



Aspen Plus.

1. Reactores en Aspen Plus
2. Simulación de un reactor CSTR.

Reactores en Aspen Plus



Hay 7 tipos de reactores en Aspen Plus:

Reactor Model

Description

RStoic

Conversion reactor with known stoichiometry

RYield

Yield reactor with known product yields

REquil

Two-phase chemical equilibrium reactor (stoichiometric)

RGibbs

Multiphase chemical equilibrium reactor (non-stoichiometric)

RCSTR

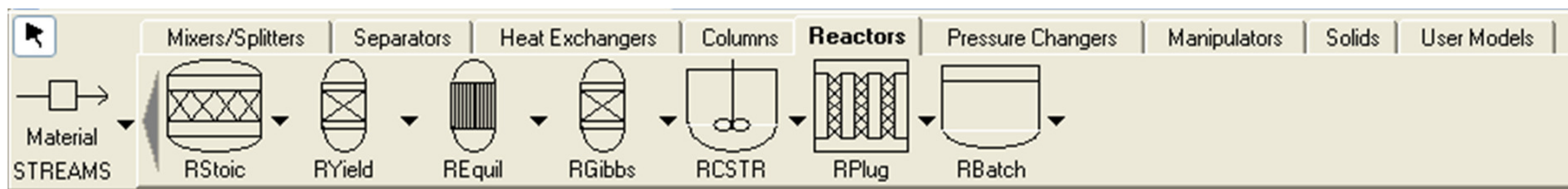
Continuous stirred-tank reactor with known kinetics

RPlug

Plug-flow reactor with known kinetics

RBatch

Batch or semi-batch reactor with known kinetics



Reactores en Aspen Plus



Rstoic

La cinética no se conoce o no es importante

Se conoce la estequiometría de la reacción

Se conoce la extensión de la reacción o la conversión.

Rcstr

Modelan de forma rigurosa reactores de mezcla perfecta.

La cinética se define de forma separada en el bloque Reactions

Rplug

Modelan de forma rigurosa reactores de flujo pistón (suponiendo mezcla perfecta en la dirección radial y no mezcla en la axial).

La cinética se define de forma separada en el bloque Reactions

Rbatch

Modela de forma rigurosa reactores tipo batch o semi-batch

La cinética se define de forma separada en el bloque Reactions

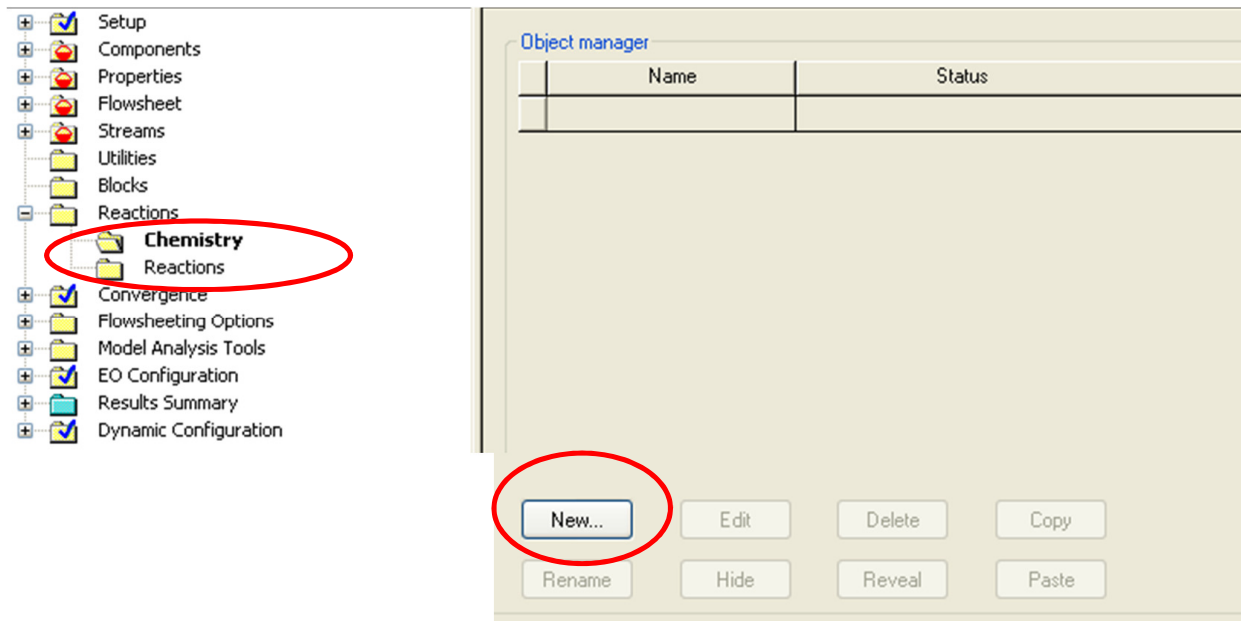
Reacciones en Aspen Plus



Tipo de Reacción:

Con electrolitos --- especies iónicas --- Seleccionar: Chemistry

Sin electrolitos --- Velocidades de reacción /equilibrios --- Seleccionar: Reactions



Reactions



Para especificar reacciones con cinéticas de reacción o equilibrios es sistemas sin electrolitos. Se identifican mediante un ID (R-1,R-2etc.)

Pueden usarse en:

Reactores: Rbatch, RCSTR, Rplug

Columnas : Radfrac

Permite usar:

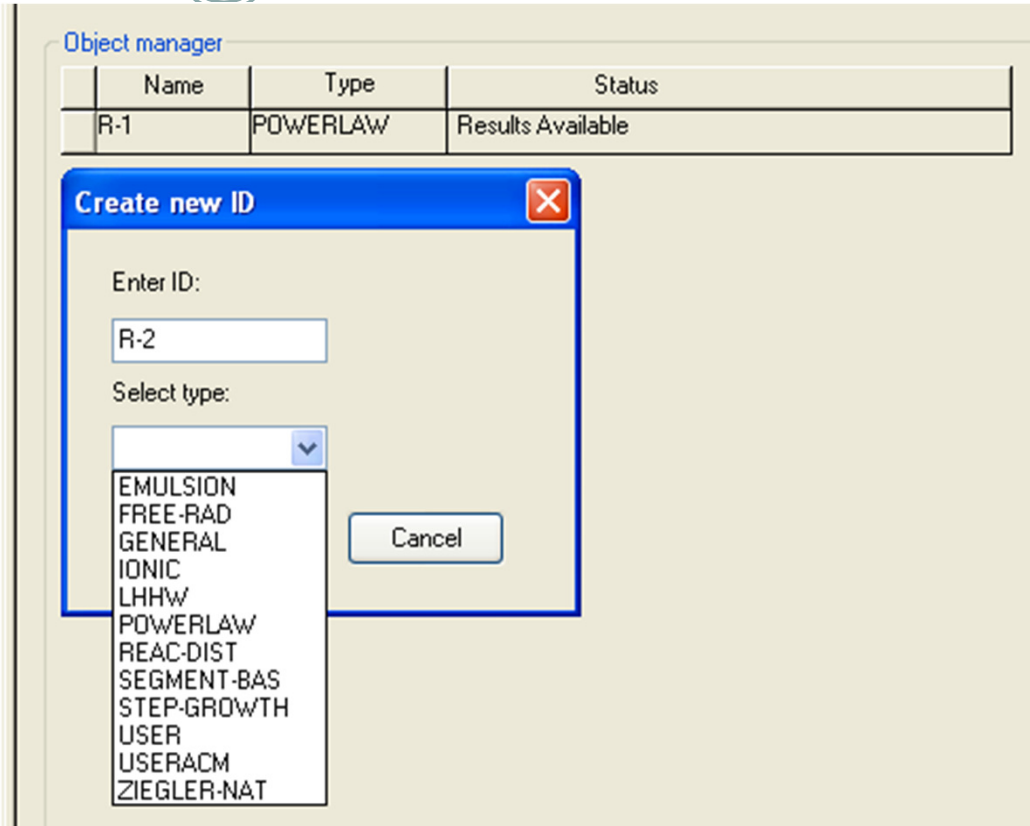
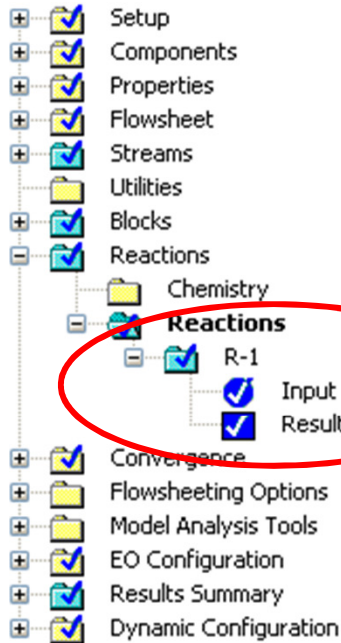
Modelo cinético Power Law (de Arrhenius)

Modelo LHHW (Langmuir-Hinshelwood-Hougen-Watson)

Modelo de equilibrio

Cinéticas de usuario

Reactions: selección del tipo



Reactions: Power Law model



$$r = k \left(\frac{T}{T_0} \right)^n e^{-\left(\frac{E}{R} \right) \left[\frac{1}{T} - \frac{1}{T_0} \right]} \prod_{i=1}^N C_i^{\alpha_i}$$

If T_0 is not specified the model reduces to:

$$r = kT^n e^{-\frac{E}{RT}} \prod_{i=1}^N C_i^{\alpha_i}$$

r = rate of reaction

k = pre-exponential factor

T = absolute temperature

T_0 = reference temperature

n = temperature exponent

E = activation energy

R = gas law constant

\prod = product operator

N = number of components

C_i = concentration of component i

α_i = exponent of component i

Reactions: Power Law model

Setup
Components
Properties
Flowsheet
Streams
Utilities
Blocks
Reactions
 Chemistry
 Reactions
 R-1
 Input
 Results
Convergence
Flowsheeting Options
Model Analysis Tools
EO Configuration
Results Summary
Dynamic Configuration

| Rxn No. | Reaction type | Stoichiometry |
|---------|---------------|--|
| 1 | Kinetic | $C_6H_6 \rightarrow .5 C_{12}H_{10} + .5 H_2$ |
| 2 | Kinetic | $.5 C_{12}H_{10} + .5 H_2 \rightarrow C_6H_6$ |
| 3 | Kinetic | $C_6H_6 + C_{12}H_{10} \rightarrow C_{18}H_{14} + H_2$ |
| 4 | Kinetic | $C_{18}H_{14} + H_2 \rightarrow C_6H_6 + C_{12}H_{10}$ |

Edit Reaction

Reaction No.: 1 Reaction type: Kinetic

Reactants

| Component | Coefficient | Exponent |
|-----------|-------------|----------|
| C6H6 | -1 | 2 |
| * | | |

Products

| Component | Coefficient | Exponent |
|-----------|-------------|----------|
| C12H10 | 0,5 | |
| H2 | 0,5 | |
| * | | |

Let's you select the reaction type.

New... Edit Delete Copy Paste

No olvidar poner el orden de la reacción (exponent)

Reactions: Power Law model



- Setup
- Components
- Properties
- Flowsheet
- Streams
- Utilities
- Blocks
- Reactions
 - Chemistry
 - Reactions
 - R-1
 - Input
 - Results
- Convergence
- Flowsheeting Options
- Model Analysis Tools

Stoichiometry **Kinetic** Equilibrium Activity

1) C6H6 -> .5 C12H10 + .5 H2

Reacting phase: Vapor Rate basis: Reac (vol)

Power Law kinetic expression

Kinetic factor = $k(T/T_0)^n e^{-(E/R)(1/T-1/T_0)}$

| | | |
|-------------|------------------|---------|
| k: | 3,235E-06 | |
| n: | 0 | |
| E: | 30190 | cal/mol |
| To: | | C |
| [Ci] basis: | Partial pressure | |

Edit reactions

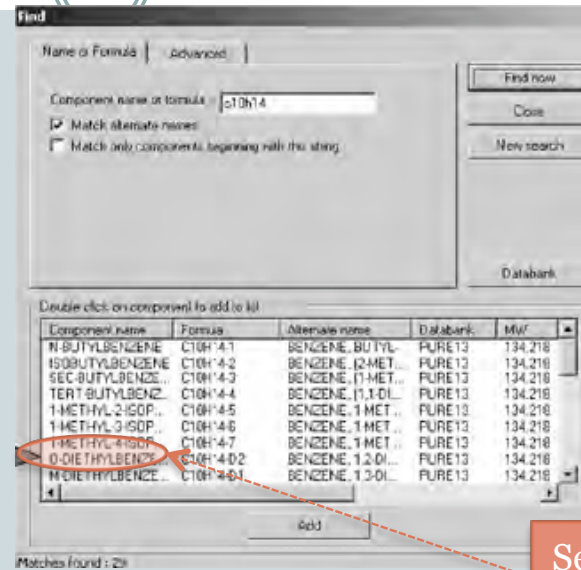
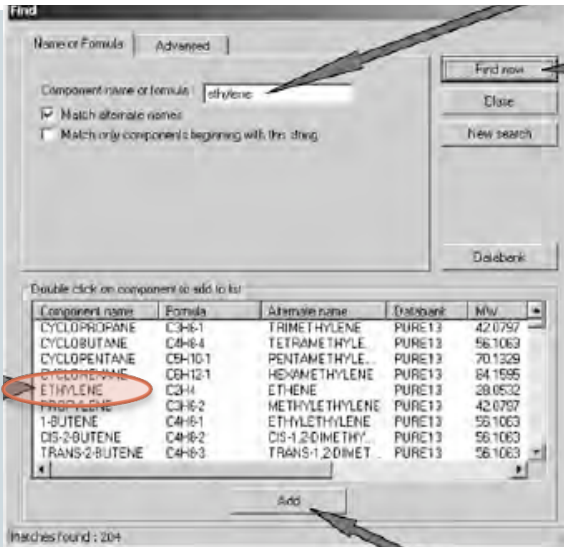
Solids

Ejemplo

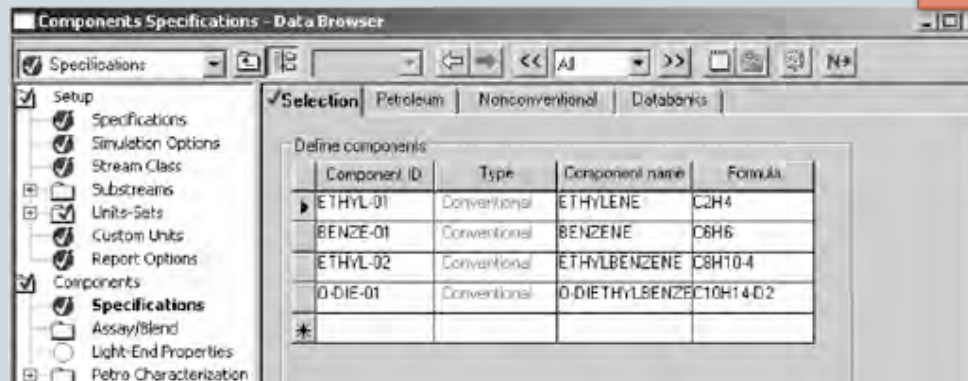


- Modelado de un Reactor CSTR

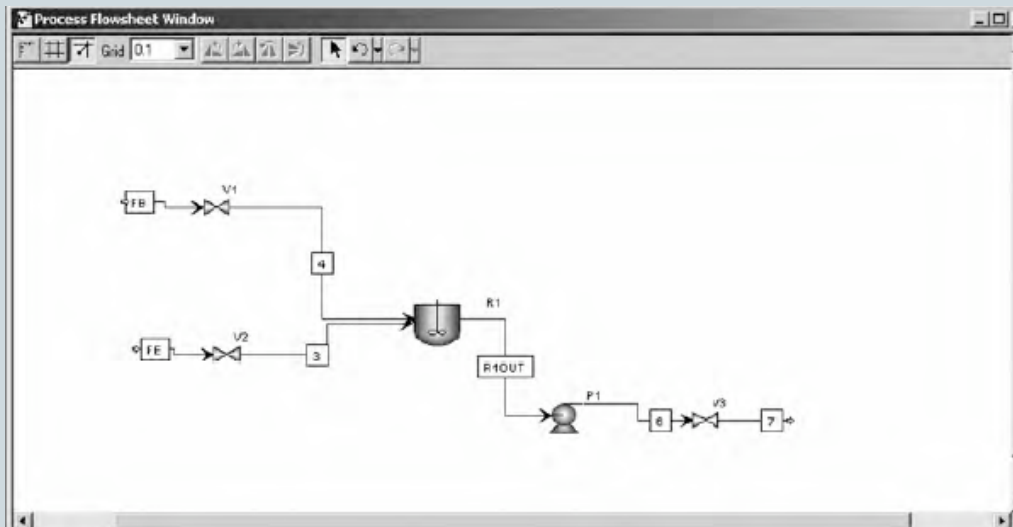
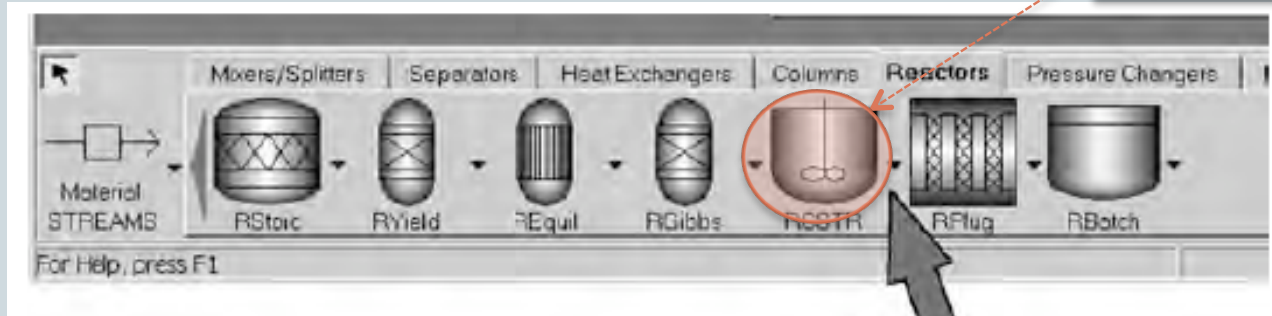
1. Establecer componentes, y propiedades físicas (Chao-Seader)



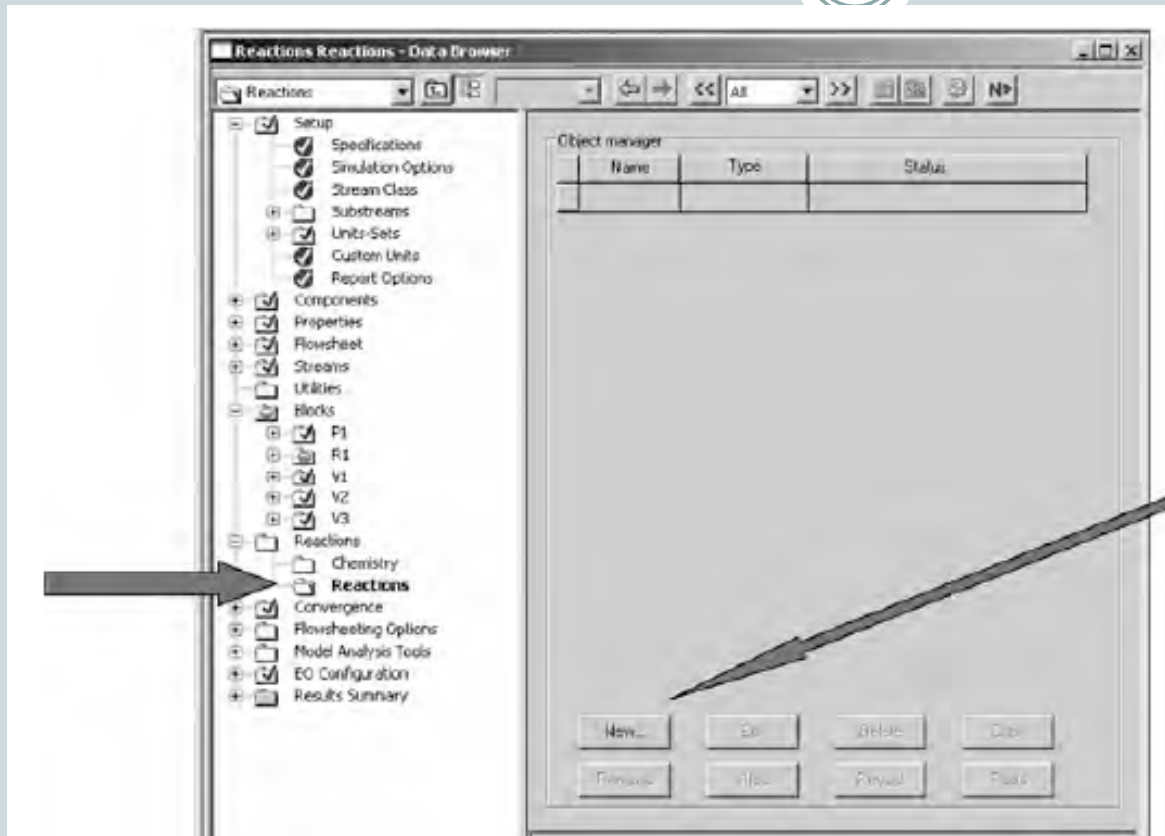
Se puede escoger cualquier Isómero del dietilbenzeno.



2. Seleccionar el equipo, hacer el diagrama de proceso y rellenar datos de las corrientes de entrada

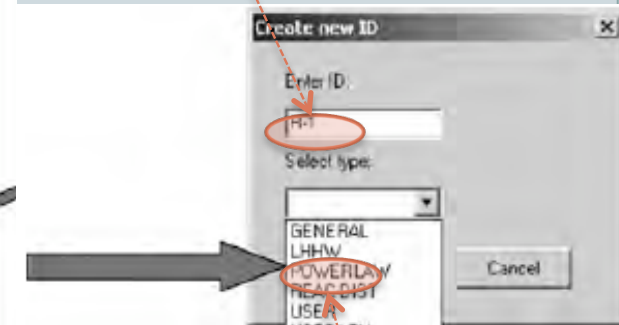


3. Definir las reacciones



Nueva reacción

Se pueden poner en un único grupo (R-1) las tres reacciones



Como la cinética viene dada en exponencial (Arrhenius) escoger POWERLAW

4. Poner la estequiometría de las reacciones

Reaction No.: 1 Reaction type: Kinetic

| Reactants | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| E | -1 | 1 | |
| B | -1 | 1 | |
| * | | | |

| Products | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| | | | |
| | | | |
| * | | | |

Reaction No.: 2 Reaction type: Kinetic

| Reactants | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| E | -1 | 1 | |
| EB | -1 | 1 | |
| * | | | |

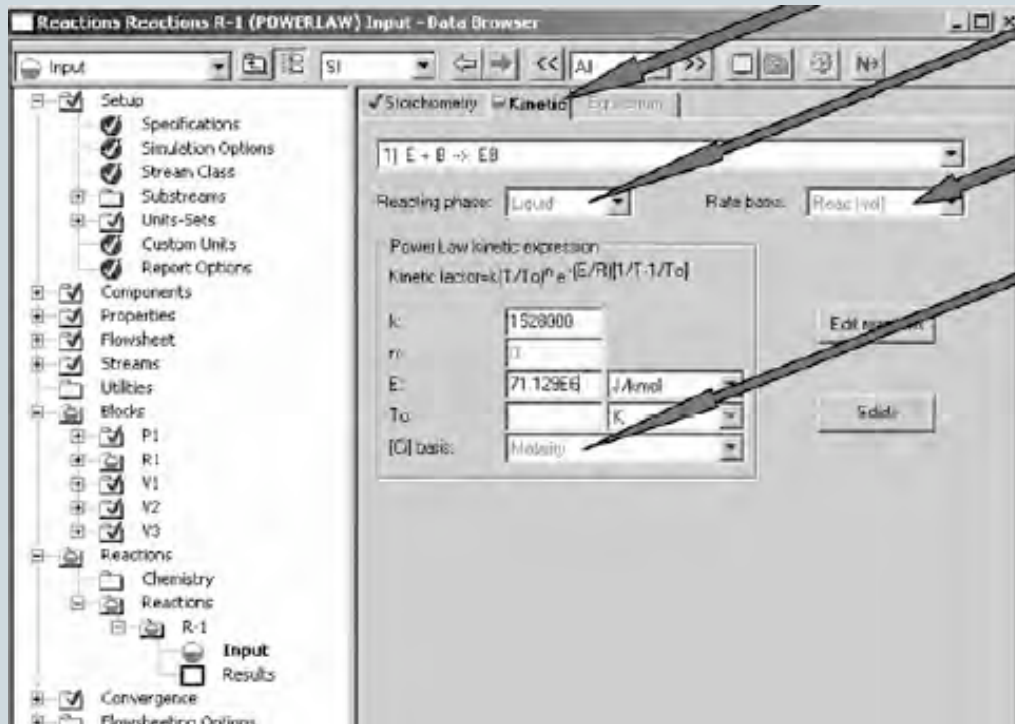
| Products | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| DEB | 1 | | |
| * | | | |

Reaction No.: 3 Reaction type: Kinetic

| Reactants | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| DEB | 1 | 1 | |
| B | -1 | 1 | |
| * | | | |

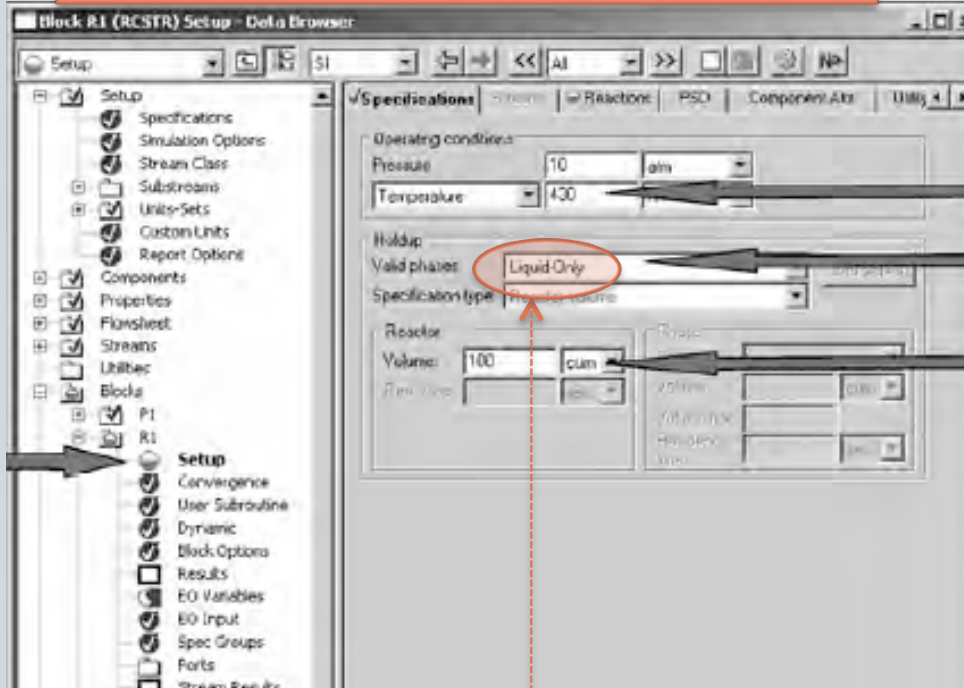
| Products | | | |
|-----------|-------------|----------|--|
| Component | Coefficient | Exponent | |
| EB | 2 | | |
| | | | |
| | | | |
| * | | | |

No olvidar los exponentes que indican el orden de la reacción



Poner los datos de la cinética de la reacción
(con la formulación dada no es necesario poner
nada en To)

Poner las condiciones de operación del reactor.



Nótese que en este caso se debe poner líquido únicamente

Añadir el grupo de reacciones que tiene lugar

