DSOySP

Módulos de DWSIM (III)
Equipos con reacción química en DWSIM

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Modelos de reactores presentes en DWSIM

Continous Stirred Tank Reactor

CSTR model, supports Kinetic and HetCat reactions

Conversion Reactor

Supports reactions defined by amounts of reactant converted as a function of

Equilibrium Reactor

Supports equilibrium constant-defined reactions

Gibbs Reactor

Calculates chemical/atomic equilibrium for a Material Stream

Plug-Flow Reactor (PFR)

Plug-Flow Reactor model, supports Kinetic and HetCat reactions

Reacciones químicas soportadas por DWSIM

Las reacciones pueden se de 4 tipo:

Equilibrio (*Equilibrium*): Se definen a partir de una constante de equilibrio (K). La fuente de información para la constante de equilibrio puede ser un cálculo directo de energía Gibbs, una expresión definida por el usuario o un valor constante. Pueden utilizarse en reactores de Equilibrium y Gibbs.

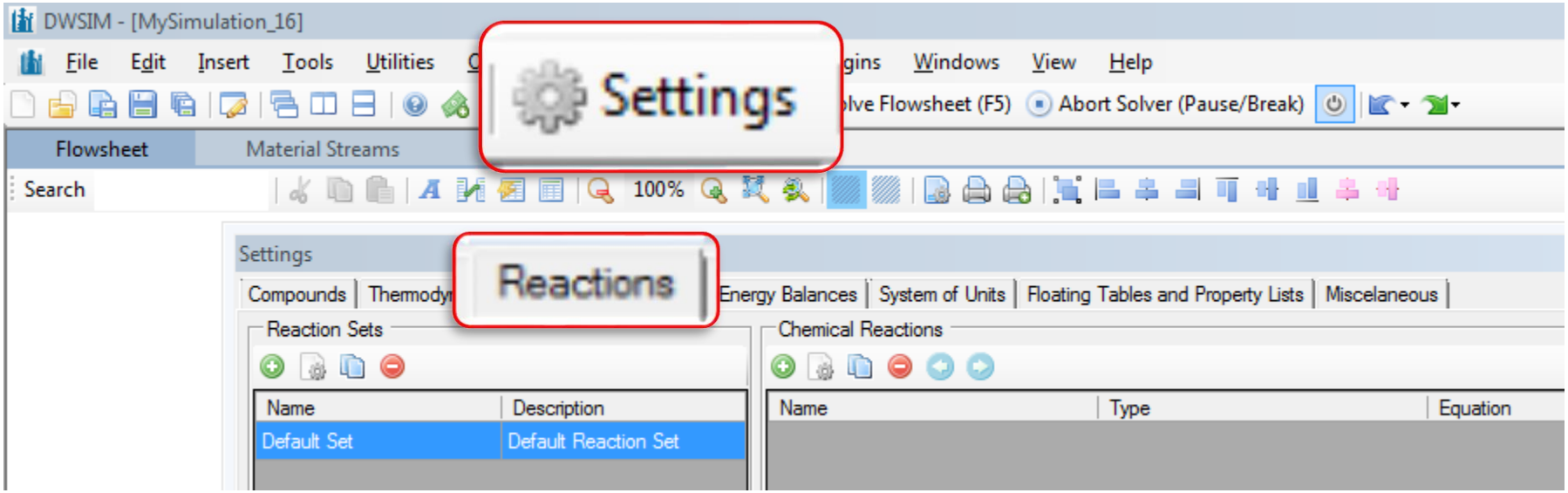
Conversión (*Conversion*): Se definen por la cantidad de un compuesto básico que se consume en la reacción. Esta cantidad puede ser un valor fijo o una función de la temperatura del sistema. Son soportadas por el reactor de Conversión.

Cinética (*Kinetic*): Se definen a partir de una expresión cinética. Son soportadas por los reactores PFR y CSTR.

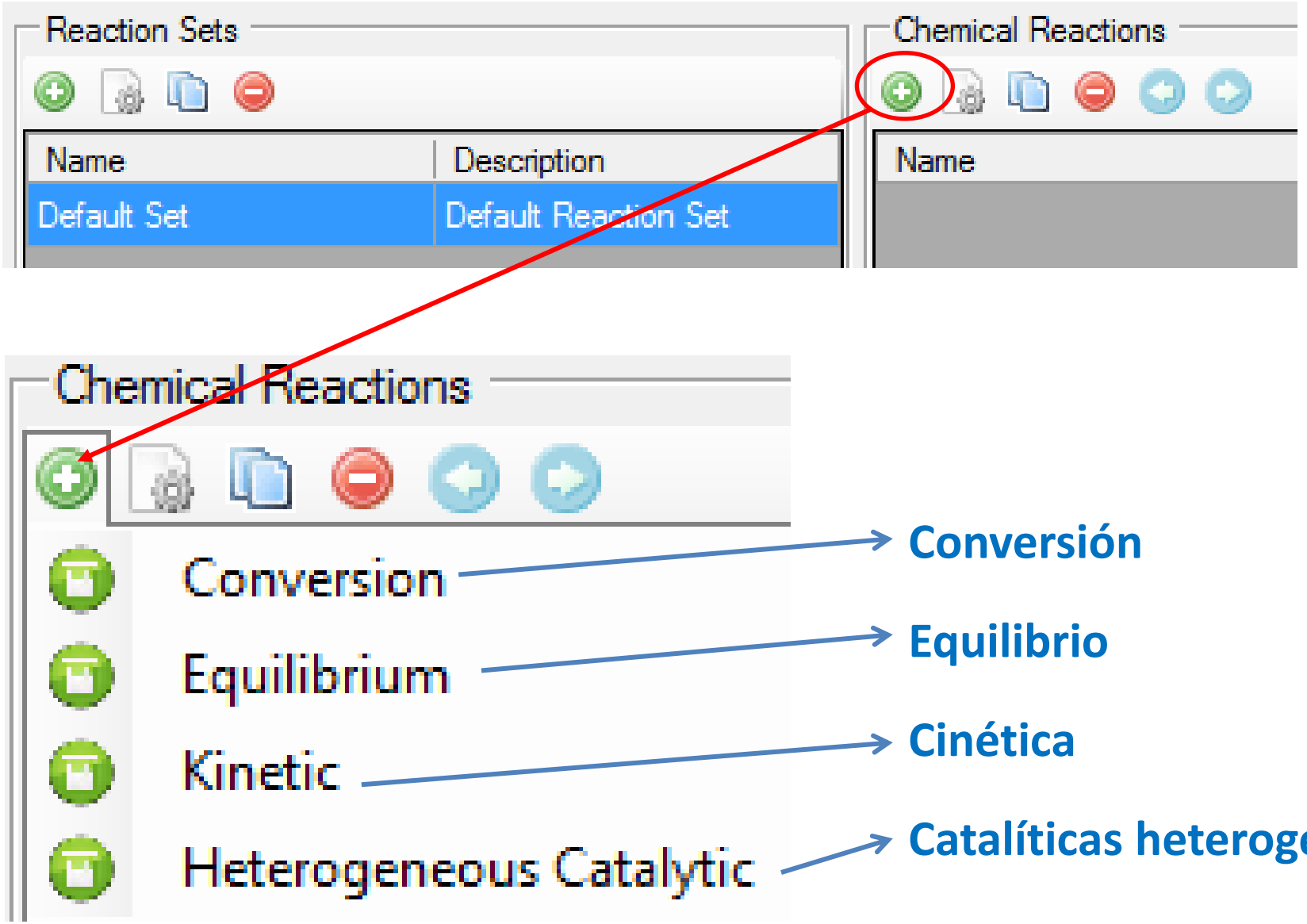
Catalíticas heterogéneas (*Heterogeneous Catalytic*): Obedecen al mecanismo de Langmuir-Hinshelwood, donde los compuestos reaccionan sobre una superficie sólida de catalizador. En este modelo, las velocidades de reacción son una función de la cantidad de catalizador (es decir, mol/kg cat.s). Son soportadas por los reactores PFR y CSTR.

Modelos de reactores presentes en DWSIM

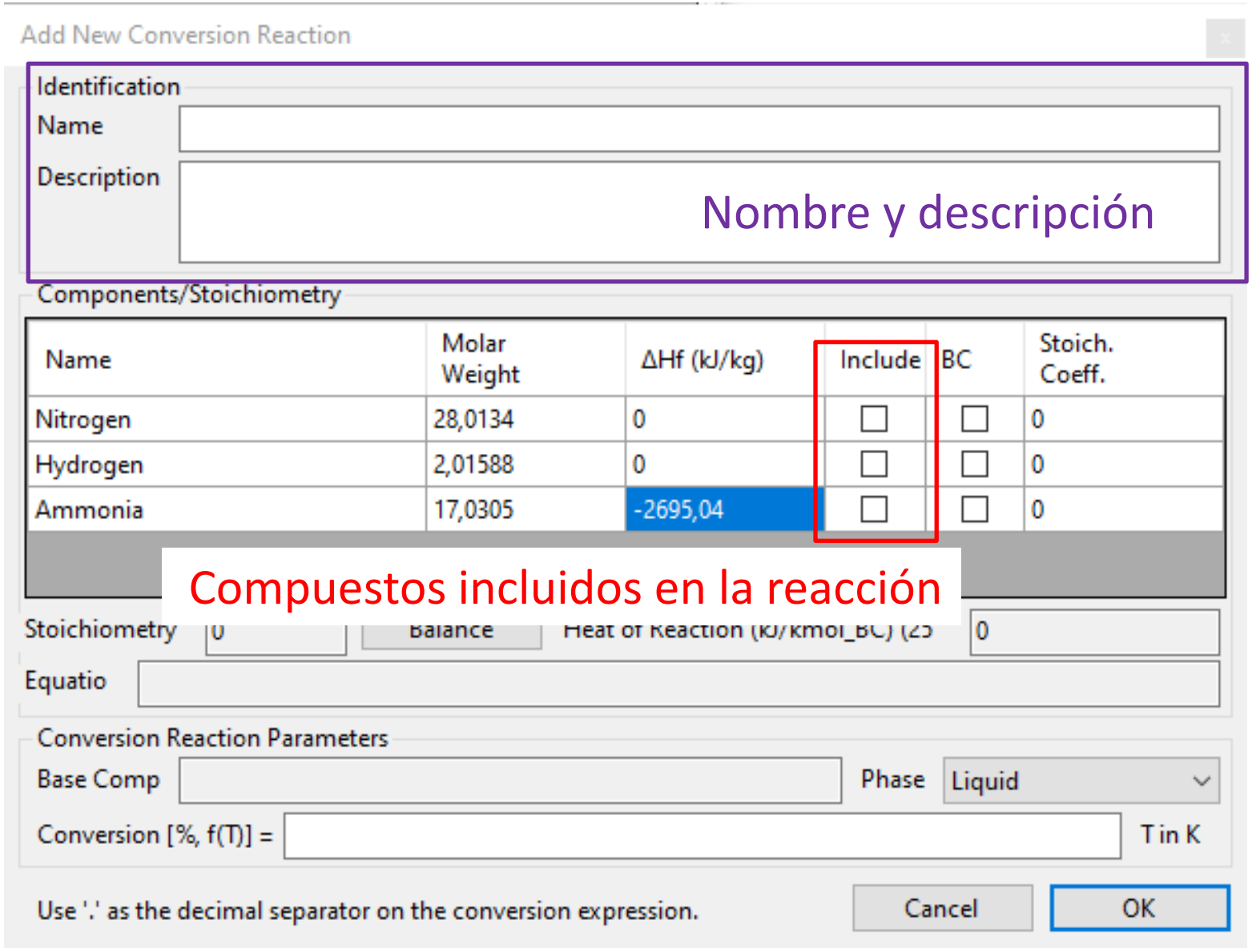
Para realizar una simulación de un reactor, se necesitan definir las reacciones químicas que tendrán lugar en el reactor. Esto se realiza a través del Administrador de Reacciones (Reactions Manager).



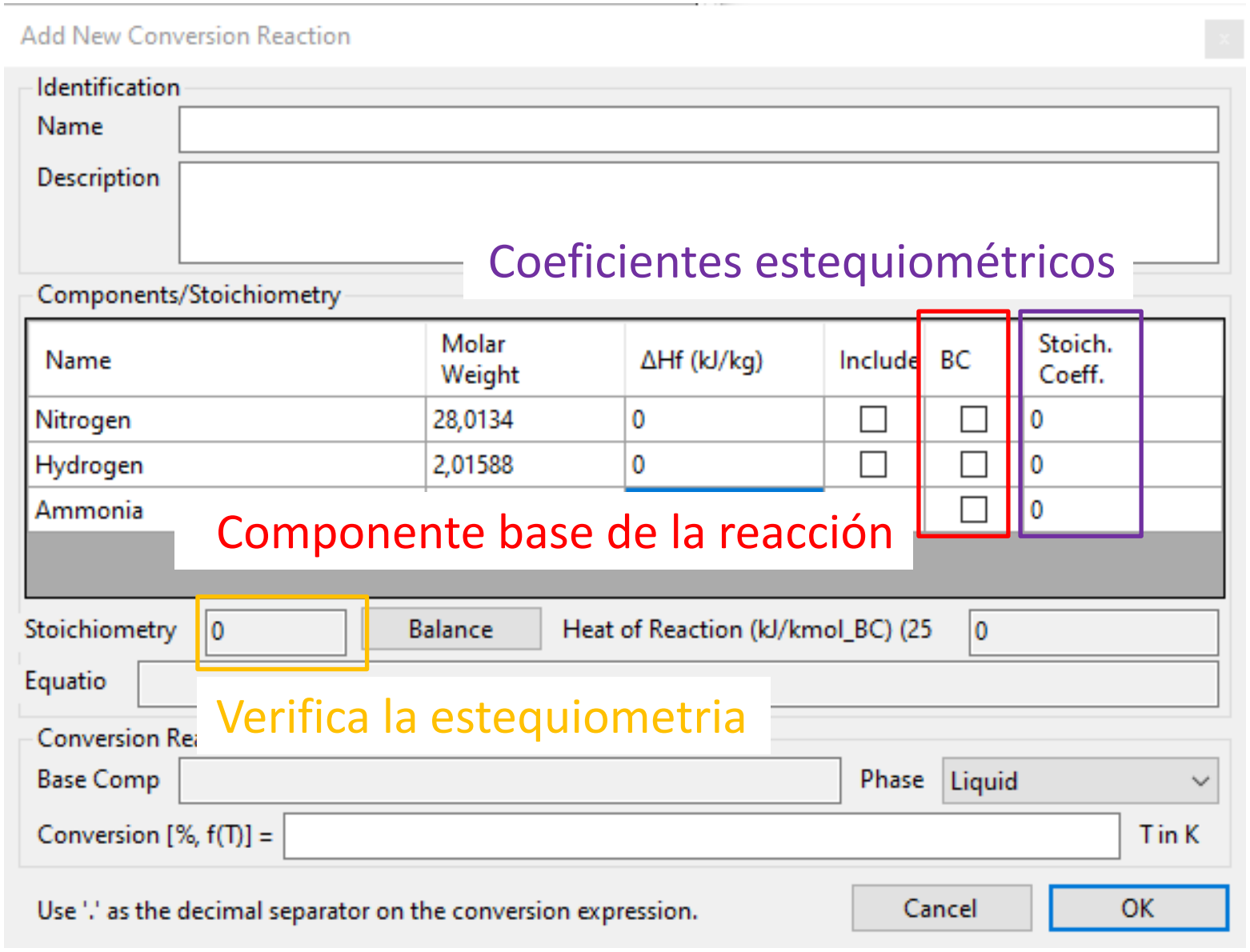
Administrador de Reacciones químicas (Chemical Reactions Manager).



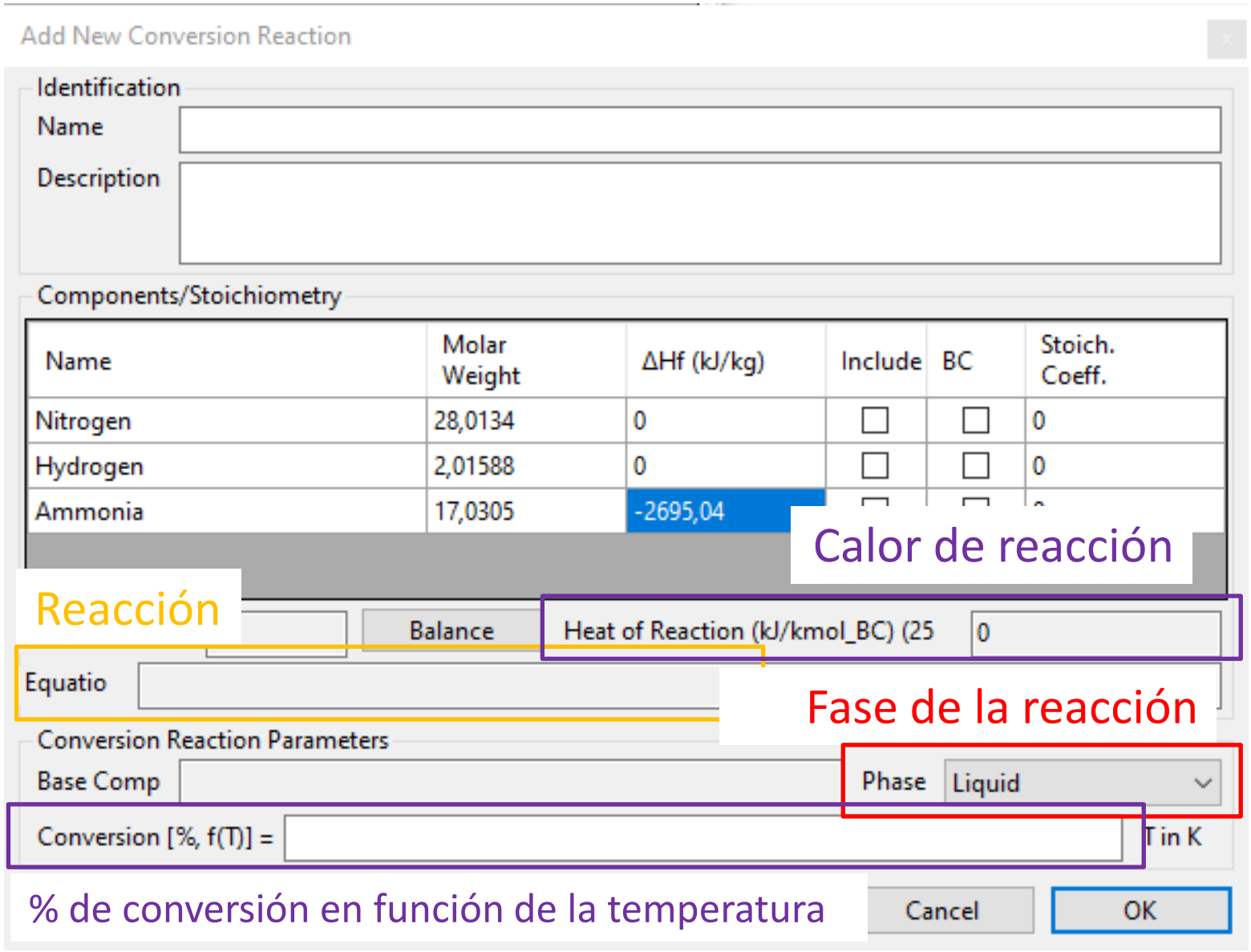
Reacciones de Conversión



Reacciones de Conversión

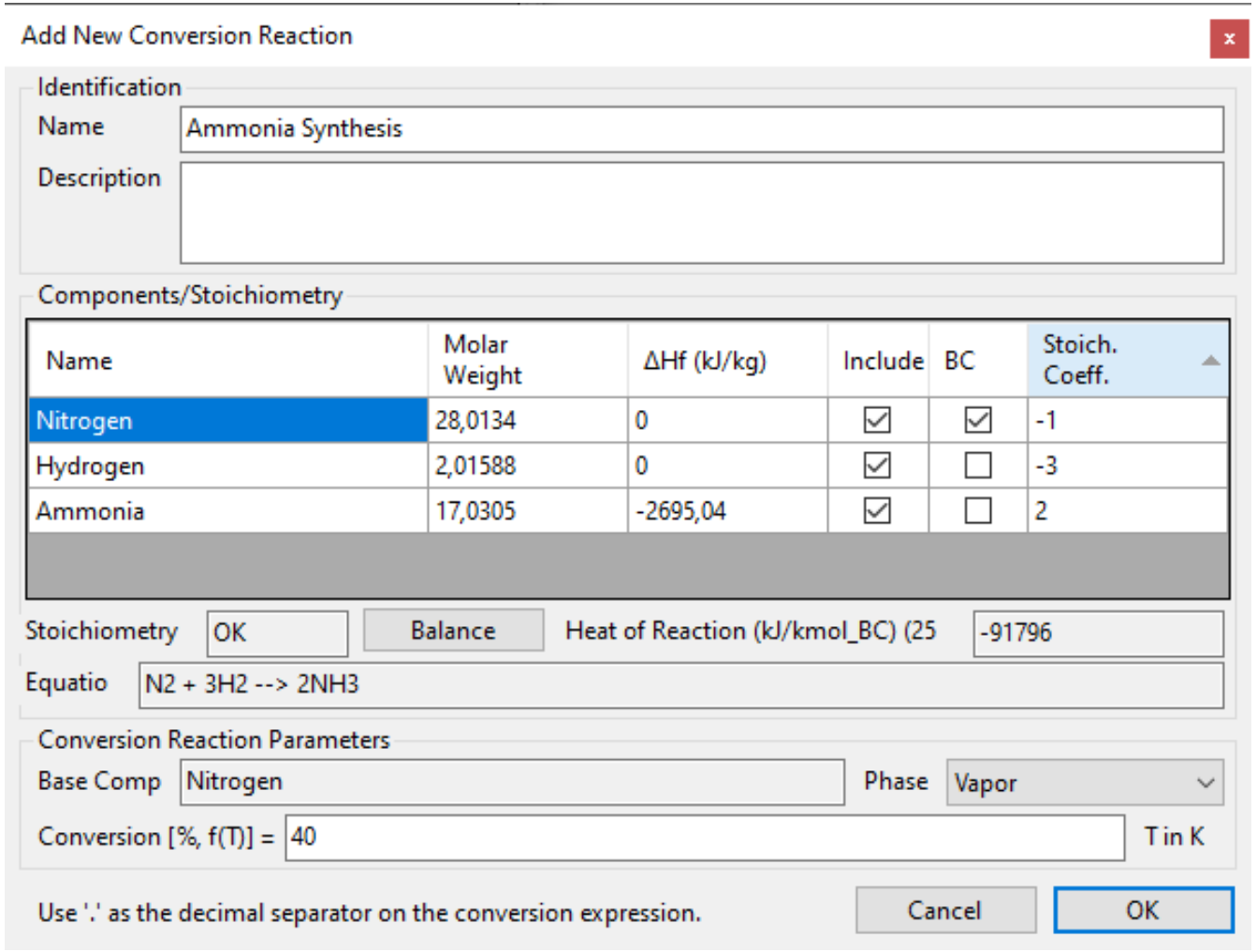


Reacciones de Conversión



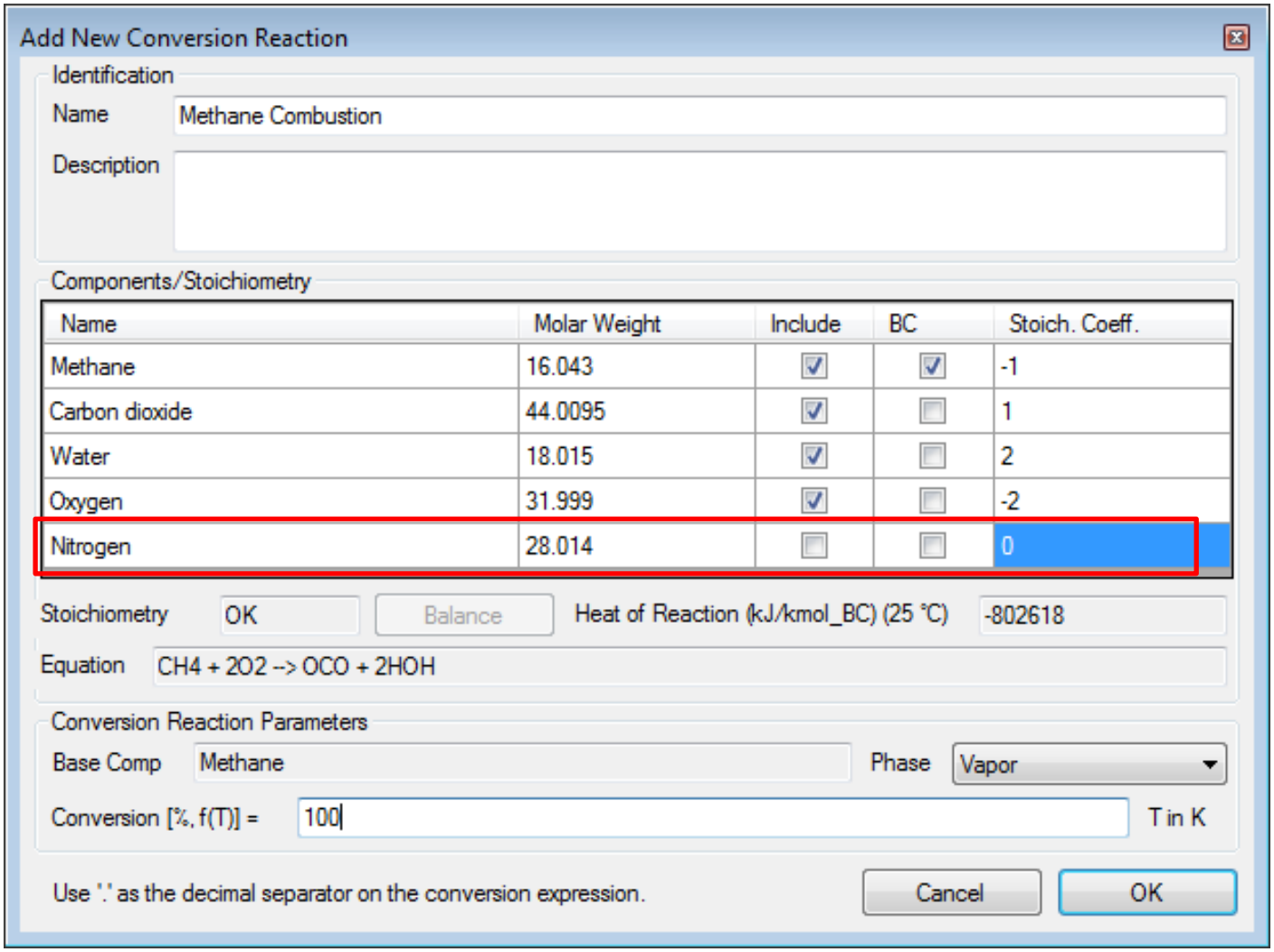
Ejemplos de Reacciones de Conversión

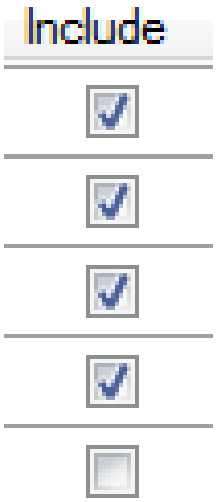
$$3H_2 + N_2 \Leftrightarrow 2NH_3$$ Conversión del 40% del Nitrógeno



Ejemplos de Reacciones de Conversión

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$ Combustión del 100 %

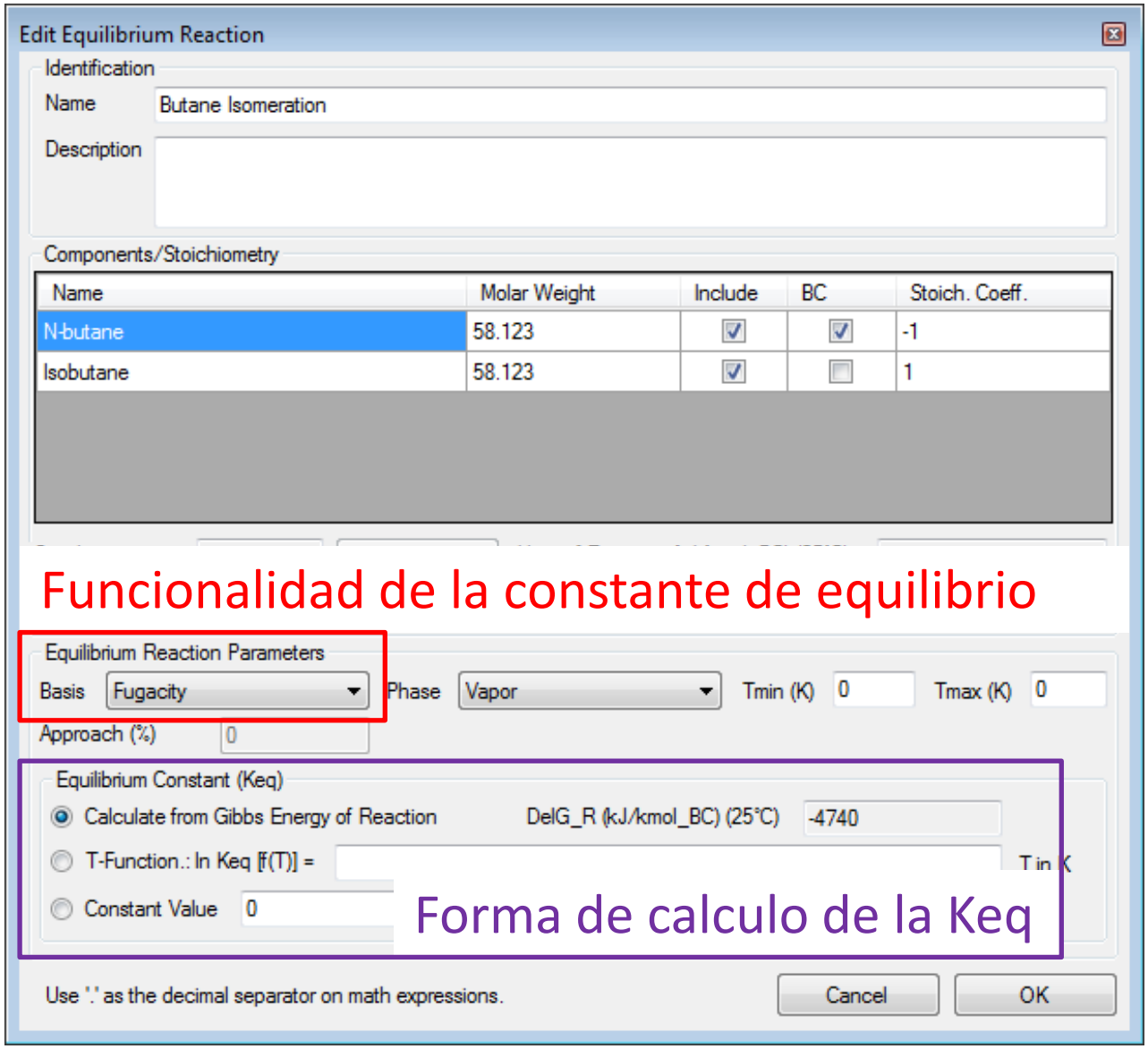




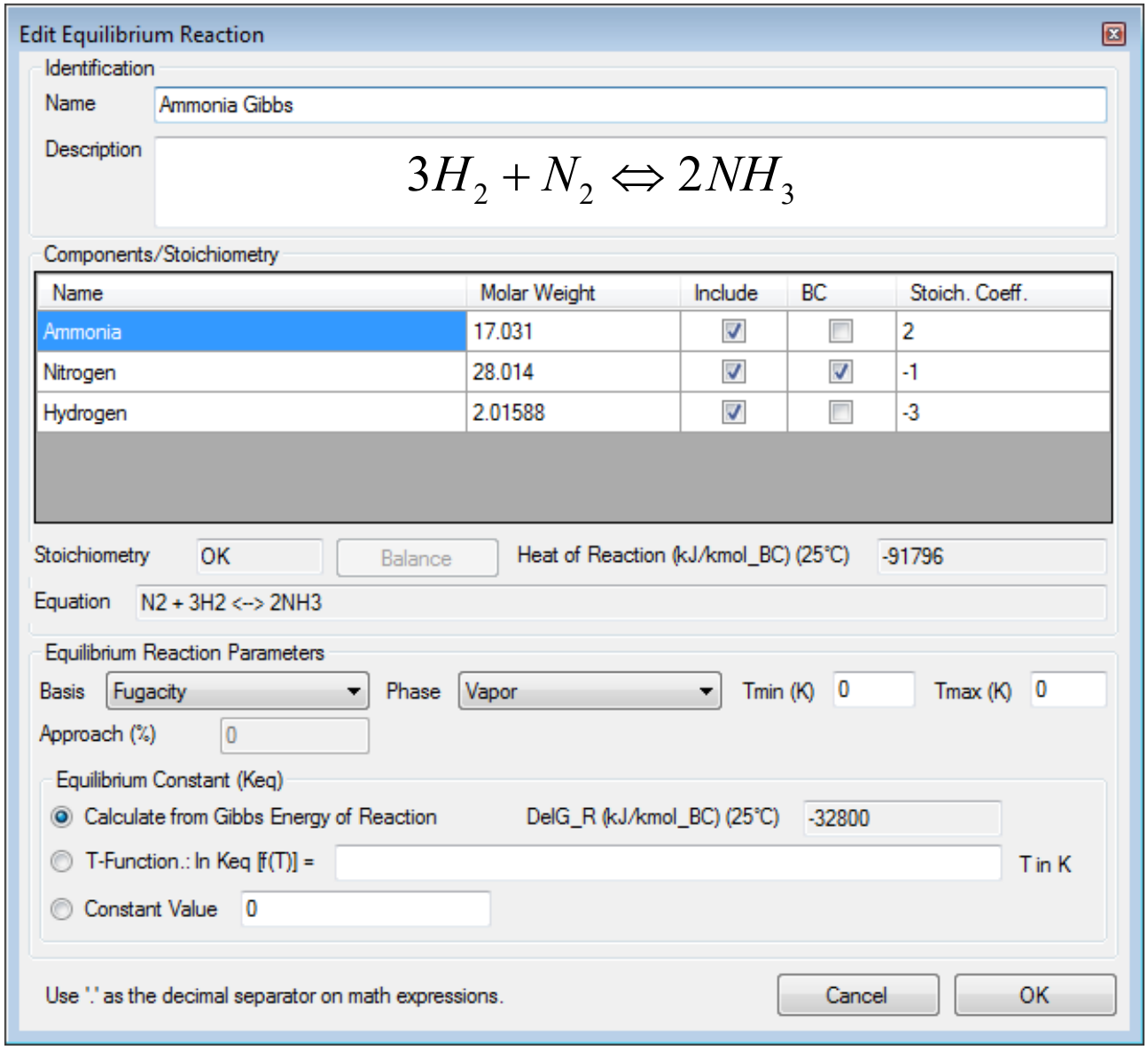
El N_2 no interviene en la reacción.

Suele aparecer porque se utiliza aire para la combustión.

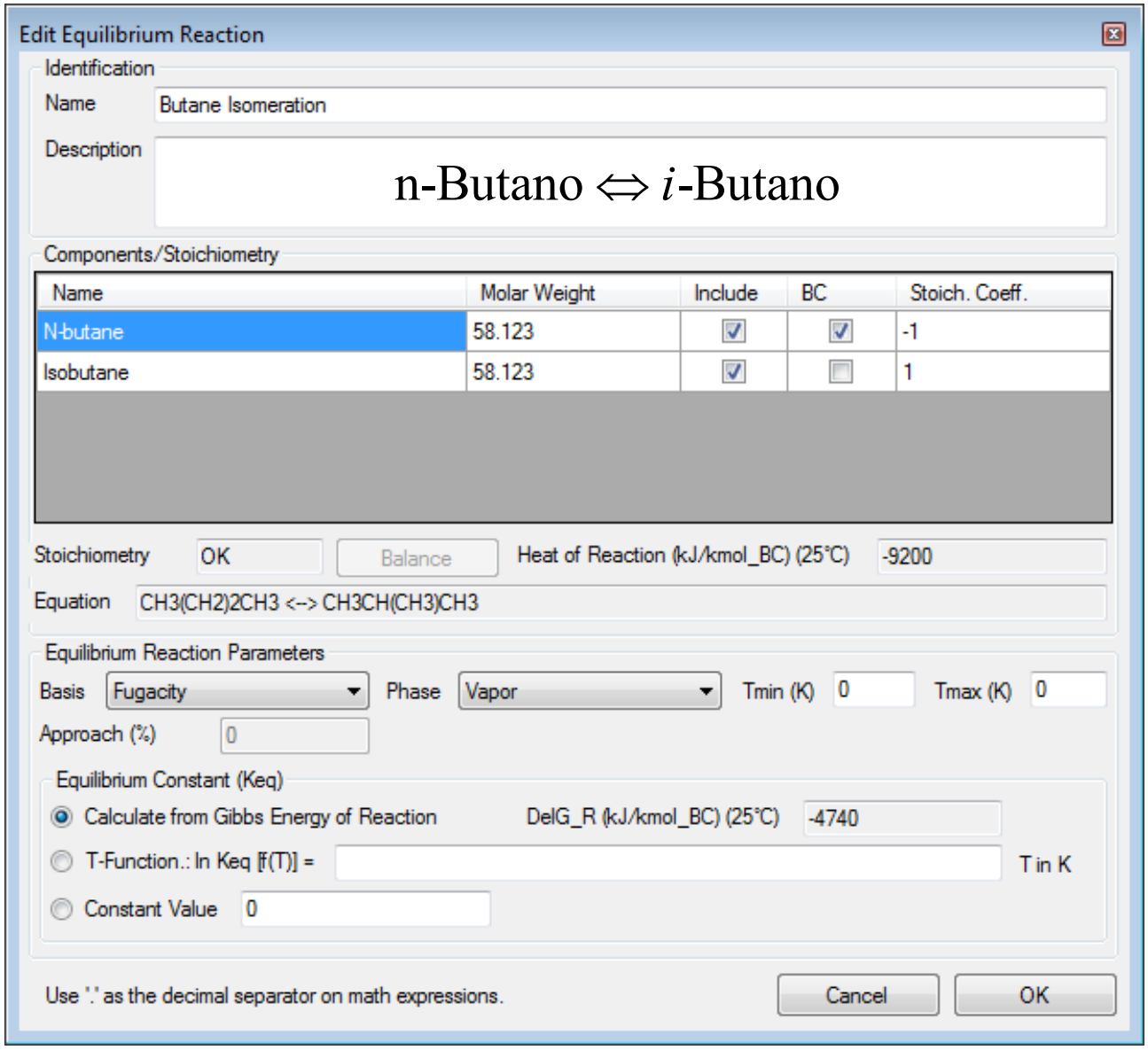
Reacciones de Equilibrio



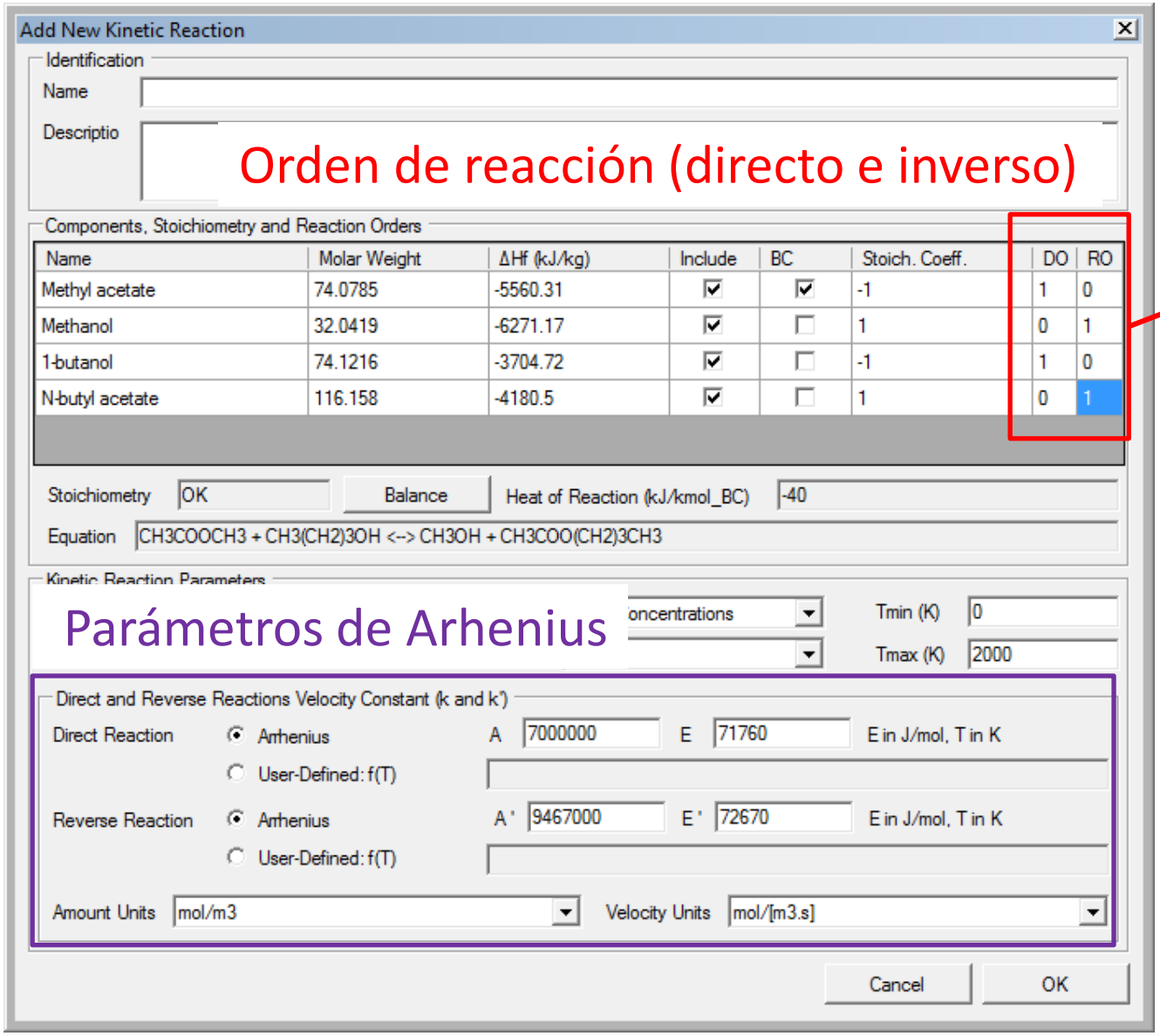
Ejemplos de Reacciones de Equilibrio



Ejemplos de Reacciones de Equilibrio



Reacciones de Cinética



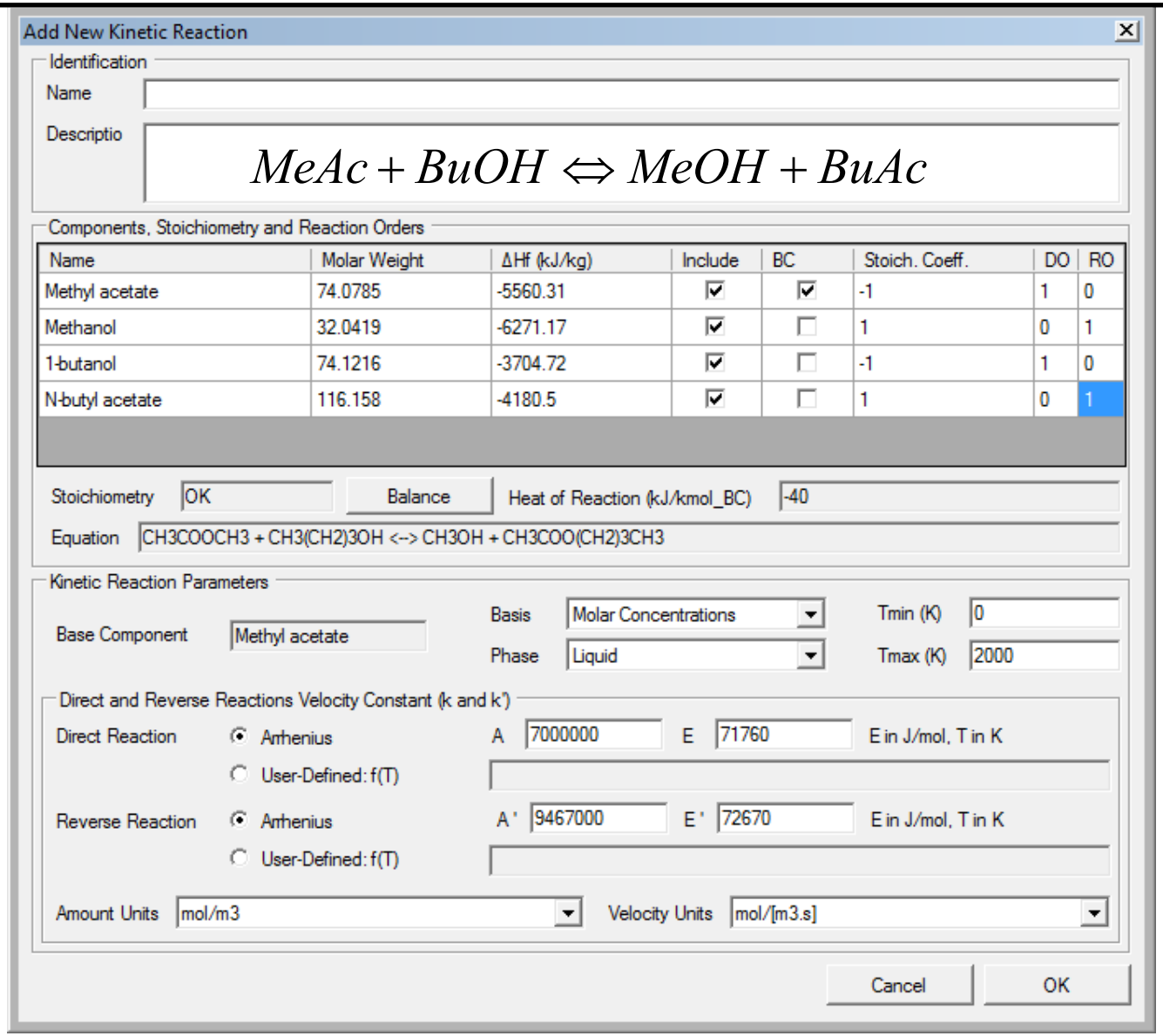
DO	RO
1	0
0	1
1	0
0	1

$$A \underset{k'}{\overset{k}{\rightleftharpoons}} B$$

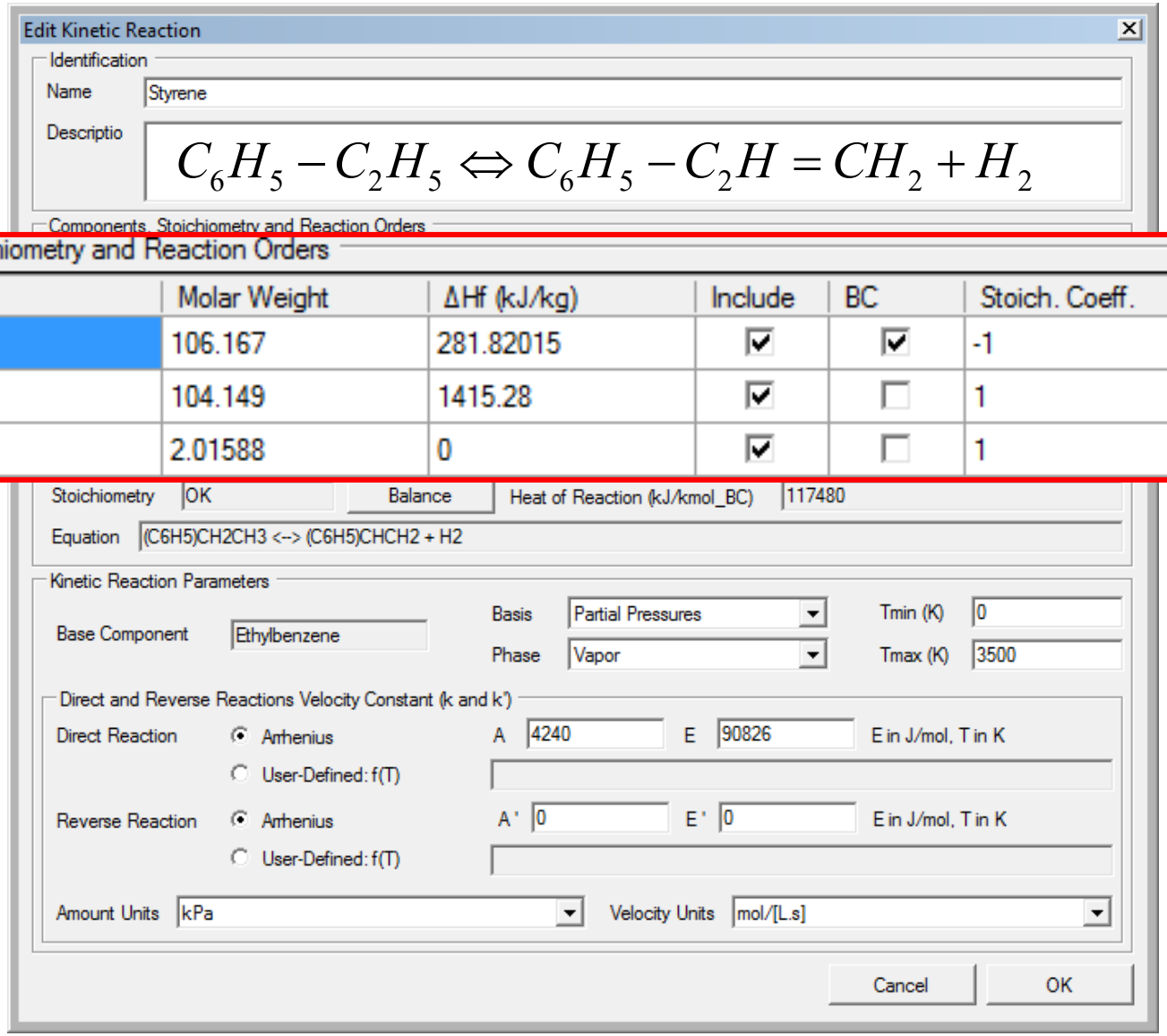
$$k = Ae^{-\frac{E}{RT}}$$

$$k' = A'e^{-\frac{E'}{RT}}$$

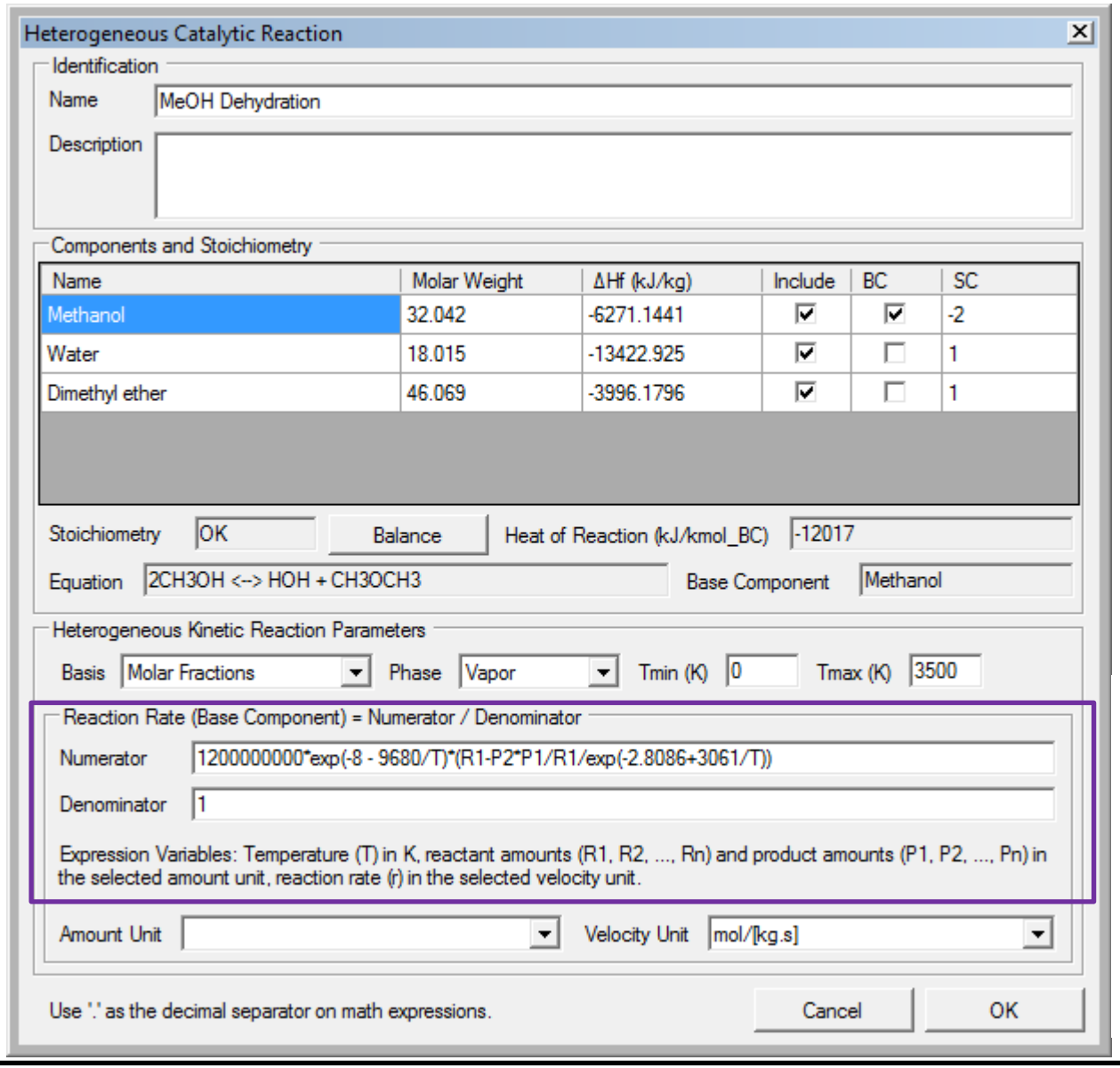
Ejemplos de Reacciones de Cinética



Ejemplos de Reacciones de Cinética



Reacciones Heterogéneas Catalíticas



Ley funcional de la velocidad de reacción

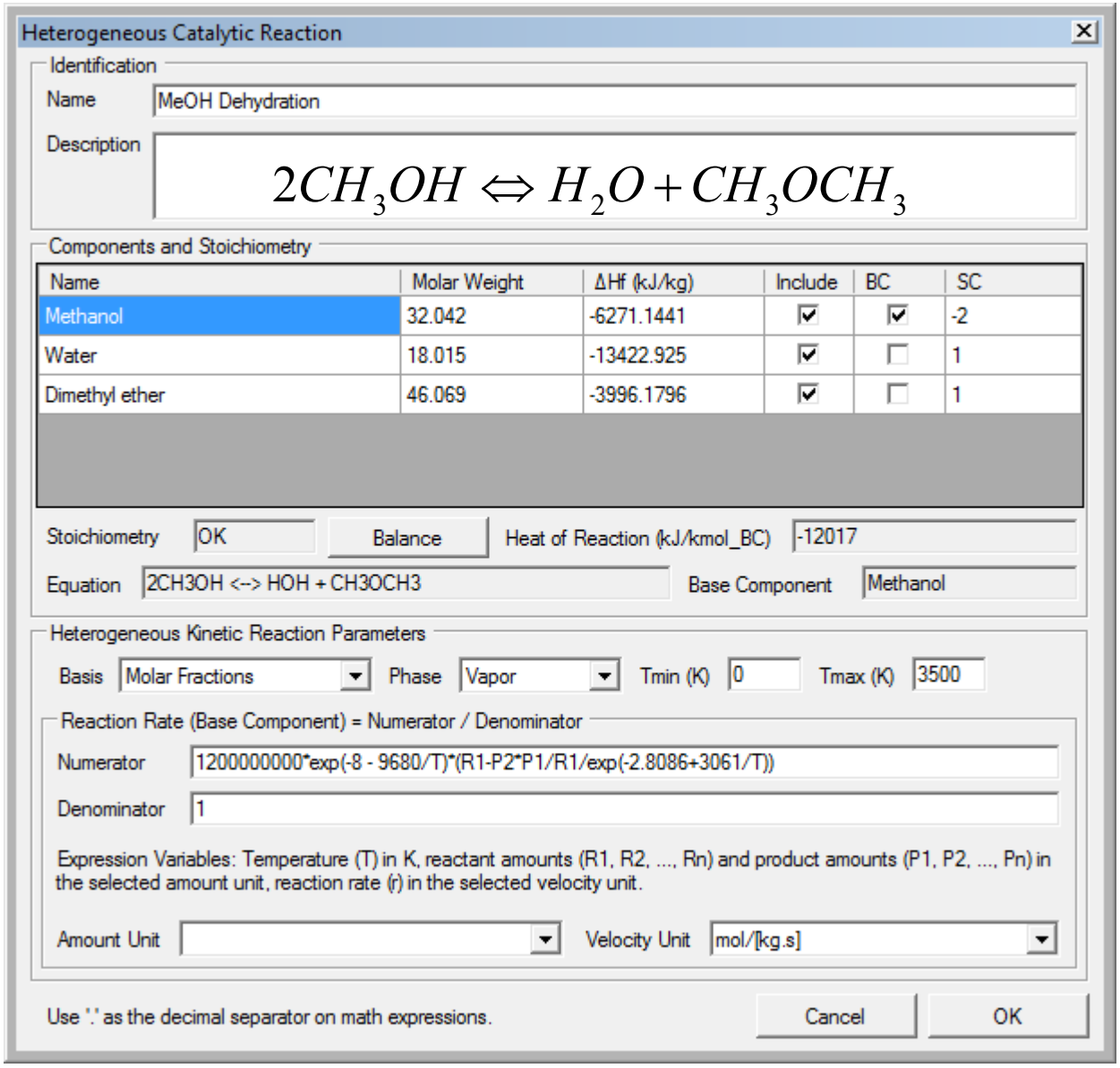
Las variable son:

T

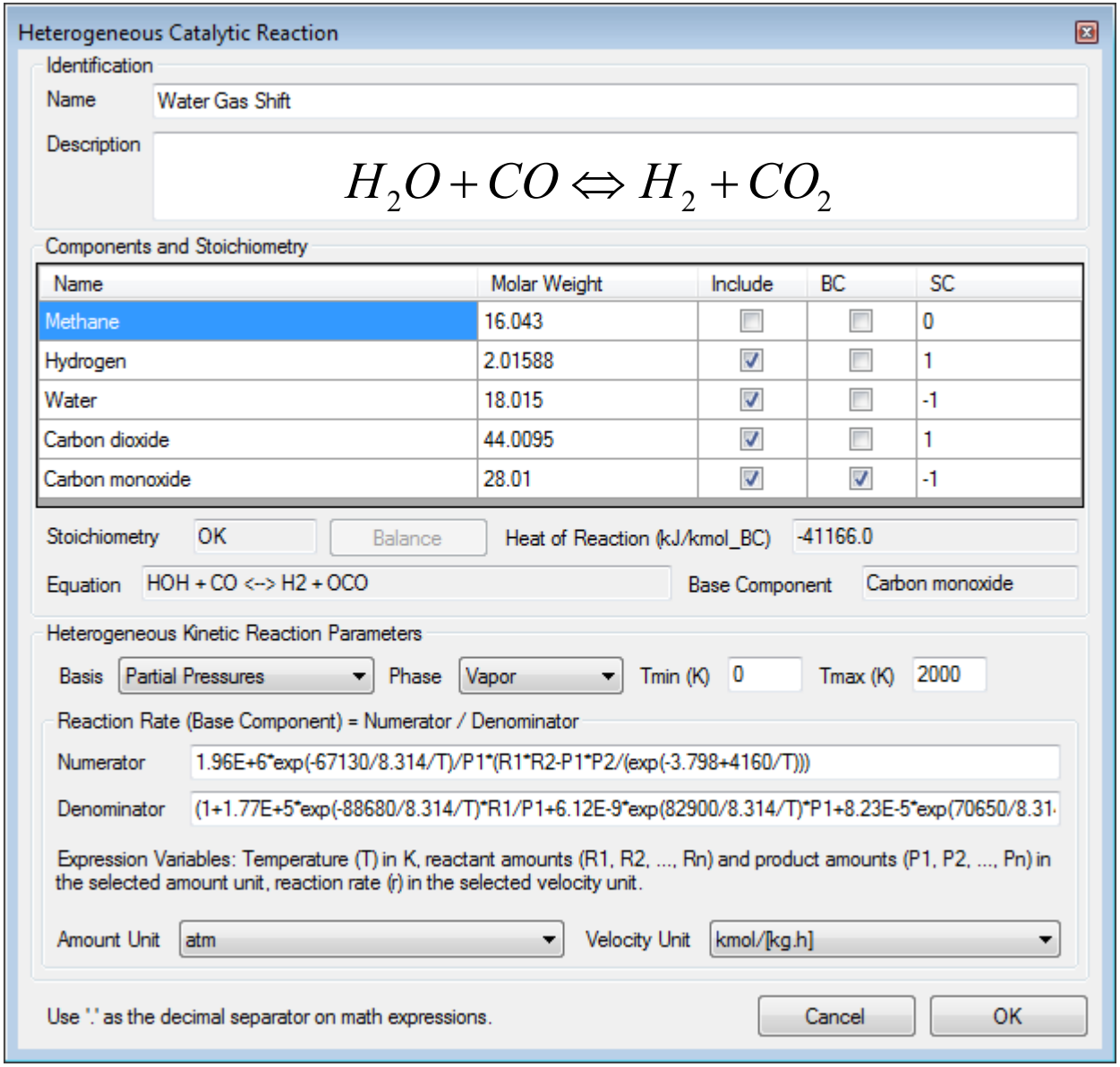
R1, R2, …, Rn

P1, P2, …, Pn

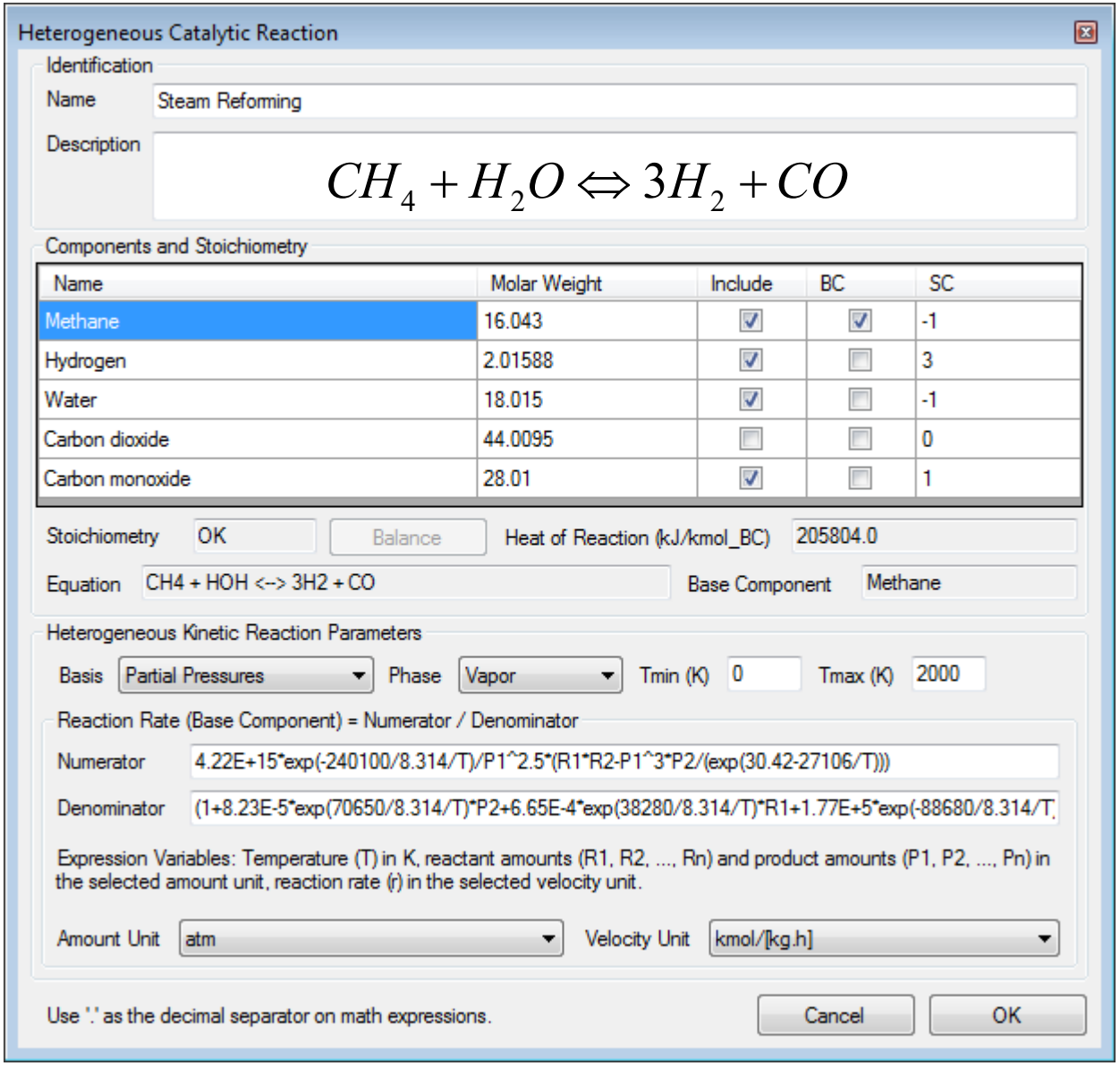
Reacciones Heterogéneas Catalíticas



Reacciones Heterogéneas Catalíticas



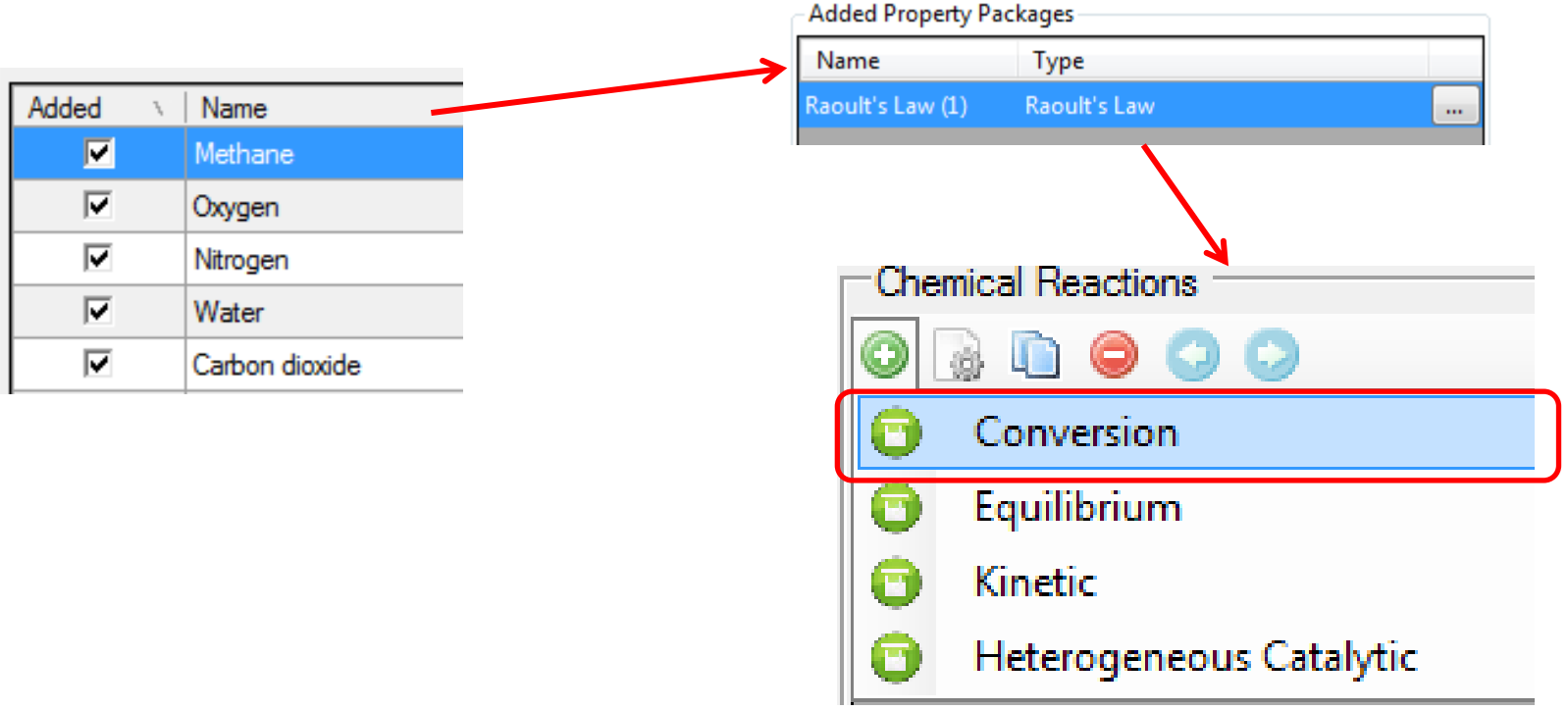
Reacciones Heterogéneas Catalíticas



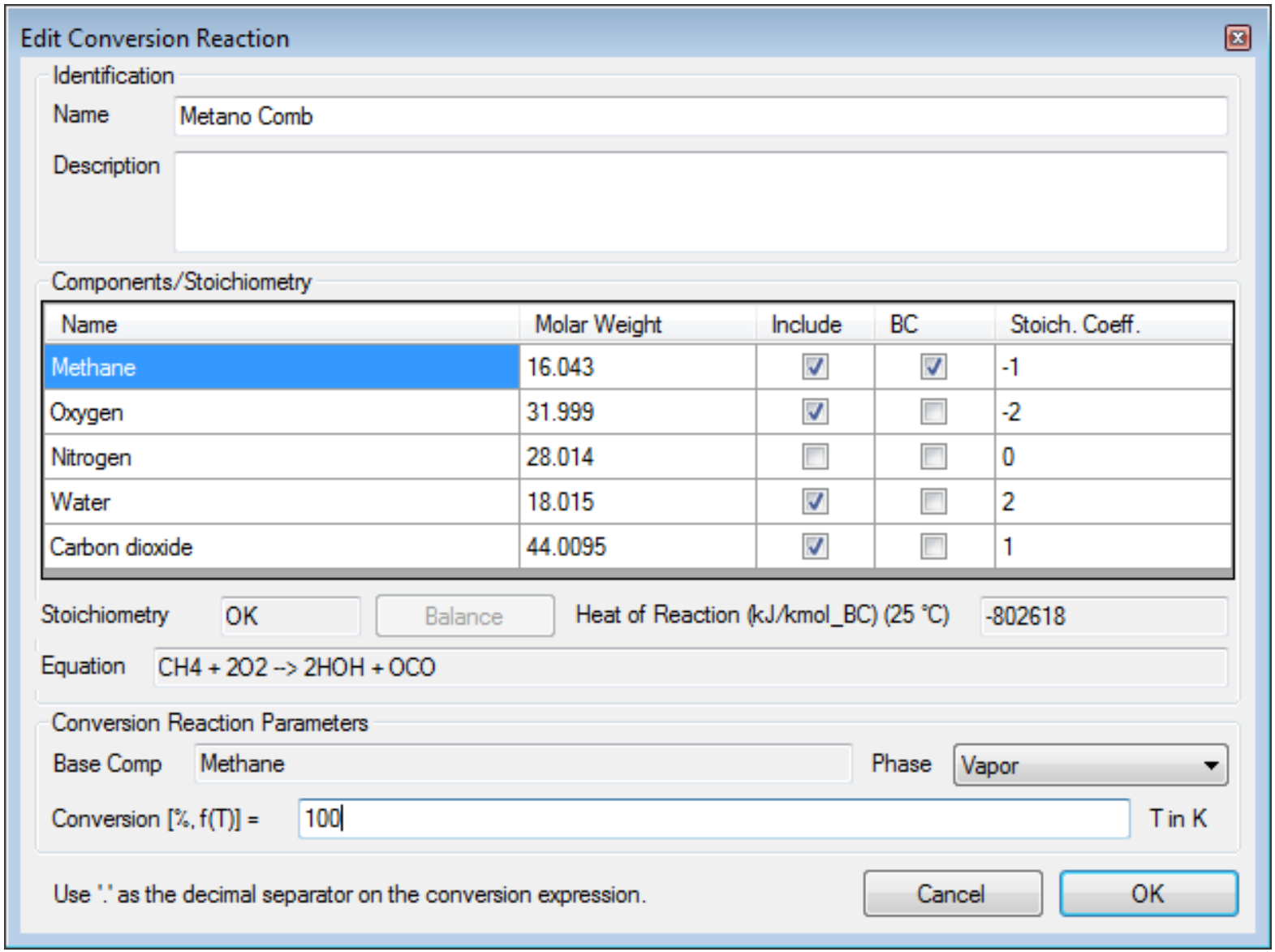
Ejemplo: Combustión de gas natural

Se desea conocer la temperatura de llama que se alcanza al quemar 1 kg/s de gas natural (suponemos metano puro) con una relación másica de 1:40 fuel-aire. Se considera que el gas y el aire ingresan a 298.15 y 1 atm.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$



Reacción de combustión del metano



Corriente de combustible

Input Data | Results | Annotations | Floating Tables

Stream Conditions | Compound Amounts

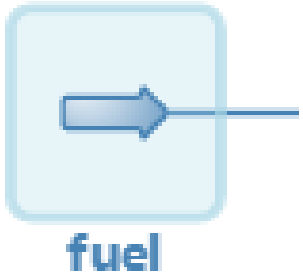
Flash Spec	Temperature and Pressure (TP)	
Temperature	298.15	K
Pressure	101325	Pa
Mass Flow	1	kg/s
Molar Flow	62.332481	mol/s
Volumetric Flow	1.5249045	m3/s
Specific Enthalpy	0	kJ/kg
Specific Entropy	0	kJ/[kg.K]
Vapor Phase Mole Fraction	1	

Stream Conditions | Compound Amounts

Basis: Mole Fractions

Solvent:

Compound	Amount
Methane	1
Oxygen	0
Nitrogen	0
Water	0
Carbon dioxide	0



Corriente de aire

Input Data | Results | Annotations | Floating Tables

Stream Conditions | Compound Amounts

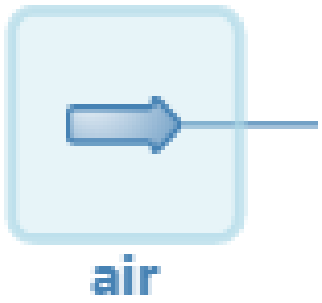
Flash Spec	Temperature and Pressure (TP)	
Temperature	298.15	K
Pressure	101325	Pa
Mass Flow	40	kg/s
Molar Flow	1386.441	mol/s
Volumetric Flow	33.91795	m3/s
Specific Enthalpy	0	kJ/kg
Specific Entropy	0.14041917	kJ/[kg.K]
Vapor Phase Mole Fraction	1	

Stream Conditions | Compound Amounts

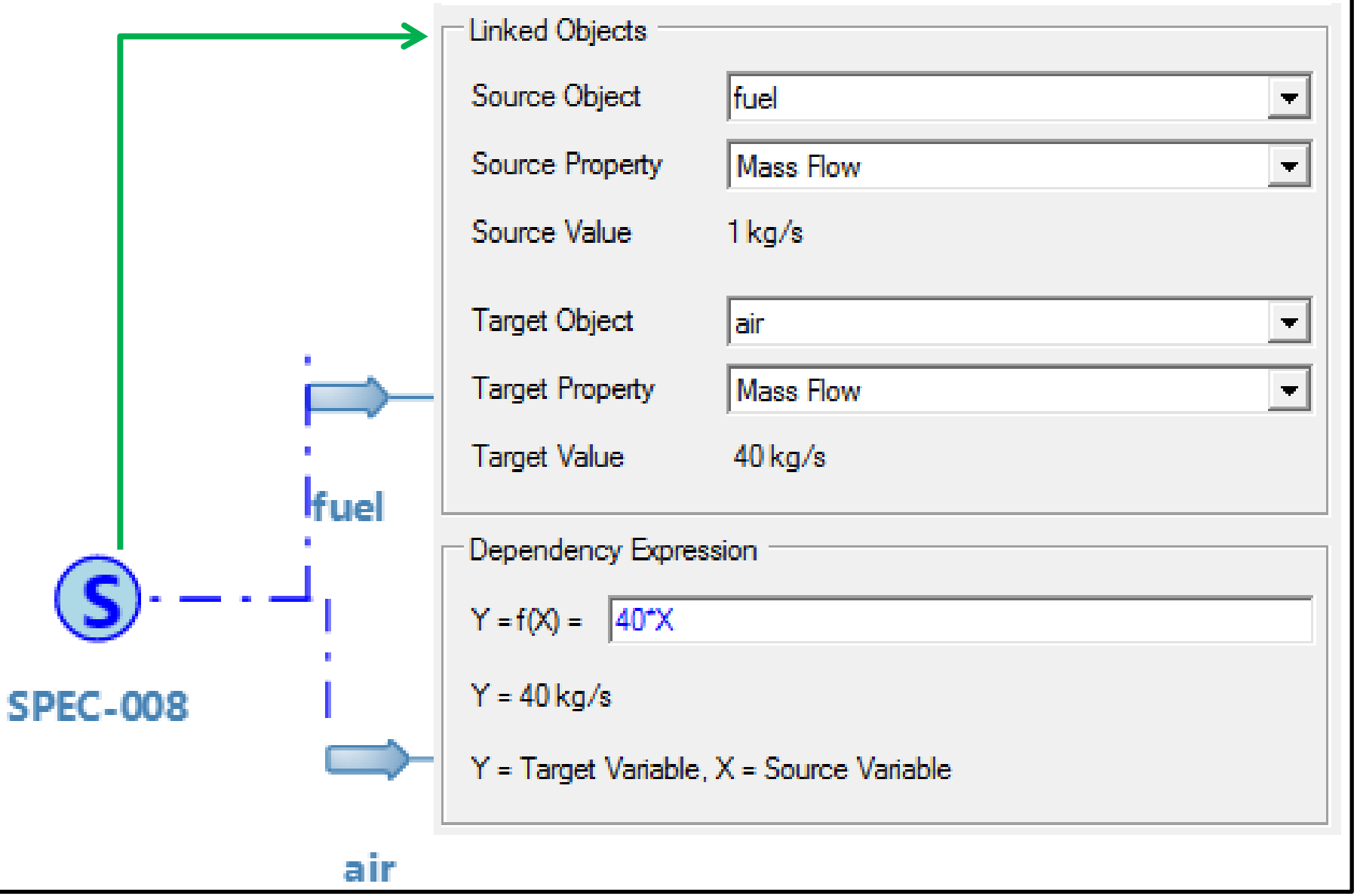
Basis: Mole Fractions

Solvent:

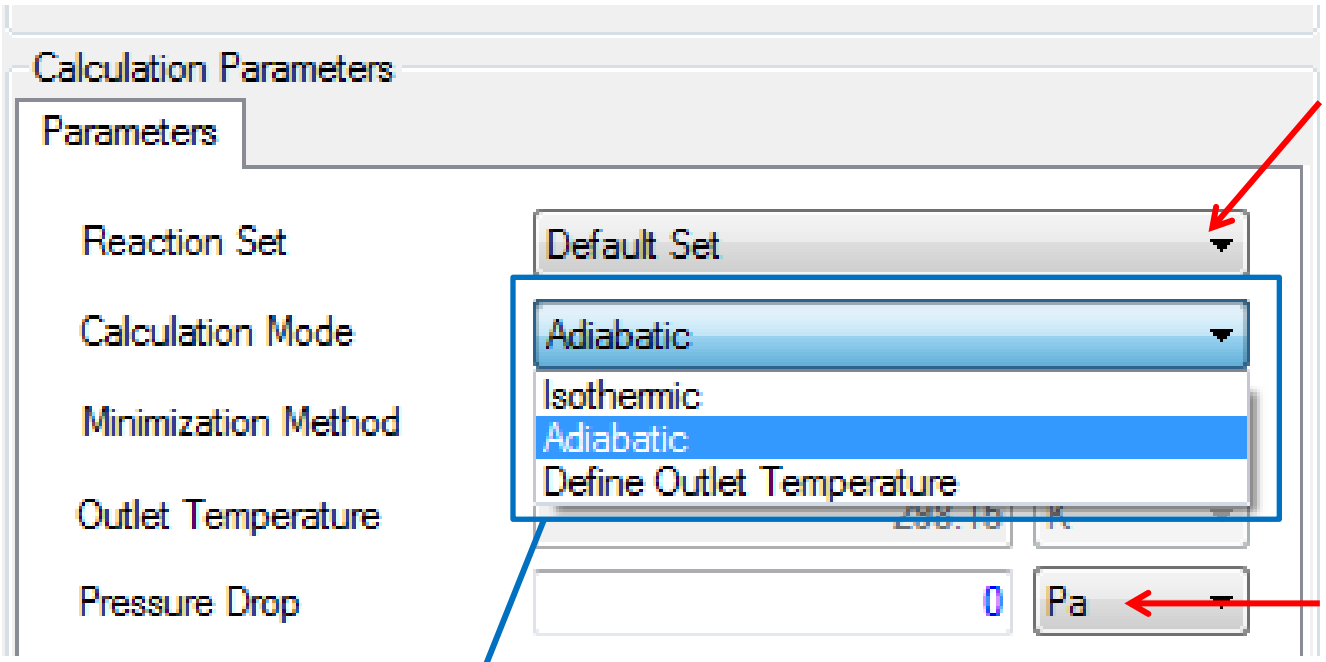
Compound	Amount
Methane	0
Oxygen	0.21
Nitrogen	0.79
Water	0
Carbon dioxide	0



Mezcla para ingresar al reactor



Reactor de conversión

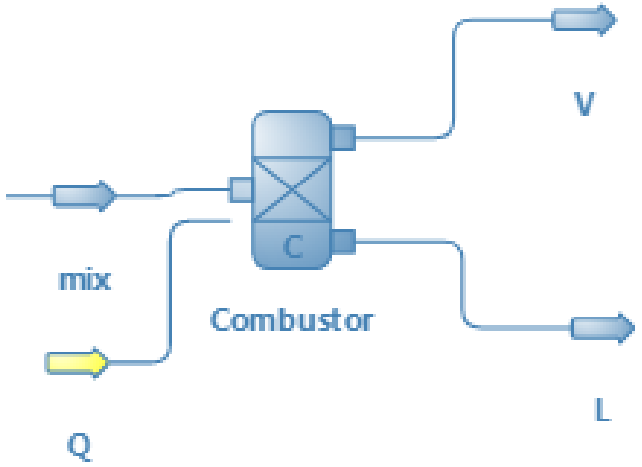


Paquete de reacciones que intervienen en el reactor

Caída de presión

Métodos de calculo disponibles:

- Isotérmico
- Adiabático
- Con temperatura de salida definida



Reactor de conversión

Calculation Parameters

Parameters

Reaction Set	Default Set	
Calculation Mode	Adiabatic	
Minimization Method		
Outlet Temperature	298.15	K
Pressure Drop	0	Pa

Results

General | Reactions | Conversions

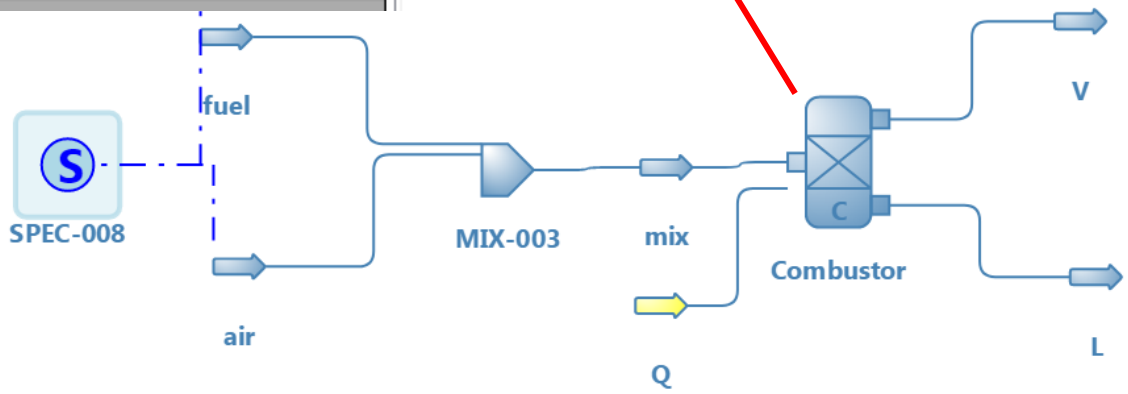
Property	Value	Units
Delta-T	1039.9984	K.
Heat Load	0	kW

General | Reactions | Conversions

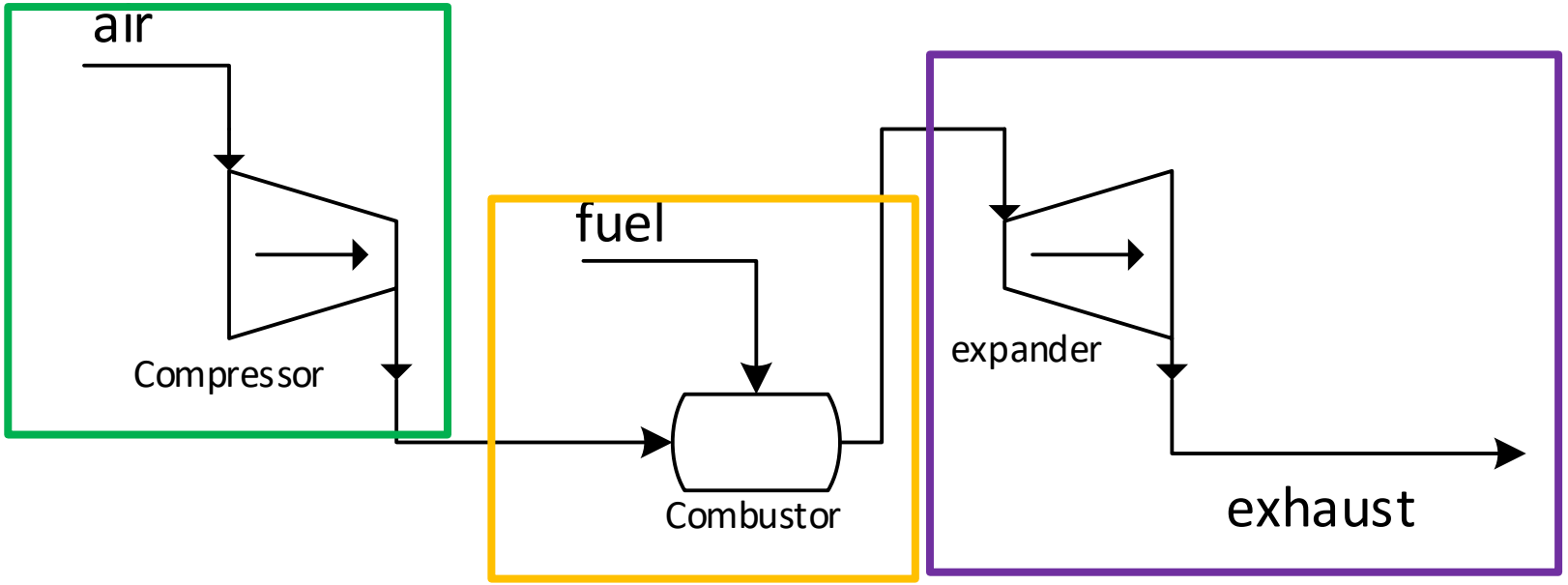
Reaction	Property	Value	Units
Metano Comb	Conversion	100	%

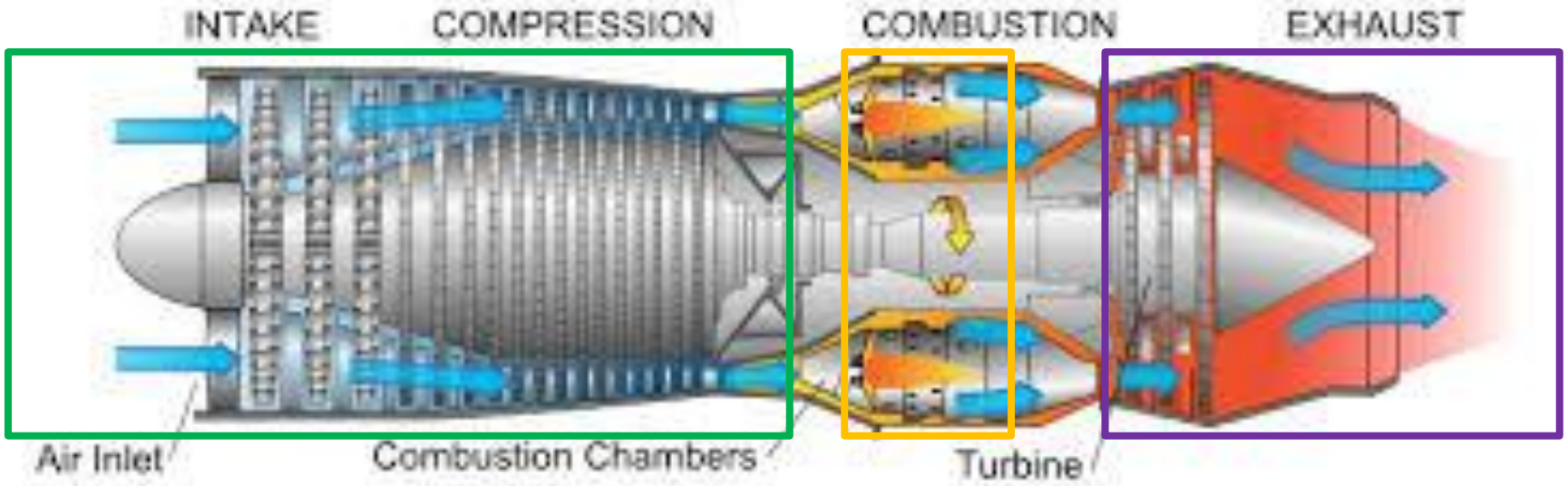
Temperature	1338.1484	K
Pressure	101325	Pa
Mass Flow	41	kg/s
Molar Flow	1448.7767	mol/s

Compound	Amount
Methane	0
Oxygen	0.11491627
Nitrogen	0.75601079
Water	0.086048626
Carbon dioxide	0.043024313

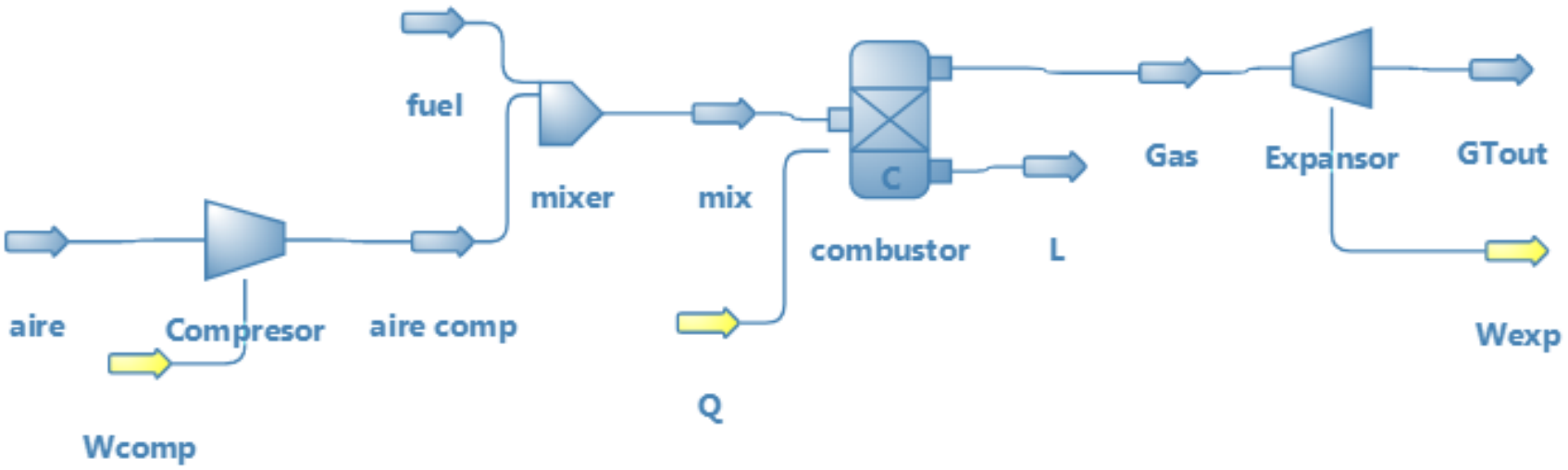


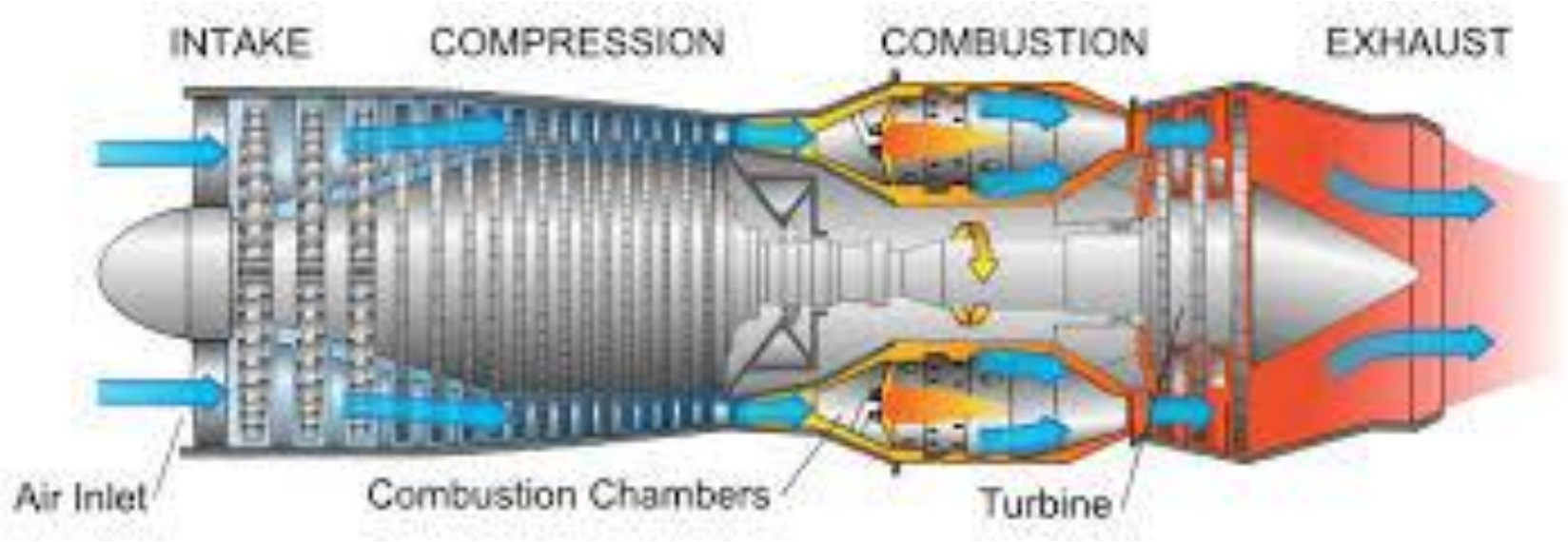
Ejemplo: Simulación de una turbina de Gas



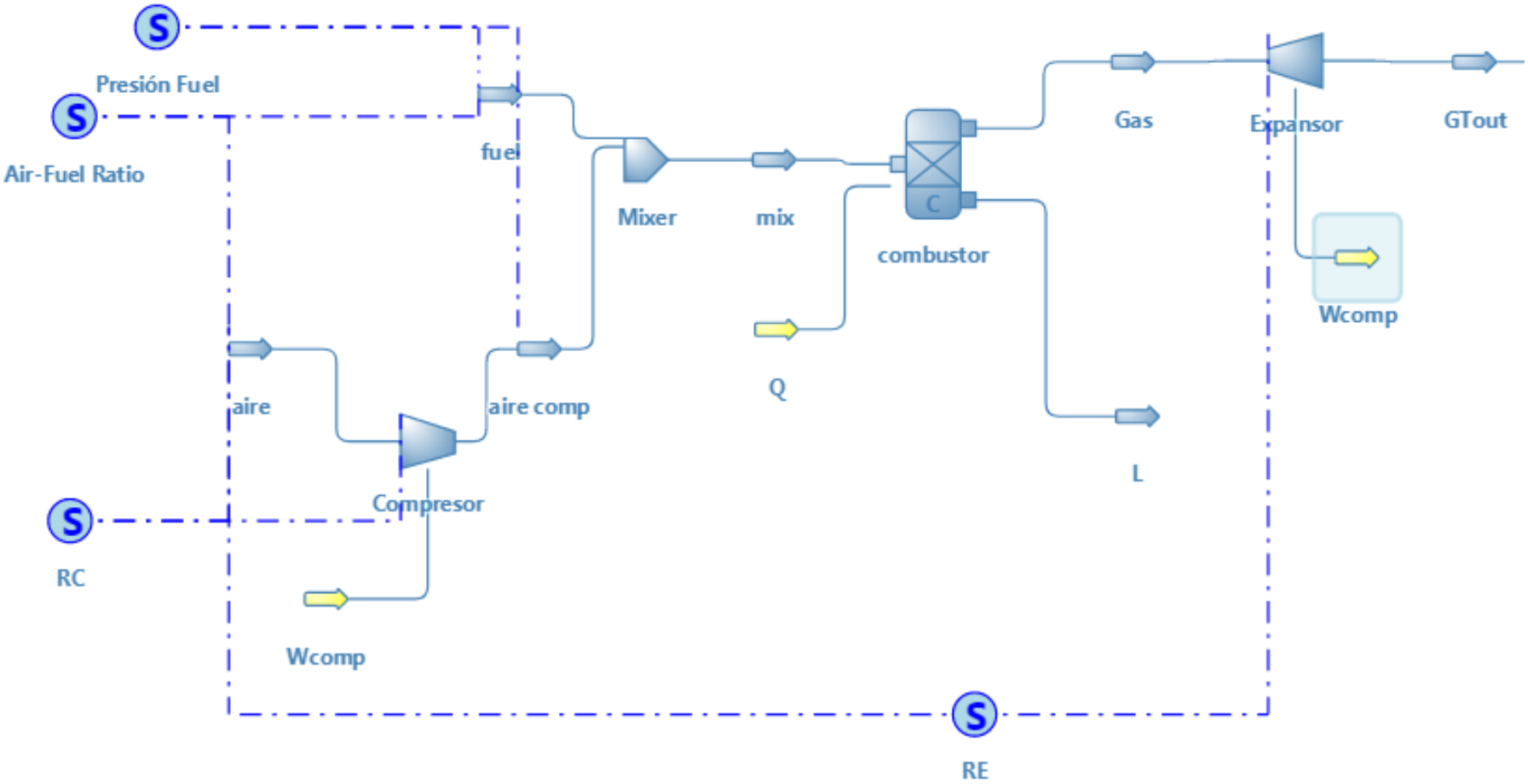


Ejemplo: Simulación de una turbina de Gas





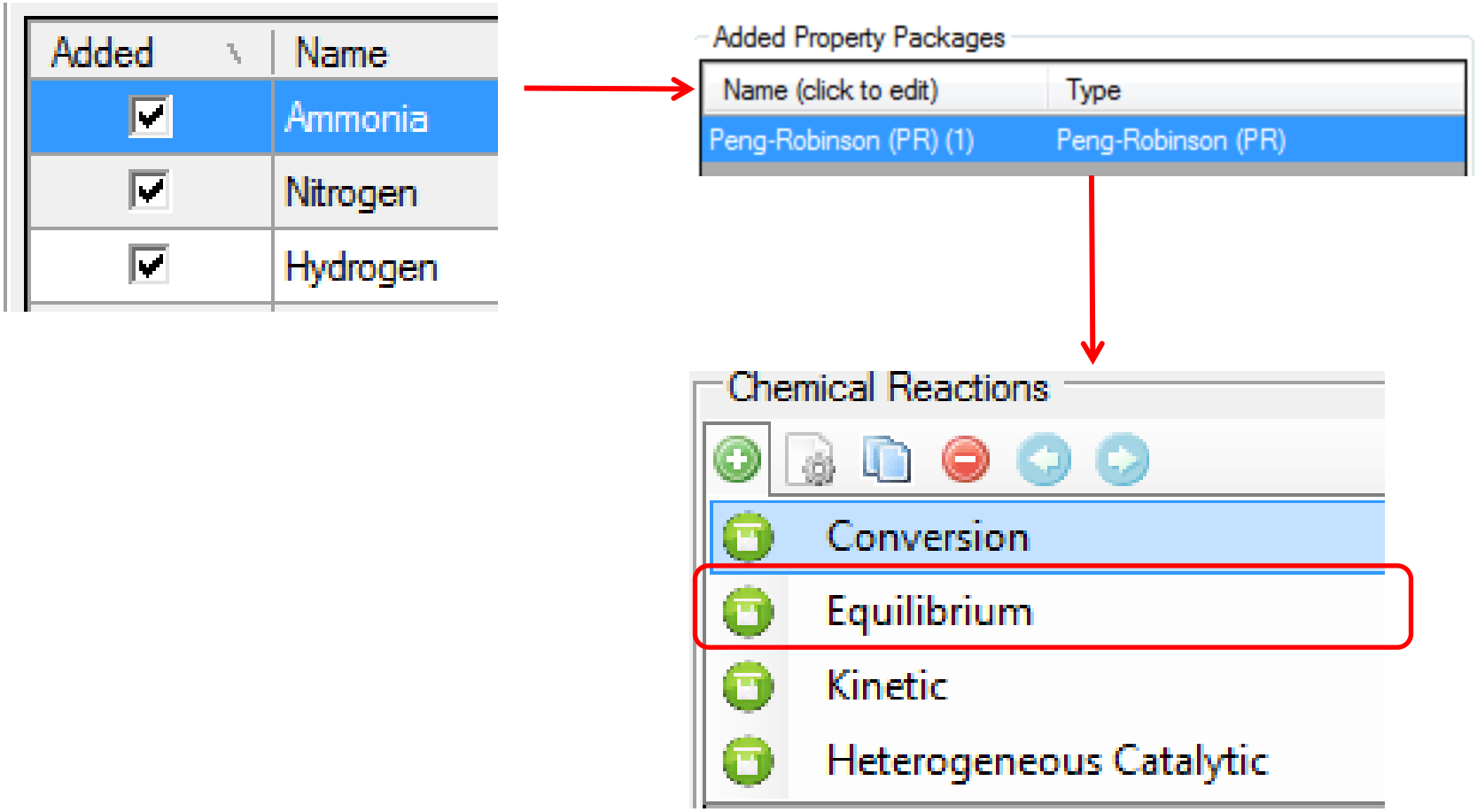
Ejemplo: Simulación de una turbina de Gas



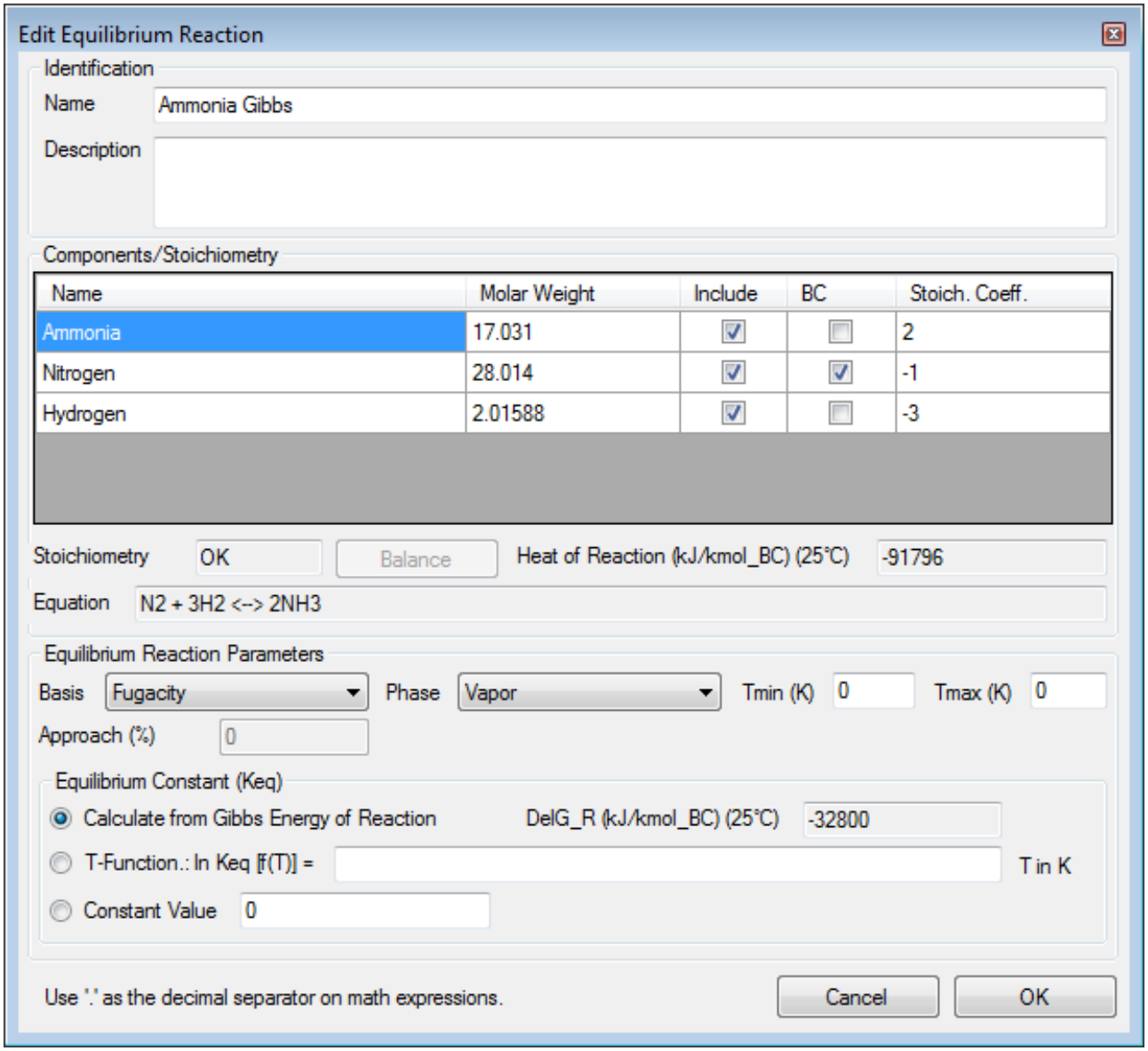
Ejemplo: Reactor de equilibrio

$$3H_2 + N_2 \Leftrightarrow 2NH_3$$

Alimentación estequiométrica



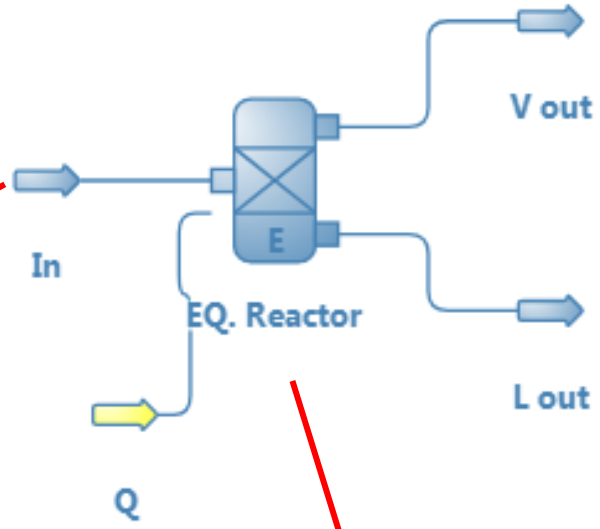
Reacción de equilibrio



Reactor de equilibrio 450 ºC 100 atm

Stream Conditions | Compound Amounts

Flash Spec	Temperature and Pressure (TP)	
Temperature	723.15	K
Pressure	10132500	Pa
Mass Flow	0.0851541	kg/s
Molar Flow	10	mol/s
Volumetric Flow	0.0060835443	m3/s
Specific Enthalpy	1480.9576	kJ/kg
Specific Entropy	-0.45617289	kJ/[kg.K]
Vapor Phase Mole Fraction	1	



Stream Conditions | Compound Amounts

Basis: Mole Fractions

Solvent:

Compound	Amount
Ammonia	0
Nitrogen	0.25
Hydrogen	0.75

Calculation Parameters

Parameters | Convergence

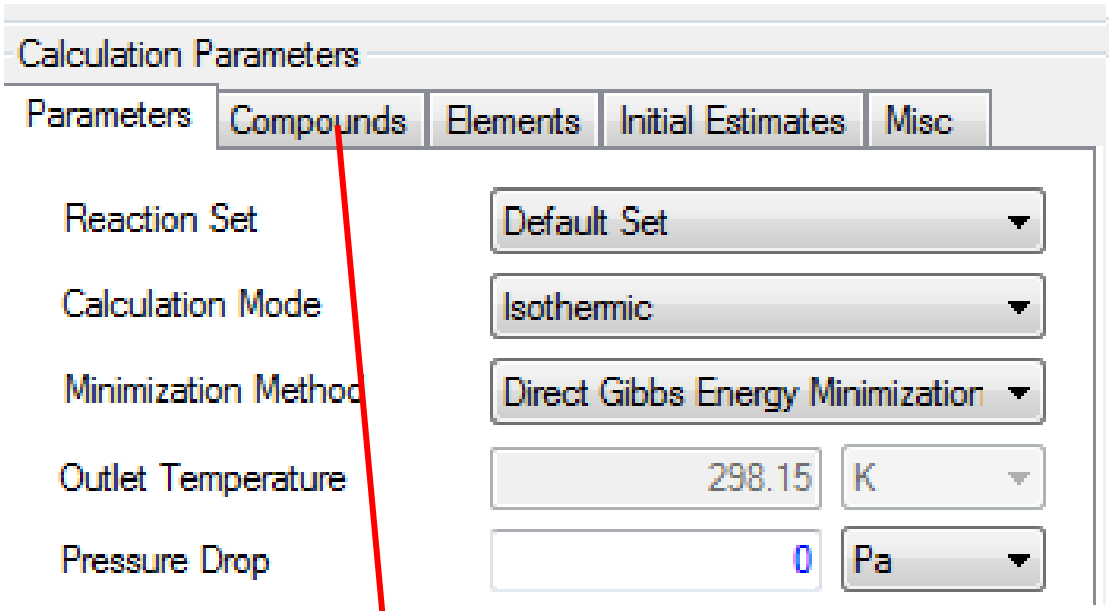
Reaction Set	Default Set	
Calculation Mode	Isothermic	
Minimization Method		
Outlet Temperature	298.15	K
Pressure Drop	0	Pa

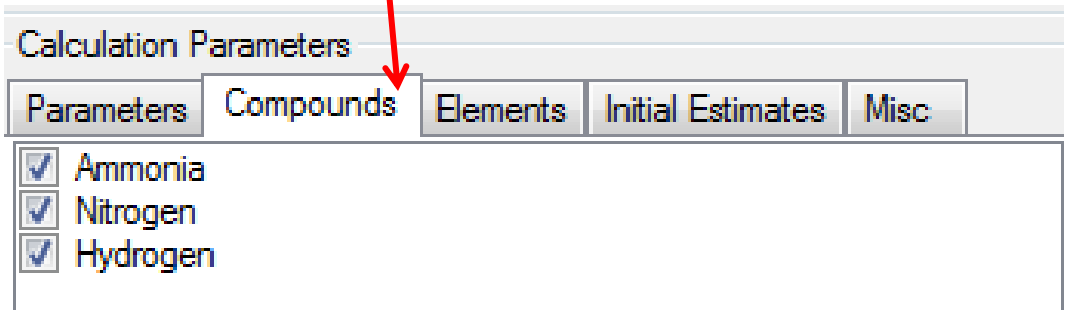
Results

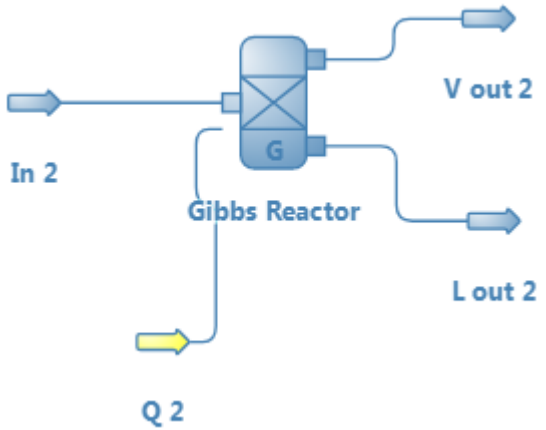
General | Reactions | Conversions

Compound	Conversion (%)
Nitrogen	28.759722
Hydrogen	28.759722

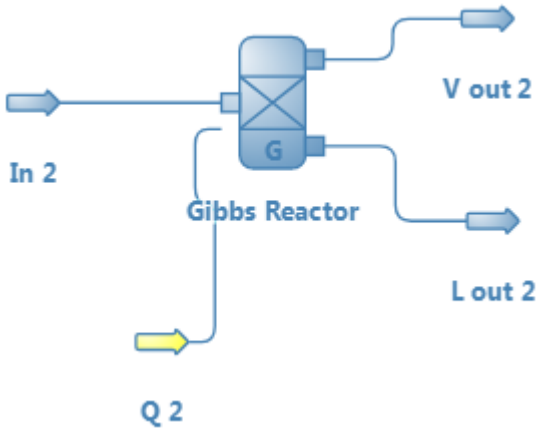
Reactor de Gibbs







Reactor de Gibbs



Calculation Parameters

Parameters | Compounds | Elements | Initial Estimates | Misc

Configuration

Add Element | Remove Selected Element

Save Changes | Create from Selected Components

Matrix

Element	Ammonia	Nitrogen	Hydrogen
N	1	2	0
H	3	0	2

Reactor de Gibbs

Calculation Parameters

Parameters | Compounds | Elements | Initial Estimates | Misc

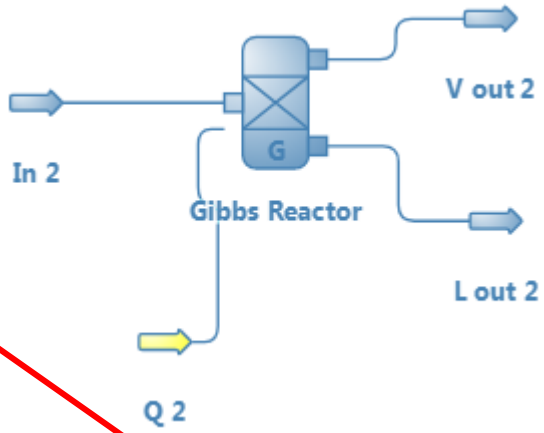
Configuration

Copy from inlet stream | Copy from outlet liquid stream

Copy from outlet vapor stream

Initial Estimates

Compound	Estimates for Outlet Mole Flows (mol/s)
Ammonia	0
Nitrogen	0
Hydrogen	0



Calculation Parameters

Parameters | Compounds | Elements | Initial Estimates | Misc

Use Damping Factor (Newton's Method)

Lower Limit	0.001
Upper Limit	2
Max. Internal Loop Iterations	20000
Max. External Loop Iterations	50
Internal Loop Tolerance	1E-06
External Loop Tolerance	0.001

Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)}$$

$$MEG_{(l)} + EtO_{(l)} \xrightarrow{k_2} DEG_{(l)}$$

$$DEG_{(l)} + EtO_{(l)} \xrightarrow{k_3} TEG_{(l)}$$

Added	Name
☑	Ethylene oxide
☑	Water
☑	Ethylene glycol
☑	Diethylene glycol
☑	Triethylene glycol

$$k_1/[\text{L}/(\text{mol}\cdot\text{min})] = \exp(13.62 - 8220/T)$$

$$k_2/[\text{L}/(\text{mol}\cdot\text{min})] = \exp(15.57 - 8700/T)$$

$$k_3/[\text{L}/(\text{mol}\cdot\text{min})] = \exp(16.06 - 8900/T)$$

CAChemE

A. Carrero, N. Quirante, J. Javaloyes

October 2016

Feed in

x_{water}: 0.7

x_{EtO}: 0.3

P: 20 atm

T: 100 ºC

m: 100 mol/s

Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)} \qquad k_1/[\mathrm{L/(mol \cdot min)}] = \exp(13.62 - 8220/T)$$

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔHf (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylene oxide	44.0526	-1194.7081	☑	☑			
Water	18.015	-13422.925	☑	☐			
Ethylene glycol	62.0678	-6318.8964	☑	☐			
Diethylene glycol	106.12	-5148.8881	☐	☐			
Triethylene glycol	150.173	-4828.4312	☐	☐			

Kinetic Reaction Parameters

Base Component: Ethylene oxide

Basis: Molar Concentrations

Phase: Liquid

Tmin (K): 0

Tmax (K): 3500

Direct and Reverse Reactions Velocity Constant (k and k')

Direct Reaction: (•) Arrhenius — A: — E: — E in J/mol, T in K

( ) User-Defined: f(T)

Reverse Reaction: (•) Arrhenius — A': 0 — E': 0 — E in J/mol, T in K

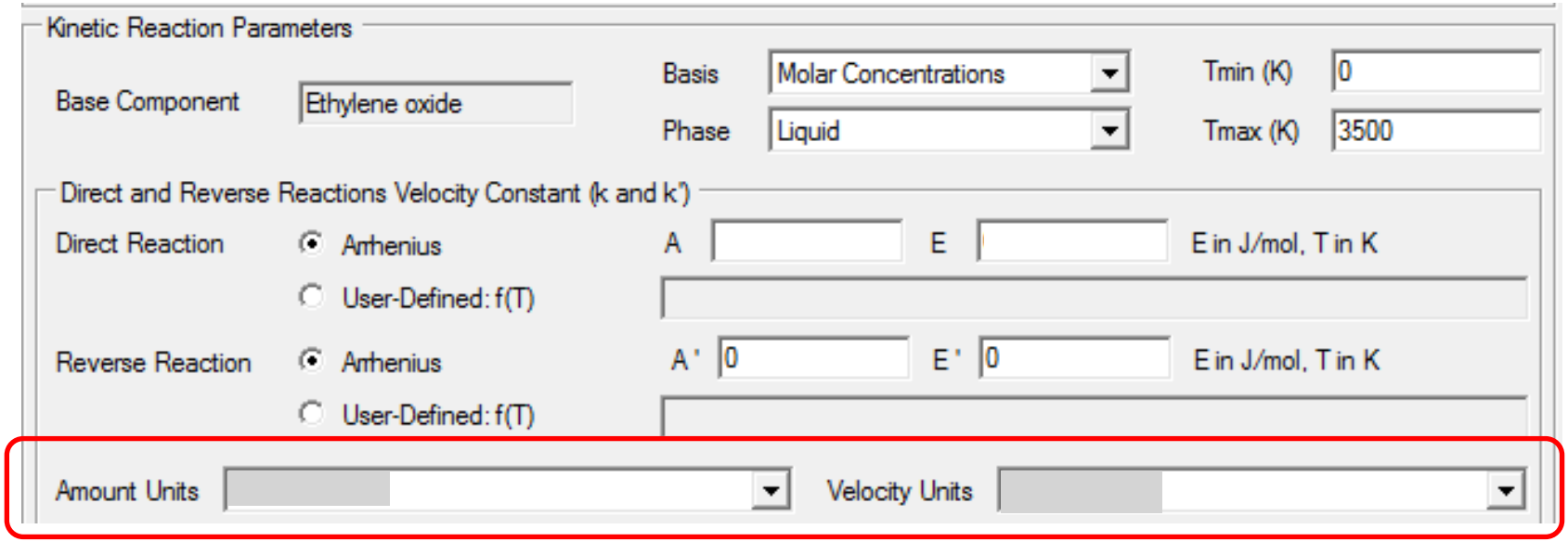
( ) User-Defined: f(T)

Amount Units: — Velocity Units: —

Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)} \qquad k_1/[\mathrm{L/(mol \cdot min)}] = \exp(13.62 - 8220/T)$$

$$\left(-r_{EtO}\right) = k_1 C_{EtO} C_{H_2O} \qquad k_1 = A_1 e^{-\frac{E_1}{RT}}$$



Define las unidades de la expresión cinética

Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)} \qquad k_1/[\mathrm{L/(mol \cdot min)}] = \exp(13.62 - 8220/T)$$

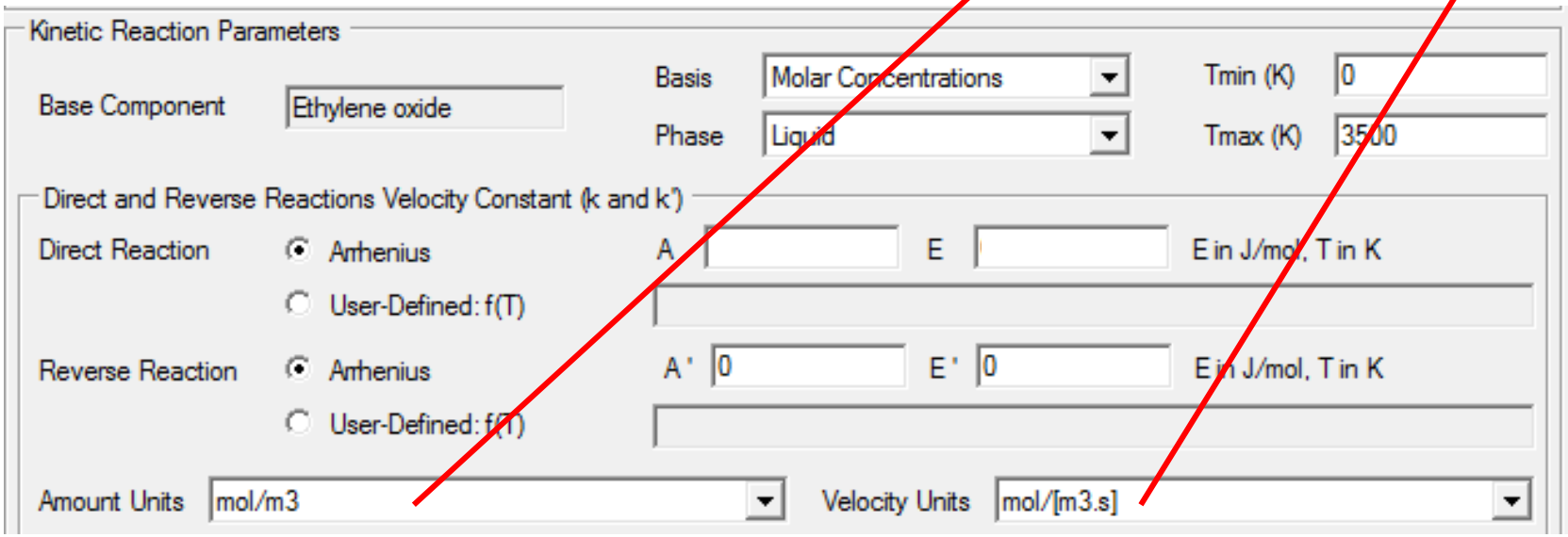
$$\left(-r_{EtO}\right) = k_1 C_{EtO} C_{H_2O}$$

$$k_1 = A_1 e^{-\frac{E_1}{RT}}$$

$$k_1 \left[\ \text{¿?}\ \right]$$

$$C_{EtO}; C_{H_2O} \left[\frac{mol}{m^3}\right]$$

$$\left(-r_{EtO}\right) \left[\frac{mol}{m^3 s}\right]$$



Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)}$$

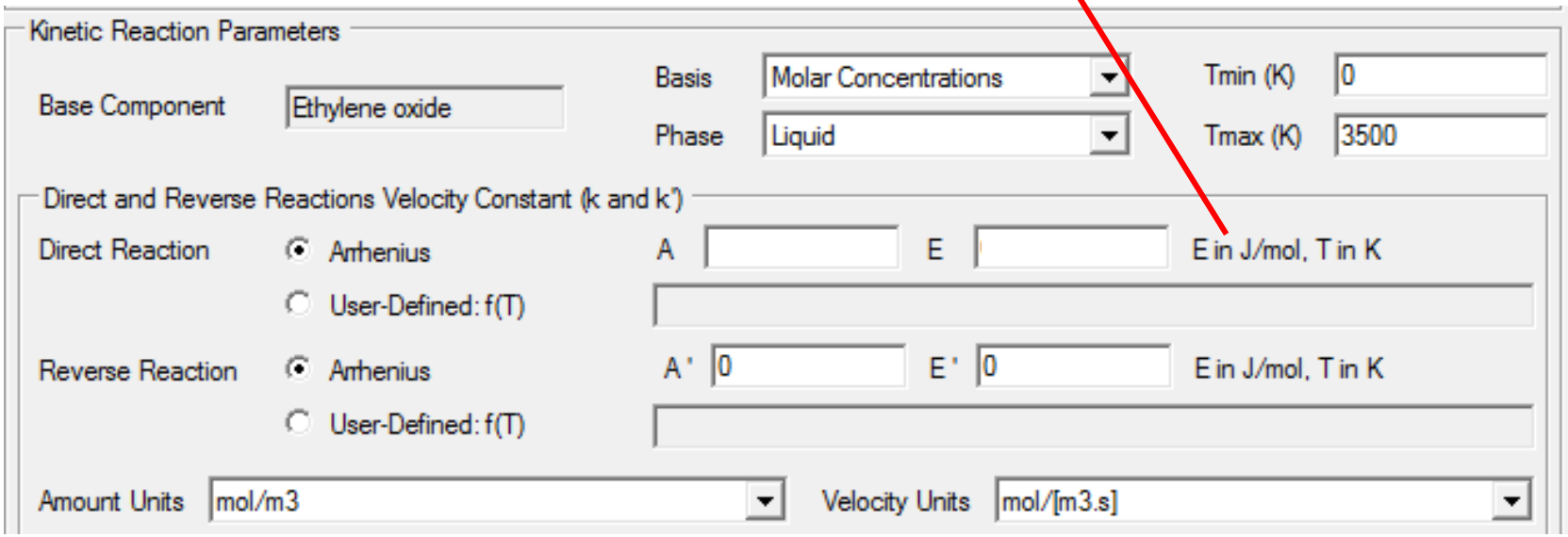
$$k_1/[\mathrm{L/(mol \cdot min)}] = \exp(13.62 - 8220/T)$$

$$k_1 = A_1 e^{-\frac{E_1}{RT}}$$

$$E_1\left[\frac{J}{mol}\right] \quad T[K]$$

$$A_1\left[\frac{m^3}{mol.s}\right]$$

$$k_1\left[\frac{m^3}{mol.s}\right]$$



Ejemplo: Reactor CSTR y PFR

$$EtO_{(l)} + H_2O_{(l)} \xrightarrow{k_1} MEG_{(l)} \qquad k_1/[\mathrm{L/(mol \cdot min)}] = \exp(13.62 - 8220/T)$$

$$k_1 = \exp\left(13.62 - 8220/T\right)$$

$$k_1 = \mathrm{e}^{13.62}\, e^{-8220/T} \left[\frac{L}{mol.\mathrm{min}}\right]$$

$$k_1 = \underbrace{\frac{\mathrm{e}^{13.62}}{60\times 1000}}_{A_1} \underbrace{e^{-8220/T}}_{e^{-\frac{E_1}{RT}}} \left[\frac{m^3}{mol.\mathrm{s}}\right]$$

$$A_1 = \frac{\mathrm{e}^{13.62}}{60\times 1000}\left[\frac{m^3}{mol.\mathrm{s}}\right]$$

$$-\frac{E_1}{RT} = -\frac{8220}{T}$$

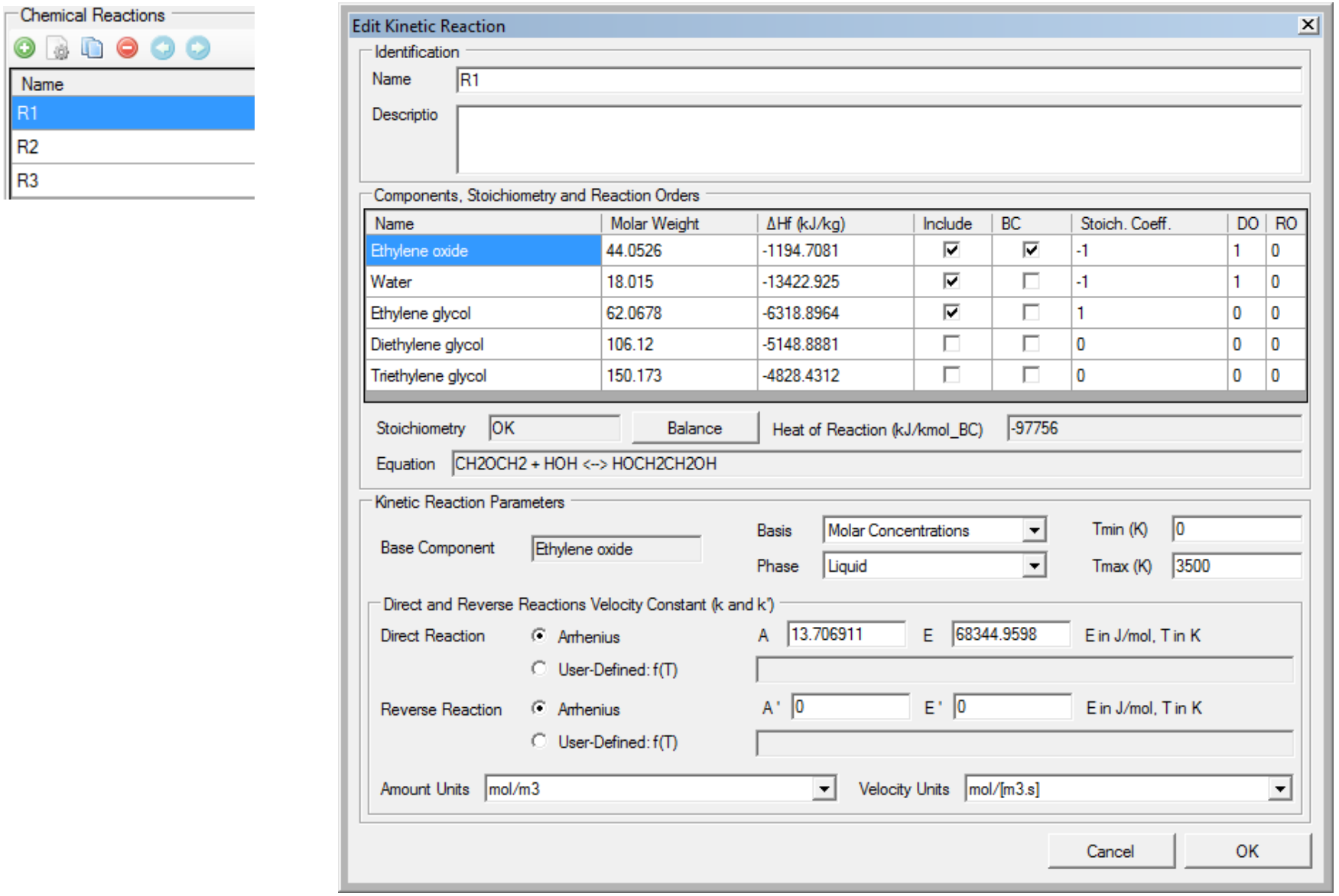
$$E_1 = 8220R$$

$$E_1 = 8220\left[K\right]\times 8.314472\left[\frac{J}{mol.K}\right]$$

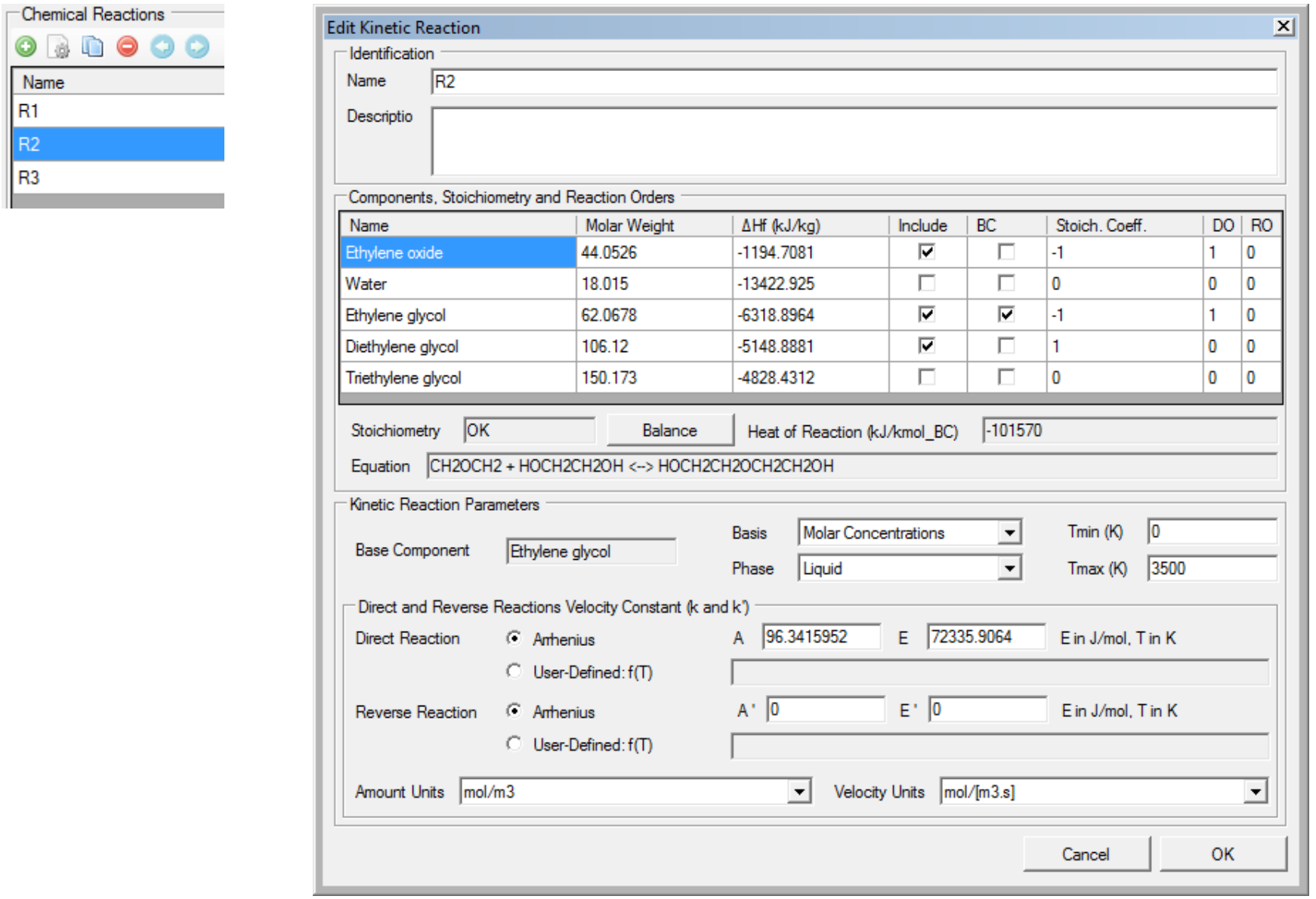
$$A_1 = 13.7069\left[\frac{m^3}{mol.\mathrm{s}}\right]$$

$$E_1 = 68344.9598\left[\frac{J}{mol}\right]$$

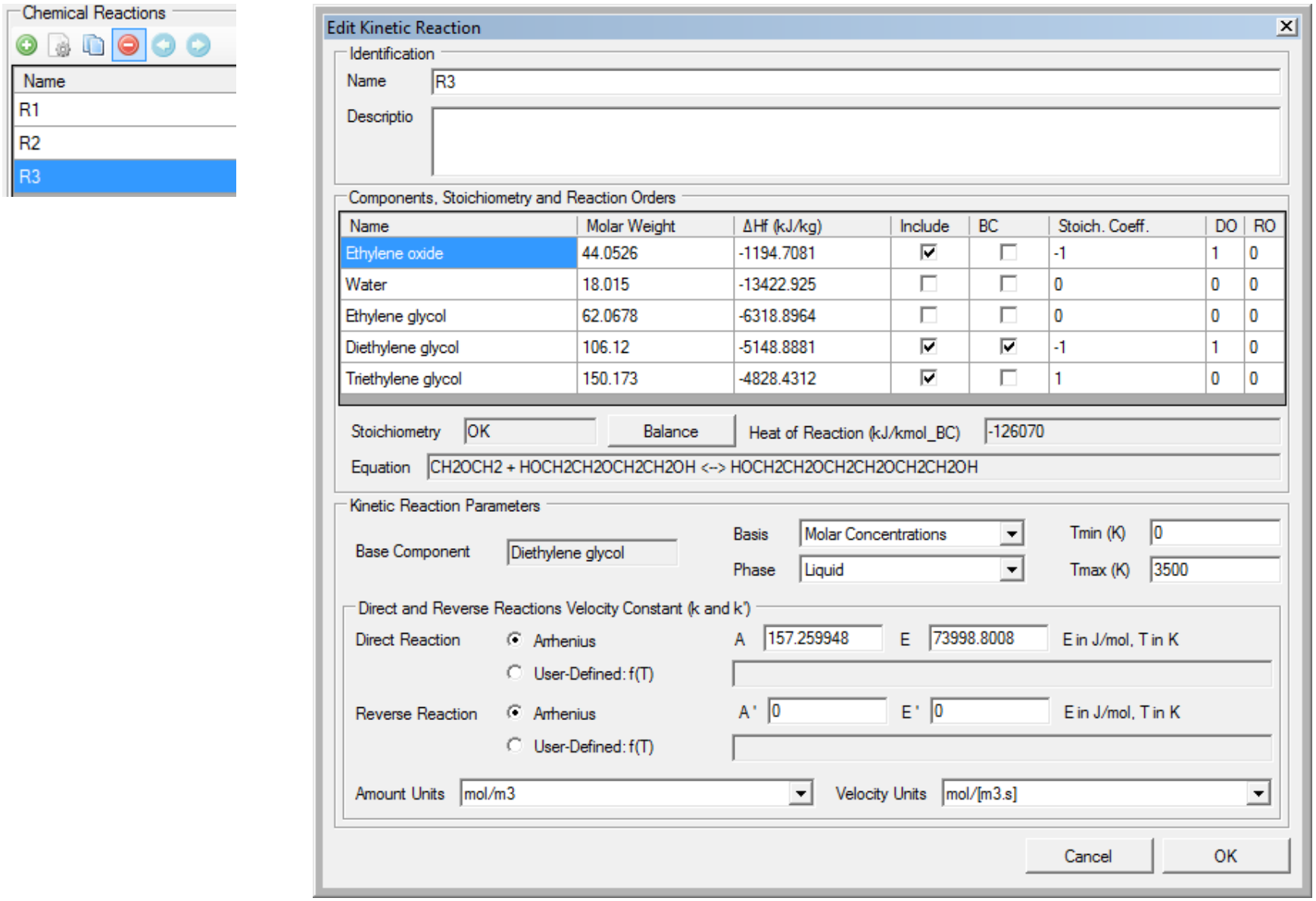
Ejemplo: Reactor CSTR y PFR



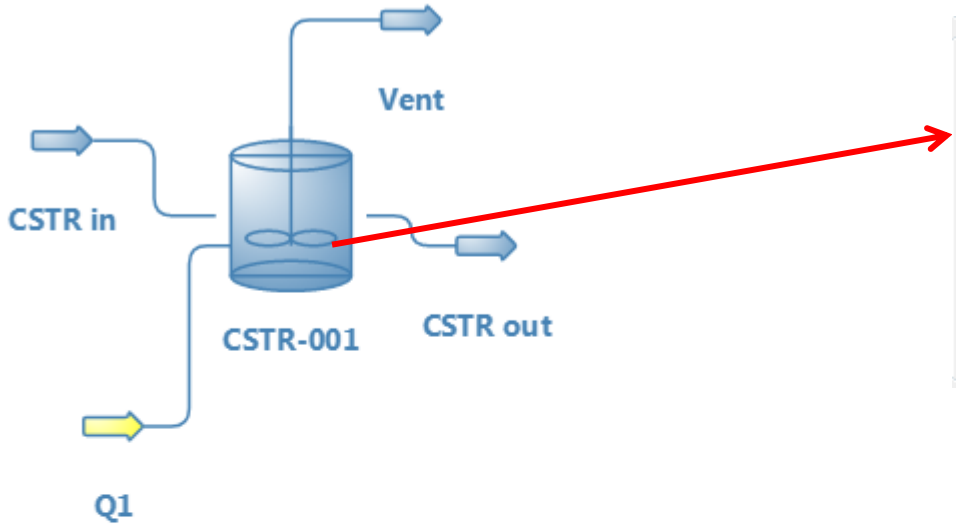
Ejemplo: Reactor CSTR y PFR



Ejemplo: Reactor CSTR y PFR

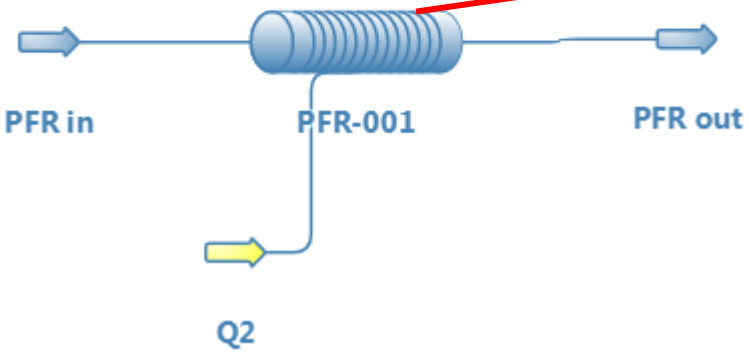


Ejemplo: Reactor CSTR y PFR



Calculation Parameters

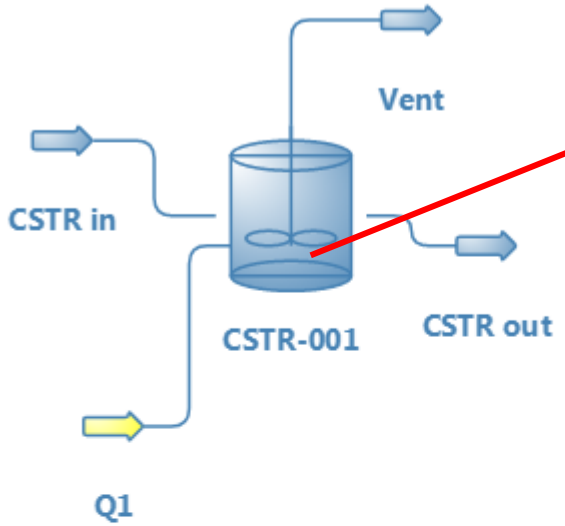
Reaction Set	Default Set	
Calculation Mode	Isothermic	
Outlet Temperature	25	C
Reactor Volume	4	m3
Headspace	0	m3
Reactor Pressure Drop	0	kgf/cm²
Catalyst Amount	0	kg



Calculation Parameters

Reaction Set	Default Set	
Calculation Mode	Isothermic	
Outlet Temperature	25	C
Reactor Volume	4	m3
Reactor Length	10	m
Catalyst Loading	0	kg/m3
Catalyst Particle Diameter	0	mm
Catalyst Void Fraction	0	

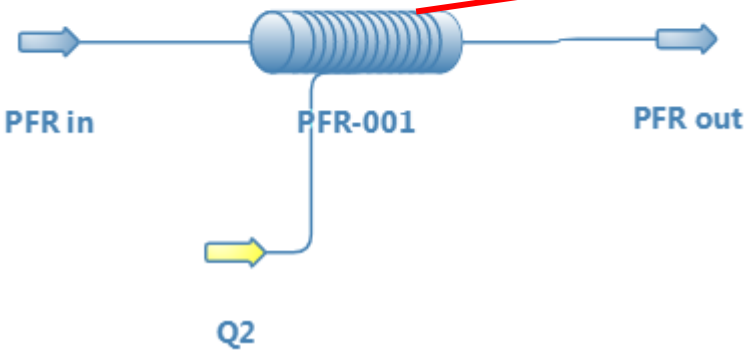
Ejemplo: Reactor CSTR y PFR



Results

General | Reactions | Conversions

Compound	Conversion (%)
Water	4.37499
Ethylene oxide	11.0937
Ethylene glycol	0
Diethylene glycol	0
Triethylene glycol	0

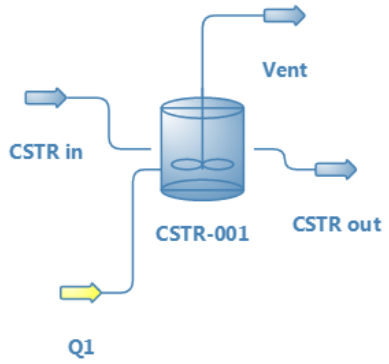


Results

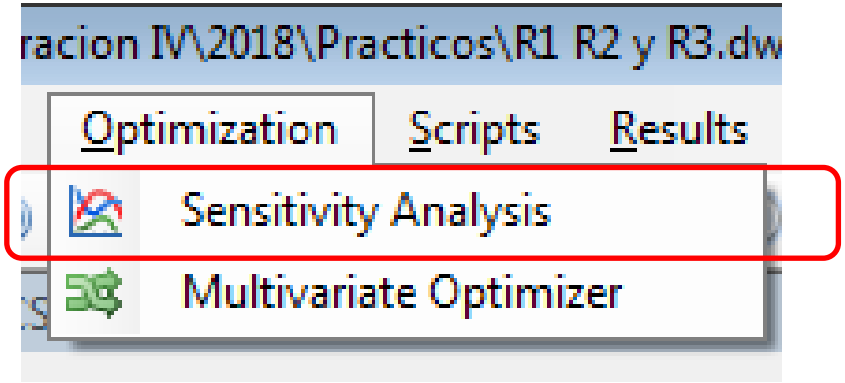
General | Reactions | Conversions | Concentration Profile

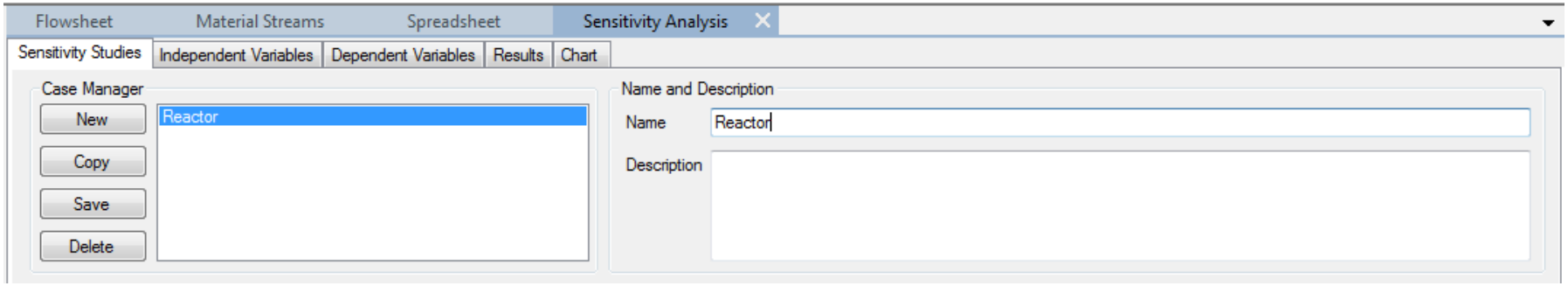
Compound	Conversion (%)
Water	4.72378
Ethylene oxide	11.5431

Análisis Paramétrico

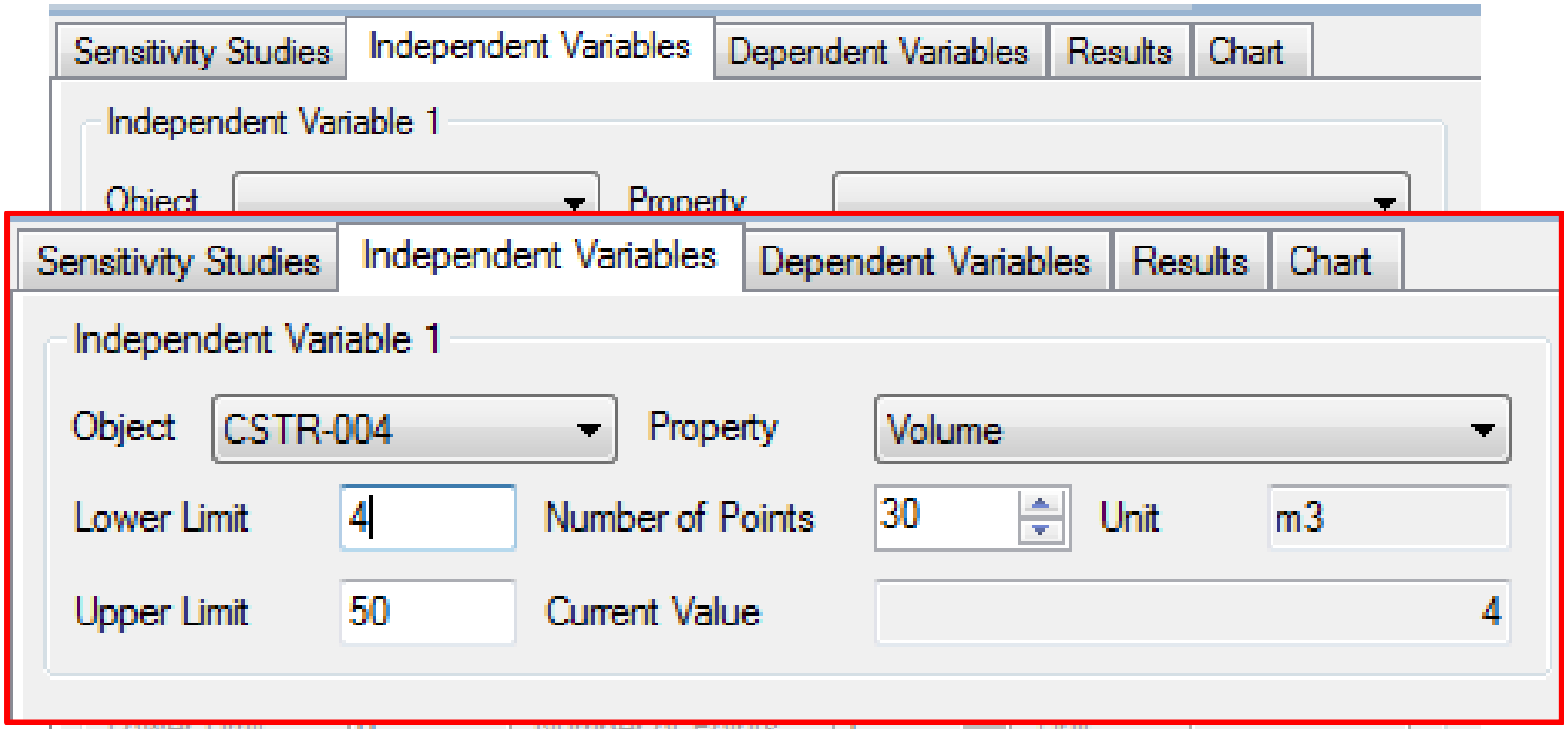


Se analizara de manera automática la variación de la composición de salida con el tamaño del reactor

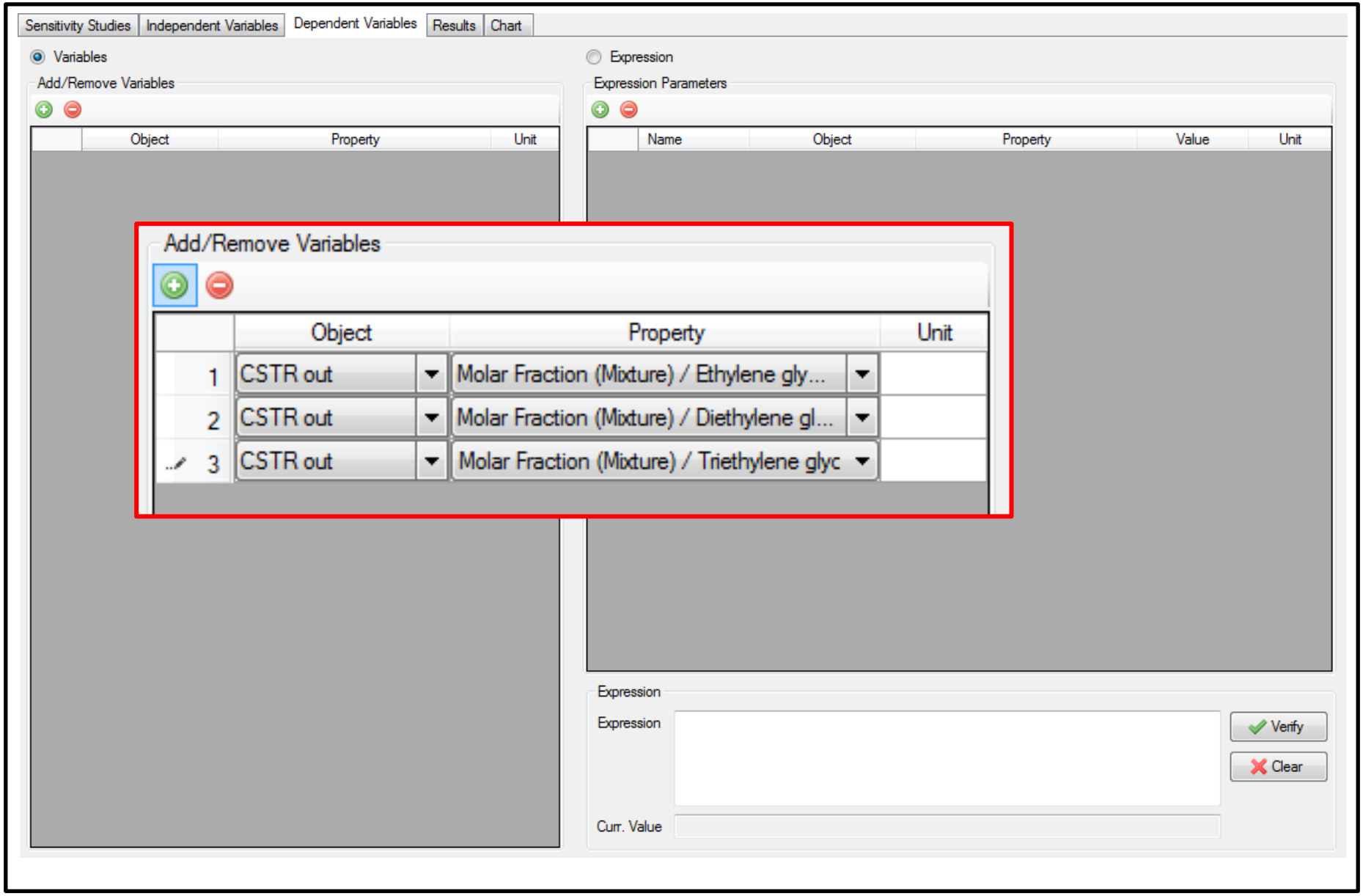




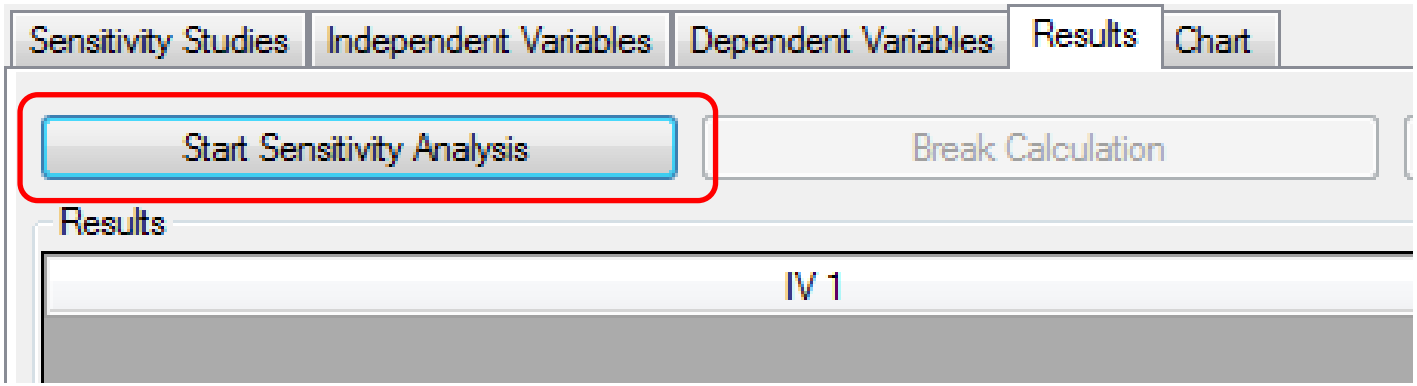
Análisis Paramétrico

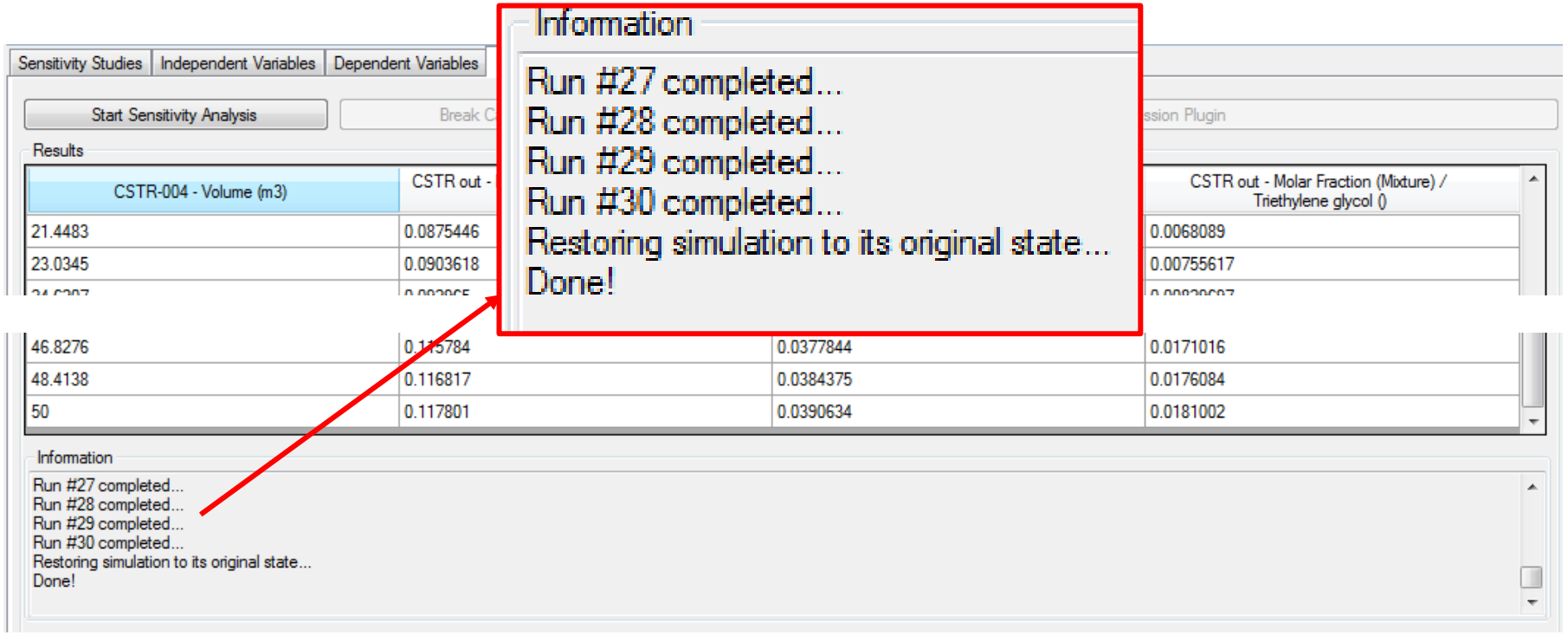


Análisis Paramétrico

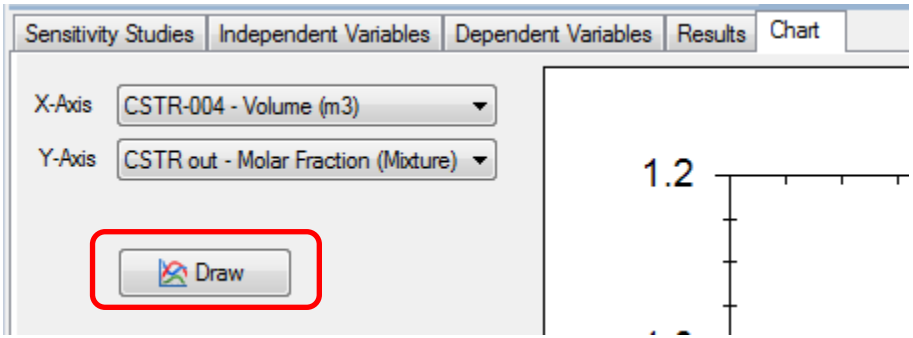


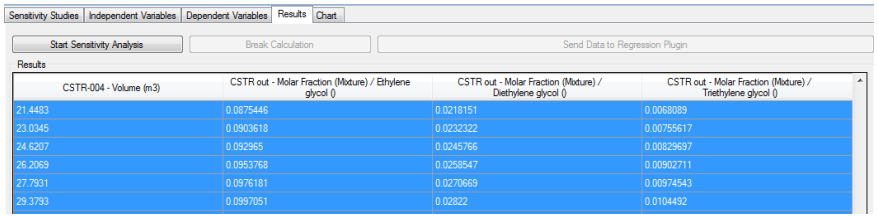
Análisis Paramétrico



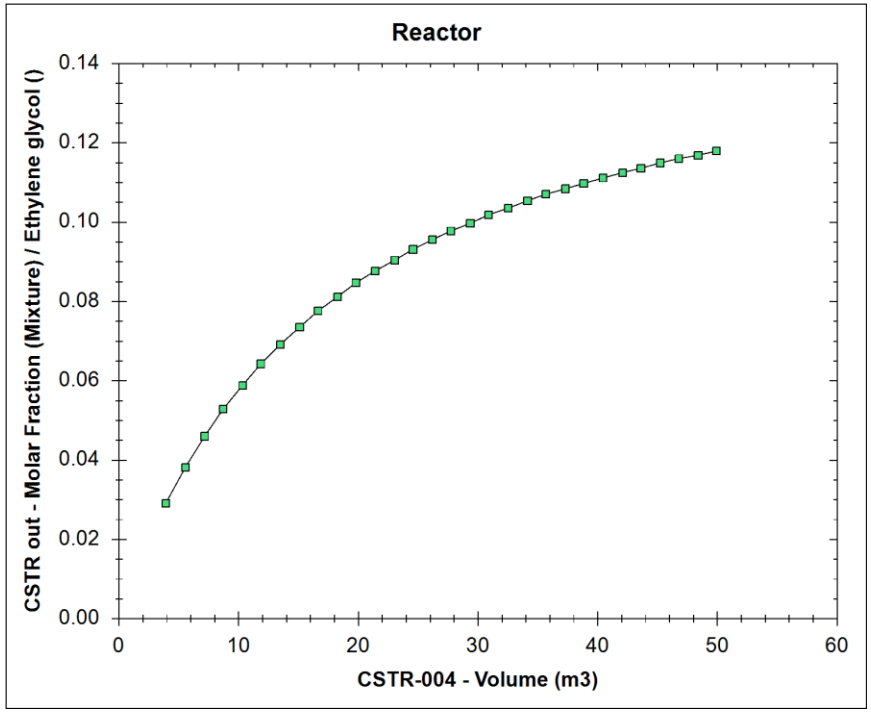


Análisis Paramétrico





Copiamos los datos y los pegamos en Excel



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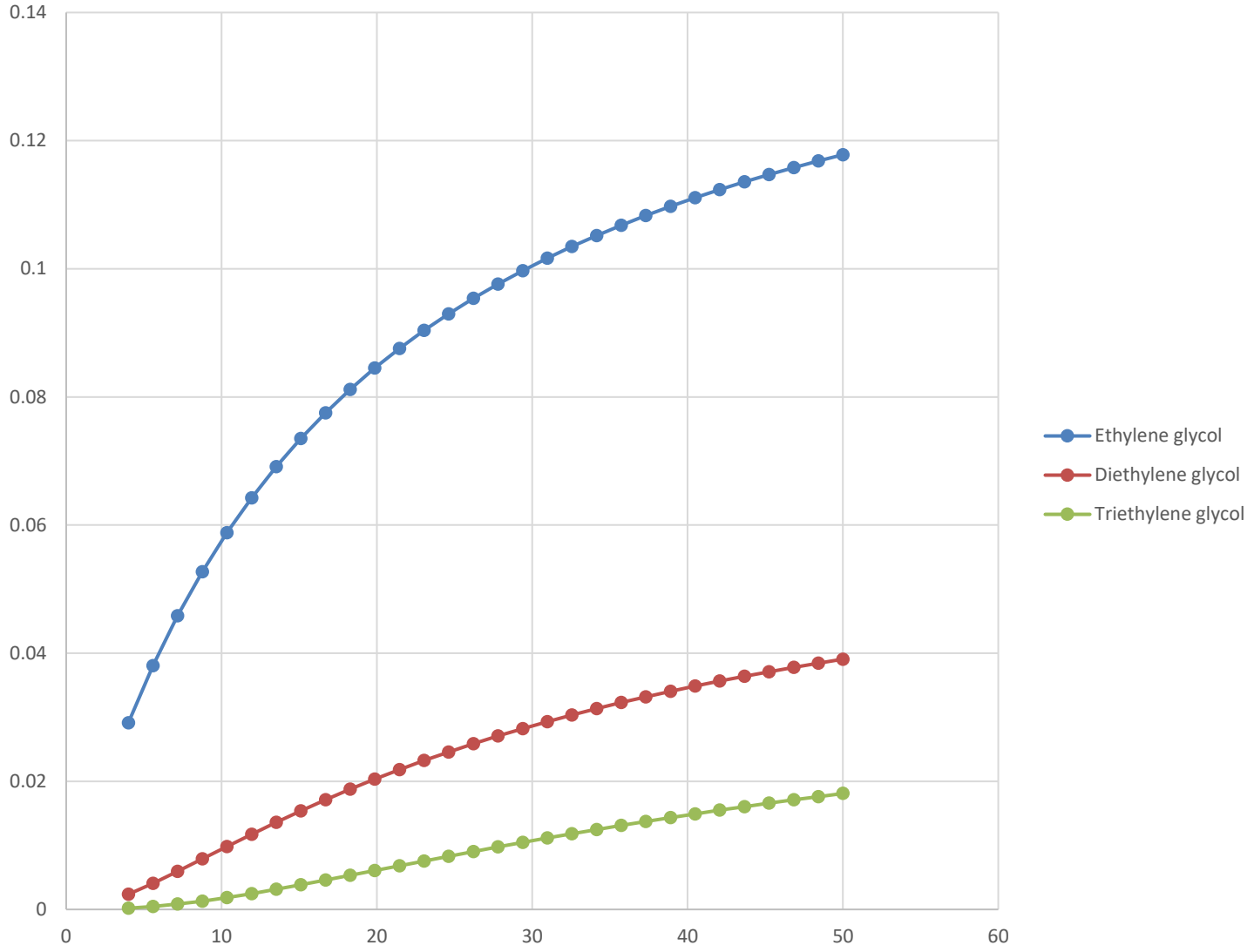
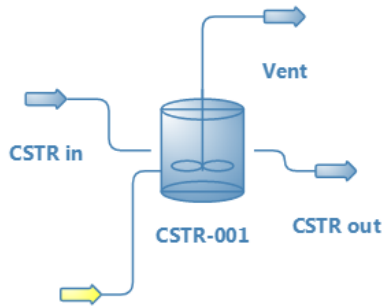


Análisis Paramétrico



Se analizara la variación de la conversión del EtO con el tamaño del reactor

Sensitivity Studies | Independent Variables | Dependent Variables | Results | Chart

Case Manager

New
Copy
Save
Delete

Reactor
Conversión

Name and Description

Name: Conversión

Description:

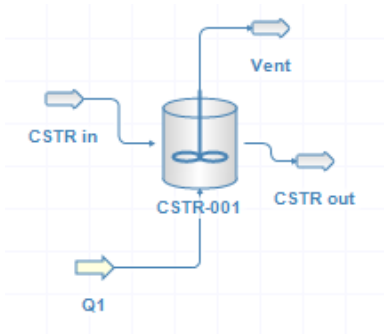
Independent Variable 1

Object: CSTR-004 Property: Volume

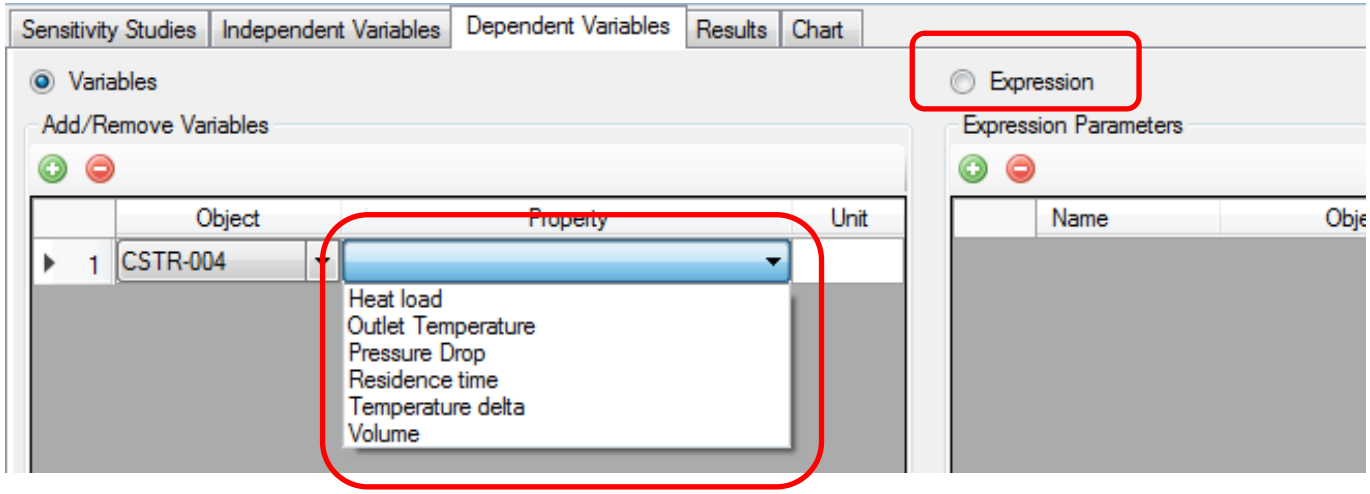
Lower Limit: 4 Number of Points: 40 Unit: m3

Upper Limit: 150 Current Value: 4

Análisis Paramétrico



Se analizara la variación de la conversión del EtO con el tamaño del reactor

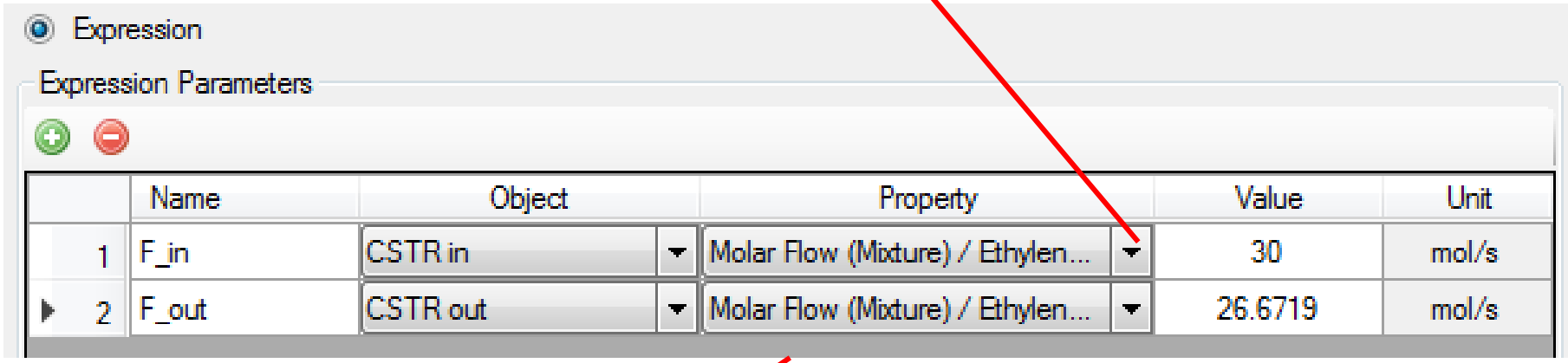


¿Conversión?

$$x_{EtO} =$$

Análisis Paramétrico

Molar Flow (Mixture) / Ethylene Oxide

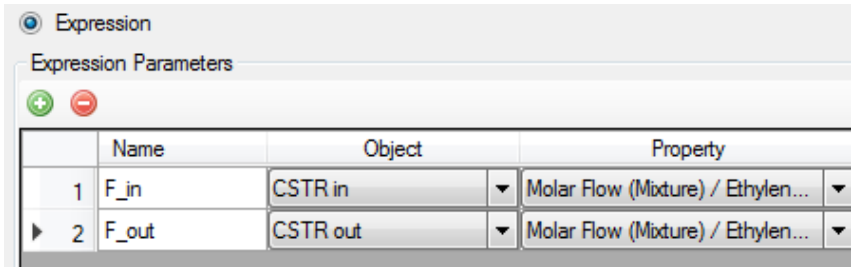


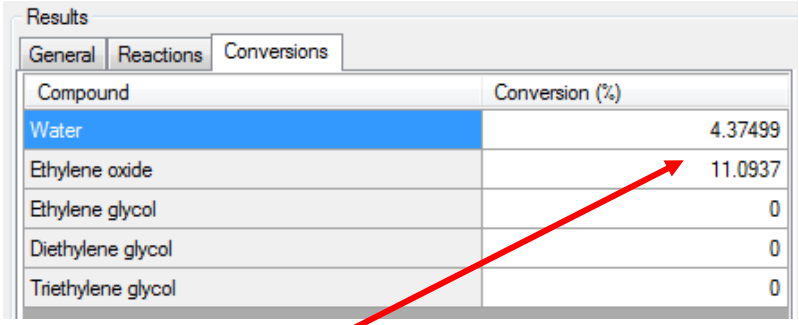
Variables del flowsheets que necesito para la expresión de la conversión

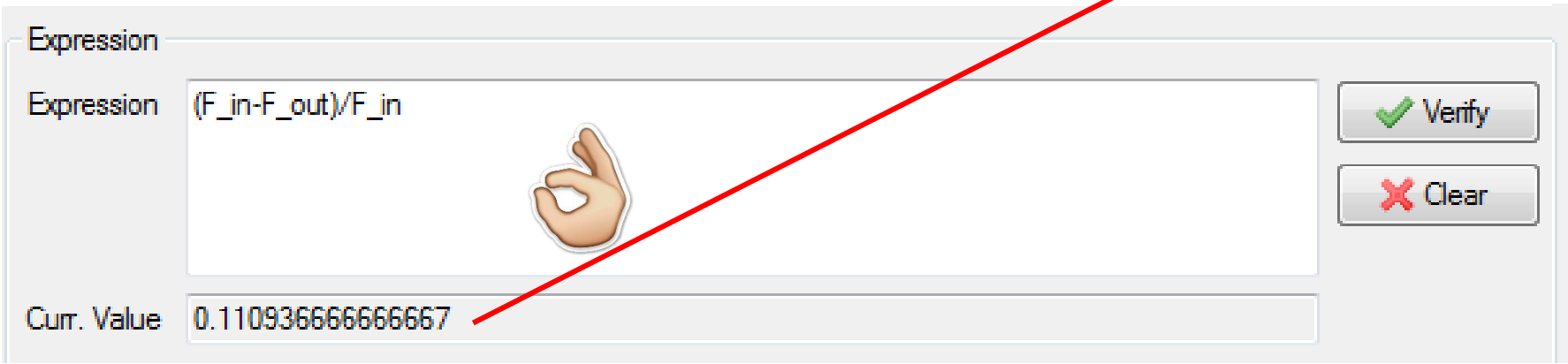
$$x_{EtO} = \frac{F_{EtO_{in}} - F_{EtO_{out}}}{F_{EtO_{in}}}$$

$$\frac{\text{Moles consumidos de EtO}}{\text{Moles alimentados de EtO}}$$

Análisis Paramétrico



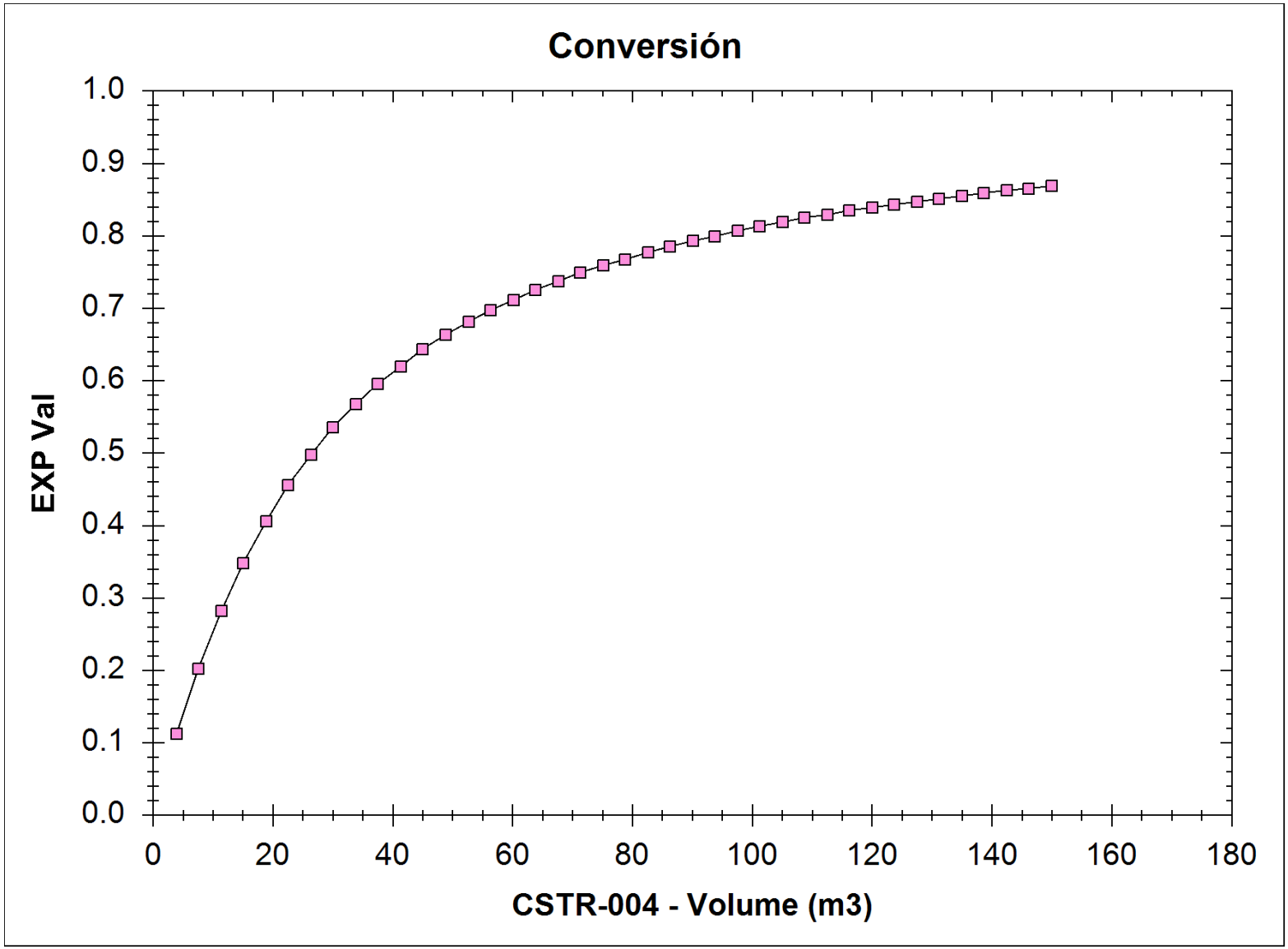




$$x_{EtO} = \frac{F_{EtO_{in}} - F_{EtO_{out}}}{F_{EtO_{in}}}$$

$$\frac{\text{Moles consumidos de EtO}}{\text{Moles alimentados de EtO}}$$

Análisis Paramétrico



Estudio paramétrico del reactor de equilibrio

$$3H_2 + N_2 \Leftrightarrow 2NH_3$$

Edit Equilibrium Reaction

Identification

Name: Ammonia Gibbs

Description:

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Ammonia	17.031	☑	☐	2
Nitrogen	28.014	☑	☑	-1
Hydrogen	2.01588	☑	☐	-3

Stoichiometry: OK | Balance | Heat of Reaction (kJ/kmol_BC) (25°C): -91796

Equation: N2 + 3H2 <--> 2NH3

Equilibrium Reaction Parameters

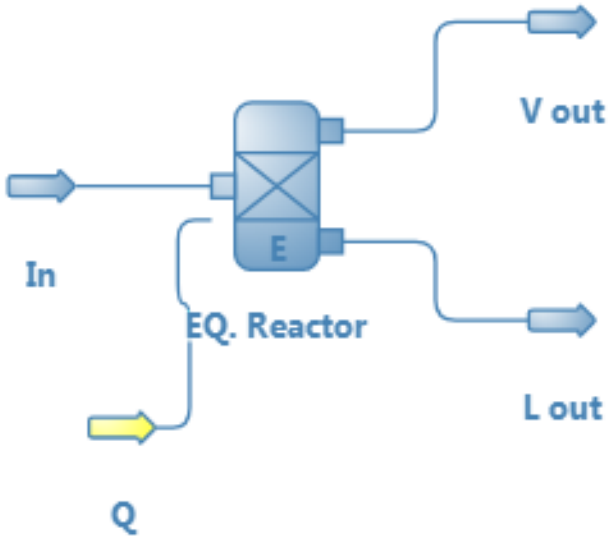
Basis: Fugacity | Phase: Vapor | Tmin (K): 0 | Tmax (K): 0

Approach (%): 0

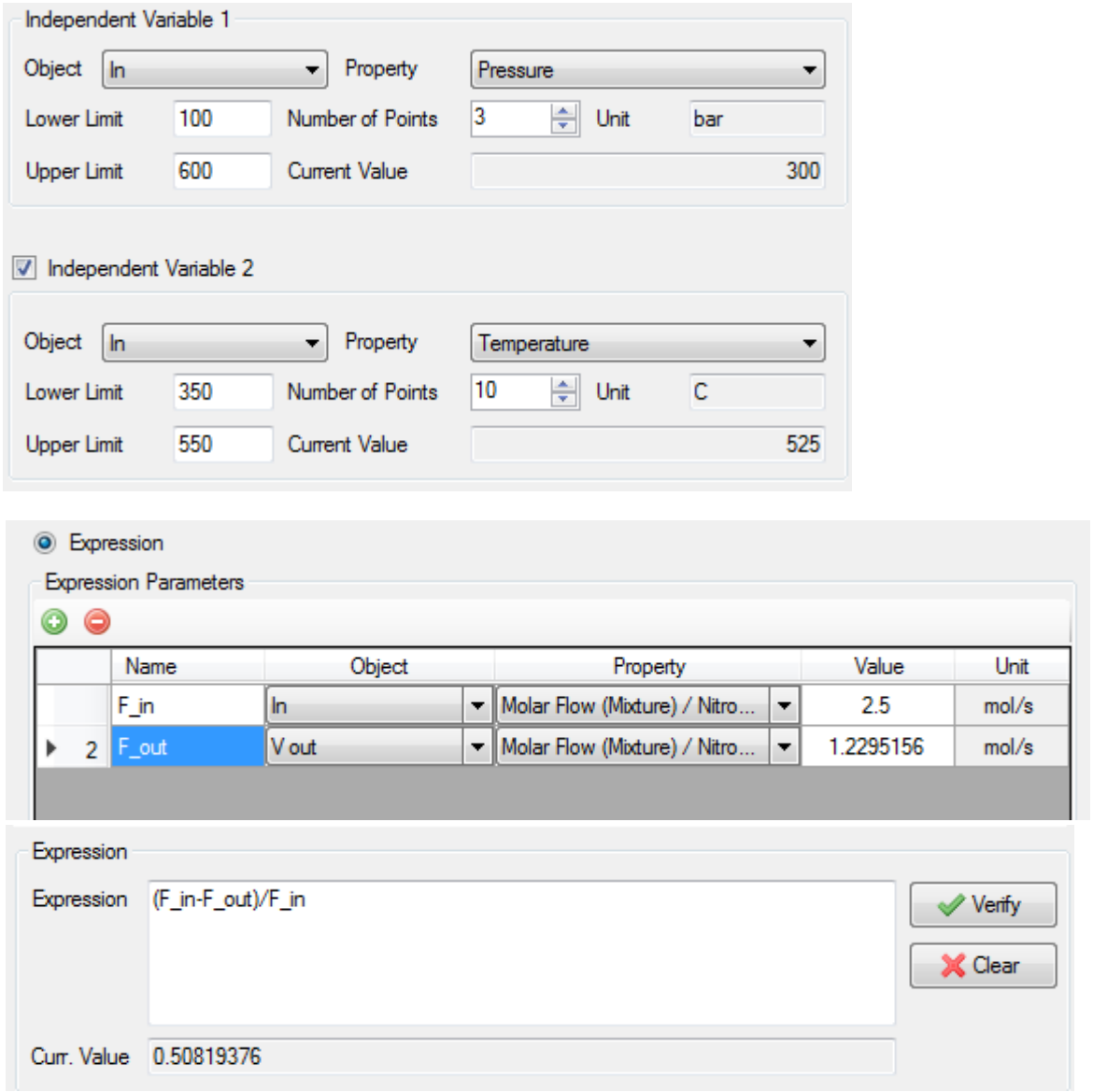
Equilibrium Constant (Keq)

- (•) Calculate from Gibbs Energy of Reaction — DelG_R (kJ/kmol_BC) (25°C): -32800
- ( ) T-Function.: ln Keq [f(T)] = — T in K
- ( ) Constant Value: 0

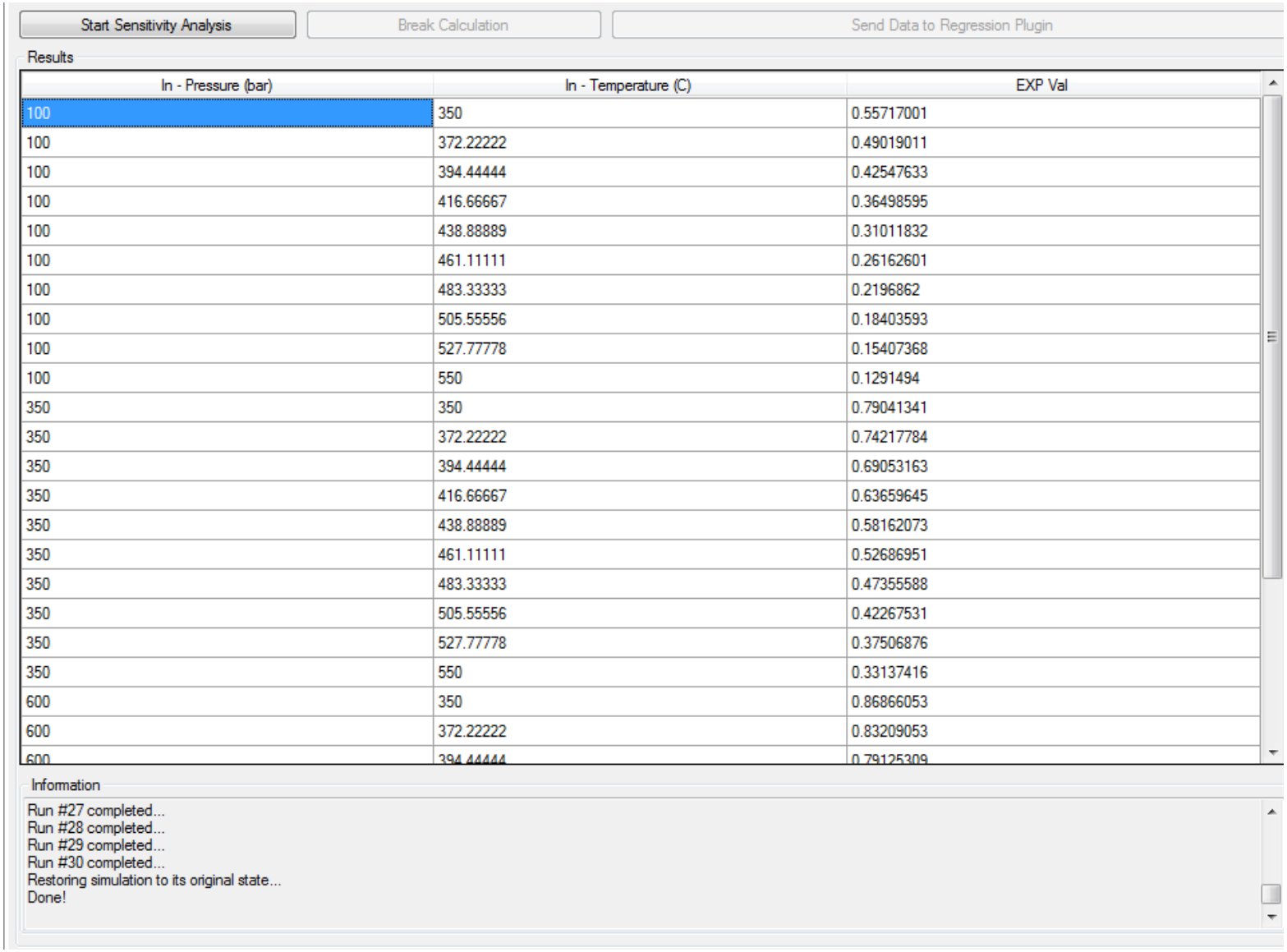
Use '.' as the decimal separator on math expressions. | Cancel | OK



Estudio paramétrico del reactor de equilibrio



Estudio paramétrico del reactor de equilibrio



Estudio paramétrico del reactor de equilibrio

$$3H_2 + N_2 \Leftrightarrow 2NH_3$$