![pvtsim nova CCS logo]

PVTsim Nova CCS – Specialized PVT Software for CCS Simulations

Calsep introduces the CCS module, a software specialized in simulation models and features needed for CCS projects.

Specialized Models for Complex Challenges

The PVTsim Nova CSS module offers specialized models to simulate and understand complex phase equilibrium problems related to Carbon Capture and Storage (CCS). This includes analyzing the phase equilibrium challenges that CO_2-rich fluids with impurities will face during transport in pipelines, through the well, and into the depleted reservoir or saline aquifer.

The PVTsim Nova CCS module provides features that makes it a one-stop solution for modeling and evaluating CO_2 rich systems.

Thermodynamic Models
Span-Wagner, GERG-2008, Cubic EoS and Leachman.

Viscosity/Thermal Conductivity
Laesecke/Huber, CSP (CO_2), CSP, LBC, Muzny/Assael.

Verification
The accuracy of the simulations in the CCS module are documented in a comprehensive CCS report.

Simulation Options
- Flash
- Phase Envelope
- PH Phase Envelope
- Saturate with Water / Brine
- Critical Point
- Property Generator
- Hydrate
- Hydrate Phase Mapping
- Unit Operations
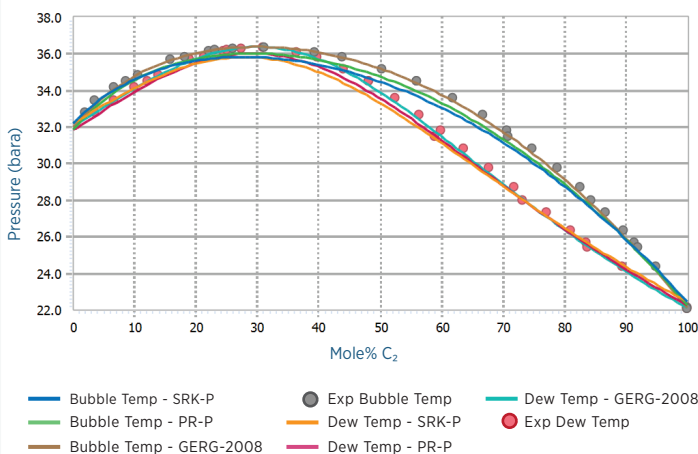- SO_x, NO_x, and NH_3 Available

CO_2 Simulation Tools
- Impact of Impurities (P-xy / T-xy plots)
- Density Tuning
- Saturate Brine with CO_2/ Impure CO_2
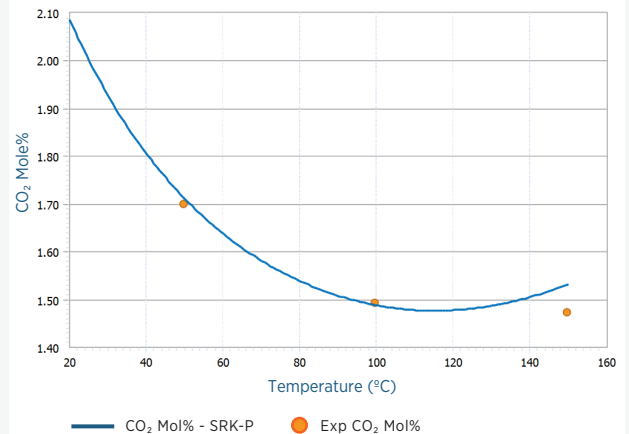- CO_2 Brine Solubility Tables

Interfaces
- OLGA and LedaFlow
- PH tables for OLGA
- HYSYS and UniSim

CO₂ Pxy plot at -3.15ºC

Legend:
- Bubble Temp - SRK-P
- Bubble Temp - PR-P
- Bubble Temp - GERG-2008
- Exp Bubble Temp
- Dew Temp - SRK-P
- Dew Temp - PR-P
- Dew Temp - GERG-2008
- Exp Dew Temp

X-axis: Mole% C₂ | Y-axis: Pressure (bara)

CO₂ solubility vs. Temperature @ 200.00 bara
NaCl + KCl + CaCl₂

Legend:
- CO₂ Mol% - SRK-P
- Exp CO₂ Mol%

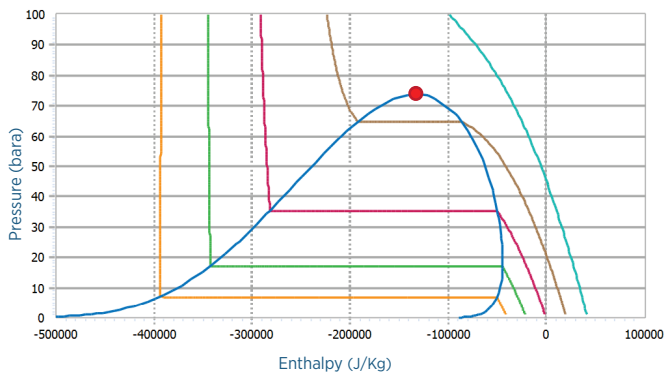X-axis: Temperature (ºC) | Y-axis: CO₂ Mole%

Updated Parameters in the CCS Module

Research and development undertaken for the CCS module has led to the estimation of new parameters, aimed at modeling the phase behavior and hydrate formation in systems involving CO_2 and water. The new parameters improve the accuracy with hydrate formation for CO_2-rich systems with very low water amounts (Corrêa and Sørensen, 2023). New parameters improving CO_2 solubility in brine calculations, as well as updated CO_2 binary interaction coefficients for better modeling of fluids with H_2, Ar, and O_2, are also included in the CCS module.
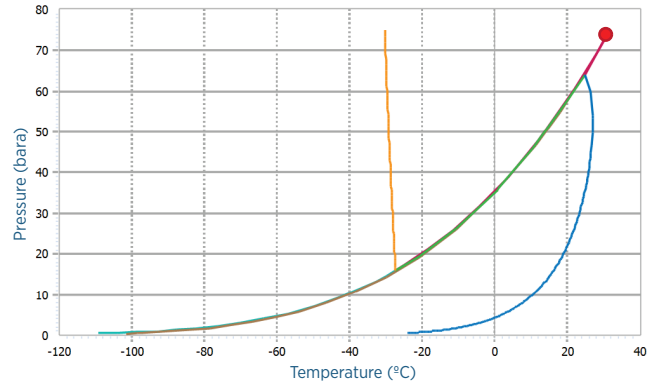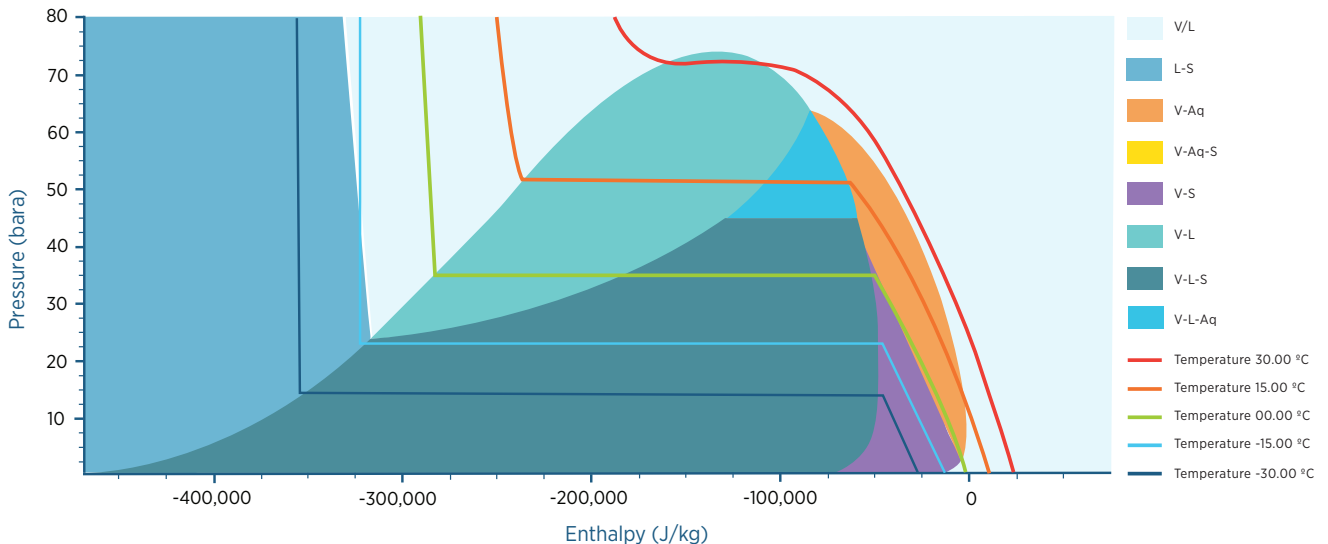
PH Phase Envelope with isotherms
CO_2 + C1

— Vap/liq mol frac 1.000	— Temperature -50.00ºC	— Temperature -25.00ºC
— Temperature 0.00ºC	— Temperature 25.00ºC	— Temperature 50.00ºC
● Critical Point		

PT Phase Envelope
CO_2 + H_2O + C1

— 2-aq	— 2-aq	— 3-aq	● Critical Point
— 2-HC	— 3-HC	— 3-HC	

Hydrate PH Phase Mapping
CO_2 + H_2O + C1

- V/L
- L-S
- V-Aq
- V-Aq-S
- V-S
- V-L
- V-L-S
- V-L-Aq
- — Temperature 30.00 ºC
- — Temperature 15.00 ºC
- — Temperature 00.00 ºC
- — Temperature -15.00 ºC
- — Temperature -30.00 ºC

Reference

Corrêa, L. F. F., & Sørensen, H. (2023). Extension of models to cover the phase behavior and hydrate formation potential of humid CO_2-rich streams at conditions relevant to CCS. 20th International Conference on Multiphase Production Technology, Nice, France. ISAVFT Ltd.

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