

Predict

SC-CO₂ modeling and simulation software



Overview

Predict is a modeling and simulation software developed for the calculations of various physical properties in the case of processes using supercritical CO₂

Predict has been developed after several years of academic research. It consists in several tools which can be used for the calculations or modeling of various properties

- Sovova's mathematical parameters in the case of SC-CO₂ extraction
- Chrastil, Adachi, Mendez-Santiago, Gordillon and Del Valle model parameters for the modeling of solute solubility in SC-CO₂
- Prediction of vegetable oils and various other solutes (Argan oil, grape seeds oil, beta carotene, etc.) in SC-CO₂
- Hansen parameters for the choice of co-solvent
- CO₂-Solvent LVE at high pressure
- CO₂-solvent mixture properties (density, Cp, etc.)
- Scale-up calculations for SC-CO₂ extraction process
- And more !

It can be used as well as for academic studies as for industrial applications (select the optimal operating conditions parameters and avoid or reduce the costs of experimental studies)

SC-CO₂ extraction kinetics modeling

SC-CO₂ experimental extraction kinetics can be modelled using the Sovova's mathematical model
 The model parameters as well as the calculated points can be exported in Excel file

Experimental values

Data	Value
N (g)	7
P (bar)	300
T (K)	333
Q (kg/h)	0
mu CO ₂ (Pa.S)	0
rho CO ₂ (kg/m ³)	827
Cu 1	0

First estimation

Deviation ys(%) : 0
 Cu (kg(solute)/kg(solid)) : 0.25
 position end solubility : 4
 offset : 100
 xu (kg(solute)/kg(insoluble solid)) : 0.3333
 slope : 0.005137

Modelling

qc estimation : 32.1
 C1 : 1, C2 : 0.01
 end ratio CO₂/biomass (kg/kg) : 100
 oil MW (g/mol) : 800

Parameters	Values
ys (kg solute / kg CO ₂)	0.0051
R ²	0.9993
C1	1.2815
C2	0.0290
ksas	0.0001
r	0.2057
AARD (%)	2.0665
qc	24.7059

Experimental values

Data	Value
N (g)	300
P (bar)	300
T (K)	332
Q (kg/h)	26.9311
Visco CO ₂ (Pa.S)	32.0066
rho CO ₂ (kg/m ³)	49.7813
Cu 1	73.5415

First estimation

position first part solubility (%) : 0
 Cu (kg(solute)/kg(solid)) : 0.64
 xu (kg(solute)/kg(insoluble solid)) : 1.778
 slope : 0.006857
 Ys (kg solute / kg CO₂) : 0.006857
 Deviation with linear part (%) : 10
 q1 estimation : 15.8

Modelling

qc : 338, C1 : 0.1, C2 : 0.001, xt : 0.1
 end ratio CO₂/biomass (kg/kg) : 300
 solute MW (g/mol) : 800

Parameters	Values
ys (kg solute / kg solve...)	0.0069
R ²	1
C1	1.5065
C2	0.0073
ksas	1.2384e-05
r	0.8462
xt	1.7129
K	0.0027
qc (kg CO ₂ / kg insolubl...)	314.0600
AARD(%)	4.6472

Experimental values

Column 1	Column 2
N (g)	7.2680
P (bar)	300.0000
T (K)	333.1500
Q (kg/h)	0.1400
Visco CO ₂ (Pa.S)	0.0001
rho CO ₂ (kg/m ³)	827.0291

Solubility part

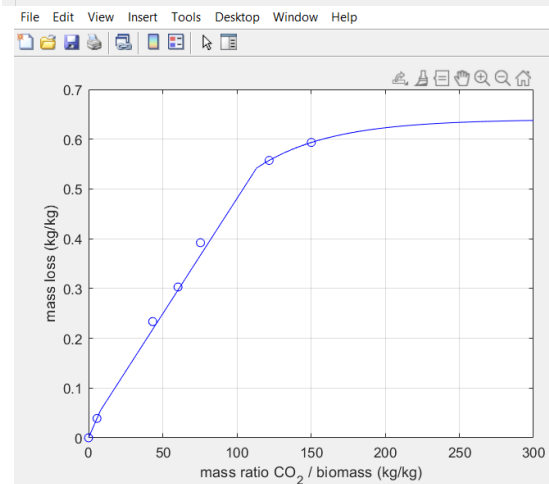
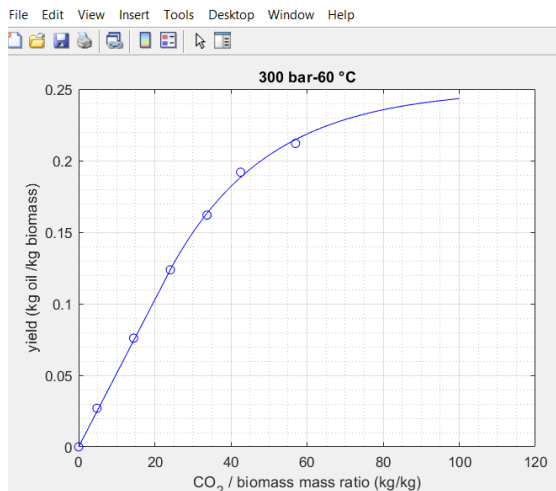
Cu (kg oil/kg biomass) : 0.23
 ys (kg oil/kg CO₂) : 0.00513

Prediction

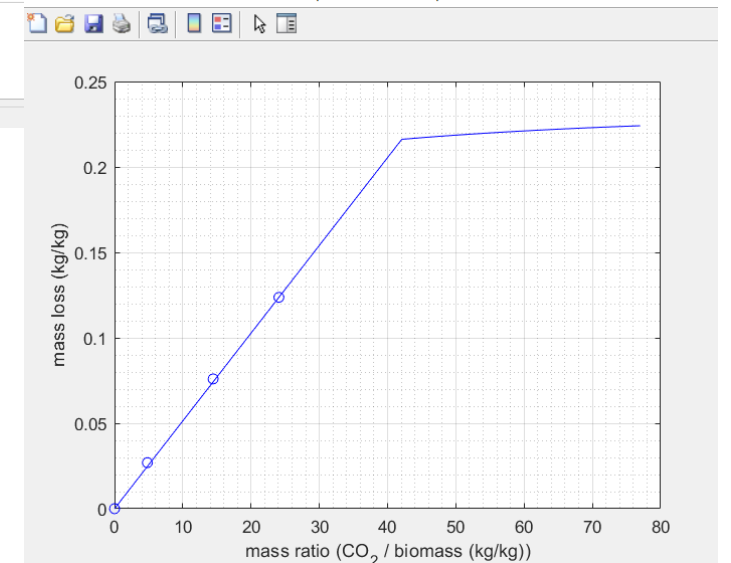
r : 0.9, qc : 55, qend : 100
 C1 : 0.1, C2 : 0.1

Parameters	Values
C1	0.1684
C2	0.0188
qc (kg CO ₂ / kg inso...)	54.6687
ksas (10 ⁻⁵)	0.4877
r	0.899

When SC-CO₂ experimental extraction kinetics is not complete, it is possible to predict a possible end of the extraction curve



Can be used for theoretical purposes and for scale up calculations



SC-CO₂ extraction scale up

Considering the extraction kinetic established at laboratory scale, this tool is used for the calculation of SC-CO₂ flow rate which can be applied in pilot or industrial scale

The MATLAB App interface is divided into two main sections: 'Flow rate calculation' and 'Autoclave dimension calc'. The 'Autoclave dimension calc' section is further divided into 'Small scale (Lab scale)' and 'Large scale (pilot scale)'. The 'Small scale' section includes input fields for L ss (cm), D ss (cm), L / D ss, sample bed porosity, d mean (μm), Q ss (kg/h), tr ss (min), Rep ss, CO₂/biomass mass ratio (kg/kg), P (bar), and T (°C). The 'Large scale' section includes a 'selection' dropdown (Dimension or volume), L ls (cm), D ls (cm), Volume (cm³), V (L), app density (kg/m³), mass of sample (kg), Filling rate, CO₂ velocity constant in the extraction autoclave (Q ls (kg/h), t (h), tr (min), Rep LS), CO₂ residence time in the extraction autoclave constant (Q ls (kg/h), t (h), tr (min), Rep LS), and Same CO₂/biomass mass ratio (extraction time (h), Q ls (kg/h)). A 'Calculate' button is located at the bottom of the 'Small scale' section.

SC-CO₂ diffusion and transfer properties

Knowing the molecular weight of solute in a porous media, this tool can calculate the diffusion and transfer properties of this solute in SC-CO₂. It can also be used for the calculation of flow regime in an autoclave.

The Prop CO₂ interface is divided into three tabs: 'Diffusion / transfer', 'Thermophysical properties CO₂', and 'Thermodynamic properties SC-CO₂'. The 'Diffusion / transfer' tab is active and shows 'Diffusion coefficient solute/CO₂ (D21)'. It is divided into 'Operating conditions' and 'Properties'. The 'Operating conditions' section includes input fields for P (bar), T (°C), MW (g/mol), dmean (μm), Q (kg/h), ε, L autoclave (cm), and D autoclave (cm). The 'Properties' section includes input fields for D21 (m²/s), kf (m/s), Dax (m²/s), Sc, Sh, tr (min), tr full auto (min), u (m/s), Pe, ρ (kg/m³), ν (Pa.s), Rep, Re, and u inters (m/s). A 'Calculate' button is located at the bottom of the 'Operating conditions' section.

Modeling and prediction of the solubility in SC-CO₂ of various solutes

Experimental results of solute solubilities in SC-CO₂ can be modelled considering 5 models : Chrastil, Adachi & Lu, Mendez-Santiago & Teja, Gordillo, Del Devalle & Aguilera

Prediction of vegetable oils solubilities in SC-CO₂ according the correlations of Sovova and Del Valle

The screenshot displays the 'Modelling' tab of the 'Solubility SC-CO2' software. It features five model configuration panels:

- Chrastil:** Parameters a = -5688, k = 7.67, b = -39.52, AARD (%) = 1.072.
- Adachi & Lu:** Parameters e0 = -371.5, A = -5195, e1 = 0.1274, B = 1999, e2 = -4.375e-05, AARD (%) = 0.6222.
- Mendez-Santiago & Teja:** Parameters A = -1.182e+04, C = 24.9, B = 4.515, AARD (%) = 1.086.
- Gordillo:** Parameters c0 = -13.47, c3 = 0.0001978, c1 = -0.03049, c4 = 0.06121, c2 = -4.534e-05, c5 = -0.0001655, AARD (%) = 0.1145.
- Del Valle & Aguilera:** Parameters A = -28.88, k = 7.671, B = -1.256e+04, C = 1.11e+06, AARD (%) = 1.073.

Additional features include an 'Import Excel Data' button, a 'Name' field set to 'Sample', and an 'Export to Excel' button.

The screenshot shows the 'Prediction vegetable oils' tab with the following data:

Model	Operating conditions	solubility (y _s in g oil / kg CO ₂)
Solubility of vegetable oils Del Valle 1988	P (bar) = 220, T (°C) = 40, ρ CO ₂ (kg/m ³) = 857.4	4.152
Solubility of Vegetable oils at high pressure Del Valle 2012		4.476
Solubility of two Vegetable oils Sovova 2001		3.927

Can be used for the selection of experimental operating conditions in the case of SC-CO₂ extraction or fractionation

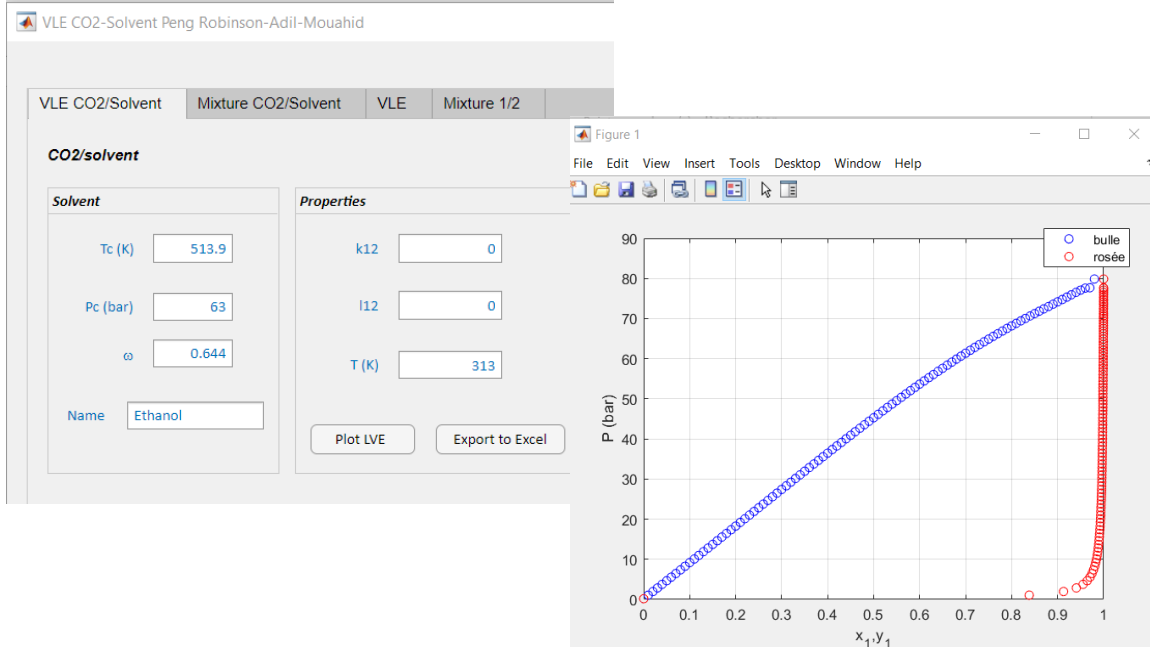
Calculation of the solubility of various types of oil in SC-CO₂ over a wide range of pressures and temperatures

The screenshot shows the 'Prediction vegetable oils' tab with a dropdown menu for solute selection. The selected solute is 'Grape seeds' at P = 350 bar and T = 45°C, resulting in a solubility of 10.47 g oil / kg SC-CO₂.

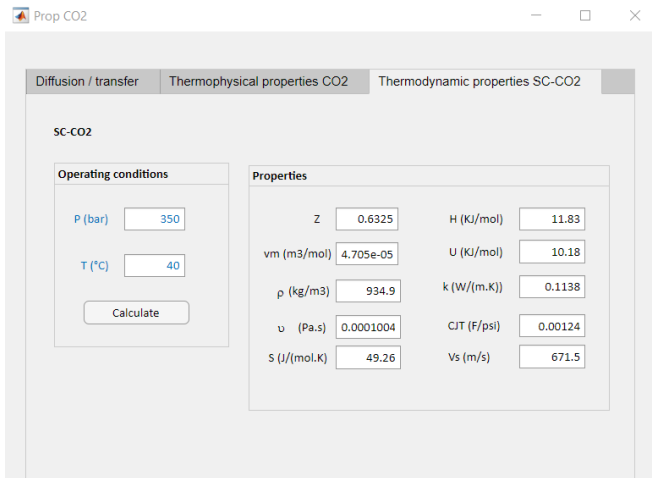
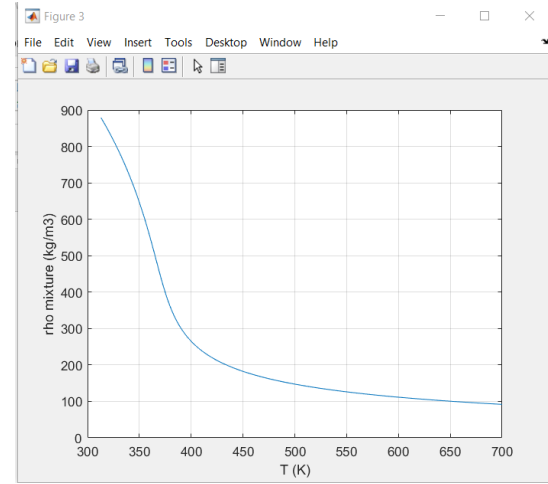
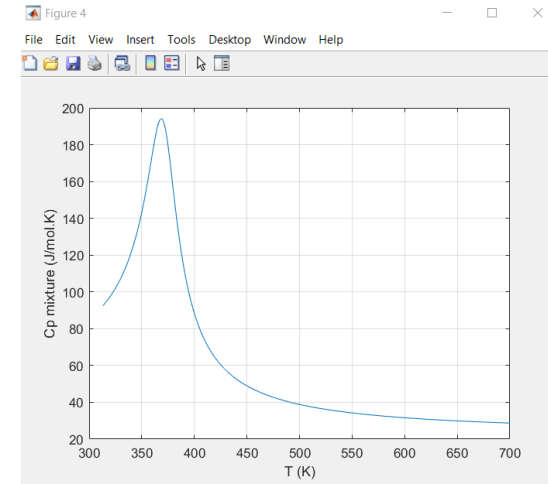
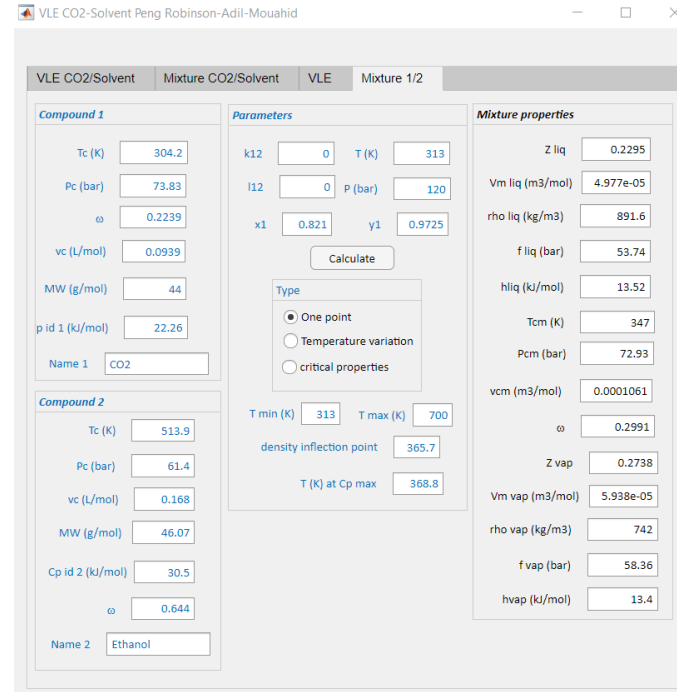
Properties	min	max
ρ (kg/m ³)	200	450
ρ _{CO2} (kg/m ³)	913	833

Calculation of pure SC-CO₂ and CO₂-solvent mixtures properties at high pressure

CO₂-solvent liquid-vapor equilibrium at high pressure and temperature



CO₂-solvent mixtures physical properties calculations : density, heat capacity, enthalpy



Calculation of pure SC-CO₂ physical properties

Can be used for particle generation process, co-solvent extraction, etc.

Determination of the best co-solvent and the optimal experimental operating conditions using Hansen method

Hansen method is applied in the case of SC-CO₂ extraction with a co-solvent

Various co-solvent can be selected and various operating conditions can be chosen

This tool help to find the best co-solvent and the optimal operating conditions for the extraction of a known compound

MATLAB App

co-solvent: ETHANOL (dropdown menu with options: ACETIC ACID, ACETONE, ACETONITRILE, DIETHYL ETHER, ETHANOL, ETHYL ACETATE, METHANOL, n-HEXANE)

P (bar): 100

T (°C): 40

volume fraction (%): 5

dispersion: 16.2

polar: 3.1

hydrogen: 5.5

vm (cm3/mol): 320

acentric factor: 1.18

Tc (°C): 497

Pc (bar): 13.9

RO: 1

Column 1	Column 2
TOLUENE	
Ra mixture	12.4757
RED mixture	12.4757
Ra SC-CO2	13.2220
RED SC-CO2	13.2220
Ra co-solvent	15.1592
RED co-solvent	15.1592
enhancement factor	5.6445

Joback method can also be used if necessary for the calculation of thermophysical properties

MATLAB App

Non ring groups:

- CH3: 2
- CH2-: 0
- >CH-: 0
- >C<: 0
- =CH2-: 0
- =CH-: 0
- =C<: 0
- =C=: 0
- =CH: 0
- =C-: 0

Ring groups:

- CH2-: 0
- >CH-: 0
- >C<: 0
- =CH-: 0
- =C<: 0

Halogen groups:

- F: 0
- Cl: 0
- Br: 0
- I: 0

Sulfur groups:

- SH: 0
- S- (non ring): 0
- S- (ring): 0

Oxygene groups:

- OH (alcohol): 0
- OH (phenol): 0
- O- (non ring): 0
- O- (ring): 0
- >C=O (non ring): 1
- >C=O (ring): 0
- O=CH- (aldehyde): 0
- COOH (acid): 0
- COO- (ester): 0
- =O (other than above): 0

Nitrogen groups:

- NH2: 0
- >NH (non ring): 0
- >NH (ring): 0
- >N- (non ring): 0
- N- (non ring): 0
- N= (ring): 0
- =NH: 0
- CN: 0
- NO2: 0

T (K): 273.15

Name: Sample

Buttons: Calculate, Export to Excel

Column 1	Column 2
T ebullition (K)	322.1100
T fusion (K)	173.5000
Tc (K)	500.5590
Pc (bar)	48.0250
Vc (cm3/mol)	209.5000

Predict

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