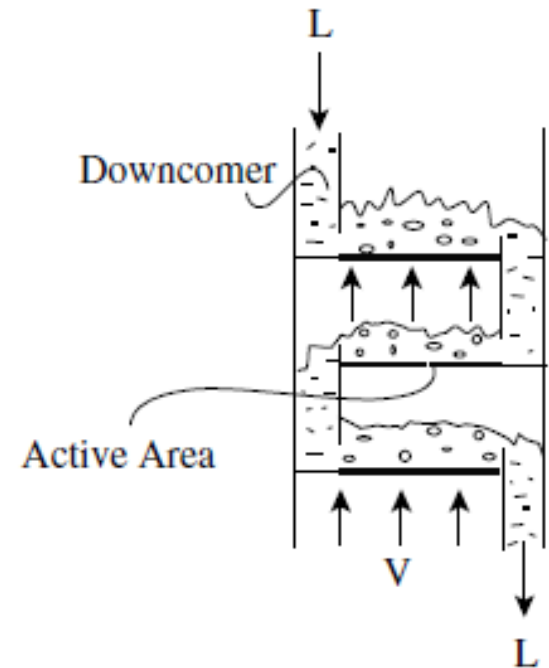
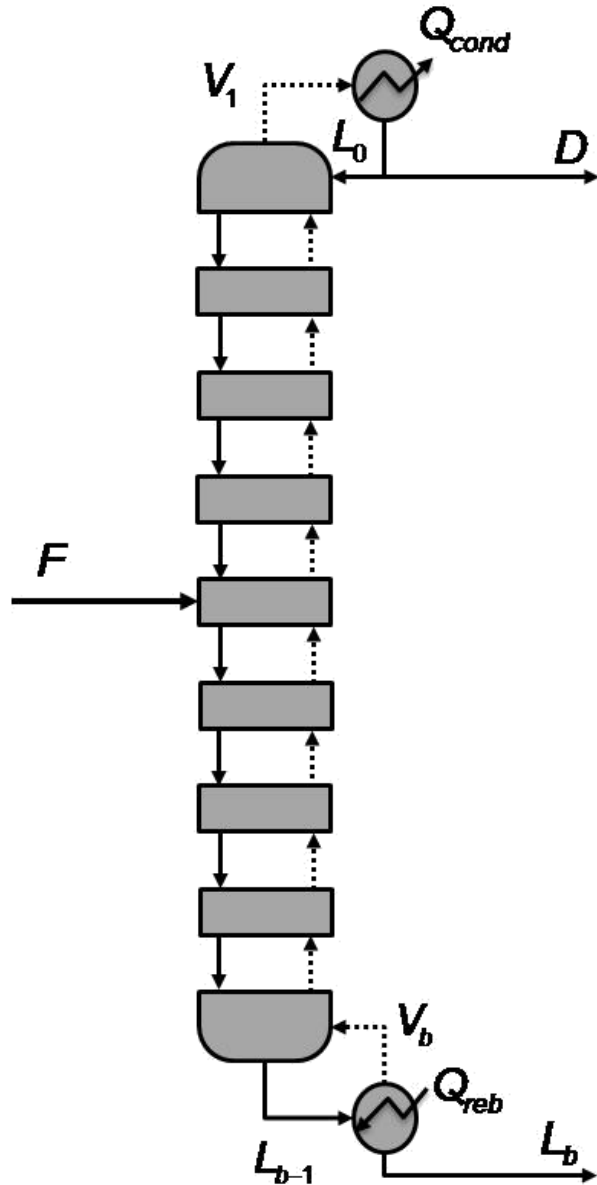
Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

# DSOySP

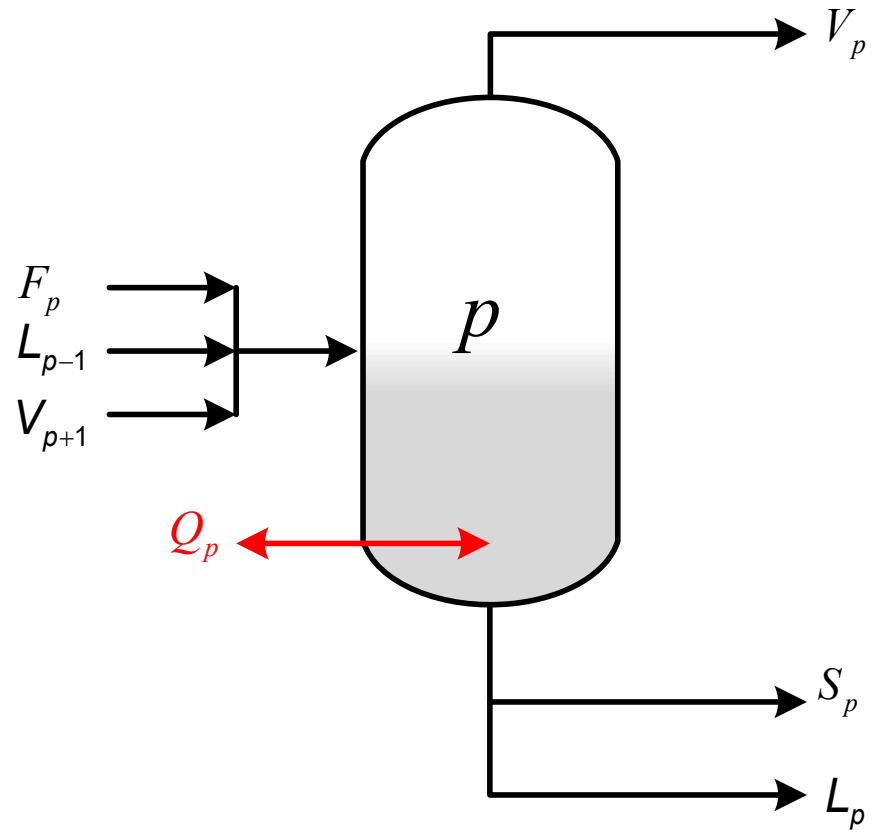
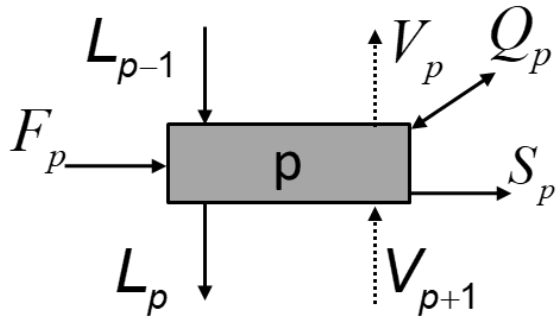
Modelado matemático de una columna de  
destilación simple

Profesor: Dr. Nicolás J. Scenna  
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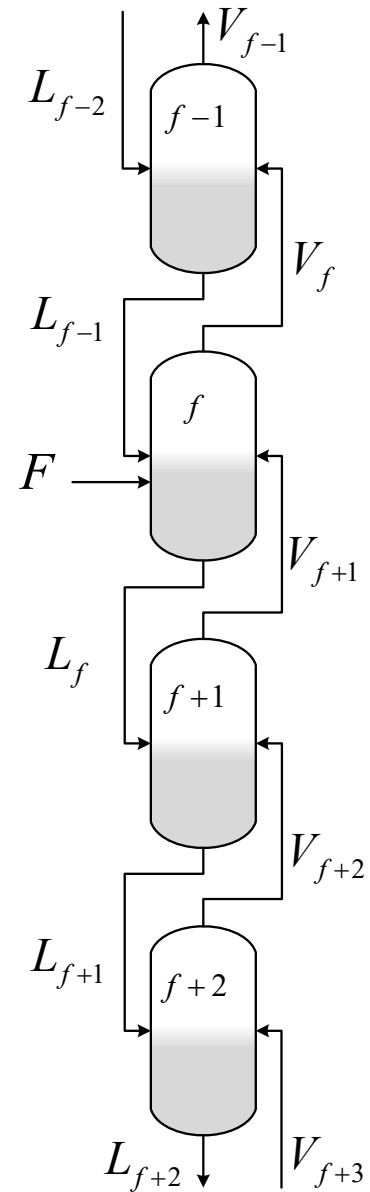
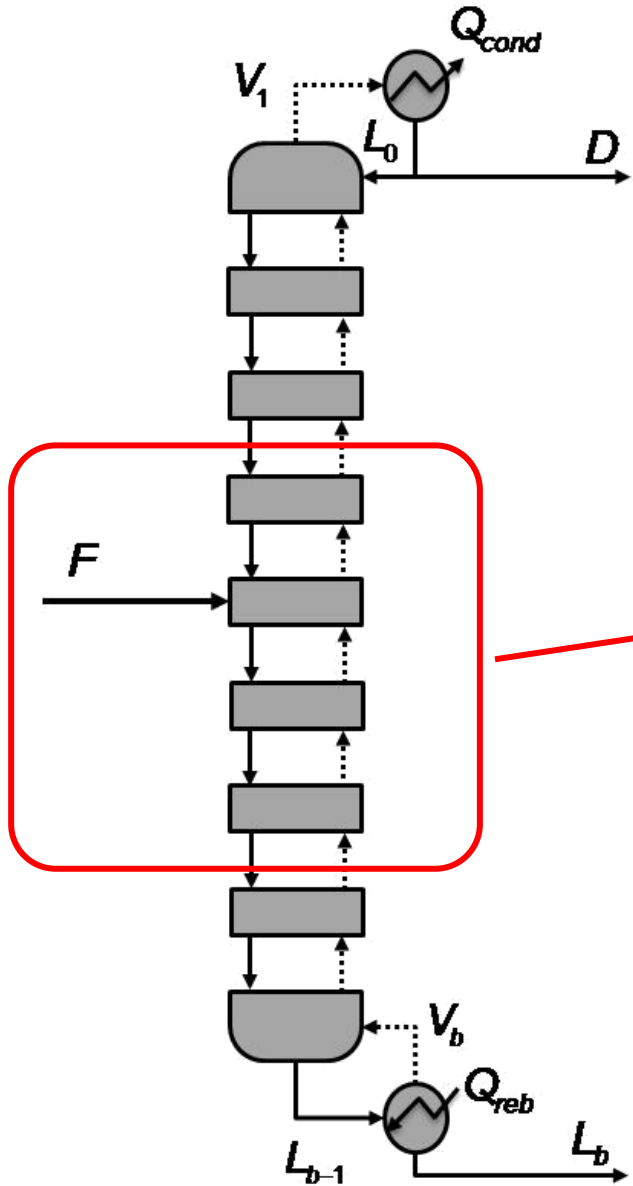
# Columna de Destilación simple (con condensador total)



# Etapa ideal de equilibrio



# Etapa ideal de equilibrio



# Etapa ideal de equilibrio

## MESH equation

(Material balance, phase Equilibrium, molar fraction Summation, entHalpy balance)

## Balances de Materia y Energía

$$F_p x_f^i + L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i = V_p y_p^i + (L_p + S_p) x_p^i \quad ; \forall i$$

$$F_p h_f + L_{p-1} h_{p-1} + V_{p+1} H_{p+1} + Q_p^{in} = V_p H_p + (L_p + S_p) h_p + Q_p^{out}$$

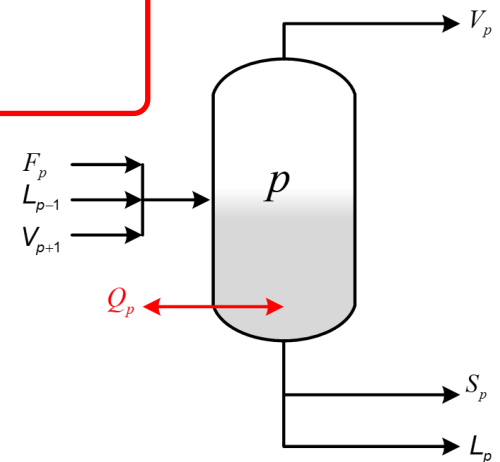
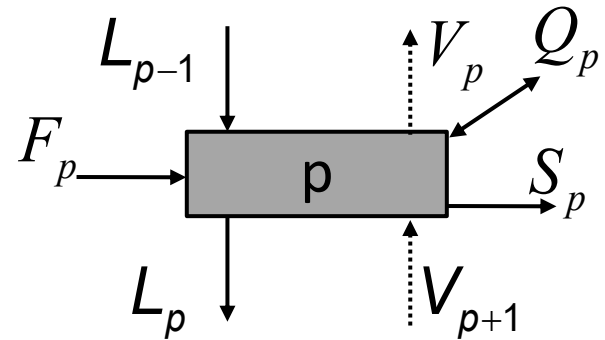
$$\sum_i x_p^i = 1$$

$$\sum_i y_p^i = 1$$

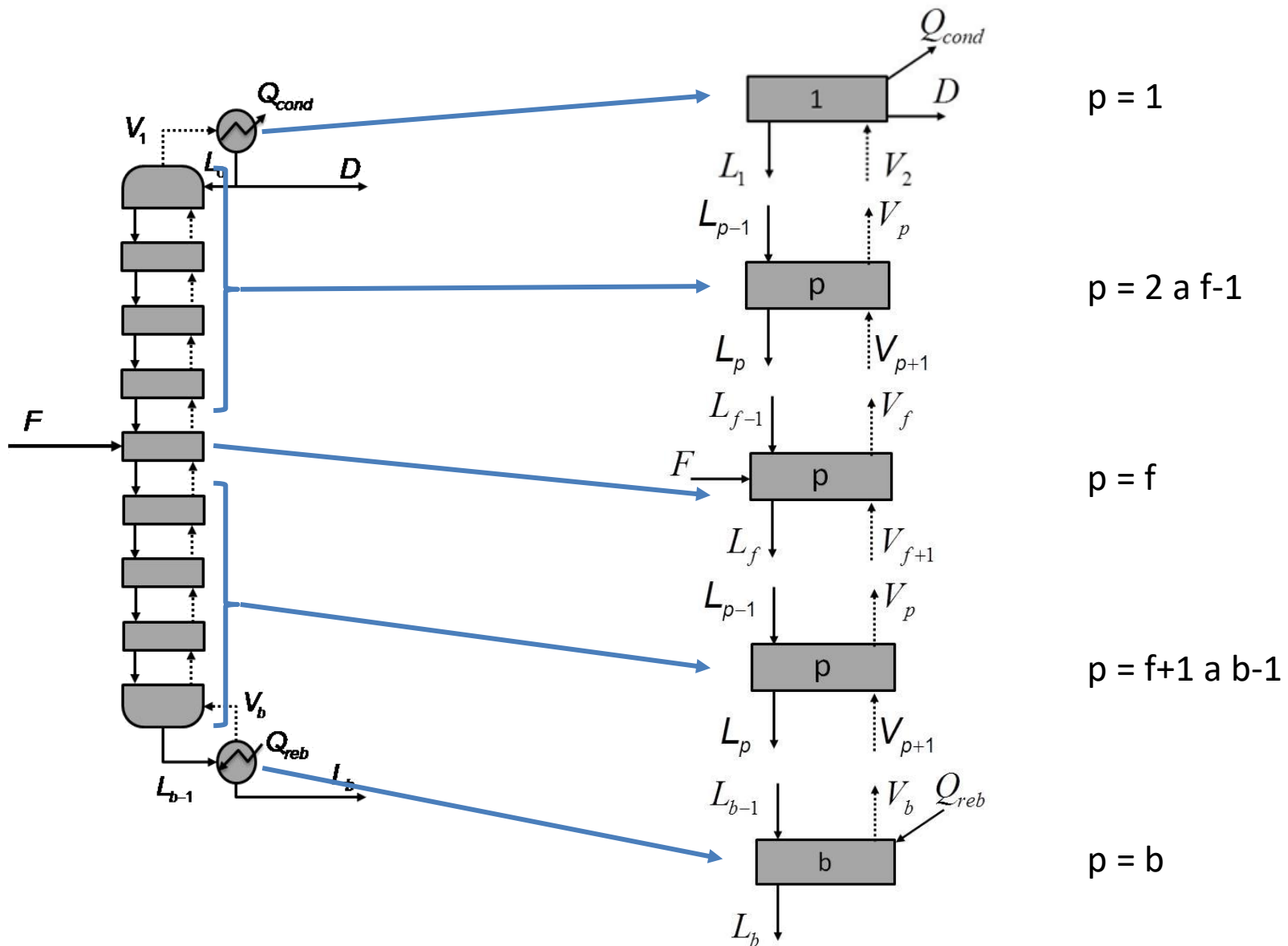
## Modelo fisicoquímico

$$h_p = f(x_p, T_p, P_p) \quad H_p = f(y_p, T_p, P_p)$$

$$y_p^i = K_p^i x_p^i \quad \forall i \quad K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i$$



# Columna de destilación a partir etapas de equilibrio



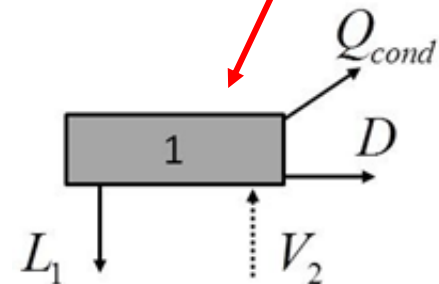
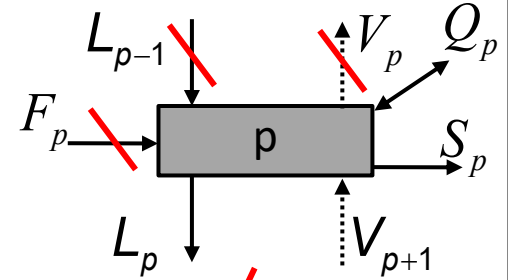
# Condensador

$$\cancel{F_p} x_f^i + \cancel{L_{p-1}} x_{p-1}^i + V_{p+1} y_{p+1}^i = \cancel{V_p} y_p^i + (L_p + S_p) x_p^i ; \forall i$$

$$\cancel{F_p} h_f + \cancel{L_{p-1}} h_{p-1} + V_{p+1} H_{p+1} + \cancel{Q_p^{in}} = \cancel{V_p} H_p + (L_p + S_p) h_p + Q_p^{out}$$

$$V_2 y_2^i = (L_1 + D) x_1^i ; \forall i$$

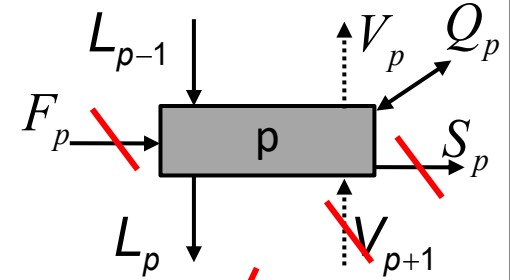
$$V_2 H_2 = (L_1 + D) h_1 + Q_{cond}$$



# Rehervidor

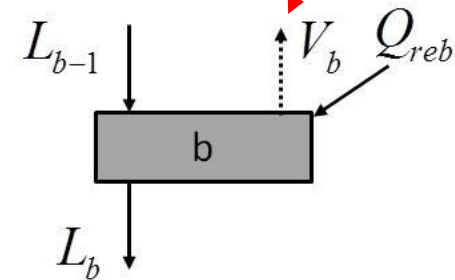
$$\cancel{F_p} x_f^i + L_{p-1} x_{p-1}^i + \cancel{V_{p+1}} y_{p+1}^i = V_p y_p^i + (L_p + \cancel{S_p}) x_p^i ; \forall i$$

$$\cancel{F_p} h_f + L_{p-1} h_{p-1} + \cancel{V_{p+1}} H_{p+1} + Q_p^{in} = V_p H_p + (L_p + \cancel{S_p}) h_p + \cancel{Q_p}^{out}$$



$$L_{b-1} x_{b-1}^i = V_b y_b^i + L_b x_b^i ; \forall i$$

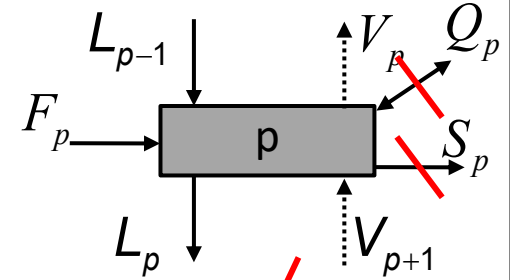
$$L_{b-1} h_{b-1} + Q_{reb} = V_b H_b + L_b h_b$$



# Plato de Alimentación

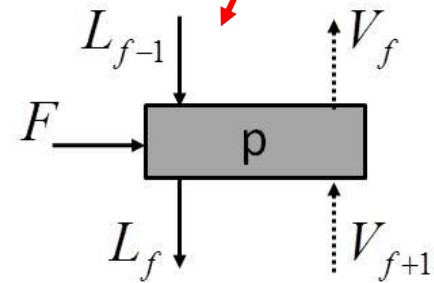
$$F_p x_f^i + L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i = V_p y_p^i + (L_p + S_p) x_p^i ; \forall i$$

$$F_p h_f + L_{p-1} h_{p-1} + V_{p+1} H_{p+1} + Q_p^{in} = V_p H_p + (L_p + S_p) h_p + Q_p^{out}$$



$$F x_{feed}^i + L_{f-1} x_{f-1}^i + V_{f+1} y_{f+1}^i = V_f y_f^i + L_f x_f^i ; \forall i$$

$$F h_{feed} + L_{f-1} h_{f-1} + V_{f+1} H_{f+1} = V_f H_f + L_f h_f$$



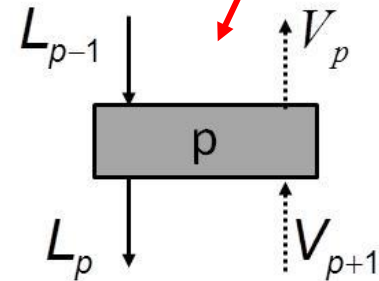
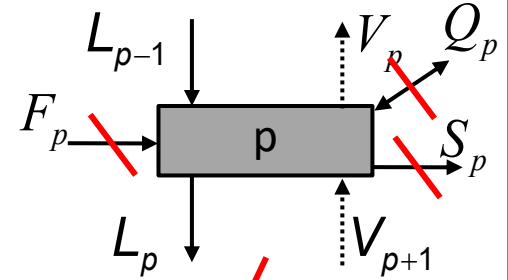
# Platos intermedios

$$\cancel{F_p} x_f^i + L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i = V_p y_p^i + (L_p + \cancel{S_p}) x_p^i ; \forall i$$

$$\cancel{F_p} h_f + L_{p-1} h_{p-1} + V_{p+1} H_{p+1} + \cancel{Q_p^{in}} = V_p H_p + (L_p + \cancel{S_p}) h_p + \cancel{Q_p^{out}}$$

$$L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i = V_p y_p^i + L_p x_p^i ; \forall i$$

$$L_{p-1} h_{p-1} + V_{p+1} H_{p+1} = V_p H_p + L_p h_p$$



## Modelo final para $b$ etapas y $n$ componentes

$$V_2 y_2^i = (L_1 + D) x_1^i \quad \forall i$$

$$V_2 H_2 = (L_1 + D) h_1 + Q_{cond}$$

$$L_{b-1} x_{b-1}^i = V_b y_b^i + L_b x_b^i \quad \forall i$$

$$L_{b-1} h_{b-1} + Q_{reb} = V_b H_b + L_b h_b$$

$$F x_{feed}^i + L_{f-1} x_{f-1}^i + V_{f+1} y_{f+1}^i = V_f y_f^i + L_f x_f^i \quad \forall i$$

$$F h_{feed} + L_{f-1} h_{f-1} + V_{f+1} H_{f+1} = V_f H_f + L_f h_f$$

$$\left. \begin{aligned} L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i &= V_p y_p^i + L_p x_p^i \quad \forall i \\ L_{p-1} h_{p-1} + V_{p+1} H_{p+1} &= V_p H_p + L_p h_p \end{aligned} \right\} \begin{aligned} 2 \leq p \leq f-1 \\ f+1 \leq p \leq b-1 \end{aligned}$$

$$\sum_i x_p^i = 1 \quad \forall p$$

$$\sum_i y_p^i = 1 \quad \forall p$$

$$h_p = f(x_p, T_p, P_p) \quad \forall p$$

$$H_p = f(y_p, T_p, P_p) \quad \forall p$$

$$y_p^i = K_p^i x_p^i \quad \forall i; \forall p$$

$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

**Número de variables:  $6 \times b + 3 \times b \times n + 2$**

$L_p$	$V_p$	$x_p^i$	$y_p^i$	$Q_{reb}$	$Q_{cond}$	$h_p$	$H_p$	$D$	$K_p^i$	$T_p$	$P_p$
$b$	$b-1$	$b \times n$	$b \times n$	1	1	$b$	$b$	1	$b \times n$	$b$	$b$

# Modelo final para $b$ etapas y $n$ componentes

$$V_2 y_2^i = (L_1 + D) x_1^i \quad \forall i$$

$$V_2 H_2 = (L_1 + D) h_1 + Q_{cond}$$

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$$L_{b-1} h_{b-1} + Q_{reb} = V_b H_b + L_b h_b$$

$$F x_{feed}^i + L_{f-1} x_{f-1}^i + V_{f+1} y_{f+1}^i = V_f y_f^i + L_f x_f^i \quad \forall i$$

$$F h_{feed} + L_{f-1} h_{f-1} + V_{f+1} H_{f+1} = V_f H_f + L_f h_f$$

$$L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i = V_p y_p^i + L_p x_p^i \quad \forall i \quad \left. \begin{array}{l} 2 \leq p \leq f-1 \\ f+1 \leq p \leq b-1 \end{array} \right\}$$

$$L_{p-1} h_{p-1} + V_{p+1} H_{p+1} = V_p H_p + L_p h_p$$

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$$y_p^i = K_p^i x_p^i \quad \forall i; \forall p$$

$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

Número de ecuaciones:  $b \times n + b + 4 \times b + 2 \times b \times n$

$$= 5 \times b + 3 \times b \times n$$

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$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

$$\left. \begin{aligned} \text{Número de variables: } & 6 \times b + 3 \times b \times n + 2 \\ \text{Número de ecuaciones: } & 5 \times b + 3 \times b \times n \end{aligned} \right\} \begin{aligned} & \text{Grados de libertad} \\ & b + 2 \end{aligned}$$

# Modelo final para $b$ etapas e $i$ componentes

$$V_2 y_2^i = (L_1 + D) x_1^i \quad \forall i$$

$$V_2 H_2 = (L_1 + D) h_1 + Q_{cond}$$

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$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

Grados de libertad

~~$b + 2$~~



Perfil de presiones conocido

Grados de libertad

2

# Modelo final para $b$ etapas e $i$ componentes

$$V_2 y_2^i = (L_1 + L_1/RR) x_1^i \quad \forall i$$

$$V_2 H_2 = (L_1 + L_1/RR) h_1 + Q_{cond}$$

$$L_{b-1} x_{b-1}^i = V_b y_b^i + L_b x_b^i \quad \forall i$$

$$L_{b-1} h_{b-1} + Q_{reb} = V_b H_b + L_b h_b$$

$$F x_{feed}^i + L_{f-1} x_{f-1}^i + V_{f+1} y_{f+1}^i = V_f y_f^i + L_f x_f^i \quad \forall i$$

$$F h_{feed} + L_{f-1} h_{f-1} + V_{f+1} H_{f+1} = V_f H_f + L_f h_f$$

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$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

Grados de libertad

2

$$RR = L_1/D \implies D = L_1/RR$$

$L_b$  y  $RR$

Variables habituales para cerrar los grados de libertad (column spec)

## Modelo final para 10 etapas y mezcla binaria (b=10 y n=2)

$$V_2 y_2^i = (L_1 + L_1/RR) x_1^i \quad \forall i$$

$$V_2 H_2 = (L_1 + L_1/RR) h_1 + Q_{cond}$$

$$L_{b-1} x_{b-1}^i = V_b y_b^i + L_b x_b^i \quad \forall i$$

$$L_{b-1} h_{b-1} + Q_{reb} = V_b H_b + L_b h_b$$

$$F x_{feed}^i + L_{f-1} x_{f-1}^i + V_{f+1} y_{f+1}^i = V_f y_f^i + L_f x_f^i \quad \forall i$$

$$F h_{feed} + L_{f-1} h_{f-1} + V_{f+1} H_{f+1} = V_f H_f + L_f h_f$$

$$\left. \begin{aligned} L_{p-1} x_{p-1}^i + V_{p+1} y_{p+1}^i &= V_p y_p^i + L_p x_p^i \quad \forall i \\ L_{p-1} h_{p-1} + V_{p+1} H_{p+1} &= V_p H_p + L_p h_p \end{aligned} \right\} \begin{aligned} 2 \leq p \leq f-1 \\ f+1 \leq p \leq b-1 \end{aligned}$$

$$\sum_i x_p^i = 1 \quad \forall p$$

$$\sum_i y_p^i = 1 \quad \forall p$$

$$h_p = f(x_p, T_p, P_p) \quad \forall p$$

$$H_p = f(y_p, T_p, P_p) \quad \forall p$$

$$y_p^i = K_p^i x_p^i \quad \forall i; \forall p$$

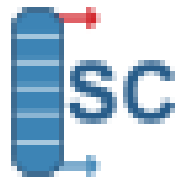
$$K_p^i = f(x_p, y_p, T_p, P_p) \quad \forall i; \forall p$$

Número de ecuaciones:  $5 \times b + 3 \times b \times n \Rightarrow 5 \times 10 + 3 \times 10 \times 2$

Se debe resolver un sistema de  
110 ecuaciones y 110 incógnitas



# DSOySP



## Shortcut Column

Model for quick sizing of distillation columns

Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

## Shortcut Column - Introducción

La columna debe tener una entrada, dos salidas (tope y fondo), un condensador (total o parcial) y un rehervidor.

Se basa en el método de Fenske-Underwood-Gilliland y los resultados que arroja son:

- Reflujo mínimo
- Carga calórica y temperaturas del condensador y rehervidor para un reflujo dado.
- Lugar óptimo de alimentación para un reflujo dado
- Mínimo número de etapas de equilibrio



**Shortcut Column**

Model for quick sizing of distillation columns

# Shortcut Column



## Shortcut Column

Model for quick sizing of distillation columns

Shortcut Column: SC column

### General Info

Object

Nombre

SC column

Status

Calculated (05/09/2017 05:03:20)

Linked to

### Connections

### Conexiones

Feed Stream

Distillate Stream

Bottoms Stream

Condenser Duty

Reboiler Duty

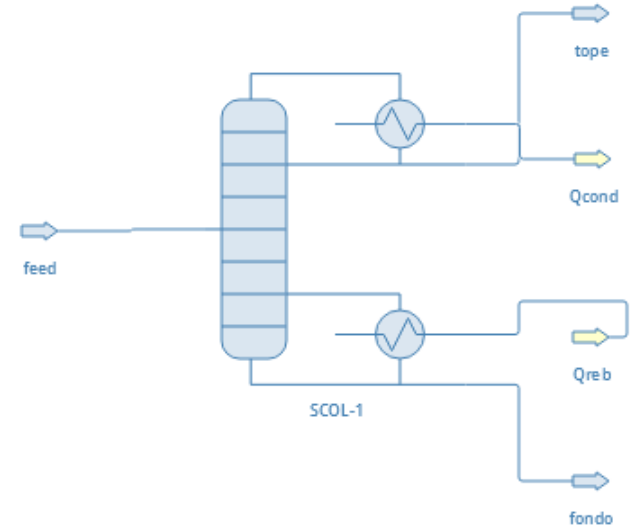
feed

Tope

Fondo

Qcond

Qreb



Se deben conectar una corriente de entrada, dos de salida y dos corrientes energéticas (entrada y salida)

Detalle de las conexiones

# Parámetros de calculo (Shortcut Column)

Clave liviano

Clave pesado

Fracción molar del LK en el fondo

Fracción molar del HK en el tope

Relación de reflujo

Tipo de condensador

Presión en el condensador

Presión en el rehervidor

Calculation Parameters

Light Key Compound (LK)	Benzene
Heavy Key Compound (HK)	Toluene
LK Mole Fraction in Bottoms	0.01
HK Mole Fraction in Distillate	0.01
Reflux Ratio	1.5
Condenser Type	<input checked="" type="radio"/> Total <input type="radio"/> Partial
Condenser Pressure	1 atm
Reboiler Pressure	1 atm

# Resultados utilizando FUG (Shortcut Column)

- Relación mínima de reflujo
- Mínimo número de etapas
- Etapas para la relación de reflujo actual
- Ubicación de la alimentación
- Flujo molar de líquido (agotamiento)
- Flujo molar de líquido (rectificación)
- Flujo molar de vapor (agotamiento)
- Flujo molar de vapor (rectificación)
- Calor que se extrae en el condensador
- Calor que se ingresa en el rehervidor

Results		
Property		Units
Minimum Reflux Ratio	1,28624	
Minimum Number of Stages	10,0277	
Actual Number of Stages	24,2878	
Optimal Feed Stage	12,1439	
Stripping Liquid	20,558	mol/s
Rectify Liquid	8,81056	mol/s
Stripping Vapor	14,6843	mol/s
Rectify Vapor	14,6843	mol/s
Condenser Duty	452,4	kW
Reboiler Duty	461,104	kW

## Ejemplo de aplicación (Shortcut model)

Se desea separar una corriente de 10 mol/s de una mezcla equimolar de N-hexano y N-heptano a 1 atm en condiciones de líquido saturado.

- La destilación se realiza en condiciones atmosféricas.
- La pureza de cada producto se desea de 0.99 en fracción molar.
- Se propone una relación de reflujo de 1.5 veces la mínima.
- La simulación de un proceso de destilación está fuertemente condicionada con el paquete fisicoquímico que se utiliza para el cálculo de las condiciones de equilibrio.
- DWSIM permite comparar los modelos teóricos disponibles con datos experimentales.
- De no ser satisfactoria la predicción también cuenta con herramientas de regresión para ajustar los modelos de equilibrio a datos experimentales.

# Armado del Caso de estudio

Calculation Parameters

Light Key Compound (LK) N-hexane

Heavy Key Compound (HK) N-heptane

LK Mole Fraction in Bottoms 0,01

HK Mole Fraction in Distillate 0,01

Reflux Ratio 2,106 **x1.5**

Condenser Type  Total  Partial

Condenser Pressure 101325 Pa

Reboiler Pressure 101325 Pa

Property Package Settings

Results

Property	Value	Units
Minimum Reflux Ratio	1,404	
Minimum Number of Stages	10,6173	
Actual Number of Stages	30,5506	
Optimal Feed Stage	15,2753	
Stripping Liquid	17,5	mol/s
Rectify Liquid	7,5	mol/s
Stripping Vapor	12,5	mol/s
Rectify Vapor	12,5	mol/s
Condenser Duty	362,319	kW
Reboiler Duty	372,067	kW

Results

Property	Value	Units
Minimum Reflux Ratio	1,404	
Minimum Number of Stages	10,6173	
Actual Number of Stages	19,2803	
Optimal Feed Stage	9,64014	
Stripping Liquid	20,53	mol/s
Rectify Liquid	10,53	mol/s
Stripping Vapor	15,53	mol/s
Rectify Vapor	15,53	mol/s
Condenser Duty	450,145	kW
Reboiler Duty	459,893	kW

# DSOySP



## Distillation Column

Rigorous model for simulation of distillation columns

Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

## Distillation Column - Introducción

- Es una operación unitaria que representa a las torres de fraccionamiento.
- Los componentes de una mezcla se separan a través de sucesivas etapas de equilibrio.
- El módulo se considera riguroso debido a los modelos termodinámicos utilizados en la solución de los balances de masa y energía a lo largo de la columna.
- Soporta varios flujos de alimentación
- Soporta varias salidas laterales
- Soporta corrientes de energía que representan intercambiadores de calor en cada etapa
- Requiere definición de presión y eficiencia por etapa



### Distillation Column

Rigorous model for simulation of distillation columns

# Distillation Column



## Distillation Column

Rigorous model for simulation of distillation columns

1 (Distillation Column) **Nombre**

General Info

Object: 1

Status: Calculated (27/7/2022 11:33:47) ✓

Linked to

General Specifications Stages Connections Estimates Results **Column Configuration**

Absorber Operating Mode: [dropdown]

Number of Stages: 18

Condenser/Top Pressure: 101325 Pa

Column Pressure Drop: 0 Pa

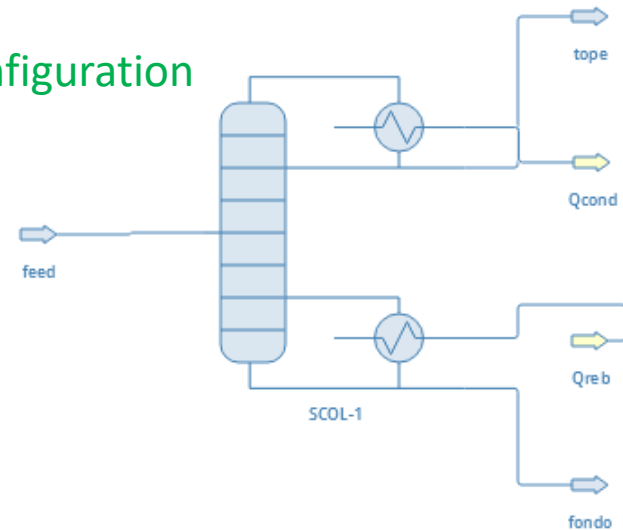
Maximum Number of Iterations: 100

Convergence Tolerance: 1E-05

Property Package: Peng-Robinson (PR) (1)

Solving Method: Wang-Henke (Bubble Point)

External Solver: [dropdown]



# Distillation Column (Column Specs > General)

General Specifications

Número de etapas de equilibrio (incluidas el condensador y rehervidor)

Absorber Operating Mode

Number of Stages 18

Condenser/Top Pressure 101325 Pa

Column Pressure Drop 0 Pa

Perfil de presiones

Maximum Number of Iterations 100

Convergence Tolerance 1E-05

Property Package Peng-Robinson (PR) (1)

Solving Method Wang-Henke (Bubble Point)

External Solver

Algoritmo y esquema de resolución

The image shows a software interface for configuring a distillation column. The 'Specifications' tab is active. A green box highlights the 'Number of Stages' field, which is set to 18, with an annotation 'Número de etapas de equilibrio (incluidas el condensador y rehervidor)'. Another green box highlights the 'Condenser/Top Pressure' and 'Column Pressure Drop' fields, with an annotation 'Perfil de presiones'. A third green box highlights the 'Solving Method' dropdown menu, which is set to 'Wang-Henke (Bubble Point)', with an annotation 'Algoritmo y esquema de resolución'. Other visible fields include 'Absorber Operating Mode', 'Maximum Number of Iterations' (100), 'Convergence Tolerance' (1E-05), 'Property Package' (Peng-Robinson (PR) (1)), and 'External Solver'.

# Distillation Column (Column Specs > Condenser)

General Specifications Stages Connections Estimates Results

Condenser Reboiler

No Condenser (Reboiled Absorber)

Condenser Type Total

Condenser Pressure Drop 0 Pa

Specification **Reflux Ratio**

Compound

1,93

Vapor Product Flow Rate 0 mol/s

Total Condenser Subcooling 0 K.

Tipo de condensador

- Total
- Total
- Partial
- Full Reflux

Presión y caída de presión en el condensador

Reflux Ratio

- Heat Load
- Product Molar Flow
- Compound Molar flow in Product Stream
- Product Mass Flow
- Compound Mass Flow in Product Stream
- Compound Fraction in Product Stream
- Compound Recovery
- Reflux Ratio
- Temperature

Variable y valor de la especificación para el condensador

Variables de especificación. Su disponibilidad depende del algoritmo seleccionado.

# Distillation Column (Column Specs > Reboiler)

General Specifications Stages Connections Estimates Results

Condenser Reboiler

No Reboiler (Refluxed Absorber)

Specification Product Molar Flow

Compound

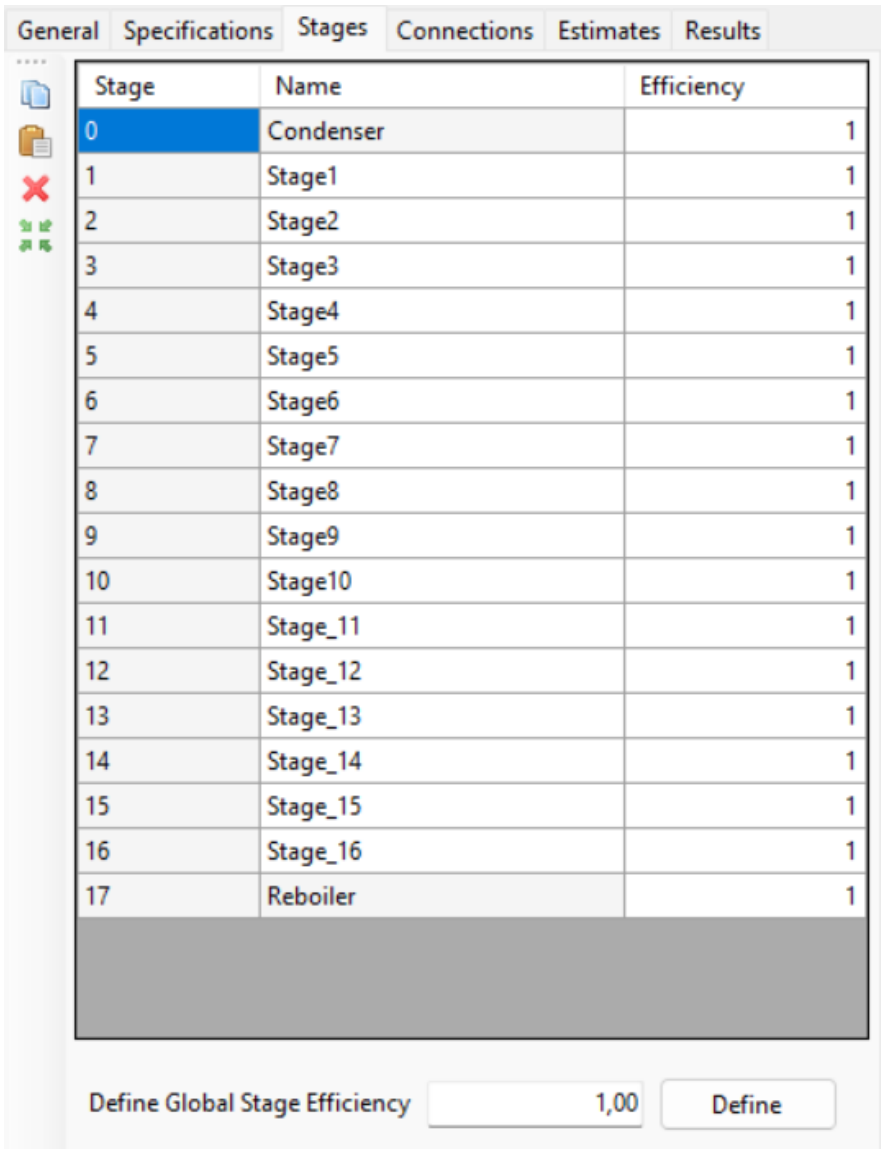
5 mol/s

Product Molar Flow  
Heat Load  
Product Molar Flow  
Compound Molar flow in Product Stream  
Product Mass Flow  
Compound Mass Flow in Product Stream  
Compound Fraction in Product Stream  
Compound Recovery  
Boil-Up Ratio  
Temperature

Variables de especificación.  
Su disponibilidad depende del  
algoritmo seleccionado.

Variable y valor de la especificación para el rehervidor

# Distillation Column (Column Configuration > Stages)



Stage	Name	Efficiency
0	Condenser	1
1	Stage1	1
2	Stage2	1
3	Stage3	1
4	Stage4	1
5	Stage5	1
6	Stage6	1
7	Stage7	1
8	Stage8	1
9	Stage9	1
10	Stage10	1
11	Stage_11	1
12	Stage_12	1
13	Stage_13	1
14	Stage_14	1
15	Stage_15	1
16	Stage_16	1
17	Reboiler	1

Define Global Stage Efficiency

Permite definir las eficiencias de cada etapa

# Distillation Column (Column Configuration > Connections)

Entradas

Salidas (Productos)

Name	Material Stream
Column Feed Port #1	feed
Column Feed Port #2	
Column Feed Port #3	
Column Feed Port #4	
Column Feed Port #5	
Column Feed Port #6	
Column Feed Port #7	
Column Feed Port #8	
Column Feed Port #9	
Column Feed Port #10	

Name	Material Stream
Distillate	tope
Bottoms	fondo
Overhead Vapor	

Name	Energy Stream
Condenser Duty	Qcond
Reboiler Duty	Qreb

Corrientes de energía

Salidas laterales

Name	Material Stream
Side Draw #1	
Side Draw #2	
Side Draw #3	
Side Draw #4	
Side Draw #5	
Side Draw #6	
Side Draw #7	

# Distillation Column (Column Configuration > Connections)

## Asociación Corriente-Etapa



General	Specifications	Stages	Connections	Estimates	Results
Stream Connections		Stream-Stage Associations		Side Draw Specs	
Port Type	Stream Name	Stage Location			
Feed	feed	Stage9	▼		
Distillate	tope	Condenser	▼		
Bottoms Product	fondo	Reboiler	▼		

## Especificación de las salidas laterales

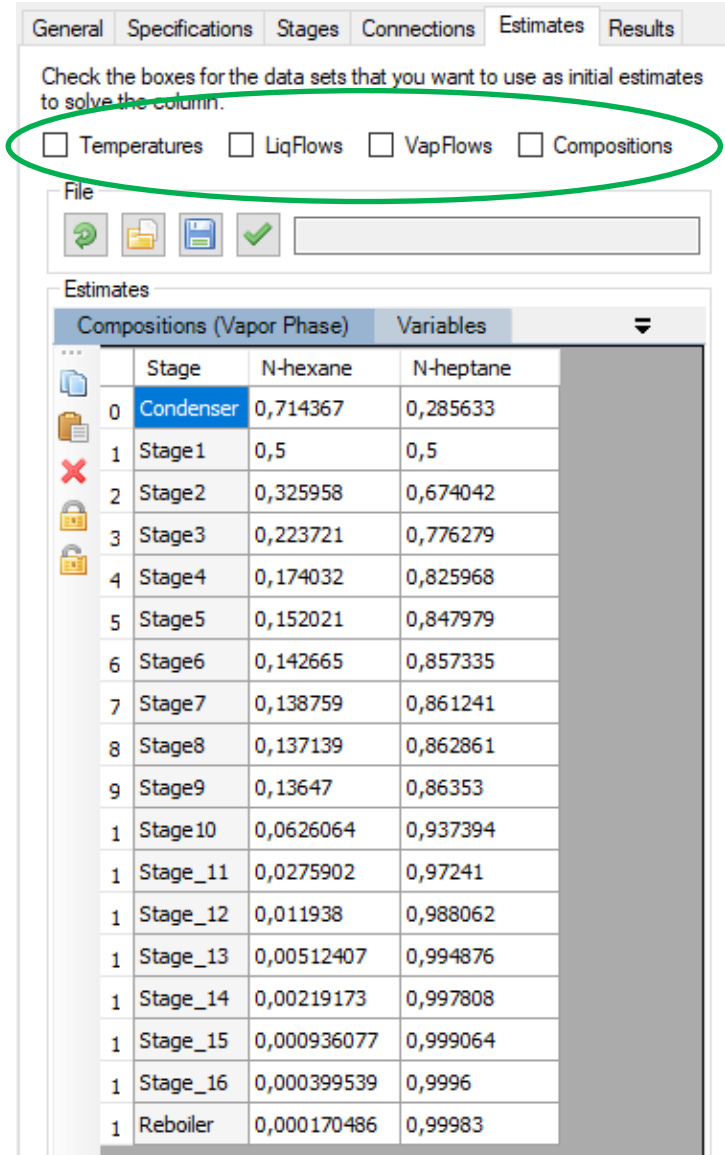


General	Specifications	Stages	Connections	Estimates	Results
Stream Connections		Stream-Stage Associations		Side Draw Specs	
Stream Name	Draw Phase	Molar Flow (mol/s)			

# Distillation Column (Column Configuration > Initial Estimate)

Se puede introducir una estimación inicial de algunas variables para mejorar el valor de arranque

Activa la inicialización de variables



General Specifications Stages Connections **Estimates** Results

Check the boxes for the data sets that you want to use as initial estimates to solve the column.

Temperatures  LiqFlows  VapFlows  Compositions

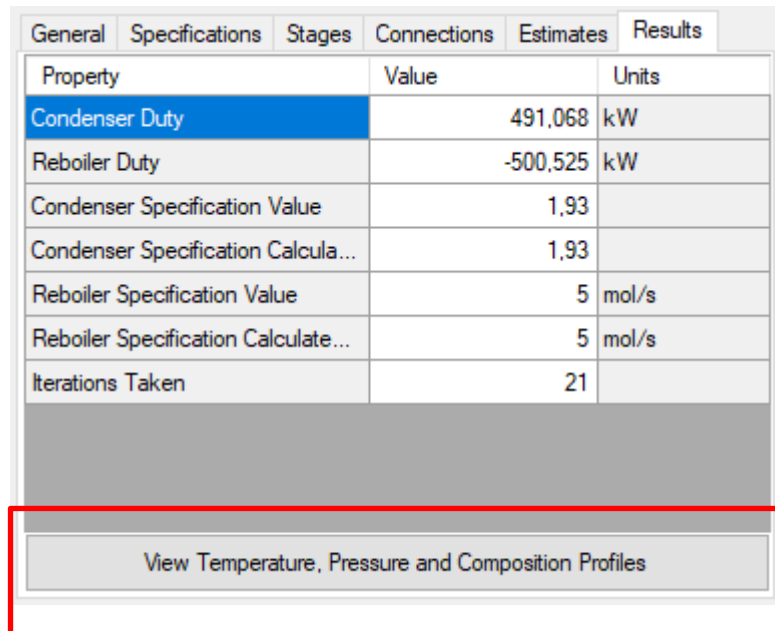
File

Estimates

Compositions (Vapor Phase)		Variables	
Stage	N-hexane	N-heptane	
0	Condenser	0,714367	0,285633
1	Stage1	0,5	0,5
2	Stage2	0,325958	0,674042
3	Stage3	0,223721	0,776279
4	Stage4	0,174032	0,825968
5	Stage5	0,152021	0,847979
6	Stage6	0,142665	0,857335
7	Stage7	0,138759	0,861241
8	Stage8	0,137139	0,862861
9	Stage9	0,13647	0,86353
1	Stage10	0,0626064	0,937394
1	Stage_11	0,0275902	0,97241
1	Stage_12	0,011938	0,988062
1	Stage_13	0,00512407	0,994876
1	Stage_14	0,00219173	0,997808
1	Stage_15	0,000936077	0,999064
1	Stage_16	0,000399539	0,9996
1	Reboiler	0,000170486	0,99983

## Distillation Column (Results)

- Una vez definidos todos los parámetros y conexiones de la columna se debe presionar (como siempre) F5 para la resolución del flowsheet.
- Si se llega a una solución que cumple con las especificaciones y tolerancias establecidas, en la solapa Results se presentaran los resultados.



Property	Value	Units
Condenser Duty	491,068	kW
Reboiler Duty	-500,525	kW
Condenser Specification Value	1,93	
Condenser Specification Calcula...	1,93	
Reboiler Specification Value	5	mol/s
Reboiler Specification Calculate...	5	mol/s
Iterations Taken	21	

View Temperature, Pressure and Composition Profiles

Permite observar los perfiles dentro de la columna

## Ejemplo de aplicación

Se desea separar una corriente de 10 mol/s de una mezcla equimolar de N-hexano y N-heptano a 1 atm en condiciones de líquido saturado.

- La destilación se realiza en condiciones atmosféricas.
- La pureza de cada producto se desea de 0.99 en fracción molar.

Un análisis FUG (shortcut) arrojó los siguientes resultados:

Property	Value	Units
Minimum Reflux Ratio	1,404	
Minimum Number of Stages	10,6173	
Actual Number of Stages	19,2803	
Optimal Feed Stage	9,64014	
Stripping Liquid	20,53	mol/s
Rectify Liquid	10,53	mol/s
Stripping Vapor	15,53	mol/s
Rectify Vapor	15,53	mol/s
Condenser Duty	450,145	kW
Reboiler Duty	459,893	kW

## Armado del Caso

- Se crea el caso de estudio y se seleccionan los componentes.
- Se utiliza Peng Robinson.
- Se propone una torre de 20 etapas alimentada en la etapa 9
- Como especificación en el condensador se establece una relación de reflujo de 2.106
- Como especificación en el rehervidor se ingresa un flujo molar de producto de 5 mol/s

# Armado del Caso

## Property Package Settings

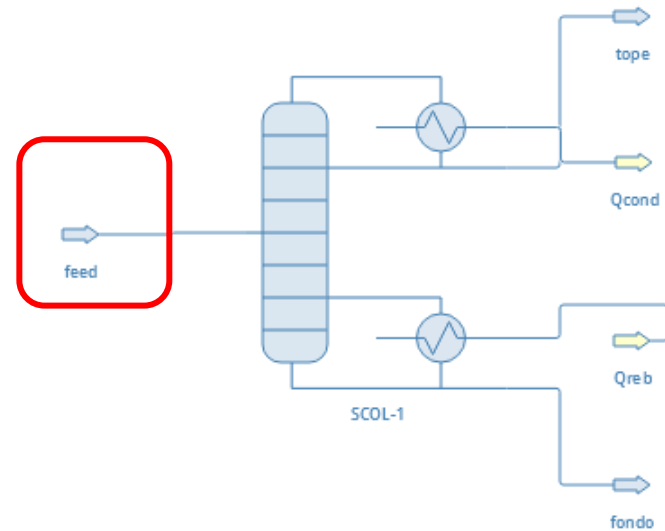
Property Package Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Flash Spec	Pressure and Vapor Fraction (PVF) ▾	
Temperature	354,612	K ▾
Pressure	101325	Pa ▾
Mass Flow	0,931887	kg/s ▾
Molar Flow	10	mol/s ▾
Volumetric Flow	0,00151208	m <sup>3</sup> /s ▾
Specific Enthalpy	-232,394	kJ/kg ▾
Specific Entropy	-0,556482	kJ/[kg.K] ▾
Vapor Phase Mole Fraction	0	
Force Stream Phase	Global Definition ▾	

Do not change this setting unless you know what you're doing.



# Armado del Caso

General Specifications Stages Connections Estimates Results

Absorber Operating Mode ▼

Number of Stages

Condenser/Top Pressure  Pa ▼

Column Pressure Drop  Pa ▼

Tray Spacing (Sizing)  m ▼

Maximum Number of Iterations

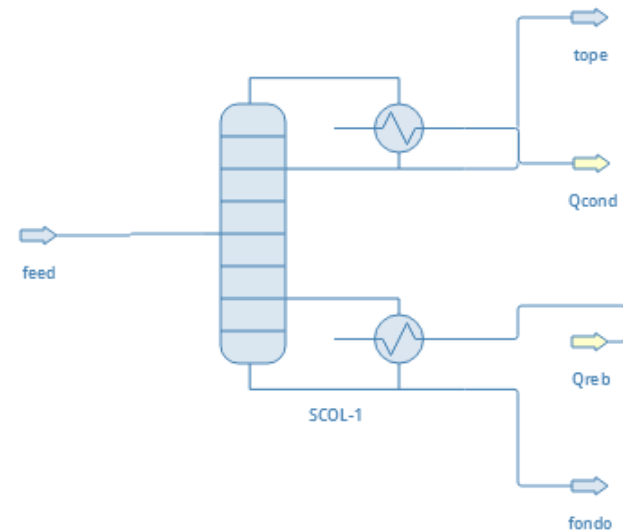
Convergence Tolerance

Property Package Peng-Robinson (PR) (1) ▼

Solving Method Wang-Henke (Bubble Point) ▼

External Solver ▼

Generate Convergence Report



# Armado del Caso

General Specifications Stages Connections Estimates Results

Condenser Reboiler

No Condenser (Reboiled Absorber)

Condenser Type Total

Condenser Pressure Drop 0 Pa

Specification Reflux Ratio

Compound

2,106

Vapor Product Flow Rate 0 mol/s

Total Condenser Subcooling 0 K.



General Specifications Stages Connections Estimates Results

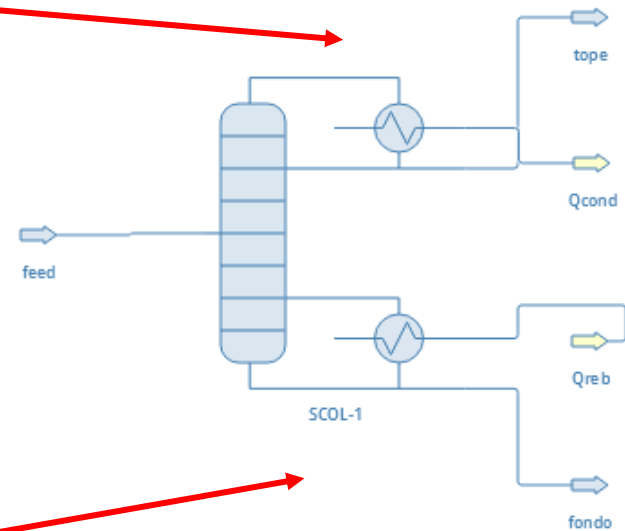
Condenser Reboiler

No Reboiler (Refluxed Absorber)

Specification Product Molar Flow

Compound

5 mol/s



# Armado del Caso

General Specifications Stages **Connections** Estimates Results

Stream Connections Stream-Stage Associations Side Draw Specs

Feeds Products Duties Side Draws

Name	Material Stream
Column Feed Port #1	feed
Column Feed Port #2	

General Specifications Stages **Connections** Estimates Results

Stream Connections Stream-Stage Associations Side Draw Specs

Feeds Products Duties Side Draws

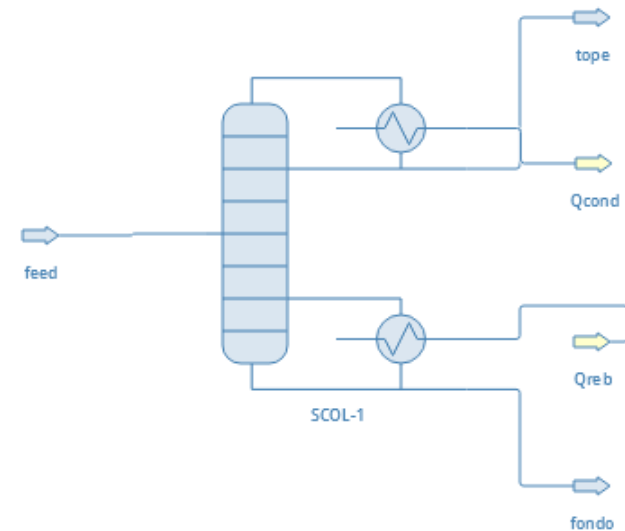
Name	Material Stream
Distillate	Tope
Bottoms	Fondo
Overhead Vapor	

General Specifications Stages **Connections** Estimates Results

Stream Connections Stream-Stage Associations Side Draw Specs

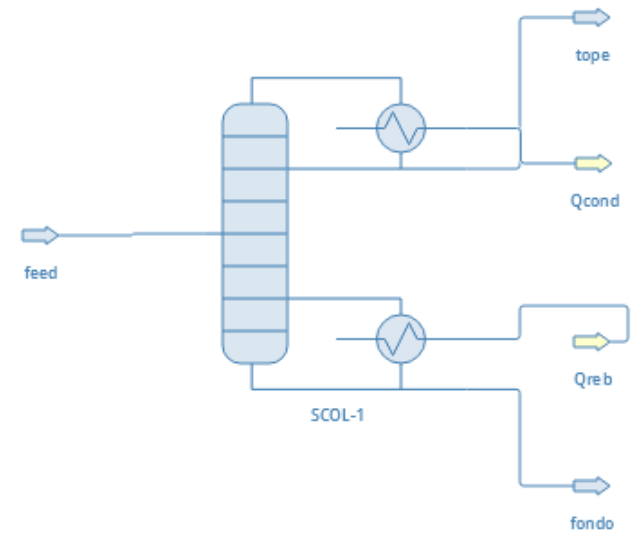
Feeds Products Duties Side Draws

Name	Energy Stream
Condenser Duty	Qcond
Reboiler Duty	Qreb



# Armado del Caso

Port Type	Stream Name	Stage Location
Feed	feed	Stage9
Distillate	Tope	Condenser
Bottoms Product	Fondo	Reboiler



# Resultados

General Specifications Stages Connections Estimates Results

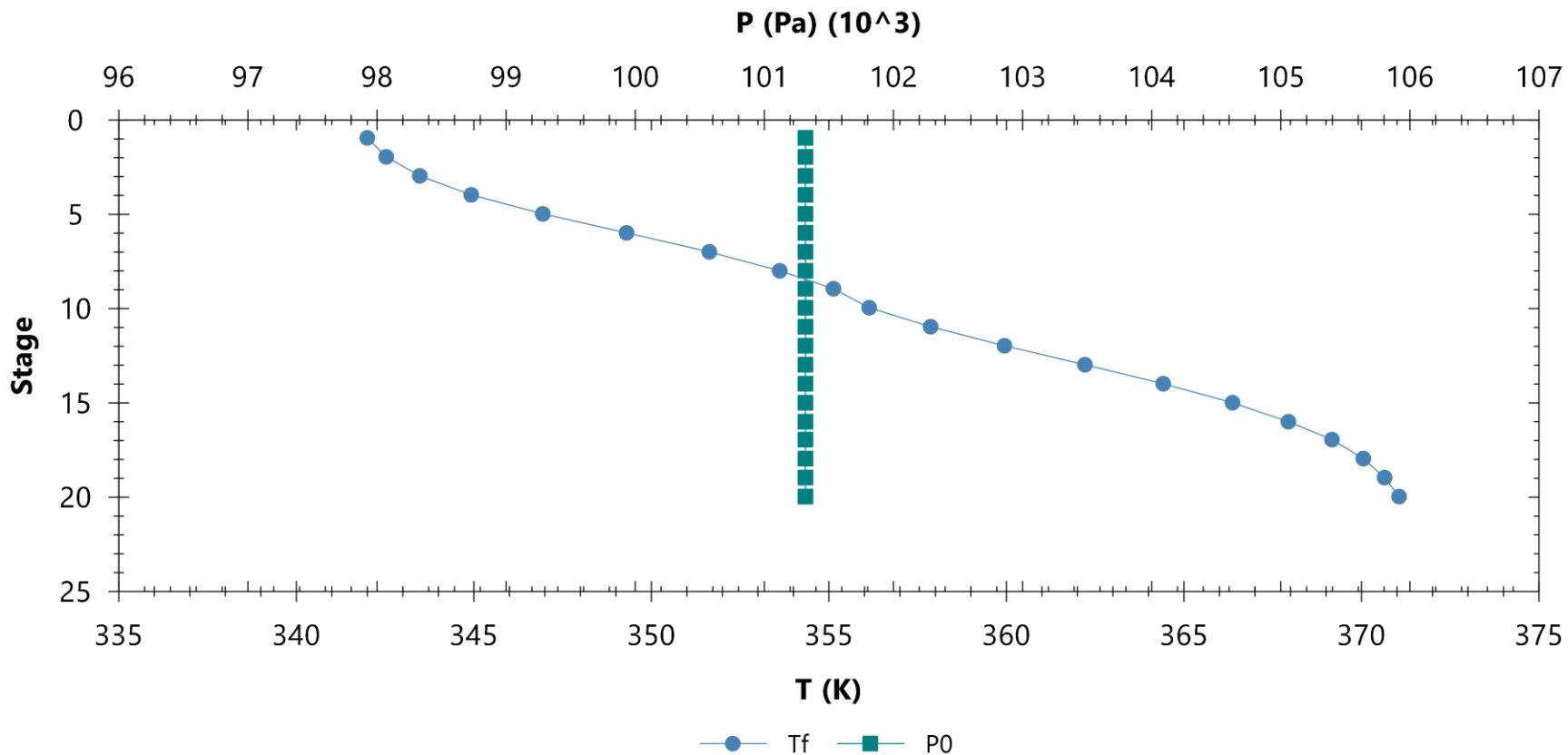
View Temperature, Pressure and Composition Profiles

View Properties Profile

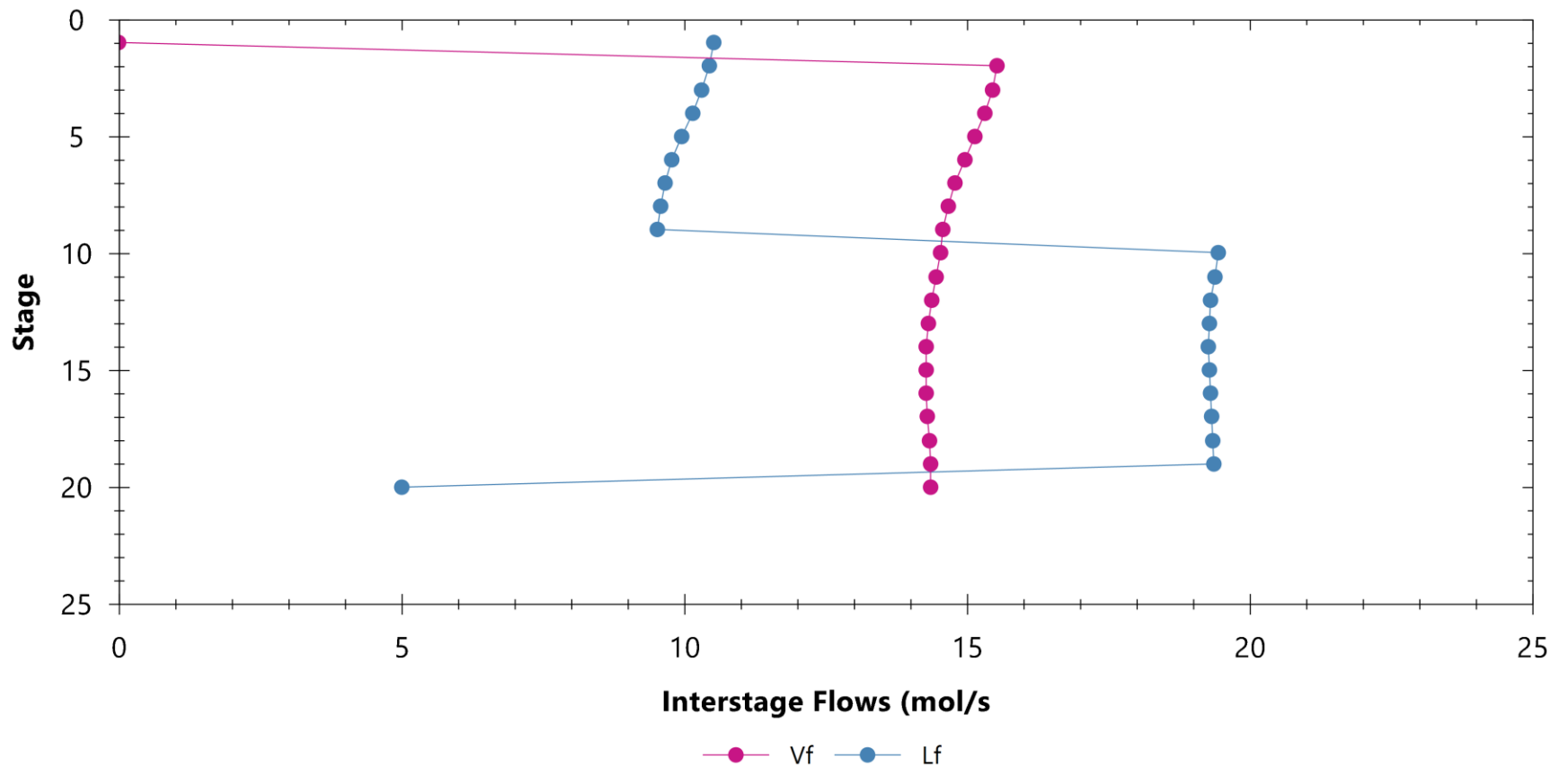
View Convergence Report

Property	Value	Units
Condenser Duty	450,822	kW
Reboiler Duty	-459,194	kW
Condenser Specification Value	2,106	mol/s
Condenser Specification Calculat...	2,106	
Reboiler Specification Value	5	mol/s
Reboiler Specification Calculated...	5	mol/s
Iterations Taken	48	
Estimated Height	11000	mm
Estimated Diameter	940,176	mm

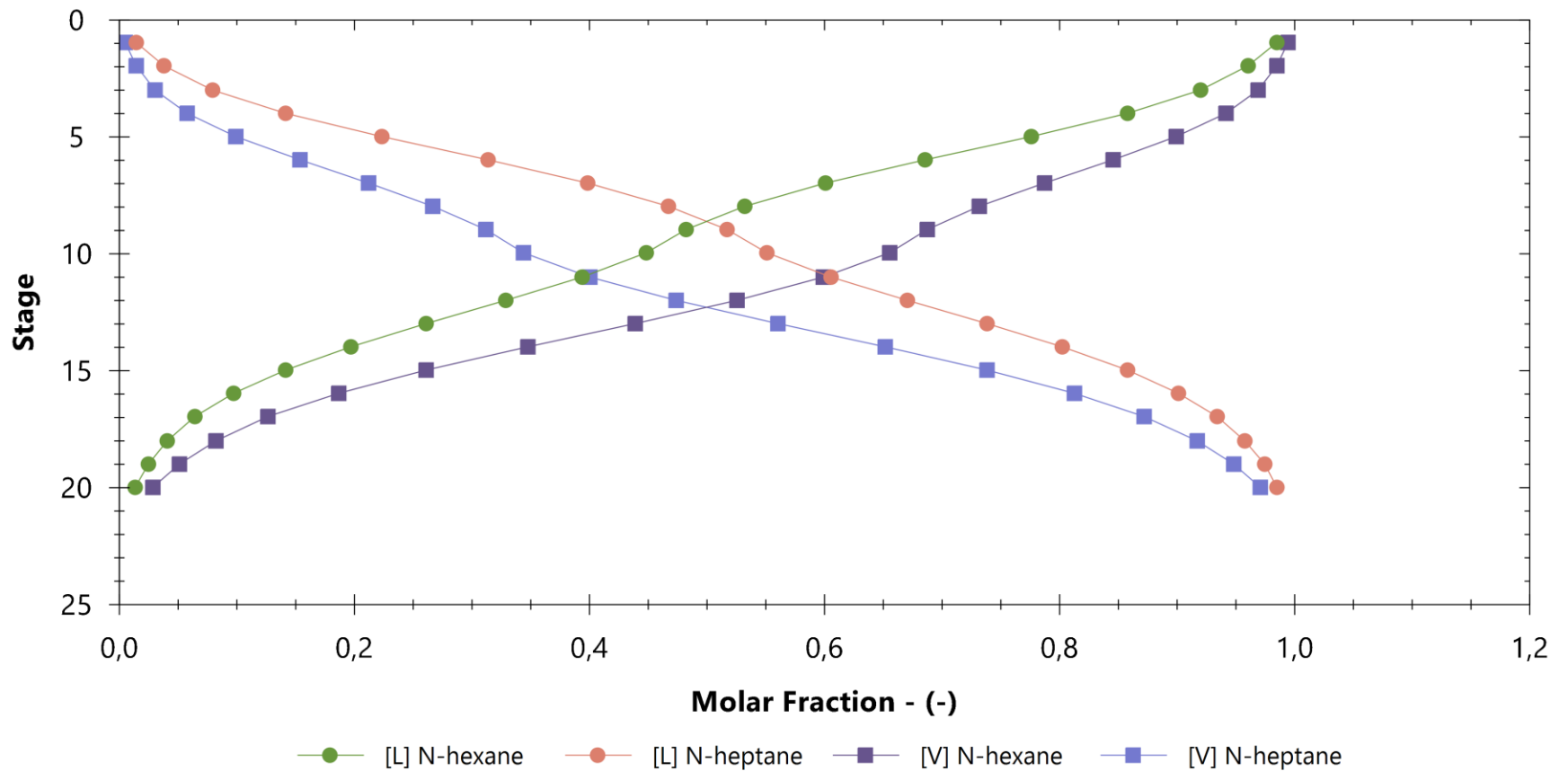
# Resultados (perfil de composiciones)



# Resultados (perfil de presión y temperatura)



# Resultados (perfil de presión y temperatura)



## Resultados (perfil de flujo molar)

	Feed	Tope	Fondo
Temperature (K)	354.612	342.026	371,081
Pressure (Pa)	101325	101325	101325
Molar Flow (mol/s)	10	5	5
Molar Fraction (Mixture) / N-hexane	0.5	0.98566	0.01432
Molar Fraction (Mixture) / N-heptane	0.5	0.01434	0.98568

La composición de salida no es la deseada.



Los valores de diseño del análisis shortcut son aproximados

¿Cómo se puede mejorar la separación?

## Resultados (perfil de flujo molar)

	Feed	Tope	Fondo
Temperature (K)	354.612	341.923	371,259
Pressure (Pa)	101325	101325	101325
Molar Flow (mol/s)	10	5	5
Molar Fraction (Mixture) / N-hexane	0.5	0.99034	0.00963
Molar Fraction (Mixture) / N-heptane	0.5	0.00966	0.99037

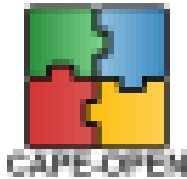
**Etapas constantes:** Se aumenta la relación de reflujo hasta obtener la composición deseada. Se puede realizar de forma manual o utilizando un bloque controlador.

**RR=2.4 y 20 etapas**

## Resultados (perfil de flujo molar)

	Feed	Tope	Fondo
Temperature (K)	354.612		
Pressure (Pa)	101325		
Molar Flow (mol/s)	10		
Molar Fraction (Mixture) / N-heptane	0.5		
Molar Fraction (Mixture) / N-hexane	0.5		

Relación de reflujo constante: Se aumenta la cantidad de etapas hasta obtener la composición deseada. Se debe realizar si o si de forma manual (completar)



## CAPE-OPEN Unit Operation

Model for utilization of a CAPE-OPEN  
Unit Operation in the flowsheet



**ChemSep  
Column**

- En las versiones recientes Chemsep ya cuenta con un quipo propio.
- El procedimiento es similar ya que se trata de una conexión directa a ChemSep mediante Cape Open

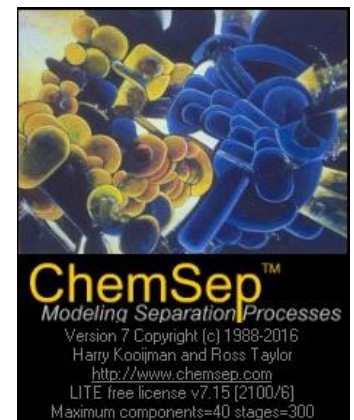
Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

# Simulación Mediante el protocolo CAPE OPEN (ChemSep)

- El estándar de interfaz CAPE-OPEN consiste en una serie de especificaciones para ampliar el rango de aplicación de las tecnologías de simulación de procesos.
- Las especificaciones CAPE-OPEN comprenden un conjunto de interfaces de software que permiten la interoperabilidad plug and play entre un entorno de modelado de proceso (PME) y un componente de modelado de proceso (PMC) de terceros.



**CAPE-OPEN Unit Operation**  
Model for utilization of a CAPE-OPEN  
Unit Operation in the flowsheet

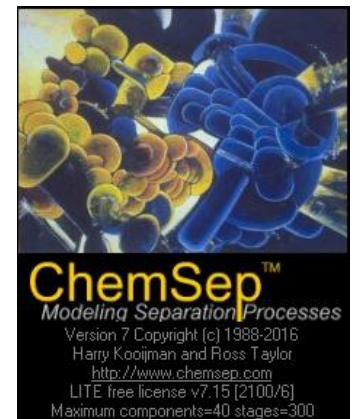


# Conexión Mediante el protocolo CAPE OPEN (ChemSep)

- ChemSep es un simulador de columnas para operaciones de destilación, absorción y extracción.
- Puede ser utilizado de manera aislada (solo columnas) o integrado a un flowsheet en un simulador de procesos.
- ChemSep LITE permite modelar columnas de equilibrio con hasta 40 componentes y 300 etapas utilizando una base de datos que cubre más de 400 productos químicos.



**CAPE-OPEN Unit Operation**  
Model for utilization of a CAPE-OPEN  
Unit Operation in the flowsheet



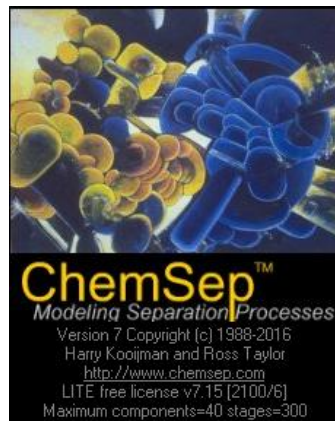
# DSOySP



Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

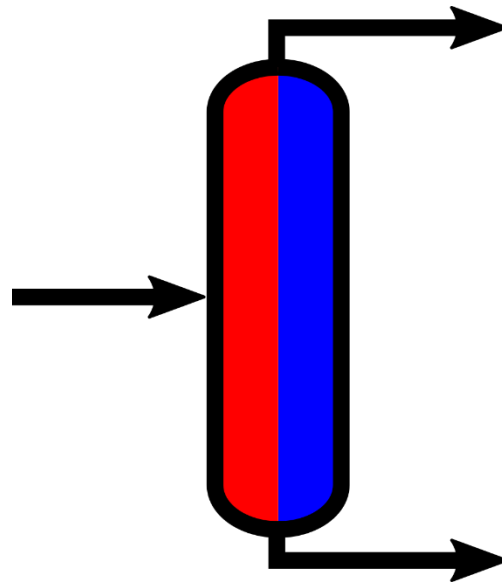
# ChemSep

- ChemSep is a column simulator for distillation, absorption, and extraction operations.
- It combines the classic equilibrium stage column model with a nonequilibrium (rate-based) column model in one easy and intuitive interface.
- Test-drive the equilibrium column model and convince yourself with the free ChemSep LITE with up to 40 components and 300 equilibrium stages using a database covering 400+ chemicals.



# ChemSep

- Es posible utilizar Chemsep desde su interfaz (sin CAPE-OPEN).
- Solamente se puede simular una columna de destilación.
- La única diferencia respecto de lo anterior es que se deben seleccionar los compuestos y las corrientes de entrada dentro de la interfaz de ChemSep.

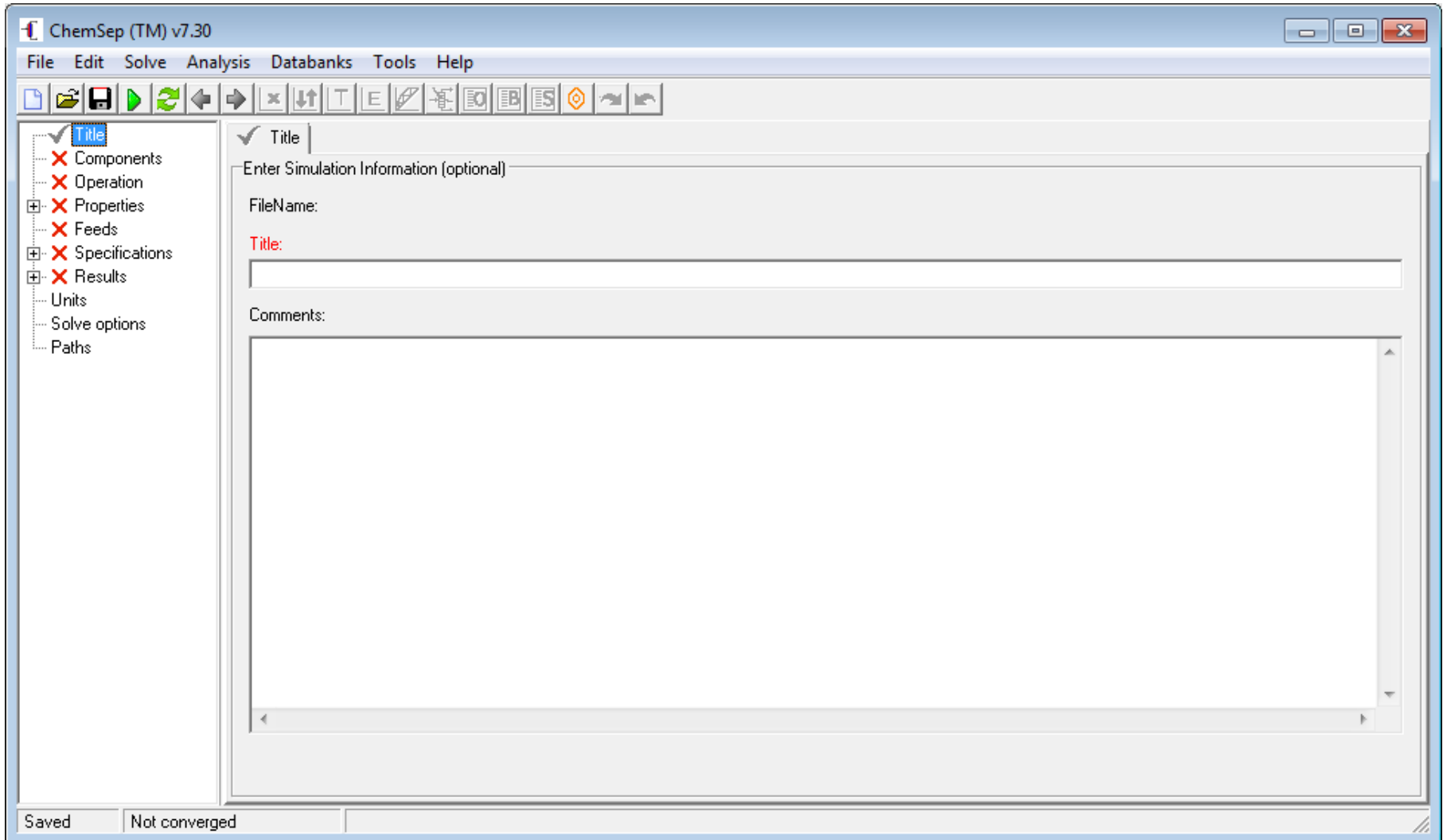


## Ejemplo de aplicación de ChemSep

Se desea separar una corriente de 10 mol/s de una mezcla equimolar de N-hexano y N-heptano a 1 atm en condiciones de liquido saturado.

- La destilación se realiza en condiciones atmosféricas.
- La pureza deseada de cada producto es de 0.99 en fracción molar.
- Se propone una columna de destilación simple de 20 etapas de equilibrio con un condensador total.
- La alimentación se introduce 9 etapas por debajo del condensador

# Ejemplo de aplicación de ChemSep



# Ejemplo de aplicación de ChemSep

The screenshot displays the ChemSep (TM) v7.30 software interface. The main window is titled "ChemSep (TM) v7.30" and features a menu bar with "File", "Edit", "Solve", "Analysis", "Databanks", "Tools", and "Help". Below the menu bar is a toolbar with various icons for file operations and simulation control.

The interface is divided into several sections:

- Left Panel:** A tree view showing the project structure with the following items: Title (checked), Components (checked), Operation (unchecked), Properties (unchecked), Feeds (unchecked), Specifications (unchecked), Results (unchecked), Units, Solve options, and Paths.
- Components Section:** A tab labeled "Components" is active. It includes a "Select Components" area with a "Component databank" field set to "c:\users\jmanassald\appdata\local\chemsepl7v30\" and a "Browse" button. There is also an "Advanced search" checkbox and a "Sort" button.
- Find Field:** A text input field for searching components, currently containing "ChemSep v7.30 pure component data - Copyright (c) Harry Kooijman and Ross Tayl...".
- Component Lists:** Two lists are shown: "Components in databank" and "Selected components in simulation".
- Component Lists Table:** A table with columns: Identifier, L#, File, Loc., CAS, and SMILES. The "Selected components in simulation" list contains two entries: hexane (L# 11, CAS 110-54-3, SMILES CCCCCC) and heptane (L# 17, CAS 142-82-5, SMILES CCCCCC).
- Control Buttons:** A set of buttons for managing the component lists: Add, Remove, Substitute, Remove All, Up, Down, Add New, Pseudo's, and Show.
- Checkboxes:** A checkbox labeled "Separate Apparent and True species" is checked.
- Status Bar:** At the bottom, there are two indicators: "Changed" and "Not converged".

# Ejemplo de aplicación de ChemSep

ChemSep (TM) v7.30

File Edit Solve Analysis Databanks Tools Help

✓ Title  
✓ Components  
✓ Operation  
✗ Properties  
✗ Feeds  
✗ Specifications  
✗ Results  
Units  
Solve options  
Paths

✓ Operation

Select Type of Simulation

Flash  
 Equilibrium column  
 Nonequilibrium column

Configuration

Operation: Simple Distillation

Condenser: Total (Liquid product)

Reboiler: Partial (Liquid product)

Number of stages (e.g. 10) 20

Feed stage(s) (e.g. 5,7) 10

Sidestream stage(s) (e.g. 2,9)

Pumparound(s) (e.g. 6>8, 9>1)

Changed Not converged

# Ejemplo de aplicación de ChemSep

The screenshot displays the ChemSep (TM) v7.30 software interface. The window title is "ChemSep (TM) v7.30". The menu bar includes "File", "Edit", "Solve", "Analysis", "Databanks", "Tools", and "Help". The toolbar contains various icons for file operations, solving, and analysis.

The main window is divided into several sections:

- Left Panel (Tree View):** A list of configuration categories with checkboxes and expand/collapse icons. The categories are: Title (checked), Components (checked), Operation (checked), Properties (checked), Feeds (unchecked), Specifications (unchecked), Results (unchecked), Units, Solve options, and Paths.
- Top Navigation:** Three tabs are visible: "Thermodynamics" (checked), "Physical properties" (checked), and "Reactions" (checked).
- Select Thermodynamic Models:** A section with two columns of dropdown menus:
  - Column 1: K-value (Raoult's law), Equation of state (Ideal gas law), Activity coefficient (Ideal solution), Vapour pressure (Antoine), Enthalpy (Ideal).
  - Column 2: Enthalpy / Exergy (Reference state: Vapour, 298.1 (K); Heat of formation: Excluded; Surroundings T: 298.150 (K); Heat Capacity IG: T correlation; Heat Capacity L: Mole fraction a<sup>v</sup>).
- Henry's law components:** A checkbox labeled "Henry's law components" which is currently unchecked.
- Enter Thermodynamic Model Parameters (when required):** A large empty text area for entering specific model parameters.

At the bottom of the window, there are two status indicators: "Changed" and "Not converged".

# Ejemplo de aplicación de ChemSep

The screenshot displays the ChemSep (TM) v7.30 software interface. The window title is "ChemSep (TM) v7.30". The menu bar includes "File", "Edit", "Solve", "Analysis", "Databanks", "Tools", and "Help". The toolbar contains various icons for file operations, solving, and analysis. The left sidebar shows a tree view with the following items: Title (checked), Components (checked), Operation (checked), Properties (checked), Feeds (checked), Specifications (unchecked), Results (unchecked), Units, Solve options, and Paths. The main area is titled "Feeds" and contains a "Feed Stream(s) Specifications" section. This section includes "Insert" and "Remove" buttons, and a dropdown menu set to "Molar flows". Below these controls is a table with the following data:

Feed:	1
Name	Feed1
Stage	10
Two-phase feed	Split
State	p & V
Pressure (N/m <sup>2</sup> )	101325
Vapour fraction (-)	0.000000
Temperature (K)	
Flowrates (kmol/s):	
hexane	0.00500000
heptane	0.00500000
Total flowrate	0.01000000

At the bottom of the window, there are two status indicators: "Changed" and "Not converged".

# Ejemplo de aplicación de ChemSep

The screenshot displays the ChemSep (TM) - test.sep application window. The interface includes a menu bar (File, Edit, Solve, Analysis, Databanks, Tools, Help) and a toolbar with various icons. A tree view on the left shows the project structure, with 'Column specs' highlighted in blue. The main workspace is divided into two sections: 'Column Product Specifications' and 'Product Guesses (optional)'. The 'Column Product Specifications' section contains fields for 'Top product name' (Top), 'Condenser duty name' (Qcondenser), 'Top specification' (Mole fraction of a component = 0.990000), and 'Bottom product name' (Bottom), 'Reboiler duty name' (Qreboiler), 'Bottom specification' (Mole fraction of a component = 0.990000). The 'Product Guesses (optional)' section includes a checkbox for 'Use guesses for initialization', a 'Reset' button, and an 'Add variable to monitor' dropdown menu. The status bar at the bottom indicates 'Changed', 'Not converged', and the file path 'C:\Users\jmanassaldi\Desktop\test.sep'.

ChemSep (TM) - test.sep

File Edit Solve Analysis Databanks Tools Help

Column Product Specifications

Top product name: Top Condenser duty name: Qcondenser

Top specification: Mole fraction of a component = 0.990000 (-)  
hexane

Bottom product name: Bottom Reboiler duty name: Qreboiler

Bottom specification: Mole fraction of a component = 0.990000 (-)  
heptane

Product Guesses (optional)

Use guesses for initialization Reset Add variable to monitor

Changed Not converged C:\Users\jmanassaldi\Desktop\test.sep

# Ejemplo de aplicación de ChemSep

The screenshot displays the ChemSep software interface. The main window shows a table of results for a distillation column simulation. The table is organized into sections: physical properties, flow rates, and mass flows. The columns represent different stages: Feed1, Top, and Bottom. The 'Results' section is highlighted in the left-hand navigation pane.

Table 1: Physical Properties

Stream	Feed1	Top	Bottom
Stage	10	1	20
Pressure (Pa)	101325	101325	101325
Vapour fraction (-)	0.000000	0.000000	0.000000
Temperature (K)	353.821	342.236	371.196
Enthalpy (J/kmol)	-2.120E+07	-2.202E+07	-1.847E+07
Entropy (J/kmol/K)	-17920.2	-31124.1	-11305.4

Table 2: Flow Rates

Property	Feed1	Top	Bottom
Total molar flow (mol/s)	10.0000	5.00000	5.00000
Total mass flow (kg/s)	0.931905	0.431586	0.500319
Vapour std.vol.flow (m <sup>3</sup> /s)			
Liquid std.vol.flow (m <sup>3</sup> /s)	0.00138045	6.5136E-04	7.2907E-04

Table 3: Mole Flows (mol/s)

Component	Feed1	Top	Bottom
hexane	5.00000	4.95000	0.0500000
heptane	5.00000	0.0500000	4.95000

Table 4: Mole Fractions (-)

Component	Feed1	Top	Bottom
hexane	0.500000	0.990000	0.01000000
heptane	0.500000	0.01000000	0.990000

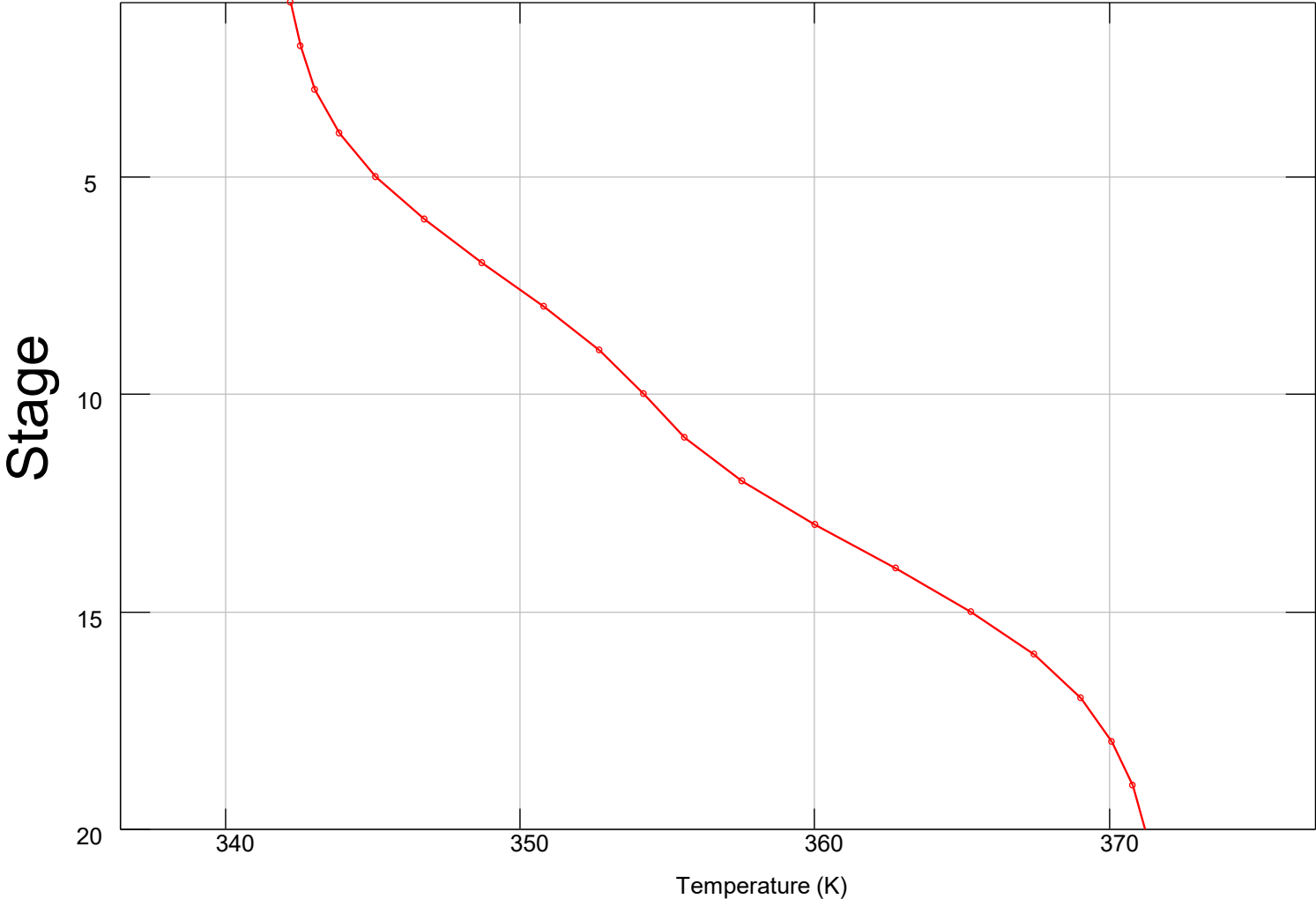
Table 5: Mass Flows (kg/s)

Component	Feed1	Top	Bottom
hexane	0.430885	0.426576	0.00430885

At the bottom of the window, the status bar indicates: Saved, Converged 6 iterations, and the file path C:\Users\jmanassaldi\Desktop\test.sep.

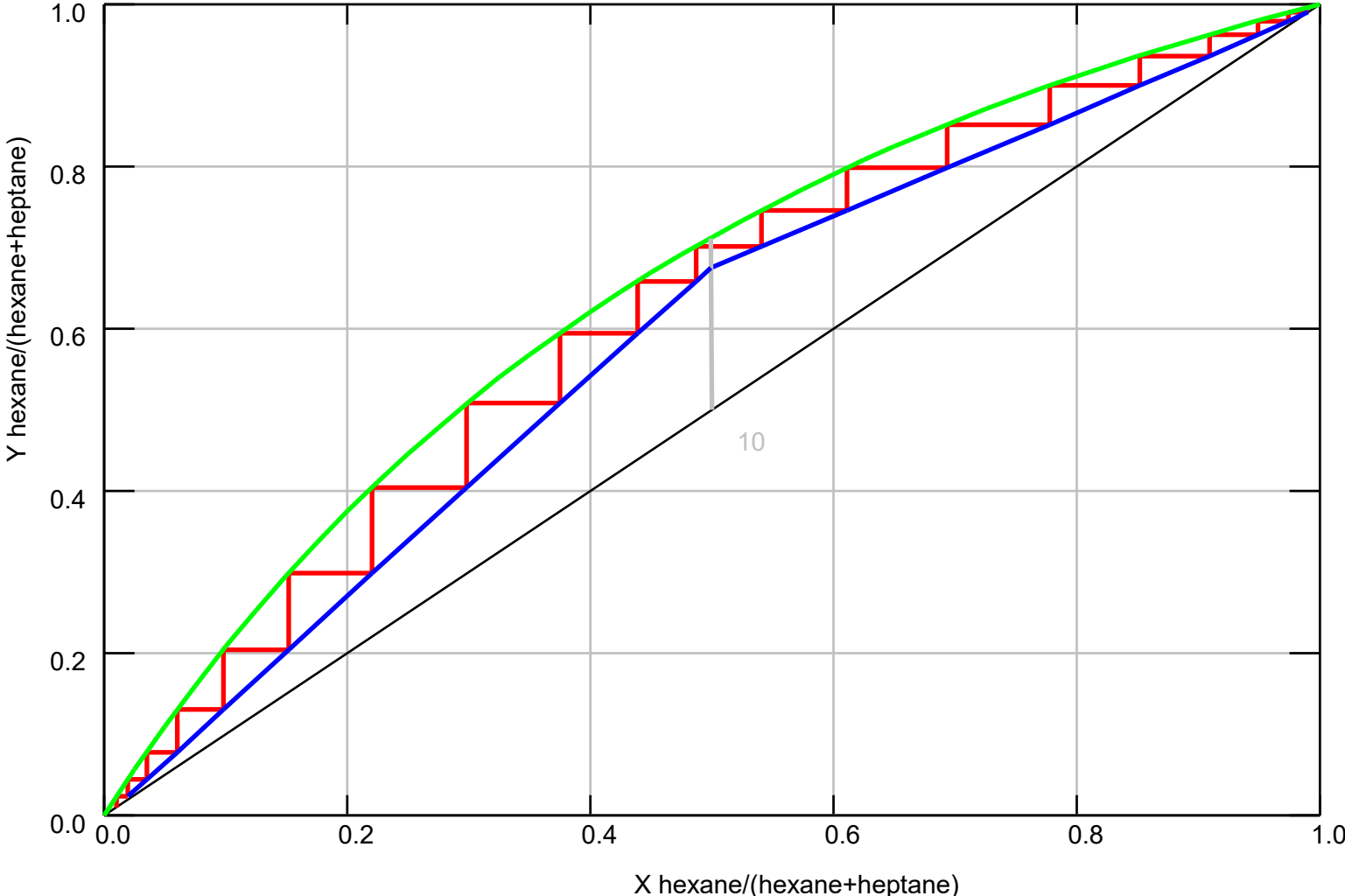
# Ejemplo de aplicación de ChemSep

Temperature profile



# Ejemplo de aplicación de ChemSep

McCabe-Thiele diagram hexane - heptane



# DSOySP

## Pressure Swing Distillation Separación de Metanol y Acetona

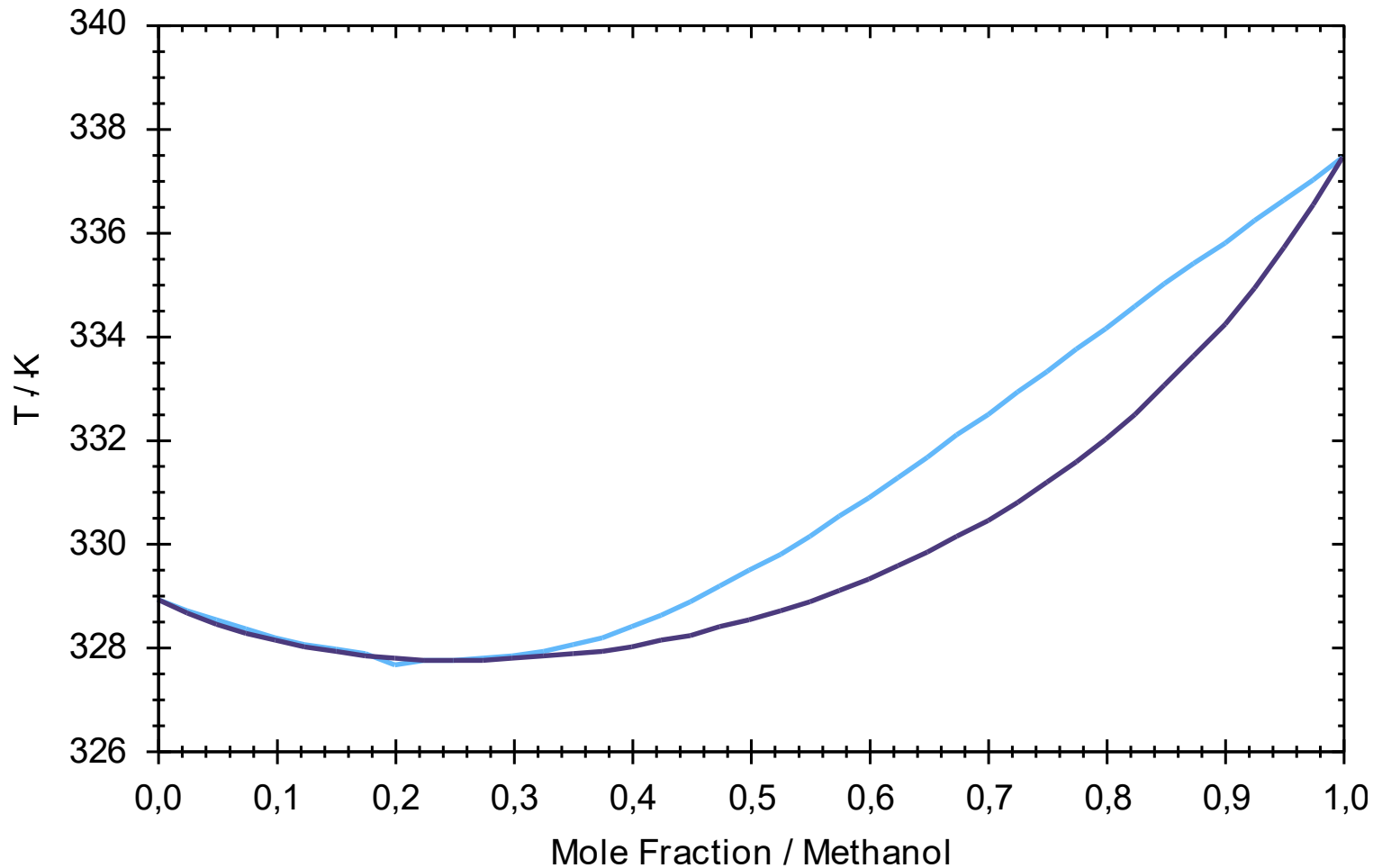
Profesor: Dr. Nicolás J. Scenna  
JTP: Dr. Néstor H. Rodríguez  
Aux. 1ra: Dr. Juan I. Manassaldi

# Pressure Swing Distillation

- Es un método para separar un azeótropo sensible a la presión utilizando dos columnas operadas en secuencia a dos presiones diferentes.
- El método aprovecha el “corrimiento” del azeótropo para poder obtener ambos componentes puros.

# Pressure Swing Distillation

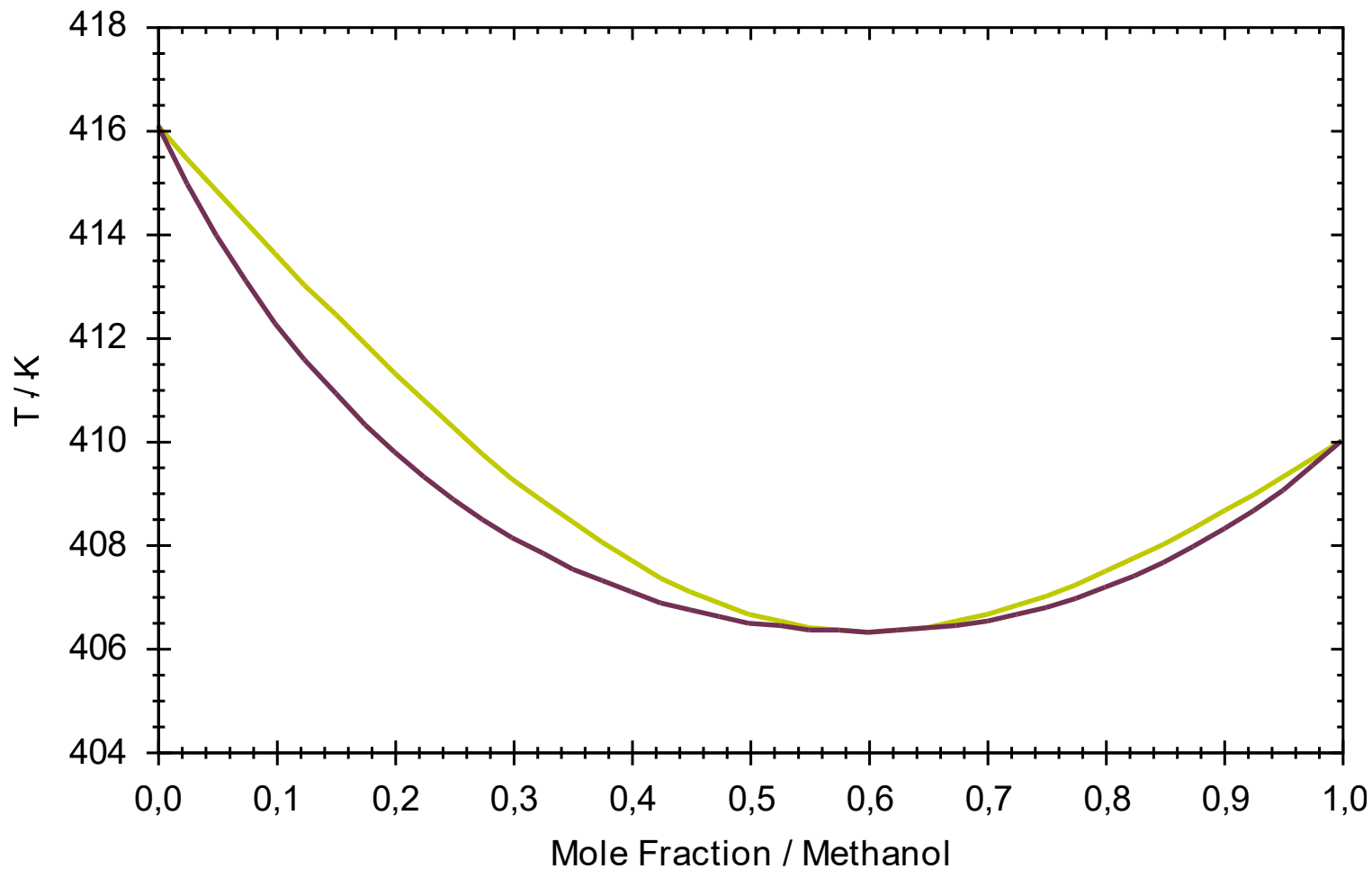
Methanol / Acetone  
P = 1 bar



— [NRTL] Bubble Points — [NRTL] Dew Points

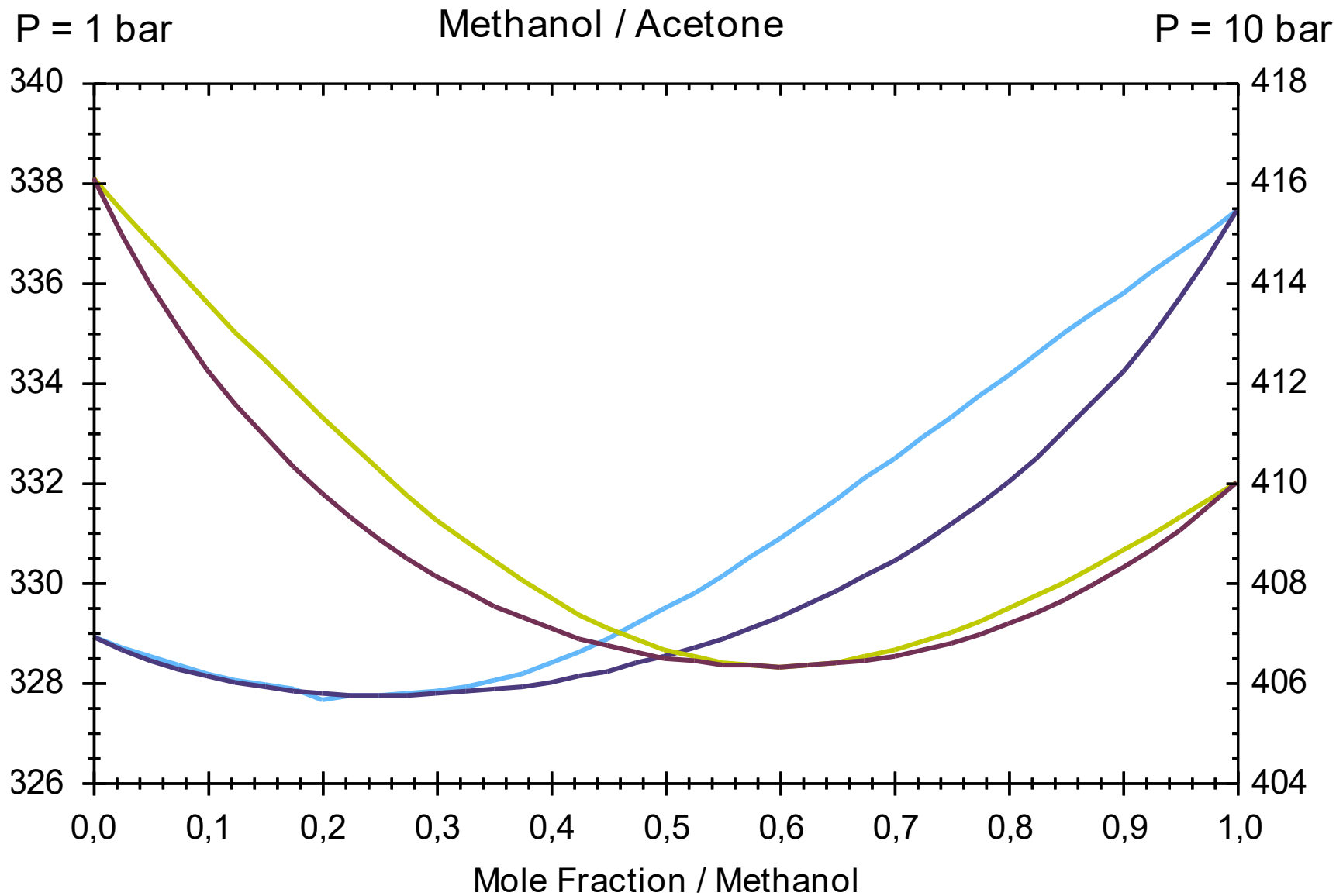
# Pressure Swing Distillation

Methanol / Acetone  
P = 10 bar



— [NRTL] Bubble Points — [NRTL] Dew Points

# Pressure Swing Distillation



# Pressure Swing Distillation

