

DSOySP

Módulos de DWSIM (III)

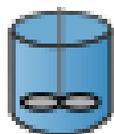
Equipos con reacción química en DWSIM

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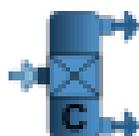
Aux. 1ra: Dr. Juan I. Manassaldi

Modelos de reactores presentes en DWSIM



Continuous 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 ser de 4 tipos:

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.

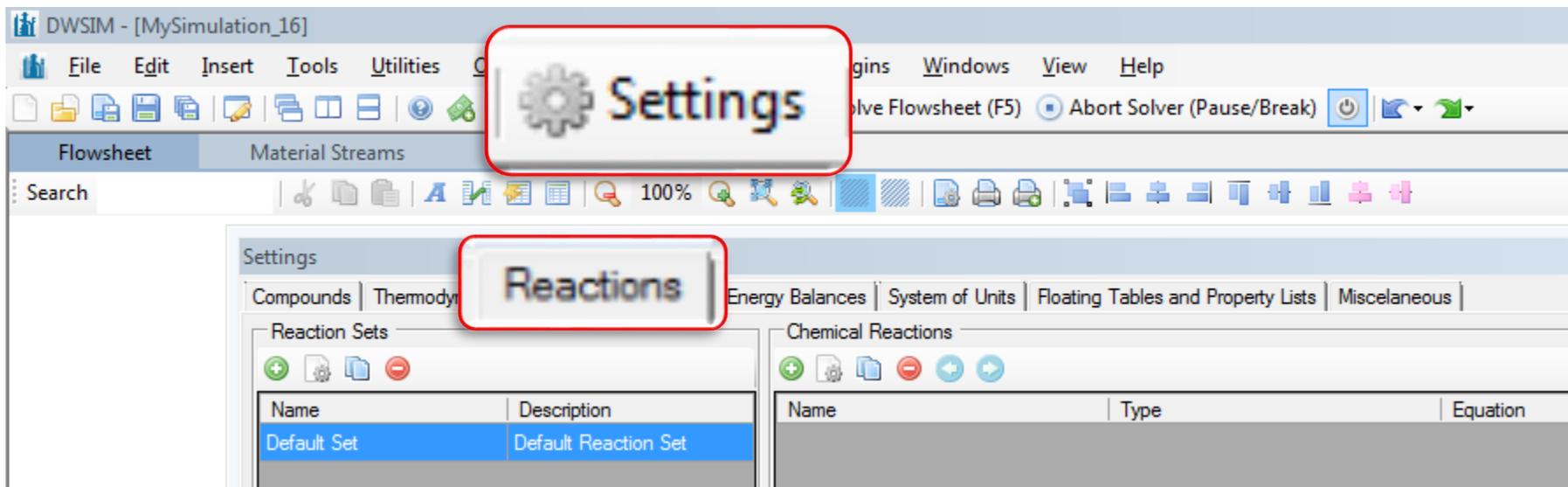
Conversión (*Conversion*): Se definen por la cantidad de un compuesto básico que se consume en la reacción. Esta cantidad puede ser un valor fijo o una función de la temperatura del sistema. Son soportadas por el reactor de Conversión.

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).

The screenshot shows two panels. The 'Reaction Sets' panel on the left has a toolbar with a green plus icon, a gear icon, a blue folder icon, and a red minus icon. Below the toolbar is a table with two columns: 'Name' and 'Description'. The first row is highlighted in blue and contains the text 'Default Set' and 'Default Reaction Set'. The 'Chemical Reactions' panel on the right has a toolbar with a green plus icon (circled in red), a gear icon, a blue folder icon, a red minus icon, and two blue arrow icons. Below the toolbar is a table with one column: 'Name'.

Name	Description
Default Set	Default Reaction Set

Name

The screenshot shows the 'Chemical Reactions' panel with a toolbar containing a green plus icon (circled in red), a gear icon, a blue folder icon, a red minus icon, and two blue arrow icons. Below the toolbar is a list of reaction types, each with a green icon and a text label:

- Conversion
- Equilibrium
- Kinetic
- Heterogeneous Catalytic

Conversión

Equilibrio

Cinética

Catalíticas heterogéneas

Reacciones de Conversión

Add New Conversion Reaction

Identification

Name

Description

Nombre y descripción

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.
Nitrogen	28,0134	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2,01588	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Ammonia	17,0305	-2695,04	<input type="checkbox"/>	<input type="checkbox"/>	0

Compuestos incluidos en la reacción

Stoichiometry

0

Balance

Heat of Reaction (kJ/kmol_BC) (ΔH)

0

Equatio

Conversion Reaction Parameters

Base Comp

Phase

Liquid

Conversion [%, f(T)] =

T in K

Use '.' as the decimal separator on the conversion expression.

Cancel

OK

Reacciones de Conversión

Add New Conversion Reaction

Identification

Name

Description

Coeficientes estequiométricos

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.
Nitrogen	28,0134	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2,01588	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Ammonia				<input type="checkbox"/>	0

Componente base de la reacción

Stoichiometry

0

Balance

Heat of Reaction (kJ/kmol_BC) (25

0

Equatio

Verifica la estequiometria

Conversion Re:

Base Comp

Phase Liquid

Conversion [%, f(T)] =

T in K

Use '.' as the decimal separator on the conversion expression.

Cancel

OK

Reacciones de Conversión

Add New Conversion Reaction

Identification

Name

Description

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.
Nitrogen	28,0134	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2,01588	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Ammonia	17,0305	-2695,04	<input type="checkbox"/>	<input type="checkbox"/>	1

Calor de reacción

Reacción

Balance

Heat of Reaction (kJ/kmol_BC) (25

0

Equatio

Fase de la reacción

Conversion Reaction Parameters

Base Comp

Phase Liquid

Conversion [%, $f(T)$ =

T in K

% de conversión en función de la temperatura

Cancel

OK

Ejemplos de Reacciones de Conversión



Add New Conversion Reaction ✕

Identification

Name

Description

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.
Nitrogen	28,0134	0	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2,01588	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-3
Ammonia	17,0305	-2695,04	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2

Stoichiometry Heat of Reaction (kJ/kmol_BC) (25)

Equatio

Conversion Reaction Parameters

Base Comp Phase

Conversion [%, f(T)] = T in K

Use '.' as the decimal separator on the conversion expression.

Ejemplos de Reacciones de Conversión



Add New Conversion Reaction

Identification

Name: Methane Combustion

Description:

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Methane	16.043	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Carbon dioxide	44.0095	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Water	18.015	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Oxygen	31.999	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-2
Nitrogen	28.014	<input type="checkbox"/>	<input type="checkbox"/>	0

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC) (25 °C): -802618

Equation: CH4 + 2O2 -> CO2 + 2H2O

Conversion Reaction Parameters

Base Comp: Methane Phase: Vapor

Conversion [%, f(T)] = 100 T in K

Use '.' as the decimal separator on the conversion expression.

Cancel OK

Include



El N₂ no interviene en la reacción.



Suele aparecer porque se utiliza aire para la combustión.

Reacciones de Equilibrio

Edit Equilibrium Reaction

Identification

Name: Butane Isomeration

Description:

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
N-butane	58.123	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Isobutane	58.123	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Equilibrium Reaction Parameters

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

Approach (%): 0

Equilibrium Constant (Keq)

Calculate from Gibbs Energy of Reaction ΔG_R (kJ/kmol_BC) (25°C): -4740

T-Function.: $\ln Keq [f(T)] =$ T in K

Constant Value: 0

Forma de calculo de la Keq

Use '.' as the decimal separator on math expressions.

Cancel OK

Ejemplos de Reacciones de Equilibrio

Edit Equilibrium Reaction

Identification

Name Ammonia Gibbs

Description $3H_2 + N_2 \rightleftharpoons 2NH_3$

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Ammonia	17.031	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Nitrogen	28.014	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2.01588	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-3

Stoichiometry 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.

Ejemplos de Reacciones de Equilibrio

Edit Equilibrium Reaction

Identification

Name

Description

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
N-butane	58.123	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Isobutane	58.123	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Stoichiometry Heat of Reaction (kJ/kmol_BC) (25°C)

Equation

Equilibrium Reaction Parameters

Basis Phase Tmin (K) Tmax (K)

Approach (%)

Equilibrium Constant (Keq)

Calculate from Gibbs Energy of Reaction

T-Function.: $\ln Keq [f(T)] =$ T in K

Constant Value

Use '.' as the decimal separator on math expressions.

Reacciones de Cinética

Add New Kinetic Reaction

Identification

Name

Descriptio

Orden de reacción (directo e inverso)

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Methyl acetate	74.0785	-5560.31	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Methanol	32.0419	-6271.17	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	1
1-butanol	74.1216	-3704.72	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1	1	0
N-butyl acetate	116.158	-4180.5	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	1

Stoichiometry Balance Heat of Reaction (kJ/kmol_BC)

Equation

Kinetic Reaction Parameters

Parámetros de Arrhenius

concentrations

Tmin (K)

Tmax (K)

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)

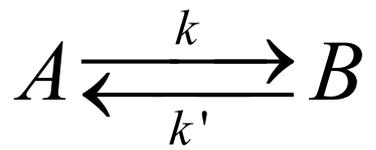
Reverse Reaction Arrhenius A' E' E in J/mol, T in K

User-Defined: f(T)

Amount Units Velocity Units

Cancel OK

DO	RO
1	0
0	1
1	0
0	1



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

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

Ejemplos de Reacciones de Cinética

Add New Kinetic Reaction

Identification

Name

Description

$$MeAc + BuOH \rightleftharpoons MeOH + BuAc$$

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Methyl acetate	74.0785	-5560.31	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Methanol	32.0419	-6271.17	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	1
1-butanol	74.1216	-3704.72	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1	1	0
N-butyl acetate	116.158	-4180.5	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	1

Stoichiometry Heat of Reaction (kJ/kmol_BC)

Equation

Kinetic Reaction Parameters

Base Component Basis Tmin (K)

Phase Tmax (K)

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' E' E in J/mol, T in K

User-Defined: f(T)

Amount Units Velocity Units

Ejemplos de Reacciones de Cinética

Edit Kinetic Reaction

Identification

Name: Styrene

Description: $C_6H_5 - C_2H_5 \Leftrightarrow C_6H_5 - C_2H = CH_2 + H_2$

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylbenzene	106.167	281.82015	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Styrene	104.149	1415.28	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	0
Hydrogen	2.01588	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	0

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC): 117480

Equation: $(C_6H_5)CH_2CH_3 \leftrightarrow (C_6H_5)CHCH_2 + H_2$

Kinetic Reaction Parameters

Base Component: Ethylbenzene

Basis: Partial Pressures Tmin (K): 0

Phase: Vapor Tmax (K): 3500

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

Direct Reaction: Arrhenius A: 4240 E: 90826 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: kPa Velocity Units: mol/[L.s]

Cancel OK

Reacciones Heterogéneas Catalíticas

Heterogeneous Catalytic Reaction

Identification

Name: MeOH Dehydration

Description:

Components and Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	SC
Methanol	32.042	-6271.1441	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-2
Water	18.015	-13422.925	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Dimethyl ether	46.069	-3996.1796	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC): -12017

Equation: $2\text{CH}_3\text{OH} \leftrightarrow \text{HOH} + \text{CH}_3\text{OCH}_3$ Base Component: Methanol

Heterogeneous Kinetic Reaction Parameters

Basis: Molar Fractions Phase: Vapor Tmin (K): 0 Tmax (K): 3500

Reaction Rate (Base Component) = Numerator / Denominator

Numerator: $1200000000 \cdot \exp(-8 - 9680/T) \cdot (R1 - P2 \cdot P1/R1 / \exp(-2.8086 + 3061/T))$

Denominator: 1

Expression Variables: Temperature (T) in K, reactant amounts (R1, R2, ..., Rn) and product amounts (P1, P2, ..., Pn) in the selected amount unit, reaction rate (r) in the selected velocity unit.

Amount Unit: Velocity Unit: mol/[kg.s]

Use '.' as the decimal separator on math expressions.

Cancel OK

Ley funcional de la velocidad de reacción

Las variables son:

T

R_1, R_2, \dots, R_n

P_1, P_2, \dots, P_n

Reacciones Heterogéneas Catalíticas

Heterogeneous Catalytic Reaction [X]

Identification

Name:

Description: $2CH_3OH \rightleftharpoons H_2O + CH_3OCH_3$

Components and Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	SC
Methanol	32.042	-6271.1441	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-2
Water	18.015	-13422.925	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Dimethyl ether	46.069	-3996.1796	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Stoichiometry: Heat of Reaction (kJ/kmol_BC):

Equation: Base Component:

Heterogeneous Kinetic Reaction Parameters

Basis: Phase: Tmin (K): Tmax (K):

Reaction Rate (Base Component) = Numerator / Denominator

Numerator:

Denominator:

Expression Variables: Temperature (T) in K, reactant amounts (R1, R2, ..., Rn) and product amounts (P1, P2, ..., Pn) in the selected amount unit, reaction rate (r) in the selected velocity unit.

Amount Unit: Velocity Unit:

Use '.' as the decimal separator on math expressions.

Reacciones Heterogéneas Catalíticas

Heterogeneous Catalytic Reaction

Identification

Name: Water Gas Shift

Description:

$$H_2O + CO \rightleftharpoons H_2 + CO_2$$

Components and Stoichiometry

Name	Molar Weight	Include	BC	SC
Methane	16.043	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2.01588	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Water	18.015	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1
Carbon dioxide	44.0095	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Carbon monoxide	28.01	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC): -41166.0

Equation: HOH + CO <-> H2 + OCO Base Component: Carbon monoxide

Heterogeneous Kinetic Reaction Parameters

Basis: Partial Pressures Phase: Vapor Tmin (K): 0 Tmax (K): 2000

Reaction Rate (Base Component) = Numerator / Denominator

Numerator: $1.96E+6 \cdot \exp(-67130/8.314/T) / P1 \cdot (R1 \cdot R2 \cdot P1 \cdot P2 / (\exp(-3.798+4160/T)))$

Denominator: $(1 + 1.77E+5 \cdot \exp(-88680/8.314/T) \cdot R1 / P1 + 6.12E-9 \cdot \exp(82900/8.314/T) \cdot P1 + 8.23E-5 \cdot \exp(70650/8.314/T) \cdot P1 \cdot P2)$

Expression Variables: Temperature (T) in K, reactant amounts (R1, R2, ..., Rn) and product amounts (P1, P2, ..., Pn) in the selected amount unit, reaction rate (r) in the selected velocity unit.

Amount Unit: atm Velocity Unit: kmol/[kg.h]

Use '.' as the decimal separator on math expressions.

Cancel OK

Reacciones Heterogéneas Catalíticas

Heterogeneous Catalytic Reaction

Identification

Name: Steam Reforming

Description:

$$CH_4 + H_2O \rightleftharpoons 3H_2 + CO$$

Components and Stoichiometry

Name	Molar Weight	Include	BC	SC
Methane	16.043	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2.01588	<input checked="" type="checkbox"/>	<input type="checkbox"/>	3
Water	18.015	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1
Carbon dioxide	44.0095	<input type="checkbox"/>	<input type="checkbox"/>	0
Carbon monoxide	28.01	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC): 205804.0

Equation: CH4 + HOH <-> 3H2 + CO Base Component: Methane

Heterogeneous Kinetic Reaction Parameters

Basis: Partial Pressures Phase: Vapor Tmin (K): 0 Tmax (K): 2000

Reaction Rate (Base Component) = Numerator / Denominator

Numerator: $4.22E+15 \cdot \exp(-240100/8.314/T) / P1^{2.5} \cdot (R1 \cdot R2 \cdot P1^3 \cdot P2 / (\exp(30.42 - 27106/T)))$

Denominator: $(1 + 8.23E-5 \cdot \exp(70650/8.314/T) \cdot P2 + 6.65E-4 \cdot \exp(38280/8.314/T) \cdot R1 + 1.77E+5 \cdot \exp(-88680/8.314/T))$

Expression Variables: Temperature (T) in K, reactant amounts (R1, R2, ..., Rn) and product amounts (P1, P2, ..., Pn) in the selected amount unit, reaction rate (r) in the selected velocity unit.

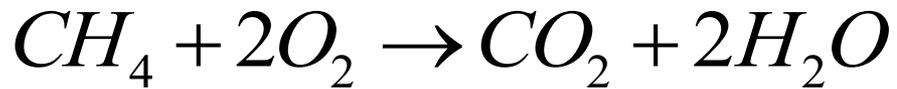
Amount Unit: atm Velocity Unit: kmol/[kg.h]

Use '.' as the decimal separator on math expressions.

Cancel OK

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.



The image shows a software interface for configuring a chemical reaction model. It consists of three main windows:

- Added Property Packages:** A table with columns 'Added' and 'Name'. The 'Name' column lists Methane, Oxygen, Nitrogen, Water, and Carbon dioxide, all with checked boxes in the 'Added' column.
- Added Property Packages (Detail):** A window showing a table with columns 'Name' and 'Type'. The entry 'Raoult's Law (1)' is selected, with 'Raoult's Law' in the 'Type' column.
- Chemical Reactions:** A window with a toolbar and a list of reaction models. The 'Conversion' model is selected and highlighted with a red box.

Red arrows indicate the flow of configuration: from the 'Added' column of the first table to the 'Added Property Packages' window, and from the 'Raoult's Law (1)' entry to the 'Conversion' model in the 'Chemical Reactions' window.

Reacción de combustión del metano

Edit Conversion Reaction ✕

Identification

Name

Description

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Methane	16.043	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Oxygen	31.999	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-2
Nitrogen	28.014	<input type="checkbox"/>	<input type="checkbox"/>	0
Water	18.015	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Carbon dioxide	44.0095	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1

Stoichiometry Heat of Reaction (kJ/kmol_BC) (25 °C)

Equation

Conversion Reaction Parameters

Base Comp Phase

Conversion [%, f(T)] = T in K

Use '.' as the decimal separator on the conversion expression.

Corriente de combustible

Input Data | Results | Annotations | Floating Tables

Stream Conditions | Compound Amounts

Flash Spec

Temperature K

Pressure Pa

Mass Flow kg/s

Molar Flow mol/s

Volumetric Flow m³/s

Specific Enthalpy kJ/kg

Specific Entropy kJ/[kg.K]

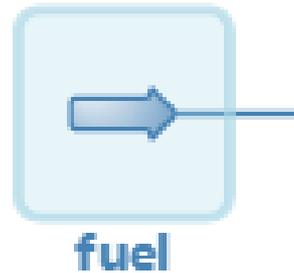
Vapor Phase Mole Fraction

Stream Conditions | Compound Amounts

Basis

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

Pressure

Mass Flow

Molar Flow

Volumetric Flow

Specific Enthalpy

Specific Entropy

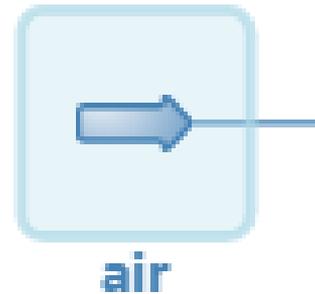
Vapor Phase Mole Fraction

Stream Conditions | Compound Amounts

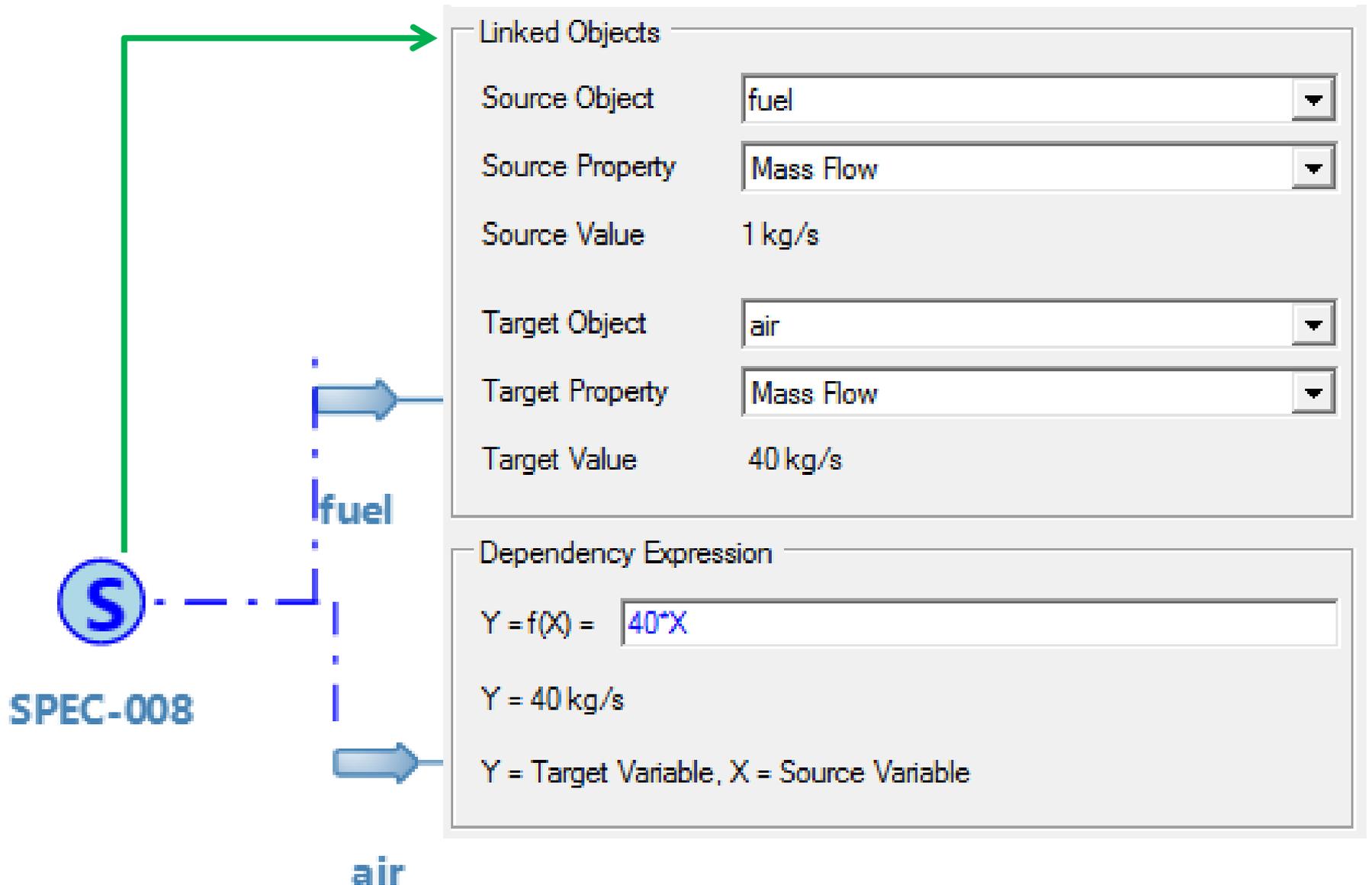
Basis

Solvent

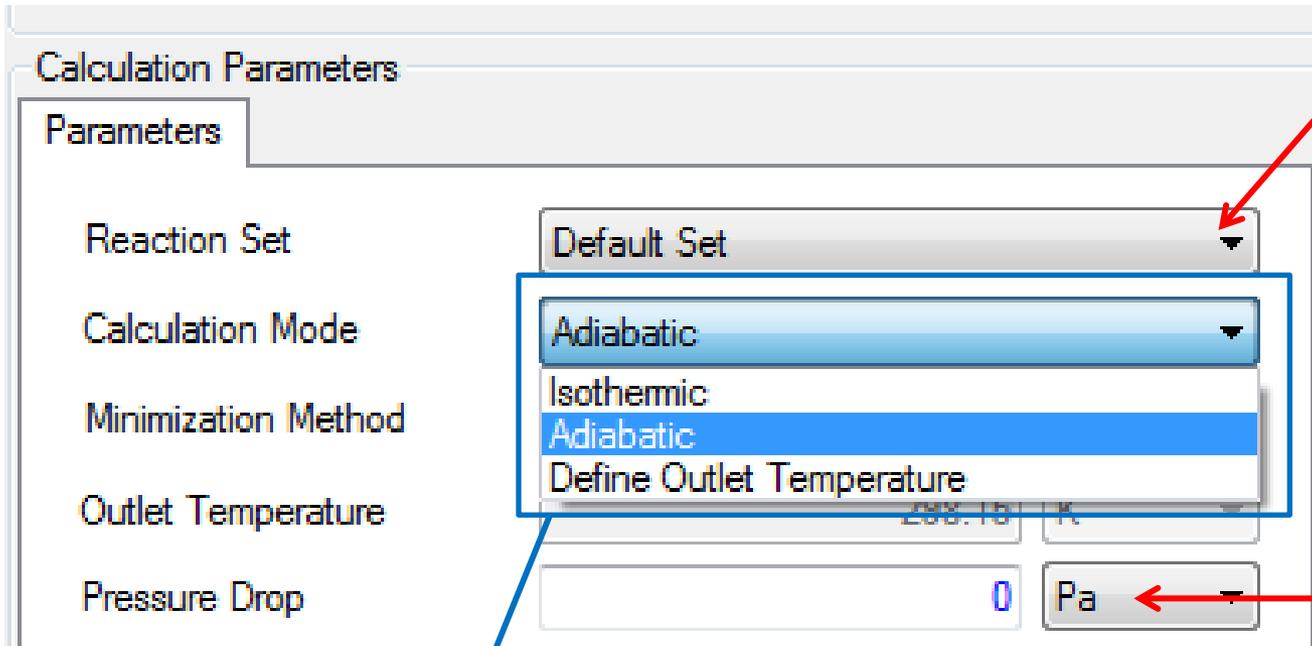
Compound	Amount
Methane	0
Oxygen	0.21
Nitrogen	0.79
Water	0
Carbon dioxide	0



Mezcla para ingresar al reactor



Reactor de conversión

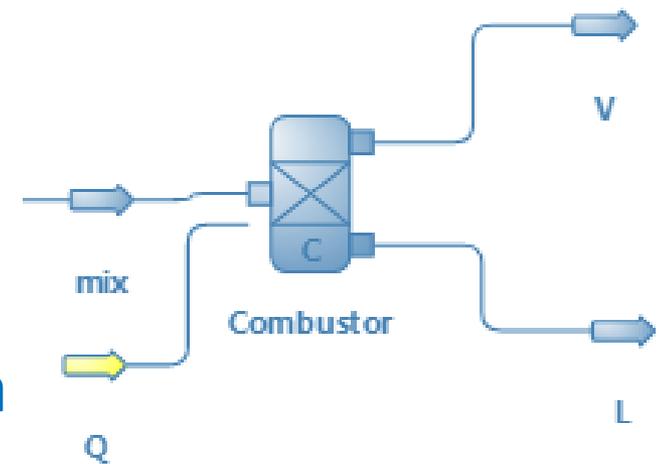


Paquete de reacciones que intervienen en el reactor

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

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

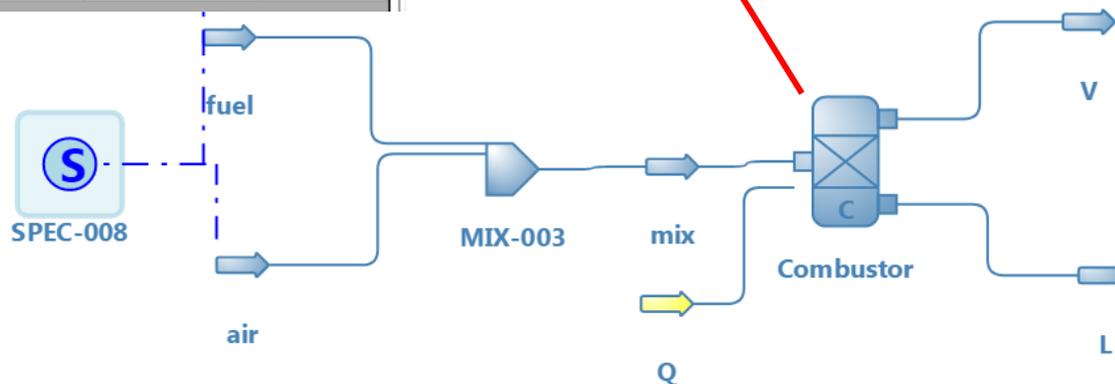
Results

General Reactions Conversions

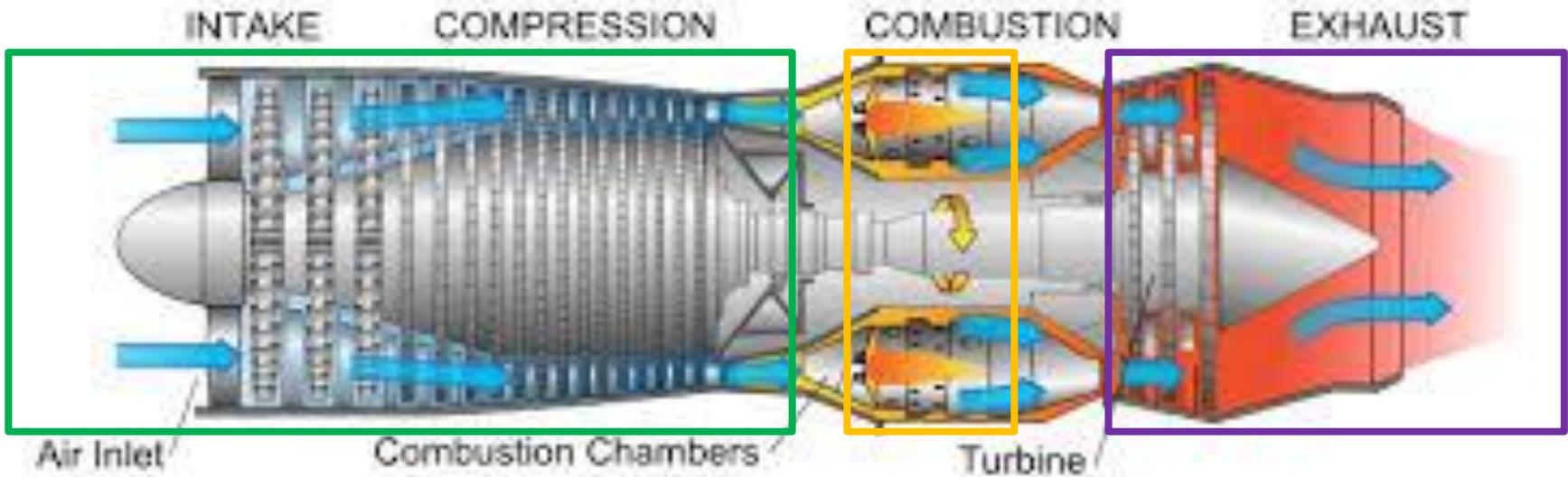
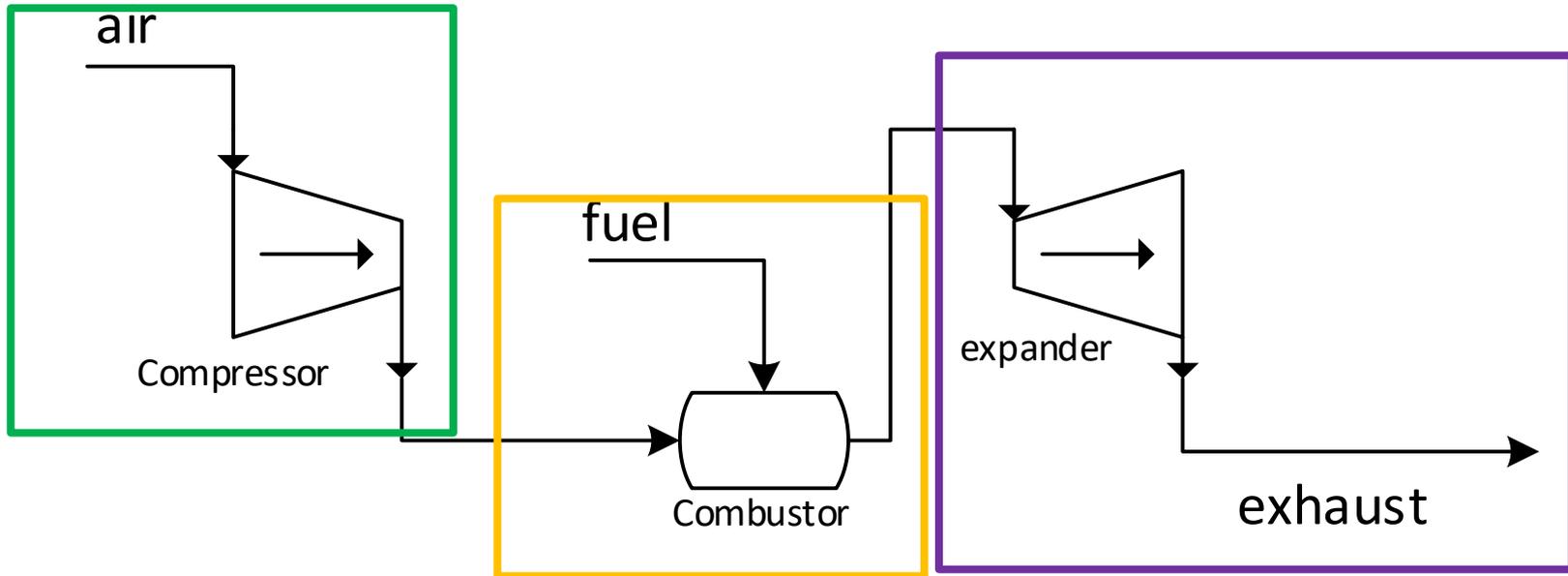
Property	Value	Units
Delta-T	1039.9984	K
Heat Load	0	kW

General Reactions Conversions

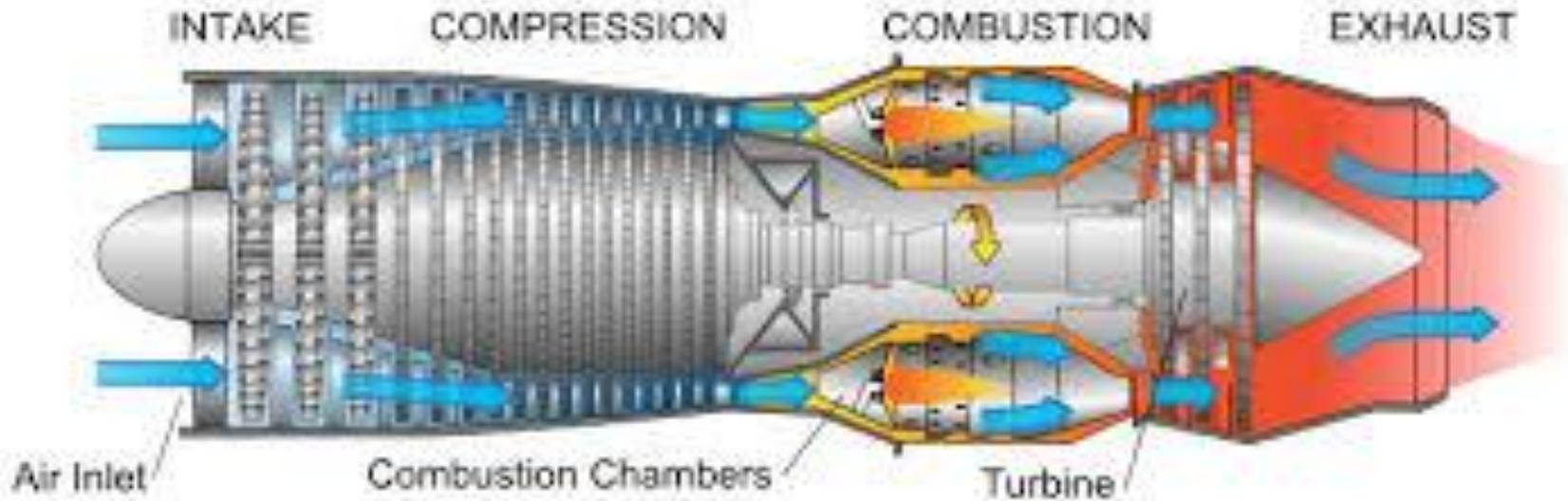
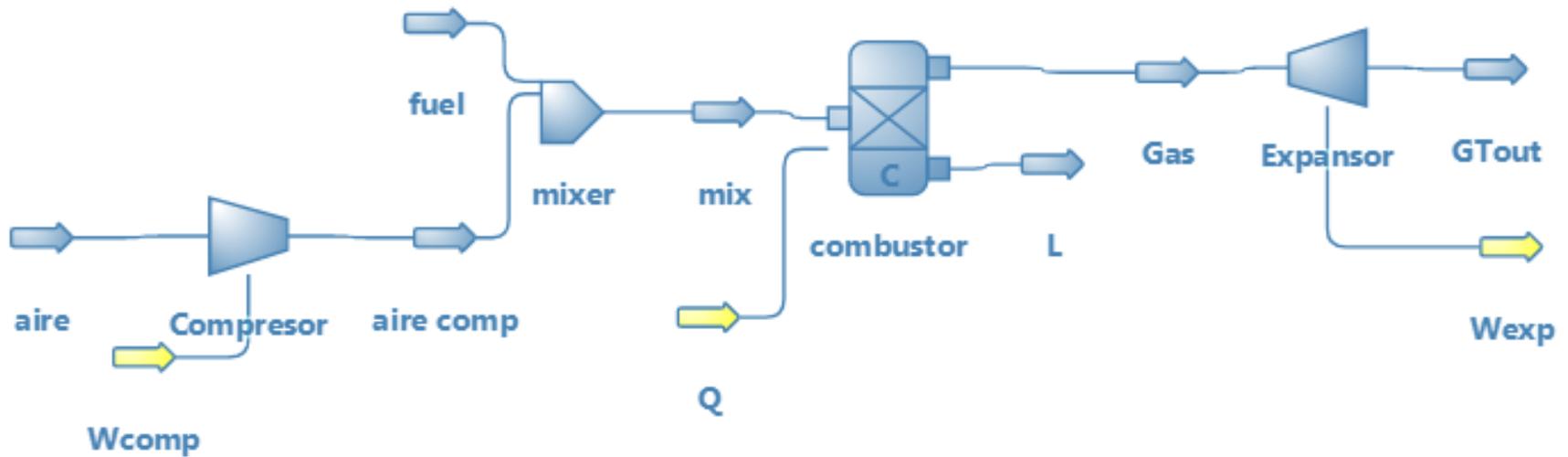
Reaction	Property	Value	Units
Metano Comb	Conversion	100	%



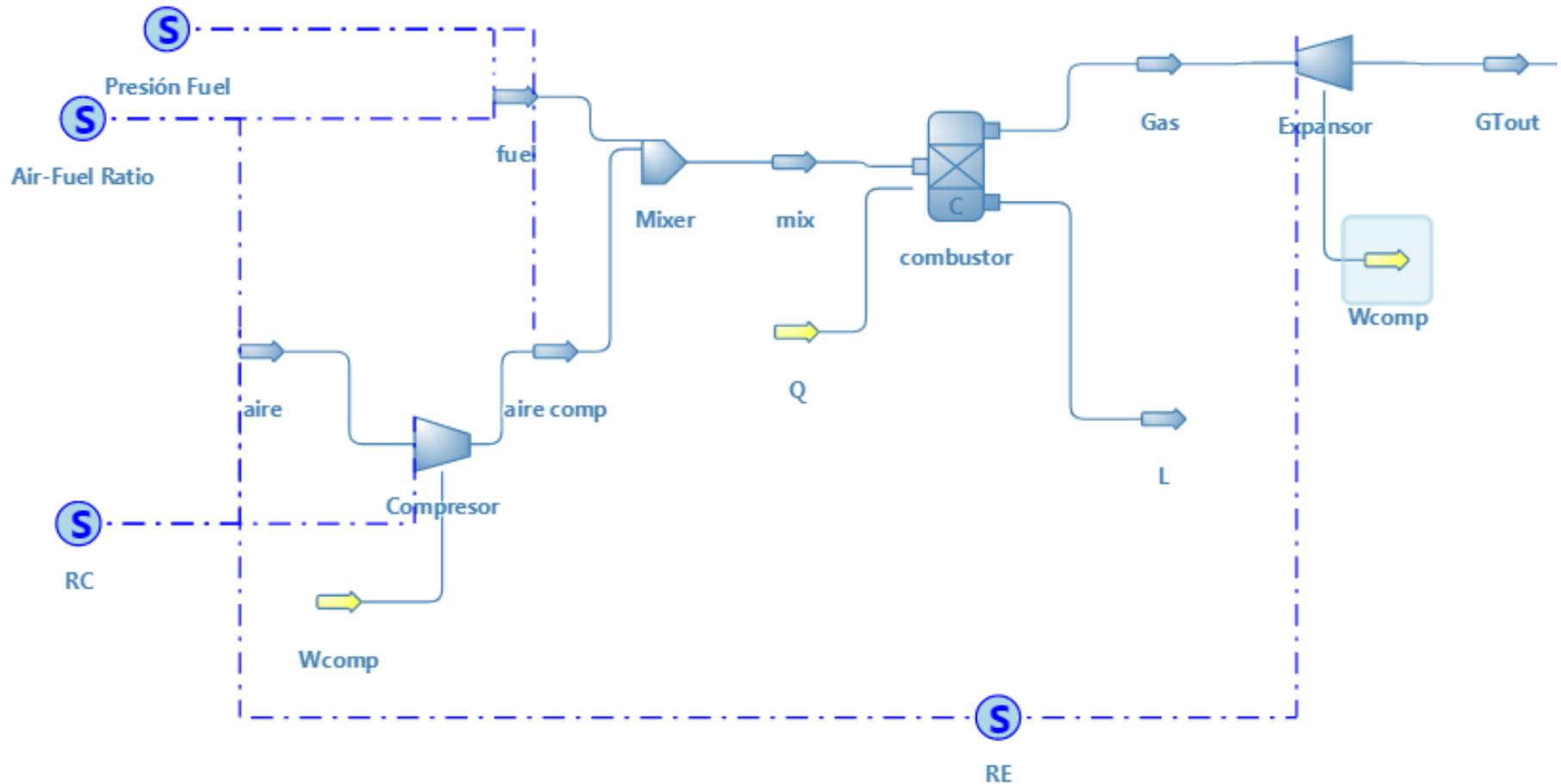
Ejemplo: Simulación de una turbina de Gas



Ejemplo: Simulación de una turbina de Gas



Ejemplo: Simulación de una turbina de Gas



Ejemplo: Reactor de equilibrio



Alimentación estequiométrica

Added	Name
<input checked="" type="checkbox"/>	Ammonia
<input checked="" type="checkbox"/>	Nitrogen
<input checked="" type="checkbox"/>	Hydrogen

Added Property Packages

Name (click to edit)	Type
Peng-Robinson (PR) (1)	Peng-Robinson (PR)

Chemical Reactions

<input checked="" type="checkbox"/>	Conversion
<input checked="" type="checkbox"/>	Equilibrium
<input checked="" type="checkbox"/>	Kinetic
<input checked="" type="checkbox"/>	Heterogeneous Catalytic

Reacción de equilibrio

Edit Equilibrium Reaction

Identification

Name: Ammonia Gibbs

Description:

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Ammonia	17.031	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Nitrogen	28.014	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2.01588	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-3

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

Equation: $N_2 + 3H_2 \leftrightarrow 2NH_3$

Equilibrium Reaction Parameters

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

Approach (%): 0

Equilibrium Constant (Keq)

Calculate from Gibbs Energy of Reaction ΔG_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

Reactor de equilibrio 450 °C 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]

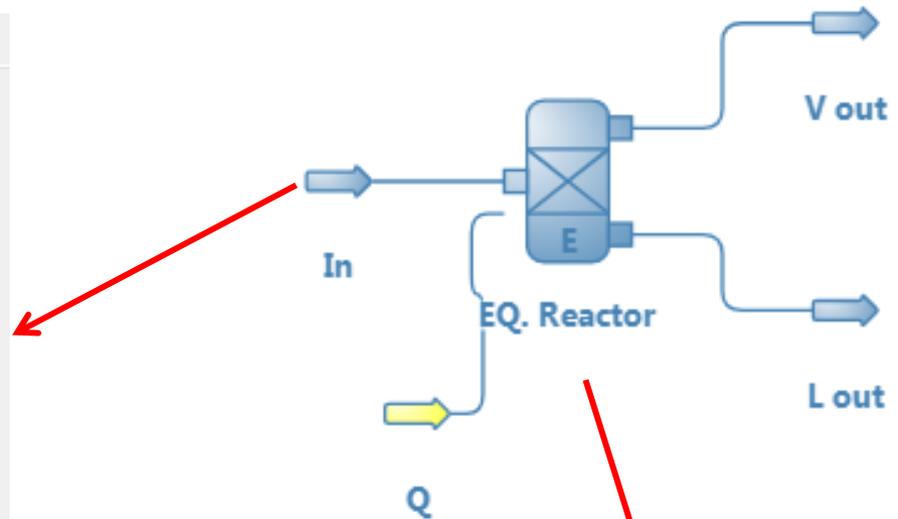
Vapor Phase Mole Fraction: 1

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

Calculation Parameters

Parameters **Compounds** Elements Initial Estimates Misc

Reaction Set Default Set

Calculation Mode Isothermic

Minimization Method Direct Gibbs Energy Minimization

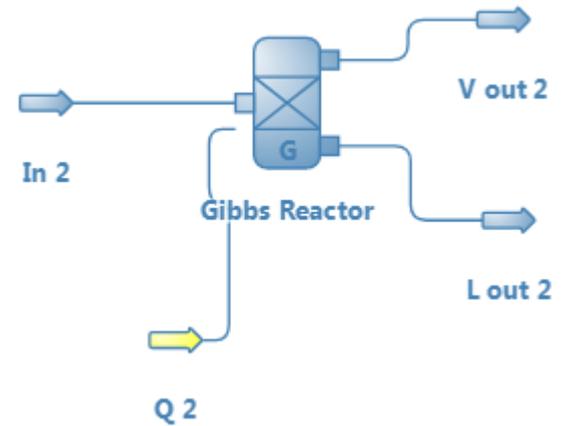
Outlet Temperature 298.15 K

Pressure Drop 0 Pa

Calculation Parameters

Parameters **Compounds** Elements Initial Estimates Misc

- Ammonia
- Nitrogen
- Hydrogen



Reactor de Gibbs

Calculation Parameters

Parameters

Compounds

Elements

Initial Estimates

Misc

Configuration

Add Element

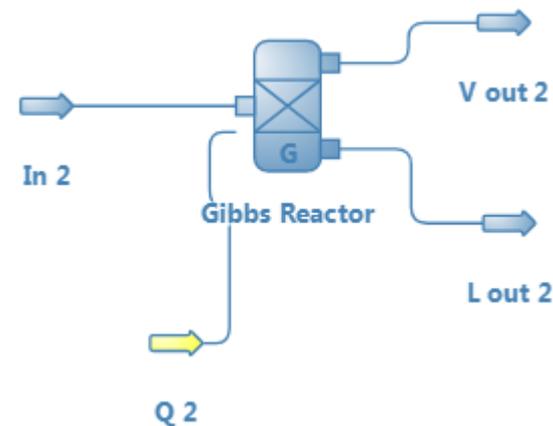
Remove Selected Element

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

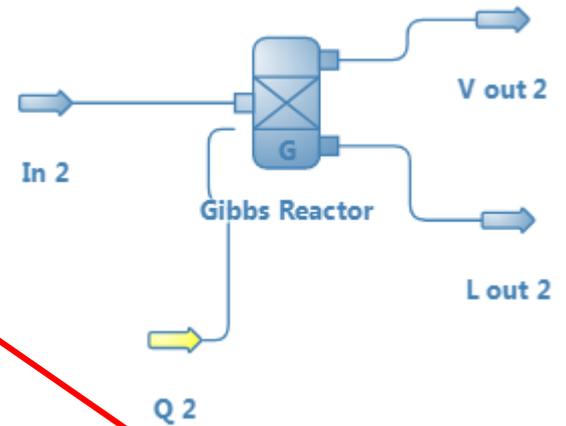
Configuration

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

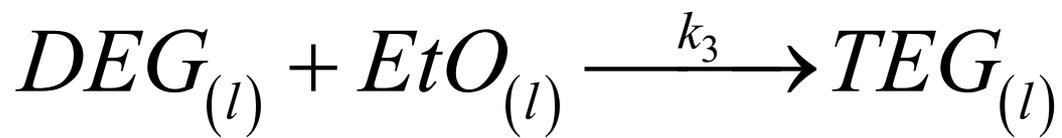
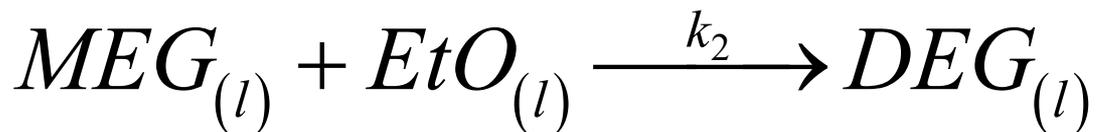
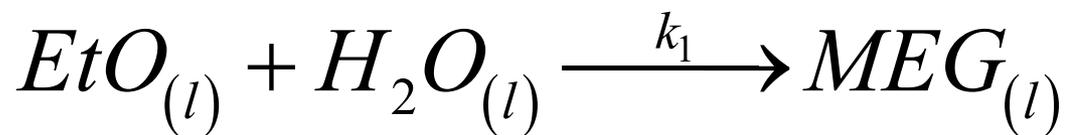
Max. Internal Loop Iterations 20000

Max. External Loop Iterations 50

Internal Loop Tolerance 1E-06

External Loop Tolerance 0.001

Ejemplo: Reactor CSTR y PFR



Added	Name
<input checked="" type="checkbox"/>	Ethylene oxide
<input checked="" type="checkbox"/>	Water
<input checked="" type="checkbox"/>	Ethylene glycol
<input checked="" type="checkbox"/>	Diethylene glycol
<input checked="" type="checkbox"/>	Triethylene glycol

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

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

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



A. Carrero, N. Quirante, J. Javaloyes
October 2016

Feed in

$x_{\text{water}}: 0.7$

$x_{\text{EtO}}: 0.3$

P: 20 atm

T: 100 °C

m: 100 mol/s

Ejemplo: Reactor CSTR y PFR



Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylene oxide	44.0526	-1194.7081	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>			
Water	18.015	-13422.925	<input checked="" type="checkbox"/>	<input type="checkbox"/>			
Ethylene glycol	62.0678	-6318.8964	<input checked="" type="checkbox"/>	<input type="checkbox"/>			
Diethylene glycol	106.12	-5148.8881	<input type="checkbox"/>	<input type="checkbox"/>			
Triethylene glycol	150.173	-4828.4312	<input type="checkbox"/>	<input type="checkbox"/>			

Kinetic Reaction Parameters

Base Component: Basis: T_{min} (K):
 Phase: T_{max} (K):

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': E': E in J/mol, T in K

User-Defined: f(T)

Amount Units: Velocity Units:

Ejemplo: Reactor CSTR y PFR



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

Kinetic Reaction Parameters

Base Component:

Basis:

Phase:

Tmin (K):

Tmax (K):

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': E': E in J/mol, T in K

User-Defined: f(T)

Amount Units:

Velocity Units:

Define las unidades de la expresión cinética

Ejemplo: Reactor CSTR y PFR



$$(-r_{EtO}) = k_1 C_{EtO} C_{H_2O} \quad k_1 \left[\begin{matrix} \text{?} \\ \text{?} \end{matrix} \right] \quad C_{EtO}; C_{H_2O} \left[\frac{mol}{m^3} \right]$$

$$k_1 = A_1 e^{-\frac{E_1}{RT}} \quad (-r_{EtO}) \left[\frac{mol}{m^3 s} \right]$$

Kinetic Reaction Parameters

Base Component:

Basis:

Phase:

Tmin (K):

Tmax (K):

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' E' E in J/mol, T in K

User-Defined: f(T)

Amount Units:

Velocity Units:

Ejemplo: Reactor CSTR y PFR



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

$$A_1 \left[\frac{m^3}{mol.s} \right] \quad E_1 \left[\frac{J}{mol} \right] \quad T [K]$$

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

Kinetic Reaction Parameters

Base Component:

Basis:

Phase:

Tmin (K):

Tmax (K):

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' E' E in J/mol, T in K

User-Defined: f(T)

Amount Units:

Velocity Units:

Ejemplo: Reactor CSTR y PFR



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

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

$$k_1 = \frac{e^{13.62}}{60 \times 1000} e^{-\frac{E_1}{RT}} \left[\frac{m^3}{mol \cdot s} \right]$$

A_1

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

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

$$E_1 = 8220R$$

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

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

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

Ejemplo: Reactor CSTR y PFR

Chemical Reactions

Name
R1
R2
R3

Edit Kinetic Reaction

Identification

Name: R1

Descriptio:

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylene oxide	44.0526	-1194.7081	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Water	18.015	-13422.925	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1	1	0
Ethylene glycol	62.0678	-6318.8964	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	0
Diethylene glycol	106.12	-5148.8881	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0
Triethylene glycol	150.173	-4828.4312	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0

Stoichiometry: Heat of Reaction (kJ/kmol_BC): -97756

Equation: CH2OCH2 + HOH <=> HOCH2CH2OH

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: 13.706911 E: 68344.9598 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: mol/m³ Velocity Units: mol/[m³.s]

Ejemplo: Reactor CSTR y PFR

Chemical Reactions

+ - < >

Name

R1

R2

R3

Edit Kinetic Reaction

Identification

Name R2

Descriptio

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylene oxide	44.0526	-1194.7081	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1	1	0
Water	18.015	-13422.925	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0
Ethylene glycol	62.0678	-6318.8964	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Diethylene glycol	106.12	-5148.8881	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	0
Triethylene glycol	150.173	-4828.4312	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0

Stoichiometry Heat of Reaction (kJ/kmol_BC) -101570

Equation CH2OCH2 + HOCH2CH2OH <-> HOCH2CH2OCH2CH2OH

Kinetic Reaction Parameters

Base Component Ethylene glycol

Basis Molar Concentrations

Phase Liquid

Tmin (K) 0

Tmax (K) 3500

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

Direct Reaction Arrhenius A 96.3415952 E 72335.9064 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 mol/m3

Velocity Units mol/[m3.s]

Ejemplo: Reactor CSTR y PFR

Chemical Reactions

+ - + -

Name
R1
R2
R3

Edit Kinetic Reaction ✕

Identification

Name

Descriptio

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethylene oxide	44.0526	-1194.7081	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1	1	0
Water	18.015	-13422.925	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0
Ethylene glycol	62.0678	-6318.8964	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0
Diethylene glycol	106.12	-5148.8881	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1	1	0
Triethylene glycol	150.173	-4828.4312	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1	0	0

Stoichiometry Heat of Reaction (kJ/kmol_BC)

Equation

Kinetic Reaction Parameters

Base Component

Basis Tmin (K)

Phase Tmax (K)

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

Direct Reaction Arrhenius A E E in J/mol, T in K

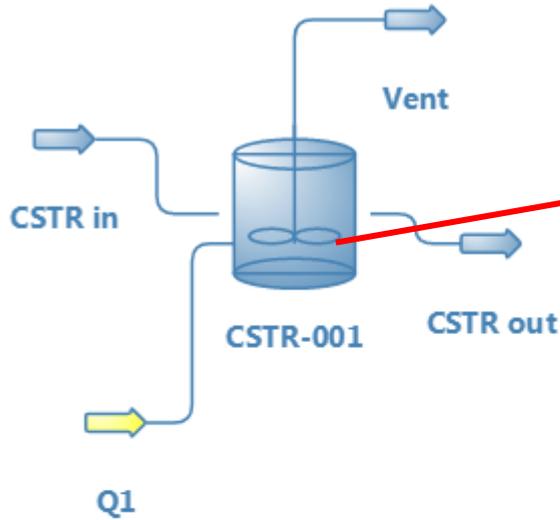
User-Defined: f(T)

Reverse Reaction Arrhenius A' E' E in J/mol, T in K

User-Defined: f(T)

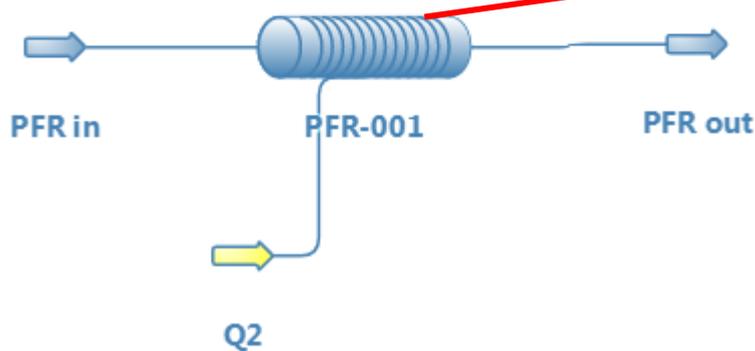
Amount Units Velocity Units

Ejemplo: Reactor CSTR y PFR



Calculation Parameters

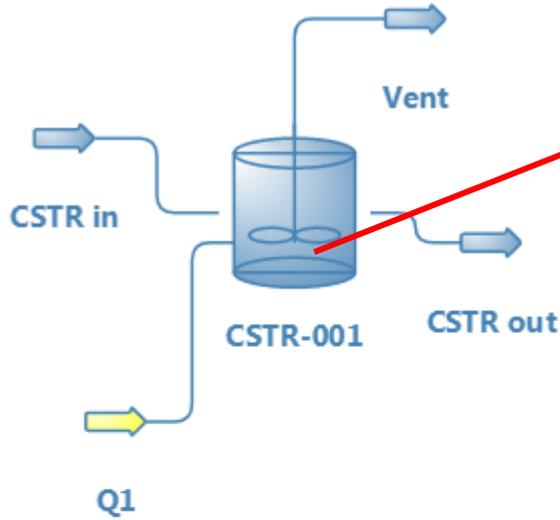
Reaction Set	Default Set	
Calculation Mode	Isothermic	
Outlet Temperature	25	C
Reactor Volume	4	m ³
Headspace	0	m ³
Reactor Pressure Drop	0	kgf/cm ²
Catalyst Amount	0	kg



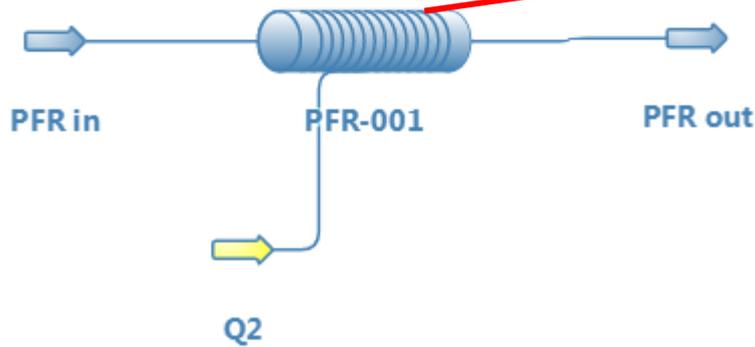
Calculation Parameters

Reaction Set	Default Set	
Calculation Mode	Isothermic	
Outlet Temperature	25	C
Reactor Volume	4	m ³
Reactor Length	10	m
Catalyst Loading	0	kg/m ³
Catalyst Particle Diameter	0	mm
Catalyst Void Fraction	0	

Ejemplo: Reactor CSTR y PFR

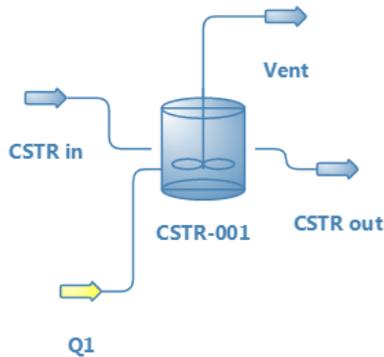


Results		
General	Reactions	Conversions
Compound	Conversion (%)	
Water	4.37499	
Ethylene oxide	11.0937	
Ethylene glycol	0	
Diethylene glycol	0	
Triethylene glycol	0	



Results			
General	Reactions	Conversions	Concentration Profile
Compound	Conversion (%)		
Water	4.72378		
Ethylene oxide	11.5431		

Análisis Paramétrico



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

Practico IV\2018\Practicos\R1 R2 y R3.dwg

Optimization

Scripts

Results



Sensitivity Analysis



Multivariate Optimizer

Flowsheet Material Streams Spreadsheet Sensitivity Analysis ×

Sensitivity Studies Independent Variables Dependent Variables Results Chart

Case Manager

New Copy Save Delete

Reactor

Name and Description

Name Reactor

Description

Análisis Paramétrico

Sensitivity Studies Independent Variables Dependent Variables Results Chart

Independent Variable 1

Object Property

Sensitivity Studies Independent Variables Dependent Variables Results Chart

Independent Variable 1

Object Property

Lower Limit Number of Points Unit

Upper Limit Current Value

Lower Limit Number of Points Unit

Upper Limit Current Value

Análisis Paramétrico

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

Variables Expression

Add/Remove Variables

	Object	Property	Unit
+			
-			

Expression Parameters

	Name	Object	Property	Value	Unit
+					
-					

Add/Remove Variables

+

-

	Object	Property	Unit
1	CSTR out	Molar Fraction (Mixture) / Ethylene gly...	
2	CSTR out	Molar Fraction (Mixture) / Diethylene gl...	
3	CSTR out	Molar Fraction (Mixture) / Triethylene glyc	

Expression

Expression

Verify

Clear

Curr. Value

Análisis Paramétrico

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

Start Sensitivity Analysis | Break Calculation

Results

IV 1

Sensitivity Studies | Independent Variables | Dependent Variables

Start Sensitivity Analysis | Break Calculation

Results

CSTR-004 - Volume (m3)	CSTR out - Molar Fraction (Mixture) / Triethylene glycol (0)		
21.4483	0.0875446		
23.0345	0.0903618		
24.6207	0.0931790		
46.8276	0.115784	0.0377844	0.0171016
48.4138	0.116817	0.0384375	0.0176084
50	0.117801	0.0390634	0.0181002

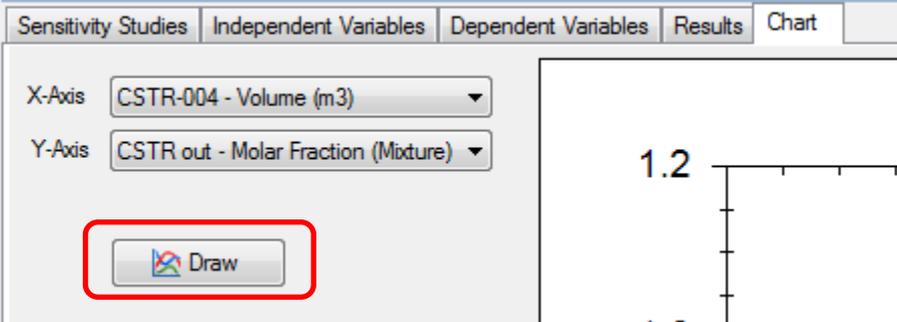
Information

Run #27 completed...
Run #28 completed...
Run #29 completed...
Run #30 completed...
Restoring simulation to its original state...
Done!

Information

Run #27 completed...
Run #28 completed...
Run #29 completed...
Run #30 completed...
Restoring simulation to its original state...
Done!

Análisis Paramétrico



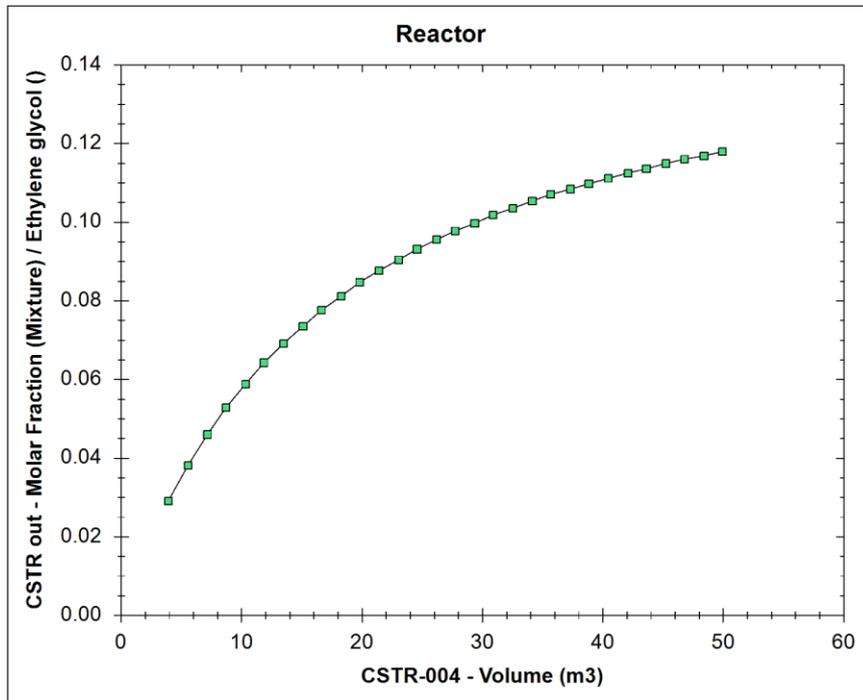
Sensitivity Studies | Independent Variables | Dependent Variables | Results | Chart

Start Sensitivity Analysis | Break Calculation | Send Data to Regression Plugin

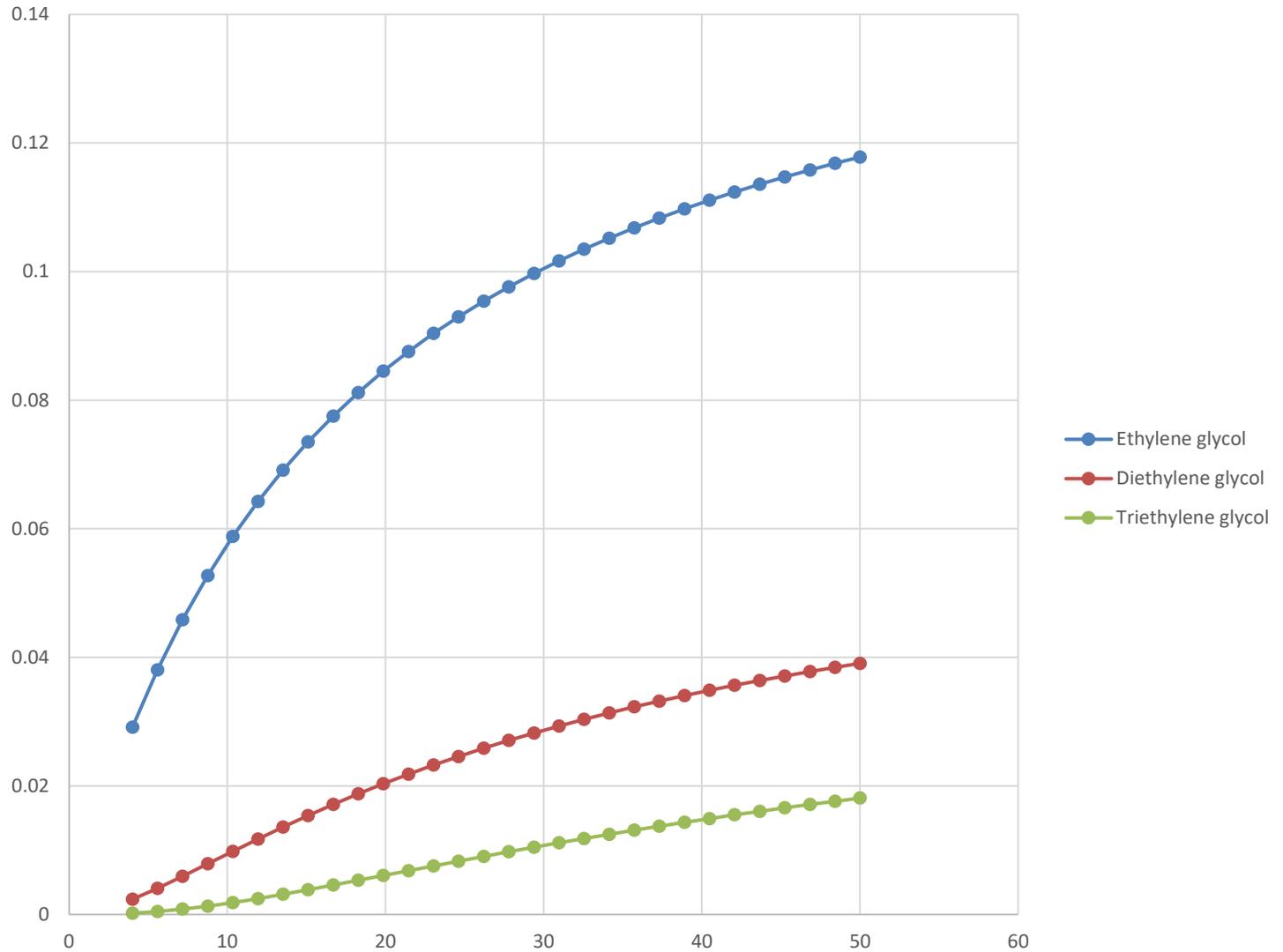
Results

CSTR-004 - Volume (m3)	CSTR out - Molar Fraction (Mixture) / Ethylene glycol ()	CSTR out - Molar Fraction (Mixture) / Diethylene glycol ()	CSTR out - Molar Fraction (Mixture) / Triethylene glycol ()
21.4483	0.0875446	0.0218151	0.0068089
23.0345	0.0903618	0.0232322	0.00755617
24.6207	0.092965	0.0245766	0.00828637
26.2069	0.0953788	0.0258547	0.00902711
27.7931	0.0976181	0.0270663	0.00974543
29.3793	0.0997051	0.02822	0.0104492

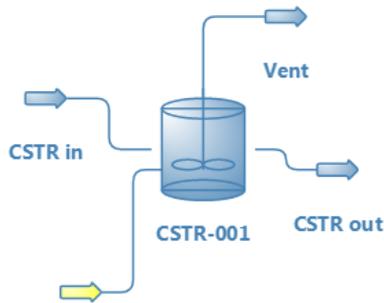
Copiamos los datos y los pegamos en Excel



Análisis Paramétrico



Análisis Paramétrico



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

O1
Sensitivity Studies

Independent Variables | Dependent Variables | Results | Chart

Case Manager

New | Copy | Save | Delete

Reactor
Conversión

Name and Description

Name: Conversión

Description:

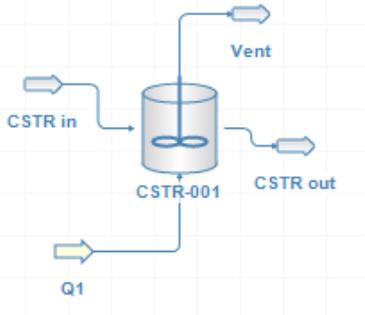
Independent Variable 1

Object: CSTR-004 | Property: Volume

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

Upper Limit: 150 | Current Value: 4

Análisis Paramétrico



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

The screenshot shows a software interface for sensitivity studies. The 'Variables' tab is active. A table lists the object 'CSTR-004' with a dropdown menu for selecting properties. The 'Expression' radio button is selected. The 'Expression Parameters' table is empty.

Object	Property	Unit
1	CSTR-004	

- Heat load
- Outlet Temperature
- Pressure Drop
- Residence time
- Temperature delta
- Volume

Name	Object
------	--------

¿Conversión?

$$x_{EtO} =$$

Análisis Paramétrico

Molar Flow (Mixture) / Ethylene Oxide

Expression

Expression Parameters

	Name	Object	Property	Value	Unit
1	F_in	CSTR in	Molar Flow (Mixture) / Ethylen...	30	mol/s
2	F_out	CSTR out	Molar Flow (Mixture) / Ethylen...	26.6719	mol/s

Variables del flowsheets que necesito para la expresión de la conversión

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

Moles consumidos de EtO
Moles alimentados de EtO

Análisis Paramétrico

Expression

Expression Parameters

	Name	Object	Property
1	F_in	CSTR in	Molar Flow (Mixture) / Ethylen...
2	F_out	CSTR out	Molar Flow (Mixture) / Ethylen...

Results

General Reactions Conversions

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

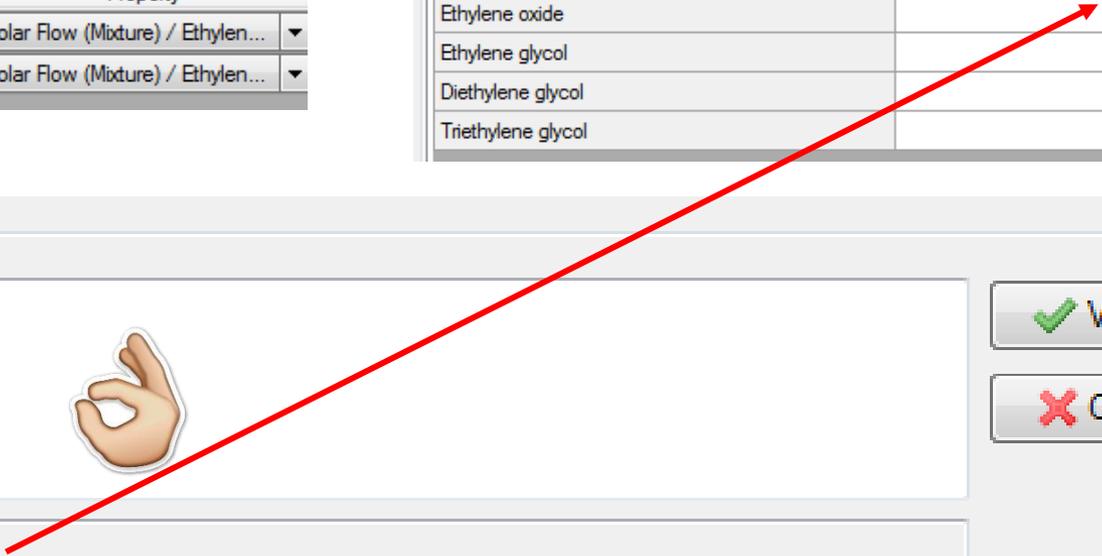
Expression

Expression (F_in-F_out)/F_in

Cur. Value 0.110936666666667

Verify

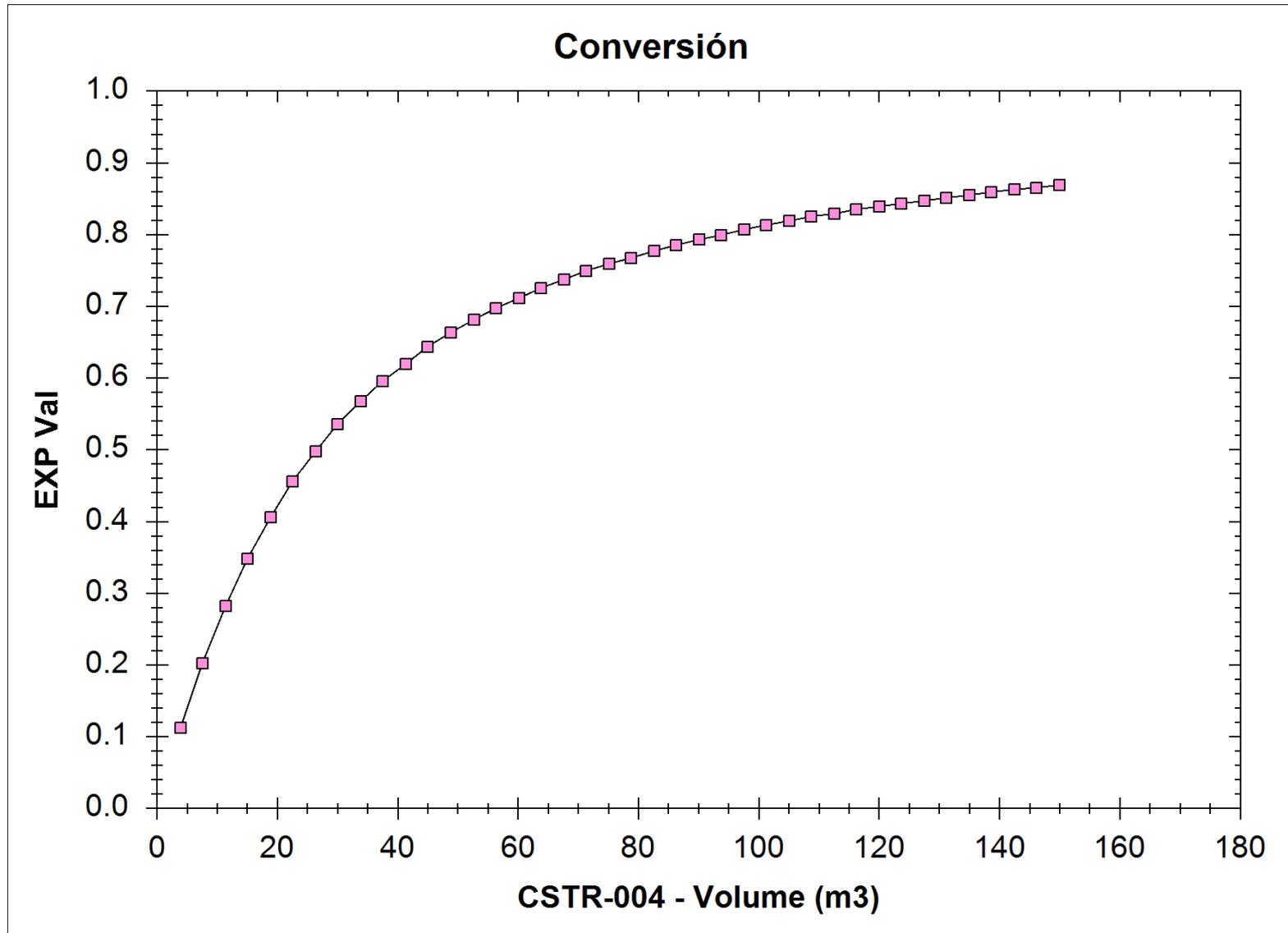
Clear



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

Moles consumidos de EtO
Moles alimentados de EtO

Análisis Paramétrico



Estudio paramétrico del reactor de equilibrio



Edit Equilibrium Reaction

Identification
Name: Ammonia Gibbs
Description:

Components/Stoichiometry

Name	Molar Weight	Include	BC	Stoich. Coeff.
Ammonia	17.031	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Nitrogen	28.014	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2.01588	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-3

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

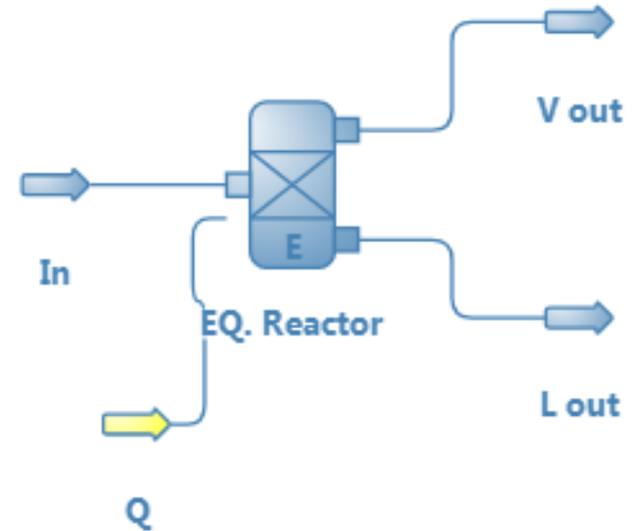
Equation: N2 + 3H2 <-> 2NH3

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

Independent Variable 1

Object Property

Lower Limit Number of Points Unit

Upper Limit Current Value

Independent Variable 2

Object Property

Lower Limit Number of Points Unit

Upper Limit Current Value

Expression

Expression Parameters

	Name	Object	Property	Value	Unit
	F_in	<input type="text" value="In"/>	<input type="text" value="Molar Flow (Mixture) / Nitro..."/>	2.5	mol/s
▶ 2	F_out	<input type="text" value="V out"/>	<input type="text" value="Molar Flow (Mixture) / Nitro..."/>	1.2295156	mol/s

Expression

Expression

Verify

Clear

Curr. Value

Estudio paramétrico del reactor de equilibrio

Start Sensitivity Analysis			Break Calculation			Send Data to Regression Plugin		
Results								
In - Pressure (bar)		In - Temperature (C)		EXP Val				
100		350		0.55717001				
100		372.22222		0.49019011				
100		394.44444		0.42547633				
100		416.66667		0.36498595				
100		438.88889		0.31011832				
100		461.11111		0.26162601				
100		483.33333		0.2196862				
100		505.55556		0.18403593				
100		527.77778		0.15407368				
100		550		0.1291494				
350		350		0.79041341				
350		372.22222		0.74217784				
350		394.44444		0.69053163				
350		416.66667		0.63659645				
350		438.88889		0.58162073				
350		461.11111		0.52686951				
350		483.33333		0.47355588				
350		505.55556		0.42267531				
350		527.77778		0.37506876				
350		550		0.33137416				
600		350		0.86866053				
600		372.22222		0.83209053				
600		394.44444		0.79125309				

Information

Run #27 completed...
Run #28 completed...
Run #29 completed...
Run #30 completed...
Restoring simulation to its original state...
Done!

Estudio paramétrico del reactor de equilibrio

