

Introducción a DWSIM

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- DWSIM is an open-source CAPE-OPEN compliant chemical process simulator for Windows and Linux.
- DWSIM is built on top of the Microsoft .NET and Mono Platforms and features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools.
- DWSIM is able to simulate steady-state, vapor-liquid, vapor-liquidliquid, solid-liquid and aqueous electrolyte equilibrium processes.

- Thermodynamic models:
 - PC-SAFT, FPROPS
 - CoolProp
 - Peng–Robinson
 - Peng–Robinson-Strÿjek-Vera (PRSV2)
 - Soave–Redlich–Kwong
 - Lee-Kesler
 - Lee-Kesler-Plöcker
 - UNIFAC(-LL)
 - Modified UNIFAC (Dortmund)
 - Modified UNIFAC (NIST)
 - UNIQUAC

- NRTL
- COSMO-SAC
- Chao-Seader
- Grayson-Streed
- Extended UNIQUAC
- Raoult's Law
- IAPWS-IF97 Steam Tables
- IAPWS-08 Seawater
- Black-Oil
- Sour Water

- Unit operations:
 - Mixer
 - Splitter
 - Separator
 - Pump
 - Compressor
 - Expander
 - Heater
 - Cooler
 - Valve
 - Pipe Segment

- Shortcut Column
- Heat Exchanger
- Reactors
- Component Separator
- Orifice Plate
- Distillation/Absorption
 Columns
- Solids Separator
- Cake Filter

- Utilities:
 - Binary Data Regression
 - Phase Envelope
 - Natural Gas Hydrates
 - Pure Component Properties
 - True Critical Point
 - PSV Sizing
 - Vessel Sizing
 - Spreadsheet and Petroleum Cold Flow Properties
- Tools:
 - Hypothetical Component Generator
 - Bulk C7+/Distillation Curves Petroleum Characterization
 - Petroleum Assay Manager
 - Reactions Manager and Compound Creator;
 - Process Analysis and Optimization:
 - Sensitivity Analysis Utility
 - Multivariate Optimizer with bound constraints;
- Extras:
 - Support for Runtime Scripts
 - Plugins and CAPE-OPEN Flowsheet Monitoring Objects.



Feature-Complete

DWSIM is a CAPE-OPEN compliant Chemical Process Simulator and has an easy-to-use graphical interface with many features previously available only in commercial chemical process simulators.



Support DWSIM open-source development

Support the DWSIM open-source development with a single, one-time donation or with a monthly subscription!

By becoming a patron, you will support me (Daniel Wagner) directly and shape the future development of DWSIM while getting access to exclusive goodies, depending on your subscription tier. You can also say thank you with a one-time donation by getting me a coffee or, if you're from Brazil, you can do me a Pix transfer and I'll buy the coffee myself. So in



MORE INFORMATION

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Instalación del software

Check the components you wan Click Next to continue.	t to install and uncheck the components you don't want	to install.
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Tildar todas las opciones

Inicio del software



Ventana de bienvenida

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Asistente de configuración

Simulation Configuration Wizard
 Simulation Wizard
 Simulation Configuration Wizard
 Simulation Wizard

Introduction

Introduction

Welcome to the simulation configuration wizard.

- Compounds
- Property Packages
- System of Units
- Behavior
- Undo/Redo

In the next pages you will be able to add compounds, property packages, set the system of units and configure specific parameters for a new simulation.

Click "Next" to continue.

Puede cerrarse y configurarse manualmente

Close Wizard and go to the Simulation Configuration Window

Selección de compuestos

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	СР	^
	Methane	74-82-8	CH4	ChemSep		
	Ethane	74-84-0	СНЗСНЗ	ChemSep		
	Propane	74-98-6	СН3СН2СН3	ChemSep	\checkmark	
	N-butane	106-97-8	CH3(CH2)2CH3	ChemSep		
	N-pentane	109-66-0	CH3(CH2)3CH3	ChemSep		
	N-hexane	110-54-3	CH3(CH2)4CH3	ChemSep		
	N-heptane	142-82-5	CH3(CH2)5CH3	ChemSep		
	N-octane	111-65-9	CH3(CH2)6CH3	ChemSep		
	N-nonane	111-84-2	CH3(CH2)7CH3	ChemSep		
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Next > Cancel

Selección de paquetes de propiedades fisicoquímicas

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.

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

Next >	Cancel
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Selección de unidades

Click "Finish" to exit the wizard and start designing the simulation model.

Simulation Configuration Wizard

than SI, CGS or ENG).

System of Units

Introduction

Compounds

Property Packages

System of Units

Behavior

Undo/Redo

System of Units SI		~	Clone Create	Set as Default		
Property	Unit		Property	Unit	1	^
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Volumetric flow rate	m3/s	~	Specific Enthalpy	kJ/kg	~	
Specific Entropy	kJ/[kg.K]	~	Molecular Weight	kg/kmol	~	
Density	kg/m3	~	Surface Tension	N/m	~	
Heat Capacity	kJ/[kg.K]	~	Thermal Conductivity	W/[m.K]	~	
Kinematic Viscosity	m2/s	~	Dynamic Viscosity	Pa.s	~	
Temperature Difference	К.	~	Pressure Difference	Pa	~	
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Time	s	~	Volume	m3	~	
Molar Volume	m3/kmol	~	Area	m2	~	
Diameter/Thickness	mm	~	Force	N	~ ~	,

Select the desired System of Units for your simulation. You can change individual units by selecting a custom system (other

Next > Cancel

Opciones del software

🗧 🚹 Simulation Configuration Wizard

Behavior

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

Smart Object Solving

DWSIM can skip calculations of flowsheet objects if none of its input parameters (including inlet streams) have changed since the last successful calculation. This feature is disabled by default. You can change it later in Edit > Simulation Settings > Behavior.

Activate Smart Object Solving

Fail-Safe Flash Calculations

If the selected equilibrium calculation method fails, DWSIM can try it again using a simple VLE procedure assuming ideal behavior for the mixture. Would you like to enable this feature? This is a Property Package-level setting and can be changed later in the Property Package Settings editor > Equilibrium Calculation Settings.

Activate Fail-Safe Flash Calculations

Object Editing Behavior

The default behavior for editing flowsheet objects is single-click to open the editor. Would you like to switch this to double-click editing? This is a global setting that can be changed later in Edit > Global Settings > Flowsheet.

Activate Double-Click to Open Editors

Next > Cancel

Opciones del software

Simulation Configuration Wizard
 Simulation W

Undo/Redo

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

Undo/Redo Operations

Would you like to enable full Undo/Redo capabilities? This feature is disabled by default and can make the interface less responsive on complex flowsheets.

You can enable or disable this feature later in the 'Simulation Settings' > 'Behavior' panel.

Enable Undo/Redo Operations



Finish Cancel

Entorno del software

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Entorno del software

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Listado de objetos disponibles para agregar al flowsheet



Energy Stream Splitter

Listado de objetos disponibles para agregar al flowsheet



Listado de objetos disponibles para agregar al flowsheet



Material Stream

- Es uno de los módulos de cálculo más importantes ya que se utiliza para representar el ingreso y egreso de materia a un proceso, así como también la interconexión de equipos dentro del mismo.
- Para poder ejecutarse requiere la siguiente información (inputs):
 - Composición global de la mezcla (base molar, másica o volumétrica).
 - Dos propiedades intensivas (por ejemplo, Presión y Temperatura).
 - Una magnitud de flujo de materia (base molar, másica o volumétrica).

Secuencia de cálculo realizada por el módulo Material Stream:

- Realiza la estimación del estado de agregación de la mezcla, identificando la presencia de fase liquida, vapor o mezcla de ambas (FLASH problem).
- 2. Calcula de manera individual las propiedades de la/s fase/s.
- 3. Calcula las propiedades globales de la corriente (si existe una única fase las propiedades son idénticas a las del paso 2).

Se calculan las siguientes propiedades:

- 1. Distribución de los componentes entre las fases.
- 2. Propiedades de cada fase (entalpía, entropía, peso molecular, densidad, etc).
- 3. Calcula las propiedades globales de la corriente (entalpía, entropía, peso molecular, densidad, etc).

Dada de la corriente de gas cuyo Flujo es de 100 kg/h, y de composición:

C1	C2	C3
0.6	0.2	0.2

- Utilizar el paquete termodinámico Peng-Robinson.
- Ajuste una presión de 7500 kPa y una temperatura de 10º C. ¿Cuál es la fracción de vapor?
- Realice el cálculo de punto de rocío a esta corriente. Fije una presión de 7500 kPa. ¿Cual es la temperatura de rocío?

Simulation Configuration Wizard

Compounds

En lo posible utilizar la misma base de datos (ChemSep en este ejemplo)

- 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		СР	^
\checkmark	Methane		74-82-8	CH4	ChemSep		\checkmark	
	Ethane		74-84-0	СНЗСНЗ	ChemSep			
	Propane		74-98-6	СН3СН2СН3	ChemSep			
	N-butane		106-97-8	CH3(CH2)2CH3	ChemSep			
	N-pentane		109-66-0	CH3(CH2)3CH3	ChemSep		\checkmark	
	N-hexane		110-54-3	CH3(CH2)4CH3	ChemSep			
	N-heptane		142-82-5	CH3(CH2)5CH3	ChemSep			
	N-octane		111-65-9	CH3(CH2)6CH3	ChemSep			1
	N-nonane		111-84-2	CH3(CH2)7CH3	ChemSep			
	N-decane		124-18-5	CH3(CH2)8CH3	ChemSep			
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Next > Cancel

Selección del paquete fisicoquímico

🗧 👔 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.

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🚹 R	EFPROP					
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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)
VLE/LLE
Do not calculate

Next >	Cancel
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Selección del paquete fisicoquímico

🗧 👔 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		
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Added Property Packages

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)
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Do not calculate

Selección del paquete fisicoquímico

Unidades

🗧 🚹 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).

 \sim

Clone

Create

Set as Default

Click "Finish" to exit the wizard and start designing the simulation model.

SI

System of Units

Property	Unit		Property	Unit		^
Temperature	К	~	Pressure	Pa	~	1
Mass Flow Rate	kg/s	~	Molar Flow Rate	mol/s	~	1
Volumetric flow rate	m3/s	~	Specific Enthalpy	kJ/kg	~	
Specific Entropy	kJ/[kg.K]	~	Molecular Weight	kg/kmol	~	1
Density	kg/m3	~	Surface Tension	N/m	~	
Heat Capacity	kJ/[kg.K]	~	Thermal Conductivity	W/[m.K]	~	
Kinematic Viscosity	m2/s	~	Dynamic Viscosity	Pa.s	~	
Temperature Difference	К.	~	Pressure Difference	Pa	~	
Length/Head	m	~	Energy Flow	kW	~	
Time	s	~	Volume	m3	~	
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Next > Cancel

Comienzo de la simulación

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Modulo "Material Stream" (corriente de materia)

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Do not chan	ge this setti	ng unle	ss you know	what yo	ou're doin	g.					

Al agregar una corriente sus datos se completan con valores por defecto



Propiedades de las corrientes de materia

nformation Connectio	ons				S	se puede	cambia	ar el	
General Info					→ ~				
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Stream Conditions Co	ompound Am	iou nte		Input	t Data	Results Annota	tions Dynam	nics Floating	Tables
Flash Spec	[Temperature and P	ressure (TP)	Stre	am Con	ditions Compo	und Amounts		
Temperature	[298.15	K						
Pressure	[101325	Pa	Ba	asis	Mole Fractions			
Mass Flow	[1	kg/s	S	olvent				
Molar Flow	[0	mol/s		Compou	ind	Amount		Normalize
Volumetric Flow	[0	m3/s		lethane			0.33333333	E
Specific Enthalpy		0	kJ/kg	E	thane			0.33333333	Equalize
Specific Entropy	[0	kJ/[kg.K]	P	ropane			0.33333333	Clear
Vapor Phase Mole Fra	action	0							Complete
				,					Accept

Es conveniente comenzar definiendo la composición de la corriente. Por defecto es una mezcla equimolar de todos los compuestos.

Input Data	Results	Annotatio	ons Dy	namics	Floating) Tables										
Stream Co	nditions	Compoun	d Amou	nts												
Basis Solvent	Mole F	ractions														
Compo	ound	A	mount			No	rmalize					1				
Methan Ethane	e				0.6	Eq	ualize									
Propan	e				0.2	(Clear									
						Co	mplete									
						A	ccept	\supset								
						-										
									Se i	ngre ace	esa la epai	a cor n los	npos cam	ición bios	y se	

FLASH Spec (Especificaciones para el calculo del flash)

Input Data	Results	Annotations	Dynamics	Floating Tables	
Stream Cor	nditions	Compound Ar	nounts		
Flash Spe	ec		Temperatu	re and Pressure (TP)	\sim

FLASH Spec (Especificaciones para el calculo del flash)



Resolución del ejercicio propuesto

Ajuste una presión de 7500 kPa y una temperatura de 10º C ¿Cuál es la fracción de vapor? 10 K к Input Data Results Annotations Dynamics Floating Tables R Stream Conditions Compound Amounts Flash Spec Temperature 298.15 7500 Pa Pa Pressure 101325 Pa atm kaf/cm2 Mass Flow kg/s kgf/cm2g lbf/ft2 cPa. Molar Flow 40.8857 mol/s \sim kPag bar Volumetric Flow 0.995099 m3/s \sim barg ftH2O Specific Enthalpy -1.58673 kJ/kg \sim inH20 inHg Specific Entropy 0.305015 kJ/[kg.K] mbar \sim mH20 mmH2O Vapor Phase Mole Fraction mmHg MPa psi psig

Ajuste una presión de **7500 kPa** y una temperatura de **10º C** ¿Cuál es la fracción de vapor?



Clonamos la corriente para no volver a definir la composición





Realice el cálculo de punto de rocío a esta corriente. Fije una presión de 7500 kPa ¿Cual es la temperatura de rocío?



Realice el cálculo de punto de rocío a esta corriente. Fije una presión de 7500 kPa ¿Cual es la temperatura de rocío?

Input Data	Results	Annotations	Dynamics	Floatin	g Tables	
Stream Co	nditions	Compound Ar	nounts			
Flash Spec			Pressure ar	nd Vapor	r Fraction	(PVF) ~
Temperat	ture		2	93.104	К	\sim
Pressure			7.	5E+06	Pa	~
Mass Flow				1	kg/s	\sim
Molar Flow			4	0.8857	mol/s	~
Volumetric Flow			0.007	744895	m3/s	~
Specific Enthalpy			-1	77.453	kJ/kg	~
Specific Entropy			-1	.61086	kJ/[kg.K]	~
Vapor Ph		1				

Pasos:

- 1. Crear un nuevo caso de simulación definiendo los compuestos intervinientes y los paquetes termodinámicos que se desean comparar.
- 2. En el flowsheet crear una nueva corriente de materia.

Ejemplo:

Metanol (1) y Agua(2) usando NRTL y Ley de Raoult.

Added	 Name
1	Methanol
V	Water

Added Property Packages

Name	Туре	
Raoult's Law (1)	Raoult's Law	
NRTL (2)	NRTL	

- 3. Seleccionar la corriente de materia creada y agregar una "utility".
- 4. Seleccionar las siguientes opciones:

Material Stream > Binary Phase Envelope > MSTR-000 (nombre de la corriente creada)

Utilities Octimination	Add Utility		x
Optimization	Add an Utility and associa	ate it with an object on the Flowsheet.	
	Object Type:	Utility Type:	Flowsheet Object:
	Material Streams Separator Vessels Valves	Phase Envelope <u>Binary Phase Envelope</u> Ternary Phase Envelope True Critical Point Petroleum Cold Flow Properties Natural Gas Hydrates	Cancel Add Utility

En la ventana principal se deben seleccionar las opciones del diagrama 5. Files Flowsheet Dynamics Manager Material Streams Spreadsheet Charts Script Manager GHG Emissions Costing BinaryEnvelope1 Docking 🔄 🖪 🗭 🕞 🚯 🚱 🖶 🖺 😣 Close BinaryEnvelope1 Name Attached to 1 Update automatically **Diagram Settings** Results Compound 1 Methanol Graph Exp. Data Table Compound 2 Water \sim Title Envelope type ● Txy ○ Pxy ○ (T)xy ○ (P)xy VLE 🗌 LLE **Txy Diagram Options** 1.2 SLE Eutectic Solid Solution Critical Line X Axis Basis Mole Fraction \sim 1.0 Pressure 101325 Pa Temperature 298.15 K 0.8 Max Min Fraction Range 0 Stepcount 40 Axis 0.6 Property Package \sim Raoult's Law (1) (Raoult's Law) Compare Models Calculate 0.4 0.2 0.0 0.0 0.2 0.4 0.8 1.0 0.6 1.2 X Axis

Open Panel View History

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Diagrama T vs x/y a 1 atm utilizando NRTL

Diagram Settings			
Compound 1	Methanol \checkmark		
Compound 2	Water \checkmark		
Envelope type	● Txy ○ Pxy ○ (T)xy ○ (P)xy		
Txy Diagram Options	VLE LLE		
	□ SLE		
	Critical Line		
X Axis Basis	Mole Fraction \sim		
Pressure	101325 Pa		
Temperature	298.15 K		
	Min Max		
Fraction Range	0 1		
Stepcount	40		
Property Package	NRTL (2) (NRTL) V		
Compare Models	Calculate		



Diagrama y vs x a	1 atm	utilizando	NRTL
-------------------	-------	------------	------

Diagram Settings	
Compound 1	Methanol \checkmark
Compound 2	Water \checkmark
Envelope type	○ Txy ○ Pxy
Txy Diagram Options	VLE LLE
	□ SLE
	Critical Line
X Axis Basis	Mole Fraction \checkmark
Pressure	101325 Pa
Temperature	298.15 K
	Min Max
Fraction Range	0 1
Stepcount	40
Property Package	NRTL (2) (NRTL) V
Compare Models	Calculate



Diagramas T vs x/y a 1 atm comparando los modelos fisicoquímicos.

Diagram Settings	
Compound 1	Methanol \checkmark
Compound 2	Water \checkmark
Envelope type	● Txy ○ Pxy ○ (T)xy ○ (P)xy
Txy Diagram Options	VLE 🗌 LLE
	SLE Eutectic Solid Solution
	Critical Line
X Axis Basis	Mole Fraction \sim
Pressure	101325 Pa
Temperature	298.15 K
	Min Max
Fraction Range	0 1
Stepcount	40
Property Package	Raoult's Law (1) (Raoult's Law) $\qquad \qquad \qquad$
Compare Models	Calculate



Diagramas y vs x a 1 atm comparando los modelos fisicoquímicos.

Diagram Settings	
Compound 1	Methanol \checkmark
Compound 2	Water \checkmark
Envelope type	○ Txy ○ Pxy
Txy Diagram Options	VLE LLE
	SLE Eutectic Solid Solution
	Critical Line
X Axis Basis	Mole Fraction \sim
Pressure	101325 Pa
Temperature	298.15 K
	Min Max
Fraction Range	0 1
Stepcount	40
Property Package	Raoult's Law (1) (Raoult's Law) $\qquad \qquad \qquad$
Compare Models	Calculate



Inclusión de datos experimentales

Res	sults					
G	raph	Exp. Data	Table			
		x1 (Molar Fract	ion)	y1 (Molar Fraction)	Т (К)	P (Pa)

Results					
Graph	Exp. Data	Table		\sim	
	x1 (Molar Fract	ion)	y1 (Molar Fraction)	т (К)	P (Pa)
	0.04780		0.25590	312.91	9079
	0.09250		0.45620	312.91	11412
	0.13350		0.6214	312.91	13012
	0.3065		0.76120	312.91	19025
				\smile	

Inclusión de datos experimentales

Diagram Settings	
Compound 1	Methanol \checkmark
Compound 2	Water ~
Envelope type	○ Txy ● Pxy ○ (T)xy ○ (P)xy
Txy Diagram Options	VLE LLE
	SLE Eutectic Solid Solution
	Critical Line
X Axis Basis	Mole Fraction $$
Pressure	101325 Pa
Temperature	312,91) К
	Min Max
Fraction Range	0 1
Stepcount	40
Property Package	Raoult's Law (1) (Raoult's Law) $\qquad \qquad \qquad$
Compare Models	Calculate





