PVTsim Technical Overview

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INTRODUCTION

WHAT IS PVTSIM?

PVTsim is a versatile equation of state (EOS) modeling software that allows the user to simulate fluid properties and experimental PVT data. PVTsim is the primary commercial software owned, marketed, and developed by Calsep thereby ensuring continued and long term improvements to the software. PVTsim is divided into a number of modules. Clients can purchase Standard PVTsim Packages tailored for different application areas, or customize a package according to their actual needs.

WHY CHOOSE PVTSIM?

Since its first release in 1988, PVTsim has been used by over 300 of the world's leading oil & gas companies and PVT lab specialists. More than 30 years of extensive data collection and joint industry projects has made PVTsim one of the most versatile and reliable petroleum fluid simulators. Distinguishing PVTsim features include:

- Reliable & predictive reservoir fluid characterization with flexible component lumping.
- Separate input mode for extended GC analyses with option to lump C7+ isomers with carbon number fractions.
- Conversion of True Boiling Point Analysis to molar composition.
- Automatic fluid composition QC with auto-correction capability.
- Nine variations of cubic equations of state plus PC-SAFT, and GERG-2008.
- Model polar components using popular cubic EoS models SRK or PR with Huron-Vidal, CPA, or Classical mixing rule.
- Plus fluid regression that adjusts property correlations to actual fluid composition.
- Automated EoS builder including detailed tracking of regression settings and results for complete transparency.
- Regression history and audit trail automatically cataloged.
- Characterization of multiple fluids to a common EOS, with and without regression.
- Compositional variation with depth considering impact of T-gradient.
- Asphaltene phase tracking for full PT spectrum.
- Fully compositional simulation of wax deposition along pipelines.
- Viscosities of gas, oil, aqueous, oil with suspended wax, and water-oil emulsions.
- Export to over thirty of the most popular reservoir, pipeline, and process simulators for consistent fluid data across disciplines.
- Open structure technology to create customized software solutions using PVTsim thermodynamics in 3rd party software.

In an effort to continue providing the most advanced and accurate models, Calsep periodically updates models and parameters. Verification reports are published and available upon request. Examples of available verification reports include: Hydrate Verification, Mutual Solubility of Water-Hydrocarbon Mixtures, and Velocity of Sound.
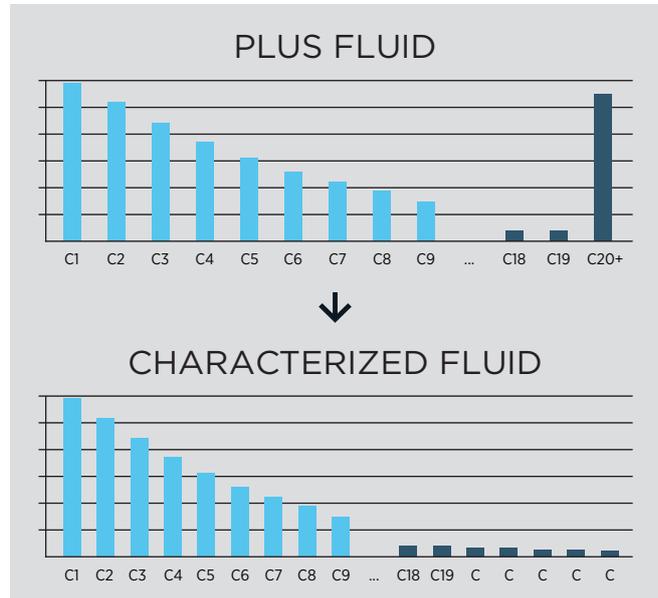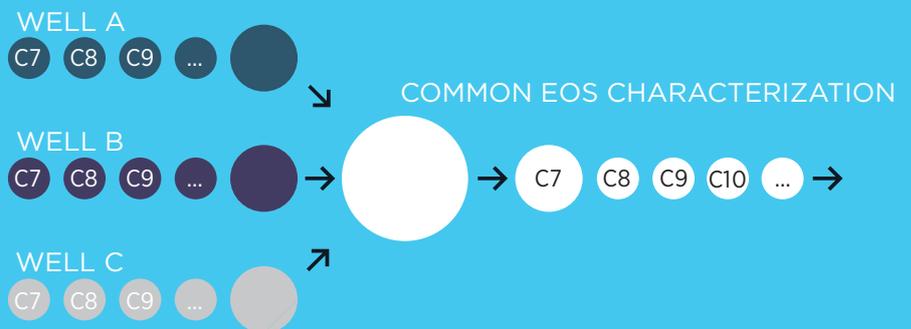
PVTsim MODULES

BASE

PVTsim provides 3 different compositional input options. One is the classical molar or weight-based fluid compositions with molecular weights and densities input for each C7+ fraction. Another input mode is for extended GC fluid analyses, which may count several C7+ isomers, but lack detailed molecular weight and density data for the heavy fractions. A True Boiling Point (TBP) Analysis for a stable oil may be converted into a molar composition and used in simulations, possibly after recombination with a gas composition to create the full reservoir fluid composition.

Nine variations of the Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) cubic equations of states (EoS) are supported with the option to use constant or temperature dependent volume translation. The PC-SAFT EoS is available for general flash and PVT simulations as well as in Asphaltene simulation. For high-accuracy gas property predictions such as gas Z-factors and dewpoints, the GERG-2008 EoS is available with non-aqueous flash calculations, phase envelope, and the property generator.

EoS models developed for reservoir fluids using a standard cubic equation of state can be readily extended to also handle water, hydrate inhibitors, and other polar components. An additional polar model

Key features included with the BASE module are:

PLUS FLUID

C1 C2 C3 C4 C5 C6 C7 C8 C9 ... C18 C19 C20+

↓

CHARACTERIZED FLUID

C1 C2 C3 C4 C5 C6 C7 C8 C9 ... C18 C19 C C C C C

can be selected from a separate drop-down menu. Both the SRK and PR EoS models can be used to model polar components using Huron-Vidal, CPA, or Classical mixing rule. Separating the model with polar components from the non-polar allows the user to first tune the fluid using the standard cubic EoS of choice followed by application of the desired polar component model.

- Fluid property database
- Input of plus, no-plus, or characterized fluid compositions
- Flexible lumping options and preset lumping schemes
- Recombination of separator oil & gas
- Mix up to 50 different fluids
- Weave up to 50 different fluids while maintaining original fluid components
- Convert ions from a standard water analysis to salt composition in mol%

WELL A
C7 C8 C9 ...

WELL B
C7 C8 C9 ...

WELL C
C7 C8 C9 ...

COMMON EOS CHARACTERIZATION
C7 C8 C9 C10 ...

OBM CLEANING

Reservoir fluid samples taken for lab analysis are sometimes contaminated with oil-based drilling mud. The Oil Based Mud (OBM) Cleaning option in PVTsim will numerically remove OBM contaminate to generate a clean reservoir fluid with the associated mud attached. It is possible to estimate the OBM contaminate composition when it is not available. PVT data measured on the contaminated fluid sample may be input for this fluid. The mud will be mixed in when simulating and regressing to experimental PVT data measured on the contaminated fluid. The resulting cleaned and possibly regressed fluid can be saved and used for reservoir fluid simulation studies.

PROPERTY GENERATOR

Customize fluid property tables to investigate trends in specific properties as a function of pressure and temperature, or generate property input for a program to which PVTsim has no dedicated interface.

Fluid properties available through the Property Generator include:

Mol %	dDensity/dT	Enthalpy	JT Coefficient
Weight %	Z-factor	Entropy	Velocity of Sound
Molar Volume	Molecular Weight	Heat Capacity (Cp)	Viscosity
Volume %	Internal Energy	Heat Capacity (Cv)	Thermal Conductivity
Density	dDensity/dP	Kappa (Cp/Cv)	Interfacial Tension

QC (QUALITY CHECK)

Ensure fluid data is reliable before characterization using this comprehensive tool, which generates a straightforward and easy to read Word report listing possible reasons for fluid quality failure. Because the reliability of PVTsim outputs depends on the quality of input fluid data, it is critical to ensure the input data is accurate and representative of the desired fluid. In case of failure, it is possible to have reasons for failure and suggested cures printed to a QC report.

Information required by the QC Module is:

• Fluid sample type: Bottomhole or separator

• Compositional analyses of the fluid samples

• Gas/oil ratio and STO oil density

• Fluid sample type: Gas, gas condensate, near-critical, oil, or heavy oil

A fully automated QC feature is also available under the PVT sim APPS section.

FLASH & UNIT OPERATIONS

Plot phase envelopes including the option to search for 3 phase regions or capture up to 5 phases in a color coded grid using Phase Mapping.

There are several different flash operations available, including:

- PT (Pressure, Temperature) including options for non-aqueous fluids, aqueous fluids, or multi-phase (up to 5 phases)
- PH (Pressure, Enthalpy)
- PS (Pressure, Entropy)
- VT (Volume, Temperature)
- UV (Internal energy, Volume)
- HS (Enthalpy, Entropy)
- K-factor (Specify K-factor)
- Split-factor (Specify split factor)
- P-Beta (Pressure, Vapor mole fraction of non-aqueous phases)
- T-Beta (Temperature, Vapor mole fraction of non-aqueous phases)
- Saturate with water (Saturate the current fluid with water at given pressure and temperature)

The PT non-aqueous, K-factor, and Split-factor flash options consider only non-aqueous components and two phases (gas and oil). The PT multi-phase option considers up to five fluid phases. The remaining flash options consider gas, oil, and aqueous phases.

Simulation results are presented in a tabular format that can be exported to a built-in worksheet where the data may be manipulated and plotted inside PVTsim or the output data can be exported to Excel. Output from a flash calculation includes:

- Phase amounts (mole%, weight%, and volume%) and compositions
- Molar volume, density, and Z-factor
- Enthalpy, entropy, Cp and Cv
- JT coefficient and velocity of sound
- Viscosity, thermal conductivity, and surface tension
- Ability to save phase compositions from a flash for use in new simulations

Volumetric properties in the output are derived from the selected equation of state. Thermal properties are derived from a combination of separate ideal gas models and the selected equation of state. The viscosity and thermal conductivity are calculated using either a corresponding states model (Pedersen modification) or the Lohrenz-Bray-Clark correlation.

It is possible to calculate viscosities of water-in-oil and oil-in-water emulsions at specified temperatures

and pressures. Users can select from the available Rønningsen (default) or Pal and Rhodes models. For each pressure and temperature input, plots will be shown of viscosity versus water volume fraction.

The Flash & Unit Operations module also includes simulation capabilities for various unit operations such as compressor, expander, valve, pump, heater, and separator. The compressor option may further be used to simulate polytropic compressions.

BASIC PVT SIMULATION & REGRESSION

Simulate standard experiments carried out in PVT laboratories including

- Constant mass (or composition) expansion

- Constant volume depletion (CVD)

- Differential liberation (DL)

- Separator test

- Viscosity experiments

Constant Volume Depletion at 82.5 °C
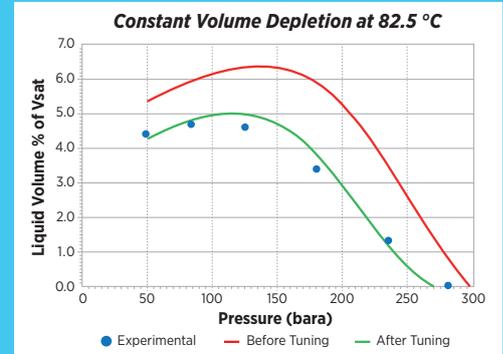
Up to five data sets for each type of experiment may be stored with each fluid composition. The data input includes measured phase compositions for experiments where phase compositions are reported. The user may define the standard (stock tank) conditions compliant with the actual PVT experiments.

In the PVT simulation input menus, the entered temperatures and pressures are shown as default values when the experiments are simulated and plots comparing experimental and simulated data are shown. However, it is important to note that no experimental data is required to simulate these experiments.

Input menus for storing the PVT data are arranged to comply with standard PVT reports, allowing for direct cut and paste of data from PVT reports available as soft copy. To get a more representative simulation of the reservoir production process, it is possible to include separator corrected values with the CVD, DL, and Depth Gradient simulations.

The output results are presented in a user-friendly format and can be exported to a worksheet where the data may be manipulated and plotted inside PVTsim or the output data can be exported to Excel. Detailed output of physical properties and compositions at each pressure stage may optionally be shown.

Using the Save Phase option, the phase composition at each stage may be stored in the database and used for subsequent calculations. This, for example, allows for studying the change in GOR of the liberated gas from a Constant Volume Depletion simulation as function of depletion pressure.

The extensive data output allows the users to cross check the experimental data with simulated values. PVTsim can generate a comparison of all experimental and simulated PVT data input for a fluid in one click using the "Compare with Experimental PVT Data" button. Plots and tables comparing simulated and measured PVT data and equilibrium phase compositions along with percent deviation are provided as output.

It is also possible to perform a mass balance check on experimental data for the Separator Test, DL, Equilibrium Contact, and Multiple Contact experiments by using the Material Balance Check button. The output from a Material Balance Check is a report providing Component Molar Balance tables which compare the difference in inlet and outlet molar compositions, and

Overall Mass Balance tables comparing the mass in at the first pressure stage vs. mass out at each subsequent pressure stage and the mass of stock tank oil in the last stage.

Regression may be needed when developing an EOS model to match available PVT data. This is a

primary step for a heavily lumped fluid model to be exported to a compositional reservoir or flow simulator. Regression in PVTsim may start with a plus fluid composition or an already characterized composition. Fluid regression results in a tree structure in the database where regressed fluids are child fluids of the original root fluid. This process allows the user to keep track of the history of tuned fluids. The child fluid is indexed in the database through a multilevel list where the result of a regression of fluid #2 would be a child fluid indexed as fluid #2.1, and so on. After each regression, the result is stored as a temporary fluid. Temporary fluids can be saved permanently in the database.

The regression history of a fluid, including adjusted parameters and selected weighting, is automatically written and kept with a fluid in the Reg History tab.

An EoS modeling tool, which has automated the fluid characterization, regression, and lumping into a single step is available under the PVTsim APPS section.

Composition varies with depth in a reservoir. Based on a sample composition, sample depth, and PT-conditions, PVTsim simulates the variation with depth in composition, pressure, GOR and a number of physical properties along with location of the gas-oil contact, if such exists. Simulations may be carried out isothermally or with application of a vertical temperature gradient modeled using the theory of irreversible thermodynamics.

For fluids with asphaltene components, the Asphaltene Tar Mat option calculates the variations in composition, saturation point, and asphaltene onset point with depth and identifies the location of a possible tar mat.

EOR, MULTIFLUID PVT & REGRESSION

Experiments used to study gas injection and miscibility of fluids are time consuming and expensive. Careful planning of which experimental conditions to use is therefore important. Standard EOR lab experiments available for simulation in PVTsim include:

- Swelling test
- Equilibrium contact
- Multiple contact
- Slim tube

Injection gases used in EOR PVT experiments can be entered with a fluid and assigned to a particular EOR PVT experiment. A swelling test may be performed to simulate the swelling of a reservoir fluid during gas injection. It is possible to include CME and viscosity data for the mixture at each stage and use this data for regression. The critical point can be input with the swelling data and used for regression. A slim tube experiment can be simulated and provide results for recovery and composition of the produced fluid at the actual reservoir pressure. The multi-component MMP option gives a fast and reliable answer about the minimum pressure required to develop a miscible drive.

In many cases, it is desired to make a single EoS model for multiple fluids, also known as a Common EoS model. In a Common EoS model, multi-

ple fluids utilize the exact same EoS parameters and differ only by the molar amounts of each component. For example, fluid compositions will vary with horizontal location and depth in the reservoir. If these fluids are from the same reservoir, though they may vary by molar composition, each fluid can be represented using the same equation of state model.

With the common EoS option in PVTsim, it is possible to characterize from 2 to 50 different plus and/or no-plus fluids to a common EoS. When developing the common EOS model, it is possible to regress to PVT data for each of the individual fluid compositions.

Common EoS models for fluid samples at varying depths can also be tuned to match the measured compositional gradient with depth.

ASPHALTENE

Simulate the conditions at which asphaltene precipitates for a given fluid composition, tune to asphaltene onset pressure, perform a PT flash, and determine weight % of asphaltene components in stock tank oil (STO). This module allows calculation of the entire asphaltene phase envelope for the complete PT spectrum. For a given temperature, you may also determine the pressure range

at which asphaltene precipitation occurs for various amounts of injection gas. The effect of gas injection on the asphaltene precipitation conditions can be studied using a Px-curve option. The asphaltene model has been developed based on experimental live oil asphaltene precipitation data and supports all Cubic EoS models, PC-SAFT, and the CPA model.

WAX

Evaluate wax formation conditions from an ordinary compositional analysis or, if available, the n-paraffin distribution may be entered with the fluid. Using the wax module, it is possible to quantify the amount of wax precipitate, run flash calculations, and plot wax formation conditions through PT curves. If data is available, it is also possible to tune the wax model to an experimental cloud point or to experimental wax content in the stock tank oil. The amount of wax precipitate may be calculated as a function of P for constant T or as a function of T for constant P and quantitative flash calculations will consider gas, oil and wax. Additionally, there is an option to account for the influence of wax inhibitors.

Oil with suspended wax particles, which exhibits a non-Newtonian viscosity behavior, can be modeled with PVTsim. Viscosity plots can be made of wax in oil suspensions for varying shear rates. Fluids tuned in the wax module may be used in the PVTsim DepoWax module, a pipeline simulator considering wax deposition and the effect on viscosity of wax particles suspended in the oil phase.

Wax PT Curve Phase Envelope (Wax)

— Wax PT Curve   — Phase Envelope (Wax)   ● Critical Point (Wax)
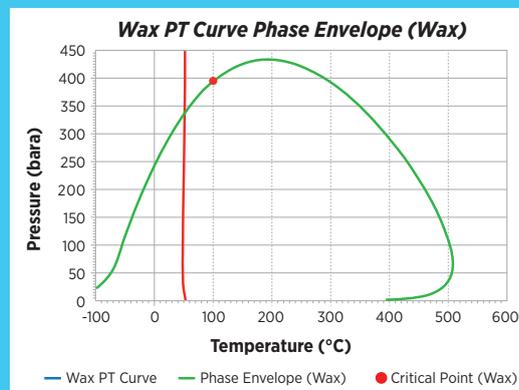
DEPOWAX

Analyze the nature and extent of wax deposition along a pipeline by calculating pressure drops, temperature profile, position and thickness of wax deposited with a fully compositional profile. Wax appearance temperature and wax amount can be tuned in the wax module prior to initiating a wax deposition simulation. The RRR and Matzain wax deposition models are available. Being fully compositional, DepoWax is well suited for pipelines with multiple inlets.

With the fluid properly characterized, all the user has to input is pipeline geometry, (xy-coordinates, inner diameter, roughness, ambient temperature, and insulation) inlet P&T, and inlet flow rate. Default values are automatically set up for remaining properties (i.e. section lengths, wax diffusion coefficients, and laminar film thickness), but the user also has the option to manually input parameters.

To properly account for the heat of phase transitions (evaporation, condensation and solidification) the temperature profile in the pipeline is determined by carrying out PH (Pressure-Enthalpy) flash calculations. The deposition mechanism is assumed to be molecular diffusion across the laminar sub-layer near the wall.

The influence on the viscosity of wax particles suspended in the oil phase is considered via a shear rate dependent (non-Newtonian) viscosity model. Influence of wax inhibitors on the viscosity can be accounted for. The module offers the choice between four different methods for calculating heat transfer:

- Sieder-Tate
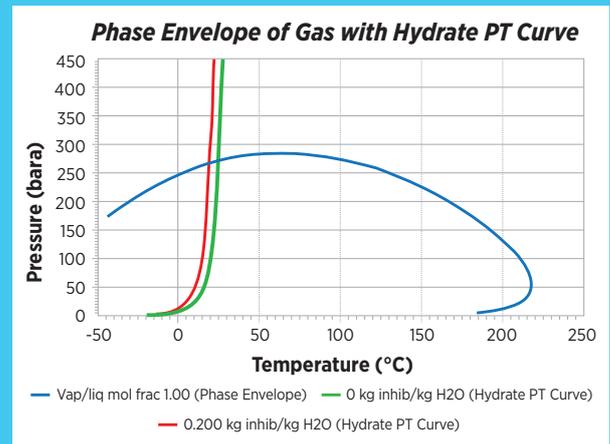- Dittus-Boelter
- Petukhov
- Petukhov-ESDU

The simulation results give information with respect to time for pressure drop, temperature profile, and position and thickness of deposited wax.

HYDRATE

PVTsim can accurately simulate hydrate formation conditions of gas and oil mixtures. Depression of hydrate formation temperature of the most commonly used hydrate inhibitors (MeOH, EtOH, MEG, DEG and TEG) can be simulated as well as the loss of inhibitors to the hydrocarbon phases.

- Hydrate formation conditions
- Amount of hydrates formed
- Amount of inhibitor needed to suppress formation
- Effect of salts on hydrate formation
- PT & PH flash options

Phase Envelope of Gas with Hydrate PT Curve

— Vap/liq mol frac 1.00 (Phase Envelope) — 0 kg inhib/kg H2O (Hydrate PT Curve)
— 0.200 kg inhib/kg H2O (Hydrate PT Curve)

The flash options automatically provide amounts and types of hydrates (structures I, II and H) as well as hydrocarbon and aqueous phases, solid salt phases, and ice. The Hydrate module supports all cubic equations and the CPA model.

SCALE

Determine the amount of scale (salt precipitate) that will emerge from formation water and seawater mixtures. This module takes into account CO2 and H2S equilibrium pressures in the water, pH, as well as the effect of the other ionic species (primarily NaCl, CaCl2, and KCl).
The PVTsim scale module considers precipitation of most common salts including:

- $BaSO_4$
- $CaSO_4$
- $SrSO_4$
- $CaCO_3$
- FeS
- $FeCO_3$

Pitzer's activity coefficient model is used. The risk of scale formation over an entire PT grid can be viewed through 2D and 3D plot options.

ALLOCATION

Allocate the export streams of gas, oil, and water (aqueous) back to 2 – 50 production streams. Export flow streams are reported at reference conditions, which by default are the selected standard conditions.

PVTsim APPS

AUTO QC & CORRECTION

Most of today's compositions come from Gas Chromatography analysis where plus fraction properties are derived from bulk fluid properties, not directly measured. This practice can result in a high degree of uncertainty on reported plus fraction properties. The process for evaluating and correcting reported compositional data has been automated into a single step, which checks whether the reported plus fraction properties of a fluid are consistent with the rest of the reported data for a fluid. In the event of failure, the composition is automatically adjusted with details of the correction procedure reported in the output datasheet. A new corrected fluid is added to the database and selected for simulations while the original fluid is preserved in the database.
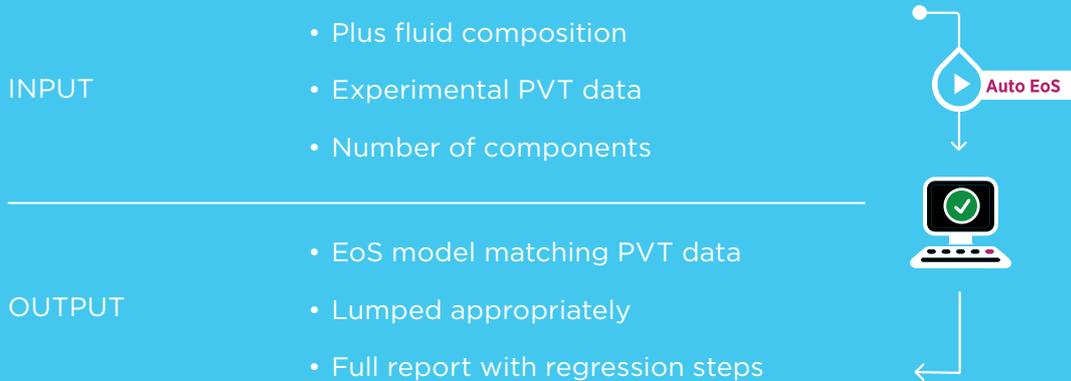
AUTO EOS

With a plus fluid in the database, Auto EoS will deliver a fully tuned and lumped EoS model. Select from a list of available EoS models, define the final number of components for the model, and PVTsim will automatically include and rank available PVT experimental data for tuning. For complete transparency, Auto EoS regression steps are reported in detail including plots and datasheets illustrating parameters adjusted and the match before and after tuning.

SEPARATION

Simulate an overall separation process in a way that is true to the actual facility design without requiring the level of detail needed for most process simulators. A characterized fluid and the temperatures and pressures of each separation stage are the only required input. Generated output includes formation volume factors (Bo, Bg), process GOR, stream compositions and PVT properties. Once a process flowsheet is created, it can be saved in a database and accessed through the PVTsim interface menus to generate black oil tables with accurate gas and oil properties.

INPUT
- Plus fluid composition
- Experimental PVT data
- Number of components

OUTPUT
- EoS model matching PVT data
- Lumped appropriately
- Full report with regression steps

Auto EoS

OPEN STRUCTURE

OPEN STRUCTURE

Open structure gives access to PVTsim thermody-namics and fluid databases without opening the PVTsim interface. Open structure code can be written in most common programming languages including Visual Basic, C++, C#, and MatLab. This allows the user to work from in-house applications and create customized solutions to unique prob-lems using PVTsim thermodynamics.

3RD PARTY SOFTWARE OPEN STRUCTURE	PVTsim NOVA

CONSISTENT RESULTS

DATA ACCESS LAYER
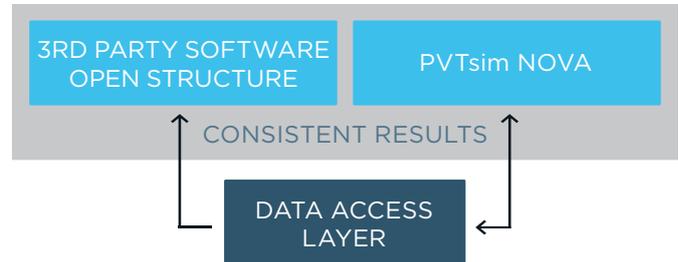
FLASH OPEN STRUCTURE

Flash Open Structure allows the following flash calculations and can also be used as a property generator:

- PT (Pressure, Temperature) including options for non-aqueous fluids, aqueous fluids,
   or multi-phase (up to 5 phases)

- PH (Pressure, Enthalpy)

- PS (Pressure, Entropy)

- VT (Volume, Temperature)

- UV (Internal energy, Volume)

- HS (Enthalpy, Entropy)

- K-factor (Specify K-factors)

- Split-factor (Specify split factors)

- P-Beta (Pressure, Vapor mole fraction of non-aqueous phases)

- T-Beta (Temperature, Vapor mole fraction of non-aqueous phases)

All open structure calculation options are fully consistent with calculations carried out in PVTsim directly.

HYDRATE OPEN STRUCTURE

Hydrate Open Structure gives access to the following calculation options:

- PT and PH hydrate flash

- Hydrate formation PT curve

- Hydrate formation pressure

- Hydrate formation temperature

- Minimum inhibitor

WAX OPEN STRUCTURE

Wax Open Structure gives access to the following calculation options:

- PT wax flash

- Wax formation PT curve

- Wax formation temperature

INTERFACES

PVTsim includes modules to generate PVT input tables to a number of external (non-Calsep) programs. Tables may contain physical, compositional, or black oil properties. Interface modules provide easy export to the following popular reservoir, process, and flow assurance programs:

- Eclipse (100, Gi (200), and 300 (incl. import))
- CMG (IMEX, GEM, and STARS)
- Nexus (Comp and Black Oil)
- VIP (Comp and Black Oil)
- More (EOS and Black Oil)
- Prosper/Mbal (incl. Prosper EOS import)
- Saphir
- tNavigator
- OLGA
- OLGA Wax
- LedaFlow
- Pipesim
- Multiphase meters
- Pipephase
- Hysys
- PRO/II
- UniSim
- WELLCAT
- WePS
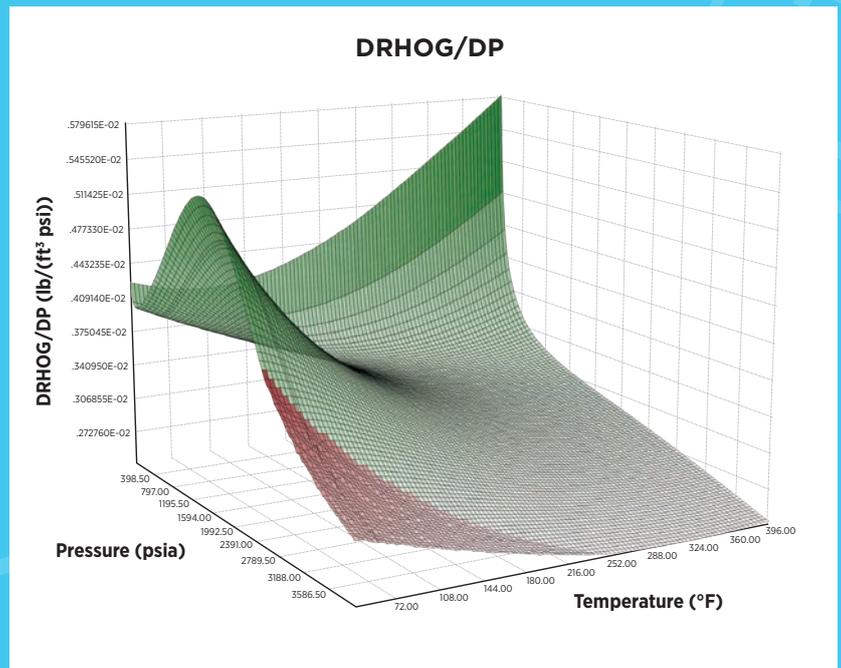
OLGA Plotting Tool

Access to each interface can be purchased as a module, individually or in packages.

It is possible to visually observe trends and identify potential problem areas in the table/black oil files for reservoir simulator Eclipse and multiphase flow simulator OLGA using the available plotting tools in PVTsim. The plotting tool for the OLGA interface allows plotting in 2D and 3D formats and provides a summary of any illegal or non-numerical values which can be corrected at the click of a button. In the plots, real data is marked with a green color, while imaginary data is marked with a red color.

LICENSING & MAINTENANCE

PVTsim licenses are available as Local Area Network (LAN) licenses which are convenient for multiple users at the same site who can access a local server. Network licenses are run using the FLEXlm license manager. Stand-alone licenses are also available as a dongle that can be plugged into the USB drive of any computer.

Calsep offers a maintenance arrangement for an annual fee. This fee covers any updates in PVTsim, bug fixes, and superior technical support from Calsep consultants.

To run PVTsim, minimum hardware requirements include: 1 Gb RAM and 1 Gb free disk space, 1280 x 800 pixels screen resolution, and a Windows operating system including Windows Vista, Windows 7, Windows 8, and Windows 10.

STANDARD PVTsim PACKAGES

Popular PVTsim modules have been collected into standard packages offered for a lower price when compared to paying for each module individually. The different packages target the needs of different application areas. The following table summarizes the modules and interfaces included with each package:

MODULES	Basic PVT	PVT Lab	Reservoir	PVTsim for OLGA/ LEDAFLOW	Flow Assurance	Wax Deposition	Premium PVT	Full Package
BASE	X	X	X	X	X	X	X	X
OBM CLEANING		X	X		X	X	X	X
PROPERTY GENERATOR		X	X		X	X	X	X
QUALITY CHECK (QC)		X	X				X	X
FLASH & UNIT OPS				X[1]	X		X	X
BASIC PVT SIMULATION & REGRESSION	X	X	X				X	X
EOR AND MULTIFLUID PVT & REGRESSION		X	X				X	X
HYDRATE				X[2]	X		X	X
WAX					X	X	X	X
ASPHALTENE					X		X	X
SCALE					X		X	X
ALLOCATION							X	X
DEPOWAX						X		X
APPS								
CREATE EOS MODEL			X				X	X
SEPARATION							X	X
OPEN STRUCTURE								
OPEN STRUCTURE FLASH								X
OPEN STRUCTURE HYDRATE								X
OPEN STRUCTURE WAX								X
INTERFACES								
ECLIPSE	X		X					X
VIP			X					X
MORE			X					X
CMG			X					X
NEXUS			X					X
PROSPER/MBAL			X					X
SAPHIR			X					X
tNavigator			X					X
OLGA				X				X
LEDAFLOW				X				X
PIPESIM								X
MULTIPHASE METERS								X
HYSYS								X
PRO/II								X
UniSim								X
PIPEPHASE								X
WePS								X
WELLCAT								X

X[1]: Includes only the 3-phase aqueous flash option.
X[2]: Includes only the Hydrate PT curve option.

For more information
please visit us at
www.calsep.com
or contact our office
in your region:

calsep