Predict

SC-CO_2 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 CO_2

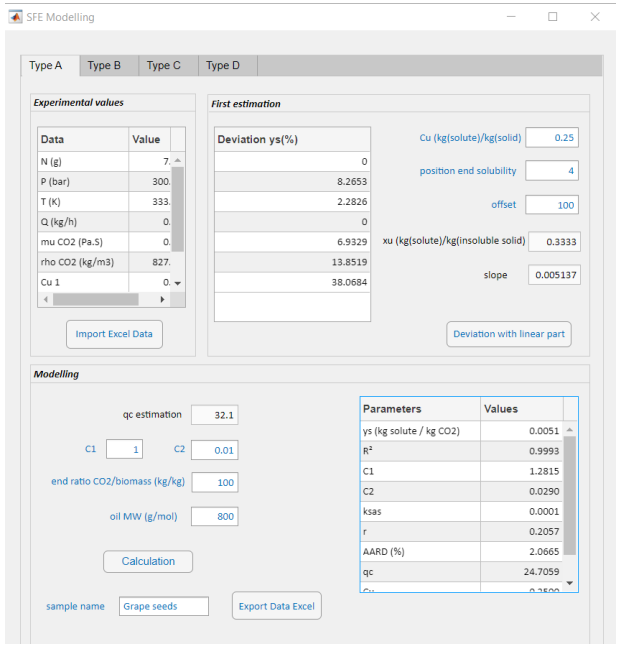
Predict has been developed after several years of academic research. It consist in several tools which can be used for the calculations or modeling of various properties

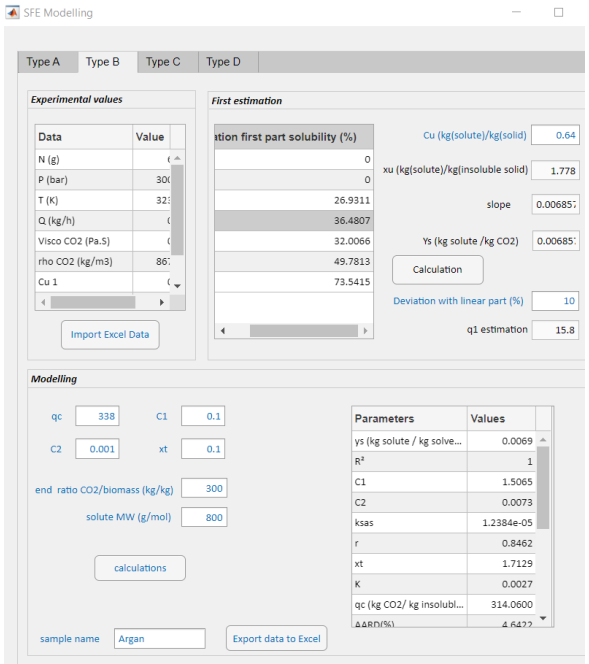
- Sovova's mathematical parameters in the case of SC-CO_2 extraction
- Chrastil, Adachi, Mendez-Santiago, Gordillon and Del Valle model parameters for the modeling of solute solubility in SC-CO_2
- Prediction of vegetable oils and various other solutes (Argan oil, grape seeds oil, beta carotene, etc.) in SC-CO2
- Hansen parameters for the choice of co-solvent
- CO_2-Solvent LVE at high pressure
- CO_2-solvent mixture properties (density, Cp, etc.)
- Scale-up calculations for SC-CO_2 extraction process
- And more !

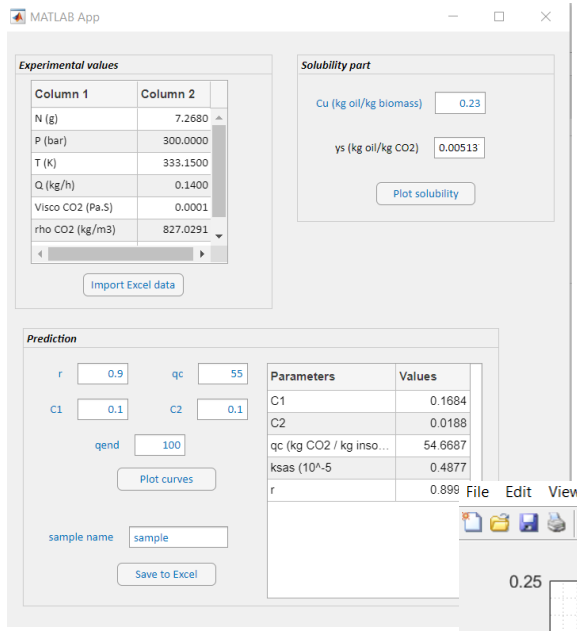
It can be used as well as for academic stuides as for industrial applications (select the optimal operating conditions parameters and avoid or reduce the ocsts of experimental studies)

SC-CO_2 extraction kinetics modeling

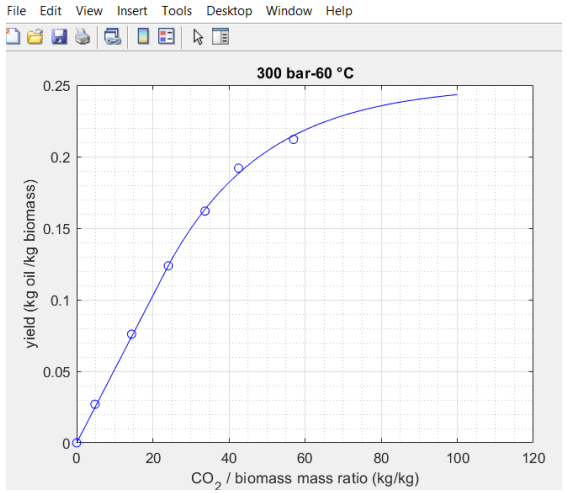
SC-CO_2 experimental extraction kinetics can be modelled using the Sovova's mathematical model
The model parameters as well as the calculated points can be exported in Excel file

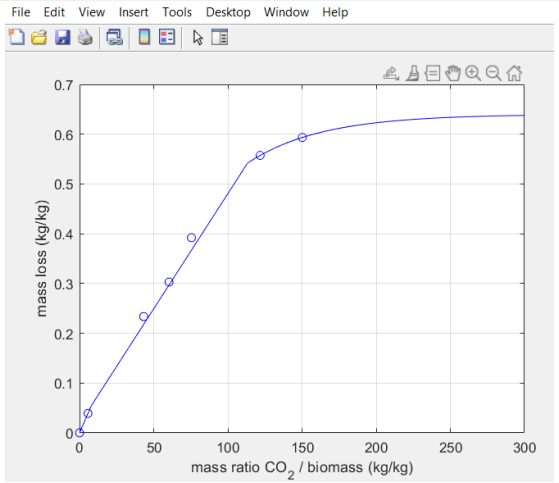




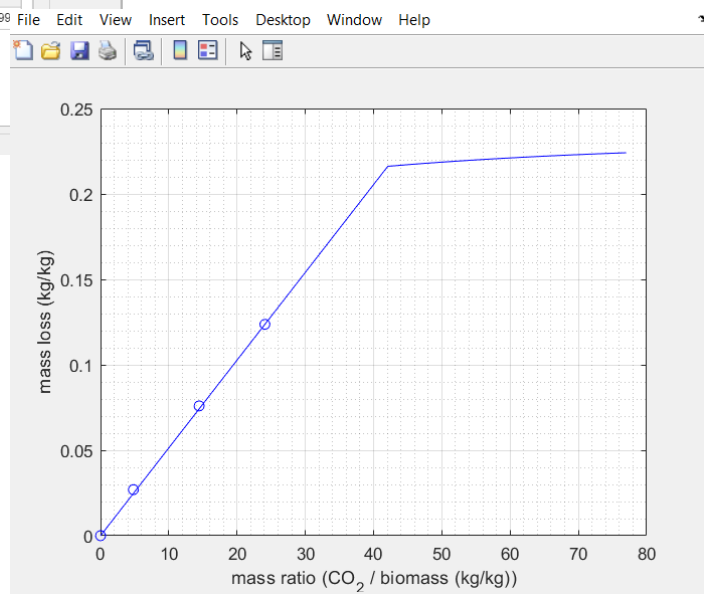


When SC-CO_2 experimental extraction kinetics is not complete, it is possible to predict a possible end of the extraction curve



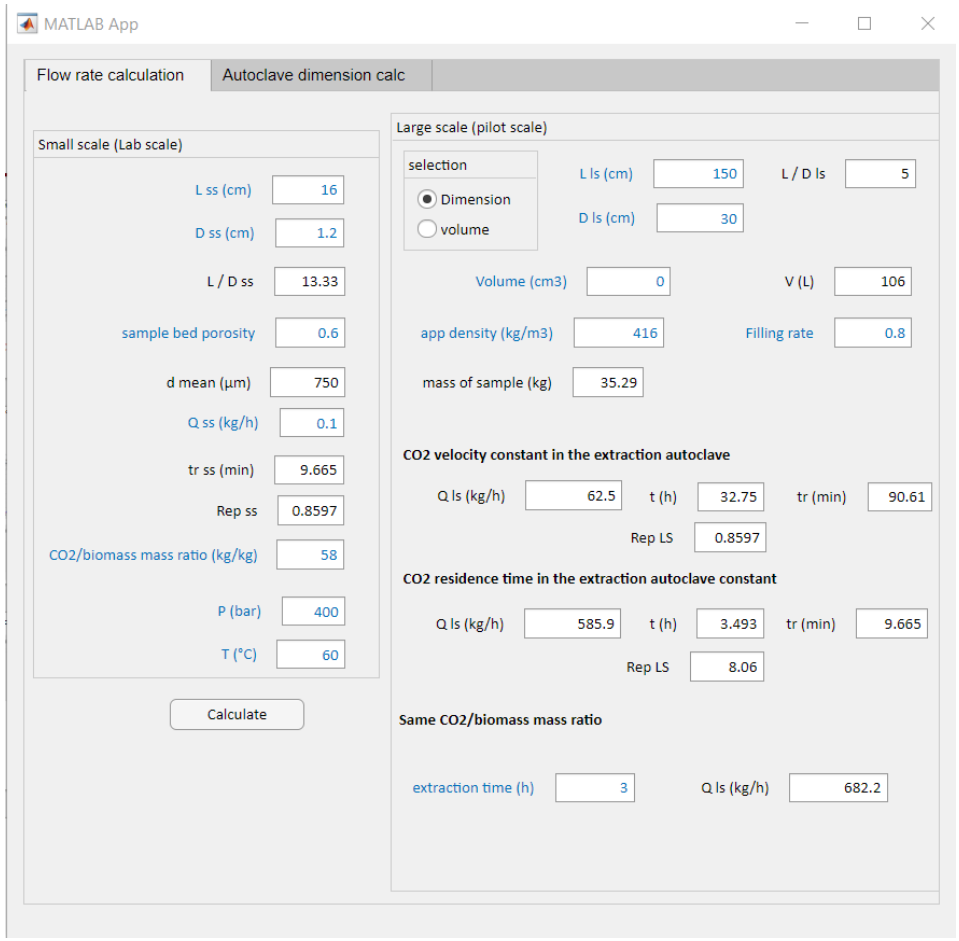


Can be used for theorical purposes and for scale up calculations



$SC\text{-}CO_2$ extraction scale up

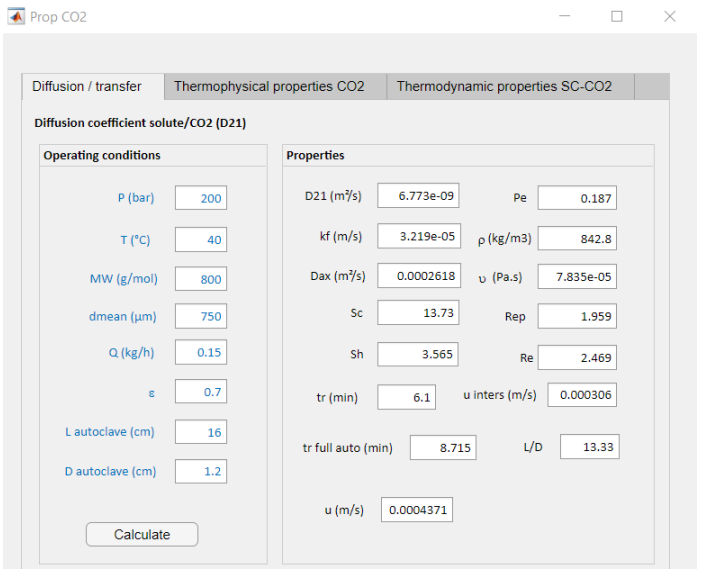
Considering the extraction kinetic established at laboratory scale, this tool is used for the calculation of $SC\text{-}CO_2$ flow rate which can be applied in pilot or industrial scale



$SC\text{-}CO_2$ diffusion and transfer properties

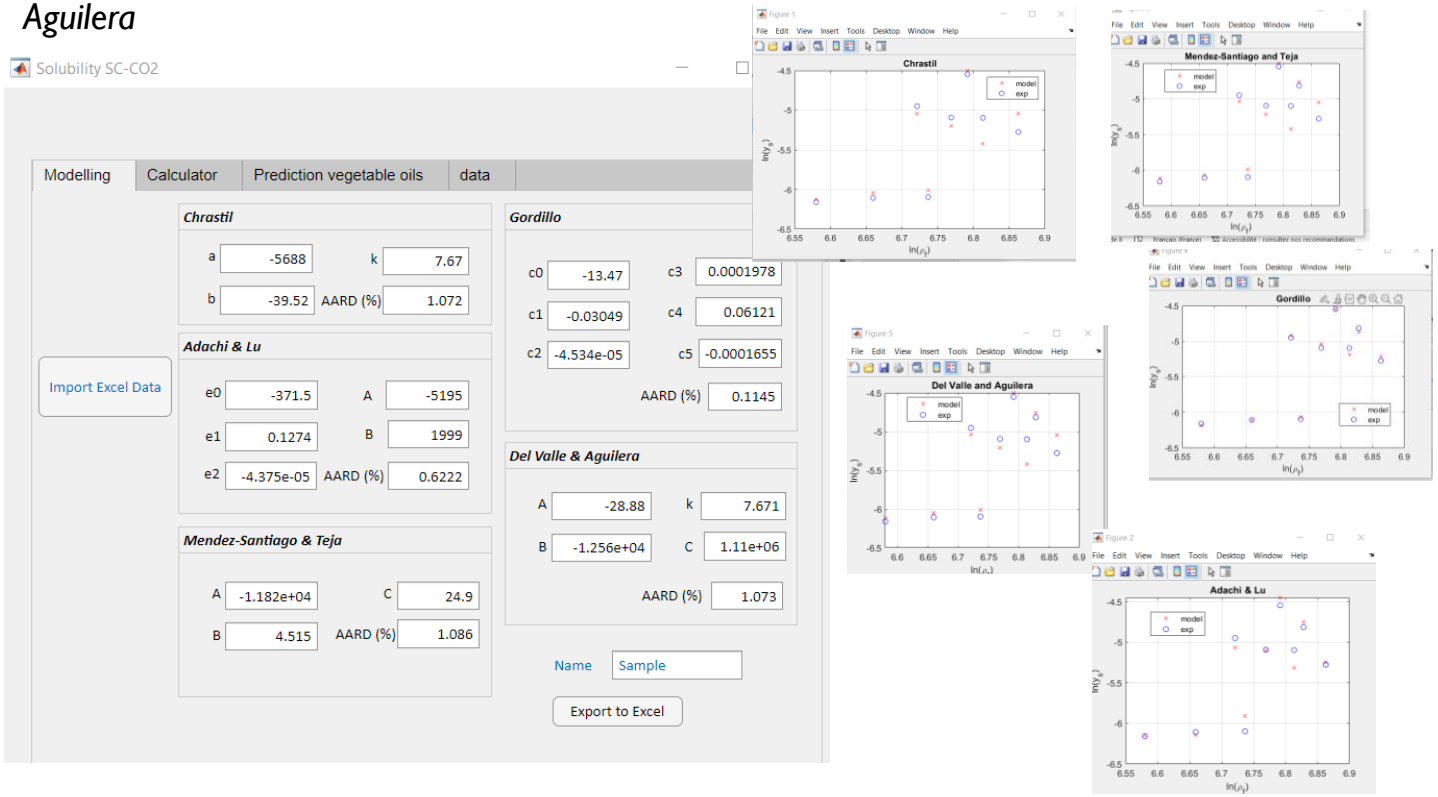
Knowing the molecular weight of solute in a porous media, this tool can calculate the diffusion and transfer properties of this solute in $SC\text{-}CO_2$

It can also be used for the calculation of flow regime in an autoclave

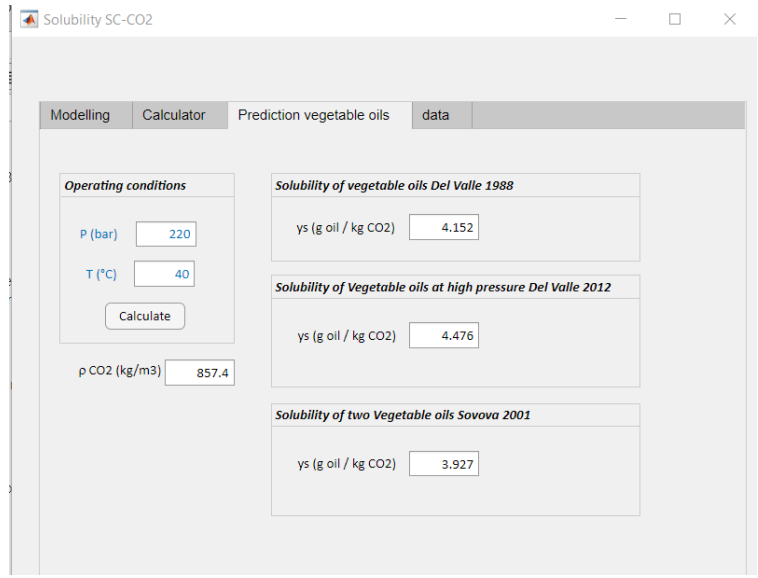


Modeling and prediction of the solubility in SC-CO_2 of various solutes

Experimental results of solute solubilities in SC-CO_2 can be modelled considering 5 models : Chrastil, Adachi & Lu, Mendez-Santiago & Teja, Gordillo, Del Devalle & Aguilera

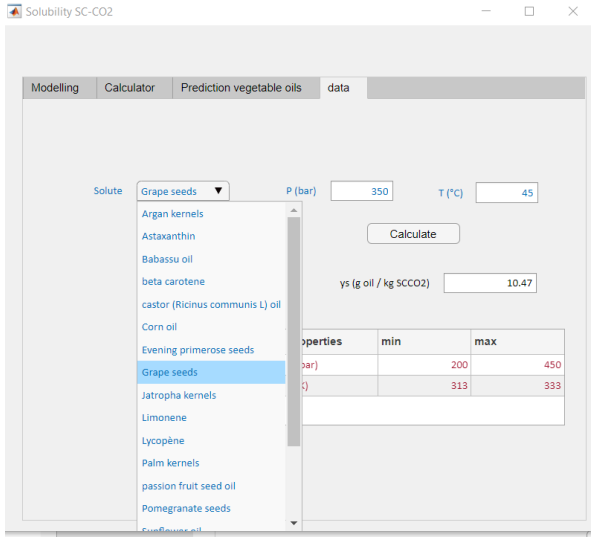


Prediction of vegetable oils solubilities in SC-CO_2 according the correlations of Sovova and Del Valle



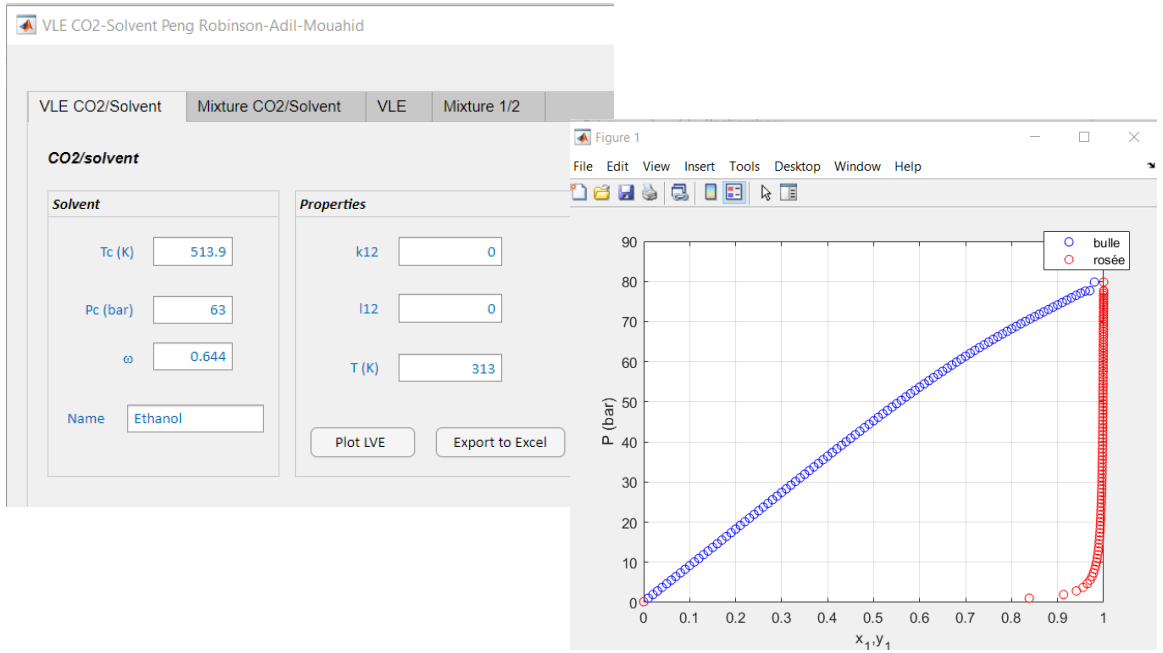
Can be used for the selection of experimental operating conditions in the case of SC-CO_2 extraction or fractionation

Calculation of the solubility of various types of oil in SC-CO_2 over a wide range of pressures and temperatures

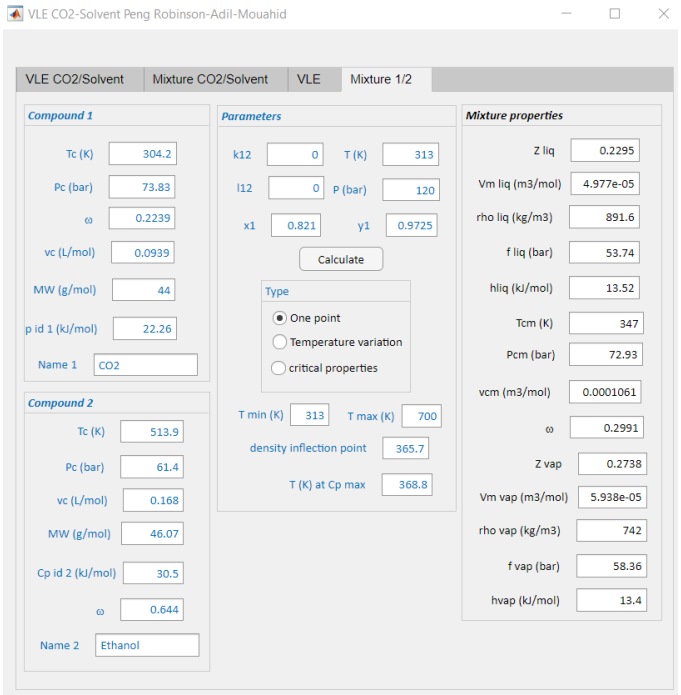


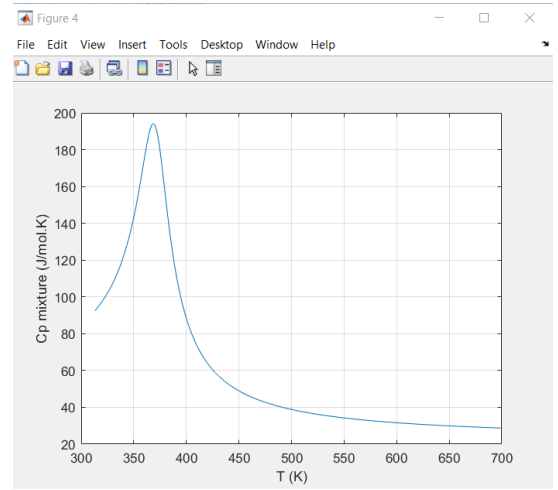
Calculation of pure SC-CO_2 and CO_2-solvent mixtures properties at high pressure

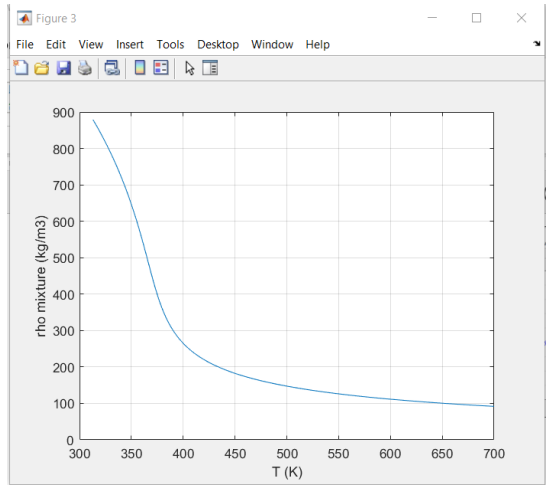
CO_2-solvent liquid-vapor equilibrium at high pressure and temperature

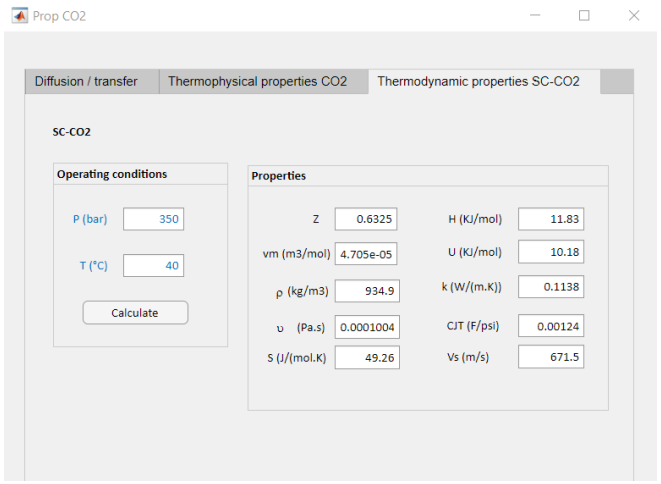


CO_2-solvent mixtures physical properties calculations : density, heat capacity, enthalpy







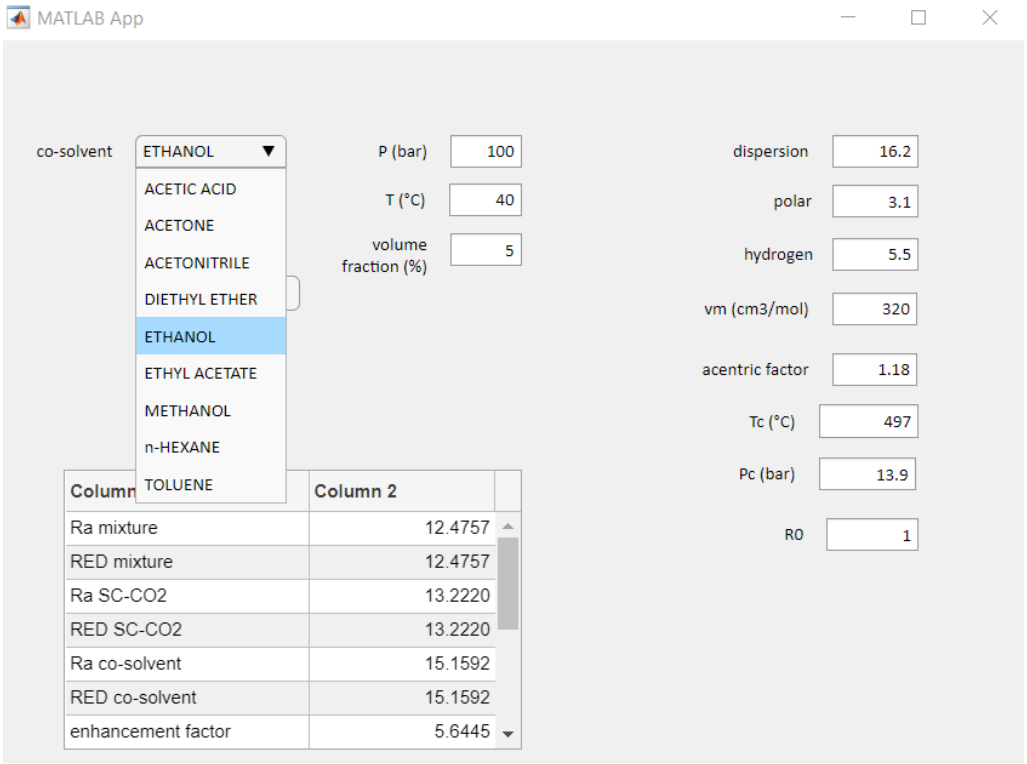


Calculation of pure SC-CO_2 physical properties

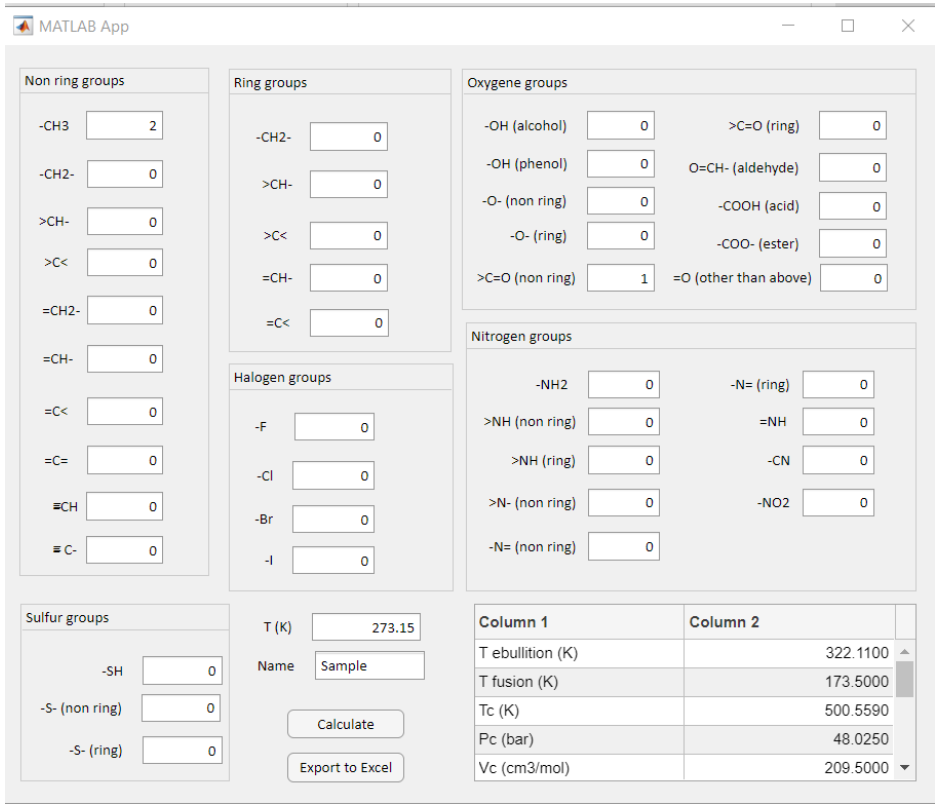
Can be used for particle generation process, co-solvent extraction, etc.

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

Hansen method is applied in the case of SC-CO_2 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



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



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SC-CO_2 modeling and simulation software

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SATT SUD-EST

ACCÉLÉRONS LE TRANSFERT DE TECHNOLOGIES

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