



UNIVERSIDADE FEDERAL DO RIO DE JANEIRO
ESCOLA DE QUÍMICA



EQE776 Modelagem e Simulação de Processos

Aula 06. Craqueamento a vapor do etano em DWSIM

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Recapitulando

- Dimensionamento de coluna desbutanizadora em Aspen Hysys

Temas da aula

- Craqueamento a vapor do etano em DWSIM

Apresentação do problema

O craqueamento a vapor consiste na quebra das moléculas de hidrocarbonetos saturados (etano, propano, etc.) para a obtenção de olefinas leves (eteno, propeno, etc.) na presença e vapor de água.

A reação acontece em fornos a altas temperaturas, sendo que o vapor de água é um inerte, utilizado somente para diminuir a pressão parcial dos compostos que participam na reação.

Será realizada uma simulação simplificada, utilizando um reator do tipo PFR e considerado apenas a reação de conversão do etano em eteno.

Apresentação do problema

Condições da corrente de alimentação de gás:

- Temperatura: 953 K
- Pressão: 303000 Pa
- Vazão: 100 mol/s
- Fração molar C_2H_6 : 1
- Fração molar de C_2H_4 : 0
- Fração molar de H_2 : 0,00
- Fração molar de H_2O : 0

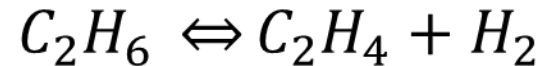
Apresentação do problema

Condições da corrente de alimentação de vapor:

- Temperatura: 953 K
- Pressão: 303000 Pa
- Vazão: 60% da vazão molar de gás
- Fração molar C_2H_6 : 0
- Fração molar de C_2H_4 : 0
- Fração molar de H_2 : 0,00
- Fração molar de H_2O : 1

Apresentação do problema

Informações da reação química:



Cujas taxas de reação ($\text{mol.m}^{-3}.\text{s}^{-1}$) direta e inversa dependem da concentração (mol. m^{-3}) segundo :

$$r_d = k_d C_{C_2H_6}$$

$$r_i = k_i C_{C_2H_4} C_{H_2}$$

Sendo que k obedece a equação de Arrhenius:

$$k = k_0 e^{\left(-\frac{Ea}{RT}\right)}$$

Com:

$$k_{d0} = 8,65E14; k_{i0} = 2,25E13; Ea = 273000 \text{ J/mol}$$

Apresentação do problema

Informações do reator:

- Reator tubular do tipo PFR
- Operação isotérmica
- Volume efetivo: 5 m³
- Comprimento do reator: 100 m

Apresentação do problema

Realize a simulação desse processo e responda:

- Qual será a conversão da reação?
- Quanta energia será necessária retirar do reator para manter a operação isotérmica?
- Troque o tipo de operação para adiabática e verifique qual o novo valor da conversão? Explique esse comportamento.
- Retome a operação isotérmica e realize uma análise de sensibilidade da conversão em função da vazão de gás. Utilize uma faixa de 10 a 100 mol/s de gás. Explique o comportamento encontrado.
- Proponha outras formas de aumentar a conversão.

Simulação em DWSIM

Criar novo caso

The screenshot displays the DWSIM software interface. The top menu bar includes File, Edit, Tools, Windows, View, and Help. A toolbar below the menu contains icons for file operations and a language dropdown set to Portuguese. The main content area is titled 'Welcome to DWSIM!' and features several sections: 'Process Modeling' (highlighted with a red box), 'Discover DWSIM Pro', 'Free Simulate 365 Dashboard for DWSIM', 'User Compound Creation / Data Regression', 'Support/Sponsor', and 'Documentation'. The 'Process Modeling' section includes the text 'Create or load chemical steady-state or dynamic process models.' and three links: 'Create New', 'Load File', and 'Load File from Simulate 365 Dashboard'. The 'Recent Files' panel on the right lists several files, including 'Ethane cracker reactor.dwxmz', '23. Simulação do processo 3.dwxmz', '22. Reatores.dwxmz', 'Actividad_7.dwxmz', 'simulation_shortcut.dwxmz', '14. Simulação do Processo 1.dwxmz', '13. Separador de componentes e separador flash.dwxmz', and another 'simulation_shortcut.dwxmz'. The bottom status bar contains links for 'Get 20th Anniversary Kit', 'Support DWSIM development', 'One-Time Donation', 'Monthly Donation', and a Pix QR code.

DWSIM

File Edit Tools Windows View Help

Access DWSIM Pro Now

Log in with Simulate 365 account

Welcome to DWSIM!

Shortcuts

Process Modeling
Create or load chemical steady-state or dynamic process models.
[Create New](#) [Load File](#) [Load File from Simulate 365 Dashboard](#)

Discover DWSIM Pro
Find out how the commercial sibling of the open-source process simulator DWSIM opens up new opportunities for you and your projects.

DWSIM and DWSIM Pro Features Comparison

Free Simulate 365 Dashboard for DWSIM
Open and save your simulation files from DWSIM to Dashboard. Achieve greater transparency over your flowsheets with built-in version control and personalized tags.
[Get Started](#)

User Compound Creation / Data Regression
[Create New Data Regression Study](#) [Load Study from File](#) [Create New Compound](#) [Quick Create New Solid](#) [Create New \(with Wizard\)](#)

Support/Sponsor
Support/Sponsor open-source DWSIM development activities.
[Sponsor on GitHub](#) [BECOME A PATRON](#) [Buy me a coffee](#)

Documentation
[User Guide](#) [User Guide \(Pro\)](#) [Learning Resources](#) [View Publications](#) [API Documentation](#)

Recent Files Samples FOSSEE Flowsheets

- Ethane cracker reactor.dwxmz
- 23. Simulação do processo 3.dwxmz
- 22. Reatores.dwxmz
- Actividad_7.dwxmz
- simulation_shortcut.dwxmz
- 14. Simulação do Processo 1.dwxmz
- 13. Separador de componentes e separador flash.dwxmz
- simulation_shortcut.dwxmz

Get 20th Anniversary Kit Support DWSIM development: One-Time Donation Monthly Donation Pix (Brasil): 0f0c6cf5-2489-4d03-b7a8-3a5fd22498a2

Simulação em DWSIM

Especificação dos componentes

← Simulation Configuration Wizard

Compounds

- ✓ Introduction
- ▶ **Compounds**
- ▶ Property Packages
- ▶ System of Units
- ▶ Behavior
- ▶ Undo/Redo

Select the compounds that you want to add to the simulation. Use the textbox to search and select a compound in the list. Click "Next" to continue.

Added	Name	CAS Number	Formula	Source Database	CP
<input checked="" type="checkbox"/>	Ethane	74-84-0	CH ₃ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Hydrogen	1333-74-0	H ₂	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Ethylene	74-85-1	CH ₂ CH ₂	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Water	7732-18-5	HOH	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Methane	74-82-8	CH ₄	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-butane	106-97-8	CH ₃ (CH ₂) ₂ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-heptane	142-82-5	CH ₃ (CH ₂) ₅ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Propane	74-98-6	CH ₃ CH ₂ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-nonane	111-84-2	CH ₃ (CH ₂) ₇ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-decane	124-18-5	CH ₃ (CH ₂) ₈ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-pentane	109-66-0	CH ₃ (CH ₂) ₃ CH ₃	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	N-dodecane	112-40-3	CH ₃ (CH ₂) ₁₀ CH ₃	ChemSep	<input checked="" type="checkbox"/>

Search

Added Compounds

Next > Cancel

Simulação em DWSIM

Especificação do pacote termodinâmico

← Simulation Configuration Wizard

Property Packages

- ✓ Introduction
- ✓ Compounds
- ▶ **Property Packages**
- ▶ System of Units
- ▶ Behavior
- ▶ Undo/Redo

Select and Add the Property Packages that you want to use in your simulation. The first on the list will be used by default by all flowsheet objects. Click "Next" to continue.

Available Property Packages

Filter By: Most Popular

- ✓ Peng-Robinson (PR)
- ✓ Soave-Redlich-Kwong (SRK)
- ✓ Soave-Redlich-Kwong (SRK) Advanced
- ✓ CoolProp
- ✓ Extended CoolProp
- ✓ Raoult's Law
- ✓ ThermoC Bridge
- ✓ Peng-Robinson-Stryjek-Vera 2 (PRSV2-VL)
- ✓ Peng-Robinson / Lee-Kesler (PR/LK)
- ✓ REFPROP
- ✓ Peng-Robinson 1979 (PR79) for Polymers and...

Buttons: Add, Info, Selection Help

Added Property Packages

Name	Type
Peng-Robinson...	Peng-Robinson (PR)

Recommended packages are marked with a ✓, but you can use all available packages without restrictions.

Override Phase Equilibria calculation settings? ☐ Leave as default (SVLLE) ☒ VLE (faster) ☐ VLLE/LLE ☐ Do not calculate

Next > Cancel

Simulação em DWSIM

Especificação do sistema de unidades SI

← Simulation Configuration Wizard

System of Units

- ✓ Introduction
- ✓ Compounds
- ✓ Property Packages
- ▶ **System of Units**
- ▶ Behavior
- ▶ Undo/Redo

Select the desired System of Units for your simulation. You can change individual units by selecting a custom system (other than SI, CGS or ENG).
Click "Finish" to exit the wizard and start designing the simulation model.


System of Units: SI Clone Create New Set as Default

Property	Unit	Property	Unit
Temperature	K	Pressure	Pa
Mass Flow Rate	kg/s	Molar Flow Rate	mol/s
Volumetric flow rate	m ³ /s	Specific Enthalpy	kJ/kg
Specific Entropy	kJ/[kg.K]	Molecular Weight	kg/kmol
Density	kg/m ³	Surface Tension	N/m
Heat Capacity	kJ/[kg.K]	Thermal Conductivity	W/[m.K]
Kinematic Viscosity	m ² /s	Dynamic Viscosity	Pa.s
Temperature Difference	K	Pressure Difference	Pa
Length/Head	m	Energy Flow	kW
Time	s	Volume	m ³
Molar Volume	m ³ /kmol	Area	m ²
Diameter/Thickness	mm	Force	N
Acceleration	m/s ²	Heat Transfer Coefficient	W/[m ² .K]

Next > Cancel



Simulação em DWSIM

Corrente de gás


Gás (Material Stream) 

Information **Connections**

General Info


Object	Gás	
Status	Calculated (24/07/2025 15:50:35)	
Linked to		








Property Package Settings

Property Package Peng-Robinson (PR) (1) 

Input Data **Results** Annotations Dynamics Floating Tables

Stream Conditions **Compound Amounts**

Flash Spec Temperature and Pressure (TP) 

Temperature	953	K 
Pressure	303000	Pa 
Mass Flow	3,0069	kg/s 
Molar Flow	100	mol/s 
Volumetric Flow	2,61673	m3/s 
Specific Enthalpy	1952,12	kJ/kg 
Specific Entropy	2,91036	kJ/[kg.K] 
Vapor Phase Mole Fraction	1	

Simulação em DWSIM

Corrente de gás

Gás (Material Stream)

Information Connections

General Info

Object Gás

Status Calculated (24/07/2025 15:50:35)

Linked to

Property Package Settings

Property Package Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Basis Mole Fractions

Solvent

Compound	Amount
Ethane	1
Ethylene	0
Hydrogen	0
Water	0

Normalize

Equalize

Clear

Complete

Accept Changes

Simulação em DWSIM

Corrente de vapor

vapor (Material Stream)

Information Connections

General Info

Object Vapor

Status Calculated (24/07/2025 15:57:58)

Linked to

Property Package Settings

Property Package Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Flash Spec Temperature and Pressure (TP)

Temperature 953 K

Pressure 303000 Pa

Mass Flow 1,1723 kg/s

Molar Flow 60 mol/s

Volumetric Flow 1,56957 m3/s

Specific Enthalpy 1900,87 kJ/kg

Specific Entropy 4,51491 kJ/[kg.K]

Vapor Phase Mole Fraction 1

Simulação em DWSIM

Corrente de vapor

Vapor (Material Stream) [Icon] [X]

Information Connections

General Info

Object Vapor [Icon]

Status Calculated (24/07/2025 16:00:04) [Icon]

Linked to

Property Package Settings

Property Package Peng-Robinson (PR) (1) [Icon]

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Basis Mole Fractions [Dropdown]

Solvent [Dropdown]

Compound	Amount
Ethane	0
Ethylene	0
Hydrogen	0
Water	1

Normalize

Equalize

Clear

Complete

Accept Changes

Simulação em DWSIM

Usando o bloque de especificação para fixar a proporção vapor/gás

SP-1 (Specification Block)

General Info

Object: SP-1

Connections

Source Object: Gás

Source Property: Molar Flow

Source Value: 100 mol/s

Target Object: Vapor

Target Property: Molar Flow

Target Value: 60 mol/s

Behavior

Calculation Mode: Global Setting

Reference Object:

Expression

$Y = f(X) = 0.6 \cdot X$

$Y = 60 \text{ mol/s}$

Y = Target Variable, X = Source Variable

Simulação em DWSIM

Misturando as correntes de gás e vapor

MIX-1 (Stream Mixer)

General

Object: MIX-1

Status: Calculated (24/07/2025 16:16:17)

Linked to:

Connections

Inlet Stream 1	Gás		
Inlet Stream 2			
Inlet Stream 3			
Inlet Stream 4			
Inlet Stream 5			
Inlet Stream 6	Vapor		
Outlet Stream	Reagentes		

Calculation Parameters

Pressure Calculation: Inlet Minimum

Property Package Settings

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

Simulação em DWSIM

Especificando a reação

Edit Kinetic Reaction

Identification

Name: R1

Description: R1

Components, Stoichiometry and Reaction Orders

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.	DO	RO
Ethane	30,069	-2787,58	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1	1	0
Ethylene	28,0532	1871,8	<input checked="" type="checkbox"/>	<input type="checkbox"/>		0	1
Hydrogen	2,01588	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>		0	1
Water	18,0153	-13422,7	<input type="checkbox"/>	<input type="checkbox"/>	0	0	0

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC): 136330

Equation: CH3CH3 <--> CH2CH2 + H2

Kinetic Reaction Parameters

Base Component: Ethane

Phase: Vapor

Basis: Molar Concentrations

Amount Units: mol/m3

Tmin (K): 0

Tmax (K): 2000

Kinetics Specification: ☒ Simple ☐ Advanced Python Script Help

Rate Constants for Direct and Reverse Reactons (k and k')

Direct Reaction: ☒ Arrhenius ☐ User-Defined: f(T), T in K

Reverse Reaction: ☒ Arrhenius ☐ User-Defined: f(T), T in K

Rate Units: mol/[m3.s]

A: 8,65E+14 E: 273000 J/mol

A': 2,25E+13 E': 273000 J/mol

Cancel OK

Simulação em DWSIM

Especificando o reator

Reator (Plug-Flow Reactor (PFR)) Translat

General Info

Object: Reator

Status: Calculated (24/07/2025 16:31:46)

Linked to:

Connections

Inlet Stream: Reagentes

Outlet Stream: Productos

Energy Stream: Calor

Calculation Parameters

General Dimensions Catalyst Info Annotations Advanced

Reaction Set: Default Set

Calculation Mode: Isothermic

Outlet Temperature: 952,893 K

Internal Solver: Implicit Runge-Kutta

External Solver:

Reator (Plug-Flow Reactor (PFR)) ↑ ×

General Info

Object: Reator

Status: Calculated (24/07/2025 16:31:46)

Linked to:

Connections

Inlet Stream: Reagentes

Outlet Stream: Productos

Energy Stream: Calor

Calculation Parameters

General Dimensions Catalyst Info Annotations Advanced

Reactive Volume: 5 m3

Sizing Information: ☒ Length ☐ Diameter

Tube Length: 100 m

Tube Diameter: 252,313 mm

Number of Tubes: 1

Simulação em DWSIM

Adicionando um indicador para apresentar a conversão

Indicador de conversão [%] (Digital Gauge) [icon] [X]

Object ID

Name

Property

Property Type

Property Units

Integer Digits

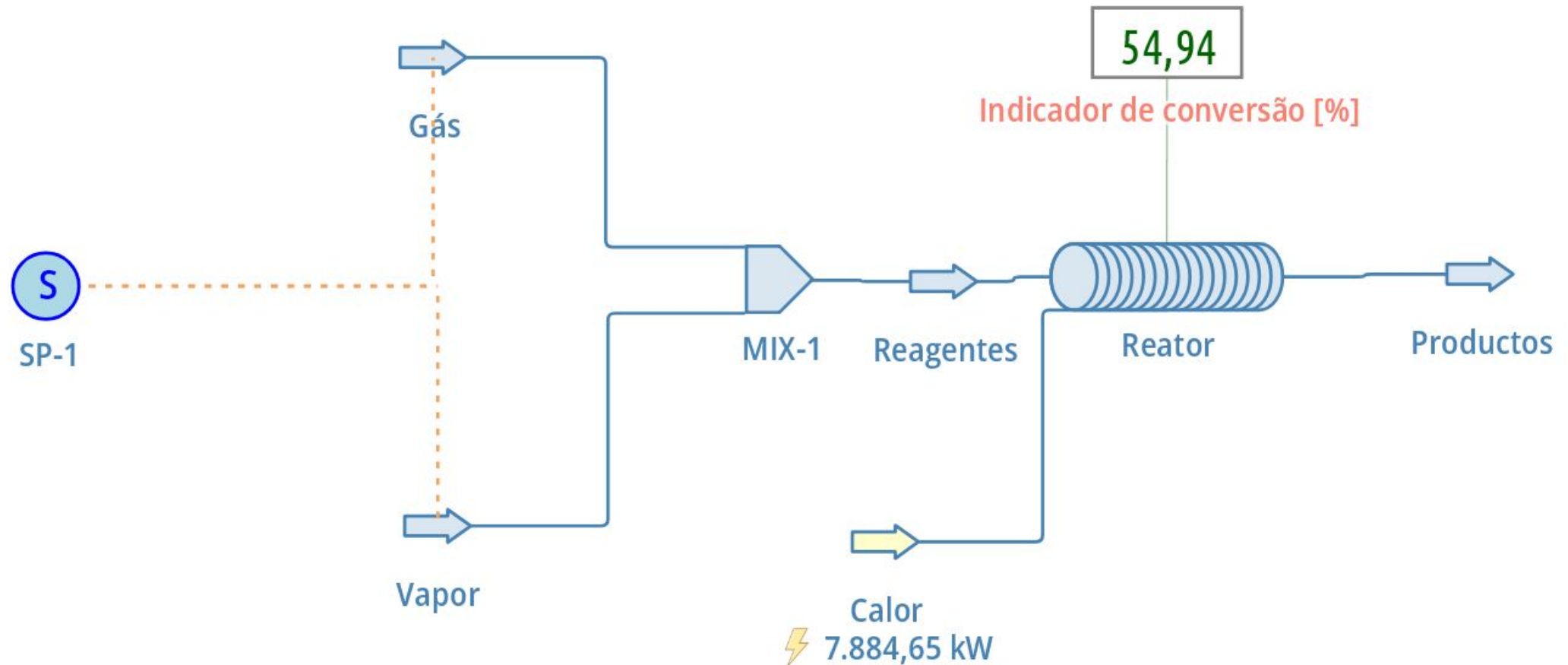
Decimal Digits

Current Value 54,9399773278386

☐ Display as Percentage

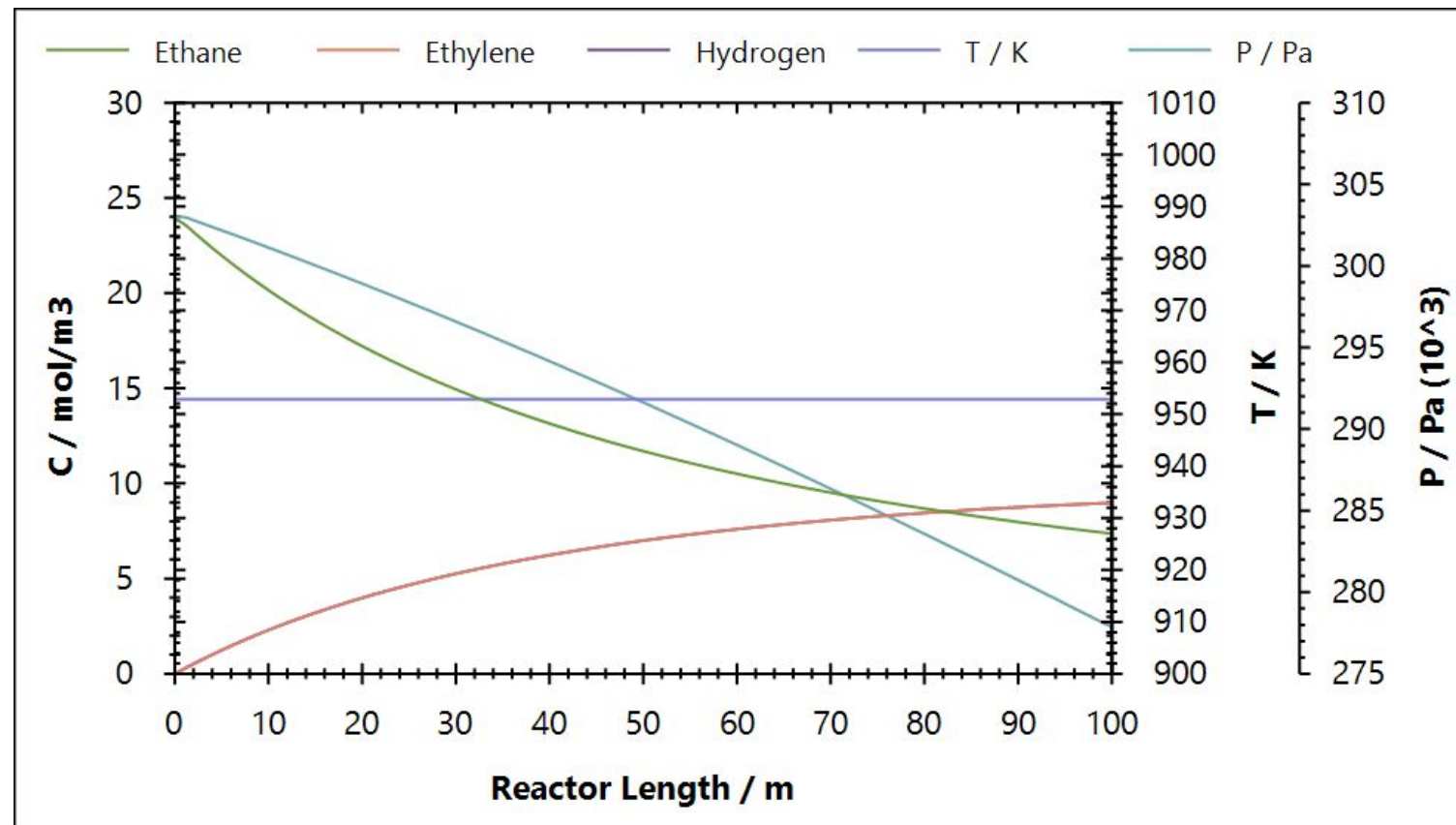
Simulação em DWSIM

Simulação convergida (operação isotérmica)



Simulação em DWSIM

Perfiles no reator (operação isotérmica)



Simulação em DWSIM

Trocando para operação adiabática no reator

Reator (Plug-Flow Reactor (PFR))

General Info

Object: Reator

Status: Calculated (24/07/2025 17:17:20)

Linked to:

Connections

Inlet Stream: Reagentes

Outlet Stream: Productos

Energy Stream: Calor

Calculation Parameters

General Dimensions Catalyst Info Annotations Advanced

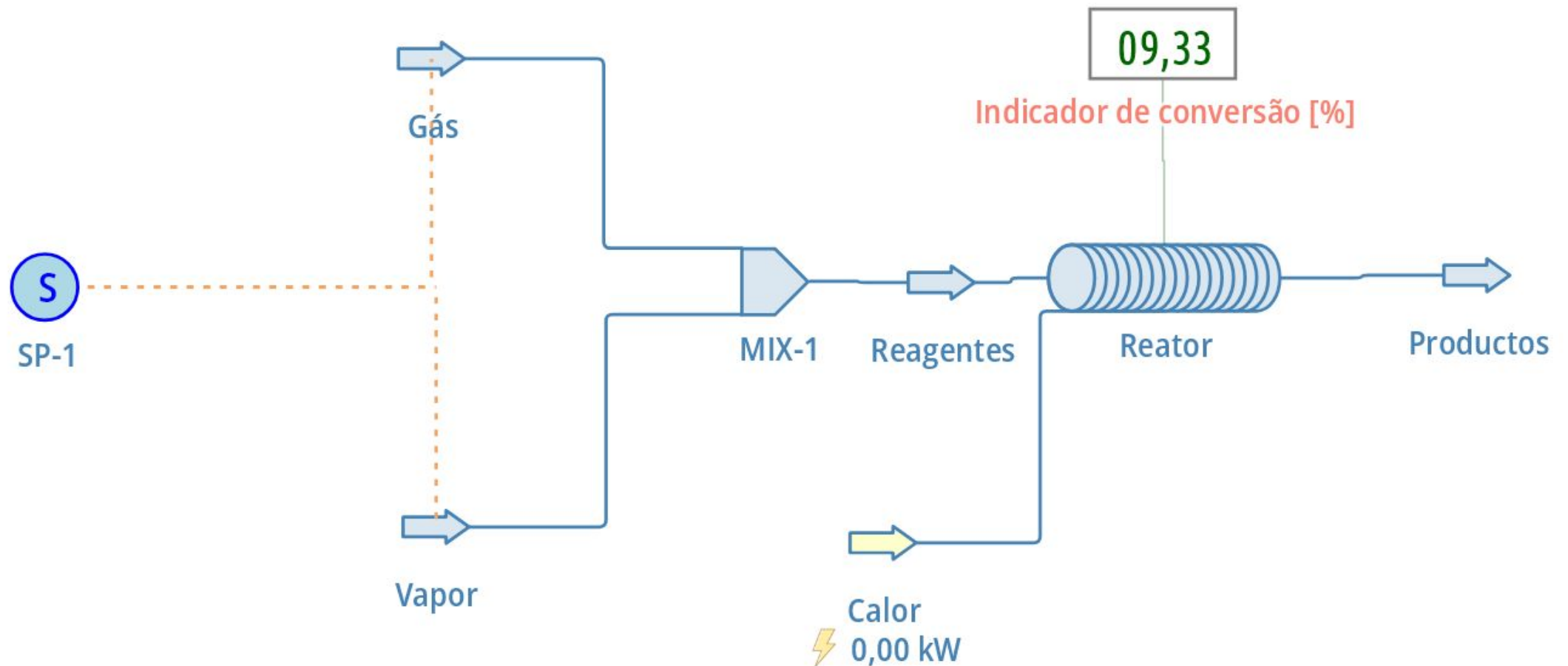
Reaction Set: Default Set

Calculation Mode: Adiabatic

Outlet Temperature: 857,542 K

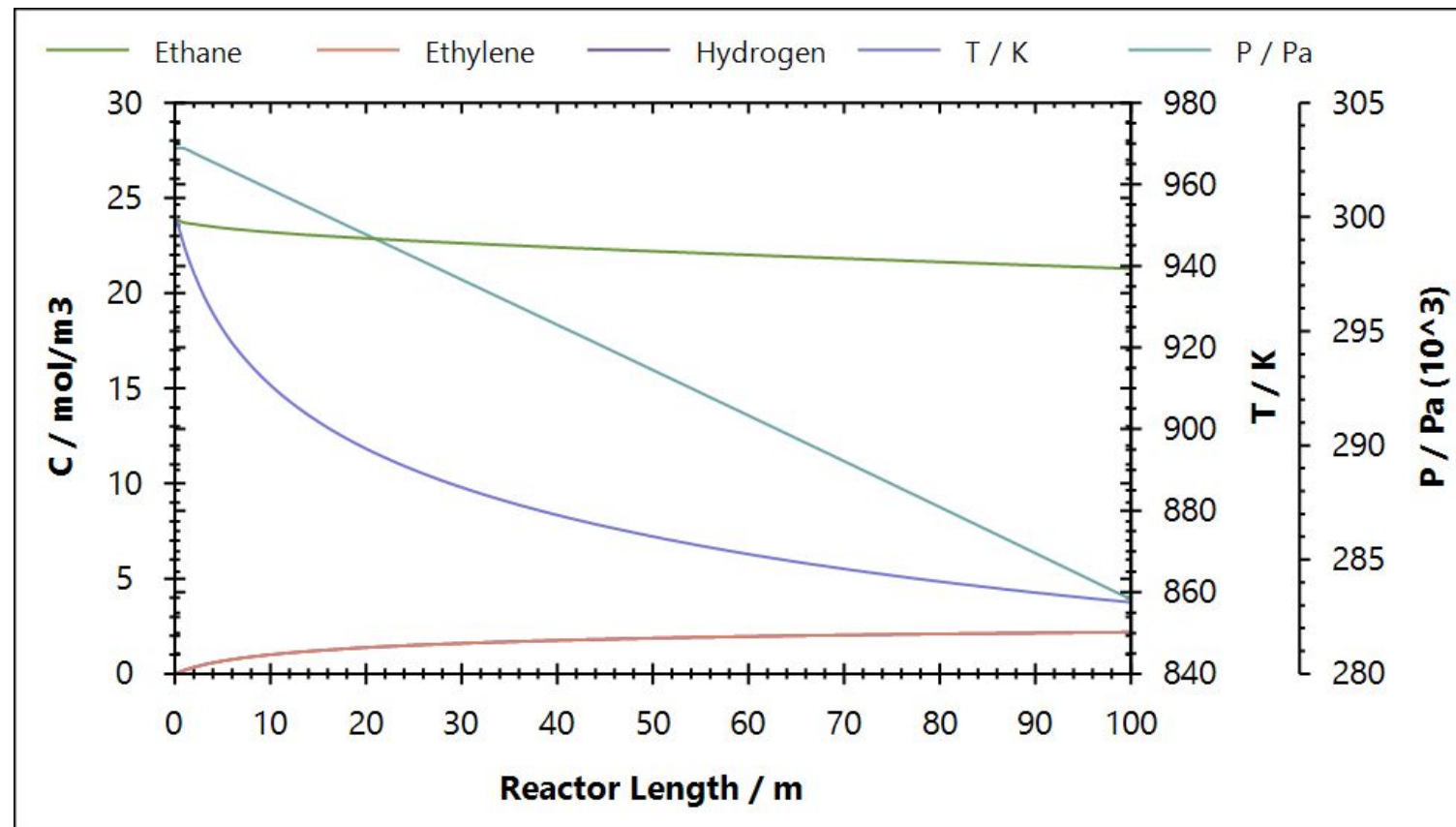
Simulação em DWSIM

Simulação convergida (operação adiabática)



Simulação em DWSIM

Perfiles no reator (operação adiabática)



Simulação em DWSIM

Configurando a variável independente na análise de sensibilidade

The screenshot displays the 'Sensitivity Study' window in DWSIM. The top menu bar includes 'Flowsheet', 'Dynamics Manager', 'Material Streams', 'Spreadsheet', 'Charts', 'Script Manager', 'GHG Emissions', 'Costing', and 'Sensitivity Study'. The 'Case Manager' section on the left shows a list with 'SACase1' selected, and buttons for 'New', 'Copy', 'Save', and 'Delete'. The 'Name and Description (Selected Case)' section on the right shows 'Name: SACase1' and an empty 'Description' field. Below these, the 'Independent Variables' tab is active, showing two configuration panels. The first panel, 'Independent Variable 1', is active and contains the following settings: Object: Gás, Property: Molar Flow, Lower Limit: 10, Upper Limit: 100, Number of Points: 10, Units: mol/s, and Current Value: 100. The second panel, 'Independent Variable 2', is inactive (checkbox not checked) and contains: Object: (empty), Property: (empty), Lower Limit: 0, Upper Limit: 0, Number of Points: 5, Units: (empty), and Current Value: (empty).

Case Manager

New Copy Save Delete

SACase1

Name and Description (Selected Case)

Name SACase1

Description

Independent Variables Dependent Variables Results Chart

Independent Variable 1

Object Gás

Property Molar Flow

Lower Limit 10 Number of Points 10

Upper Limit 100 Units mol/s

Current Value 100

☐ Independent Variable 2

Object

Property

Lower Limit 0 Number of Points 5

Upper Limit 0 Units

Current Value

Simulação em DWSIM

Configurando a variável dependente na análise de sensibilidade

Flowsheet Dynamics Manager Material Streams Spreadsheet Charts Script Manager GHG Emissions Costing Sensitivity Study X

Case Manager

New Copy Save Delete

SACase1

Name and Description (Selected Case)

Name SACase1

Description

Independent Variables Dependent Variables Results Chart

☒ Variables ☐ Expression

Add/Remove Variables

	Object	Property	Unit
▶	Reator	Ethane: Conversion	%

Expression Parameters

Name	Object	Property	Value	Unit
------	--------	----------	-------	------

Expression

Expression

Verify Clear

Curr. Value

Simulação em DWSIM

Resultados da análise de sensibilidade (tabela)

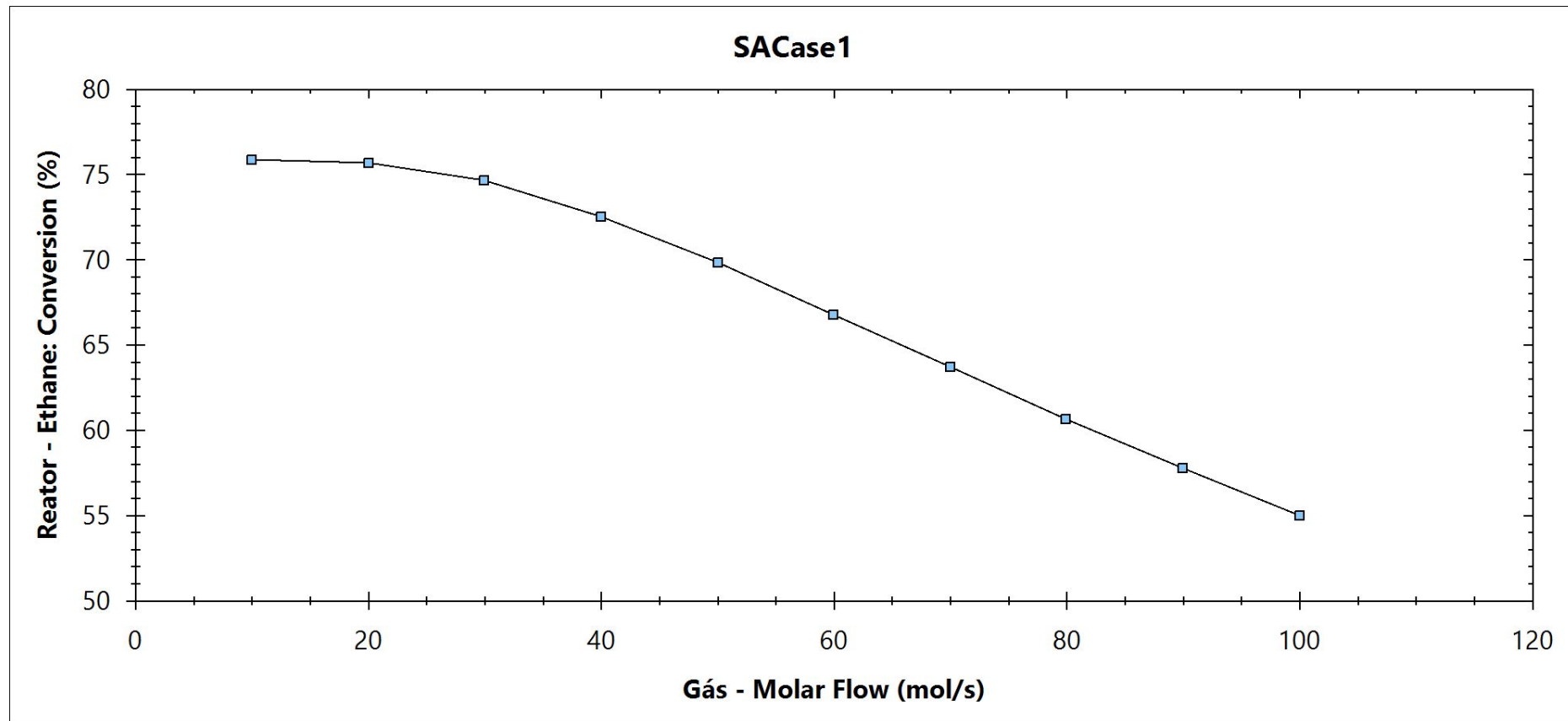
The screenshot displays the 'Sensitivity Study' window in DWSIM. The 'Case Manager' on the left shows 'SACase1' selected. The 'Name and Description (Selected Case)' panel on the right shows the case name and description. The 'Results' tab is active, showing a table of results for 'Gás - Molar Flow (mol/s)' and 'Reator - Ethane: Conversion (%)'. The table has 10 rows, with the first row (10) highlighted in blue. The 'Information' panel at the bottom shows the status of the simulation run.

Gás - Molar Flow (mol/s)	Reator - Ethane: Conversion (%)
10	75,7963
20	75,6543
30	74,6093
40	72,5272
50	69,7973
60	66,7759
70	63,6852
80	60,6472

Information
Run #10 completed...
Restoring simulation to its original state...
Done!

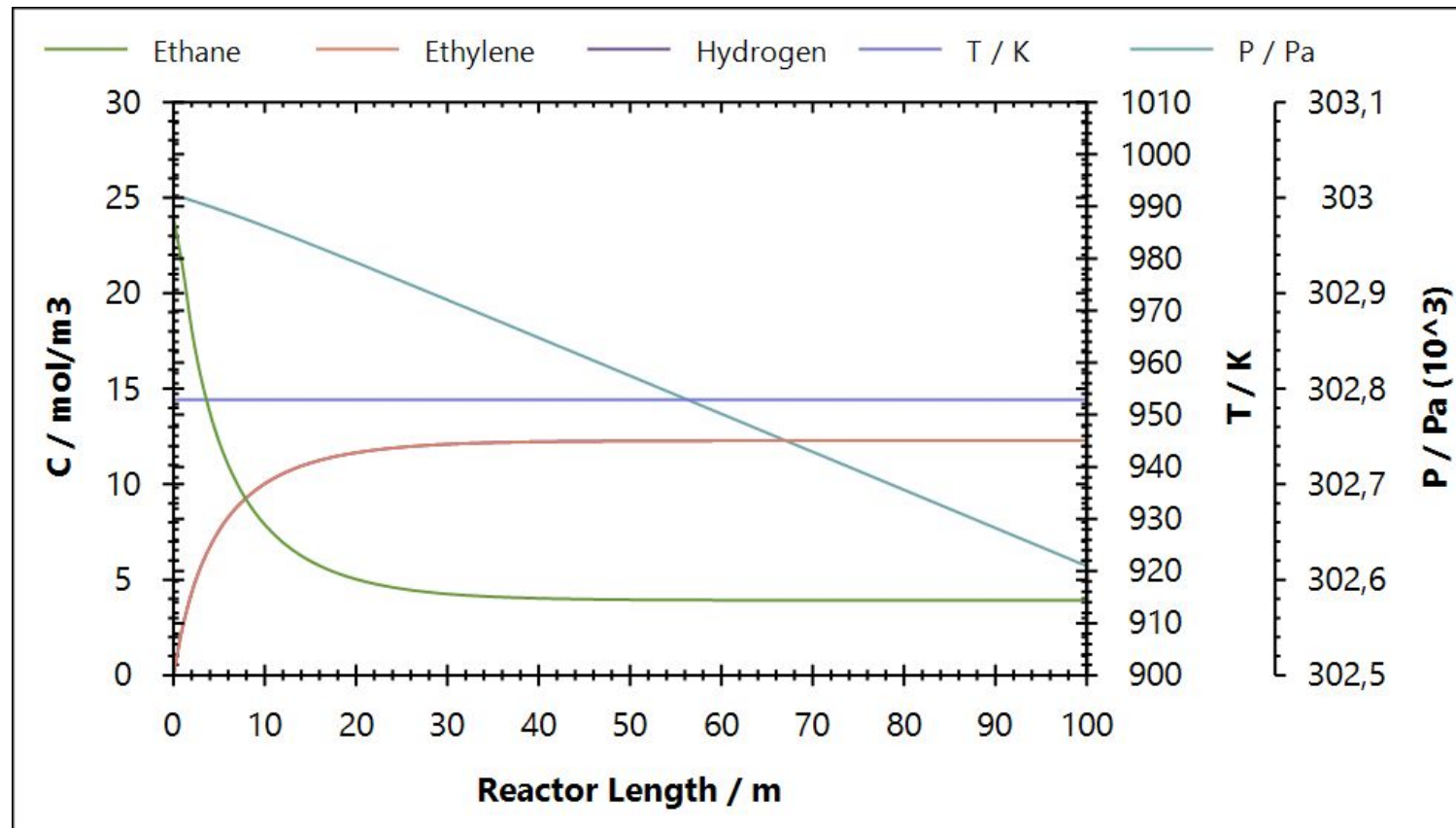
Simulação em DWSIM

Resultados da análise de sensibilidade (gráfico)



Simulação em DWSIM

Perfiles no reator para 10 mol/s de gás (operação isotérmica)



Dúvidas?



Recados importantes

- Próxima aula: Modelo customizado de separador por membrana em Aspen Plus
- Os slides desta aula estarão disponíveis no Classroom da disciplina.

“Ensinar não é transferir conhecimento, mas criar as possibilidades para a sua própria produção ou a sua construção.”

Paulo Freire