Reservoir engineering workflow to construct compositional models

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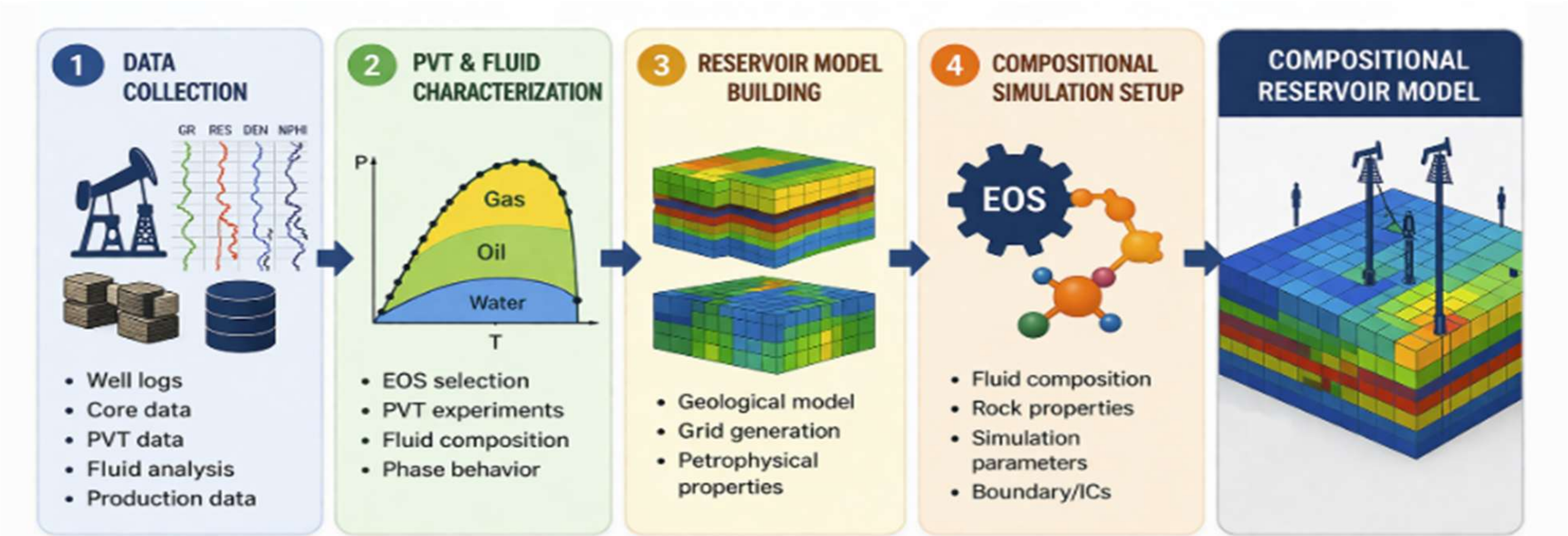

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innovation for life

Objectives

- Explain the differences and assumptions between the Black-Oil and Compositional models
- Overview on EOS theory
- Reservoir engineering workflow to construct compositional models
- Compositional PVT modeling

Compositional / Black Oil model

Compositional simulation means that the fluid properties depend on Pressure, composition (& temperature).

- **EOS parameters for each component (Pc, Tc, Vc, ...) - equilibrium between phases, phase density**
- **Flash calculation (phase fractions, compositions)**
- Reservoir rock properties
- SCAL (Kr, Pc)
- Boundary conditions (wells ((rate, pressure, temperature and composition), aquifers)
- Initial reservoir condition (pressure, temperature and composition)

Black-oil simulation means that the fluid properties depend on Pressure (& temperature). They don not depend on the composition.

- **Simplified Fluid description PVT for each phase** (PVTW, PVTO, PVTG,PVDG, PVDO....)
- Reservoir rock properties
- SCAL (Kr, Pc)
- Boundary conditions (wells (rate, pressure, temperature) , aquifers)
- Initial reservoir condition (pressure, temperature and phase saturation)

Black Oil mathematical model

Water

$$\frac{\partial}{\partial t}(\phi_{ref} m_\phi b_w s_w) + \nabla \cdot (b_w \mathbf{v}_w) + q_w = 0.$$

Oil

$$\frac{\partial}{\partial t}(\phi_{ref} m_\phi (b_o s_o + r_{og} b_g s_g)) + \nabla \cdot (b_o \mathbf{v}_o + r_{og} b_g \mathbf{v}_g) + q_o = 0.$$

Gas

$$\frac{\partial}{\partial t}(\phi_{ref} m_\phi (b_o s_o + r_{og} b_g s_g)) + \nabla \cdot (b_o \mathbf{v}_o + r_{og} b_g \mathbf{v}_g) + q_o = 0.$$

$$s_w + s_o + s_g = 1$$

$$p_{c,ow} = p_o - p_w$$

$$p_{c,og} = p_o - p_g$$

$$\mathbf{v}_g = -\lambda_g \mathbf{K}(\nabla p_g - \rho_g \mathbf{g})$$

$$\mathbf{v}_o = -\lambda_o \mathbf{K}(\nabla p_o - \rho_o \mathbf{g})$$

$$\mathbf{v}_w = -\lambda_w \mathbf{K}(\nabla p_w - \rho_w \mathbf{g})$$

Basic Assumptions:

Fluid Components: Three phase - oil, gas, and water
Phase Behavior: PVT tables
Component Transfer: Simple gas-oil ratio relationships
Compositional Changes: No real components are used. Formulation is not physically consistent.

Compositional mathematical model

$$\frac{\partial}{\partial t}\left[\phi \textstyle\sum_{\alpha=1}^{n_p} \rho_\alpha S_\alpha x_{\alpha k}\right] = -\vec{\nabla} \cdot \left[\textstyle\sum_{\alpha=1}^{n_p} \rho_\alpha x_{\alpha k} \vec{v}_\alpha\right] + q_k$$

Composition Fraction $z_k = \frac{\sum_{\alpha=1}^{n_p} \rho_\alpha S_\alpha x_{\alpha k}}{\rho}$

Mixture Density $\rho = \sum_{\alpha=1}^{n_p} \rho_\alpha S_\alpha$

Composition Conservation $\sum_{k=1}^{n_c} z_k = 1$

$$\sum_{j=1}^{np} S_j = 1 \qquad \sum_{i=1}^{nc} x_{ij} = 1 \qquad u_j = -\frac{kk_{rj}}{\mu_j} \nabla \Phi_j$$

$$P_{cog} = P_o - P_g$$

$$P_{cow} = P_w - P_o$$

$$\rho_{\alpha(P_\alpha, T, x_{\alpha k})} \qquad \mu_{\alpha(P_\alpha, T, x_{\alpha k})}$$

$$\frac{x_{gk}}{x_{ok}} = K_{kgo}\,(P, T, x_{\alpha k})$$

$x_i = \frac{z_i}{1+V(K_i-1)}$ and $y_i = \frac{K_i z_i}{1+V(K_i-1)}$

From which

$$\sum_{i=1}^{N} (y_i - x_i) = \sum_{i=1}^{N} \frac{z_i(K_i - 1)}{1 + V(K_i - 1)} = 0$$

- The equation is called **Rachford-Rice** equation

Basic Assumptions:

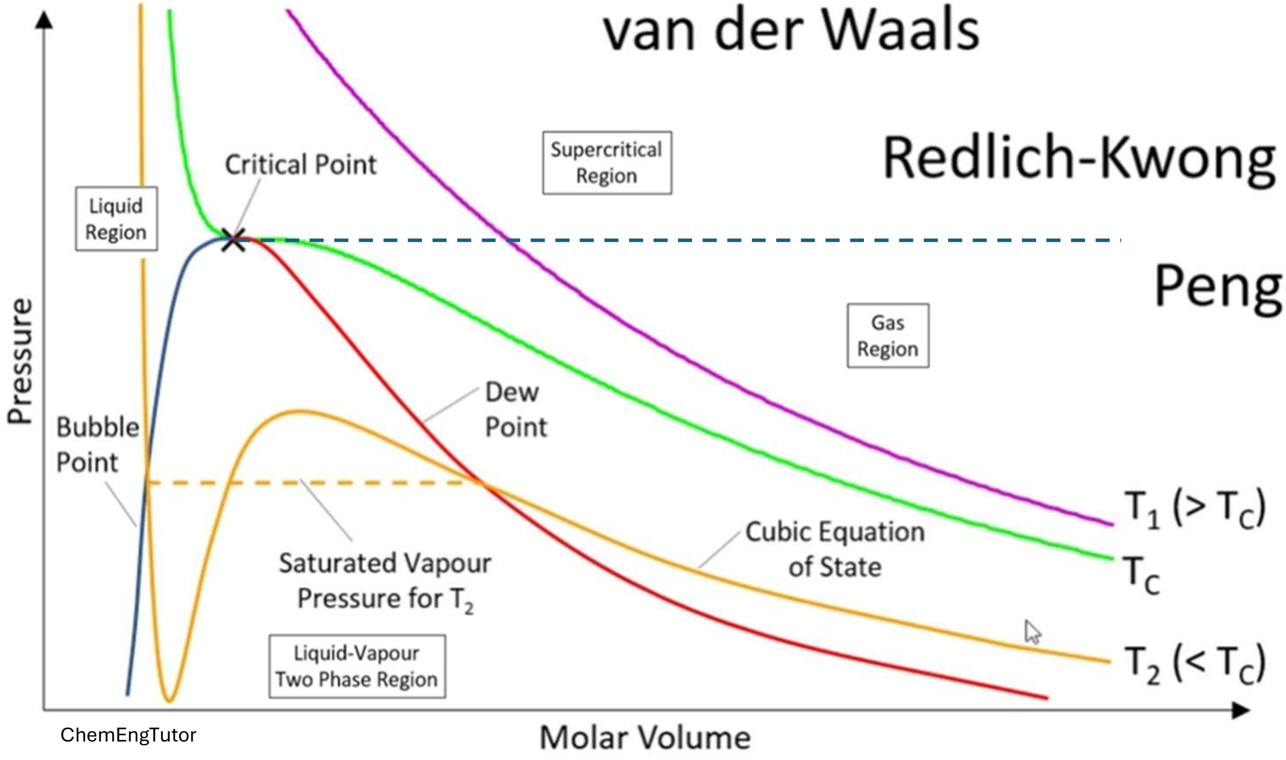
Fluid Components: Multiple individual hydrocarbon components (C1, C2, C3, etc.) plus non-hydrocarbons
Phase Behavior: Equation of State (EOS) calculations.
Component Transfer: Rigorous mass transfer between phases
Pressure-Temperature Effects: Full thermodynamic equilibrium calculations
Compositional Changes: Tracks individual component fractions
Equilibrium Calculations: Flash calculations at each time step / K-Values

Applications

- ➢ Compositional model
- ✓ Gas injection
- ✓ Miscible flooding
- ✓ Carbon dioxide flooding
- ✓ Reservoirs with fluid compositions near the bubble point
- ✓ Reservoirs with compositional gradients caused by gravity
- ✓ High T and high P reservoirs
- ✓ Thermal EOR
- ✓ Chemical EOR
- ✓ CO2 (Gas, H2) storage in depleted fields and aquifers
- ✓ Gas condensate – volatile oil reservoirs

- ➢ Black oil model
- ✓ Natural depletion
- ✓ Water injection
- ✓ Gas injection (just model displacement and pressure maintenance)

Pressure vs. volume - EOS



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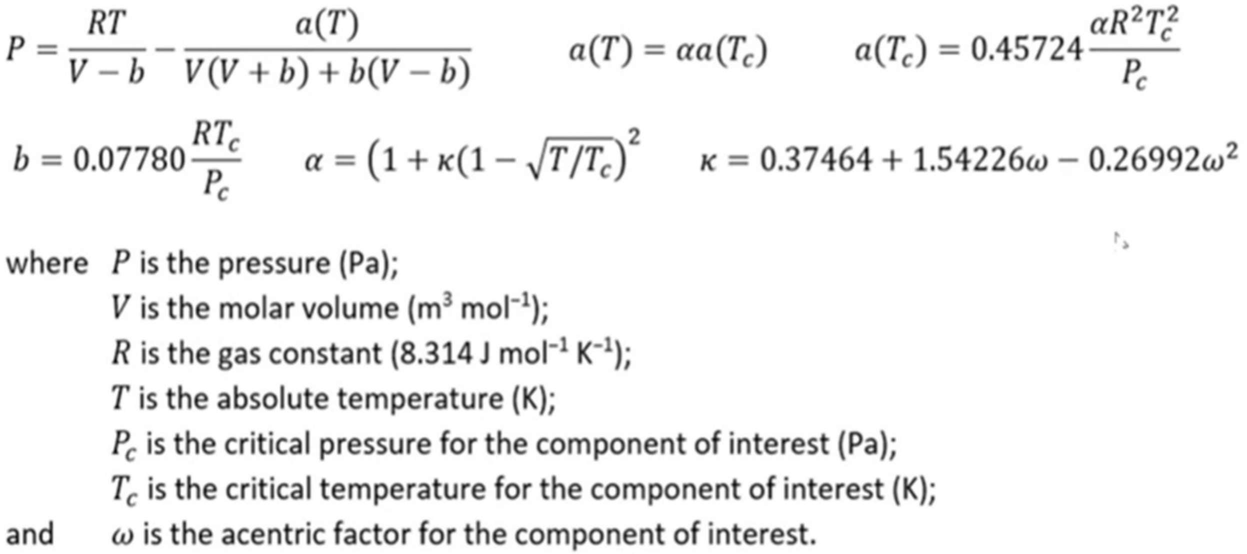
van der Waals

Redlich-Kwong

Peng-Robinson

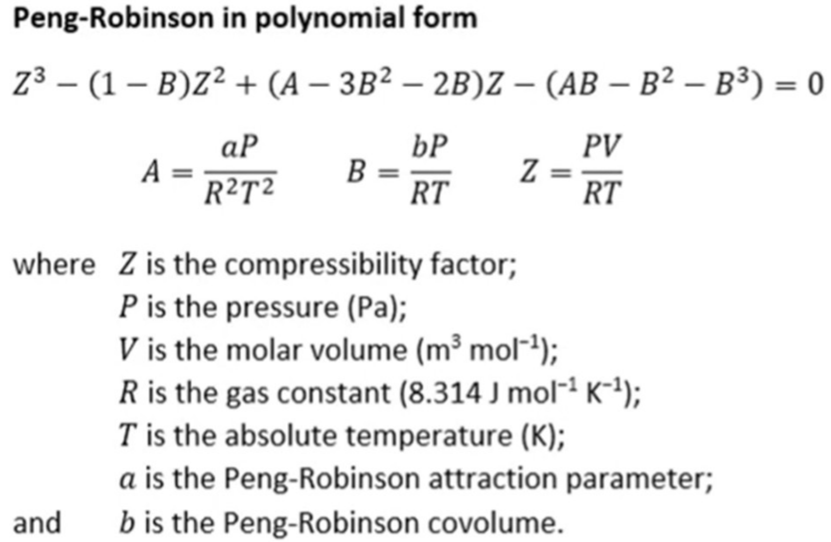
Peng-Robinson EOS



$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)} \qquad a(T) = \alpha a(T_c) \qquad a(T_c) = 0.45724\frac{\alpha R^2 T_c^2}{P_c}$$

$$b = 0.07780\frac{RT_c}{P_c} \qquad \alpha = \left(1+\kappa(1-\sqrt{T/T_c}\right)^2 \qquad \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

where P is the pressure (Pa);
V is the molar volume ($m^3\ mol^{-1}$);
R is the gas constant (8.314 $J\ mol^{-1}\ K^{-1}$);
T is the absolute temperature (K);
P_c is the critical pressure for the component of interest (Pa);
T_c is the critical temperature for the component of interest (K);
and ω is the acentric factor for the component of interest.



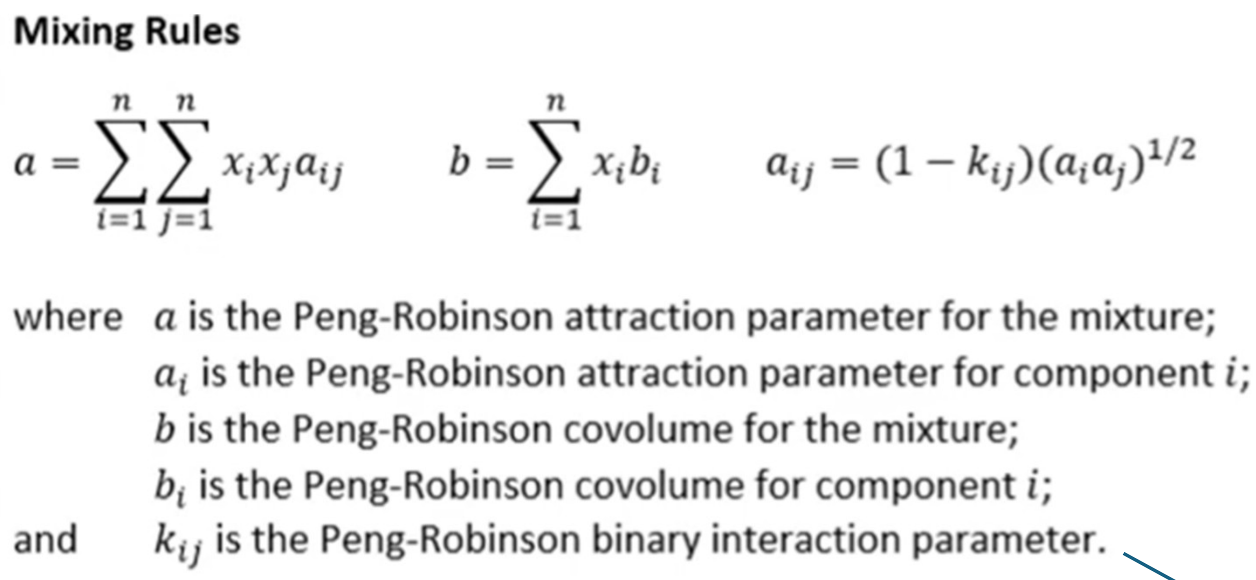
Peng-Robinson in polynomial form

$$Z^3 - (1-B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0$$

$$A = \frac{aP}{R^2T^2} \qquad B = \frac{bP}{RT} \qquad Z = \frac{PV}{RT}$$

where Z is the compressibility factor;
P is the pressure (Pa);
V is the molar volume ($m^3\ mol^{-1}$);
R is the gas constant (8.314 $J\ mol^{-1}\ K^{-1}$);
T is the absolute temperature (K);
a is the Peng-Robinson attraction parameter;
and b is the Peng-Robinson covolume.

Peng-Robinson EOS



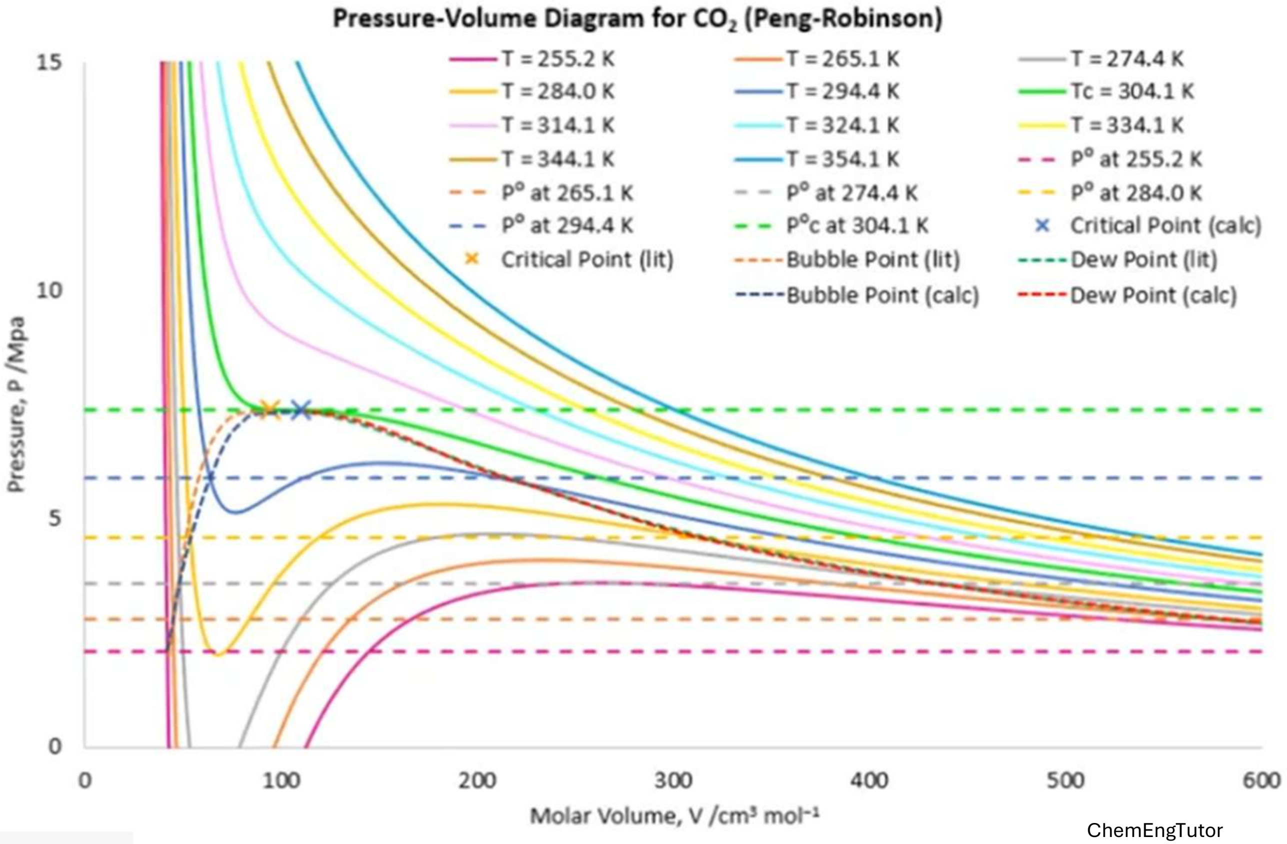
Mixing Rules

$$a = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij} \qquad b = \sum_{i=1}^{n} x_i b_i \qquad a_{ij} = (1 - k_{ij})(a_i a_j)^{1/2}$$

where a is the Peng-Robinson attraction parameter for the mixture;
a_i is the Peng-Robinson attraction parameter for component i;
b is the Peng-Robinson covolume for the mixture;
b_i is the Peng-Robinson covolume for component i;
and k_{ij} is the Peng-Robinson binary interaction parameter.

Data from:
Ohe, S. (1990). *Vapor-liquid equilibrium data at high pressure* (No. 42). Elsevier Science Limited.

Peng-Robinson EOS



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Vapor liquid equilibruim

When a system of vapour and liquid are in equilibrium, the fugacity of each component in both phase must be equal:

$$f_i^L = f_i^V$$

The fugacity of a component in a mixture can be expressed in terms of the fugacity coefficient, which applies to both the vapour and liquid phases as follows:

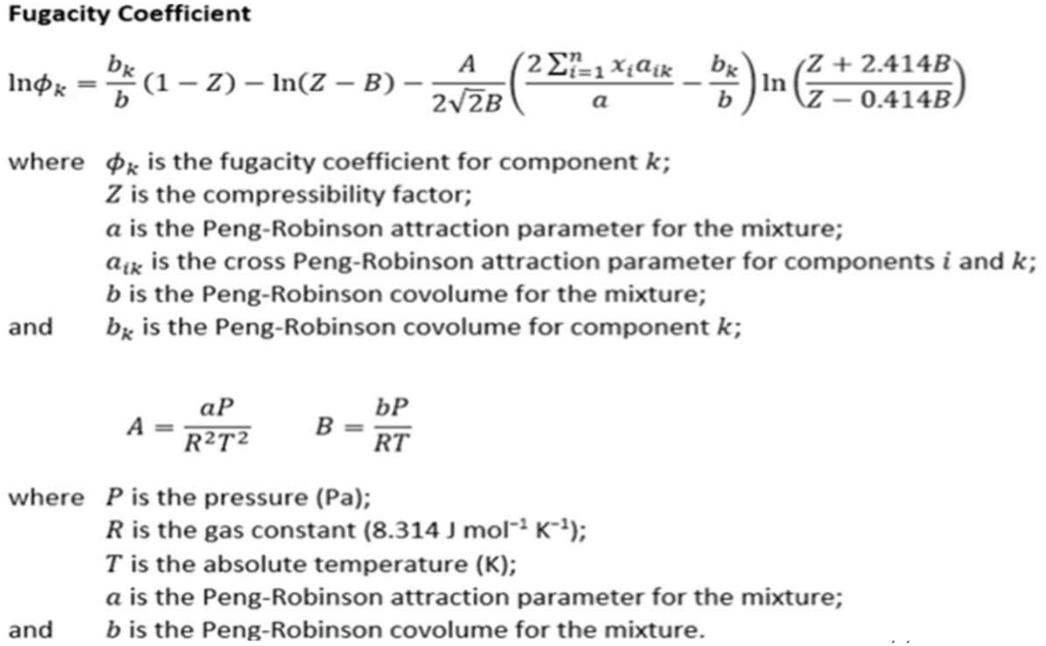
$$f_i^L = P\phi_i^L x_i$$

$$f_i^V = P\phi_i^V y_i$$

$$P\phi_i^L x_i = P\phi_i^V y_i$$

Eliminating P from the equation above, and rearranging it:

$$y_i = \frac{\phi_i^L}{\phi_i^V} x_i \qquad \text{or} \qquad y_i = K_i x_i \qquad \text{where} \qquad K_i = \frac{\phi_i^L}{\phi_i^V}$$



Fugacity Coefficient

$$\ln\phi_k = \frac{b_k}{b}(1-Z) - \ln(Z-B) - \frac{A}{2\sqrt{2}B}\left(\frac{2\sum_{i=1}^{n} x_i a_{ik}}{a} - \frac{b_k}{b}\right)\ln\left(\frac{Z+2.414B}{Z-0.414B}\right)$$

where ϕ_k is the fugacity coefficient for component k;
Z is the compressibility factor;
a is the Peng-Robinson attraction parameter for the mixture;
a_{ik} is the cross Peng-Robinson attraction parameter for components i and k;
b is the Peng-Robinson covolume for the mixture;
and b_k is the Peng-Robinson covolume for component k;

$$A = \frac{aP}{R^2T^2} \qquad B = \frac{bP}{RT}$$

where P is the pressure (Pa);
R is the gas constant (8.314 J mol^{-1} K^{-1});
T is the absolute temperature (K);
a is the Peng-Robinson attraction parameter for the mixture;
and b is the Peng-Robinson covolume for the mixture.

Commercial compositional simulators

E300

- RUNSPEC (General characteristics of model)
- GRID (geometry, grids, geological properties, rock properties)
- **PROPS (PVT model and rock-fluid interaction)**
- **SOLUTION (initialization)**
- SUMMARY (output required)
- **SCHEDULE (well data)**

CMG-GEM

- TITLE (General characteristics of model and output required)
- GRID (geometry, grids, geological properties, rock properties)
- **Fluid model (PVT model)**
- ROCKFLUID (rock-fluid interaction)
- **INITIAL (initialization)**
- NUMERICAL
- **RUN (well data)**

FLUID MODEL

- EOS TYPE
- Number of components, **Component and** user component name
- **User Component Properties**
- SG specific gravity
- *TB average normal boiling point
- ***MW*** molecular weight
- ***AC*** acentric factor
- ***PCRIT*** critical pressure
- Binary interaction coefficients
- *VCRIT critical volume
- *TCRIT critical temperature
- *ZCRIT critical compressibility factor
- *PCHOR interfacial tension (If it is not known, parachor values will be calculated from the molecular weights of the components.)
- *HCFLAG whether the user component is a hydrocarbon component

❑ A vc value is required for viscosity calculations if the Jossi-Stiel-Thodos correlation is used. A zc value can be entered in place of vc, as vc can be calculated directly from zc. If both *ZCRIT and User-defined component like C10+, MW, SG and Tb (two out of three using the correlation)

❑ *VCRIT are missing, zc will be calculated from the acentric factor.

❑ The sg and tb values are used only to calculate the required critical properties and molar volume.

❑ Volume Shift Parameters : to be applied to the equation of state molar volumes. to improve the density predictions.

❑ User-defined component like C10+, MW, SG and Tb (two out of three using the correlation)

Viscosity Correlation

- *VISCOR
- (*MIX): component viscosities to be used in a direct mixing-rule evaluation of hydrocarbon viscosities. (*coef* values for the)
- (*HZYT) Jossi-Stiel-Thodos correlation , mixing rule of Herning and Zipperer (1936), f(P, x(i))
- (*LE): Lee and Eakin (1964) absolute temperature and *M* is the average molecular weight of the mixture f(P, T, x(i))
- (*PEDERSEN): Pedersen et al, 1984, calculation is based on the reference substance property. The reference substance for the Pedersen model is methane. f(P, T, x(i)), provide good liquid viscosity predictions for light and medium gravity oils.
- (*MODPEDERSEN): Pedersen and Fredenslund (1987), f(P, T, x(i)), provide good liquid viscosity predictions for light and medium gravity oils.

Solubility of components in the aqueous phase

Thermodynamic equilibrium

$$f_{i_g} - f_{i_w} = 0 \quad for \quad i = 1, .., N_c.$$

- Henry law (Henry's constants must be specified)

$$f_{i_w} = x_{i_w} H_{h,i}.$$

$$ln(H_i) = ln(H^*_{h,i}) + \frac{\overline{V_{m,i}}(P - P^*)}{RT}.$$

In the equation the star symbol * indicates the reference condition and $\overline{V_{m,i}}$ the partial molar volume of component i.

- Ideal law is assumed in calculating the solubilities of gases in the aqueous phase.

$$z * p = x * H$$

where

z = global composition of the hydrocarbon phases in equilibrium with the aqueous phase. If both a gas and an oil phase are present, z is calculated by mixing both the oil and gas into one phase

p = pressure

In summary.....

1. Phase Equilibrium (The Flash Calculation)

The first step is determining the number of phases and their compositions. This is done via the flash calculation at a given pressure and temperature and overall composition (Zi)

- **Stability test**: determines if a single phase mixture will spilt into two phase
- **Fugacity Equality**: for equilibrium, the fugacity of each component must be equal in all phases
- **K-values**: Equilibrium ratios Ki=Yi/Xi are iteratively solved using EOS until the fugacity criteria are met.

2. Phase Density Calculation

Once phase compositions (xi, yi) re known, the EOS is used to calculate the compressibility Factor (Z)

- The EOS is solved as a cubic equation (typically) to find the roots for Z.
- **Liquid phase**: the smallest positive root of Z usually corresponds to the liquid phase.
- **Vapor phase**: the largest positive root of Z usually corresponds to the vapor phase.
- **Density** : calculated using the real gas law $\rho = \frac{P \cdot MW}{Z \cdot R \cdot T}$ where MW is the phase molecular weight
- **Volume Translation**: To improve liquid density accuracy, a volume shift is often can be added to the cubic EOS.

In summary.....

3. Phase Viscosity Calculation

Unlike density, viscosity is usually not calculated directly by the EOS itself but via semi-emperical correlations that use EOS-derived compositions and densities as inputs.

- **Lohrenz-Bray-Clark (LBC) correlation**: the industry standard for compositional simulators. It relates phase viscosity to the reduced density and the compositions of the individual phases.

4. Summary of Property Calculation Workflow

Property	Calculation Method	Key Inputs
Composition	Flash Calculation (Fugacity Equality)	P,T, overall Zi, EOS parameters
Density	EOS Z-factor root + volume shift	P,T, phase composition, critical properties
Viscosity	Empirical correlation	Phase density, T, phase composition
Fugacity	Derived from EOS integral form	P,T, phase composition, Z-factor

Initilization

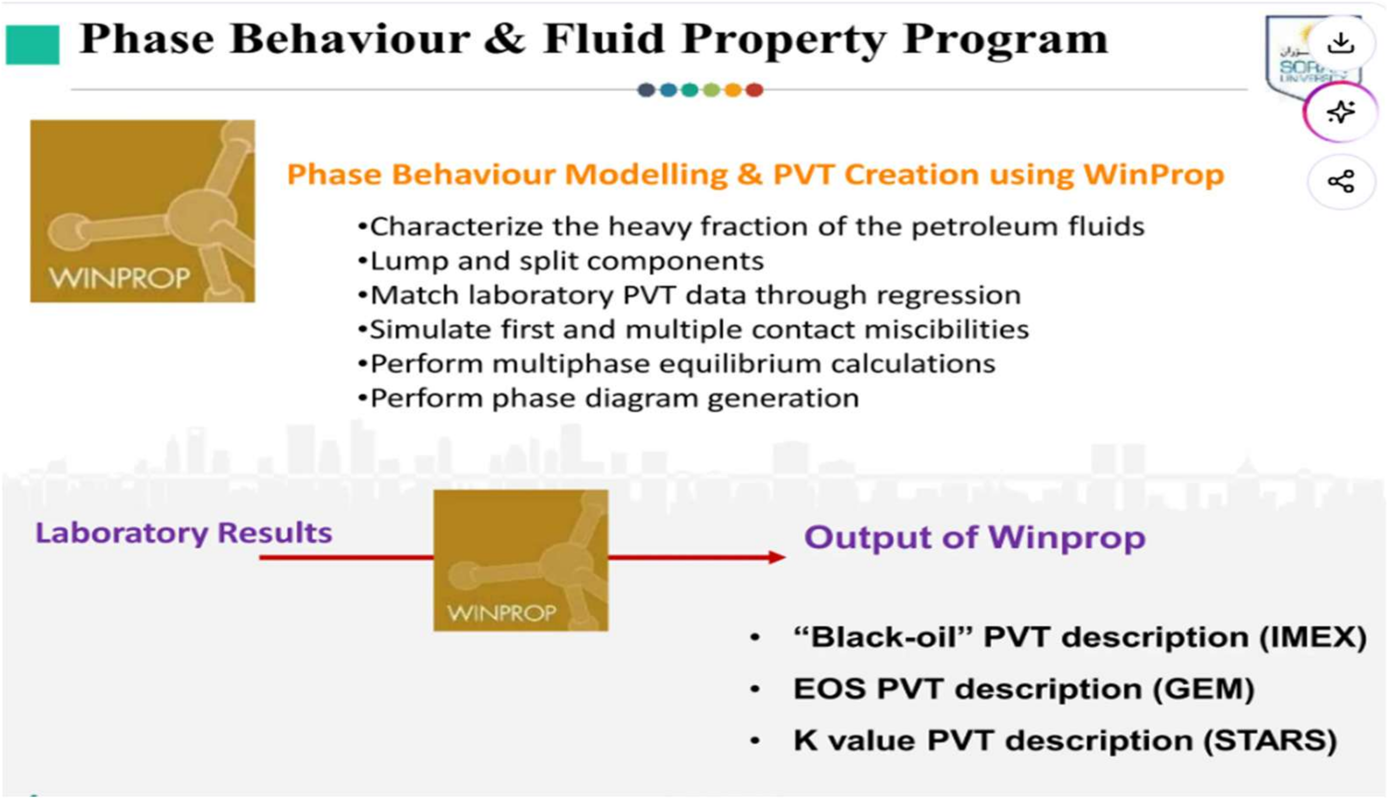
- Gravity initialization for saturated reservoirs. A gas cap in equilibrium with an oil zone is assumed (Zoil , Zgas). Gravity-capillary equilibrium calculations are performed to calculate all grid block pressures and all oil, gas and water saturations. Flash calculations are performed to determine the oil phase and gas phase compositions.

- USER_INPUT (P, sw, ZGLOBAl)

Wells

Set injection phase (water, solvent, cycling and Aqueous (soluble components)) and composition, and injection temperature

CMG-WINPROP – PVT Modelling



Phase Behaviour & Fluid Property Program

Phase Behaviour Modelling & PVT Creation using WinProp

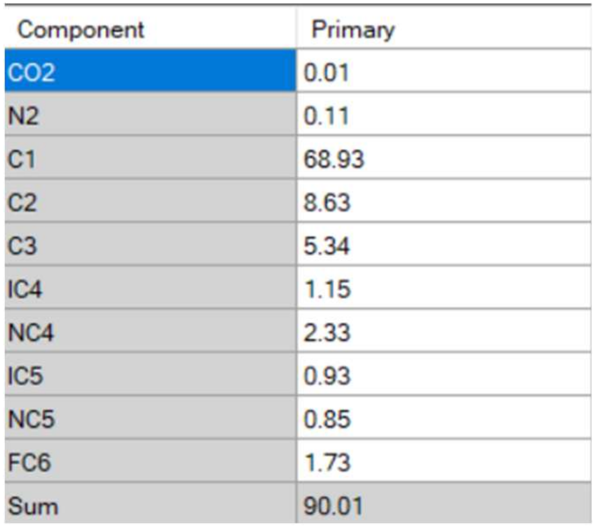
- Characterize the heavy fraction of the petroleum fluids
- Lump and split components
- Match laboratory PVT data through regression
- Simulate first and multiple contact miscibilities
- Perform multiphase equilibrium calculations
- Perform phase diagram generation

Laboratory Results → WINPROP → **Output of Winprop**

- **“Black-oil” PVT description (IMEX)**
- **EOS PVT description (GEM)**
- **K value PVT description (STARS)**

Example 1 Gas condensate modeling

- PR equation of state will be tuned via regression to match the PVT behavior of a gas condensate fluid.

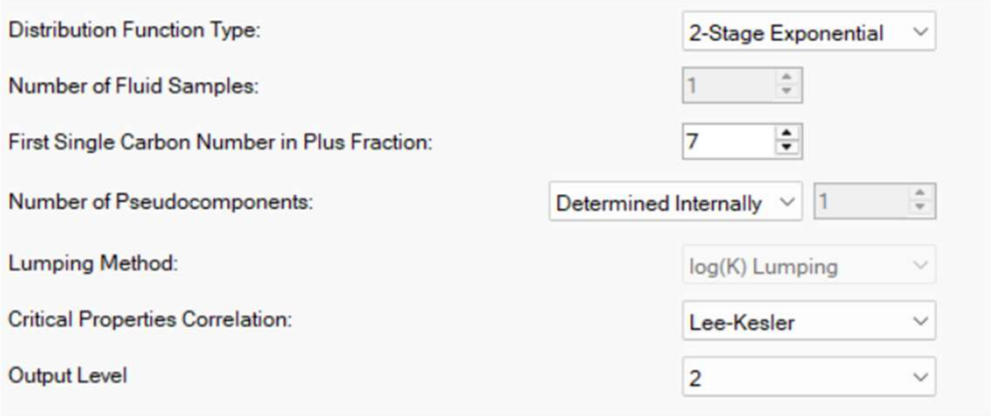


Component	Primary
CO2	0.01
N2	0.11
C1	68.93
C2	8.63
C3	5.34
IC4	1.15
NC4	2.33
IC5	0.93
NC5	0.85
FC6	1.73
Sum	90.01

C7+ : 0.0999

Plus fraction splitting to pseudo components

WINPROP
2024.10



Distribution Function Type: 2-Stage Exponential

Number of Fluid Samples: 1

First Single Carbon Number in Plus Fraction: 7

Number of Pseudocomponents: Determined Internally 1

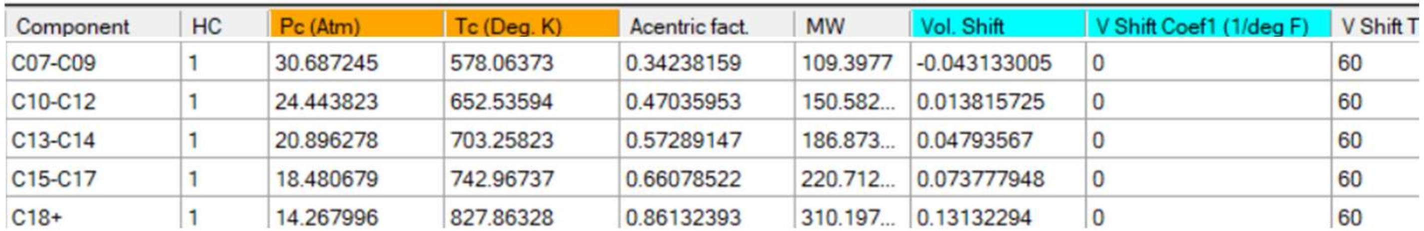
Lumping Method: log(K) Lumping

Critical Properties Correlation: Lee-Kesler

Output Level 2

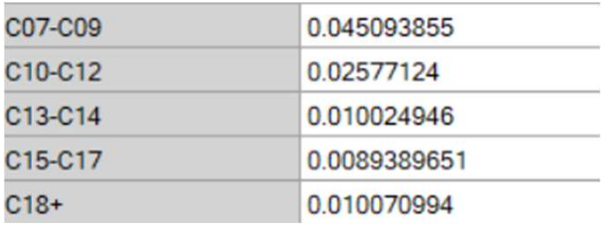
Example 1 Gas condensate modeling

C7+ →



Component	HC	Pc (Atm)	Tc (Deg. K)	Acentric fact.	MW	Vol. Shift	V Shift Coef1 (1/deg F)	V Shift T
C07-C09	1	30.687245	578.06373	0.34238159	109.3977	-0.043133005	0	60
C10-C12	1	24.443823	652.53594	0.47035953	150.582...	0.013815725	0	60
C13-C14	1	20.896278	703.25823	0.57289147	186.873...	0.04793567	0	60
C15-C17	1	18.480679	742.96737	0.66078522	220.712...	0.073777948	0	60
C18+	1	14.267996	827.86328	0.86132393	310.197...	0.13132294	0	60

C7+ : 0.0999 →

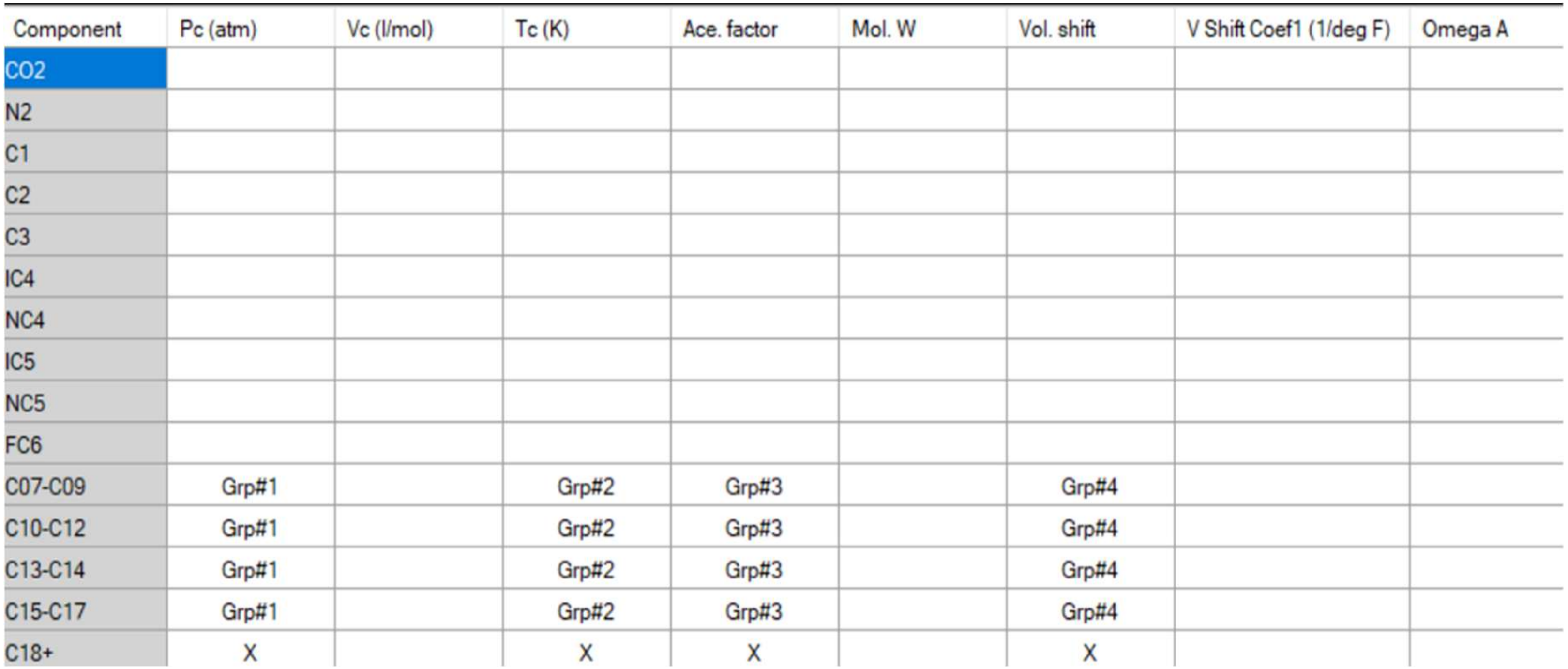


C07-C09	0.045093855
C10-C12	0.02577124
C13-C14	0.010024946
C15-C17	0.0089389651
C18+	0.010070994

Add regression parameters , initial value for parameters (min and max) and then the available lab experiments and data such as saturation pressure, CCE(constant composition expansion) pressure levels and volume data, CVD (constant volume depletion) pressure levels and depletion data, the goal is match the experimental data by tunning the regression parameters

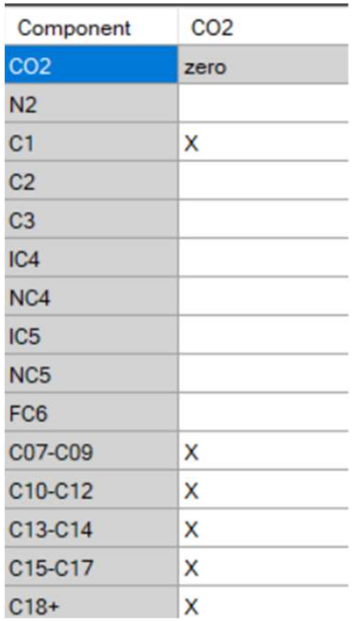
Example 1 Gas condensate modeling

Regression parameters



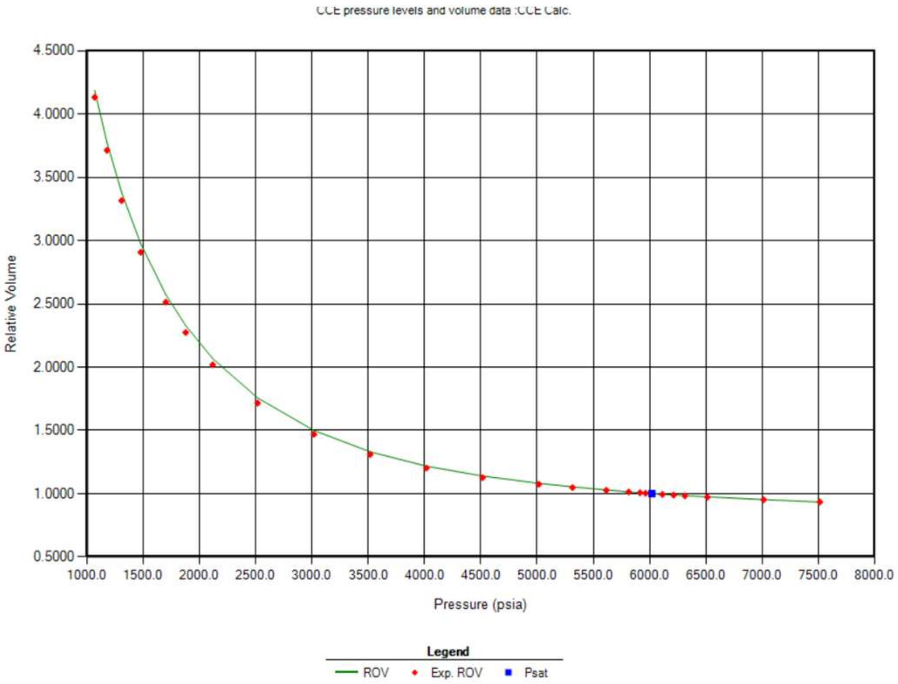
Component	Pc (atm)	Vc (l/mol)	Tc (K)	Ace. factor	Mol. W	Vol. shift	V Shift Coef1 (1/deg F)	Omega A
CO2								
N2								
C1								
C2								
C3								
IC4								
NC4								
IC5								
NC5								
FC6								
C07-C09	Grp#1		Grp#2	Grp#3		Grp#4		
C10-C12	Grp#1		Grp#2	Grp#3		Grp#4		
C13-C14	Grp#1		Grp#2	Grp#3		Grp#4		
C15-C17	Grp#1		Grp#2	Grp#3		Grp#4		
C18+	X		X	X		X		

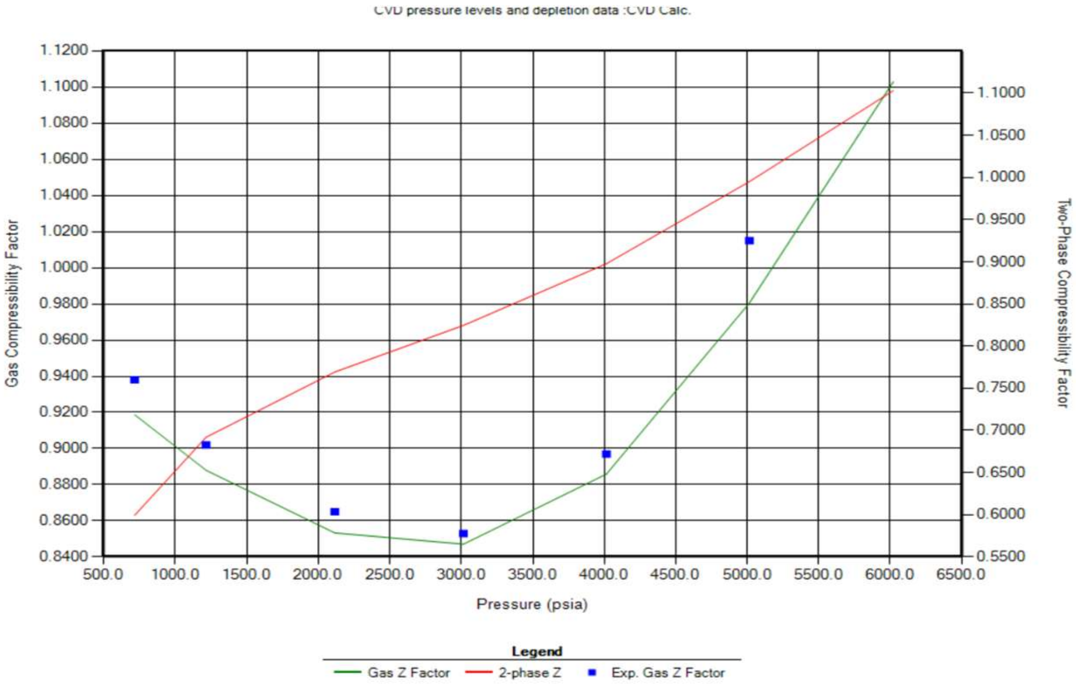
Binary interaction coeff



Component	CO2
CO2	zero
N2	
C1	X
C2	
C3	
IC4	
NC4	
IC5	
NC5	
FC6	
C07-C09	X
C10-C12	X
C13-C14	X
C15-C17	X
C18+	X

Example 1 (gas condensate modeling)





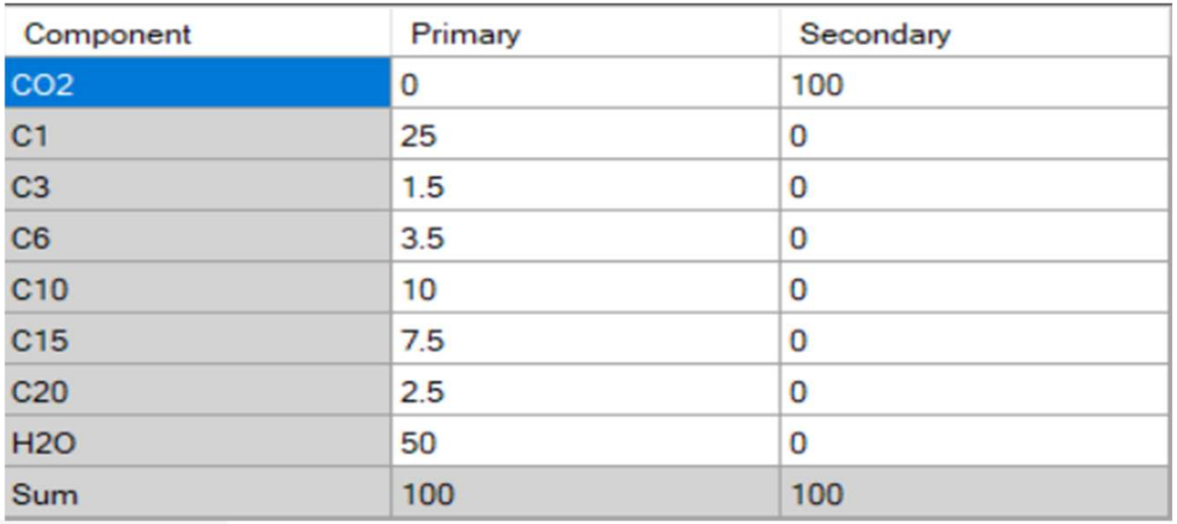
Example 1 (gas condensate modeling)

```
*COMPNAME
 'CO2'  'N2'  'C1'  'C2'  'C3’  'IC4'  'NC4'  'IC5'  'NC5'  'FC6’ 'C07-C09'  'C10-C12'  'C13-C14'
'C15-C17'  'C18+'
 *PCRIT
  72.8   33.5   45.4   48.2   41.9  36   37.5   33.4   33.3   32.46  29.543017   23.299595
19.75205   17.336451   16.27404
  *TCRIT
  304.2   126.2   190.6   305.4   369.8  408.1   425.2   460.4   469.6   507.5  559.25414
633.72635   684.44864   724.15778   905.02494
 *AC
  .225   .04   .008   .098   .152  .176   .193   .227   .251   .27504  .31048   .43845794
.54098988   .62888363   1.03359
*VSHIFT
 -.09434672  -.12838834  -.1538605  -.10210346  -.07330094 -.05706875  -.05705589  -
.03446267  -.03446267  -.004992  .056589963  .082818413  .10091836  .11610532
.18918042
```

```
*BIN
 -.02   0
.2     .031
.13   .042
.135  .091
.13    .095
.13    .095
.125   .095
.125   .095
.15     .12
.14982356   .12
0   .12
0   .12
.031305998   .12
.2   .12
```

Example 2 Solubility of CO2 in Brine

- Estimation of CO_2 solubility in brine at several pressures using WinProp’s internal model for calculation of Henry’s constants for gaseous components in aqueous brines.
- Fitting the parameters for the Henry’s law solubility model used in GEM to the predicted CO_2 solubilities via regression.



Component	Primary	Secondary
CO2	0	100
C1	25	0
C3	1.5	0
C6	3.5	0
C10	10	0
C15	7.5	0
C20	2.5	0
H2O	50	0
Sum	100	100

Example 2 Solubility of CO2 in Brine

- Add regression parameters to match the experimental CO2 solubility data using OGW/multi-phase flash calculation

WINPROP
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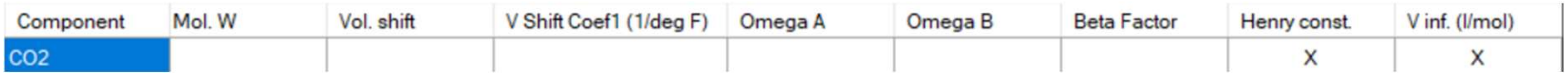
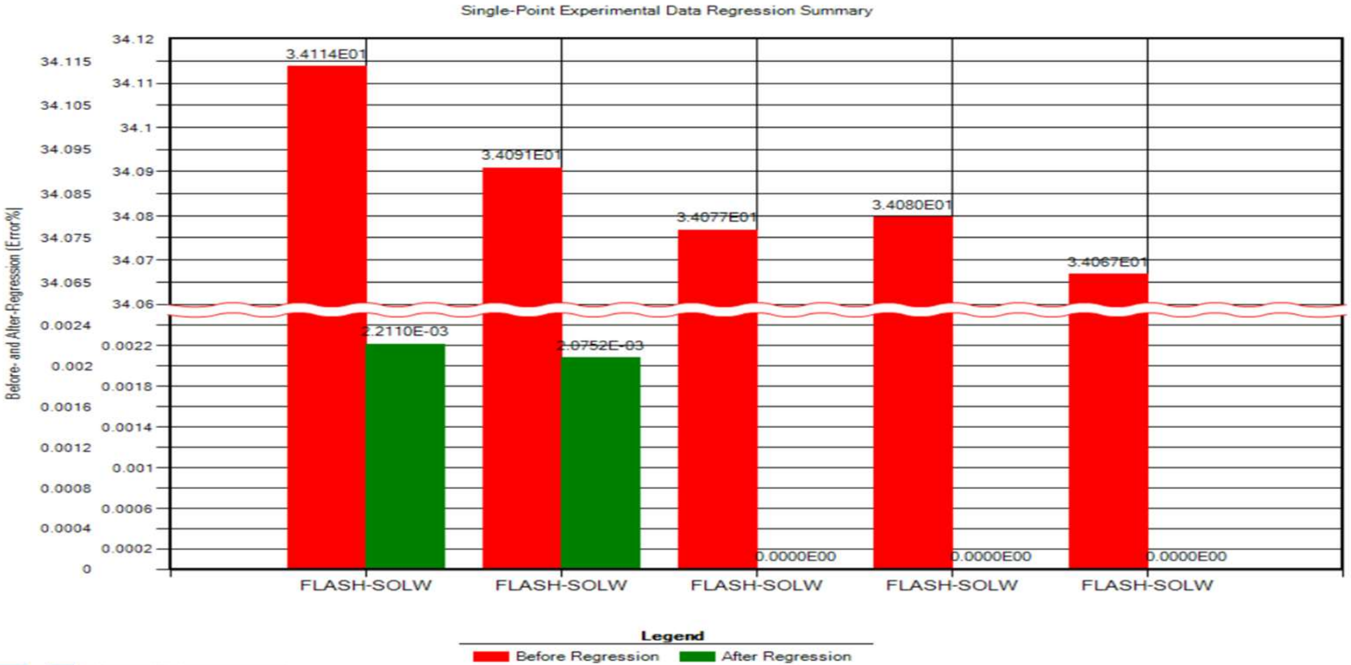


Component	Mol. W	Vol. shift	V Shift Coef1 (1/deg F)	Omega A	Omega B	Beta Factor	Henry const.	V inf. (l/mol)
CO2							X	X

VINFINITY



Example 2 Solubility of CO2 in Brine

Ready to be imported to GEM

$$\ln(H) = \ln(hens) + v8 * (p - refph) / RT$$

- *HENRYC

5.1517160E+03 1.0000000E+20 1.0000000E+20 1.0000000E+20 1.0000000E+20 1.0000000E+20
1.0000000E+20 3.2888300E-01

- *VINFINITY

3.5649862E-02 3.5774100E-02 7.1812100E-02 1.3612310E-01 2.3581460E-01 4.0723540E-01
5.4544700E-01 1.8407800E-02

- *REFPH

3.4023000E+01 3.4023000E+01 3.4023000E+01 3.4023000E+01 3.4023000E+01 3.4023000E+01
3.4023000E+01 3.4023000E+01

Open source tools – PVT modeling

- ➢ DWSIM (Chemical Process Simulation)
- EOS-based thermodynamics (PR, SRK, etc.)
- Petroleum characterization (pseudo-components, assays)
- Phase equilibrium (flash, phase envelope)
- Some regression / fitting capabilities
- CAPE-OPEN compliant (can integrate with other tools)
- ➢ No full PVT lab workflow
- Missing:
- CCE simulation
- CVD simulation
- Differential liberation
- Swelling tests

Open source tools – PVT modeling

➢Python-based EOS / PVT libraries EOS-based thermodynamics (PR, SRK, etc.)

Examples (not a single product):

- thermo (Python thermodynamics) , EOS Engine
- CoolProp (fluid properties)
- phasepy (phase equilibrium, EOS), EOS Engine
- pyEOS / custom PR/SRK implementations
- scipy.optimize: Regression Engine
- **What they can do:**
- Flash calculations
- EOS tuning (if you code regression)
- Phase envelope generation

What they can not do:

- Very limited Lab experiments modeling

Wrap up

- To expand support for oil, gas, and energy transition applications—including CO_2 storage, gas storage, and hydrogen (H_2) storage—thermal compositional modeling capabilities should be incorporated into OPM.
- To enable PVT modeling for compositional simulation, a dedicated PVT package is required to translate and integrate laboratory data into the OPM compositional simulator, ensuring it can be properly updated and utilized.

Thanks

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