PVTi and ECLIPSE 300

An Introduction to PVT analysis and compositional simulation

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1. Course Introduction

Learning Objectives

This course will give you an understanding in how to set up and run a compositional simulation model using ECLIPSE 300 Compositional.

A pre-requisite for the course is that you already understand black-oil simulation and can create and run ECLIPSE 100 black-oil models. We will therefore concentrate on the differences between black oil simulation and compositional simulation, and between ECLIPSE 100 and ECLIPSE 300.

The course contains a number of exercises during which you will practice specific topics in the presentations. These exercises build up to a small study in which you will be able to apply all that you have learnt during the course.

Course Guidelines

In this training material, you will encounter the following:

1. Overview of the course
2. When you need to use compositional simulation
3. PVT properties of hydrocarbon fluids: Background and Theory
4. The main steps involved in a PVT analysis of a hydrocarbon fluid
5. The different sections of the PVTi program
6. The differences between black oil and compositional simulation
7. How to use ECLIPSE 300
8. Advanced and specialized compositional topics
9. Practical exercises
10. A scenario-based study
11. Summary

You will also encounter notes and best practices.

Outline of Lecture Topics

Part 1: PVTi and ECLIPSE 300

- Introduction
- Overview of Black Oil and Compositional Simulation
- PVT background
    - Components
    - Equations of State
    - Flash
    - Viscosity
- Practical Exercises
    - Phase Diagrams
    - Ternary Diagrams
    - Splitting and Grouping
    - Regression
    - Output to ECLIPSE

Part 2: From PVTi to ECLIPSE 300

- PVTi Experiments
- Using Ternary Diagrams
    - Condensing Gas Drives
    - Vaporizing Gas Drives
- Miscibility: FCMP and MCMP experiments
- Flash:
    - Flash Theory
    - Flash Example
    - Difficulties in Flash
- Demo: simulation of gas injection
- Composition *vs.* depth

Part 3: From ECLIPSE 100 to ECLIPSE 300

- ECLIPSE 100 Program Usage
- Differences between ECLIPSE 100 and 300
- Keyword Review
- ECLIPSE workshop

Part 4: Advanced Topics

- Grid Orientation, 9-point and MPFA
- Numerical Dispersion
- Near-Critical Oil and Gas Relative Permeabilities
- Convergence Reports

Part 4: Optional Advanced Topics

- ECLIPSE 100/200 pseudo-compositional Models
- Diffusion
- Components in water
    - CO2 Solution in water
    - CO2 Sequestration
    - Gas-Water Systems
        - Calorific values
    - Multi-component water
- Tracers
- Transport Coefficients
- Gas flow near wells
    - Non-Darcy flow
    - Gas pseudo-pressure
    - Velocity-dependent rel perms
- Multi-Phase Flash
- Solids

- **Aziz's Ten Golden Rules**
- Glossary

Outline of Workshop Problems

1. Introduction to PVTi
    - PVT Analysis of an Oil
    - PVT Analysis of a Gas Condensate
    - PVT - Development Fluids

      Slim tube oil

      Field scale oil

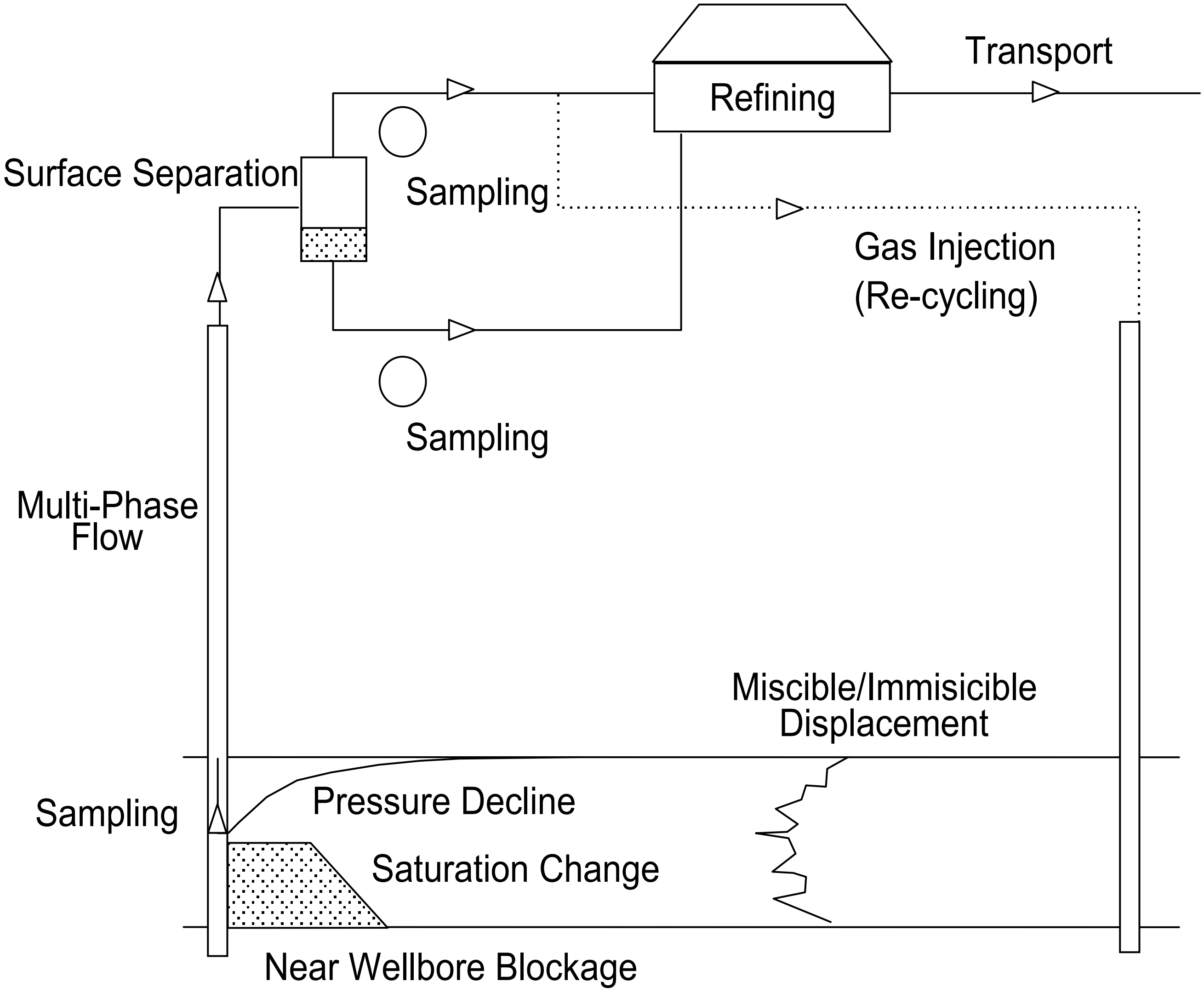
      Gas Condensate
2. Slim Tube Studies of Miscibility
3. Development of ECLIPSE 300 Field Scale Input Data Set
4. Study of Miscible Processes
5. Study of Gas Condensates

2. Introduction to Compositional Simulation

In this section we will introduce the uses and advantages of compositional simulation and the limitations of a black oil model.

Why analyse PVT data?

We start by asking why we need PVT properties of fluids. More precisely, where in the study of oil production do we need PVT properties of the hydrocarbon fluids?



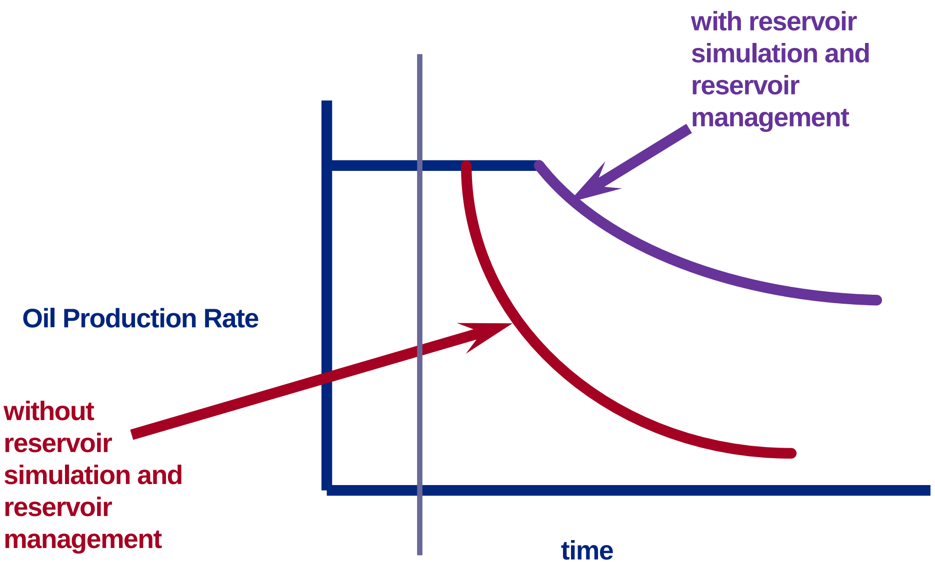
The answer is that we need to know how the fluids behave within the reservoir, within the wells, at surface conditions, in the network and at the refinery. The fluid properties need to be known over a wide range of temperatures and pressures. When gas is injected into the reservoir, we also need to know how the properties of the original reservoir fluid will change as the composition of the mixture changes.

We also need PVT fluid properties to predict:

1 The composition of well stream as a function of time
2 Completion design, which depends on the properties of the well-bore liquids
3 The effect of injecting or re-injecting gas, and
    - o The detailed specification of the injected gas - how much C3, 4, 5's to leave in
    - o separator configuration and stage from which to get the injection gas
4 Miscibility effects that may result from the injected gas
5 The amounts and composition of liquids left behind in the reservoir and their properties: density, surface tension, viscosity.
6 H2S and N2 concentration in produced gas
7 Product values and how they change with time

Why simulate?

Compositional simulation however also has a number of features in common with black-oil simulation. In both cases one of the main reasons for reservoir simulation is economic. We usually want to increase the net value of the hydrocarbon recovered from the reservoir. For a field that is already producing, for instance, we want to extend the oil plateau at minimum cost:

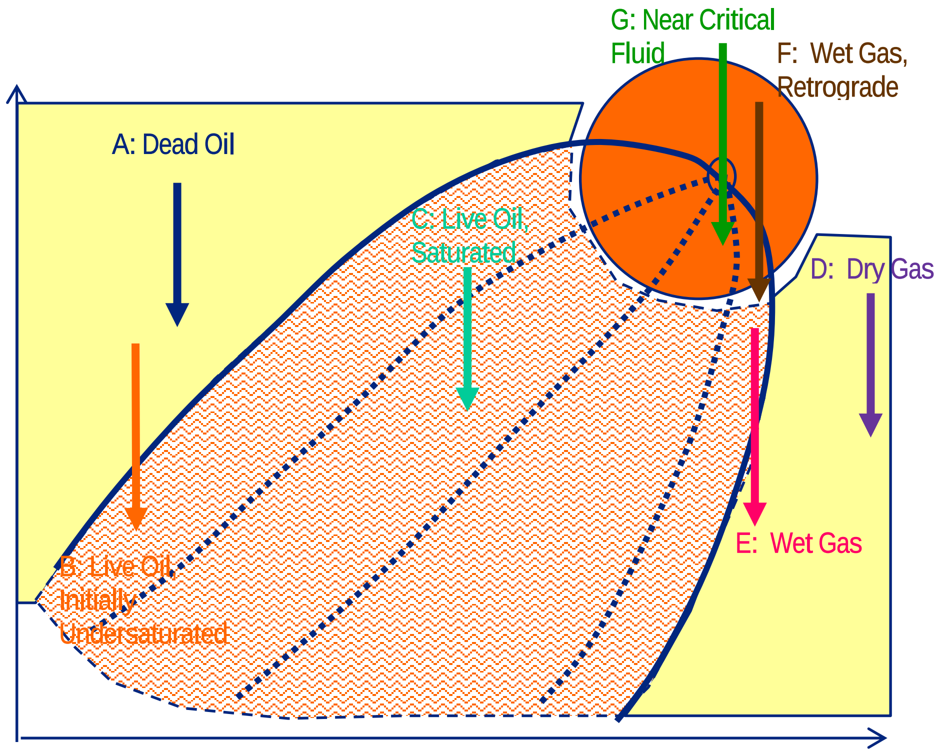


Uses of Compositional Simulation

Black-oil simulation does not provide a good enough description of reservoir processes in a number of situations. Compositional simulation has to be used for instance

1. For Enhanced Oil Recovery (EOR) processes that involves a miscible displacement
2. For cases where gas injection/re-injection into an oil produces a large compositional changes in the fluids
3. If condensates are recovered using gas cycling. In general, compositional simulation has to be used if the composition of the injected gas is significantly different from the composition of any free gas in the reservoir.
4. Because surface facilities designers need detailed compositions of the production stream.

If the hydrocarbon in the reservoir stays as a single-phase oil during its entire history, away from the critical point, then it can in general be modeled with a black-oil simulator. If the hydrocarbon is a single-phase gas, compositional simulation may have to be used if you are injecting a different gas, or if you are interested in the detailed solubility of components (such as CO2) in water.



If the reservoir is two-phase at any time during the simulation then there will be some compositional effects. In many cases however these can be approximated by varying gas/oil and oil/gas ratios to mimic small compositional changes.

- Condensate dropout or gas liberation should be a small part of the hydrocarbon in place.
- Remaining hydrocarbon composition should not change significantly when gas is liberated or condensate drops out

If the initial reservoir temperature and pressure are close to the critical point of the reservoir fluid, or if they get close during the simulation (for instance due to gas injection), then we may have to use a compositional model.

Even if we are not injecting gas into a reservoir, we may still need to consider compositional simulation if there are:

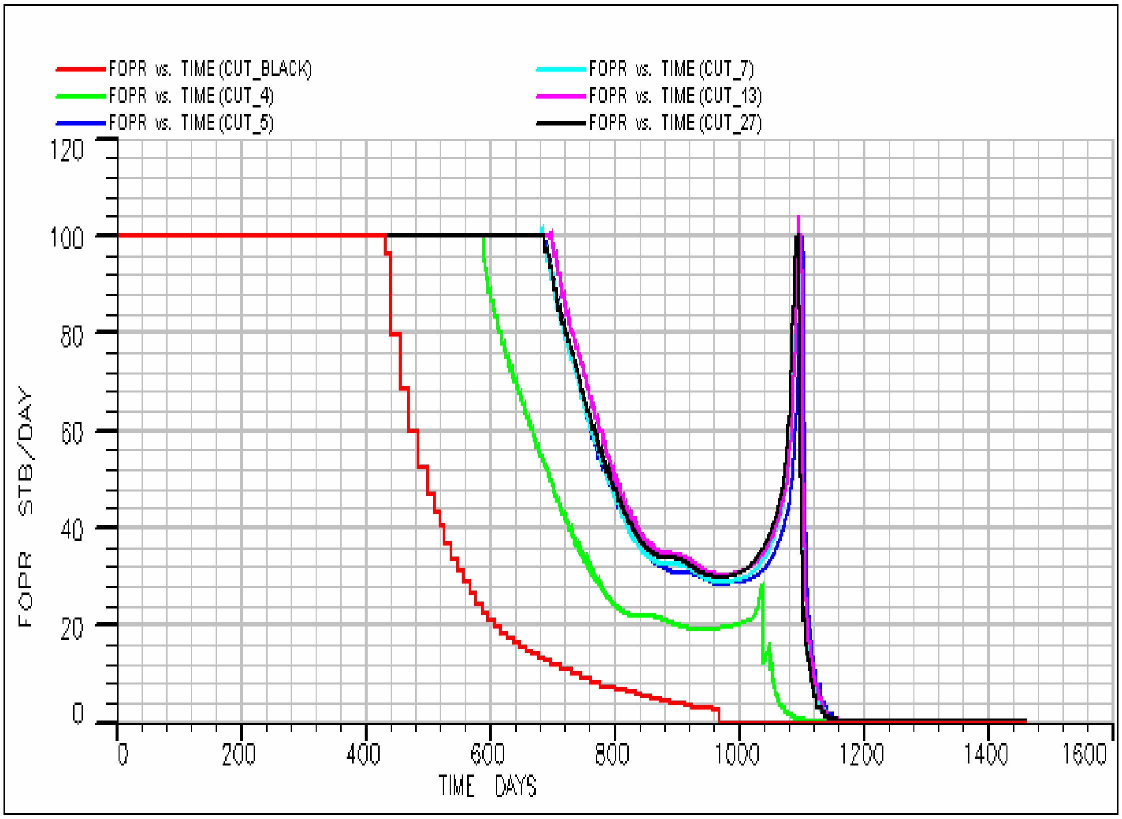
1 Large compositional variations with depth
2 Large temperature variations with depth
3 Large compositional variations in the x-y direction

Advantages of Compositional Simulation

Compositional simulators can account for the effects of composition on:

1. Phase behavior
2. Multi-contact miscibility
3. Immiscible or near-miscible displacement behavior in compositionally-dependent mechanisms such as vaporisation, condensation, and oil swelling
4. Composition-dependent phase properties such as viscosity and density on miscible sweep-out
5. Interfacial Tension (IFT) especially the effect on residual oil saturation.

These effects can have a major effect on production. Consider the picture below, which shows condensate recovery using different PVT descriptions of the fluid:



The PVT laboratory report described the fluid using 27 components. ECLIPSE 300 was first run with all 27 of these components, and the results of that simulation are shown as the black line marked CUT_27. The simulator was then run after grouping the 27 components down to 13 components. The oil production rates are labeled CUT_13 and are the same as those for CUT_27 to within engineering accuracy. The runs were repeated with 7 and 5 components and again the results are essentially the same.

The production using a 4-component description of the fluid is different. Less oil is recovered and production comes off plateau about 50 days early. Using a black-oil approximation in this model, recovery is considerably less than that from a more accurate multi-component description. As we will show later, the black oil model can be considered as a 2-component model of the fluid.

The minimum number of components needed in a reservoir simulation will depend on the hydrocarbon fluids and on the production scenarios being simulated. For this fluid and this model, 5 components are enough, but the minimum number of components will vary from case to case.

Difficulties with Compositional Simulation

There are a number of issues that may need to be considered when running any compositional simulator. These are discussed in more detail during the course, but a brief summary is:

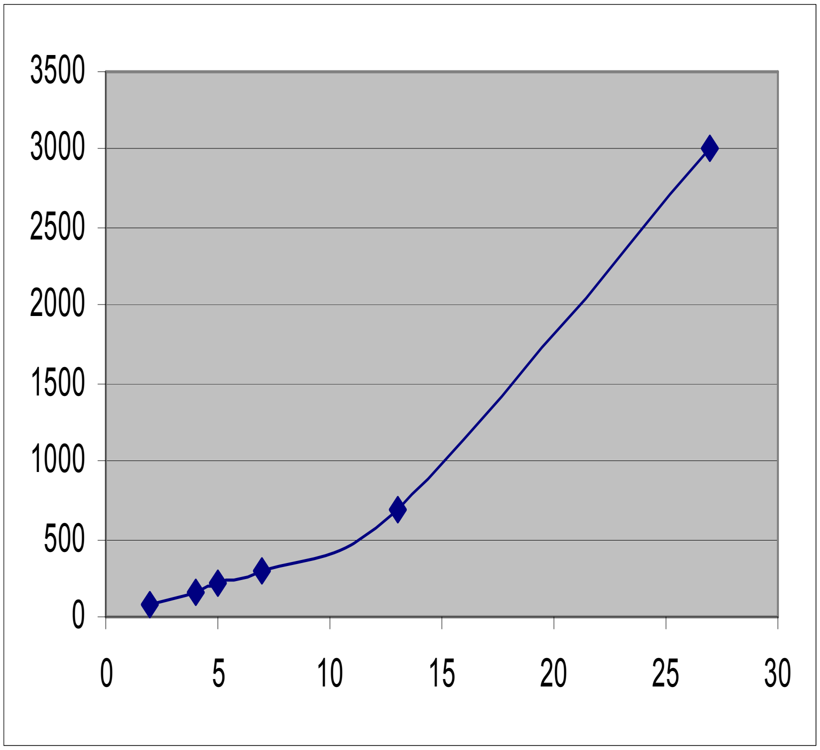
- Calculating phase composition around the critical point or in the plait-point region can be difficult. K-values and physical property calculations (as well as the equation of state) are less accurate in plait - point region. Experimental data in this region (used to calibrate EOS) are often lacking.

- Modeling viscous fingering in large grid blocks is not easy. The effects are usually ignored and complete mixing of fluids within a grid block assumed. ECLIPSE 300 contains a model based on papers by Barker and Fayers. Transport coefficients using ALPHA and TRCOEFF keywords will boost or hold back component flow as function of mole fraction

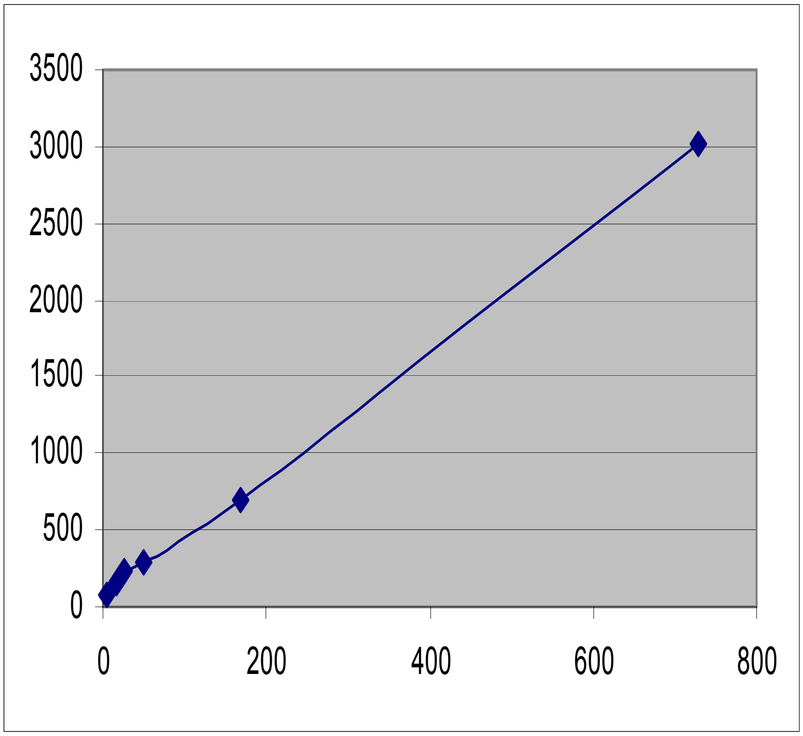
- Numerical dispersion is an issue in both black-oil and compositional simulation, but can have a greater effect in compositional. Grid orientation effects are also common to both types of simulation. Techniques exist within ECLIPSE 300 to overcome some of the effects, but they need extra computing time.

- Computing time is one of the reasons why reservoir engineers have been traditionally reluctant to run compositional instead of black-oil reservoir models. With the advent of faster computers and improved software programs (such as ECLIPSE 300), this is less of an issue. It is still true that running a multi-component simulation will take more time than a black-oil simulation. Compositional simulation needs more time than black-oil simulation because:
    - calculations are needed to work out how many phases are present and what the composition and properties of those phase are
    - there are more equations to solve because there are more components.

  We can investigate the dependence of computing time on the number of components by looking at a plot of the computing time for the different condensate models above. This shows computing time for 27 components, for 13, 7, 5, 4 components and the black-oil model (considered as 2 components). We can see that the computing time for a simulation increases approximately linearly with the number of components up to about 10 components.



Beyond about 10 components, in this model, the computing time increases much more steeply. The plot shows that computing time increases as approximately the square of the number of components.



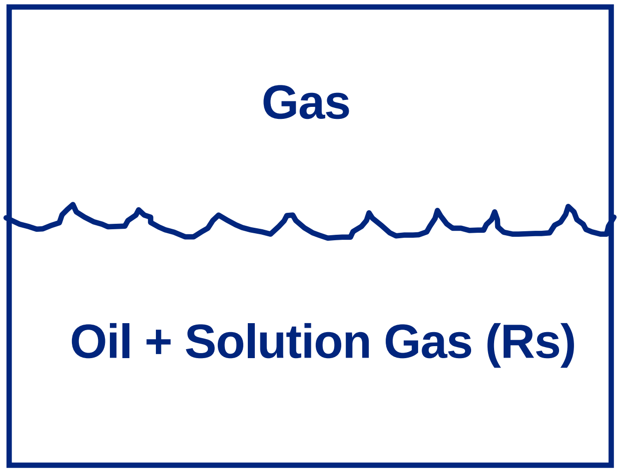
The detailed way in which computing time increases as a function of the number of components will vary from one study to another; in all cases however computing time will increase as the number of components increases. The greater the number of components, the greater the increase.

3. Black Oil and Compositional Fluid Models

In this section you will learn the key difference between black-oil and compositional simulation.

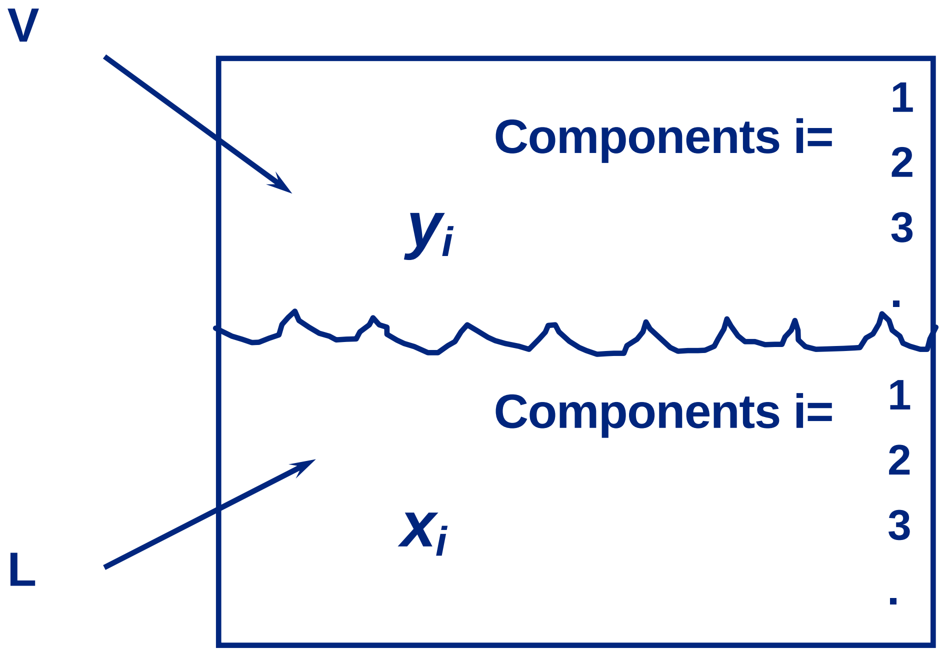
ECLIPSE 100 (and all Black-Oil Simulators)

Oil and Gas phases are represented by two components: one ‘component’ called oil and one ‘component’ called gas.



ECLIPSE 300 (and all Compositional Simulators)

Oil and Gas phases are represented by multicomponent mixtures.



Fluid Description

In a black-oil model, the oil 'component' is in the oil phase and the gas 'component' is in the gas phase. In the case of live oil, the oil phase also contains some dissolved gas 'components' and in the case of rich gas or a gas condensate the gas phase also contains some vaporized oil 'components'.

Consider a volatile oil case.

The black-oil model is that a certain volume of gas (defined by the value of Rs) has dissolved in the oil. The dissolved gas is the same as any free gas in contact with the oil. If gas is injected into the reservoir, it too will be the same gas as the dissolved gas and the gas cap gas. Any produced gas will also be the same. All these gases will have the same physical properties.

The compositional model is very different. Both the oil phase and the liquid phase are made up of the different amounts of the same components. Methane for instance will be present in both phases, but the gas phase may be 80% methane whereas the oil phase could be only 20% methane. The composition of injected gas could be completely different, for instance injected gas could be 95% methane. The composition of the produced gas is likely to vary with time. The physical properties of all these gases will be different.

Physical Properties

In a black-oil model, the physical properties of the oil and the gas are a function of pressure and of nothing else.

$$\left\{\begin{matrix} B_o \\ B_g \\ R_s \\ \mu \end{matrix}\right\} = f(p)$$

The only input needed by a black-oil simulator is therefore a table of physical properties versus pressure. For example, you have to provide ECLIPSE with a table of oil viscosity at different pressures then for any given pressure the simulator can easily look up the oil viscosity.

In a compositional model, all we know is what components are present. We first have to calculate how many phases are present at the given pressure and temperature. If there are both oil and gas phases, we have to calculate the composition of each phase. Given these compositions we then have to calculate the physical properties, for instance the oil viscosity.

$$\left.\begin{array}{l} K_i = \dfrac{y_i}{x_i} \\ \mu \\ \rho \end{array}\right\} f(p, x_i, y_i)$$

The process of deciding how many phases are present is called a "Flash". We shall show later in the course how to perform a Flash calculation. To calculate the physical properties of the oil and gas, we have to calibrate an Equation of State (EoS) using a PVT package such as PVTi.

The Flash calculations in compositional simulation take up much more computing time than a table look-up in black-oil simulation.

Variables

If a simulation model has oil, water and gas phases, then a black-oil simulator such as ECLIPSE 100 will use three variables to describe the state of the fluid.

$$\begin{pmatrix} P \\ S_w \\ S_g \end{pmatrix}$$

If all three phases are present in a grid block then the variables are the oil pressure, the water saturation, and the gas saturation. If there is no gas phase in the grid block then R_s is used instead of S_g, and if there is no oil phase then R_v is used instead of S_o. In all cases, three variables are used.

More variables are needed in compositional simulation.

$$P$$

$$z_w$$

$$z_i, \quad i = 1, \ldots n_c$$

In ECLIPSE 300 we use the oil pressure (as in ECLIPSE 100), the water molar density z_w (instead of S_w in ECLIPSE 100), and the molar densities of each hydrocarbon component z_i. If there are n_c hydrocarbon components, then there are $n_c + 2$ variables to solve. For instance, if we model our hydrocarbon fluid with 7 components then we will have 9 variables, instead of 3 in a black-oil model. We would expect this to take more computing time.

Summary

The key difference between black-oil and compositional simulation is the PVT description of the fluid. In black-oil we can fully describe the fluid properties with a table of properties vs. pressure. In compositional we need to solve both a flash equation and an Equation of State.

4. PVT analysis and PVTi

In this section we will define what we mean by the word “component”, and look at component series and heavy components.

Starting PVTi

We need to use PVTi:

- To match an Equation of State to observations

  This is done to compensate for the inability to measure directly all the things we need to know about the hydrocarbons
- To Create
  - “Black-Oil” PVT tables for a Black Oil model
  - “Modified Black-Oil” PVT tables for an ECLIPSE 100 GI Pseudo-compositional Model or an ECLIPSE 100 Solvent Model
  - Compositional PVT parameters for a Compositional Model

PVTi has 1 main panel, and can be considered as 5 modules:

1. Fluid model and Samples
2. Experiments and Observations
3. COMB: Material Balance (optional)
4. Regression to match EoS
5. Export of results to simulators

We will:

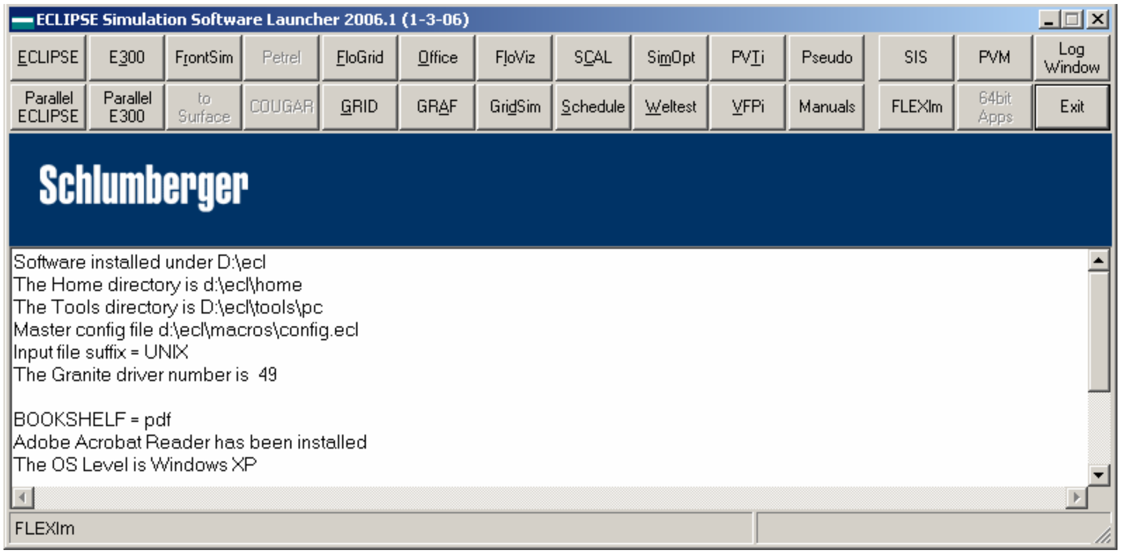
1 Discuss the background to the expected input data

2 Summarise some theory

3 Demonstrate how to input the data

4 Go through one or more practical examples

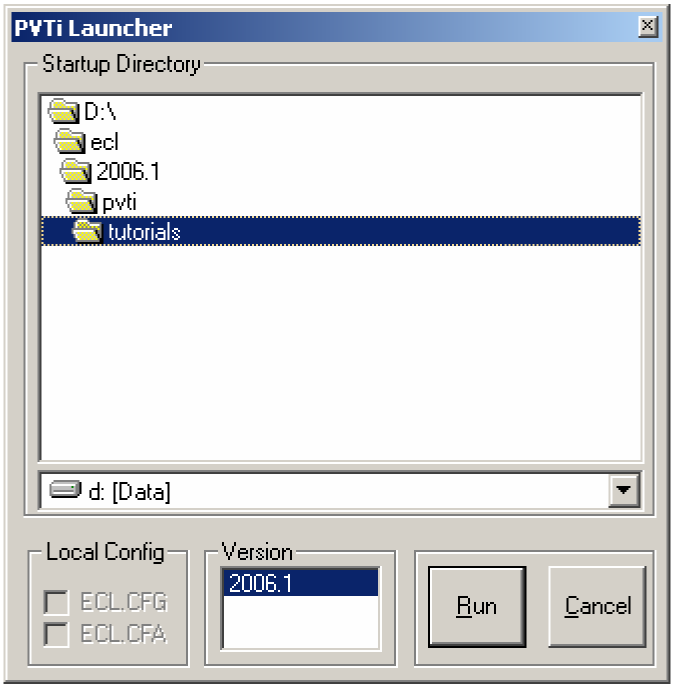
You can launch PVTi either from the Launcher on a PC GeoQuest Launcher.lnk or from a command line. The panels below are taken from a PC.



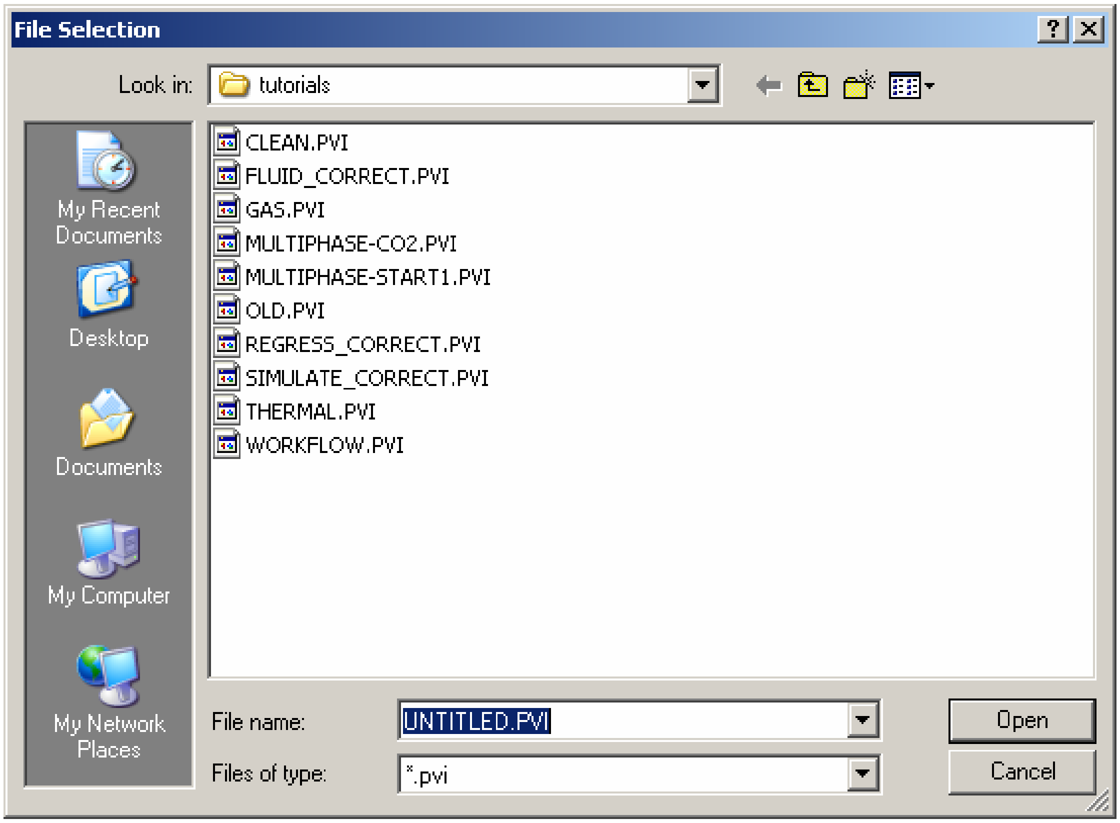
```
Software installed under D:\ecl
The Home directory is d:\ecl\home
The Tools directory is D:\ecl\tools\pc
Master config file d:\ecl\macros\config.ecl
Input file suffix = UNIX
The Granite driver number is  49

BOOKSHELF = pdf
Adobe Acrobat Reader has been installed
The OS Level is Windows XP
```

PVTi will then ask you to choose a working directory and a version.



After you have launched PVTi and specified the working directory, PVTi will ask for the name of the project. This can either be an existing project or a new one.



Look in: tutorials

CLEAN.PVI
FLUID_CORRECT.PVI
GAS.PVI
MULTIPHASE-CO2.PVI
MULTIPHASE-START1.PVI
OLD.PVI
REGRESS_CORRECT.PVI
SIMULATE_CORRECT.PVI
THERMAL.PVI
WORKFLOW.PVI

File name: UNTITLED.PVI

Files of type: *.pvi

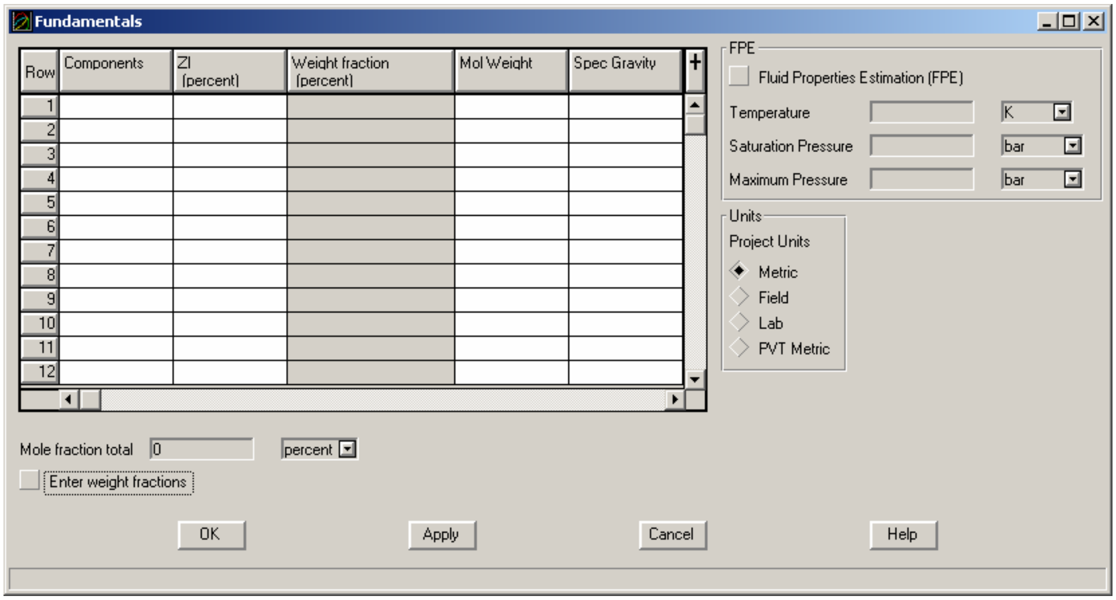
This name will be used to create a number of files. If for example the name of the project is XXX, then PVTi will create:

XXX.PVI these store the PVT data that you input to PVTi and are used whenever you want to save the data.

XXX.PVO these are the output files from PVTi and are designed to be included without the need for any change in an ECLIPSE model.

XXX.PVP these contain the detailed results of the experiments that you have run in PVTi and are the equivalent of the ECLIPSE PRT files.

Once you have given your project a name, PVTi will display the Fundamentals Panel. The fundamentals panel is a quick and easy way of defining your sample components and composition.



☐ Fluid Properties Estimation (FPE)

Temperature: K

Saturation Pressure: bar

Maximum Pressure: bar

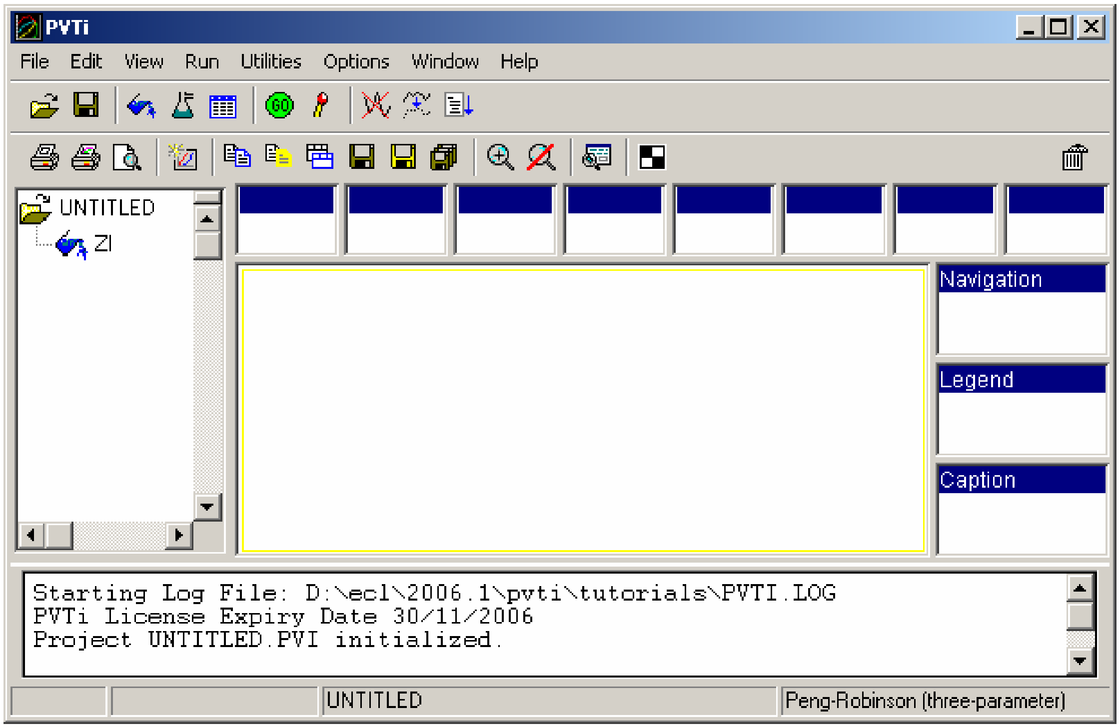
Project Units: ● Metric ○ Field ○ Lab ○ PVT Metric

Mole fraction total: 0 percent

☐ Enter weight fractions

Fluid properties estimation can provide quick-look PVT tables given a sample composition and no laboratory experiment results. A saturation pressure (bubble or dew-point) together with a reservoir composition are sufficient inputs to provide an initial estimate of fluid properties in advance of a full fluid analysis in the lab.

After the Fundamentals Panel, the main PVTi panel will appear.



```
Starting Log File: D:\ecl\2006.1\pvti\tutorials\PVTI.LOG
PVTi License Expiry Date 30/11/2006
Project UNTITLED.PVI initialized.
```

UNTITLED | Peng-Robinson (three-parameter)

Before working with PVTi, we need to first understand what we mean by a component and by sample compositions.

Components and Composition

Genesis

Petroleum hydrocarbon reservoirs have as their origin organic matter that has been preserved in sedimentary rocks. This organic matter is invariably a mixture of both animal and plant remains which have avoided the normal fate of oxidation and decay. In the presence of an anoxic basin or oxygen deficient environment (such as a stagnant lagoon, the deep sea or an oxbow lake), dead plant and animal matter will accumulate along with silt to create organically-rich sediment. This may later become “black” shale, a potential petroleum source rock.

Whether or not this happens will depend on the subsequent burial and temperature history of the sediment. At relatively modest depths and temperatures (less than 5000 feet) anaerobic bacterial action forms kerogen from the remains. The subsequent effect of temperature on the kerogen determines the properties of the resulting petroleum system; pressure and time have relatively little effect on the outcome. At temperatures about 120 F, kerogen begins to create crude oil, rich in asphaltenes. As the temperature is increased further to about 200 F, the system will begin to generate lighter hydrocarbons, and hence lighter oil. At around 350 F the amount of remaining C_{7+} molecules in the system will be small, and it will have the properties of a gas condensate. A further increase in temperature will further break down the intermediate paraffins to methane, which will be all that remains above 400 F. Under normal geothermal gradients therefore the “oil window” will occur between the depths 5000 - 21000 feet. Any organic material descending below 21000 feet is likely to produce only methane and coal-like residues. The properties of the fluids in any oil or gas reservoir therefore depend, amongst other things, on the nature of the organic source material and the degree of “cooking” to which it has been subjected.

The migration history is also critically important, as the reservoir rock in which the system is found may not necessarily be contiguous with the source material, and it may be that the constituents of the reservoir arrived at different times, or from separate sources. This can have important consequences on the initial conditions to be expected upon discovery - for instance certain migration conditions will pre-dispose a gas-condensate reservoir to be exactly at its dew point at initial reservoir conditions, even if there is little evidence of a liquid phase in the reservoir.

Components Fundamentals

- Outline
- Homologous Series
- Single carbon Numbers
- Components and Samples
- Phase plots and Ternary diagrams
- Splitting
- Grouping

Because of the organic nature of their source, all petroleum accumulations have hydrocarbons as their predominant constituents. However, there are many instances of accumulations containing significant percentages of inorganic components, the most common being the so-called “acid” gases, carbon dioxide and hydrogen sulphide. Systems containing acid gases are also referred to as being “sour.” The hydrocarbon constituents of petroleum systems are classified into the following categories, most of which describe series (known as homologous series) of compounds having a common basic characteristic or structure, and differing only in the number of structural carbon atoms (and hence molecular weight).

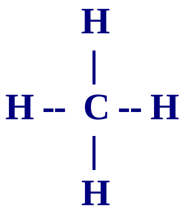
Homologous Series

- Compounds having a common basic characteristic
- Paraffin Hydrocarbons
- Cycloparaffins
- Aromatic Hydrocarbons
- Polynuclear Hydrocarbons
- Above Categories containing additional atoms:
- Sulphur
- Nitrogen
- Oxygen
- Metals

Paraffin hydrocarbons

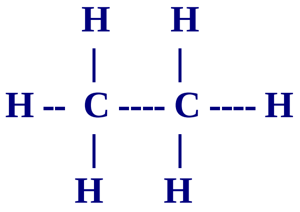
These compounds[1], also known as aliphatic hydrocarbons, and generically referred to as “alkanes”, are the simplest and often the most abundant constituents of petroleum systems. . They are stable and unreactive, and all have the general chemical formula C_nH_{2n+2}. Methane, CH_4 is the first member of the series, having n=1. The first few members of the series are as follows:

1. Methane



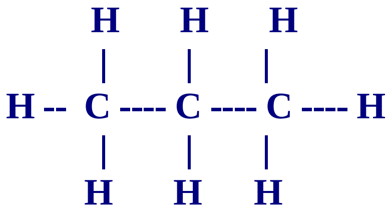
$$\begin{array}{ccc} & H & \\ & | & \\ H\text{ -- } & C & \text{ -- }H \\ & | & \\ & H & \end{array}$$

2. Ethane



$$\begin{array}{ccccc} & H & & H & \\ & | & & | & \\ H\text{ -- } & C & \text{ ---- } & C & \text{ ---- }H \\ & | & & | & \\ & H & & H & \end{array}$$

3. Propane



$$\begin{array}{ccccccc} & H & & H & & H & \\ & | & & | & & | & \\ H\text{ -- } & C & \text{ ---- } & C & \text{ ---- } & C & \text{ ---- }H \\ & | & & | & & | & \\ & H & & H & & H & \end{array}$$

N	Alkane Name	Formula	MW
1	Methane	C1H4	16
2	Ethane	C2H6	30
3	Propane	C3H8	44
4	Butane	C4H10	58
5	Pentane	C5H12	72
6	Hexane	C6H14	86
7	Heptane	C7H16	100
8	Octane	C8H18	114
9	Nonane	C9H20	128

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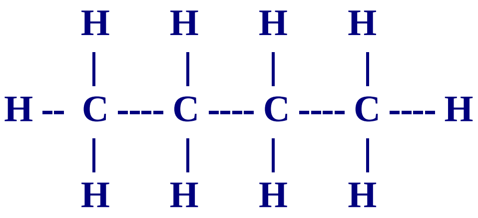
[1] The name is from the Latin *parum* and *affinis* meaning "little" and "affinity", respectively

Carbon always exhibits a valency of 4, and hence all the carbon-carbon bonds in paraffin hydrocarbons are single bonds. In chemical nomenclature, this condition is referred to as saturation and is in no way related to the meaning of saturation as related to the PVT behavior of oil and gas systems.

For n=4, (Butane) and above, the molecules may have different possible structures despite having the same formula and molecular weight.

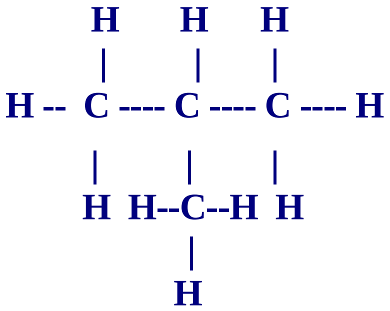
Problems start with C4H10: iso- and normal-butane

Butane



$CH_3-CH_2-CH_2-CH_3$

or Butane?



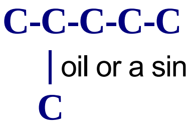
In addition to having a straight chain structure, a particular formula may also represent molecules that are branched, and the potential number of variants increases rapidly with n. The straight chain molecules are referred to as normal paraffins and the branched molecules are generically grouped as iso-paraffins. The physical properties of the iso-paraffins (such as boiling point, liquid density and critical properties) may differ substantially from those of the normal paraffin having the same molecular weight, and these variations having the same formula are called isomers. At low values of n, the isomers of a given paraffin can be distinguished by gas chromatography analysis, as it is at low n values that the physical property differences between isomers are greatest. As n increases, so the differences diminish and the paraffins themselves become much less volatile, and therefore more difficult to resolve using gas chromatography.

Systems containing significant amounts of high molecular weight paraffins will be waxy, and will precipitate out wax as temperature decreases. Rather than exhibiting a continuous reduction in viscosity with temperature, such systems will have a tendency to “set” at a given temperature.

Carbon atoms can form single or double bonds

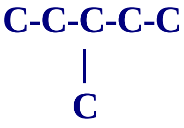
C-C-C-C-C-C

C-C-C-C-C=C

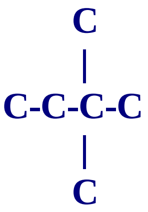


$\text{C-}\underset{\text{C}}{\underset{|}{\text{C}}}\text{-C-C-C}$

oil or a single-phase gas



$\text{C-C-}\underset{\text{C}}{\underset{|}{\text{C}}}\text{-C-C}$



$\text{C-C-}\overset{\text{C}}{\overset{|}{\underset{\text{C}}{\underset{|}{\text{C}}}}}\text{-C}$

Cycloparaffins

These are compounds where the chain structures of normal paraffins have been formed into rings. All the carbon-carbon bonds are still single and they are therefore, from a chemical nomenclature viewpoint, saturated. It is possible to form a ring paraffin from three or more carbon atoms, the first member of the series being cyclopropane, C_3H_6. All the simple cycloparaffins have the chemical formula C_nH_{2n}, which is the same generic form as the olefins, or alkenes. These compounds are characterised by having one or more carbon-carbon double bonds, the simplest olefin being ethylene. Olefins are not naturally occurring, but they have considerable importance in the downstream petroleum business.

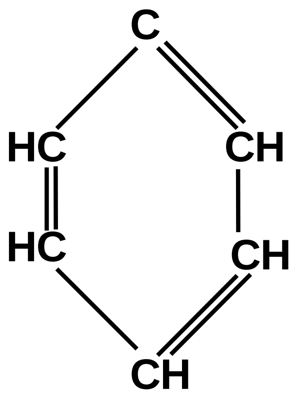
At low carbon numbers, cycloparaffins are significantly less stable than their normal paraffin counterparts (i.e., molecules having the same carbon number) and are therefore present in much smaller amounts. However, in gas/condensate systems in particular, reactive species can have a significant effect on phase behavior even in relatively small amounts.

As the molecular weight of cycloparaffins increase, they form collections of contiguous rings of five or six carbon atoms per ring, rather than single rings of ever increasing size. These are collectively known as naphthenes, and are as stable as their chain paraffin counterparts.

Aromatic Hydrocarbons

Aromatic hydrocarbons are compounds containing one or more benzene rings, these being stable ring compounds with the formula C_6H_6, and are normally represented by the structural formula shown.

BENZENE



The benzene molecule has three double carbon-carbon bonds and the molecule is therefore unsaturated. Despite the superficial resemblance to olefinic hydrocarbons, benzene and its derivatives are highly stable due to the very different structure of its electron orbits. The basic benzene ring can be attached to paraffin based chains, the most common derivatives being toluene and xylene. In the case of xylene, there can be three possible structural forms of this molecule, the meta form, the ortho- and para- forms which all have slightly different properties from one another. Benzene rings also coalesce into multi-ring structures as molecular weight increases. The aromatic content of a hydrocarbon fluid has a significant effect on its phase behavior.

Single Carbon Numbers

You can see from the previous sections that there is a considerable diversity of components in natural hydrocarbon fluids. The organic source material, the burial and temperature history, and the action of microbes all affect the composition of the fluid, and the relative amounts of the different components.

The API of oil is often quoted and used as a general description of the oil.

$$\gamma = \frac{141.5}{(API + 131.5)}$$

API however is not a good indicator of the detailed composition of the oil.

We need a more precise way of summarizing the extreme variety of components that we can find in our hydrocarbon fluid.

Knowing that an oil is 5% C9 helps, but what do we mean by C9? What are the properties of this C9?

Number of isomers increases rapidly above SCN of 6

Estimate: between 1×10^9 and 3×10^9 isomers of C30

For the lower molecular weights, modern analytical methods can identify individual components, and also the isomers of these basic components. However, as the molecular weights of the hydrocarbon components rise, it becomes less easy to discriminate them using routine analytical methods.

Naturally occurring oil and gas mixtures are usually too complex for a complete classification of all constituent components. Standard laboratory analyses usually only identify three non-hydrocarbons, namely N_2, H_2S, CO_2 and the hydrocarbons C_1, C_2, C_3, iC_4, iC_5, nC_5 and components called C_6, C_7, etc. The number of isomers increases rapidly for carbon number six and above. - it has been estimated that there are between 10^9 and $3*10^9$ isomers of C_{30}!

The most usual compromise is to report the composition of the higher molecular weight residues in terms of boiling point fractions, which are the amounts of fluid that distil between two specified temperatures.

Proliferation of isomers with increasing carbon number makes individual identification impossible.

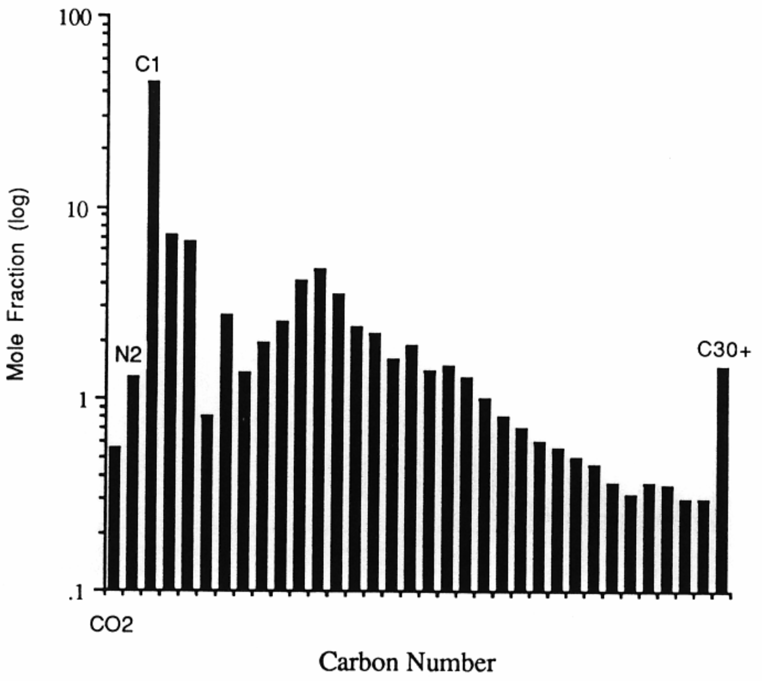
Introduce Single Carbon Number (SCN) Groups

SCN group n: all hydrocarbons with

$$T_b(C_n) < T_b < T_b(C_{n+1})$$

Benzene (C6H6) is usually found in SCN Group 7 as its boiling point is higher than that of the paraffin Heptane (C7H16).

The temperature intervals are usually chosen to be between the boiling points of each member of the series of normal paraffins, and the fractions are referred to by the number of carbon atoms in the relevant normal paraffin. Thus, the fraction which is referred to as the C9 fraction includes compounds which may have less than nine carbon atoms, but have a higher boiling point than the normal paraffin with the same number of carbon atoms. For example benzene, which has only six carbon atoms, would be included in the C7 boiling point fraction. These groups are referred to as single carbon number (SCN) groups, which is therefore misleading. PVT laboratory reports will provide the distribution of SCN groups in the reservoir oil or gas.



The distribution for a typical North Sea oil

Predicting the properties of the reservoir fluids given this composition is not straightforward, as we don't in general know the properties of the SCNs in the reservoir. For example SCN 9 in one reservoir is likely to have different properties from SCN 9 in another reservoir.

Only in the case of an extremely paraffinic fluid would the reported SCN groupings have the properties of the corresponding normal paraffin, such as molecular weight or P_c or T_c. For carbon number above which analysis for individual components becomes impractical, (around C10+) it is important to know the relative amounts of paraffinic, naphthenic, and aromatic compounds in each of the single carbon number groupings, in order that better estimates of group properties can be made. If true distillations are performed, as against simulated distillations using gas chromatography, this can be partially achieved by measuring the molecular weight and specific gravity of each true boiling point (TBP) fraction. A paraffin, naphthalene, and aromatic (PNA) breakdown has to be performed via mass spectrometry methods for the heavier fractions, and this is not a routine procedure. PVTi can perform a PNA split of the heavier components, and these can then be used to predict wax and asphaltenes precipitation.

Laboratory reports

In PVT laboratory reports, components called hexane, heptanes, etc., are SCN groups. Tables of the properties of SCN groups for "typical" fluids are widely available (Whitson, 1983). Ideally the density and molecular weight of such "lumped" components should be reported in a laboratory analysis.

All PVT reports should have a component analysis up to some upper carbon number to be specified by the owner of the fluid, say 6, 11 or 19 or 29. The residual hydrocarbon fluid is usually referred to as the plus fraction, i.e., C_{7+}, C_{12+} or C_{20+}.

Detailed component analysis is made of pure component and SCN fractions up to a PLUS fraction

- **C7+ - old/cheap**
- **C12+**
- **C20+**
- **C30+ - expensive**

Older laboratory reports will probably only contain an analysis up to C6. Current reports with details up to C30 (or even higher SCNs) are becoming more common, but are also more expensive to produce.

For the plus fraction, only a limited set of information will be made available, usually the molecular weight M_{N+} and the specific gravity γ_{N+}. For use in an EoS model, it is necessary to calculate the EoS parameters, such as T_c, P_c, etc., via correlations depending on M_{N+} and γ_{N+}. The process of obtaining EoS properties from the M_{N+} and γ_{N+} of the plus component is called "Characterisation of the Plus fraction".

Mole Weight of C+ fraction is made by freezing point depression or boiling point elevation.

- **For C7+, C12+ C20+ or C30+ only a limited set of information available, usually the molecular weight M_{N+} and sometimes the specific gravity γ_{N+}**
- **These are obtained from correlations depending on M_{N+} and γ_{N+}, for example the Kesler-Lee Correlation.**
- **This is called "Characterization of the Plus fraction".**

A correlation for the plus fraction

Several authors have generated correlations for calculating the EOS parameters T_c, P_c, etc., from mole weight and specific gravity. A popular correlation is that of Kesler-Lee (1976):

$$
\begin{aligned}
p_c = {} & 8.3634 - \frac{0.0566}{\gamma} \\
& - \left(0.24244 + 2.2989\gamma + \frac{0.11857}{\gamma^2} \right) \text{ x } 10^{-3}\, T_b \\
& + \left(1.4685 + \frac{3.648}{\gamma} \right) \; \frac{0.47227}{\gamma^2} x 10^{-7}\, T_b^2 \\
& - \left(0.42019 + \frac{1.6977}{\gamma^2} \right) x 10^{-10}\, T_b^3
\end{aligned}
$$

$$
\begin{aligned}
T_c = {} & 341.7 + 811.0\gamma + (0.4244 + 0.1174\gamma) T_b \\
& + \frac{(0.4669 - 3.26223\gamma) x 10_5}{T_b}
\end{aligned}
$$

$$
\omega = \frac{\left(-\ln\left(\frac{Pc}{14.696} \right) - 5.92714 + \frac{6.09648}{T_{b,r}} + 1.28862 \ln T_{b,r} - 0.169347 T_{b,r}^6 \right)}{\left(15.2518 - \frac{15.6875}{T_{b,r}} - 13.4721 \ln T_{b,r} + 0.43577 T_{b,r}^6 \right)}
$$

$$
(T_{b,r} < 0.8)
$$

$$
\begin{aligned}
\omega = {} & -7.904 + 0.1352 K_w - 0.007465 K_w^2 + 8.359 T_{b,r} \\
& + \frac{(1.408 - 0.01065 K_w)}{T_{b,r}} \quad (T_{b,r} > 0.8)
\end{aligned}
$$

where

T_b and T_c are the main text boiling point and critical temperatures, in degrees Rankin, respectively,

γ is the 60/60 specific gravity (density of the fraction at atmospheric pressure and 60 F divided by the density of water in g/cm^3 at the same conditions),

p_c is the critical pressure in psia,

K_w is the Watson characterisation factor, $K_w = T_b^{1/3}/\gamma$ and

$T_{b,r}$ is the reduced boiling point temperature, $T_{b,r} = T_b/T_c$.

Other correlations are available due to Cavett (1962) for P_c, T_c and Edmister (1984) for ω. The correlations of Riazi-Daubert (1980, 1987) are particularly attractive since they are of the form $\theta = aT_b^b \gamma^c$ where the set of properties θ that can be estimated are mole weight, M_w, critical temperature (T_c) and pressure, ($P_{c,}$), molar volume (V_m) and density, (γ). The values for the three coefficients (a, b, c) are given in Whitson (1983).

Summary: Components and Compositions

- **We don't know the properties of the SCNs.**
- **We don't know the properties of the plus fraction.**
- **Therefore we can't predict fluid behavior.**
- **This is where regression comes in: we adjust the fluid properties to match the observations.**

We will do this later in the Regression Module.

We have seen that the laboratory reports give the composition of the fluid in terms of Single Carbon Numbers (SCNs). We have also shown that we don't know the detailed make-up and therefore the detailed properties of these SCNs.

The reports will only quote SCNs up to a plus fraction. For the plus fraction, very limited information is available, so we have to use correlations to characterise their properties.

As we don't know the detailed properties of either the SCNs or the plus fraction, it is not possible to calculate the properties of the mixture of these SCNs and plus fraction. This is why we need to regress our equation of state to match the experimental observations given in the laboratory reports.

5. Components and Samples in PVTi

In this section we shall learn how the properties of components are defined in PVTi.

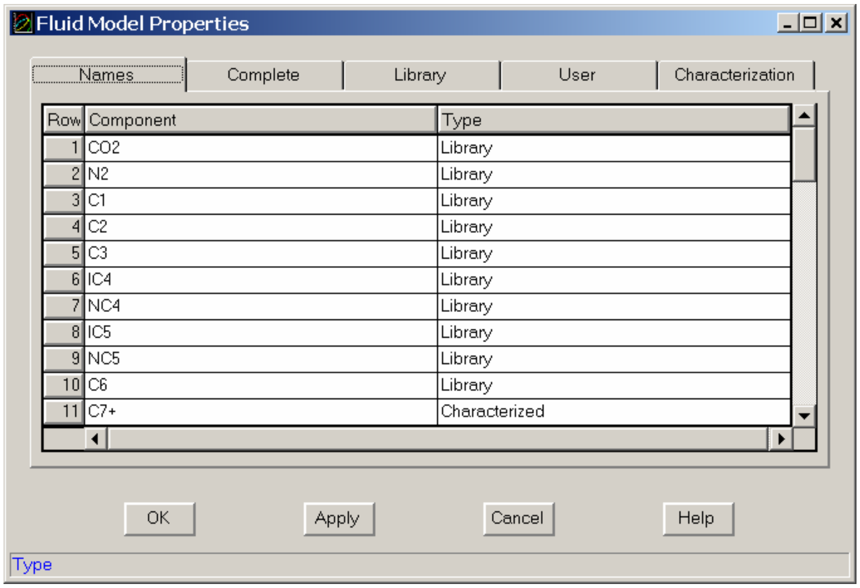
Defining Components in PVTi

If you haven't already defined your sample composition using the fundamentals panel, the first step in using PVTi is to define the components[2] that we are going to deal with. Edit | Fluid Model |Components shows that components can be defined as one of 3 possible types:

1 Library is the default. PVTi has a built-in tables of properties of the common hydrocarbons up to C_{45} and of the non-hydrocarbons H_20, H_2S, CO_2, N_2, H_2 and CO,

2 Characterise is usually reserved for the plus component

3 User-defined properties are for the cases where you wish to supply your own non-library properties for a component.

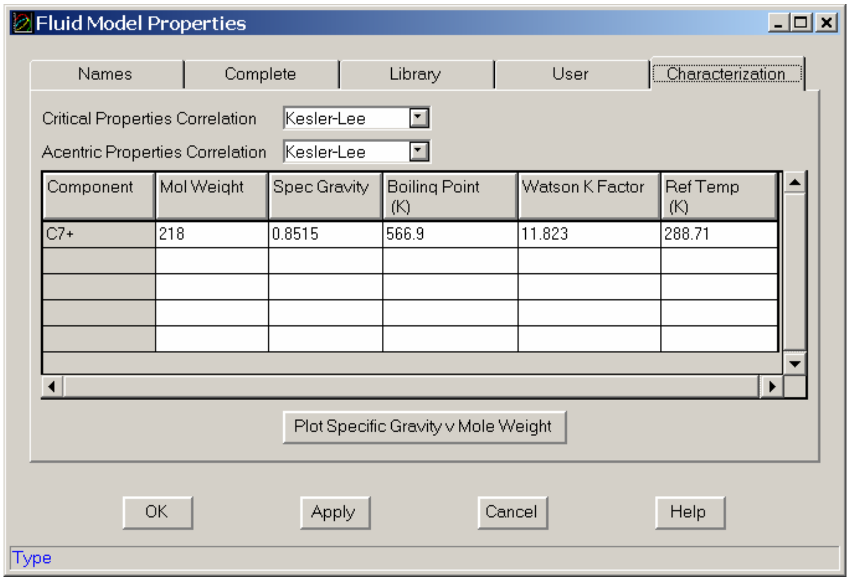


Row	Component	Type
1	CO2	Library
2	N2	Library
3	C1	Library
4	C2	Library
5	C3	Library
6	IC4	Library
7	NC4	Library
8	IC5	Library
9	NC5	Library
10	C6	Library
11	C7+	Characterized

---

[2] From now on, when we talk about PVTi components we include components, pseudo-components and merged components.

After choosing “characterise”, click Apply then the Characterise Tab. You will then have a choice of methods.



Critical Properties Correlation: Kesler-Lee
Acentric Properties Correlation: Kesler-Lee

Component	Mol Weight	Spec Gravity	Boiling Point (K)	Watson K Factor	Ref Temp (K)
C7+	218	0.8515	566.9	11.823	288.71

PVTi has five correlations for generating critical and other properties

- Kesler and Lee
- Cavett
- Riazi and Daubert
- Winn
- Pedersen

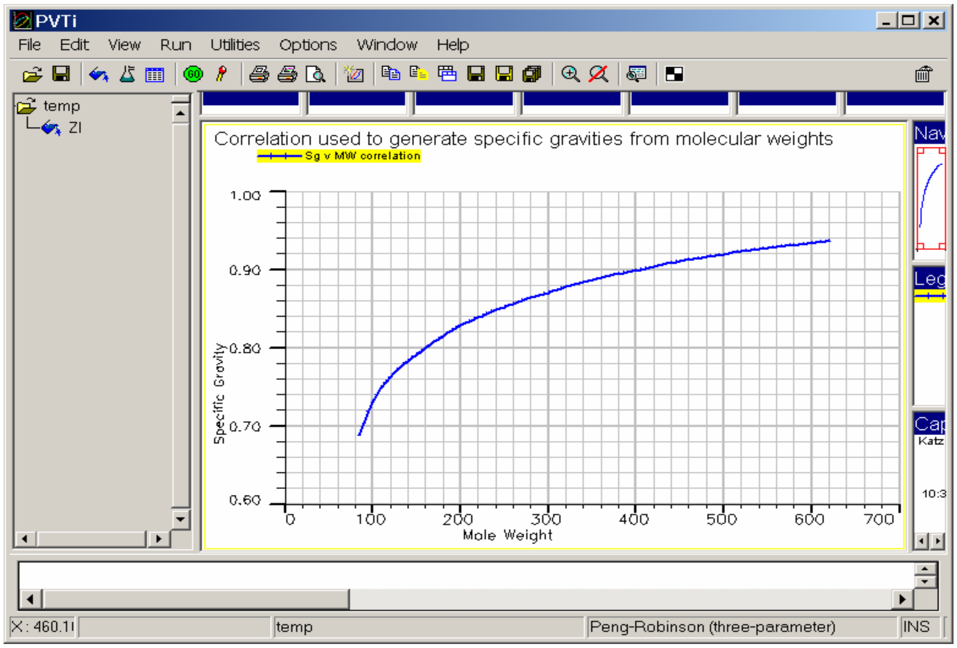
and four sets of correlations for acentric factors:

- Kesler and Lee
- Edmister
- Thomassen
- Pedersen

Unless you have a very good reason to do otherwise, choose the defaults.

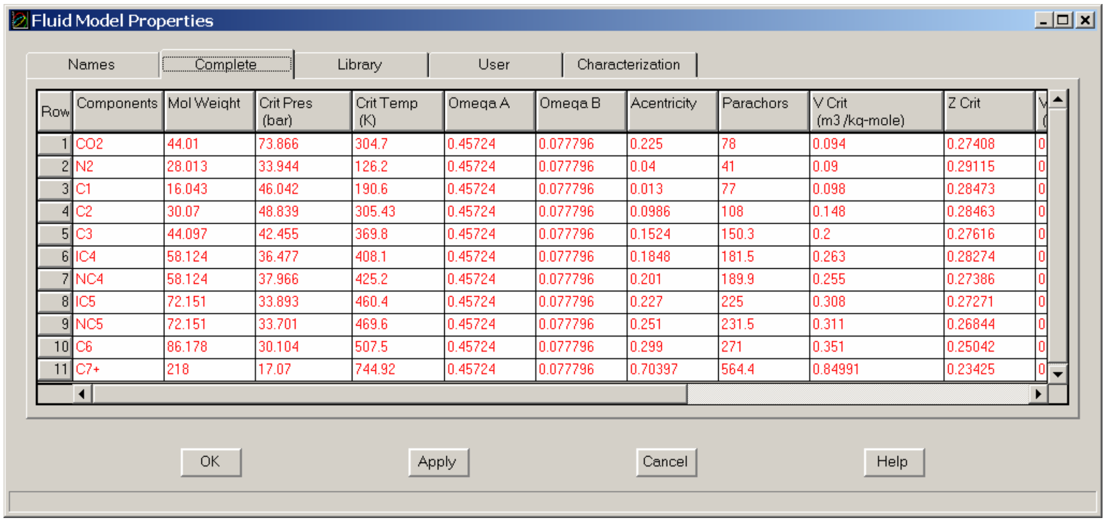
All characterisations start with the molecular weight of the plus component, which is usually provided in the laboratory report. If you don’t have that molecular weight then it is possible to start with an estimate of the molecular weight then regress using Special Regression (see later in the course).

Characterisation also needs the density of the plus component, but if this not available then another correlation will estimate it from the molecular weight.



Once both the molecular weight and the density are available then clicking the Characterise button will generate the other quantities. Looking ahead to regression: the properties of the + component are the least well-known and therefore the best candidates for adjustment

To view the complete set of properties for all the components that have been chosen, click on the Complete Tab.



Row	Components	Mol Weight	Crit Pres (bar)	Crit Temp (K)	Omega A	Omega B	Acentricity	Parachors	V Crit (m3 /kg-mole)	Z Crit
1	CO2	44.01	73.866	304.7	0.45724	0.077796	0.225	78	0.094	0.27408
2	N2	28.013	33.944	126.2	0.45724	0.077796	0.04	41	0.09	0.29115
3	C1	16.043	46.042	190.6	0.45724	0.077796	0.013	77	0.098	0.28473
4	C2	30.07	48.839	305.43	0.45724	0.077796	0.0986	108	0.148	0.28463
5	C3	44.097	42.455	369.8	0.45724	0.077796	0.1524	150.3	0.2	0.27616
6	IC4	58.124	36.477	408.1	0.45724	0.077796	0.1848	181.5	0.263	0.28274
7	NC4	58.124	37.966	425.2	0.45724	0.077796	0.201	189.9	0.255	0.27386
8	IC5	72.151	33.893	460.4	0.45724	0.077796	0.227	225	0.308	0.27271
9	NC5	72.151	33.701	469.6	0.45724	0.077796	0.251	231.5	0.311	0.26844
10	C6	86.178	30.104	507.5	0.45724	0.077796	0.299	271	0.351	0.25042
11	C7+	218	17.07	744.92	0.45724	0.077796	0.70397	564.4	0.84991	0.23425

Properties of hydrocarbon series

For the hydrocarbon series, most physical properties are found to either increase of decrease.

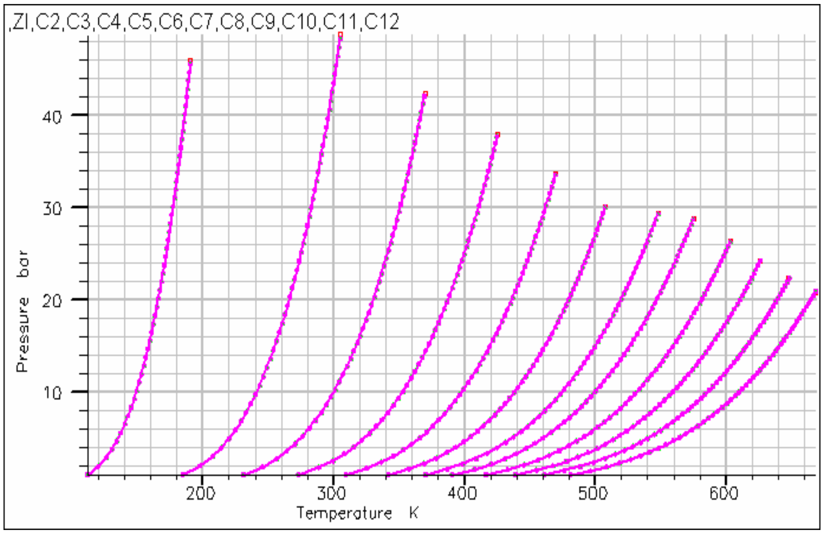
Properties increasing with increasing molecular weight are:

1. Tc Critical Temperature
2. Tb Normal Boiling Point
3. Vc Critical Volume
4. ω Acentric Factor
5. ρo Liquid Density
6. Pa Parachor

Properties decreasing with increasing molecular weight are:

1. Pc Critical Pressure
2. Zc Critical Z-Factor

It is the monotonicity of these properties that is used as the basis for the characterisation of “unknown” components such as the plus fraction. During regression the monotonicity should be maintained, and if any of these properties are changed in such a way that they are no longer monotonic with molecular weight then PVTi will give a warning message.

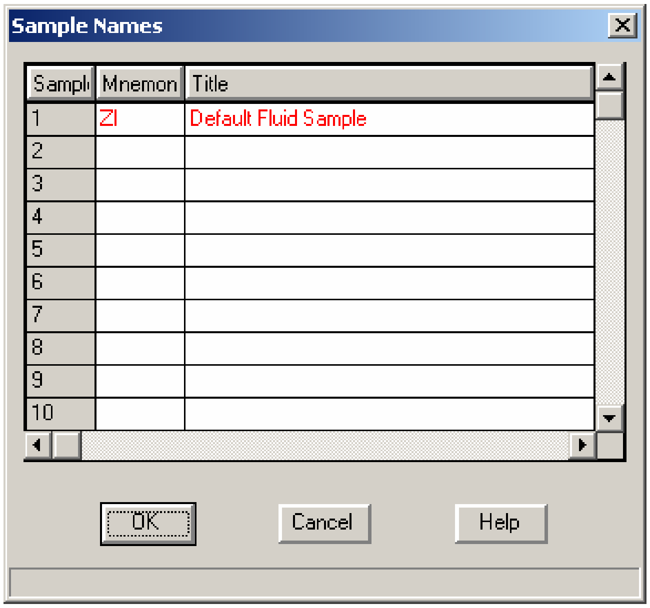


Note that the critical pressure of C_1 (labeled Z1 in the plot above) is an exception to the general rule that P_c decreases with increasing molecular weight.

Defining Samples

Having defined the components that we are going to use and their properties, we can now define the composition of our fluid sample in terms of these components.

Main Panel | Edit | Sample | Names displays the following panel:

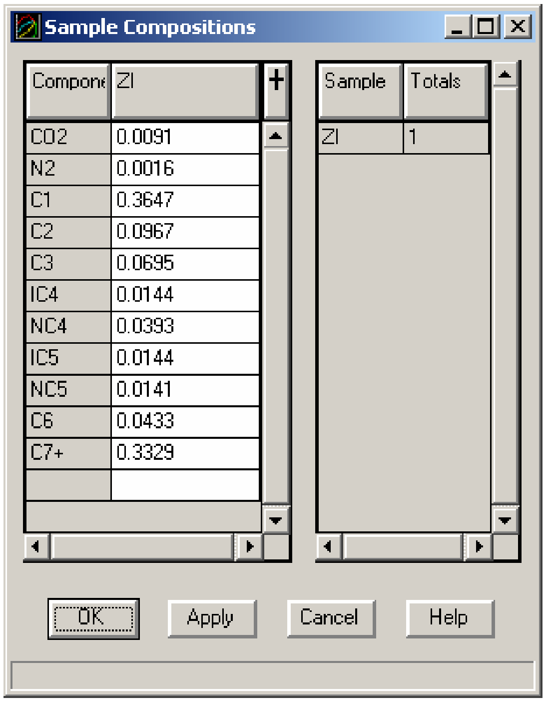


Sampl	Mnemon	Title
1	ZI	Default Fluid Sample
2		
3		
4		
5		
6		
7		
8		
9		
10		

By default, a sample always exists with the name ZI. You can define as many other samples as you wish. Sample names can be any name you want, and a description is optional.

Note the difference between “components” and “samples”. Suppose you wanted to model a gas made up entirely of carbon dioxide. You can have a component called CO2 and a sample called CO2. The component name CO2 is known to the program and PVTi will assign the appropriate properties to that component. You can call the gas “CO2” or “Carbon_Dioxide” or “Gas1” and none of these names will change the properties of the gas.

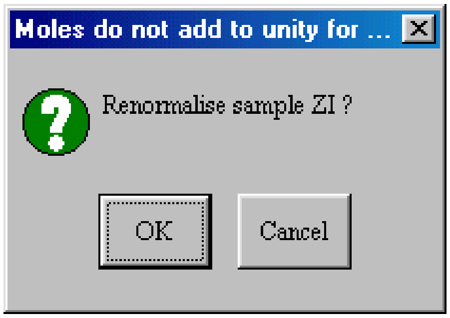
Having defined the sample name, or used the default name ZI, you can then define the composition of the sample by Edit | Samples | Compositions



Compone	ZI
CO2	0.0091
N2	0.0016
C1	0.3647
C2	0.0967
C3	0.0695
IC4	0.0144
NC4	0.0393
IC5	0.0144
NC5	0.0141
C6	0.0433
C7+	0.3329

Sample	Totals
ZI	1

Once you have specified the composition of the sample by giving either the model fraction or the percentage of each component (depending on the units chosen) then clicking on Apply will make PVTi check that the sum of the mole fractions is 1 (or that the sum of the percentages is 100%). If the sum is not correct, then you will get a message:



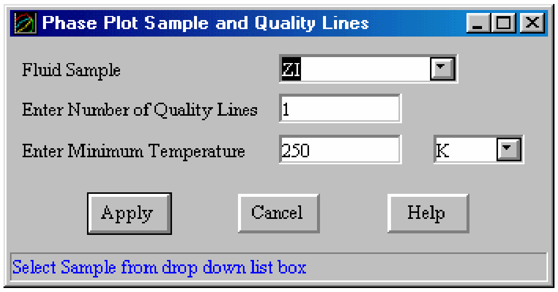
Moles do not add to unity for ...

Renormalise sample ZI ?

If the sum is close to 1 (or 100%) then choosing OK will renormalise the compositions. Otherwise correct your data and try again.

At this stage, a useful check on the data entry so far is to plot a phase diagram. This can be done either by

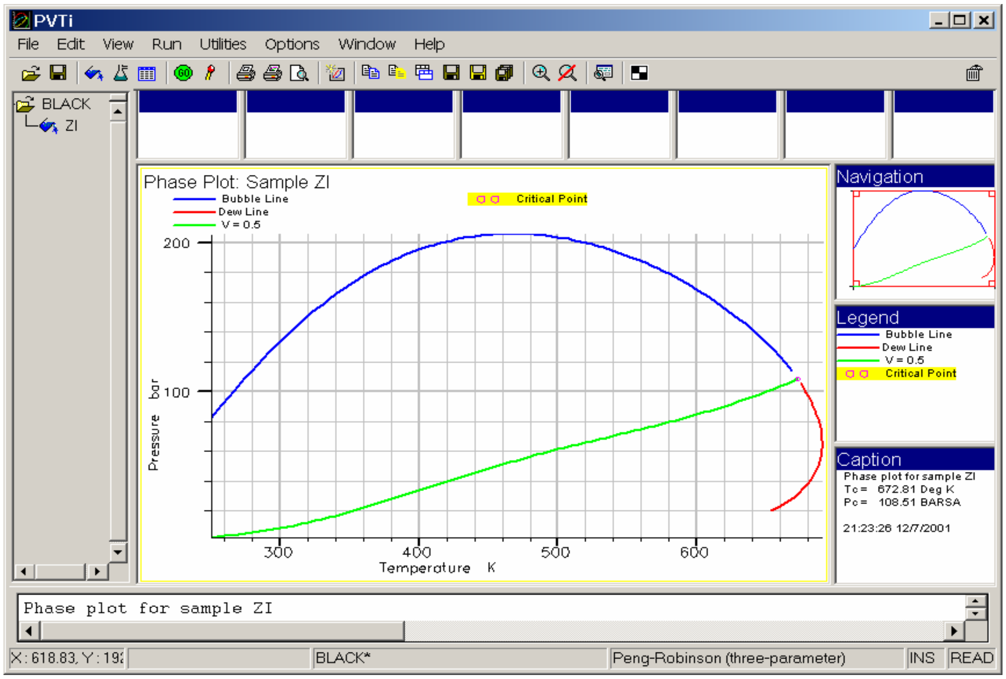
- dragging and dropping the sample name (ZI) from the left-hand column onto the main plotting area,
- or by right clicking on the sample name and choosing “phase plot”
- or by View | Samples | Phase Plot.



Fluid Sample: ZI
Enter Number of Quality Lines: 1
Enter Minimum Temperature: 250 K

Select Sample from drop down list box

The advantage of the last of these methods is that it enables you to display more than one quality line on the phase plot, should you wish to do so.



Phase plot for sample ZI
Tc = 672.81 Deg K
Pc = 108.51 BARSA
21:23:26 12/7/2001

Phase plot for sample ZI

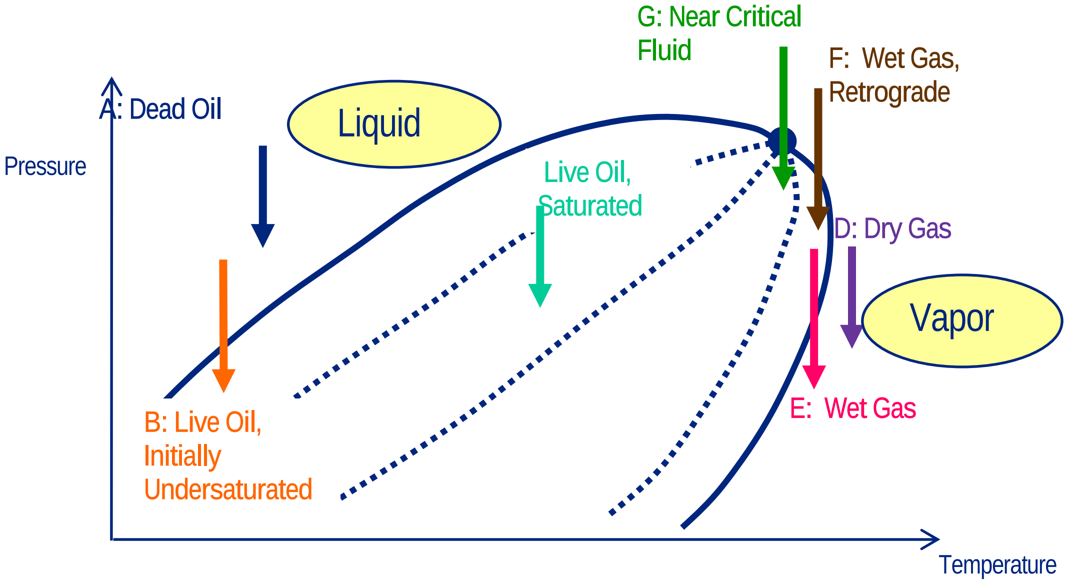
X: 618.83, Y: 19
BLACK*
Peng-Robinson (three-parameter)
INS
READ

In the picture above, the 50% quality line is displayed as well as the dew-point and bubble point lines.

Types of Oil and Gas

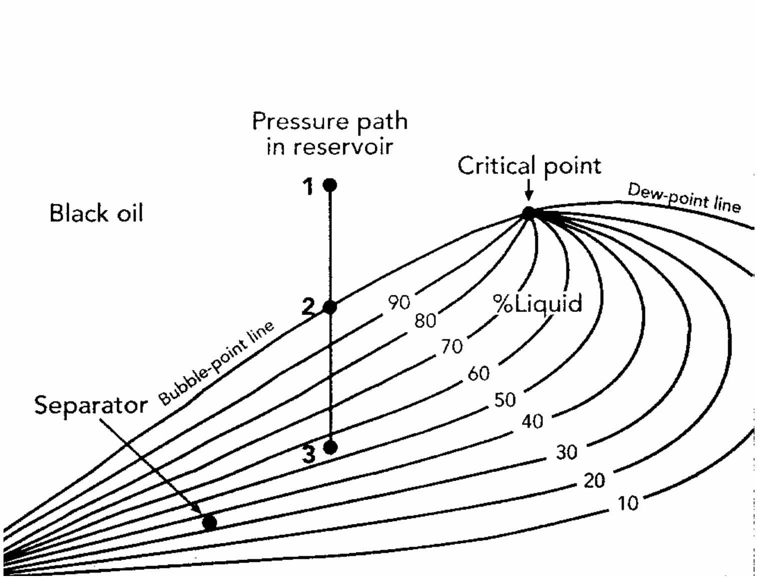
Hydrocarbon deposits are generally classified as one of the following:

1 Black Oil
2 Volatile Oil
3 Retrograde Gas / Condensate
4 Wet Gas
5 Dry Gas



Black Oil:

1 Low-shrinkage crude oil
2 Initial GOR of 2000 scf/STB or less
3 API gravity below 45°
4 Initial Bo of 2 res bbl/STB or less
5 C7+ > 20 mole %



Volatile Oil:

High-shrinkage crude oils

Near-critical oils:

Initial GORs between 2000 and 3000 scf/STB

API gravity usually 40° or higher

Initial Bo > 2 res bbl/STB

C7+ between 12.5 to 20 mole %

Associated gas is rich retrograde gas

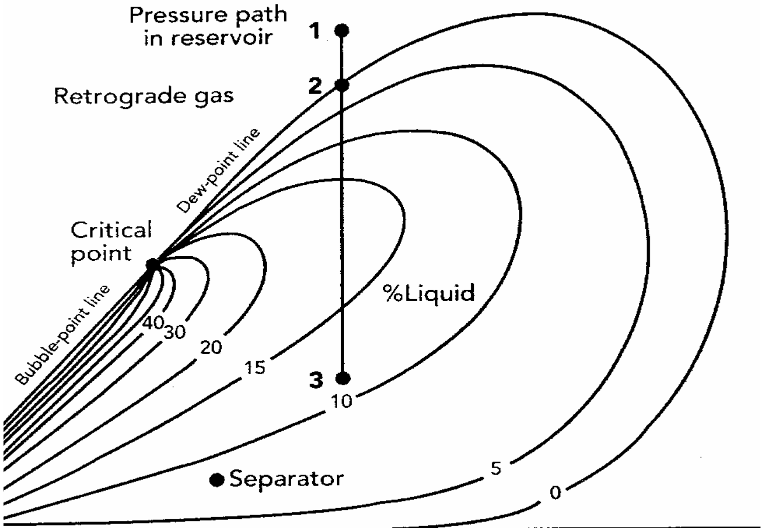
The pressure path in the reservoir is similar to that of black oil.

Retrograde Gas/ Condensate:

Initial GOR between 3300 and 150,000 scf/STB

Stock-tank liquid gravity between 40° and 60° API

C7+ < 12.5 mole %

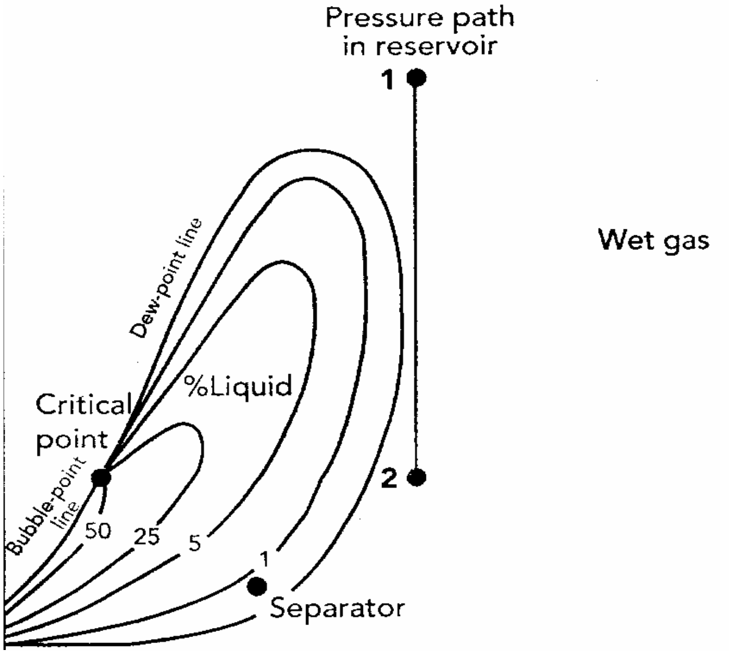


Wet Gas:

The reservoir temperature is above the Cricondentherm. The pressure path within the reservoir may or may not enter the phase envelope, but the separator output is two-phase.

Gravity of stock tank liquid same as retrograde gas - constant during life of field

Gas/Liquid production rate > 50,000 scf/STB

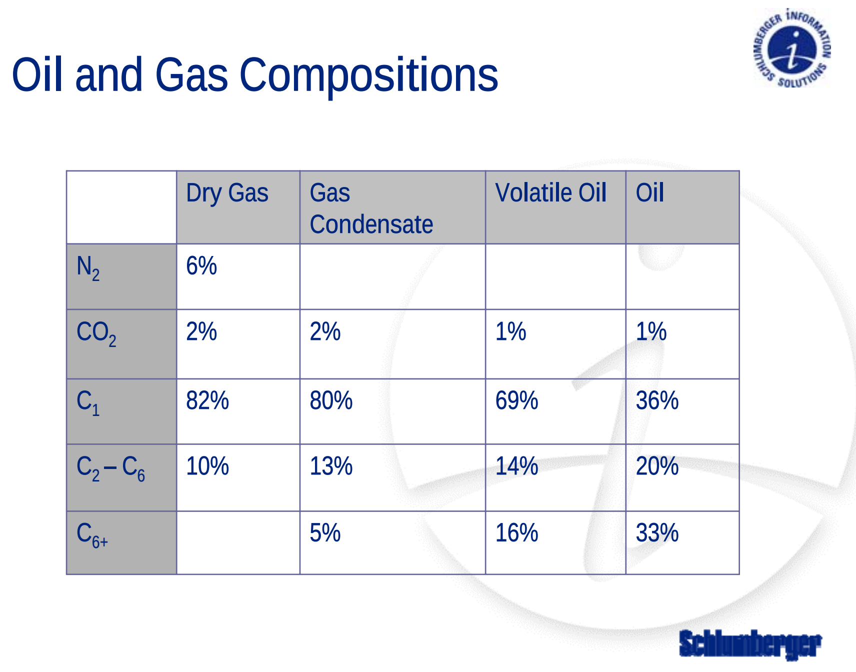


<u>Dry Gas:</u>

Primarily methane and some intermediates

No liquids formed either in reservoir or at surface

Typical compositions of the some of the types of hydrocarbon fluids are shown below.



Oil and Gas Compositions

	Dry Gas	Gas Condensate	Volatile Oil	Oil
N_2	6%			
CO_2	2%	2%	1%	1%
C_1	82%	80%	69%	36%
$C_2 – C_6$	10%	13%	14%	20%
C_{6+}		5%	16%	33%

The “nature” or “type” of a fluid is best defined by using the phase envelope and the fluid temperature. The phase envelope is unique for each particular composition of hydrocarbons and non-hydrocarbons.

<u>The distance between the critical temperature and the reservoir or surface temperature defines the fluid type.</u>

Dry Gas and Black Oil systems can be described by either EoS or non-EoS approaches. A black-oil non-EoS approach uses suitable correlations, and will work provided that fluid properties are only functions of pressure and temperature. The use of EoS to describe Dry Gases and Black Oils is usually very easy. Although many authors have generated correlations to describe particular “volatile” fluids, i.e., Gas Condensates and Volatile Oils, none of these is general and EoS methods must be used.

Exercise 1 PVTi Tutorial 1 & 2

The PVTi on-line manual contains a number of useful tutorials. We shall go through the tutorial 1 on “Fluid Properties Estimation”. The steps involved are:

1 **Introduction**
2 **Basic information - Fundamentals**
3 **Flash Calculations**
4 **Discussions**

We shall also go through Tutorial 2 on “Creating a Fluid System”. The steps involved are:

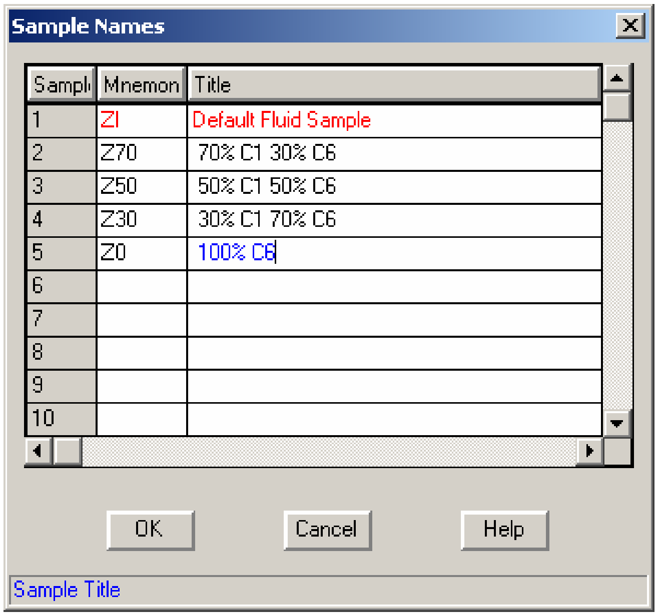
1. **Defining a fluid**
2. **Defining a fluid sample**
3. **Selecting an EoS**
4. **Program Options**
5. **Viewing fluid attributes (Phase Plots)**
6. **Saving Fluid System information**

After performing the tutorial, your display should look like this:

Exercise 2 A two-component system

The shape of the phase envelope is a function of the amount and type of components in the mixture, a phase envelope being unique to a given composition. This exercise will show how the phase envelope changes as a function of composition.

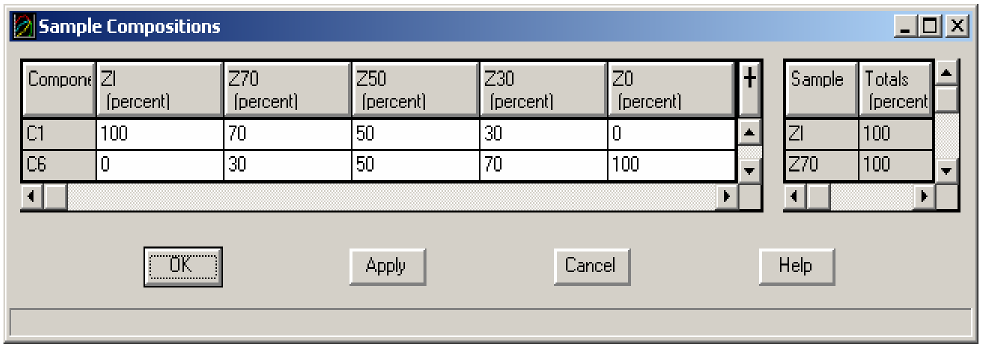
1. Click "superimpose plots"
2. For demonstration purpose define a fluid composed of only C1 and C6
3. Our first fluid is 100% C1
4. Create 4 new samples



Sampl	Mnemon	Title
1	ZI	Default Fluid Sample
2	Z70	70% C1 30% C6
3	Z50	50% C1 50% C6
4	Z30	30% C1 70% C6
5	Z0	100% C6
6		
7		
8		
9		
10		

Define the compositions of the five samples

Z 1 is 100% C1
Z70 is 70% C1, 30%C6
Z50 is 50% C1, 50%C6
Z30 is 30% C1, 70%C6
Z0 is 100%C6



Compone	ZI (percent)	Z70 (percent)	Z50 (percent)	Z30 (percent)	Z0 (percent)
C1	100	70	50	30	0
C6	0	30	50	70	100

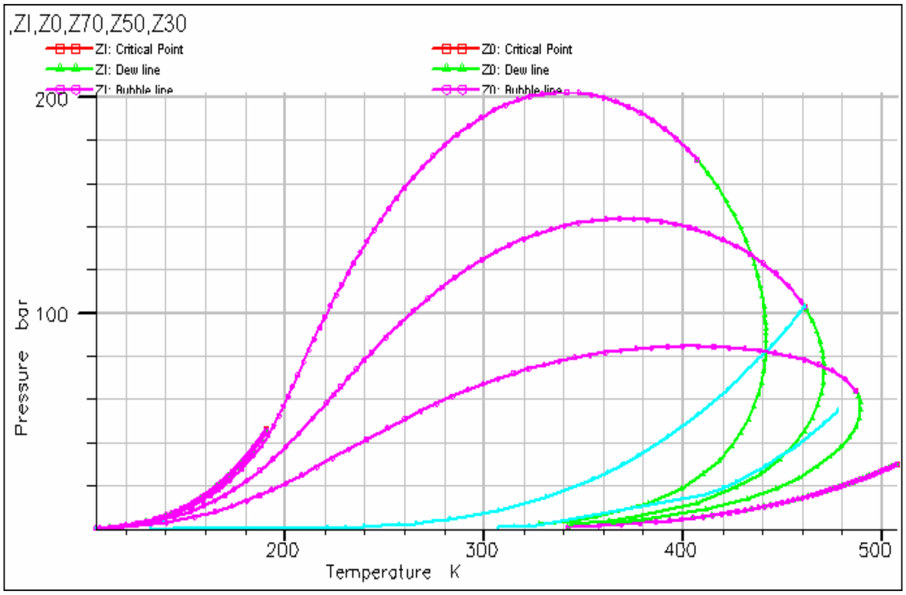
Sample	Totals (percent
ZI	100
Z70	100

Plot phase diagrams: First plot ZI, then Z0, and then the rest

Comment on:

- Shape
- Position of Critical Point
- Fluid type at 440 K
- Psat at 440 K as a function of C1 concentration

Your phase plots should look like this:



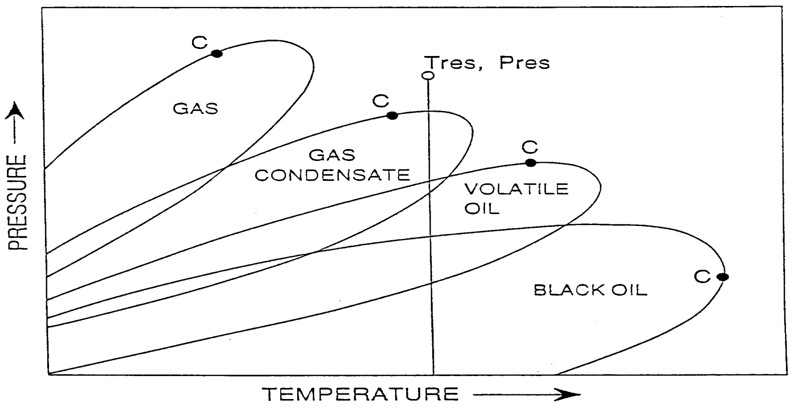
In this two component mixture, the initial composition is varied from 100% pure C_1 to 100% pure C_6. We can draw a continuous family of phase envelopes, starting from the pure component line of $C_1$and ending with the pure component line of C_6. As C_6 is the heavier component of the two, the phase envelopes described by mixtures containing very high proportions of C_6 will show bubble point behavior, that is the critical point lies on or very close to the cricondentherm, and any isothermal drop in pressure from the single-phase region will encounter the phase envelope to the left of the critical point. By contrast, mixtures rich in the lighter component will provide opportunities for isothermal decompression to take place to the right of the critical point and allow retrograde condensation behavior to occur.

The critical points of all the family of envelopes will define a curve known as the critical point locus.

The phase envelope, together with the quality lines, can be measured from experiments for any mixture but the procedure is both time consuming and expensive. The reason we regress the EoS is so that we can create a representative phase diagram based on a relatively modest experimental data set. Not only are the shape of the envelope, the position of the cricondentherm, cricondenbar and critical point important, but also the position and shape of the quality lines, as these are necessary for separator condition optimisation, and depletion performance predictions for retrograde reservoirs.

For the mixtures of C_1 and C_6 in the plot above, T_{crit} increases with increasing molecular weight and Pcrit decreases with increasing molecular weight. Note that as the mixture gets lighter (more C_1 and less C_6) then the shape of the 2-phase region appears to “balloon” out and also rise, pivoting about a low-pressure low-temperature point.

PHASE ENVELOPES FOR RESERVOIR FLUIDS.
C IS CRITICAL POINT



Summary: Components and Samples in PVTi

PVTi has built-in tables of properties of the common components

We need to characterise the plus component. Starting from the molecular weight and the density, we use a correlation to calculate other properties

In general, T_{crit} increases with increasing molecular weight, and P_{crit} decreases with increasing molecular weight

The plus component properties are the most uncertain. They are the properties most likely to be changed during regression.

If the reservoir temperature is to the left of the critical temperature then we call the fluid an oil. If it is to the right we call it a gas. Suppose that we had an oil at a reservoir temperature that was extremely close but still to the left of the critical temperature. Adding one molecule of methane may be enough to move reduce the critical temperature so that the oil now becomes a gas.

6. Ternary Diagrams

In this section we shall describe ternary diagrams and introduce some of their properties and uses.

What is a Ternary Diagram

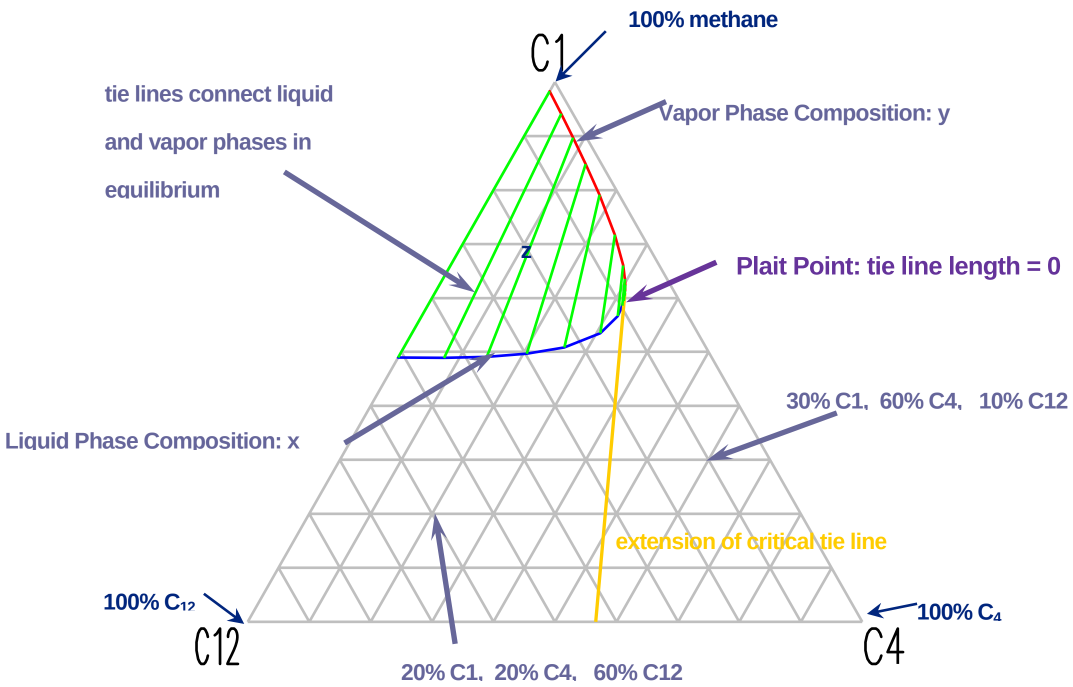
Both phase plots and ternary diagrams show the shape and size of the two-phase region.

- A phase plot (or phase diagram) is at a fixed composition and is a function of pressure and temperature.
- A Ternary plot is at fixed pressure and temperature and is a function of composition.

The ternary or triangular diagram was first introduced by Gibbs to represent phase relationships of three pure components. Multi-component fluids can be displayed on the ternary diagram by grouping the N-component system down to three components:

- A light group, consisting of C_1 and N_2
- An intermediate group, of CO_2, H_2S and the hydrocarbons C_2, C_3...C_6
- A heavy group, of all the heavy hydrocarbons, C_{7+}.

The detailed shape of the ternary plot will depend on exactly which components are grouped together, but the light group is always plotted at the top of the triangle, the intermediate at the bottom right, and the heavy group at the bottom left.



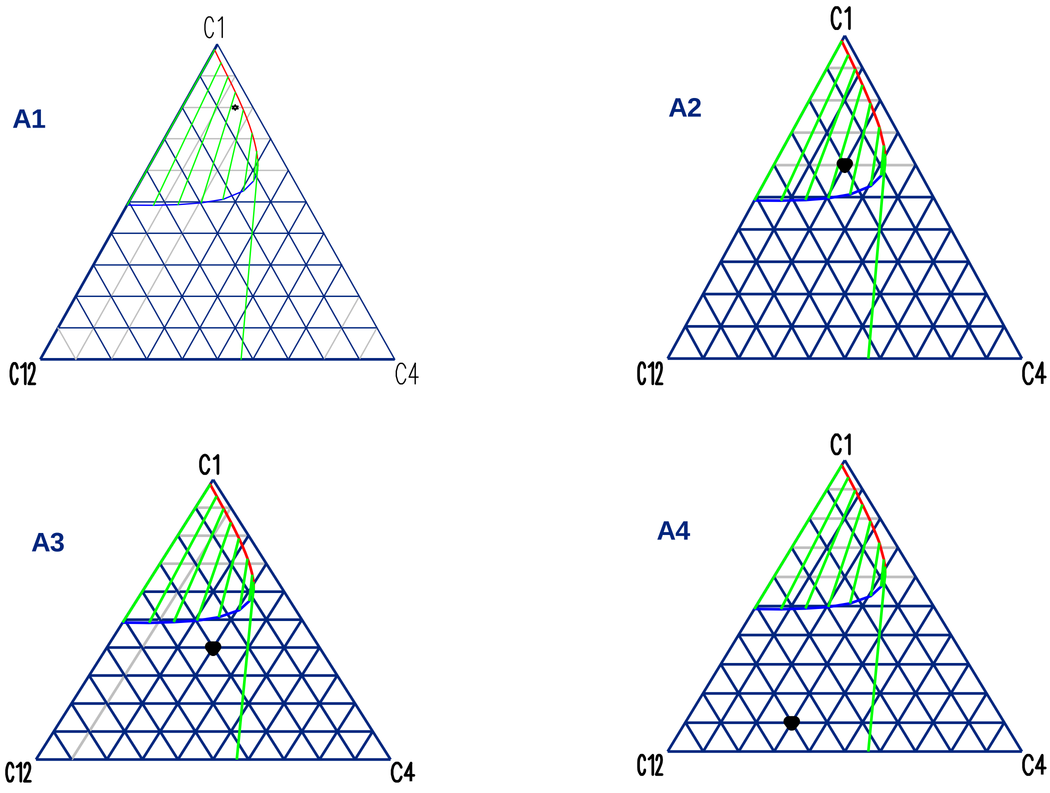
The phase envelope separates the one-phase and the two-phase region. The line at which a bubble of gas first appears is the equivalent of the bubble-point line in the phase plot, and the line at which a drop of liquid first appears is the equivalent of the dew-point line. The point at which these two lines meet is called the Plait Point, and is the equivalent of the critical point. At this point, the liquid and vapour compositions are identical.

The ternary diagram is for all compositions of those three grouped components at a fixed temperature and pressure. A fluid with composition z at that temperature and pressure is shown to be in the two-phase region. It will therefore form an oil phase and a gas phase. The oil phase will have a composition x and the gas phase a composition y. Both of these are shown on the ternary diagram. The straight line joining x, z and y is called the tie line.

The tie lines get shorter as they get closer to the Plait point. The tangent from the plait point to bottom axis effectively divides the fluid compositions into miscible and immiscible regions. More information on miscible/immiscible phase behaviour is given in the chapter on miscibility.

Ternary Diagrams as a function of composition

Ternary Diagrams at 150°C and 200 Bar



The four ternary diagrams above show four different fluids.

- Sample A1 is in the two-phase region and so will form two hydrocarbon phases. The sample is mainly composed of C_1 and is close to the dew-point line, and therefore will be mainly gas with a little oil.
- Sample A2 is in also the two-phase region and so will form two hydrocarbon phases. The sample has less C_1 than sample A1 and will be more oil than gas. If A1 and A2 were on the same tie line, the composition of the oil from both samples would be the same, and the

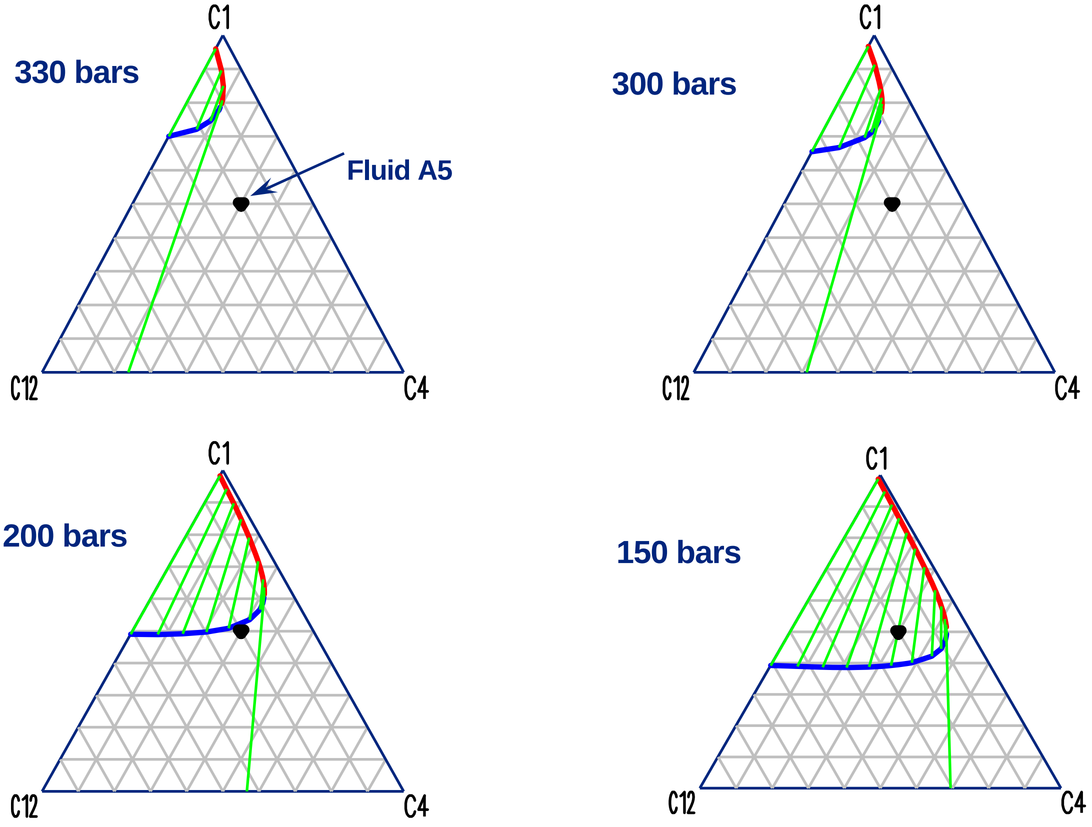
composition of the gas from both samples would be the same. The only difference would be the amounts of oil and gas.

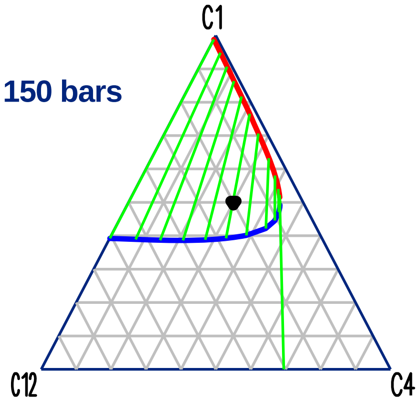
- Sample A3 is single phase. We should avoid calling it either oil or a gas: the name of the phase will depend on the value of the temperature compared to the critical temperature. This can be determined by looking at a phase diagram but not in general at a ternary diagram.
- Sample A4 is also single phase.

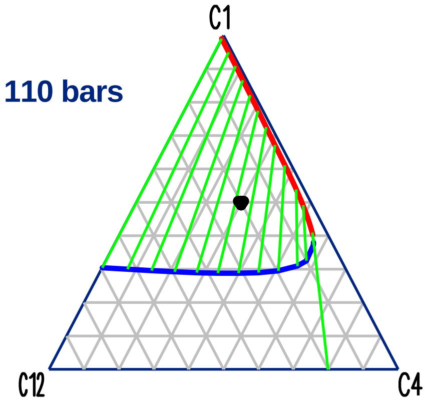
Ternary Diagrams as a function of Pressure

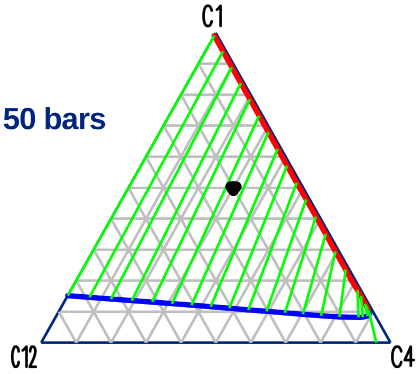
The ternary diagrams below show how the size and shape of the two-phase region changes with pressure, at a fixed temperature of 500 K. The higher the pressure, the smaller the two-phase region. At high enough pressure, the two-phase region becomes so small that it cannot in practice be plotted.

Two Phase Envelope at Various Pressures









From these ternary diagrams, we can estimate the saturation pressure of the fluid sample to be just less than 200 bars[3].

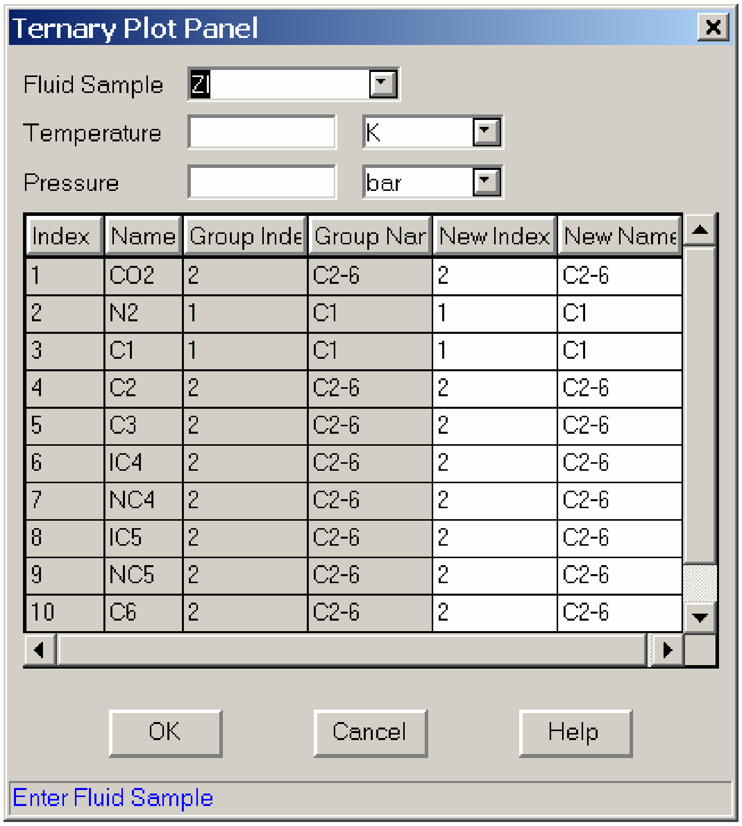
Exercise 3 Ternary Diagrams

1. Load the fluid system that you saved in Exercise 1b ; PVTi Tutorial 2 "Creating a Fluid System".
2. Plot a ternary diagram from View | Samples |Ternary Plot
3. Set the temperature to 500 K
4. Try different temperatures.

---

[3] We can also call the sample an oil instead of a single-phase hydrocarbon, as we can now see that the saturation pressure is a bubble-point pressure.

5. What is Psat?



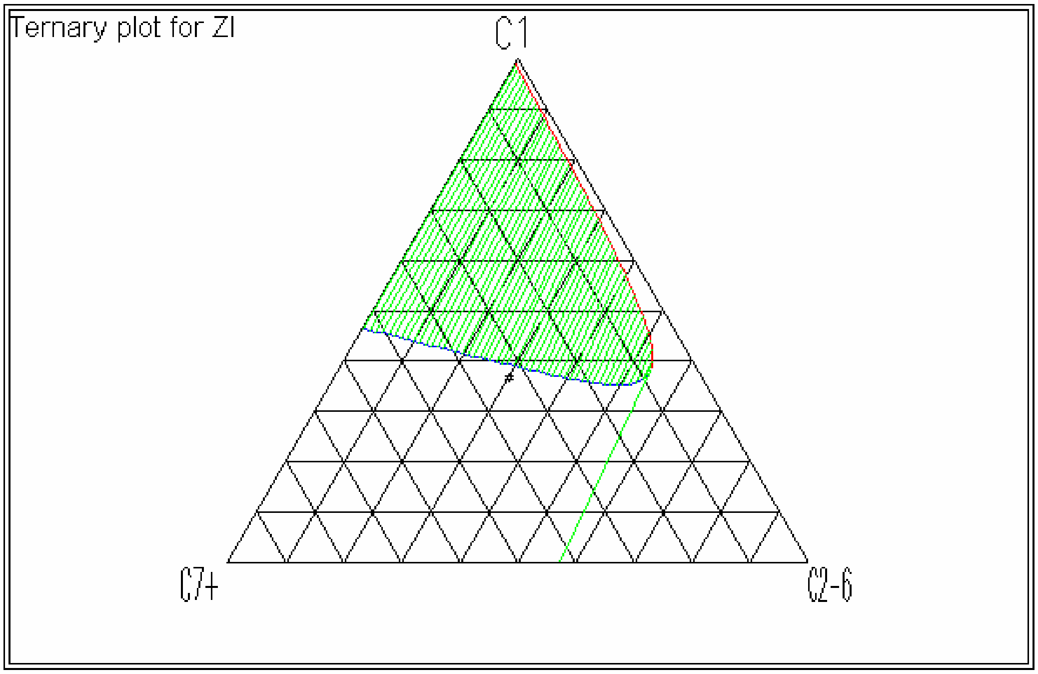
Fluid Sample: ZI

Temperature: K

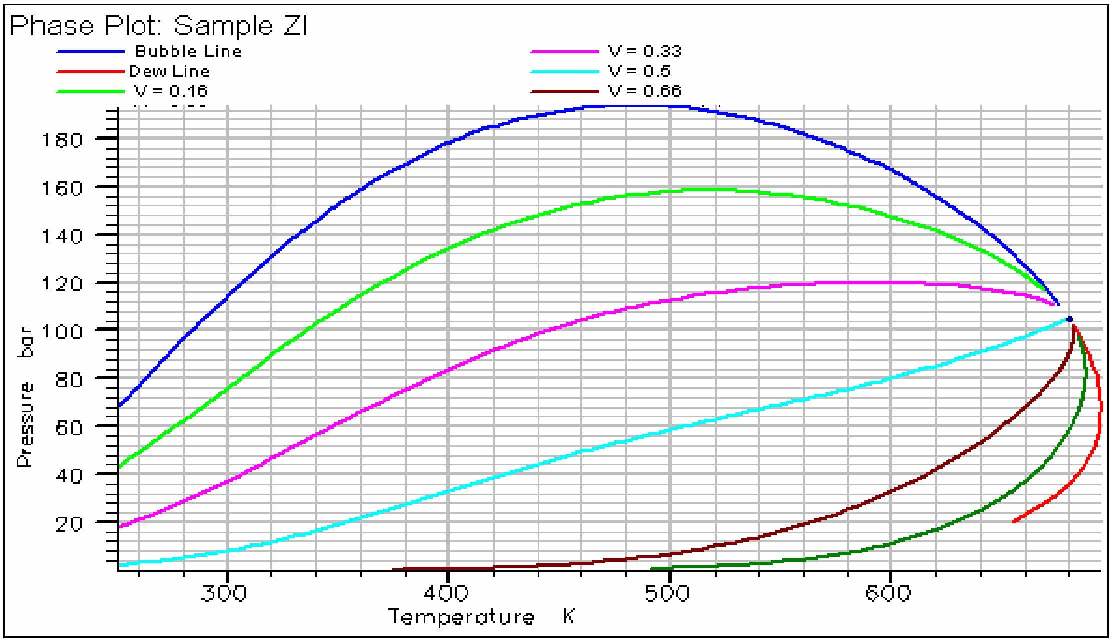
Pressure: bar

Index	Name	Group Inde	Group Nar	New Index	New Name
1	CO2	2	C2-6	2	C2-6
2	N2	1	C1	1	C1
3	C1	1	C1	1	C1
4	C2	2	C2-6	2	C2-6
5	C3	2	C2-6	2	C2-6
6	IC4	2	C2-6	2	C2-6
7	NC4	2	C2-6	2	C2-6
8	IC5	2	C2-6	2	C2-6
9	NC5	2	C2-6	2	C2-6
10	C6	2	C2-6	2	C2-6

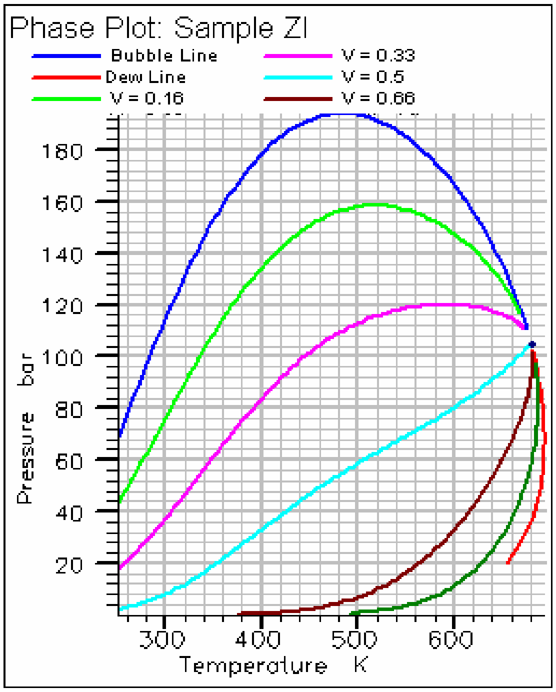
Enter Fluid Sample

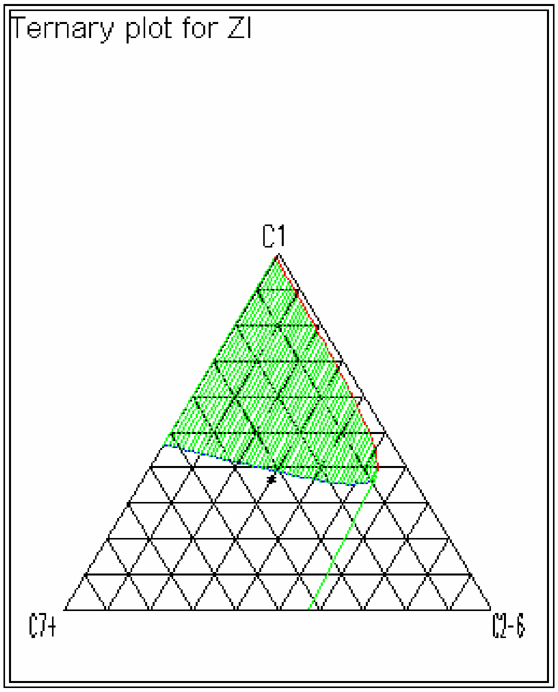


You can check your estimate of Psat by plotting the phase diagram.



We can plot both a phase diagram for the given fluid composition and a ternary diagram at 200 bars and 500 K. The phase diagram shows Psat = 192 bars, and the ternary shows that Psat is just below 200 bars.





Summary: Ternary Diagrams

- A ternary diagram is an alternative way at looking at the split between one-phase and two-phase regions. A Ternary plot is at a fixed pressure and temperature and is a function of composition. A phase diagram is for a fixed composition and is a function of pressure and temperature.
- The higher the pressure, the smaller the two-phase region. At high enough pressure, the two-phase region becomes so small that it cannot in practice be plotted.

7. Splitting and Grouping

Although many people have gone to a great deal of work and effort to obtain fluid samples, analyse them and determine their PVT behaviour, the way the data is presented is not always in the optimum format for use in an EoS model. Two extra steps that often have to be performed are splitting of the residual hydrocarbon plus fraction, and grouping of similar hydrocarbons.

Splitting

We sometimes have to split the ‘plus’ component. Splitting involves replacing for instance C7+ by two or three pseudo-components such as C7-C10, C11-C19, and C20+. The procedure is simple and fairly automatic and does not need detailed knowledge of the components. The reason we split components is that we may not able to regress without first splitting the heaviest component

- Our objective is to match all the available observations with the minimum number of (pseudo-)components.
- We therefore want to group components

but …

- We may need to split the “+” component before we start

Reasons for Splitting:

- "Insufficient description of heavier hydrocarbons reduces the accuracy of PVT predictions" (Whitson, 1983)
- Condensates and Volatile Oils are particularly sensitive to plus fraction composition and properties
- Laboratories tend to give very limited analysis to the plus fraction, i.e., M_{N+}, γ_{N+}

The plus fraction often has an importance that appears to far outweigh its relatively small mole fraction of a fluid sample[4]. In particular, saturation pressure calculations can be extremely sensitive to the mole fraction and properties of the plus fraction. More accurate predictions requiring less regression of equation of state parameters can be achieved if a thorough description of the plus fraction can be made.

From a C7+, C12+ and C20+ analysis:

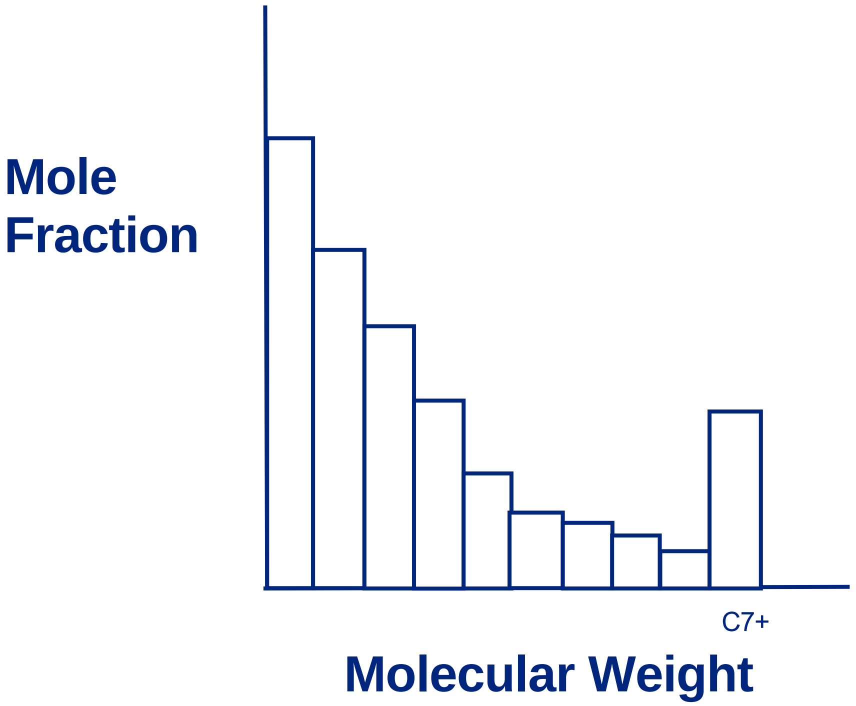
- The heavier ends tend to remain in solution during CVD Experiment
- There is a wide distribution of heavy components in the plus fraction
- No EoS model using a single component for such a plus fraction could hope to adequately model the above process, even with tuning.

A C30+ analysis may not need splitting, as there is likely to be a small percentage of C30+..

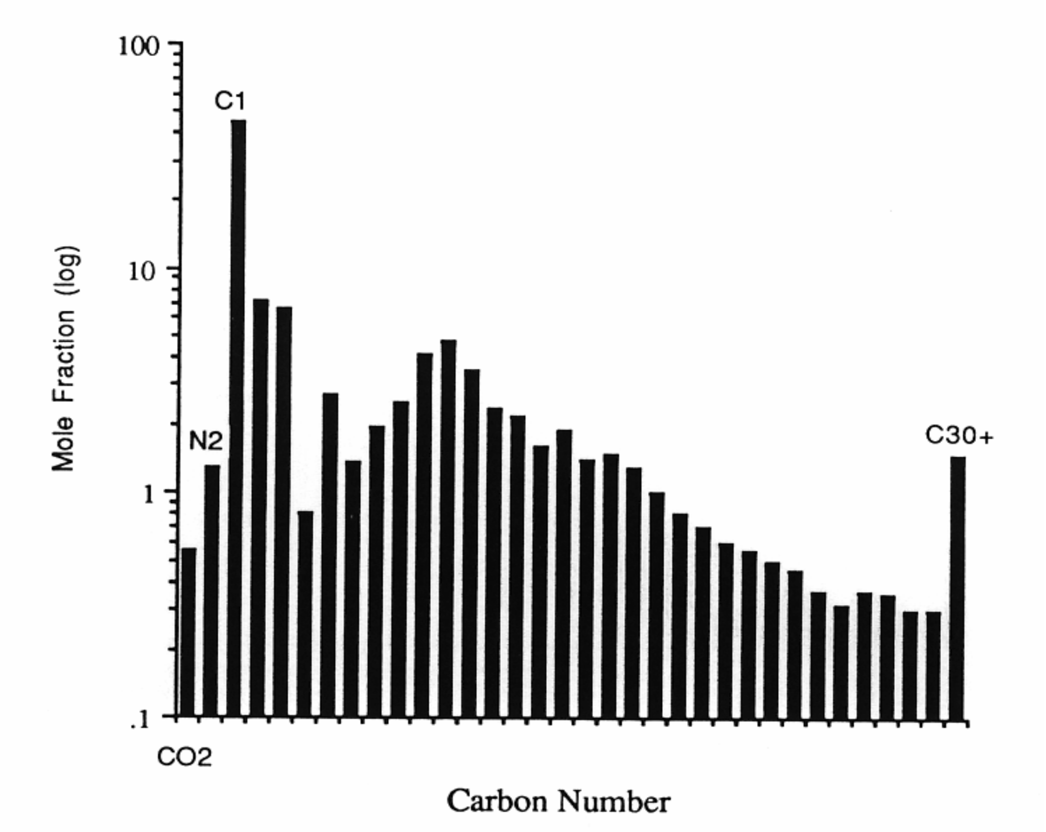
A simplified example of component mole fractions shows the relatively high percentage of C7+ in a typical oil.

---

[4] The weight fraction will of course be much greater then the model fraction, and can give a better idea of the importance of the plus component.



We can compare this with a detailed analysis up to C30+ of a North Sea oil:



Three techniques are available within PVT*i* for the splitting of the plus fraction into sub-fractions:

- Constant Mole Fraction (CMF);
- Whitson.
- Semi-Continuous Thermodynamics (Modified Whitson)

All of these techniques rely on a probability density function (PDF) to relate mole fraction to mole weight. This approach is due to Whitson.

Whitson Splitting

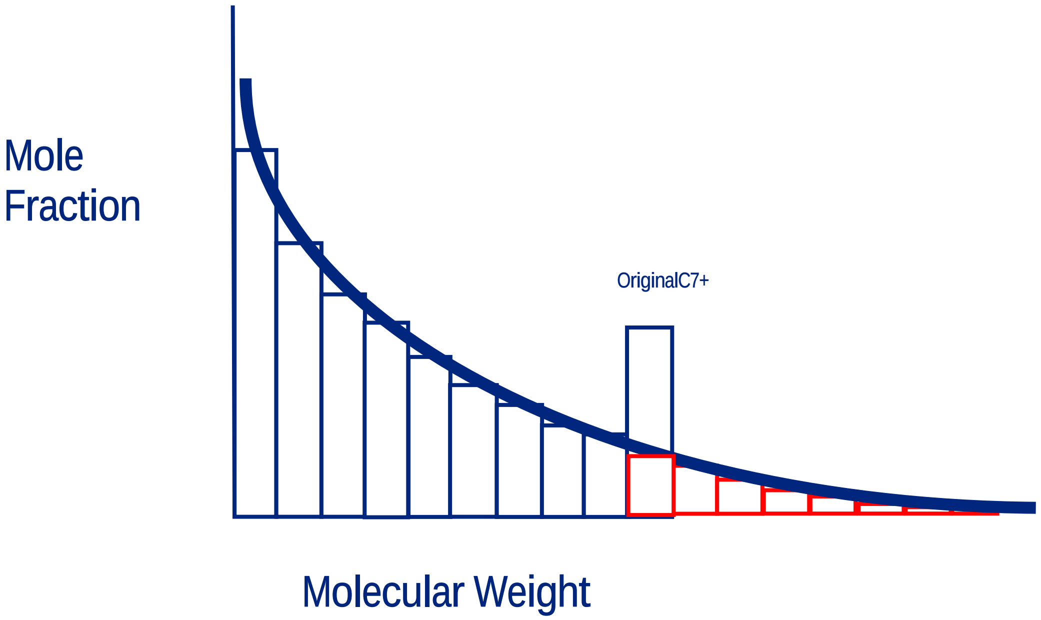
If you have a CVD[5] analysis report with the mole weight and specific gravity of the plus fraction of the removed gas then you will notice that they decrease with reducing pressure. Clearly the heavier ends tend to remain in solution so that the molar distribution of components within the plus fraction changes. As mentioned above, no EoS model using a single component for such a plus fraction could hope to adequately model the above process, even with tuning.

A numerical procedure is needed to find a correlation between mole composition and mole weight for the plus fraction, adjust that correlation to fit any available data, and then to turn it into a set of components that can be used in an EoS model. A widely used splitting procedure is that due to Whitson (1983) in which mole fraction is related to mole weight by a three parameter probability density function (PDF). The PDF is used to split the plus fraction into many (about 30 to 40) SCNs.

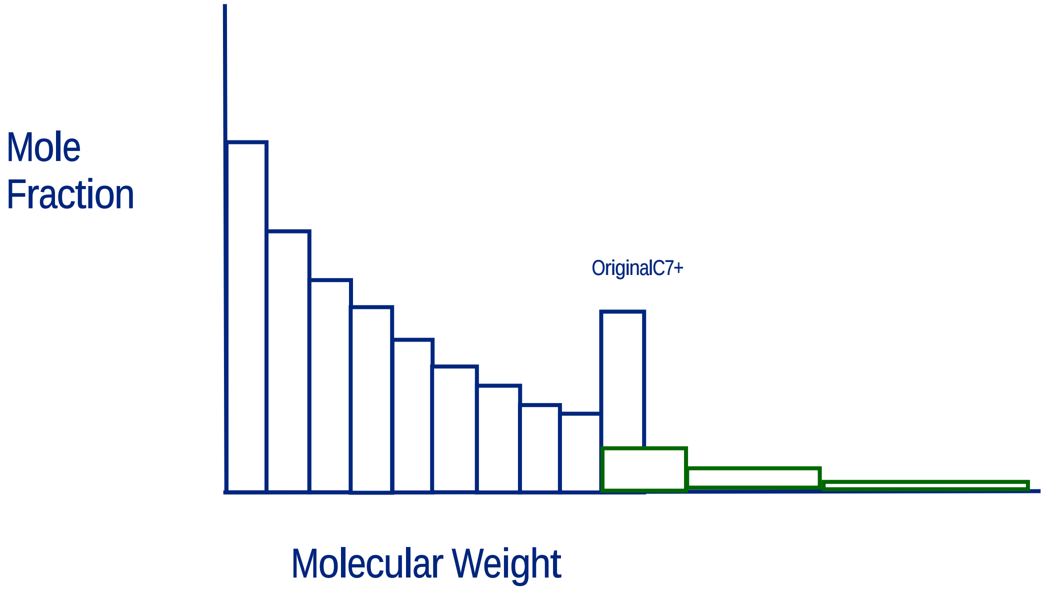
In this example, the original C7+ component split into several new (red) fractions.

---

[5] The CVD and other laboratory experiments are discussed later.

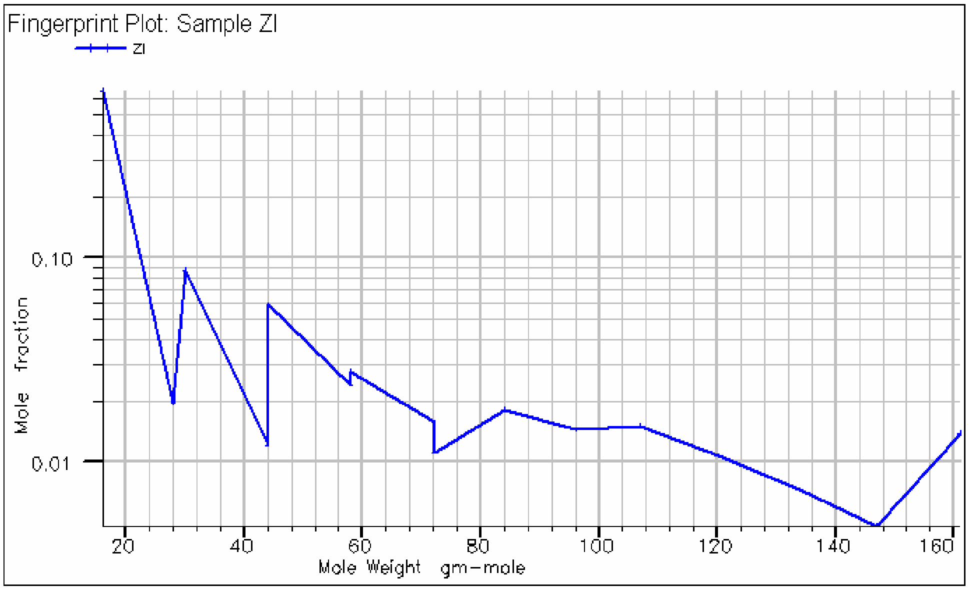


These 30 to 40 SCNs are then grouped back into the requested number of pseudo-components, usually 3. In our case, red fractions are regrouped into three (green) fractions. The net result is to split one plus component into three heavy components.

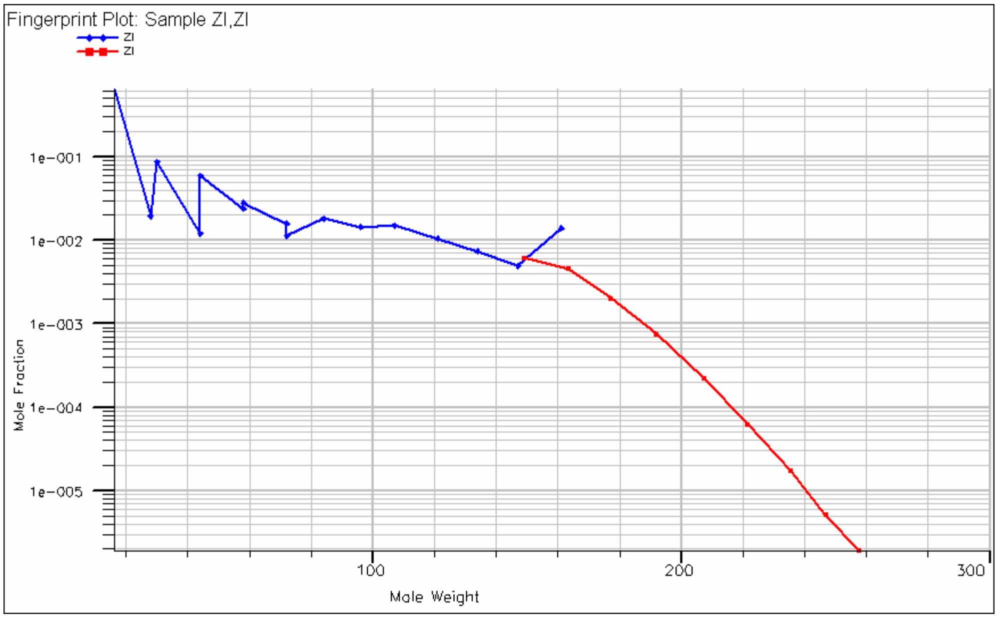


Having calculated mole compositions and mole weights, the critical properties, etc., can be calculated from the characterisation procedures discussed in the previous section.

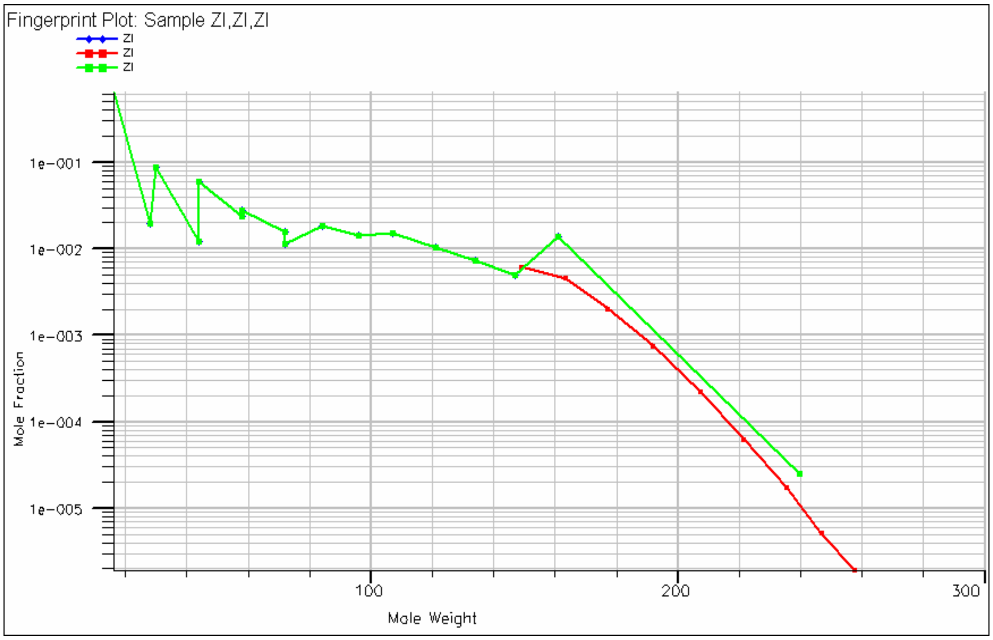
Plots of mole fraction vs. Molecular weight are known as fingerprint plots, and can be displayed in PVTi either by right clicking on the sample name and choosing “fingerprint plot” or by View | Samples | Fingerprint Plot. An example is shown below:



The first step of Whitson splitting gives:

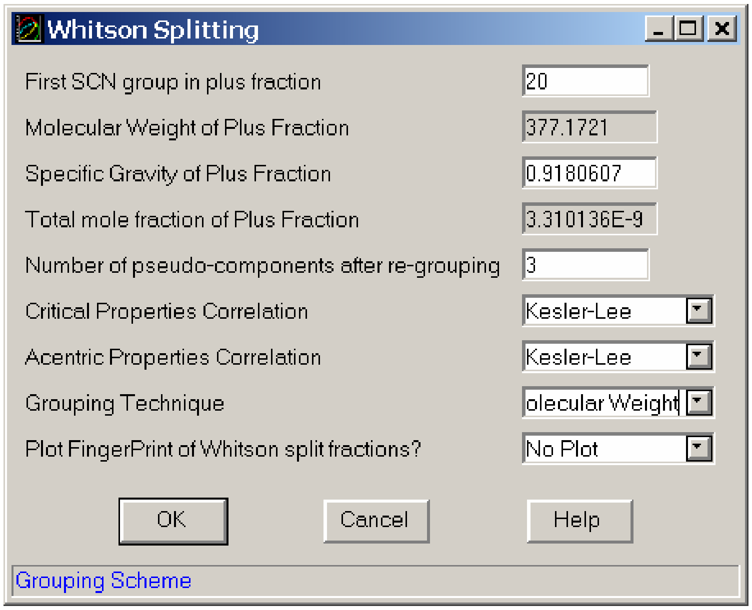


The original plus component has been split into ever-decreasing amounts of higher SCN components. The second and final step gives:



The new high-SCN components have now been regrouped into three new heavy pseudo-components.

The PVTi panel that provides Whitson splitting is set up with default values. These are probably best left unchanged.



First SCN group in plus fraction	20
Molecular Weight of Plus Fraction	377.1721
Specific Gravity of Plus Fraction	0.9180607
Total mole fraction of Plus Fraction	3.310136E-9
Number of pseudo-components after re-grouping	3
Critical Properties Correlation	Kesler-Lee
Acentric Properties Correlation	Kesler-Lee
Grouping Technique	olecular Weight
Plot FingerPrint of Whitson split fractions?	No Plot

Grouping

Why group?

The cost and resources required to simulate PVT phase behaviour increases rapidly with an increasing number of components. The main reason for grouping components is to speed-up a compositional simulator[6], such as **ECLIPSE COMPOSITIONAL**. There are two issues:

1. For large number of components, the computing time needed to solve the flash equations may be as great as the time needed to solve the flow equations.
2. If there are n_c hydrocarbon components, the number of equations to be solved per grid block is n_c+2. Therefore running a simulation with more than nine components (for example) may be impractical in computing time, especially for a fully implicit solution.

The number of grouped 'pseudo-components' needed in a compositional simulation depends on the process that is modeled:

- For depletion, 2 pseudo-components may be enough (Black-oil model)
- For miscibility, more than 10 components may sometimes be needed.

In general, 4 to 10 components should be enough to describe the phase behavior

---

[6] If you are analysing PVT data for a black-oil simulation, you do need to group components.

At one extreme, a black oil model with a gas cap can be considered as a 2-component model, and a black oil reservoir that stays above the bubble point could be thought of as a 1-component model. At the other extreme, some academic calculations may require 10s of components. In most cases between 4 and 10 components should be enough to describe most simulation processes.

How to group

Basis for grouping

- similar properties, e.g. MW
- same log(K) versus p trend
- insensitivity of experiments to trial grouping

Obvious candidates

- iC4 and nC4 → C4
- iC5 and nC5 → C5

- Add N2 to CH4, CO2 to C2H6 (at low concentrations)

The main basis for grouping is to group components with similar molecular weights. We would for instance group C7 with C8 rather that with C2, as we would expect their properties of C7 and C8 to be similar, while the properties of C7 and C2 would be very different. Obvious candidates are to group iC4 with nC4, and to group iC5 with nC5.

An exception to this rule is that N2 is usually added to C1 and CO2 is usually added to C2. Their molecular weights would suggest that we should group N2 (MW=28) with C2 (MW=20) and not with C1 (MW=16). Similarly, why are we not grouping CO2 (MW=44) with C3 (MW=44)?

Molecule	**Molecular Weight**
N2	**28**
CO2	**44**
CH4	**16**
C2H6	**30**
C3H8	**44**
C4H10	**58**

The answer is that we group components with similar molecular weights to try to group components with similar properties. Hydrocarbon molecules with similar molecular weights will have similar properties, but this will not apply to non-hydrocarbon molecules such as N2.

As an example, one property of interest is the K-value of each component[7].

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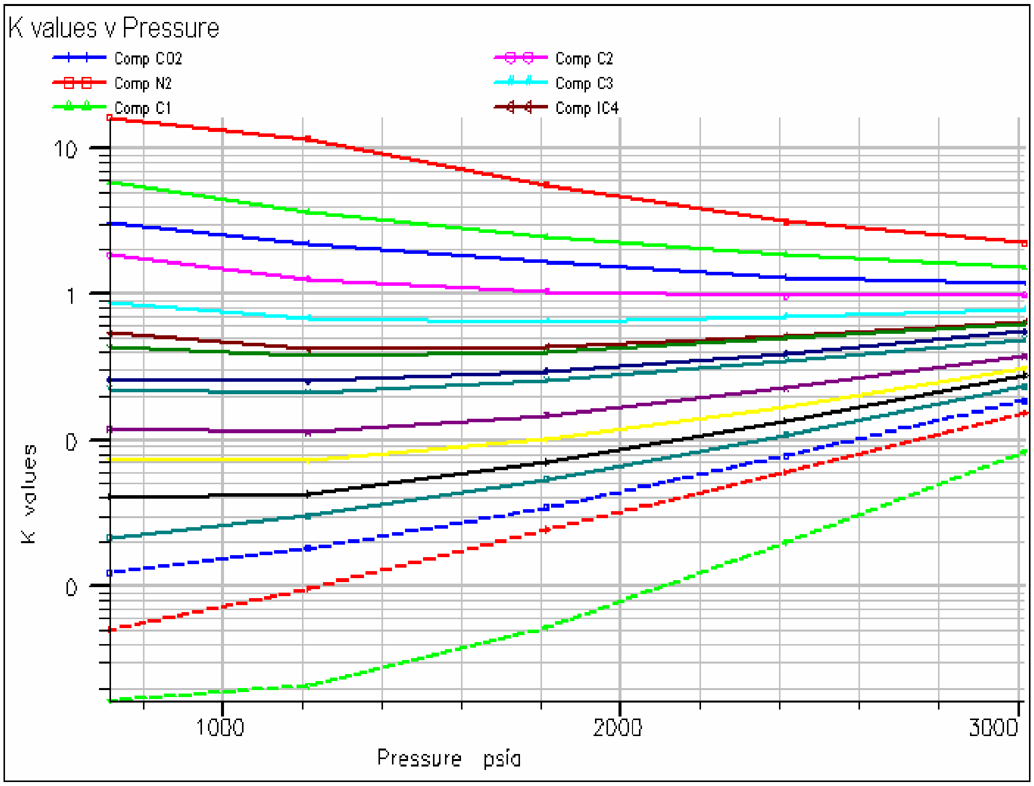
[7] The meaning and significance of the K-value will be discussed later.



A plot of the log of the K-values as a function of pressure shows a clear trend with the line for C1 being the highest, followed by C2, C3, C4, etc., in order of increasing molecular weight. The line for N2 however is some way above that for C1, while the CO2 line is between that for C1 and C2.

Success Criteria

In PVTi, the main criterion for a successful grouping is whether the new grouped components can predict observed experimental results at least as well as the original ungrouped components[8]. If a compositional simulation model is run, the results of the simulation should be independent of whether the new grouped components of the original ungrouped components are used.

---

[8] We shall discuss regression and the matching of experimental results later.

Summary of Splitting and Grouping

- We need to split the plus component if there is too much of it compared with the other components. This is because the plus component can have a disproportionate effect on the physical properties of the fluid.
- Use defaults when splitting the plus component.
- We need to group components to speed up the compositional runs that are going to use them.
- When grouping, first compare the shape of the phase diagram with the ungrouped phase diagram. If that looks OK, then you should regress to the laboratory results to achieve at least as good a match as with the ungrouped components.

8. Equations of State

In this section you will learn about some of the common equations of state.

Definition

An analytic expression relating pressure to temperature and volume is called an "Equation of State" (EoS).

Ideal Gas Law

The earliest EoS is the ideal gas law, combining of Boyle's and Charles's law.

Boyle's Law

Boyle's Law is based on observations made around 1660 that for a fixed mass of gas at a fixed temperature, the product of pressure and volume is a constant,

$pV = \text{constant}$

Charles's Law

Over a century later (1787), Charles observed that for a fixed mass of gas at constant pressure, the volume varies linearly with temperature.

$V \propto T$

If the gas has a volume V_0 at 0 °C, then at a temperature T:

$V = V_0(1 + aT)$

The gradient, a, is found to have the value 1/273, and as a consequence, when T=-273 °C, the gas volume will become zero. By re-specifying a temperature scale T' with the same spacing of degrees as the Centigrade scale, but starting with 0 at -273 °C the volume/ temperature relationship becomes:

$$V = \frac{V_0}{273} T'$$

The scale is the absolute temperature scale, measured in Kelvin (K), where

$K = C + 273$

The Fahrenheit equivalent is the Rankin scale, R, where

$$R = F + 460$$

Ideal Gas Law

Combining Boyle's Law with Charles's Law gives us the ideal gas law:

$$PV = RT$$

which is an Equation of State (EoS) for ideal gases. The constant R is defined using Avagadro's hypothesis, and in oilfield units is:

$$10.732 \frac{(psia)(ft^3)}{(lb - mole)(^o R)}$$

If 1 lb.-mole is involved, at a pressure of 14.7 psia and temperature of 60 °F, the volume occupied will be:

$$\frac{10.732x(60+460)}{14.7} ft^3 = 379.484 \text{ cu. ft.}$$

If n lb.-moles are involved, then the relationship is simply:

$$PV = n \ RT$$

This assumes that we are dealing with an ideal gas, which most gases are not, certainly not over the range of conditions encountered in oil field applications. However, many gases (including mixtures such as air) exhibit behaviour approximating closely to ideal at and around standard conditions. Ideal behaviour pre-supposes two properties of a gas, namely:

i.) The molecules are infinitely small

ii.) There are no inter-molecular forces

Condition i.) is imposed by Charles's Law, in that all volume must vanish at T=0. For condition ii.) to hold, no gaseous element or compound could ever change state into a liquid or a solid. Neither of these conditions is true. Molecules are not infinitely small, and you cannot reduce a volume down to zero by increasing pressure. Attractive intermolecular forces dominate at lower temperatures and higher pressures. They are the forces that cause condensation. i.e. a change of state from gas to liquid.

Real Gas Law

For applications where the prediction of changes of state are unimportant, such as relating the volume of a real gas at one set of temperature and pressure conditions to another set, the problem is overcome via the use of Z-factors or compressibility factors. The ideal gas law is extended to real gases (i.e. non-ideal behaviour can be incorporated) by inserting a compressibility, the Z factor

$$PV = nZRT$$

for n moles of gas. The Z-factor is a function of T and P and of the gas involved

The problem of relating the gas in state 1 to state 2 is thus:

$$\frac{P_1V_1}{T_1Z_1} = \frac{P_2V_2}{T_2Z_2}$$

The Z-factor at standard conditions (60 °F, 14.7 psia) is equated to 1, and can be calculated or measured at other pressures and temperatures[9].

These equations are only adequate for describing the behaviour of gases at relatively low pressures, since no account of change of phase or modelling of liquid behaviour is possible.

Phase Changes in EoS

To model the phase behaviour of real fluids, we have to account for attractive and repulsive forces between molecules. The pressure exerted between the molecules by a real fluid has two components:

$$P = P^{rep} - P^{att}$$

---

[9] The calculation method for the Z-factors of mixtures relies on the validity of the law of corresponding states, which is discussed later.

where P^{rep} and P^{att} are the repulsive and attractive pressure terms, respectively. The most famous relationship for describing the energy of interaction between molecules is that due to Lennard-Jones (1931):

$$\phi(r) = \left[\frac{\in_1}{r^{12}} - \frac{\in_2}{r^6}\right]$$

where r is the intermolecular separation and $\in_1$, $\in_2$ are constants.

Van der Waals EoS

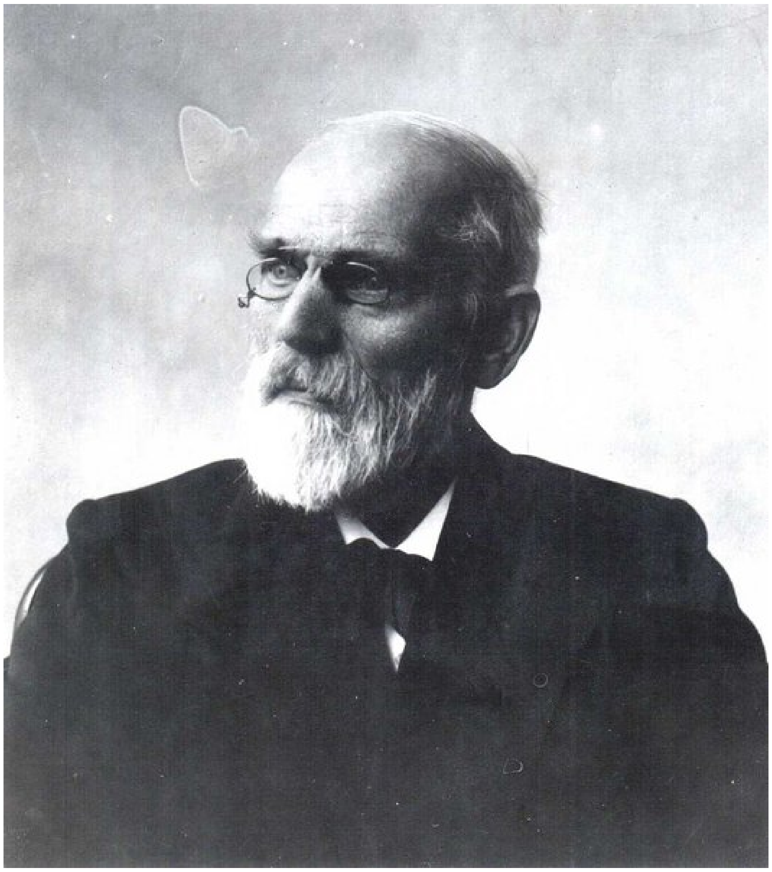
Various attempts were made in the latter half of the 19th Century to modify the ideal gas EoS to account for departures from ideal behaviour. The first EoS capable of handling the transition from vapour to liquid states was due to Van der Waals in 1873:

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT$$

or

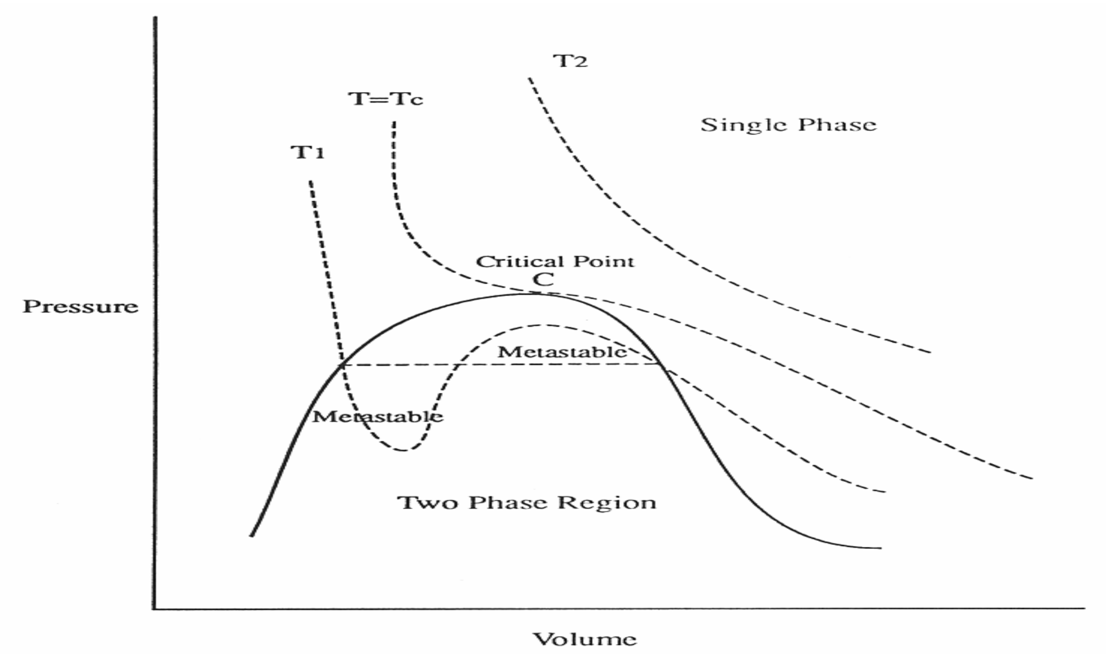
$$P = \frac{RT}{(V - b)} - \frac{a}{V^2}$$

The parameter “a” was introduced to account for the attractive force between molecules, and the “b” parameter to account for the finite (non-zero) volume of the molecules. The numerical values of the constants a and b are specific to the gas. In terms of the Lennard-Jones potential, the r^{12} term has been replaced by a “hard-sphere” approximation in the form of the b parameter whereas the attractive r^6 term is accurately represented by the a/V^2 term since the volume V ~ r^3.



Johannes Diderik van der Waals (November 23, 1837 – March 8, 1923)

At temperatures less than the critical temperature, T_c, our cubic model has three (real) roots. The lowest and highest roots correspond to the saturated liquid and vapour volumes respectively; the middle root has no physical meaning. As the temperature approaches the critical temperature from below, these three roots all converge until at the critical point, C, they are identical.



At the critical point, the intensive[10] properties of the liquid and vapour become identical. The critical point has temperature T_c and pressure P_c. At the critical point, one mole occupies a critical volume V_c. The critical Z-factor $Z_c = RT_c/P_cT_c$, which should be 1 for an ideal gas.

The values of the (a, b) coefficients can be found by noting that the point C is a point of inflection, so both the first and second derivatives with respect to V are zero:

$$\left(\frac{\partial P}{\partial V}\right)_{T_c} = -\frac{RT_c}{(V_c-b)^2} + \frac{2a}{V_c^3} = 0$$

$$\left(\frac{\partial^2 P}{\partial V^2}\right)_{T_c} = \frac{2RT_c}{(V_c-b)^3} - \frac{6a}{V_c^4} = 0$$

Rewriting these two equations as

$$\frac{2a}{V_c^3} = \frac{RT_c}{(V_c - b)^2}$$

$$\frac{3a}{V_c^4} = \frac{RT_c}{(V_c - b)^3}$$

we can solve for b in terms of V_c and get

$$b = \frac{V_c}{3}$$

We can then solve for a

$$a = \frac{27\, R^2 T_c^2}{64\, P_c}$$

and b

$$b = \frac{1\, RT_c}{8\, P_c}$$

then V_c

$$V_c = \frac{3\, RT_c}{8\, P_c}$$

Comparing the equation for V_c with the real gas law applied at the critical point

$$P_c V_c = ZRT_c$$

we see that the critical Z-factor calculated from the Van der Waals EoS is 0.375. This value is considerably larger than that of real hydrocarbon components, typically $Z_c<0.29$

The numerical constants in the equations for (a, b) are "magic numbers" of the particular EoS and are referred to as Ω_a, Ω_b. These are defined by:

$$a = \Omega_a \frac{R^2 T_c^2}{P_c}$$

$$b = \Omega_b \frac{RT_c}{P_c}$$

---

[10] Recall that an *intensive* property is independent of the amount of the substance. The opposite is an *extensive* property, which depends on the amount of the substance. For instance compressibility is an

For Van der Waals EoS,

$$\Omega_a^{VdW} = \frac{27}{64}$$

$$\Omega_b^{VdW} = \frac{1}{8}$$

Redlich-Kwong EoS

Most modifications of the original Van der Waals EoS have involved a correction of the attractive pressure term[11]. Redlich and Kwong's (RK, 1948) EoS takes the form:

$$p = \frac{RT}{(V-b)} - \frac{a}{V(V+b)}$$

where the a parameter is now a function of temperature, a(T). For the RK EoS $a = a'T^{-1/2}$, where a' is a constant. The value of a' is set by conditions imposed at the critical point. More generally, the a parameter can be written as $a= a'$f(T) so that at the critical point $a_c = a'$f(T_c) and

$$a = a_c \frac{f(T)}{f(T_c)}$$

Usually the ratio f(T)/f(T_c) is denoted by α, and $\alpha \to 1$ as $T \to T_c$. For the basic Redlich-Kwong EoS, $\alpha = T_r^{-1/2}$ where T_r is the reduced temperature, $T_r = T/T_c$.

We leave it as an exercise to show that:

---

intensive property and volume is an extensive property.

[11] Several other EoS were published at the time of Van der Waal

$$\left(p + \frac{a}{T(V+c)^2}\right)(V-b) = RT \qquad \textit{Clausius}\ (1880)$$

$$\left(p + \frac{a}{TV^2}\right)(V\text{-}b) = RT \qquad \textit{Berthelot}\ (1878)$$

$$Z_c = 0.333\ldots$$

$$a_c = 0.42748\ldots\frac{R^2 T_c^2}{p_c}$$

$$b = 0.08664\ldots\frac{RT_c}{p_c}$$

so that the Ω_a, Ω_b for the Redlich-Kwong EoS are

$$\Omega_a^{RK} = 0.42748...$$

$$\Omega_b^{RK} = 0.08664...$$

Soave Addition to RK EoS

Several authors improved on the Redlich-Kwong EoS by introducing additional functionality into the α parameter. In particular, Soave (1972) made α a function of Acentric factor[12] as well as reduced temperature, i.e.:

$$\alpha = \alpha(\omega, T_r)$$

To find the functional form for α, Soave calculated values of α at a series of temperatures for a number of pure hydrocarbons, using as a condition the equality of fugacities in the vapour and liquid phases along the saturation curve. He found that $\alpha^{1/2}$ was a linear function of $T_r^{1/2}$ with a negative slope. Noting this and the condition that α=1 at T_r=1 gives:

$$\alpha^{1/2} = 1 + m(1 - T_r^{1/2})$$

To define Acentric factor, Soave followed Pitzer's definition:

$$\omega = -(\log_{10} P_r^s + 1) \text{ at } T_r = 0.7$$

where P_r^s represents the reduced vapour pressure at a reduced temperature of T_r=0.7. Thus by assuming a value of ω we can calculate a value for P_r at a T_r of 0.7. Substituting these values into the equal Fugacity condition, we can estimate

---

[12] Acentric factor: measure of the non-sphericity of a molecule and thus of non-ideal behaviour.

a value for α and hence the slope m which can be parameterised in ω. Soave obtained:

$$\alpha^{1/2} = 1 + (0.480 + 1.574\omega - 0.176\omega^2)(1 - T_r^{1/2})$$

The values of Z_c, Ω_a and Ω_b for the SRK equation are equal to those of the original RK EoS.

Peng-Robinson EoS

The major failing of the RK and SRK EoS is the unrealistically high compressibilities Z_c=0.333... and consequent poor prediction of liquid densities. In an attempt to improve on this, Peng and Robinson modified the SRK EoS:

$$P = \frac{RT}{(V-b)} - \frac{a}{V(V+b) + b(V-b)}$$

or

$$P = \frac{RT}{(V-b)} - \frac{a}{[V + (2^{1/2}+1)b][V - (2^{1/2}-1)b]}$$

Values for Z_c, Ω_a and Ω_b from the PR EoS are:

$$Z_c = 0.307\ldots$$

$$a_c = 0.457235\ldots\frac{R^2T_c^2}{P_c}$$

$$b = 0.077796\ldots\frac{RT_c}{P_c}$$

The value of Z_c=0.307... is a significant improvement over that of the RK and SRK EoS, and consequently the PR EoS predicts liquid properties significantly better. However, this value is still larger than the Z_cs of real hydrocarbons, which are less than 0.29.

The α parameter ($a=a_c\alpha$) was assumed to have the same functionality as for the SRK EoS, and Peng and Robinson found:

$$\alpha^{1/2} = 1 + (0.37646 + 1.54226\omega - 0.26992\omega^2)\ (1 - T_r^{1/2})$$

For components with large Acentric factors, i.e., plus fractions with $\omega>0.49$, the ω term can be modified to $(0.379642+1.48503\omega-0.164423\omega^2+0.016666\omega^3)$. The use of the 3rd order expansion in ω can have significant effects on phase behaviour calculations, moving saturation pressures by 200 psia or more compared with the 2nd order expansion.

Zudkevitch-Joffe EoS

Another attempt to improve on the original RK EoS was made by Zudkevitch and Joffe (1969) who made the Ω_a, Ω_b constants into functions of temperature, i.e., $\Omega_a(T)$, $\Omega_b(T)$.

This is done on a component-by-component basis at a given set of temperatures below the critical temperature, by equating fugacities and densities for liquid and vapour phases along the saturated pressure line. The Omegas are taken as temperature-independent above the critical temperature.

3-Parameter EoS

The critical compressibilities that we can calculate from the Equations of State that we have considered so far are:

$Z_c^{VdW} = 0.375$

$Z_c^{RK} = 0.333\ldots$

$Z_c^{PR} = 0.307\ldots$

Unfortunately, hydrocarbons have $Z_c < 0.29$.

The major problem with the Van der Waals type EoS that have been examined to this point is they only have the two free parameters (a, b) and so generally the third parameter in the cubic EoS, i.e. Z_c is fixed. Several authors have attacked this problem by introducing a third parameter, usually referred to as c, and treated as a volume shift:

$$V^{(3)} = V^{(2)} - \sum_{i=1}^{N} x_i c_i$$

In this equation $V^{(2)}$ is the volume predicted by the 2-parameter EoS and $V^{(3)}$ is the corrected 3-parameter volume. This shift in volume leads to a reduced Z-factor.

Values of the coefficients c_i can be determined by a variety of techniques. The method used[13] in PVT consists of comparing the liquid molar volume $V^{Obs}(P_{st}, T_{st})$ of a component at standard conditions with that predicted by the two-parameter at the same conditions, $V^{EoS}(P_{st}, T_{st})$. The difference defines the c_i for that component.

$$c_i = V_i^{EoS}(P_{st}, T_{st}) - V_i^{Obs}(P_{st}, T_{st})$$

The shift parameters c_i are often defined[14] in terms of dimensionless shift parameters s_i where:

$$s_i = \frac{c_i}{b_i}$$

and the b_i are the EoS constants:

$$b_i = \Omega_{b,i} \frac{RT_{c,i}}{p_{c,i}}$$

---

[13] Originally due to Peneloux (1982) and used by Søreide, Reffstrup and Whitson.

[14] In ECLIPSE 300, the dimensionless volume shifts are defined using the keyword SSHIFT

The dimensionless parameters s_i of the heavier components are potentially variables for regression, and if the three-parameter EoS is used in PVT, these can be modified in order to match to measured liquid densities, etc.

This formalism is particularly appealing since the introduction of the volume shifts has no effect on the equal fugacity conditions for thermal equilibrium and hence the prediction of saturation pressures, K-values, etc. It merely modifies the molar volumes and hence Z-factors, densities, etc.

Cubic Z-factor EoS

Often when working with cubic EoS, it is more convenient to work in terms of the Z-factor rather than volume.

For the Van-der-Waals EoS, replacing V by ZRT/p and rearranging gives:

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

where:

$$A = \frac{aP}{R^2T^2}$$

$$B = \frac{bP}{RT}$$

For the Redlich-Kwong EoS,

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

For Peng-Robinson,

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

Generalized EoS

Only a very limited set of EoS have been considered here which are of the form:

$$P = \frac{RT}{(V-b)} - \frac{a(T)}{(V+m_1 b)\,(V+m_2 b)}$$

where the (a, b) are as discussed previously and (m_1, m_2) are constants.

For VdW,	m1=m2=0
For RK,	m1=0, m2=1
For PR,	$m_1=2+\sqrt{2}$, $m_2=2-\sqrt{2}$.

Martins has shown that most cubic EoS can be derived from the single generalized form:

$$P = \frac{RT}{p} - \frac{\alpha(T)}{(V+\beta)(V+\gamma)} + \frac{\delta(T)}{V(V+\beta)(V+\gamma)}$$

where α and δ are functions of temperature and β and γ are constants.

Martin's generalised form can also be written as a cubic in the Z-factor

$$Z^3 + E_2 Z^2 + E_1 Z + E_0 = 0$$

with

$$E_2 = (m_1 + m_2 - 1)B - 1$$
$$E_1 = A - (2(m_1 + m_2) - 1)B^2 - (m_1 + m_2)B$$
$$E_0 = -[AB + m_1 m_2 B^2 (B+1)]$$

For a discussion on this generalized EoS and other EoS not mentioned in this text, the reader is referred to the excellent Ph.D. thesis of Whitson.

EoS for Mixtures: Mixing Rules

The Equations of State discussed in this section have been applied to pure components, but will generally be required to describe the behaviour of mixtures. The extension to mixtures requires the use of mixing rules, which are a means of calculating mixture parameters equivalent to those of pure components.

All the EoS discussed in this section use Van der Waals original mixing rules with some slight but significant modifications. The mixture (a, b) for the EoS discussed here are:

$$a = \sum_{i=1}^{N} \sum_{j=1}^{N} x_x x_j (a_i a_j)^{1/2} (1 - k_{ij})$$

$$b = \sum_{i=1}^{N} x_i b_i$$

where the x_i are the mole fractions (in the appropriate phase), and the a_i, b_i are the component EoS parameters given by:

$$a_i = a_{c,i} \alpha_i$$

$$b_i = \Omega_{b,i} \frac{RT_{c,i}}{P_{c,i}}$$

$$a_{c,i} = \Omega_{a,i} \frac{R^2 T_{c,i}^2}{P_{c,i}}$$

and the form of the α_i depends on the particular EoS being used. The $k_{i,j}$ are usually referred to as binary interaction coefficients (BIC) or binaries for short.

Binaries are not necessarily the same for different EoS. Changing the EoS from SRK to PR or vice versa will result in a message from PVTi to say that the Ω's and binaries have changed. The values of the binaries are usually determined from experimental liquid-liquid equilibrium data on binary mixtures by using some fitting procedure. The values assigned depend on the particular scheme used and therefore it is assumed that the binaries are not altered in the presence of other components.

Traditionally, binaries are assumed to be zero except for interactions between non-hydrocarbons and hydrocarbons and between light and heavy hydrocarbons, most notably $C_1 \rightarrow C_{N+}$.

Default binaries for the Peng-Robinson EoS as defined by Katz and Firzoobadi are experimentally determined between non-hydrocarbons and hydrocarbons; for $C_1 \rightarrow C_{N+}$ they defined $k_{C_1,j} = 0.14\gamma_j - 0.06$.

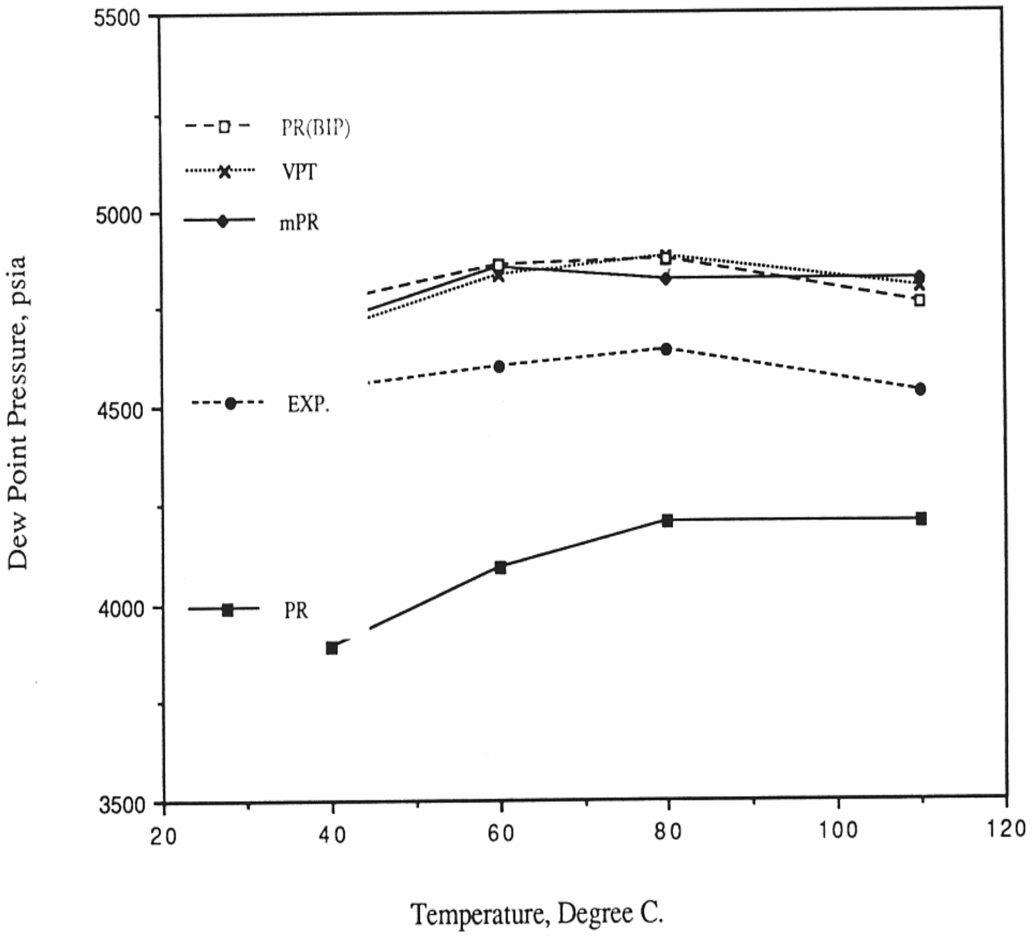
An alternative method for evaluating binaries is due to Cheuh and Prausnitz (1967), where:

$$k_{i,j} = A\left[1 - \left(\frac{2\left(V_{c,i}V_{c,j}\right)^{1/6}}{V_{c,i}^{1/3} + V_{c,j}^{1/3}}\right)^{B}\right]$$

and $V_{c,i}$ is the critical molar volume of the ith component. Generally B is set to 6.0 and A is adjusted to match the measured saturation pressure. It is found that a good match is usually obtained with $0.15 \le A \le 0.25$. There appears some physical justification for this model in that the cube root of the volume is the “radius” of the molecule, thus the equation is some weighted average of the proximity with which two unequal species can come into contact.

Examples of EoS predictions

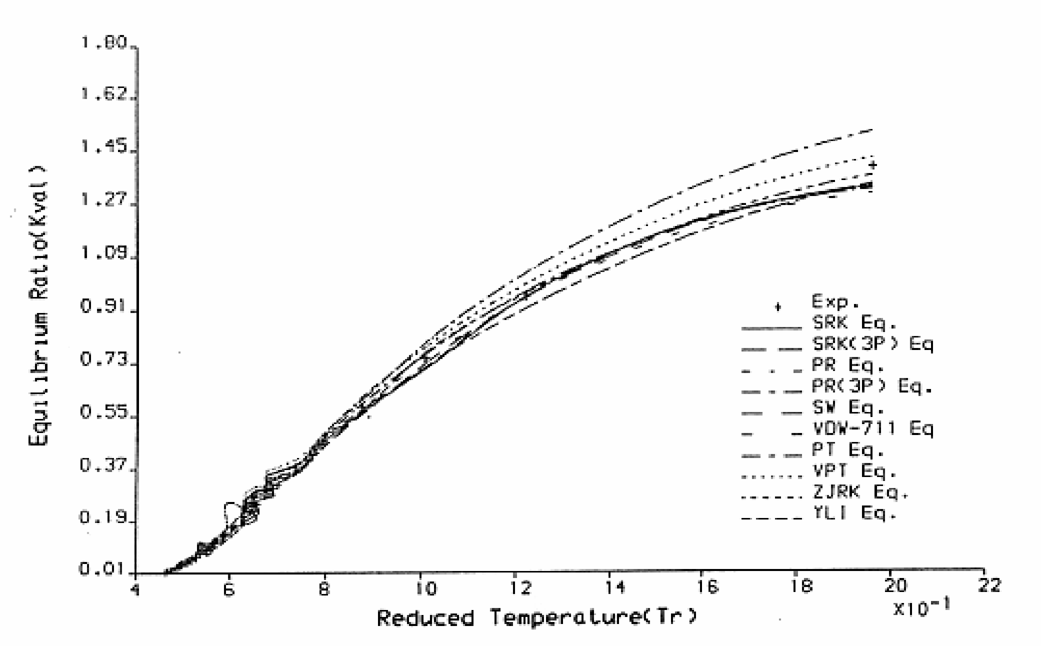
The following compare some physical properties predicted by different Equations of State and plot these with observed experimental results for particular fluids.



Predicted Dew Point Pressures by various EOS

- PR(BIP) = PR +BI Parameters
- VPT = Valderrama, Patel, Teja
- mPR = modified PR
- EXP = experimental
- PR = Peng-Robinson

The predicted dew-point pressures cover a range of 1000 psi, but not one of these four EoSs reproduces the experimental values.



Equilibrium Ratios Predicted by various EOS

The predicted condensate drop-out from a large range of EoSs again fails to reproduce the experimental data.

The reason for the lack of agreement is not a criticism of the EoS. Every hydrocarbon fluid is different as far as the detailed properties of its components and pseudo-components, especially the properties of the plus component. Any EoS can only predict properties according to the "average" properties that it has been given, and these properties have to be tuned to match the laboratory observations before valid predictions can be made. This is why we need to regress.

Summary of EoS

- **An Equation of State (EoS) is an analytic expression relating pressure to volume and temperature**
- **PV=ZRT is an equation of state**
- **Common EoS are PR, SRK**
  - **These are cubic in Z**
- **None completely satisfactory for all engineering applications**
- **They all need tuning.**

$$PV = nRT \quad \text{Ideal Gas}$$

$$PV = ZnRT \quad \text{Real Gas}$$

$$P = \frac{RT}{V-b} - \frac{a}{V(V)} \quad \text{Van der Waals}$$

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)} \quad \text{Soave-Redlich Kwong}$$

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)} \quad \text{Peng-Robinson}$$

9. Experiments, Observations and Regression

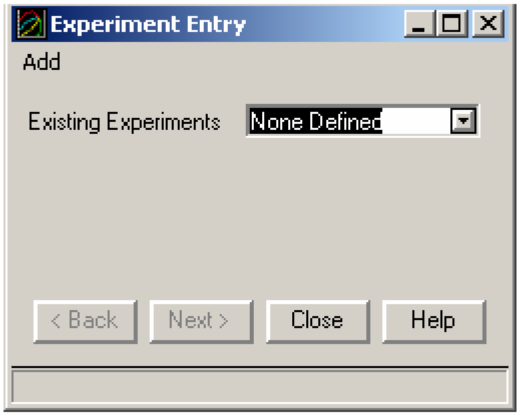
In this section we shall give a simple example of how to regress to an experimental measurement. You will learn how to use PVTi to define an experiment and the basic principles of regression in PVTi.

Bubble-point experiment

Exercise 4

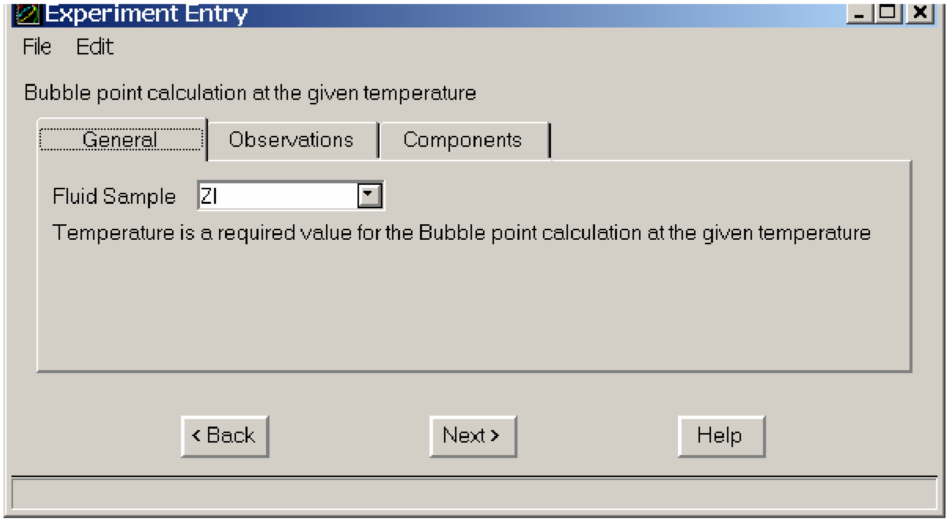
We shall define a simple bubble-point experiment in PVTi.

First load FLUID_CORRECT.PVI from the PVTi tutorial data. From the main PVTi panel, we choose "Edit | Experiments", which displays the experiment entry panel.



Existing Experiments: None Defined

From this panel, Add | New | Single Point will give us a choice of Bubble Point or Dew Point. The choice will depend on the fluid composition and the temperature, but in our case we will choose Bubble Point.

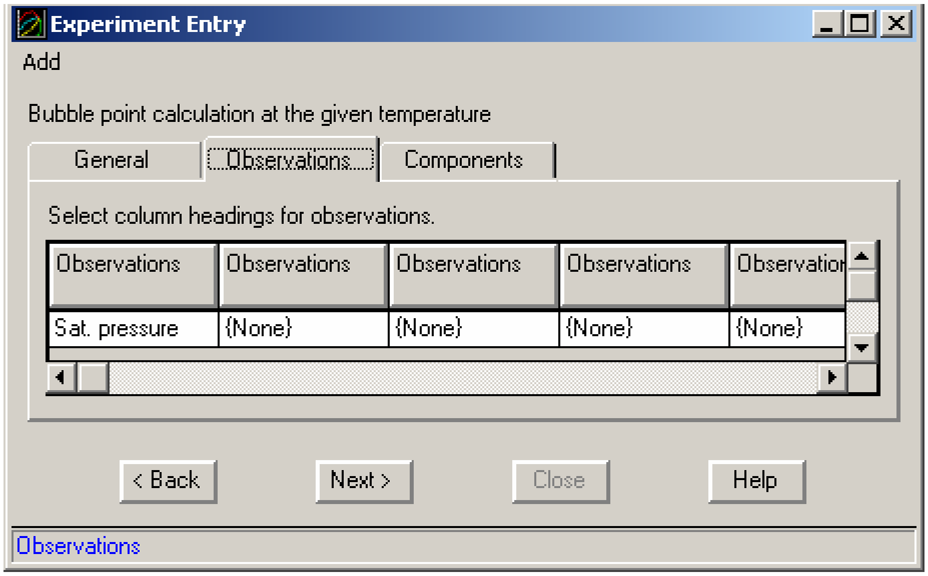


Bubble point calculation at the given temperature

Fluid Sample ZI

Temperature is a required value for the Bubble point calculation at the given temperature

Now click on the “Observations” tab to define the laboratory observations for that experiment. In fact we only have one observation, the bubble point.

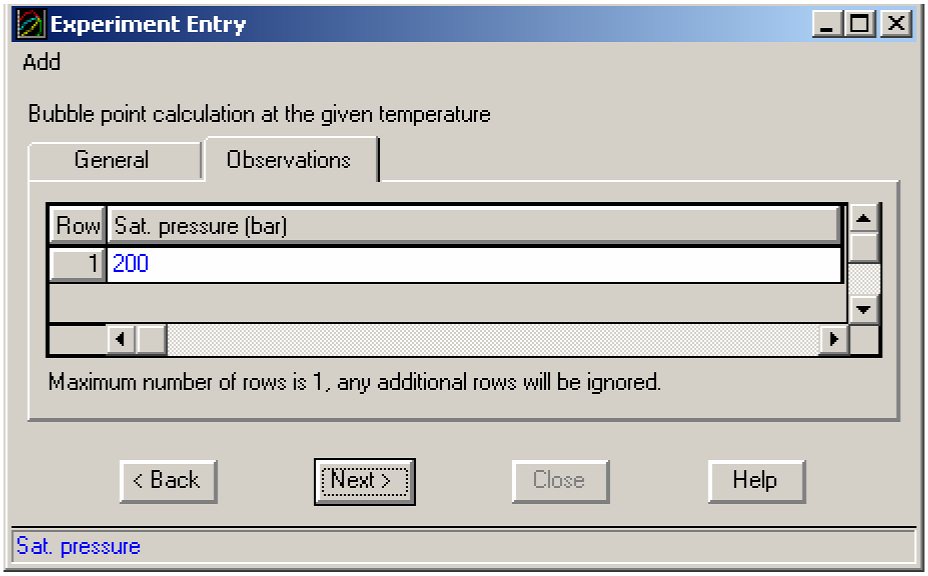


Bubble point calculation at the given temperature

Select column headings for observations.

Observations	Observations	Observations	Observations	Observatio
Sat. pressure	{None}	{None}	{None}	{None}

In the first column, choose “Sat Pressure”. Leave the other columns unchanged. “Next” allows you to enter the observed value of the bubble point. Enter a value of 200 bars.



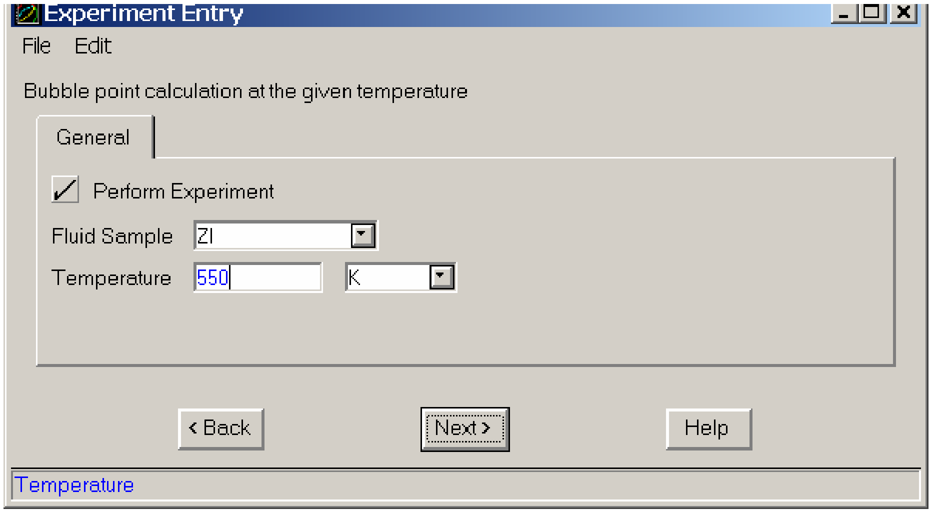
Bubble point calculation at the given temperature

Row	Sat. pressure (bar)
1	200

Maximum number of rows is 1, any additional rows will be ignored.

Sat. pressure

The “General” tab displays a panel in which we enter a temperature of 550K.



Bubble point calculation at the given temperature

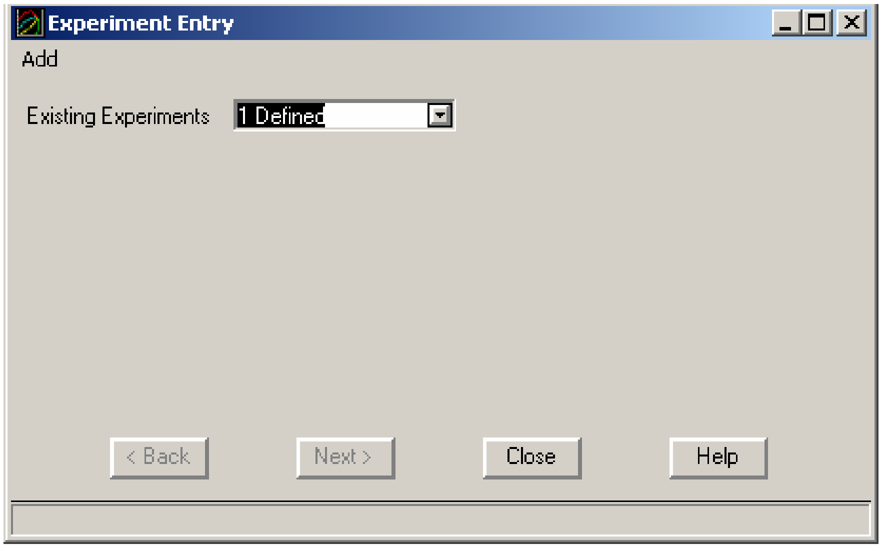
☑ Perform Experiment

Fluid Sample: ZI

Temperature: 550 K

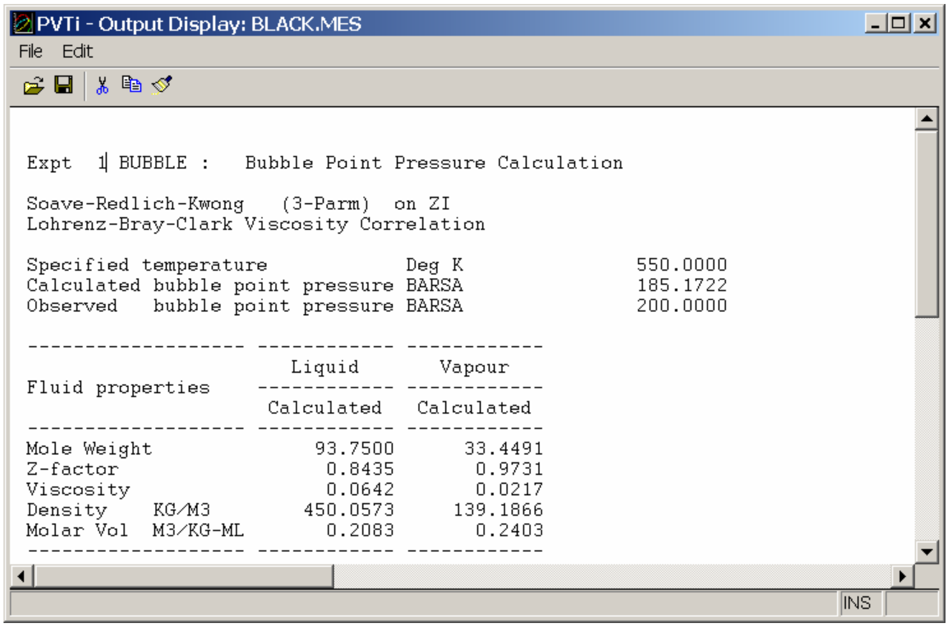
Temperature

“Next” takes us back to the Experiment Entry panel, but his time we have 1 experiment defined.



Now close this panel. We have defined our first experiment and observation.

We now calculate the result of the experiment as predicted by PVTi. This can be done by right-clicking on the BUBBLE1 experiment, or choosing Run | Simulate or the green “GO” icon.

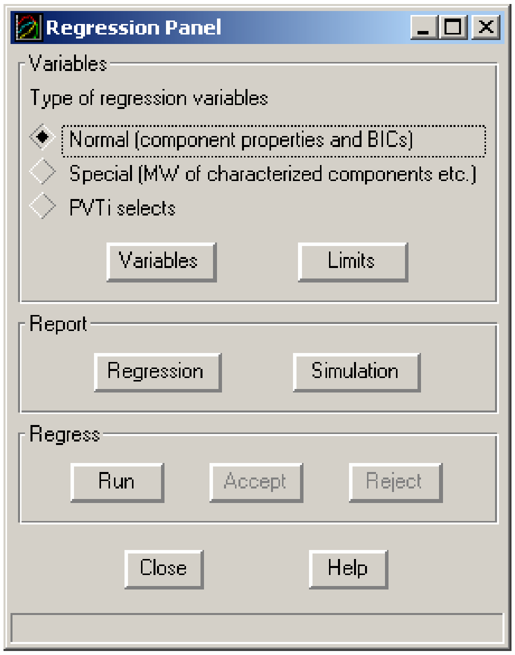


```
Expt   1 BUBBLE :   Bubble Point Pressure Calculation

Soave-Redlich-Kwong   (3-Parm)  on ZI
Lohrenz-Bray-Clark Viscosity Correlation

Specified  temperature            Deg K              550.0000
Calculated bubble point pressure BARSA              185.1722
Observed   bubble point pressure BARSA              200.0000

------------------- ------------ ------------
                       Liquid        Vapour
Fluid properties    ------------ ------------
                     Calculated   Calculated
------------------- ------------ ------------
Mole Weight              93.7500      33.4491
Z-factor                  0.8435       0.9731
Viscosity                 0.0642       0.0217
Density     KG/M3       450.0573     139.1866
Molar Vol   M3/KG-ML      0.2083       0.2403
------------------- ------------ ------------
```

PVTi has calculated a bubble point of 185 bars, based on the EoS parameters that it was given. The difference between the calculated 185 bars and the measured 200 bars is too great, so we want to adjust the EoS parameters to get a better match.

Regression to the Bubble Point

Run | Regression displays the main Regression Panel:



Regression Panel

Variables

Type of regression variables

● Normal (component properties and BICs)
○ Special (MW of characterized components etc.)
○ PVTi selects

Before regressing, we have to decide how many variables we want to modify, and which ones. In this simple example we only have one observation (the saturation pressure) so we can only choose one variable to regress[15]. Which one should we choose?

Click on the variables tab to see the possible choices.

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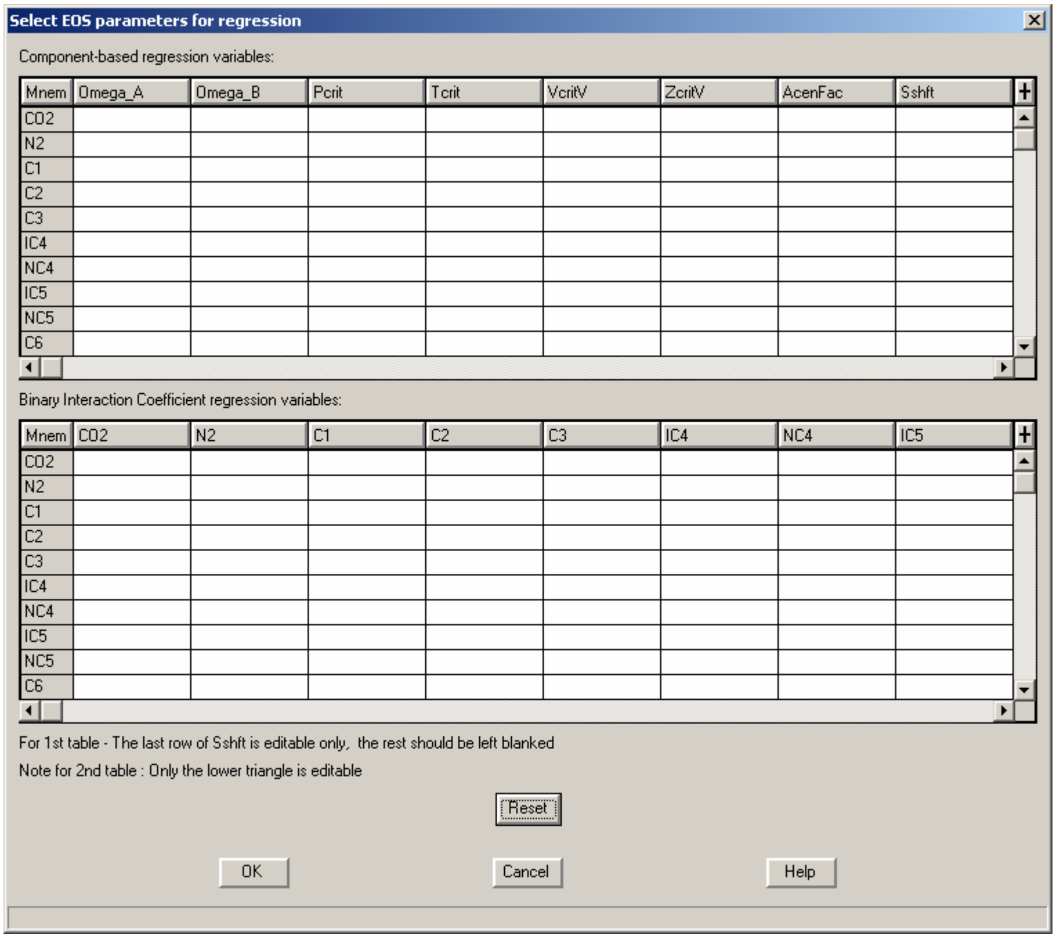
[15] In a typical laboratory report there will be over a hundred experimental observations, so we can choose as many regression variables as we want. Note however that we still want to choose a minimal set of regression variables.



Select EOS parameters for regression

Component-based regression variables:

Mnem	Omega_A	Omega_B	Pcrit	Tcrit	VcritV	ZcritV	AcenFac	Sshft
CO2								
N2								
C1								
C2								
C3								
IC4								
NC4								
IC5								
NC5								
C6								

Binary Interaction Coefficient regression variables:

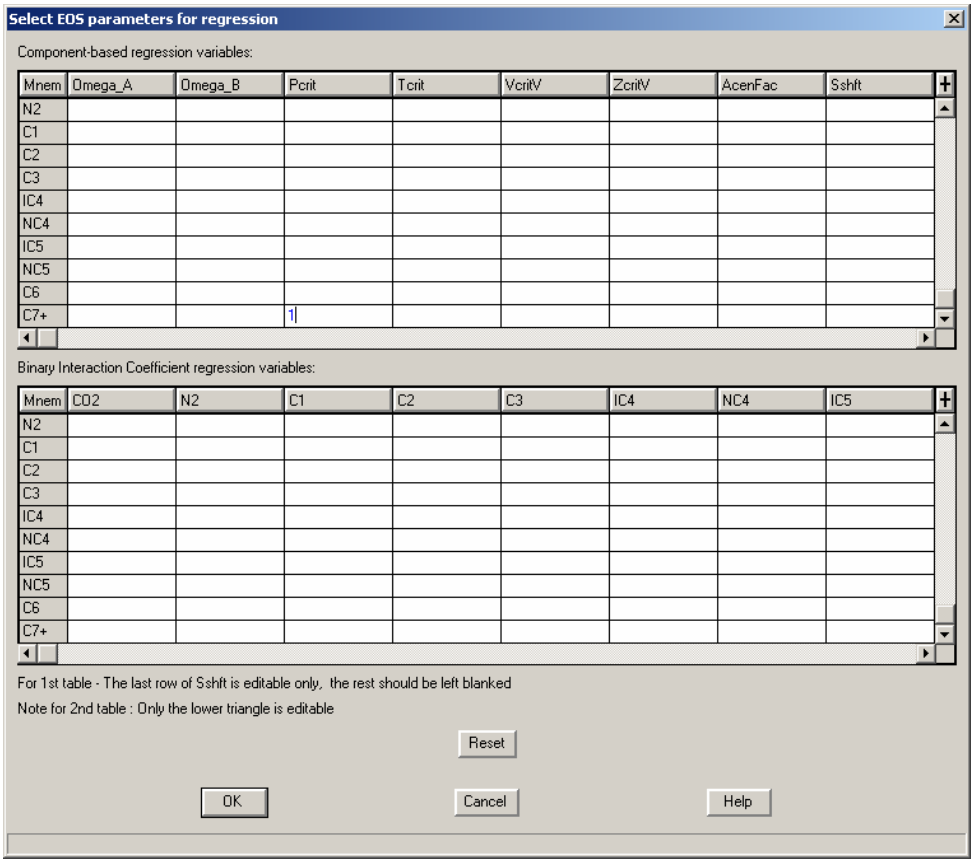
Mnem	CO2	N2	C1	C2	C3	IC4	NC4	IC5
CO2								
N2								
C1								
C2								
C3								
IC4								
NC4								
IC5								
NC5								
C6								

For 1st table - The last row of Sshft is editable only, the rest should be left blanked

Note for 2nd table : Only the lower triangle is editable

In any PVT analysis, the saturation pressure should be matched first. The saturation pressure is very sensitive to the Omega_A, Omega_B, Pcrit and Tcrit of the plus component. Recall that the properties of the plus component are the least known, so they seem obvious choices for regression.

Use the scroll bars to display the C7+ component. One at a time, choose one of these variables by putting a number 1 in the appropriate box. In the panel below, we have chosen Pcrit for C7+:



Component-based regression variables:

Mnem	Omega_A	Omega_B	Pcrit	Tcrit	VcritV	ZcritV	AcenFac	Sshft
N2								
C1								
C2								
C3								
IC4								
NC4								
IC5								
NC5								
C6								
C7+			1					

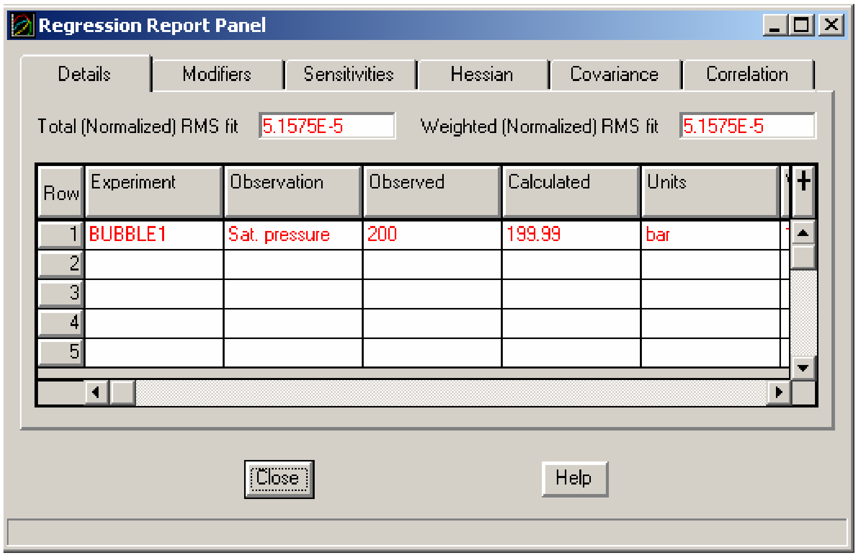
Binary Interaction Coefficient regression variables:

Mnem	CO2	N2	C1	C2	C3	IC4	NC4	IC5
N2								
C1								
C2								
C3								
IC4								
NC4								
IC5								
NC5								
C6								
C7+								

For 1st table - The last row of Sshft is editable only, the rest should be left blanked

Note for 2nd table : Only the lower triangle is editable

Click OK. This takes you back to the Regression Panel. Click Run. The main PVTi window will display the results of each regression iteration. When the regression is finished, click Report Regression to show the Regression report.

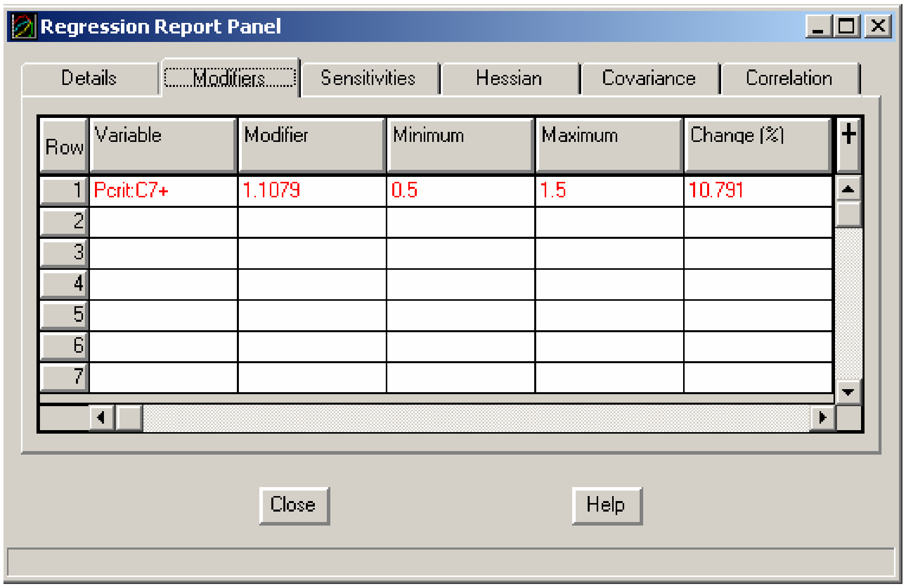


Total (Normalized) RMS fit 5.1575E-5

Weighted (Normalized) RMS fit 5.1575E-5

Row	Experiment	Observation	Observed	Calculated	Units
1	BUBBLE1	Sat. pressure	200	199.99	bar
2					
3					
4					
5					

In this case, changing Pcrit has made the calculated value of the saturation pressure equal to 199.99 bars, very close to the experimental value of 200 bars. To find out how much we had to change Pcrit, choose the Modifiers tab on the Regression Report Panel:



Row	Variable	Modifier	Minimum	Maximum	Change (%)
1	Pcrit:C7+	1.1079	0.5	1.5	10.791
2					
3					
4					
5					
6					
7					

This shows that the Pcrit value had to be increased by just over 10% to give us the excellent fit to the observed Psat.

We can now close this panel, go back to the Regression panel, and choose to accept or reject this regression.

Exercise 4 Regression

As an exercise, reject the regression and investigate the effect of regressing on the Omega_A, Omega_B and Tcrit of the plus component. Which requires the least percentage change?

What is the sensitivity to other parameters?

Viscosity correlations

Viscosity should be matched last. This is because viscosity is a flow property. The EoS will predict static equilibrium properties, but not flowing properties.

Correlations are available in PVTi to estimate viscosities, due to Lohrenz, Bray and Clark (LBC), that due to Pedersen *et al*[16].

Cannot predict viscosities from EOS: phase flow property

Two most widely used correlations

- Lohrenz-Bray-Clark (LBC)
- Pedersen et al

Aasberg-Petersen – not yet available in Eclipse Compositional

LBC OK for gases and volatile oils, very poor for heavier oils

Pedersen better for gases and oils, but not good for heavy oils (presence of asphaltenes)

AP Good over large P and T ranges. Can handle mixtures of CO2, paraffinic and aromatic components. Better than Pedersen for heavy oils

Lohrenz, Bray and Clark

The most widely used correlation for the prediction of liquid and vapour viscosities in reservoir simulators is that due to Lohrenz, Bray and Clark (LBC): the viscosity being related to a fourth-degree polynomial in reduced density, $\rho_r=\rho/\rho_c$:

$$\left[\left(\mu-\mu^*\right)\xi+10^{-4}\right]^{1/4}=a_1+a_2\rho_r+a_3\rho_r^2+a_4\rho_r^3+a_5\rho_r^4$$

where

a_1 = +0.1023000, a_2 = +0.0233640, a_3 = +0.0585330

a_4 = -0.0407580, a_5 = +0.0093324

and η^* is the low-pressure gas mixture viscosity

and ξ is the viscosity-reducing parameter, which for a fluid mixture, is given by:

$$\xi=\left[\sum_{i=1}^{N} z_i T_{ci}\right]^{1/6}\left[\sum_{i=1}^{N} z_i M_{\omega i}\right]^{-1/2}\left[\sum_{i=1}^{N} z_i P_{ci}\right]^{-2/3}$$

---

[16] PVTi also has a correlation due to Aasberg and Pedersen, but this is not yet available in ECLIPSE.

The critical density ρ_c is evaluated from:

$$\rho_c = V_c^{-1} = \left(\sum_{i=1, i \neq C_{7+}}^{N} (z_i V_{ci}) + z_{C_{7+}} V_{c_{C_{7+}}} \right)^{-1}$$

where the critical volume of the plus fraction is found from:

$$V_{cC_{7+}} = 21.573 + 0.015122 M_{\omega C_{7+}} - 27.656 \gamma_{C_{7+}} + 0.070615 M_{\omega C_{7+}} \gamma_{C_{7+}}$$

The dilute gas mixture viscosity as given by Herning and Zippener:

$$\mu^* = \left[\sum_{i=1}^{N} z_i \eta_i^* M_{\omega i}^{1/2} \right] \left[\sum_{i=1}^{N} z_i M_{\omega i}^{1/2} \right]^{-1}$$

where the dilute gas viscosities of the individual components, μ_i^* are derived from expressions due to Stiel and Thodos

$$\mu_i^* = 34x10^{-5} \frac{1}{\xi_i} T_{ri}^{0.94} \qquad T_{ri} < 1.5$$

$$\mu_i^* = 17.78x10^{-5} \frac{1}{\xi_i} \left(4.58 T_{ri} - 1.67 \right)^{0.625} \qquad T_{ri} > 1.5$$

where

$$\xi_i = T_{ci}^{1/6} M_{\omega i}^{-1/2} P_{ci}^{-2/3}$$

By making the viscosity a function of the fourth power of density, results are very sensitive to small differences in estimation of density. It is not unusual for this technique to predict a viscosity only 50% of the measured viscosity. Small changes in critical volumes or critical Z-factors will remedy the error, but it is recommended that they are changed as a single group.

- **The coefficients can be modified using the keyword LBCOEFF.**

- **A modified LBC is also available in ECLIPSE 300.**

  Using VCOMPACT, the viscosity decreases exponentially with reduced molar density.

Pedersen *et al*

Viscosities can be calculated from a modified form of the corresponding states method. A group of substances obey the corresponding states principle if the functional dependence of the reduced viscosity, μ_r, say, on reduced density and temperature, ρ_r and T_r, say, is the same for all components within the group, namely:

$$\mu_r(\rho,T) = f(\eta_r,T_r)$$

in which case comprehensive viscosity data is only needed for one component of the group which is denoted as the reference substance, to be given the subscript "o" . All other components will be identified with the subscript "x".

Generally, the critical viscosity, μ_c is not known, but can be estimated from

$$\mu_r(\rho,T) = \mu(\rho,T)T_c^{-1/2}V_c^{2/3}M_\omega^{-1/2}$$

Thus, the viscosity of component x at temperature T and a pressure where it has the density ρ is given by:

$$\mu_r(\rho,T) = {\frac{T_{cx}}{T_{co}}}^{1/2} {\frac{V_{cx}}{V_{co}}}^{-2/3} {\frac{M_{\omega x}}{M_{mo}}}^{1/2} \mu_o(\rho_o,T_o)$$

Where $\eta_o=\rho\rho_{co}/\rho_{cx}$, $T_o=TT_{co}/T_{cx}$ and η_o is the viscosity of the reference substance at T_o and ρ_o.

Oil mixtures contain a range of components with molecular weights ranging from 16 (methane) to about 1100 (C_{80}). It cannot be expected that all components from C_1 to C_{80} would belong to a group where a simple corresponding states principle applies. Generally, a third parameter must be added to account for the "shape" of molecules, such as the acentric factor. Pedersen *et al*. presented a corresponding states principle depending on reduced temperature and reduced pressure, $\mu_r=f(P_r\ ,T_r)$, where:

$$\mu_r = \mu\xi = \frac{\mu}{T_c^{-1/6}p_c^{2/3}M_\omega^{1/2}}$$

The deviation from the simple corresponding states principle is expressed in terms of a rotational coupling coefficient, denoted α, to give:

$$\mu_{mix}(P,T) = {\frac{T_{c,mix}}{T_{co}}}^{-1/6} {\frac{P_{c,mix}}{P_{co}}}^{2/3} {\frac{M_{\omega,mix}}{M_{\omega o}}}^{1/2} \frac{\alpha_{mix}}{\alpha_o}\mu_o(P_o,T_o)$$

where

$$P_o = P\frac{P_{co}\alpha_o}{P_{c,mix}\alpha_{mix}}$$

$$T_o = T\frac{T_{co}\alpha_o}{T_{c,mix}\alpha_{mix}}$$

The critical temperature and volume for unlike pairs of molecules are given by:

$$T_{c,ij} = (T_{c,i}T_{c,j})^{1/2}$$

$$V_{c,ij} = \frac{1}{8}\left(V_{c,i}^{1/3} + V_{c,j}^{1/3}\right)^3$$

where the critical volume of a component can be expressed in terms of the critical temperature and pressure via the real gas law and the critical Z-factor. Assuming a constant Z_c for all components, this becomes:

$$V_{c,ij} = \frac{1}{8}\text{constant}\left(\left(\frac{T_{c,i}}{P_{c,i}}\right)^{1/3} + \left(\frac{T_{c,j}}{p_{c,j}}\right)^{1/3}\right)^3$$

The mixture critical temperature is found from:

$$T_{c,mix} = \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j T_{c,ij} V_{c,ij}}{\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j V_{c,ij}}$$

so

$$T_{c,mix} = \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j \left[\left(\frac{T_{c,i}}{P_{c,i}}\right)^{1/3}\left(\frac{T_{c,j}}{P_{c,j}}\right)^{1/3}\right]^3 \left[T_{c,i}T_{c,j}\right]^{1/2}}{\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j \left[\left(\frac{T_{c,i}}{P_{c,i}}\right)^{1/3}\left(\frac{T_{c,j}}{P_{c,j}}\right)^{1/3}\right]^3}$$

and the mixture critical pressure is evaluated from:

$$p_{c,mix} = \frac{8\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j \left[\left(\frac{T_{c,i}}{P_{c,i}}\right)^{1/3}\left(\frac{T_{c,j}}{P_{c,j}}\right)^{1/3}\right]^3 \left[T_{c,i}T_{c,j}\right]^{1/2}}{\left(\sum_{i=1}^{N}\sum_{j=1}^{N} z_i z_j \left[\left(\frac{T_{c,i}}{P_{c,i}}\right)^{1/3}\left(\frac{T_{c,j}}{P_{c,j}}\right)^{1/3}\right]^3\right)^2}$$

The mixture mole weight is given by $M_{\omega,mix} = 1.301x10^{-4}\left(M_{\omega}^{\ 2.303} - M_{n}^{\ 2.303}\right) + M_{n}$ where M_ω and M_n are the weight average and number average mole weights, respectively. This mixing rule is derived empirically on the basis of available viscosity data and assigns a larger influence to heavier components. The α parameter for the mixture is found from:

$$\alpha_{mix} = 1.0 + 7.378x10^{-3}\rho_r^{1.847} M_{\omega,mix}^{0.5173}$$

where the α of methane, the reference substance, is given by $\alpha_o = 1.0 + 0.031\rho_r^{1.847}$ and the constants and exponents have been found from fitting to experimentally determined viscosity data.

Summary of viscosities

There are two main correlations: Pedersen and LBC.

Pedersen is based on Corresponding States Method (CSM)

A group of substances obey CSM if the functional dependence of a “reduced” quantity, such as μr, on reduced temperature and density (Tr, ρr) is same for all components in the group

Pedersen modified the CSM to use the acentric factor, which is related to the shape of the molecule.

With Pedersen you cannot regress.

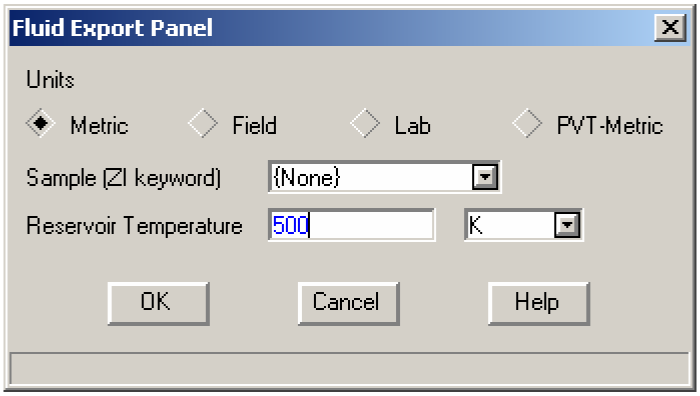
LBC viscosity is a parameterized function of reduced density

With LBC you can regress on viscosity using $V_{critvis}$ or $Z_{critvis}$ in PVTi and specifying the LBCOEFF keyword in ECLIPSE.

The method of Pedersen often gives better prediction of viscosities than does the method of Lohrenz, Bray and Clark. Neither method is particularly good, but typical calculations based on unregressed EoS data are LBC ~ 50% and Pedersen ~ 90% of the reported values. However you should treat experimentally “measured” viscosities with some caution, as these viscosities are sometimes calculated!

Exercise 5 Output of regressed properties

From the main PVTi panel, choose File|Export keywords|Eclipse Compositional Model.



Units

● Metric ○ Field ○ Lab ○ PVT-Metric

Sample (ZI keyword) {None}

Reservoir Temperature 500 K

Choose your units and temperature, choose a file name, and export the PVO file.

Rules for Regression

- Vary properties of poorly defined components, i.e., plus fraction(s)
- Choose as few properties as possible
    - “Bouncing” Rms or
    - Variables → limits ⇒
    - Redundancy in variable set: “trial and error” to find optimum set or sensitivity matrix $Aij = \partial ri/\partial xj$
- Ensure variable monotonicity

In general, when deciding which variables to choose, consider the following sensitivities:

- (Tc, pc), or Omegas of plus fraction(s): saturation pressure, liquid dropout, etc.
- Volume shift: Z-factors, densities, etc.
- Zc or Vc for LBC viscosity

Regress in the order above, so for instance first regress (Tc, Pc), accept the regression, then regress on volume shifts and accept the regression. Finally check the viscosity.

If you have reason to doubt the values of some of experimental measurements, you can choose to give them less weight in the regression. It is also good practice to set the weights of the viscosity measurements to zero until you are ready to regress on viscosity. To set the weight of an experiment, right-click on the experiment and choose “set weight”.

Summary of Regression

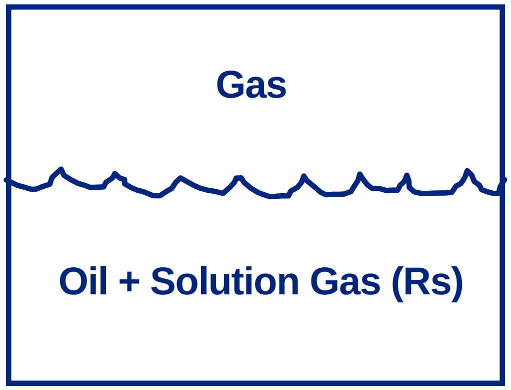
We have defined a simple bubble point experiment and compared the experimental value with the calculated value from PVTi. The comparison was poor to start with, but changing the properties of the C7+ allowed us to get a good match.

In general we will have many more observations, and the regression stage of PVT analysis will take a lot longer before an acceptable match is obtained.

10. Revision of Component Modeling

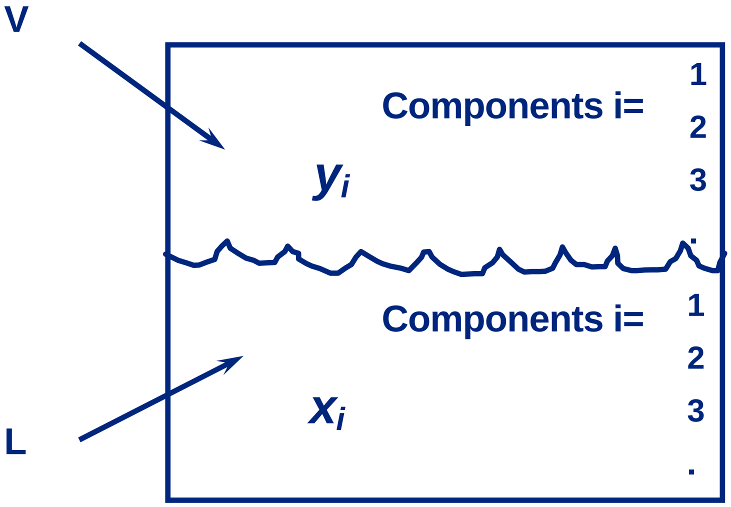
ECLIPSE 100 (& all Black-Oil Simulators)

Oil and Gas phases are represented by two components: one ‘component’ called oil and one ‘component’ called gas.



ECLIPSE 300 (& all Compositional Simulators)

Oil and Gas phases are represented by multicomponent mixtures.



Physical Properties

In a black-oil model, the physical properties of the oil and the gas are a function of pressure and of nothing else.

$$\left.\begin{matrix} B_o \\ B_g \\ R_s \\ \mu \end{matrix}\right\} = f(p)$$

In a compositional model, all we know is what components are present. We first have to calculate how many phases are present at the given pressure and temperature. If there are both oil and gas phases, we have to calculate the composition of each phase. Given these compositions we then have to calculate the physical properties.

$$\left.\begin{matrix} K_i = \dfrac{y_i}{x_i} \\ \mu \\ \rho \end{matrix}\right\} f(p, x_i, y_i)$$

The process of deciding how many phases are present is called a “Flash”.

Regression

To calculate the physical properties of the oil and gas, we have to calibrate an Equation of State (EoS) using a PVT package such as PVTi. We have to do this because we don’t know the exact properties of the SCNs, and we only have an approximate idea of the properties of the + fraction.

We have a measured value of the MW of the + fraction, and sometimes a density, and from these we have to derive all the other properties. This process is called “characterization of the plus fraction”.

Before we regress, we may need to split that + component into a number of smaller components. If we are going to run compositional simulation models we also want to group components to speed up the compositional simulations.

Once all this is done, we can regress by changing parameters in our EoS model until the predictions of the EoS model agree with the experimental observations. We then export the regressed PVT values in a form ready for input into ECLIPSE.

11. Pressure Depletion Experiments

The main experiments performed by the PVT laboratory on the fluid sample you provide are:

Single-point experiments, such as Psat

Pressure depletion experiments, such as CCE, CVD, DL

The laboratory may also perform

Swelling tests

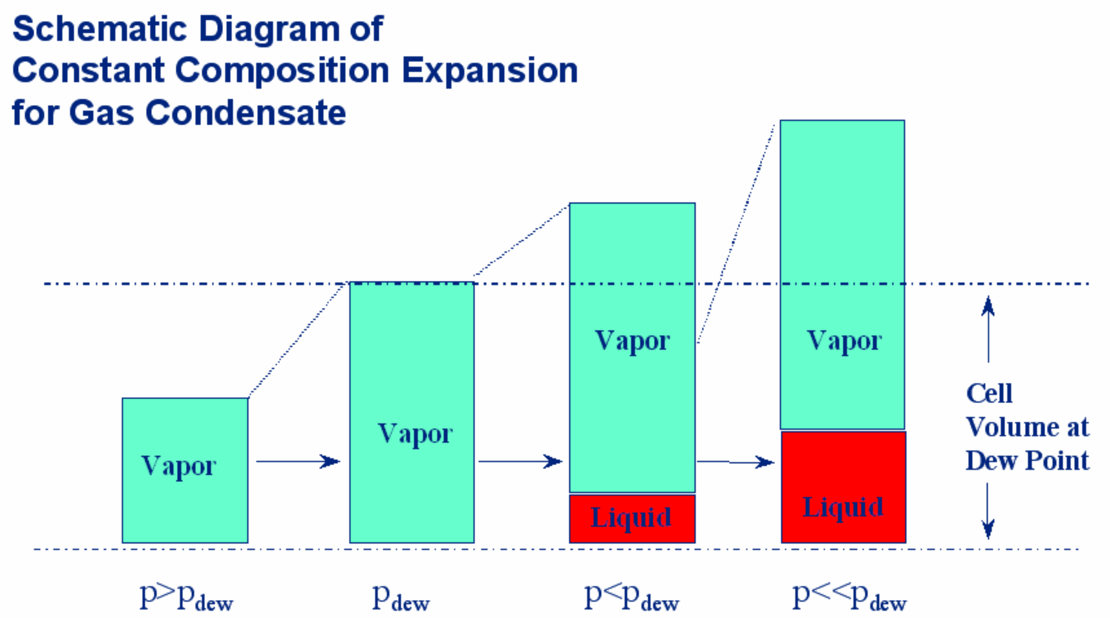
Vaporisation tests

The two fundamental experiments performed on gas-condensate systems are the constant volume depletion experiment, and the constant composition expansion experiment, often reduced and referred to by their initials, CVD and CCE respectively. For oils, a differential liberation experiment (DL) is usually performed instead of the CVD. All three experiments are the same above the saturation pressure.

A PVT cell is used for all three experiments; this is a vessel whose internal volume is known under a wide range of temperatures and pressures, and can be maintained in a constant (adjustable) temperature. The cell has a high-pressure window through which you can see (and measure) any liquids present. Pressure and volume changes are effected by introducing or withdrawing mercury at the base of the cell, or above a floating piston that forms the “roof” of the cell. Ports exist for the charging and withdrawal of fluids during the experiments. Initially the cell is charged with a mixture that we believe represents the reservoir composition. The cell is then left to attain equilibrium at the desired temperature and pressure, some cells having the ability to agitate the contents to help achieve this more rapidly.

Constant Composition Experiments (CCE)

The CCE experiment can be applied to an oil or gas sample.



Starting at a pressure above reservoir pressure, the cell pressure is gradually reduced, and the expanding volume measured. While the mixture remains above the dew point, the Z-factors can be calculated directly, as the number of moles in the cell will be known from the charging measurements. Several pressure traverses may be made to define the dew point as accurately as possible. As the pressure is reduced below the dew point, the condensed liquid volume is measured and reported as a function of the cell volume[17] at the dew point.

This measurement is all that can be obtained during the experiment[18], as the number of moles in the liquid, and the composition of the oil and gas phases are unknown below the dew point. However, it is an important set of experimental data for EoS matching purposes, as it is an independent set of observations from the CVD experiment, and given that no fluids have been withdrawn, the composition of the cell contents is known to be constant throughout.

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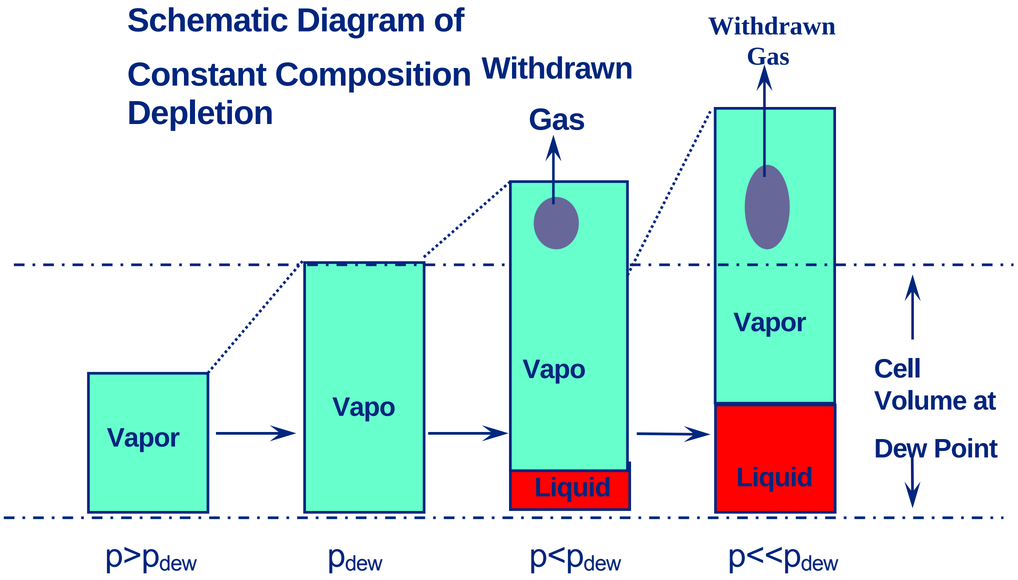
[17] Not always! Some laboratories define liquid volume in the CCE as actual liquid volume per total fluid volume.

[18] At the lowest pressure, the oil and gas properties and compositions can be measured.

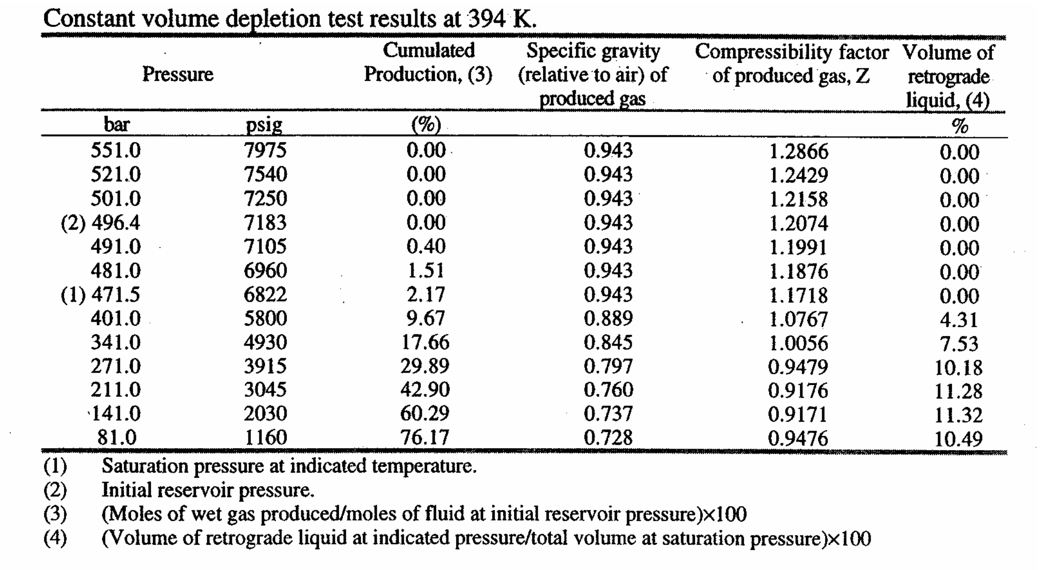
Constant Volume Depletion (CVD)

A CVD should be performed on all condensates and volatile oils, as these are the fluids that are going to undergo the greatest compositional changes if the reservoir pressure is allowed to drop below the saturation pressure.



The CVD behaves as a CCE from high pressures down to the saturation pressure (a dew point for a condensate). This experiment begins at the saturation pressure. The cell volume is noted and all subsequent volumes are referred to it. The fluid is then expanded to a new volume and pressure, and a liquid phase will condense. (On some occasions, two immiscible liquid phases may occur.) Vapour is then withdrawn at constant pressure, until the volume occupied by the cell contents is the same as the original saturation pressure cell volume. The liquid volume is recorded, and the withdrawn vapour is analysed. The process is then repeated several times until the lowest required pressure is reached. The liquid remaining in the cell is then sometimes removed and analysed.

Typical experimental results are shown below.



Constant volume depletion test results at 394 K.

Pressure		Cumulated Production, (3)	Specific gravity (relative to air) of produced gas	Compressibility factor of produced gas, Z	Volume of retrograde liquid, (4)
bar	psig	(%)			%
551.0	7975	0.00	0.943	1.2866	0.00
521.0	7540	0.00	0.943	1.2429	0.00
501.0	7250	0.00	0.943	1.2158	0.00
(2) 496.4	7183	0.00	0.943	1.2074	0.00
491.0	7105	0.40	0.943	1.1991	0.00
481.0	6960	1.51	0.943	1.1876	0.00
(1) 471.5	6822	2.17	0.943	1.1718	0.00
401.0	5800	9.67	0.889	1.0767	4.31
341.0	4930	17.66	0.845	1.0056	7.53
271.0	3915	29.89	0.797	0.9479	10.18
211.0	3045	42.90	0.760	0.9176	11.28
141.0	2030	60.29	0.737	0.9171	11.32
81.0	1160	76.17	0.728	0.9476	10.49

(1) Saturation pressure at indicated temperature.
(2) Initial reservoir pressure.
(3) (Moles of wet gas produced/moles of fluid at initial reservoir pressure)×100
(4) (Volume of retrograde liquid at indicated pressure/total volume at saturation pressure)×100

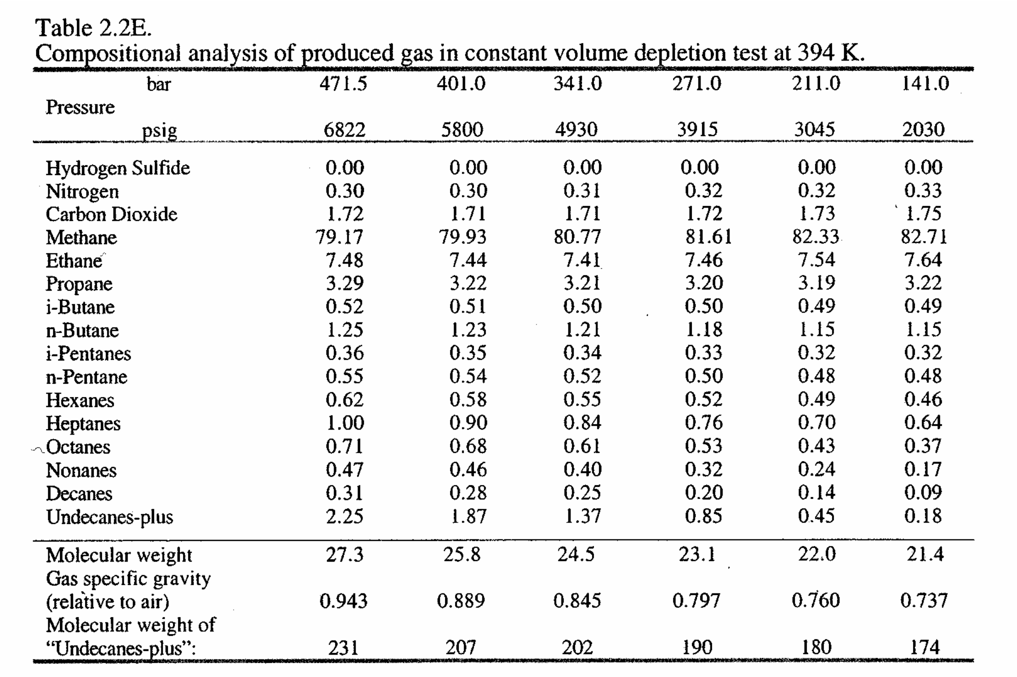


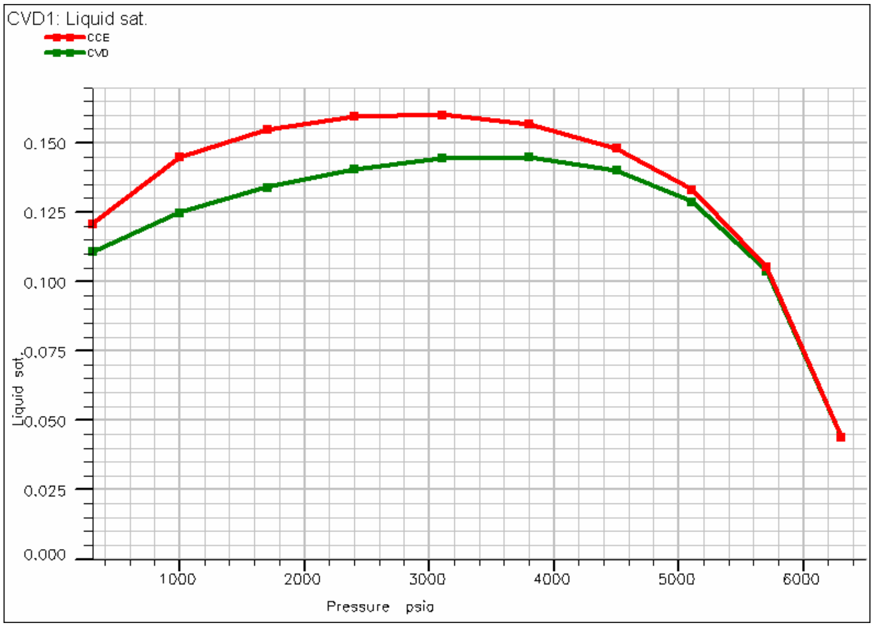
Table 2.2E.
Compositional analysis of produced gas in constant volume depletion test at 394 K.

Pressure						
bar	471.5	401.0	341.0	271.0	211.0	141.0
psig	6822	5800	4930	3915	3045	2030
Hydrogen Sulfide	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.30	0.30	0.31	0.32	0.32	0.33
Carbon Dioxide	1.72	1.71	1.71	1.72	1.73	1.75
Methane	79.17	79.93	80.77	81.61	82.33	82.71
Ethane	7.48	7.44	7.41	7.46	7.54	7.64
Propane	3.29	3.22	3.21	3.20	3.19	3.22
i-Butane	0.52	0.51	0.50	0.50	0.49	0.49
n-Butane	1.25	1.23	1.21	1.18	1.15	1.15
i-Pentanes	0.36	0.35	0.34	0.33	0.32	0.32
n-Pentane	0.55	0.54	0.52	0.50	0.48	0.48
Hexanes	0.62	0.58	0.55	0.52	0.49	0.46
Heptanes	1.00	0.90	0.84	0.76	0.70	0.64
Octanes	0.71	0.68	0.61	0.53	0.43	0.37
Nonanes	0.47	0.46	0.40	0.32	0.24	0.17
Decanes	0.31	0.28	0.25	0.20	0.14	0.09
Undecanes-plus	2.25	1.87	1.37	0.85	0.45	0.18
Molecular weight	27.3	25.8	24.5	23.1	22.0	21.4
Gas specific gravity (relative to air)	0.943	0.889	0.845	0.797	0.760	0.737
Molecular weight of "Undecanes-plus":	231	207	202	190	180	174

In theory, the composition of the final liquid can be predicted, as the composition of the vapour, and the volumes of both liquid and vapour have been recorded throughout the experiment. Knowing the number of moles that were present at the start, a material balance calculation should reveal the composition of the remaining fluid. Some laboratories do perform such a check routinely, in order to smooth the reported compositions to make the material balance. Others do not, and you can check the quality of the material balance on a CVD data set before investing a great amount of effort in EoS matching.

There are several sources of error in experiments of this kind, which contribute to material balance errors. Firstly, the initial fluid composition may be a calculated recombination composition, rather than an independent measurement. Secondly, the amounts of heavier components in the vapour can be consistently underestimated due to losses from condensation in the apparatus pipe work, and the lack of sensitivity and resolution of the gas chromatography to these heavier components.

The amount and composition of the liquid that drops out from a CVD experiment will be different from that of the liquid from a CCE experiment since the two processes are different.



Differential Liberation (DL)

The Differential Liberation experiment is usually only performed on non-volatile oils. Most crude oils analysed by this experiment generally report the so-called black oil properties of gas-oil ratio, R_s, oil formation volume factor, B_o and gas formation volume factor B_g. These are sufficient for inclusion[19] in most

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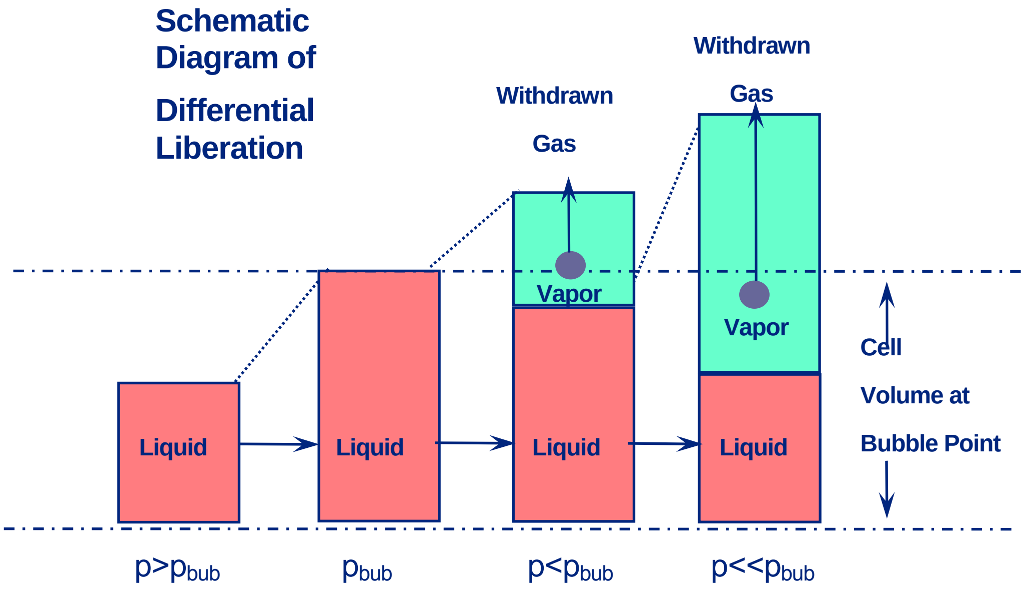
[19] This data may require modification for separator conditions. This is explained later.

simulators with black oil PVT treatments, such as ECLIPSE 100. Black oil properties of crudes (and volatile fluids using an extended black oil treatment, including a vaporising oil term R_v, the condensate-gas ratio) can be generated from a compositional description via an EoS and the simulation of suitable experiments.



Like the CVD, the DL behaves as a CCE from high pressures down to the saturation pressure. However in the DL experiment, once the pressure has dropped below the saturation pressure, then after each flash all the vapour phase is removed and the liquid composition from the flash becomes the feed for the next pressure depletion. This procedure usually terminates at standard pressure, usually 14.7 psia. A further stage is then performed, consisting of a temperature reduction from reservoir temperature to standard temperature. The volume of the oil phase at this stage is then defined to be the residual or "stock tank" oil, V_{oil}^{st}. The fraction of the initial moles that have ended up in the stock tank can be used to convert molar volumes to actual volumes and vice-versa.

In PVTi, in order to calculate the black oil properties reported on the standard DL laboratory analysis, the following calculations are done.

- Oil formation volume factors are the actual volume of oil at pressure P_j divided by the actual volume of oil that gets into the stock tank.
- The gas formation volume factor (FVF) is calculated as the volume of gas liberated at the current pressure, converted to stock tank volume using the real gas law:

$$V_{gas}^{pj} = \left(\frac{Z^{pj}}{Z^{st}}\right)\left(\frac{T^{pj}}{T^{st}}\right)\left(\frac{\mathrm{P}^{\mathrm{st}}}{\mathrm{P}_{\mathrm{j}}}\right)\mathrm{V}_{\mathrm{gas}}^{\mathrm{st}}$$

where by definition $Z^{st}=1$.

- The gas-oil ratio is calculated by summing the total volume of gas at stock tank conditions that is liberated over all stages from the current stage to the stock tank stage divided by the stock tank oil volume.

Some of these definitions can be changed in Utilities | Program | Options.

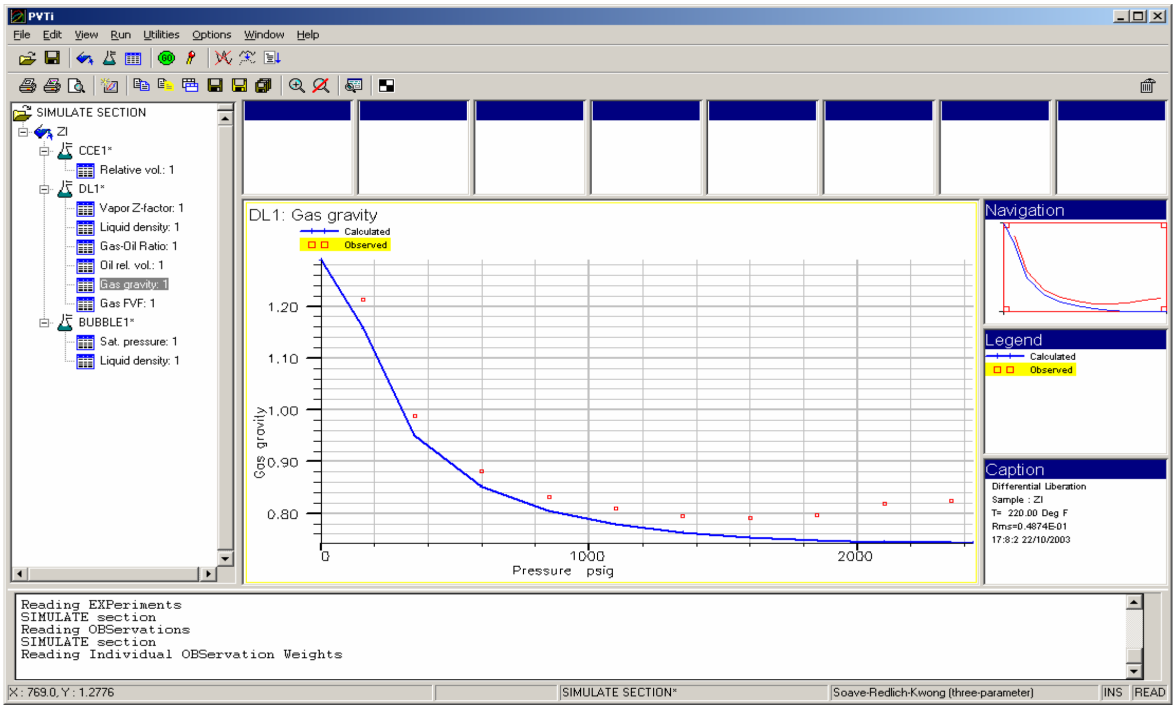
Experiments in PVTi

The Constant Composition Expansion (CCE), Constant Volume Depletion (CVD) and Differential Liberation (DL) experiments are very similar in the way they are defined and simulated by PVTi.

The first stage in all these experiments is to find the saturation pressure. To that end, you are asked to specify the nature of the fluid sample under investigation, i.e., whether it is an oil, gas (Condensate) or genuinely single phase (generally only applicable to single component fluids or fluids dominated by a single component). This tells PVTi which type of saturation pressure, i.e., bubble point, dew point or none, respectively, to look for. If you specify that the fluid is an oil and thus expect a bubble point and this cannot be found, then the dew point will automatically be searched for, and vice-versa for a Condensate/dew point system. If neither bubble nor dew points can be found, the fluid will be reported as being single phase.

For single-phase fluids, the volume of the fluid at the first (highest) pressure stage is taken as the reference (control) volume.

Example of Pressure depletion results



Differential Liberation
Sample : ZI
T= 220.00 Deg F
Rms=0.4874E-01
17:8:2 22/10/2003

```
Reading EXPeriments
SIMULATE section
Reading OBServations
SIMULATE section
Reading Individual OBServation Weights
```

X : 769.0, Y : 1.2776 | SIMULATE SECTION* | Soave-Redlich-Kwong (three-parameter) | INS | READ

Observed and predicted Gas Gravity from a DL experiment.

Summary of Pressure Depletion Experiments

Two experiments performed on gas-condensate systems are the constant volume depletion (CVD) experiment and the constant composition expansion (CCE) experiment. For oils, a differential liberation experiment (DL) is usually performed instead of the CVD.

- Separator Test - Flash conditions as the whole fluid system enters the separators immediately - i.e., reservoir fluid comes to the surface and is immediately separated into gas and oil
- Differential Liberation - models what happens in the reservoir during pressure decline
- Remember one purpose of PVTi is to model what will be simulated in ECLIPSE 100 or ECLIPSE 300

The CVD experiment is closer to what happens within the reservoir. The pore volume is approximately constant and as pressure drops below the dew point then condensate liquid is deposited and the remainder of the volume is occupied by gas. The DL experiment also reproduces reservoir behaviour in that as pressure drops below the bubble point then gas comes out of solution. This gas migrates away and the pore volume remains full of oil[20].

The CCE experiment represents in some sense what happens after the hydrocarbon enters the wells. Pressure and temperature and volume all change, but the composition remains the same – in general the composition of what enters the well is the same composition that leaves the well, but the pressure (and temperature) has changed. Similarly when the well stream enters a separator, the composition remains constant but the pressure (and temperature) changes.

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[20] One difference however is that the process is continuous in the reservoir, whereas in the lab the pressure decline is in discrete steps – typically a dozen or so.

12. Other PVT experiments

Gas Injection Experiments

There are two main gas injection experiments.

1. With a variable volume: lean gas is injected into a saturated fluid followed by a pressure change to return the mixture to saturated (single phase) conditions.
2. With a constant volume: lean gas is added to a reservoir fluid, which may or may not be at saturation pressure, followed by removal of (enriched) gas to return the mixture to the original volume.

These two experiments are known as a Swelling test and a Vaporisation test.

Swelling Tests

Gas injected into an undersaturated reservoir can go into solution, thereby swelling the oil. The injection of light components into a fluid that will be richer in heavier components also has the effect of increasing the (mixture) saturation pressure. Note that lean gas can be injected into a condensate fluid, in which case it is quite possible for the fluid to swell since additional mass is being added, but the saturation pressure may start to drop as the fluid becomes dominated by light ends.

The purpose of the experiment is to find the saturation pressure, so as usual we start with a control volume at the saturation pressure of the original reservoir fluid. Lean gas of a specified composition is then added in fixed amounts (as a mole percentage of the mixture, or as a gas-oil ratio of volume of injected gas at standard conditions per original saturation volume of reservoir fluid), the mixture is then taken to its new saturation pressure and saturation volume. The swelling factor is then defined as the new saturation volume divided by the original saturation volume with due account made of the increase in fluid moles.

Vaporisation Test

This experiment is similar to the swelling test except that it is performed at constant volume and pressure. A volume of reservoir fluid at some pressure and temperature, usually below the saturation pressure and hence two-phase, is contacted by a series of lean gas injections. After each contact, a volume of (enriched) gas and/or liquid is removed to return the system to the original volume. The composition of the removed gas is measured. The experiment seeks to measure the extent of "vaporisation" of intermediate and heavy components from the reservoir liquid phase by stripping into the injected gas stream.

The procedure is as above. One mole of reservoir fluid at a prescribed pressure and temperature is flashed to calculate the phase split and volumes of liquid and vapour. Lean gas is then added in a series of steps of moles to give a new mixture composition. This new composition is flashed at the same pressure and temperature and any excess vapour volume removed. The composition of the removed stream is noted and the resulting mixture is then subject to further lean gas injections.

Separator Experiments

Separators are essentially a sequential set of flash calculations with a specified output stream of one or more stages forming the feed for other stages. The notation we use is that a separator stage is taken to be a single “flash-box” and that a collection of stages connected in a specified order is a separator train.

Each stage in the train can be at a different pressure and temperature. The stream for the second and subsequent stages is usually a liquid stream but can be a vapour stream or both. The input stream can be a mixture of given output streams, liquid and/or vapour, of several previous or later stages.

13. Miscibility and Miscible Floods

We will now investigate in details one of the main advantages of compositional simulation: the ability to model miscible effects. In this section we will start by looking at the miscible processes that can happen within the reservoir. We will start by using PVTi to model miscibility experiments and in a later section perform the same experiments with ECLIPSE 300.

More generally, before injecting any gas into a reservoir you should be aware of the effect that gas will have on the existing fluids in the reservoir. This effect could either be to your advantage or disadvantage, as we shall see.

Definition of Miscibility

If we inject a gas into an oil then the mixture can either form

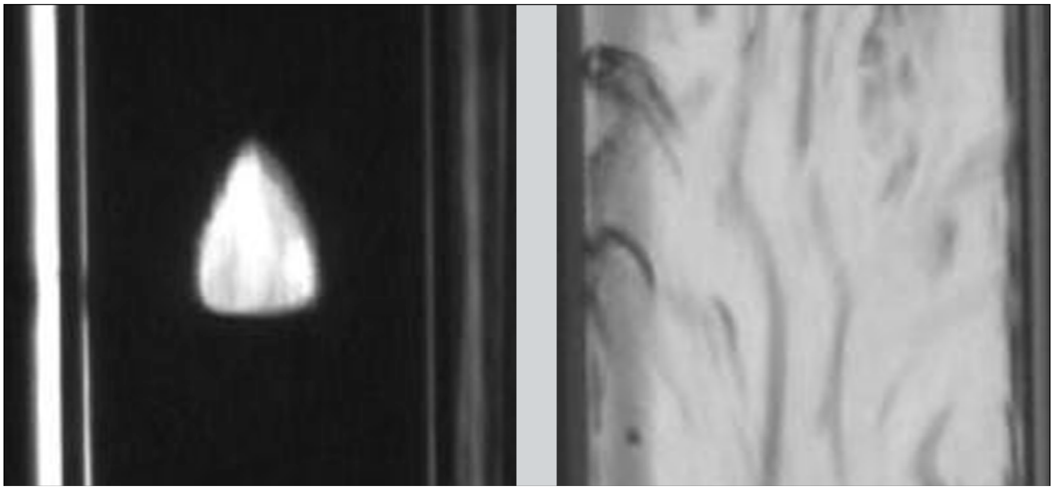
- one hydrocarbon phase or
- two separate oil and gas phases.

If the mixture is one-phase then the injection process or the displacement process is miscible. If the mixture is two-phase then the process is immiscible.

In the immiscible case, we have to use relative permeabilities when we calculate the flow of each phase, and we have to use the oil-gas capillary pressures when we calculate the vertical fluid distribution. In the miscible case, as there is only one phase, we do not consider either relative permeabilities or oil-gas capillary pressures.

From a simulation point-of-view, the main advantage of miscibility is that there is no residual oil to gas displacement. Achieving miscibility means increasing recovery.

In a reservoir with a gas-oil contact, there is an interface between the gas phase and the oil phase. This interface is associated with interfacial tension (IFT). As the IFT reduces to zero, the interface disappears and the two fluids become one: we have miscibility.



Rising bubble experiment to determine miscibility

How we get miscibility

For a given temperature, miscibility depends on the fluid composition and the pressure. There is a minimum pressure we need to achieve miscibility, and this pressure depends on the process. There are two main miscible processes:

First-contact miscibility

Multi-contact miscibility

We can divide Multi-contact miscibility into

1.1 Condensing drive

1.2 Vaporising drive

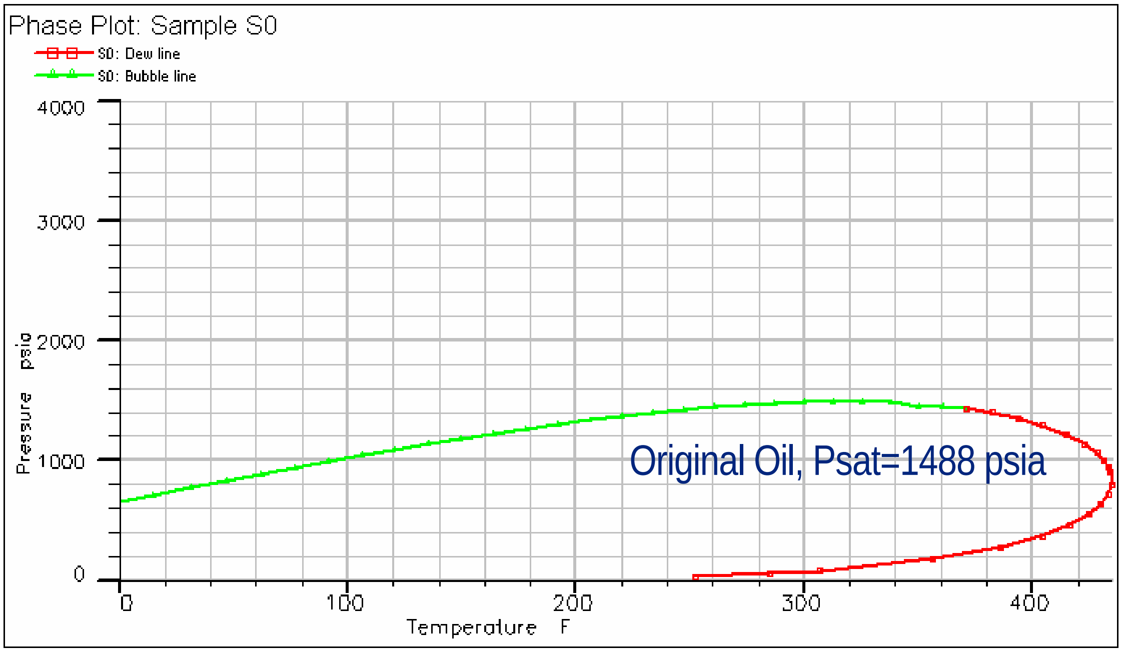
First-contact miscibility

An example of First-contact miscibility is an LPG slug - designed to achieve first-contact miscibility with oil at leading edge of slug and with driving gas at trailing edge.

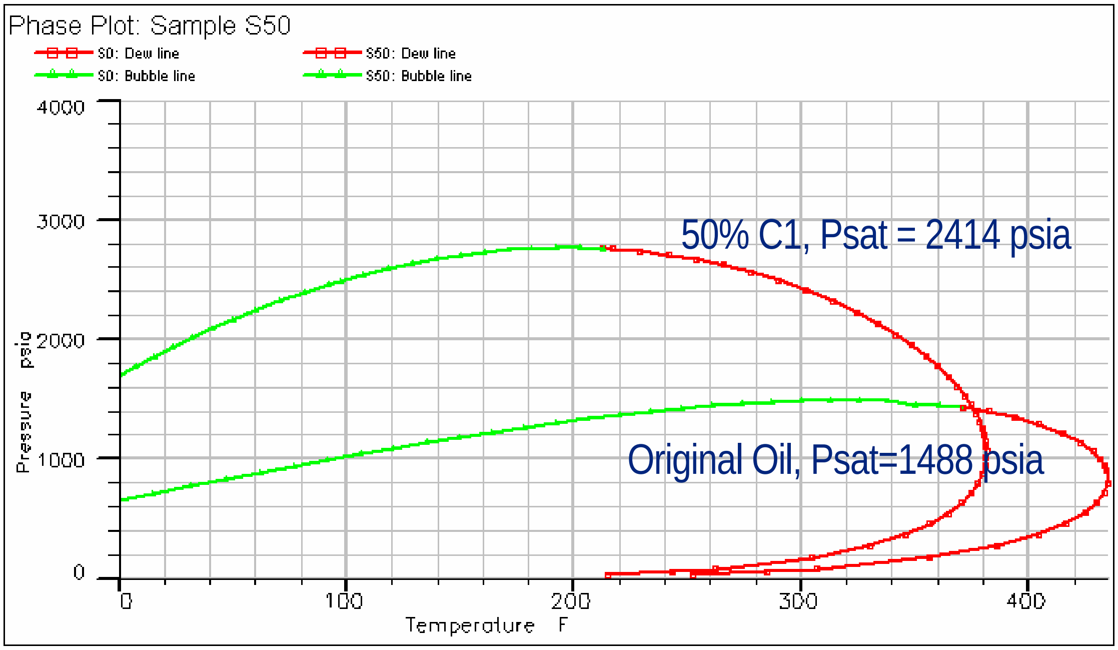
First-contact miscibility can in theory be achieved with most gases, but depends crucially on the pressure being high enough. In real life, pressures are generally too low for first-contact miscibility.

Minimum miscibility pressure

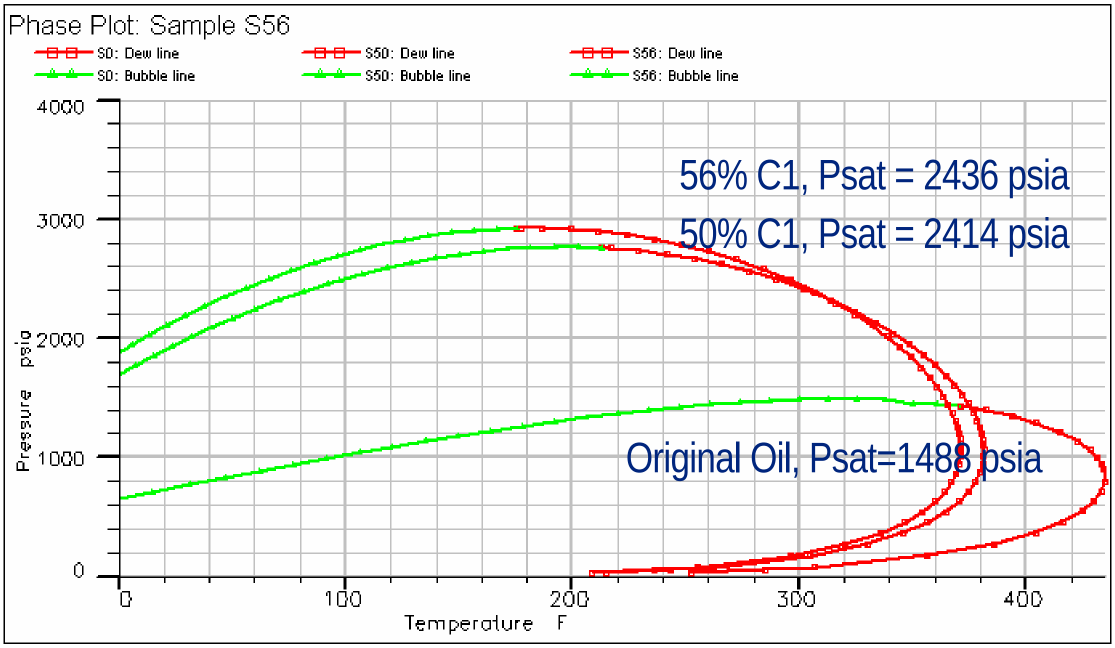
Consider an oil made up of 31% C_1, 55% iC_4 and 14% C_{10}. Let us inject methane.



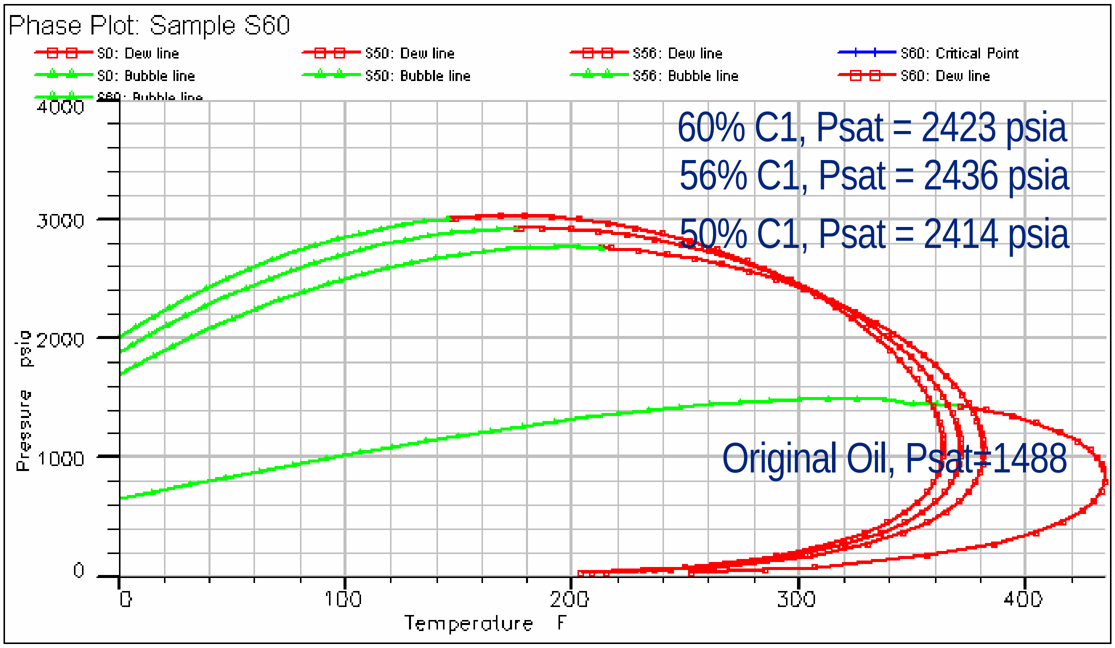
The phase diagram of the original oil is shown above. The fluid temperature is 302 F. The original saturation pressure (or bubble point) of the oil at that temperature is 1488 psia.



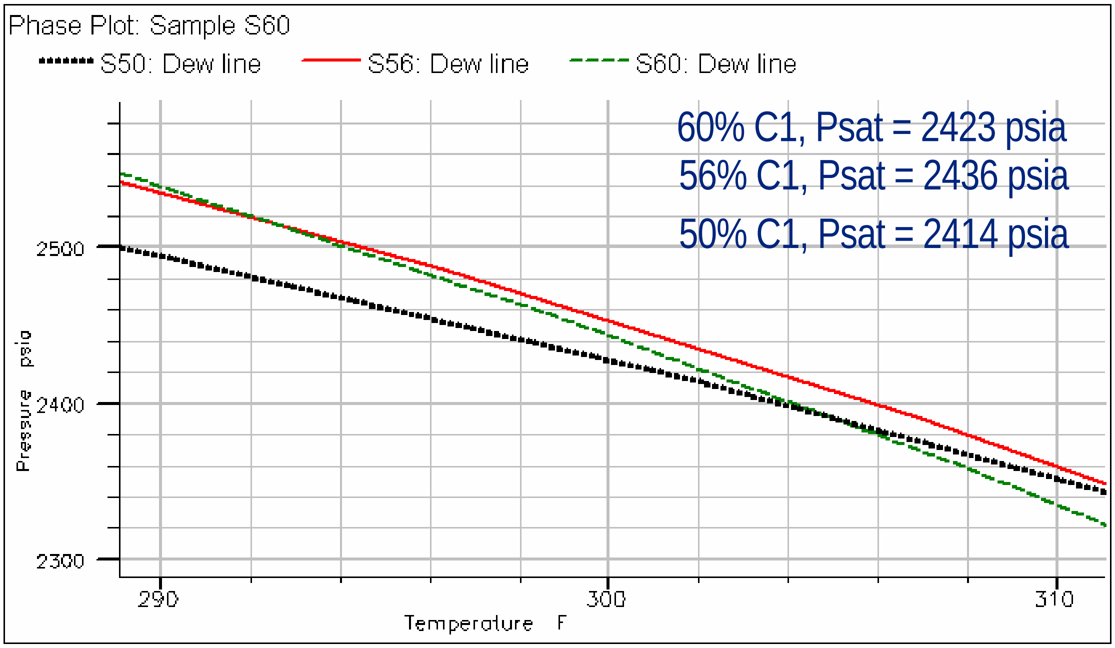
As we inject C_1 into the oil, the phase envelope changes and the saturation pressure rises. If we have injected 50% of C_1, Psat has risen to 2414 psia.



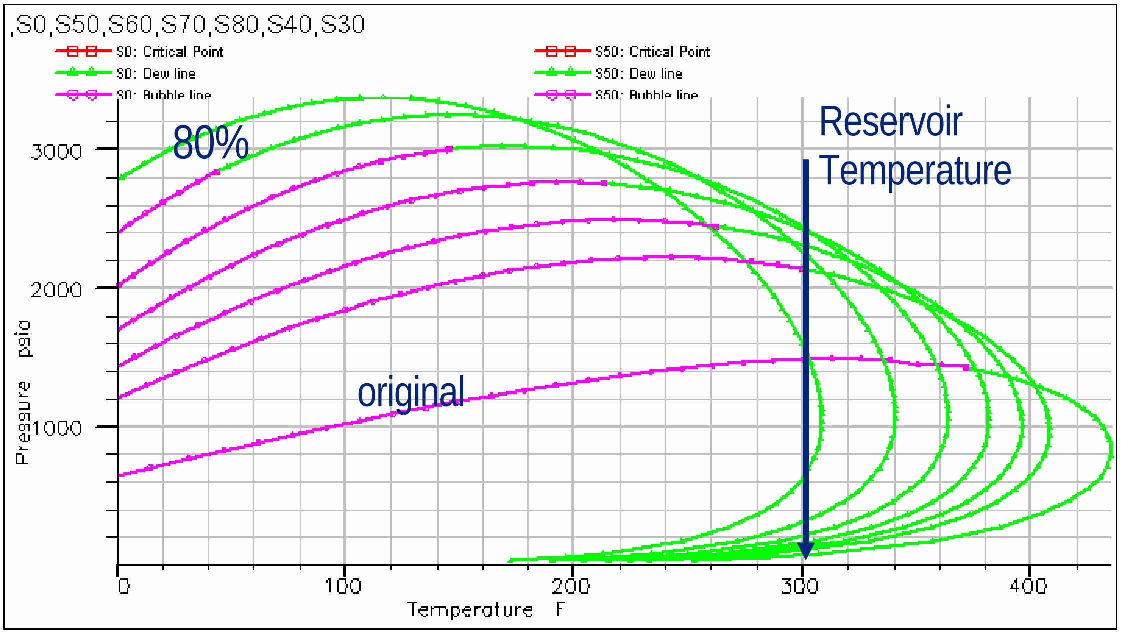
At 56% injection of C_1, Psat is 2436 psia.



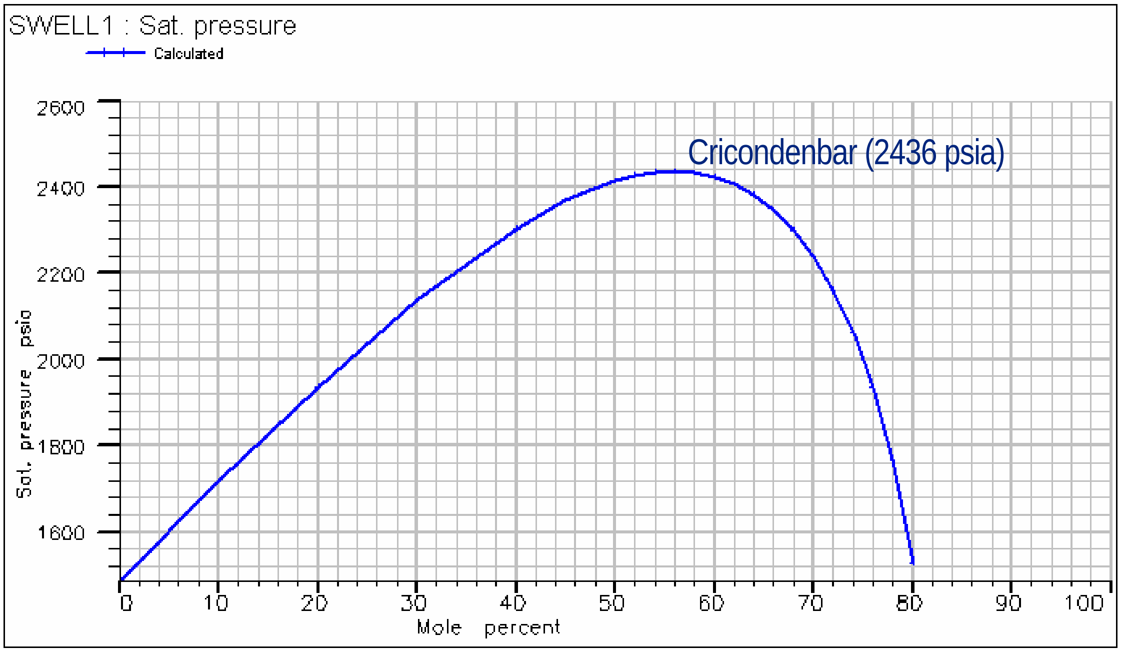
As we increase the percentage of injected C_1, Psat starts to drop. This is because we are “slipping down” the right-hand side of the dew line in the phase diagram. The picture below is a zoomed view of the dew lines at around 56% C_1 injection.



The following picture shows that at 302 F the value of Psat eventually has to decrease as the injected C1 increases. At 80% injected C1, Psat has a similar value to the Psat of the original fluid.



If we plot Psat as a function of percentage of injected C_1,

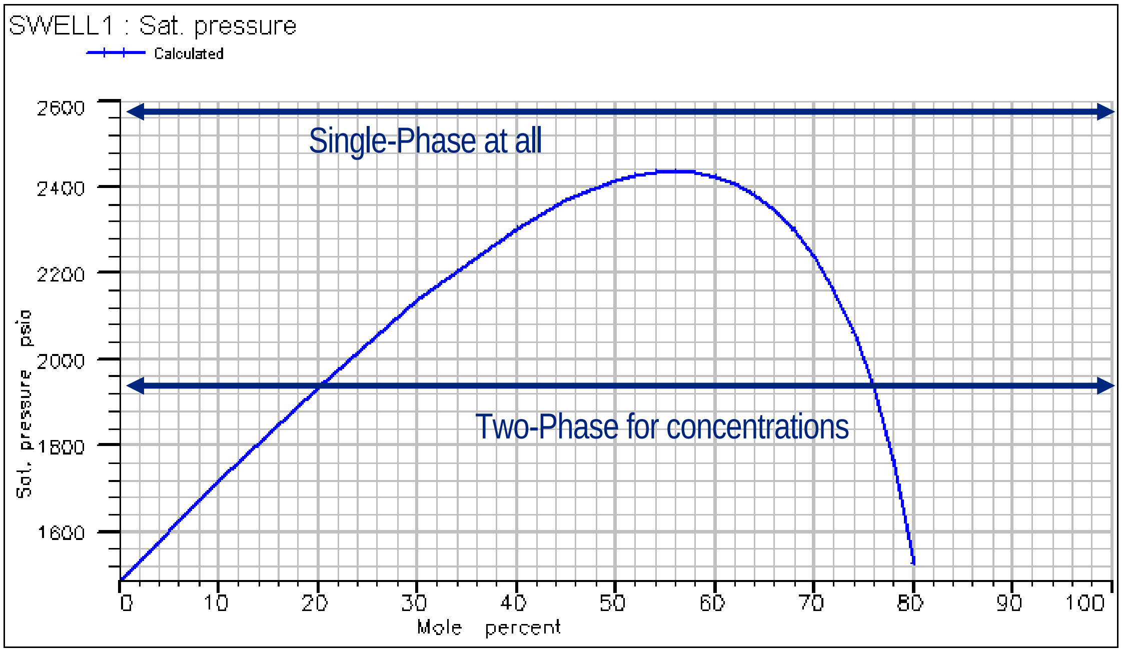


The resulting pressure-composition diagram shows that Psat starts at 1488 psia, rises to 2436 psia (the cricondenbar) then drops back. Above 80% C_1, the mixture is a dry gas with no saturation pressure.

Definition: The first contact miscibility pressure is the minimum pressure at which any mixture of the original reservoir oil and injection gas is single-phase.

We can see from the pressure-composition diagram that the minimum miscibility pressure (the FCMP) for this case is 2436 psia:

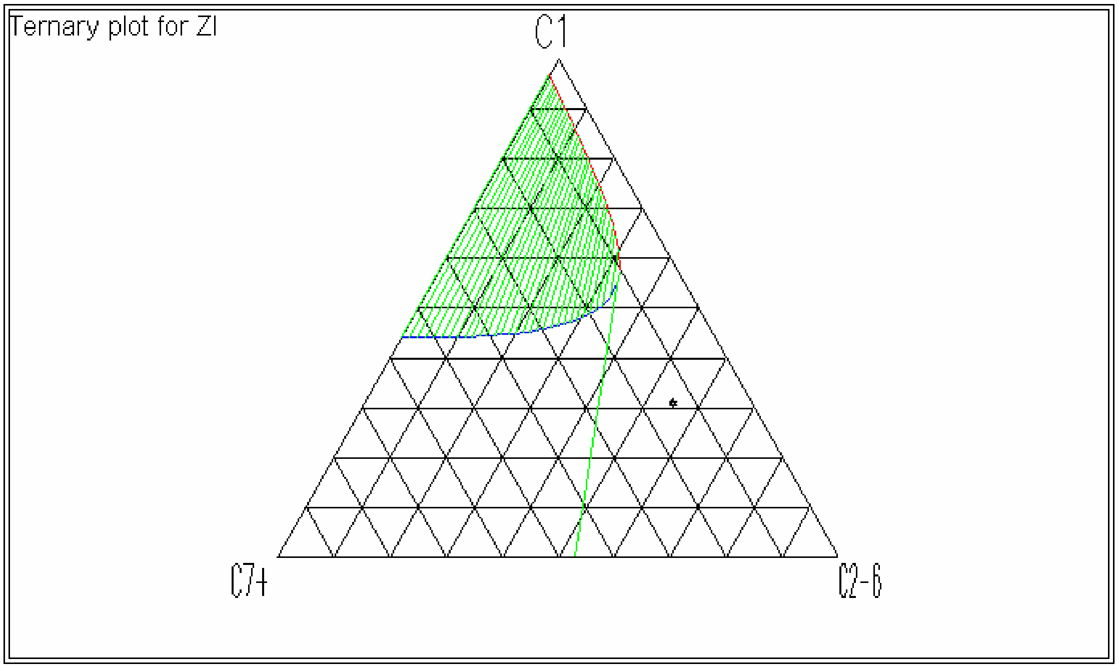
- At 2436 psia and above 2436 psia, the original oil injected with any amount of C_1 will be single phase
- Below 2436 psia, once a certain percentage of C_1 is injected, the mixture will be two-phase.



Consider for example a reservoir at an initial pressure of 2000 psia. Suppose we keep this pressure approximately constant as we inject C_1.

- The reservoir is initially more than 500 psi above the bubble point, and so is single-phase.
- As we start to inject C_1, Psat rises but the reservoir is still single-phase.
- When the oil around the injection well has 23% of injected C_1, gas and oil form two phases.
- The oil and gas two-phase region expands within the reservoir as we inject more C_1.
- Eventually at 75% injected C_1 the mixture becomes single-phase again. There is now a single phase region of enriched methane around the injection well, surrounded by a two-phase region that becomes a lighter single-phase oil, then the original single-phase reservoir oil

In terms of a ternary diagram, at the FCMP and at the reservoir temperature,



the line between the original oil composition (shown as a black dot) and the injection gas (100% C_1) is a tangent to the two-phase boundary shown in the ternary diagram. Any combination of C_1 and the original oil will lie on that line and will therefore be outside the two-phase region. At pressure above the FCMP the two-phase region will be smaller, and the line joining the oil with C_1 will be further away from the two-phase region.

For pressures below the FCMP, the two-phase region will expand and for certain oil/gas combinations we will be in the two-phase region.

Summary of FCMP

1. Pressure > MMP
2. All points between solvent and reservoir oil lie in single phase region
3. Need high concentrations of solvent - expensive

Multi-Contact Miscibility

To achieve first-contact miscibility in practice, we usually need to inject a high concentration of solvent. This is expensive. For reservoirs with an initial pressure below the FCMP, we can look at alternative processes that can also give us miscibility at a Multi-Contact Miscibility Pressure (MCMP).

Condensing Gas Drive

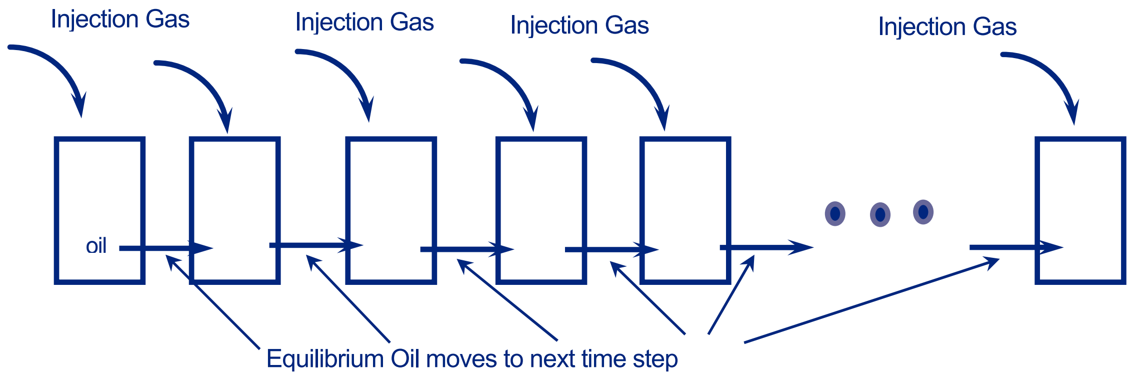
For condensing gas drive miscibility, we inject a rich gas and we look at what happens to the oil around the gas injector as more and more gas is injected into the original reservoir oil.

If our injection gas is much richer that the oil in the intermediate hydrocarbon components such as C_2, C_3, C_4 etc. then the oil will absorb some of these components from the gas and the oil will get lighter as it moves as more gas flows through it. We can say that some of the gas "condenses" into the oil. This will continue until either

1 all possible combinations of the injection gas and the lighter reservoir oil will result in a one-phase fluid. Miscibility is achieved.

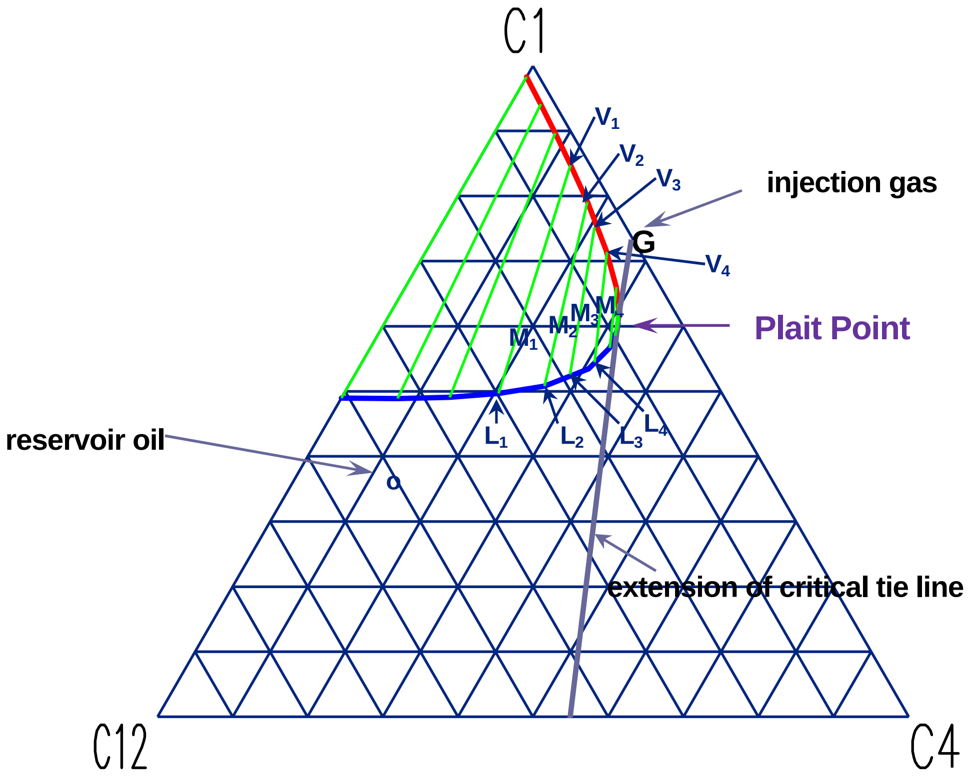
or

2 the oil lightening process will reach a steady state, and combinations of the injected gas and the lighter reservoir oil can still generate a two-phase fluid. Miscibility is not achieved.



Condensing Gas Drive

We can find out what will happen by looking at a ternary diagram:



The ternary diagram for this drive shows the original reservoir oil and an injection gas G.

- Consider an equal mixture of the original oil and the gas G. This mixture will have composition M1 and will lie in the two-phase region. It will therefore form an oil L1 and a gas V1. This oil L1 will be lighter than the original oil. The gas V1 will be more mobile than the oil, and will move away.
- The next volume of gas injected will mix with the oil L1 to form a mixture M2. M2 will split into L2 and V2. V2 will move away, leaving L2.
- The next volume of gas injected will mix with the oil L2 to form a mixture M3. M3 will split into L3 and V3. V3 will move away, leaving L3.
- Etc.

The ternary diagram shows the enrichment process moving the new equilibrium lighter oil composition toward the plait (critical) point until either:

1 Miscibility occurs when the line joining the injection gas with the lighter oil does not cross the two-phase region.

or

2 the lighter oil reaches the Plait Point and even then the line joining the injection gas with the lighter oil still crosses the two-phase region. In this case we do not get miscibility.

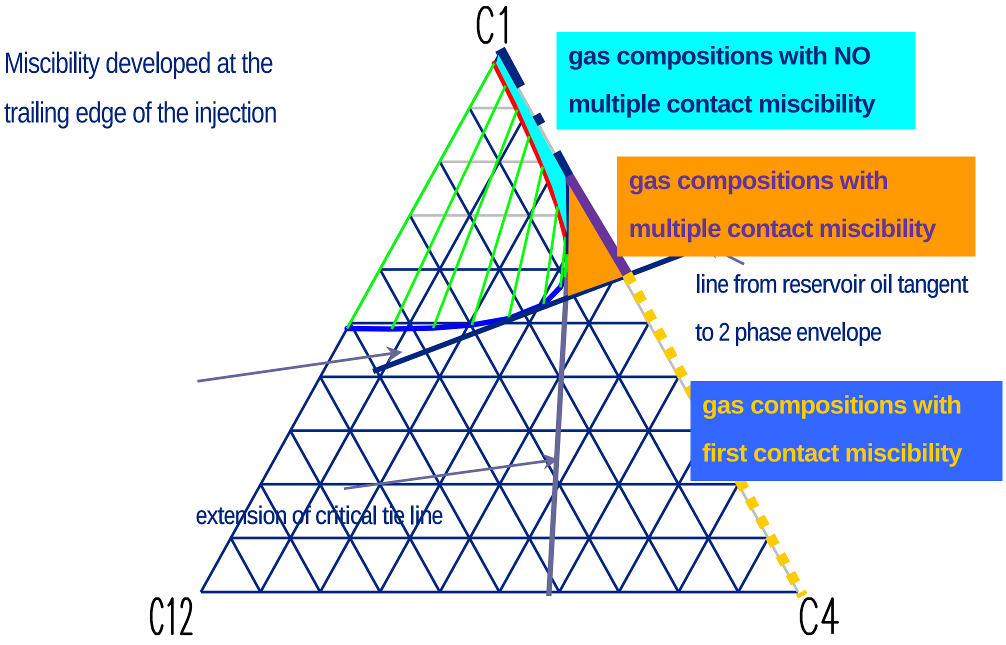
We can now see the use of the extension of the critical tie line.

Extending the critical tie line and drawing a tangent from the original reservoir oil to the two-phase region, we can define three ranges of composition for the injection gas:

1. **The injection gas composition is to the right of the tangent line from the reservoir oil:**
   A line joining the original reservoir oil to the injection gas is always in the single-phase region. We have First-Contact Miscibility.
2. **The injection gas composition is to the right of the critical tie-line extension but to the left of the tangent line from the reservoir oil:**

Transfer of intermediates from the gas to the oil continues until a line joining the equilibrium lighter oil to the injection gas is always in the single-phase region. Multi-Contact Miscibility is achieved.

3. **The injection gas composition is to the left of the critical tie-line extension:** Transfer of intermediates from the gas to the oil continues until the equilibrium oil reaches the Plait Point. At this point, injection gas contacted with this equilibrium oil would generate the same oil, the enrichment process reaches steady state, and miscibility will never be achieved.



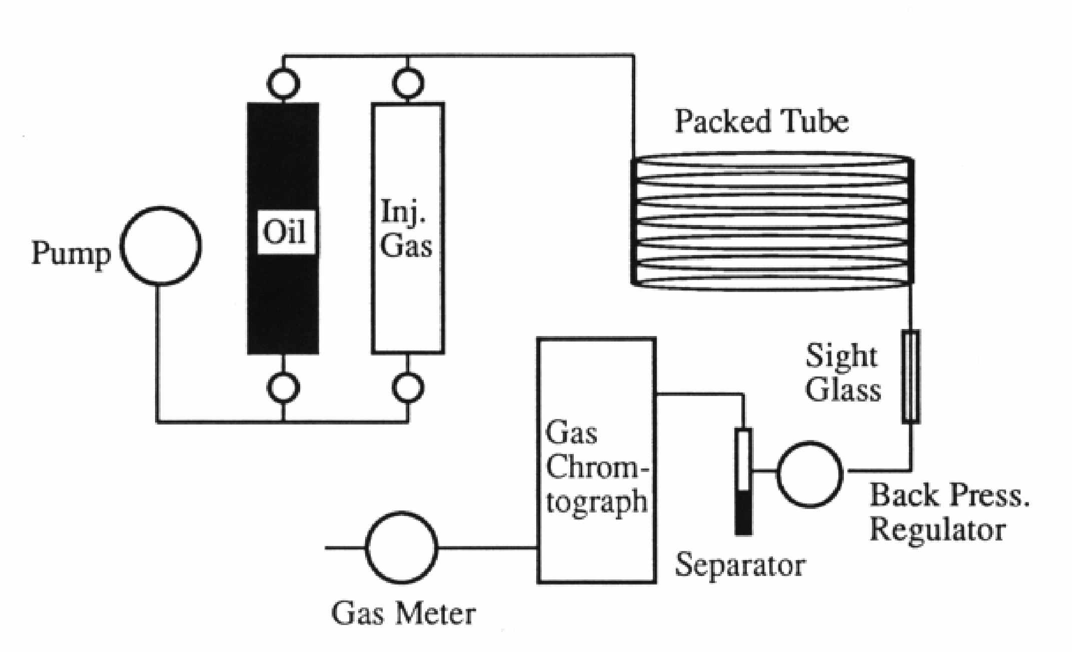
Remember that the ternary diagram is at a fixed temperature and pressure. As the pressure changes, the size and shape of the two-phase region changes, as does the position and slope of the extension of the tie-line. The ternary diagram therefore shows that a minimum pressure exists for this multiple contact miscibility process (henceforth MCMP) when the gas point lies on the critical tie-line. Pressures below this result in a steady state; pressures above this result in miscibility before the equilibrium oil reaches the plait point.

Condensing Gas Drive Summary

1 Pressure < MMP
2 Solvent and oil not miscible initially
3 Solvent components transfer to liquid oil phase
4 Repeated contact between oil and solvent moves system towards plait (critical) point (dynamic miscibility)
5 For systems with oil composition to left of tie line, solvent composition must lie to right
6 Field behavior is more complicated
7 continuous, not batch, contact
8 both phases flow
9 actual phase behavior more complicated, especially near plait point

Slim Tube experiments

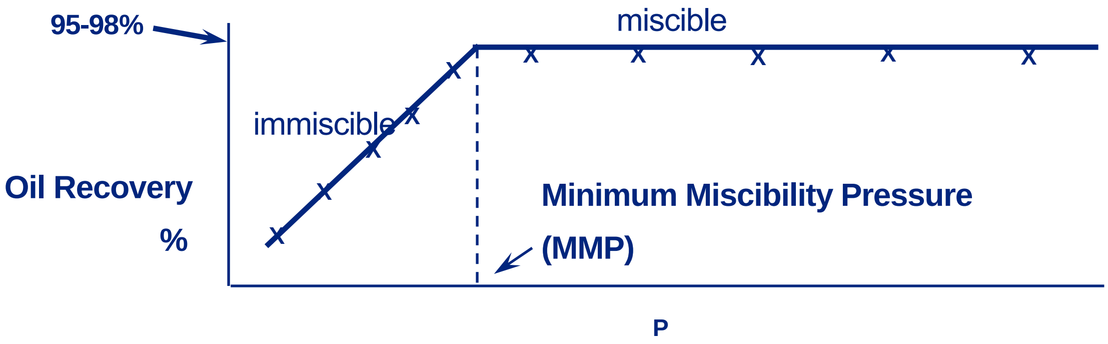
Laboratory experiments are carried out to calculate the MCMP. A slim-tube experiment is conducted by injected rich gas of a fixed composition into oil, at a number of different pressures.



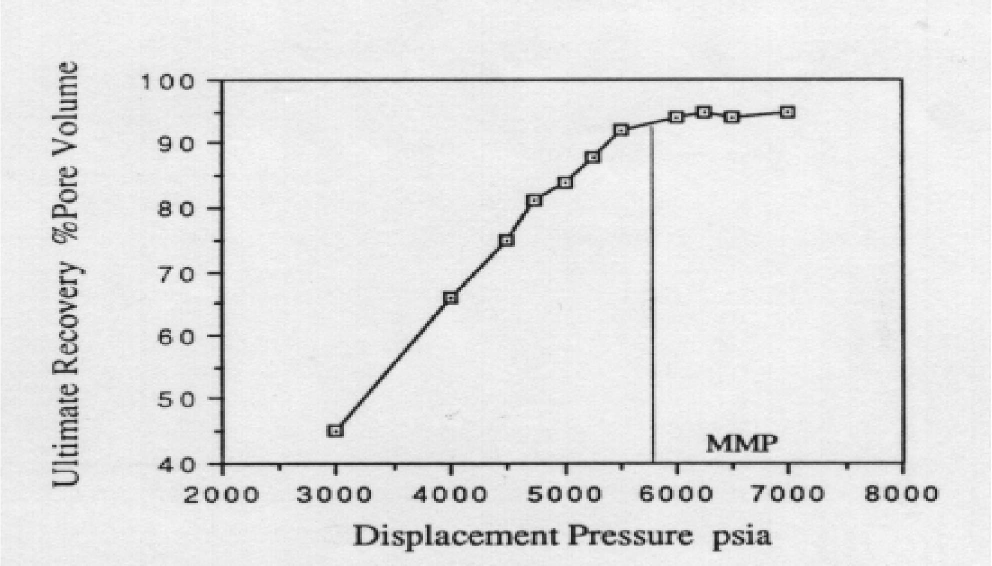
DBR (Edmonton) Slim Tube apparatus

The oil recovery is plotted as a function of pressure. At some pressure the injected gas is to the right of the limiting tie line and MCM develops.

What happens in the simulation when miscibility is achieved?

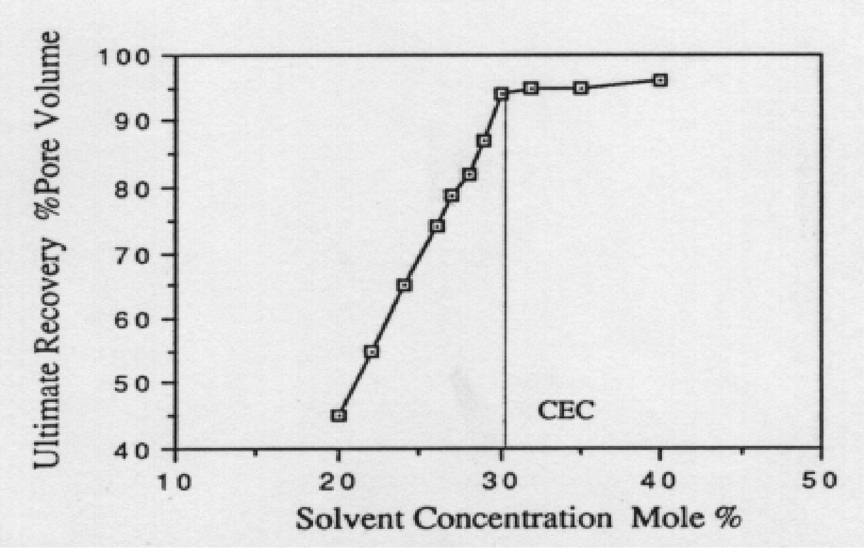


As the pressure is increased, the two-phase region becomes smaller until we reach the miscibility pressure. At that pressure the oil recovery will be a maximum as the oil and gas will form a single phase throughout the slim tube, and residual oil will drop to zero (or close to zero). The pressure at which the maximum recovery is first reached is the MCMP.



In a real laboratory experiment, the uncertainties in the measurements make it harder to determine the actual MCMP with great accuracy.

In a similar slim-tube experiment, the PVT laboratory can measure the minimum enrichment needed to achieve multi-contact miscibility at a given pressure.



This time the pressure is kept constant and a series of experiments are run, each with increasing solvent concentration. The concentration at which the oil recovery slope flattens-out is the minimum solvent concentration needed to achieve multi-contact miscibility.

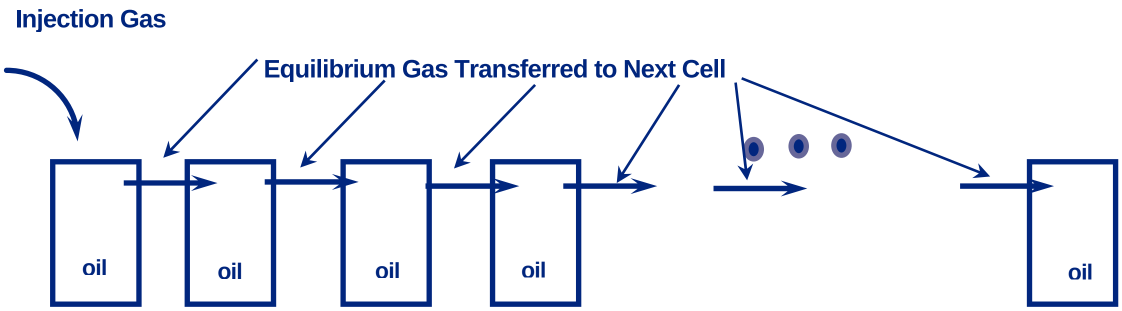
Vapourising Gas Drive

For vapourising gas drive miscibility, we inject a lean gas such as C1, CO2 or Nitrogen. We look at what happens to the gas front as it moves into the reservoir and is continually in contact with the original reservoir oil. If our injection gas is lacking in the intermediate hydrocarbon components such as C_2, C_3, C_4 etc. then the gas will pick up these components from the oil and get richer as it moves through the reservoir. We can say that the oil "vapourises" into the gas. As the gas travels over more and more oil, getting richer and richer in intermediates, until either

- all possible combinations of the enriched gas and the original reservoir oil will result in a one-phase fluid. Miscibility is achieved.

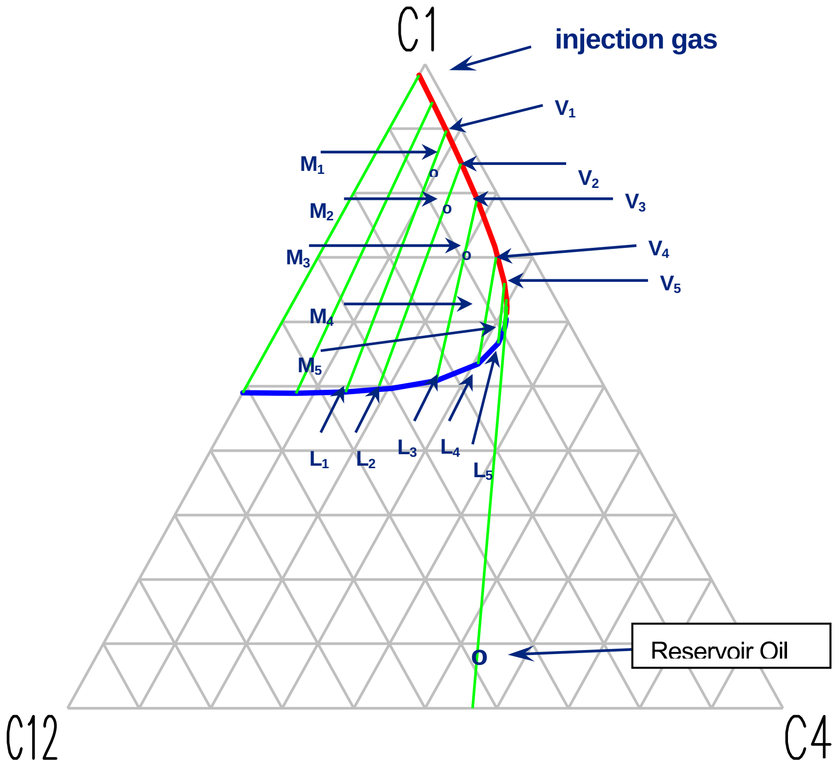
or

- the gas enrichment process will reach a steady state, and combinations of the enriched gas and the original reservoir oil can generate a two-phase fluid. Miscibility is not achieved.



Vaporizing Gas

We can find out what will happen by looking at a ternary diagram:



The ternary diagram for this drive shows the original reservoir oil and an injection gas C1. Consider a mixture of the original oil and the gas C1. This mixture will have composition M1 and will lie in the two-phase region. It will therefore form an oil L1 and a gas V1. This gas V1 will be at the leading edge of the gas front, and will meet more of the original reservoir oil, to form a mixture M2.

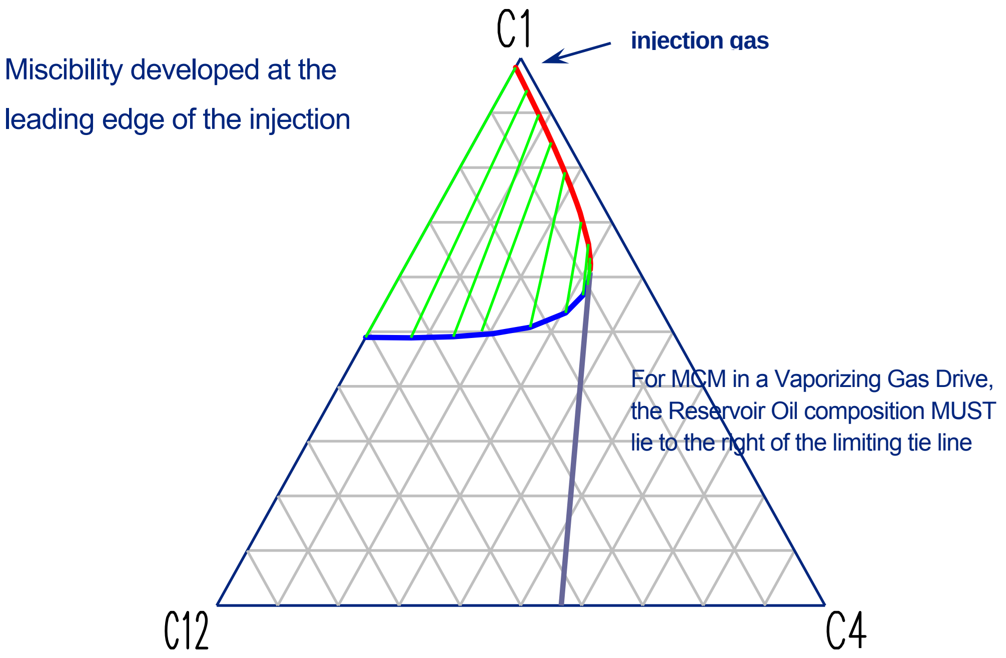
The ternary diagram shows the enrichment process moving the new equilibrium gas compositions toward the plait (critical) point until either:

- Miscibility occurs when the line joining the enriched gas with the original oil does not cross the two-phase region.

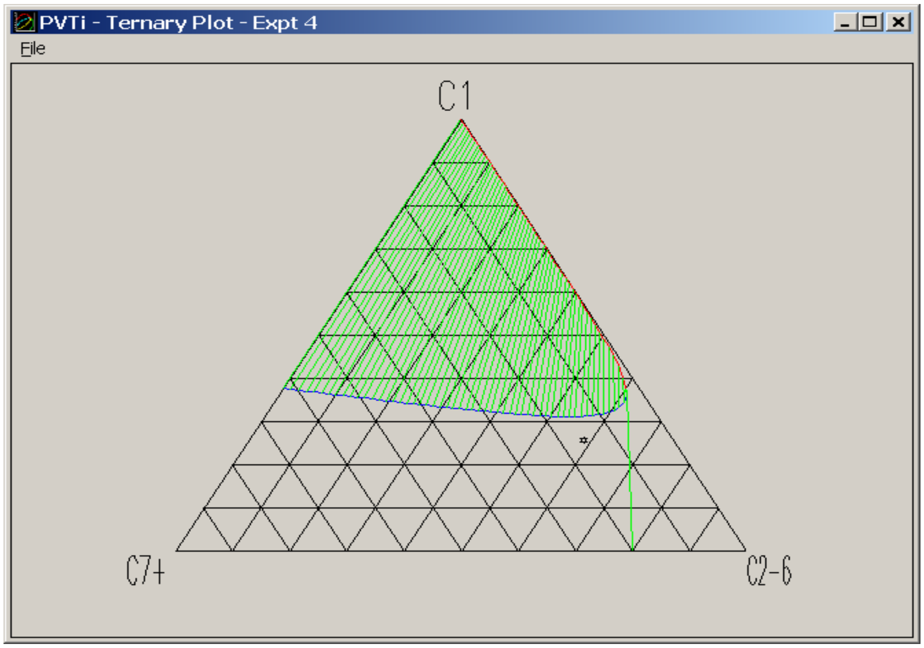
or

- the enriched gas reaches the Plait Point and even then line joining the enriched gas with the original oil still crosses the two-phase region. In this case we do not get miscibility.

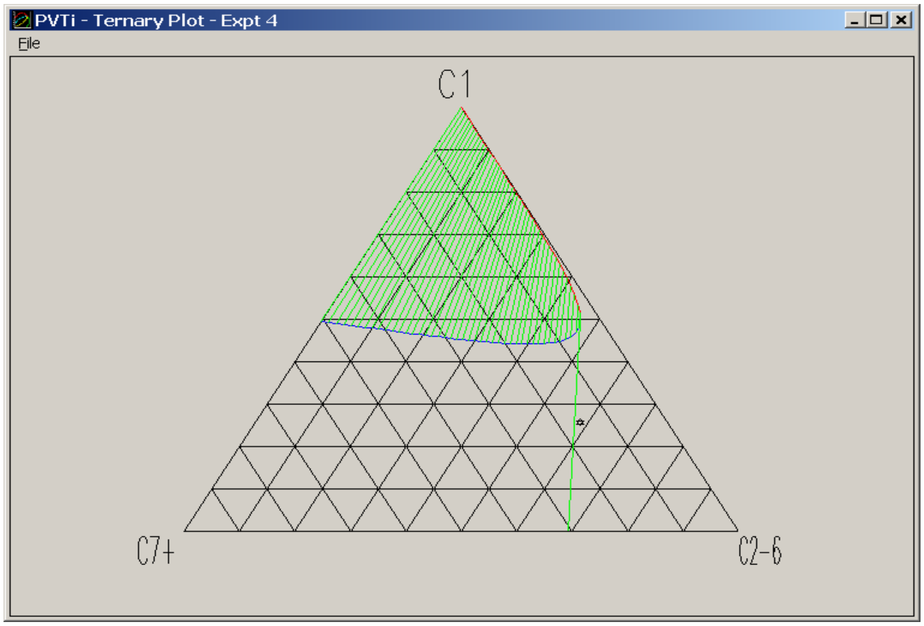
Again we can see the use of the extension of the critical tie line. For MCM in a Vaporizing Gas Drive, the Reservoir Oil composition must lie to the right of the limiting tie line.



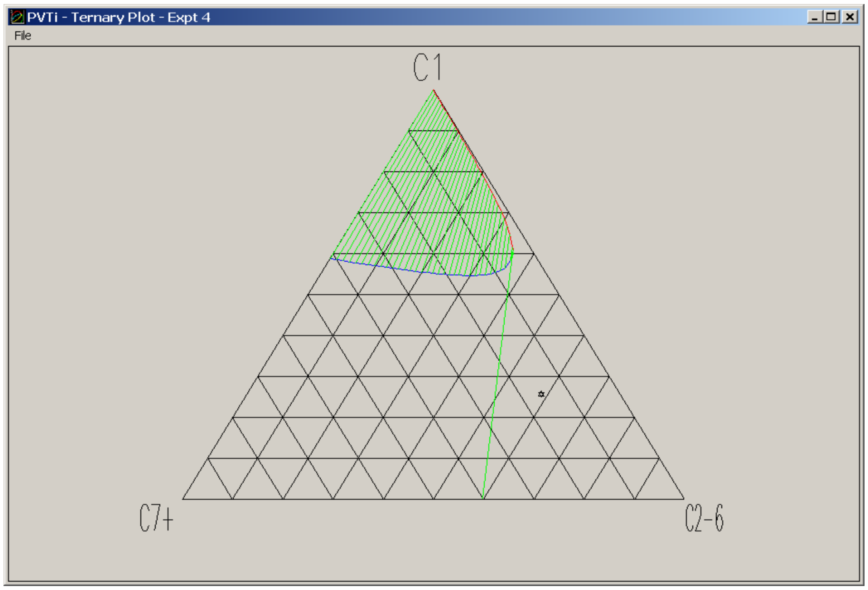
The ternary diagram reveals that a minimum pressure exists for the multiple contact miscibility process (the MCMP) when the oil point lies on the critical tie-line.



Below this pressure, the oil lies to the left of this line, and the enrichment reaches a steady state before miscibility is achieved.



At this pressure, miscibility is just achieved, as the equilibrium gas reaches the plait point.



Above this pressure, miscibility is achieved before the equilibrium gas reached the plait point.

To experimentally determine the MMP for given [oil, injection gas] combination in a slim tube, the process and results are similar to the condensing gas drive discussion

Note that the FCMP forms an upper bound for the MCMP and the larger of the original oil or gas saturation pressures forms a lower bound for the MCMP.

Exercise 6 Simple fluid MCMP

Consider the oil sample that we looked at earlier, made up of 31% C1, 55% iC4 and 14% C10. The reservoir temperature is 302F and Psat = 1488 psia. We know that the FCMP is 2436 psia.

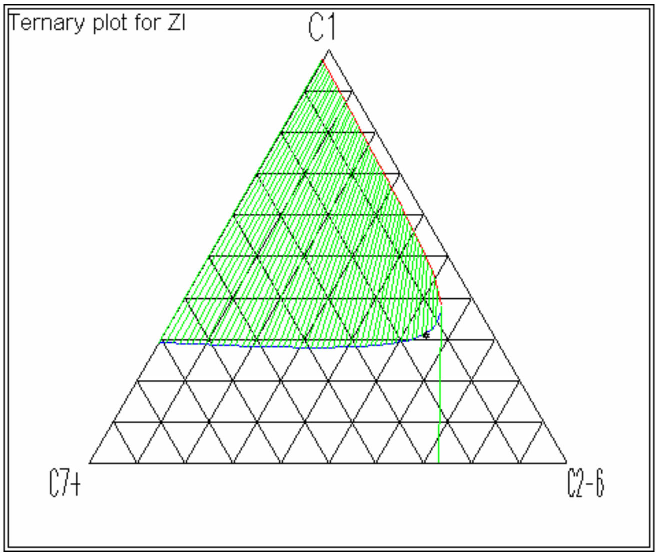
What is the MCMP if we inject C1? We know that the MCMP must be larger than the original Psat of 1488 psia, otherwise we would already be in the two-phase region[21].

---

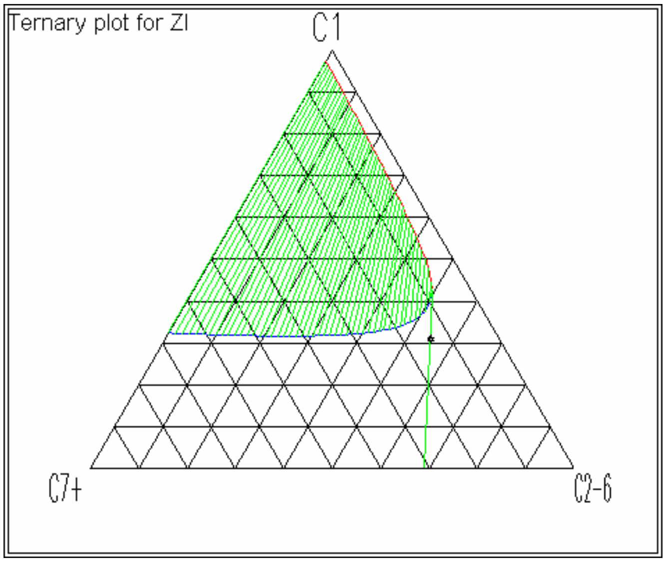
[21] The FCMP forms an upper bound for the MCMP and the larger of the original oil or gas saturation pressures forms a lower bound for the MCMP.

Plot the ternary at 1500 psia, 1687 psia and 2000 psia.

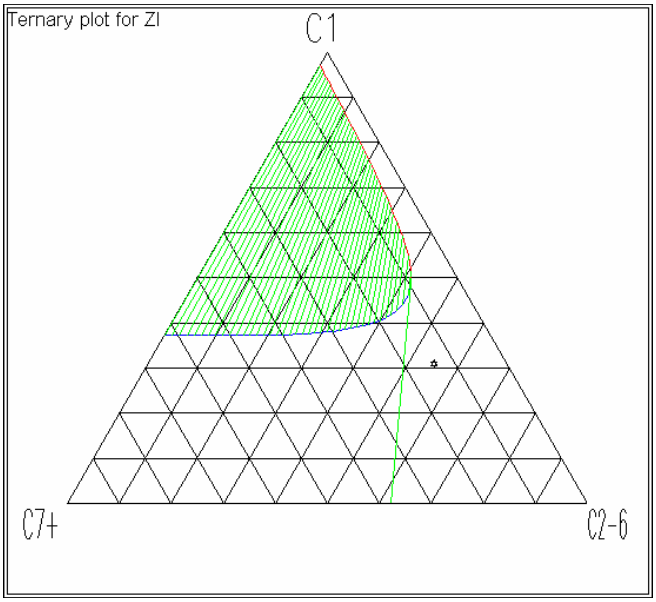
A ternary plot at 1500 psia confirms that the original reservoir fluid is single-phase. The extension of the tie line is to the right of the fluid composition so we are below the MCMP and we will never achieve miscibility. Note also that the pressure is close to Psat.



At 1687 psia, the fluid composition is on the extension of the tie-line. This is the MCMP.



At 2000 psia the extension of the tie-line has moved to the right of the fluid composition. We are in the multi-contact miscibility region, but have not yet achieved first-contact miscibility at FCMP=2436 psia.



To experimentally determine the MMP for given [oil, injection gas] combination in a slim tube, the process and results are similar to the condensing gas drive discussion.

Some questions:

1. Where does the miscibility occur? **Leading Edge or trailing edge?**
2. Which recovers most reservoir oil? **Why is not used more often?**

Condensing drive MCMP occurs at the trailing edge of the injected gas and recovers more oil since all the oil from the injector to the producer is recovered if miscibility is achieved. It is not however commonly used as there is a risk of losing the expensive hydrocarbon being injected.

Vapourising drive MCMP occurs at the leading edge of the injected gas and recovers less oil since only the oil from the miscible point to the producer is recovered if miscibility is achieved. It is however commonly used as low-cost gas is injected.

Condensing/Vapourising Drive

1 Vaporizing gas drive not strictly valid for real reservoir fluids

2 Injection gas does not generally contain middle heavy fractions which are present in the oil

3 More realistic process is called Condensing/Vaporizing Gas Drive since contains some of both processes

The processes that occur in a reservoir cannot be represented as either a vapourising process only or a condensing process only. Both are probably happening at the same time.

- Injection gas enriches the oil in the light intermediate range
- Also, it strips the heavier fractions
- Thus, reservoir in contact with fresh gas initially becomes lighter, but as it contacts more gas and loses the middle intermediates and lighter heavies, it tends to get heavier.
- This heavier oil becomes LESS miscible with the injection gas

The bubble point and the dew point curves on the pseudo-ternary diagram initially converge and then diverge. This is illustrated in papers Aaron Zick and Fred Stalkup (SPE15493, SPE16715,SPE18060) :

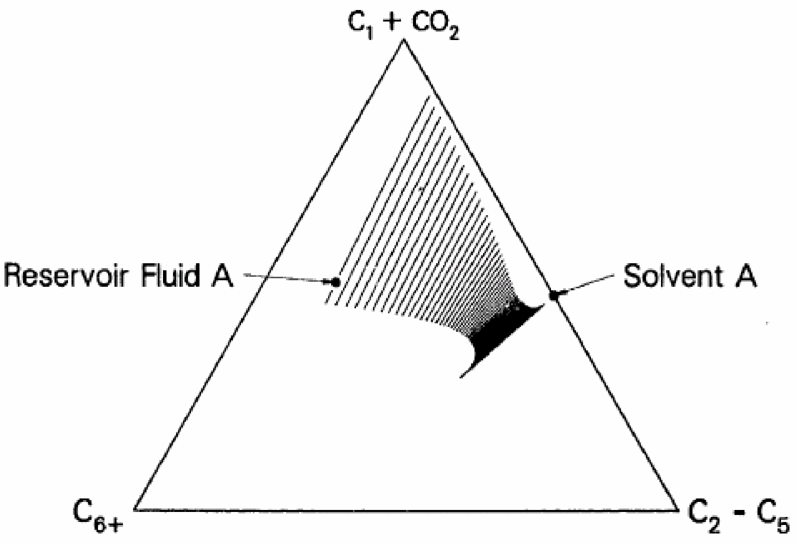
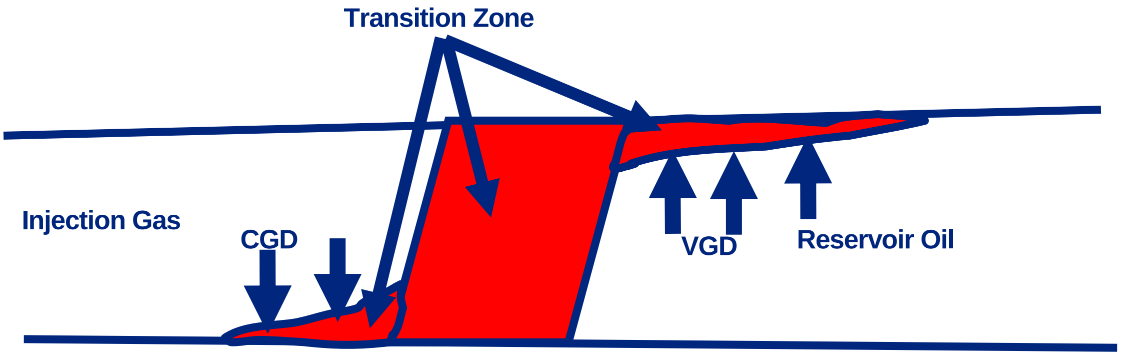


Fig. 13--Pseudoternary representation of a simulated multicontact experiment with reservoir Fluid A, 900 psi above apparent MMP.

In this Condensing/Vaporizing Gas Drive, forward moving gas (like a vaporizing gas drive) becomes richer in the middle intermediates and heavier fractions. At the same time it looses the light intermediates (like a condensing gas drive). As always, the forward moving gas becomes more similar to the reservoir oil



Miscibility (or near miscibility) is achieved within a transition zone

Front of transition zone = Vaporizing Gas Drive (VGD)

Tail of transition zone = Condensing Gas Drive (CGD)

Exercise 7 Oil MCMP

Investigate the properties of the following fluid

	Name	Mole fraction
6 components -	CO2	0.01
	N2	0.01
	C1	0.10
	C3	0.10
	C10	0.30
	C15	0.48

PR EoS

Look at the phase plot and the ternary diagram.
Determine the MCMP at the slimtube temperature with
CO_2,
Methane
Solvent (60% C1, 40% C3)
N_2

$T_{slimtube} = 38\ ^0C$
Record the results for future use.

Exercise 8 Condensate MCMP

Investigate the properties of the Condensate:

	Name	Mole fraction
6 components -	CO2	0.01
	N2	0.01
	C1	0.75
	C3	0.17
	C10	0.04
	C15	0.02

PR EOS

Field Units

$T_{RES} = 180^0$ F

Plot: Dew Pt., Ternary Diagram, any other experiments.

Run swelling experiments with N_2 and Methane to determine the effect of the injected gas on the dew point pressure. Plot the Dew Point pressure of mixtures of the condensate with increasing mole fractions of N_2 and C_1.

Record the results for future use.

Summary: Miscibility

1. If oil and gas separate into two phases then the displacement is called immiscible
2. If all possible mixtures of oil and gas are single-phase then the displacement is miscible
3. There are two kinds of miscibility: First contact (FCMP) and multi-contact (MCMP)
4. FCMP is the lowest pressure at which samples will always be single-phase in all proportions
5. MCMP is the lowest pressure at which samples will become single-phase after multiple contacts.

14. Flash calculations

In this section we will describe the flash calculations that are used by PVT packages and compositional reservoir simulators. We will demonstrate the calculations using an example with a small number of components.

- **Most EoS calculations are based on the flash**
- **The same flash library is used in both PVTi and ECLIPSE 300**

The flash calculations are used to either:

- **determine number of phases present and their split, or**
- **iterate in P or T to find P_{sat} or T_{sat}**

- **Most of the CPU time in ECLIPSE 300 can be spent on the flash calculations.**

Flash Introduction

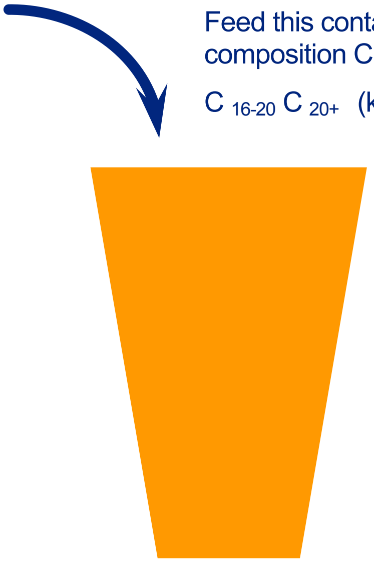
When we talk about a "flash", we usually mean calculating the number of phases present and their compositions. Consider a hydrocarbon fluid made up of known or grouped components, for instance a certain percentage of CO_2, N_2 , C_1, C_{2-3} , C_{4-6}, C_{7-10}, C_{11-15}, C_{16-20} and C_{20+}. Place this mixture in a container such as a PVT cell, a grid block, or any other volume. Fix both the temperature and the pressure within the container. Allow enough time to reach equilibrium. We know the total composition $\{z_i\}$ of the hydrocarbon mixture. We know the pressure P and the temperature T of the mixture.

What we want to know is whether there are one or two hydrocarbon phases present[22] and what the properties of the phases are:

---

[22] A mixture of hydrocarbons can form more than two phases. For simplicity we shall ignore that possibility in this discussion.

- If the mixture forms a single phase, then its composition is known and its properties can be calculated[23].
- If the mixture forms two hydrocarbon phases then we need to first calculate how much is liquid and vapour (the mole fractions L and V[24]). We then calculate the relative concentration of moles in each phase (the K-values $\{K_i\}$). From these we can work out the compositions of each phase $\{x_i\}$ and $\{y_i\}$ and from the compositions we work out the properties of each phase.



Feed this container with N moles of fluid - composition CO_2 N_2 C_1 $C_{2\text{-}3}$ $C_{4\text{-}6}$ $C_{7\text{-}10}$ $C_{11\text{-}15}$ $C_{16\text{-}20}$ C_{20+} (know Z_i mole fraction feed)

Flash: Determine amount and composition of the vapor and liquid at EQUILIBRIUM

Temperature and Pressure Set

The same flash calculations can be used to work out the bubble point Pbub or dew point Pdew of a mixture, or more generally the saturation pressure P_{sat}. In this case we know total composition $\{z_i\}$ of the hydrocarbon mixture and the temperature T of the mixture. By

---

[23] Note that we don't need to know whether this single phase is an oil or a gas. We know its composition so we can calculate it's properties.

[24] BEWARE of Notation

V = Mole fraction in Vapor

This is NOT the volume V that appears in PV=RT

z_i is mole fraction of component i in sample

. Z is compressibility form PV=ZRT

definition, we also know that at the saturation pressure is the lowest pressure at which either (L=1 and V=0) or (L=0 and V=1). We can then solve for the K-values $\{K_i\}$) and the pressure $P=P_{\mathbf{sat}}$.

Flash Equations

Consider one mole of a fluid of composition z_1, z_2... z_N that splits at some pressure and temperature (P, T) into L moles of liquid of composition x_1, x_2... x_N and V moles of vapor composition y_1, y_2... y_N.

We have the following constraints:

$$L+V=1$$

$$Lx_i+Vy_i=z_i$$

$$\sum_{i=1}^{N} x_i = \sum_{i=1}^{N} y_i = \sum_{i=1}^{N} z_i = 1$$

Substituting for L gives

$$(1-V)x_i+Vy_i=z_i$$

Define the K-value of the i^{th} component to be

$$K_i=\frac{y_i}{x_i}$$

then we can rewrite

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

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

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

is known as the Rachford-Rice equation.

K-values

Generally, we know the total mole composition $\{z_i\}$ and either the pressure and temperature or the temperature and the vapor mole fraction, i.e., V=0 at a bubble point or V=1 at a dew point[25]. This leaves as unknowns the N K-values $\{K_i\}$ and either the vapor mole fraction V or the (saturation) pressure P.

To solve the Rachford-Rice equation, we first need an estimate for the K-values.

Before the coming of powerful computer systems, the only practical way of performing compositional calculations was to assume constant K-values. Later more sophisticated models assumed that the K-value was only a function of pressure and compositional simulators would read in tables of K-values at different pressures[26]. Modern calculations start with an estimate of the K-value and refine it during the solution of the Rachford-Rice equation.

For the specified pressure, temperature and composition (P, T, $\{z_i\}$) a stability test (due to Michelsen[27]) is done to determine whether this is a one- or two-phase system. If two phases exist, then we start with an estimate for the K-values. At thermodynamic equilibrium, the component fugacities in the liquid and vapor phases must be equal, i.e. $f_i^L = f_i^V$

The equal fugacity condition can be written in terms of fugacity coefficients as:

$$Px_i\phi_i^L = Py_i\phi_i^V$$

---

[25] Strictly $V=\in$ as $\in\to 0$ at a bubble point or $V=1-\in$ as $\in\to 0$ at a dew point.

[26] ECLIPSE Compositional will accept K-value tables, but their use is not recommended except for thermal simulation.

[27] Michelsen's stability test involves calculating the minimum of the Gibbs free energy

or

$$\frac{y_i}{x_i} = K_i = \frac{\phi_i^L}{\phi_i^V}$$

Taking logs and writing in residual form:

$$R_i = \ln(K_i) + \ln(\phi_i^V) - \ln(\phi_i^L) \;\; (i = 1,2,\ldots,N)$$

The other equation is the Rachford-Rice equation. These N+1 equations are solved by Newton's method for the vapor fraction V and the N K-values, $\{K_i\}$.

Solutions near the critical point

Solving these equations close to the critical point is made more difficult because as we approach the critical point the gas and liquid compositions become very similar, so y_i becomes close to x_i, and K_i -> 1. Every term in the equation

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

can then become zero unless care is taken in the solution method.

Bubble and Dew point calculations

Saturation pressure calculations consist of performing a set of flash calculations, starting at a high pressure[28], say 500 bars, and dropping in pressure steps of say 25 bars, until a two phase system is found.

The K-values are found from the N equal fugacity equations, and the saturation pressure is found from the modified constraint equation for the bubble point (V=0).

$$R_{N+1} = \sum_{i=1}^{N} z_i(K_i - 1)$$

and for the dew point (V=1),

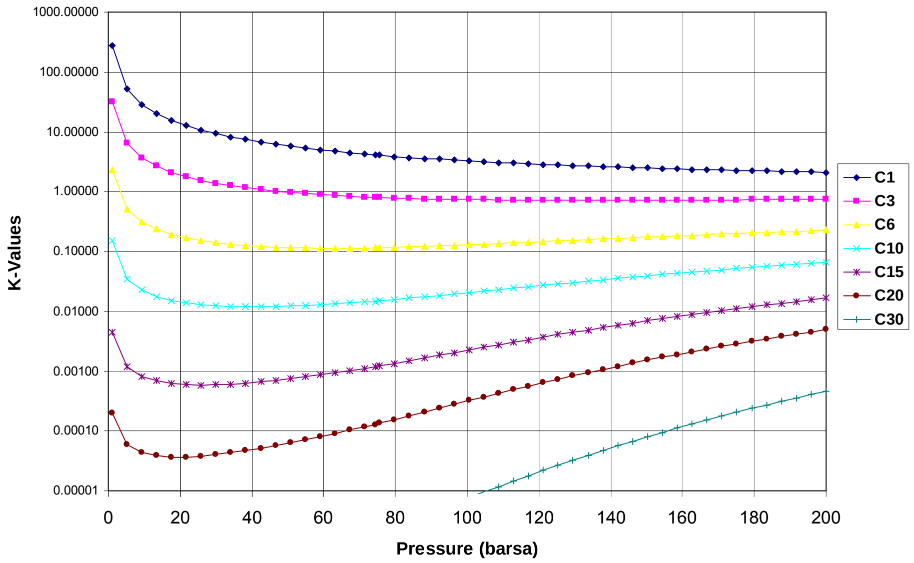
---

[28] For bubble point and retrograde dew point. For normal dew point, start low and step up in pressure.

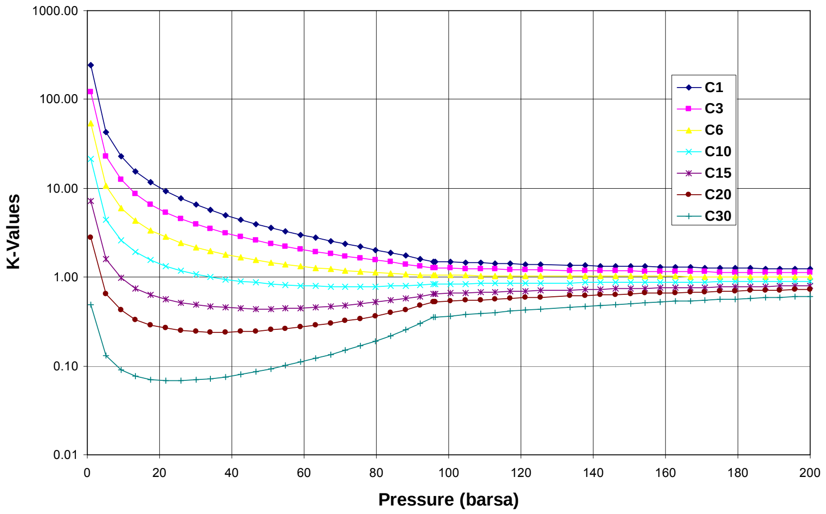
$$R_{N+1} = \sum_{i=1}^{N} z_i \left(1 - \frac{1}{K_i}\right)$$

K-values as a function of P, T

The following are some examples of K-values as a function of pressure at two different temperatures.



PR Calculated K-Values at 100° C



Note that K-values tend to get closer to 1 as pressure increases, but only at high pressures. They also tend to get closer to 1 as temperature increases. A K-value of 1 means that the concentration of that component is the same in both the liquid and the vapour phase.

Solving the Rachford-Rice equation

- In the flash calculation: we know the feed mole fractions zi and we have an estimate of the component K-Values Ki
- We do not know the molar fraction of vapour V.
- This can be found from solving the FLASH Equation usually referred to as Rachford-Rice equation:

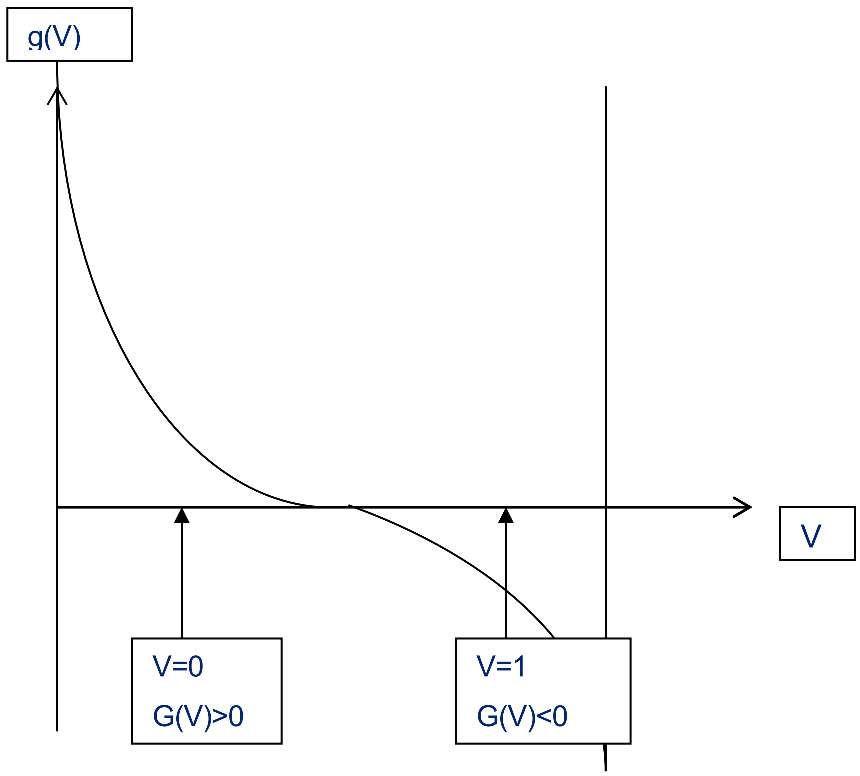
$$g(V) = \sum_{i=1}^{nc} \frac{z_i (K_i - 1)}{1 + V(K_i - 1)} = 0$$

- The root(s) of this equation will give the value of V for the hydrocarbon mixture.
- *g(V)* is a monotonically decreasing function of *V* and has the following asymptotes, where each K value gives an asymptote:

  V = 1/(1-Ki) i = 1,2,3,…nc

- If Kl is the largest K-value and Ks is the smallest K-value, then a necessary but not sufficient condition for the existence of a root between 0 and 1 is that of 0 and 1 be included in the interval

$$\left[\frac{1}{1 - K_l}, \frac{1}{1 - K_s} \right]$$



- The solution has 3 possible cases:

Case 1: $g(0) \geq 0, g(1) \leq 0$	**Root in (0,1)**	**2 phases**
Case 2: $g(0) < 0$	**Root < 0**	**1 phase**
Case 3: $g(1) > 0$	**Root > 1**	**1 phase**

If we have a single phase, then the problem is solved. We know the composition of the single phase and therefore we can calculate all the physical properties that we need. Note that, for a single-phase case, the K-value has no physical meaning, as there is no second phase and therefore there is no ratio y_i/x_i.

If we have two phases, we have to solve the Rachford-Rice equation. We know the temperature and pressure and the initial composition of the fluid. We have an estimate of the K values, usually from the previous flash results but otherwise from Wilson's formula. We can therefore solve the one equation in one unknown, V. For N components, the equation is an $(N-1)^{th}$ order polynomial and is solved iteratively.

Once V is found, then using our same estimates for the K-values we can calculate the composition of the oil phase and of the gas phase. Once we have the compositions of each phase, we can calculate their fugacities using our chosen equation of state. The Peng Robinson EoS gives a fugacity of

$$\ln\frac{f_i}{y_i p_i} = \ln \varphi_i = \frac{B_i}{B}\left(Z - B\right) - \frac{A}{2\sqrt{2}B}\ln\left[\frac{Z + \left(1+\sqrt{2}\right)B}{Z - \left(1-\sqrt{2}\right)B}\right]$$

At equilibrium, the fugacities of the liquid and vapour phases have to be the same

$$f_i^L = f_i^V \quad i = 1,2,3....n_c$$

The actual test is that the ratio of fugacities must be close to unity:

$$\sum_{i=1}^{n_c} \left(\frac{f_{iL}}{f_{iV}} - 1\right)^2 < \varepsilon$$

with

$$\varepsilon \sim 10^{-12}$$

If the ratio of fugacities is not close to 1, then the Rachford-Rice equation has to be solved with new estimates of K_i. The new estimates are the old values times the ratio of fugacities:

$$K_i^{NEW} = K_i^{OLD} \bullet \left[\frac{f_{iL}}{f_{iV}}\right]$$

We then recalculate V from g(V)=0. We use successive substitution until the ratio f_{iL}/f_{iV} is close enough to1 in which case we have equilibrium and an acceptable value for V.

Flash example problem

Consider a fluid made up of only three components, C_1, C3 and C_{10}.

The composition of the fluid is

$Z_1 = 0.8$ so we have 80% C_1
$Z_2 = 0.1$ so we have 10% C_3
$Z_3 = 0.1$ so we have 10% C_{10}

We have a good estimate of the K-values. Assume these values are correct:

$K_1 = 11$ the concentration of C_1 in the gas is 10 times that in the oil
$K_2 = 1$ the concentration of C_3 in the gas is equal to that in the oil
$K_3 = 0.1$ the concentration of C_{10} in the gas is 1/10 times that in oil

Substitute those values in the Rachford-Rice equation:

$$g(V) = \sum_{i=1}^{nc} \frac{z_i(K_i - 1)}{1 + V(K_i - 1)} = 0$$

How many phases are present?

If there are two phases, what is the value of V?

From V, what is the value of L?

What is the composition of the oil and of the gas?

Multiphase flash

The conventional two phase flash calculation starts with a stability test for the feed composition, based on Michelsen’s (1982) stability criterion. If unstable, a flash phase split calculation is performed to determine the two phase compositions.

A multiphase flash analysis is available in PVTi, and can be used before an ECLIPSE simulation. The multiphase flash continues from the two-phase flash in a step-wise fashion: if any one of the current N phases exhibits instability, an N+1 phase flash split calculation is performed, the resulting tested for stability.

In PVTi the maximum allowed number of phases is five, after that no more phases are split off.

The PVTi Multiphase flash has three modes:

1. Conventional two-phase mode.
2. Three phase mode, one of which is restricted to water.
3. The full multiphase flash mode.

The full multiphase flash is the default. In this mode there are two different ways of performing a multiphase flash calculation.

The standard method initially assumes a single phase equal to the feed. Stability checks are performed and subsequent phases are split off if the system is unstable.

Instead of the flash starting with the feed, initial guesses can be used assuming there are 4 phases present that are initially undetermined.

We mentioned previously that more than one liquid oil phase can exist in some circumstances. The following phase diagram is for Schrader Bluff Oil Mixed with Miscible Injection (MI) Gas

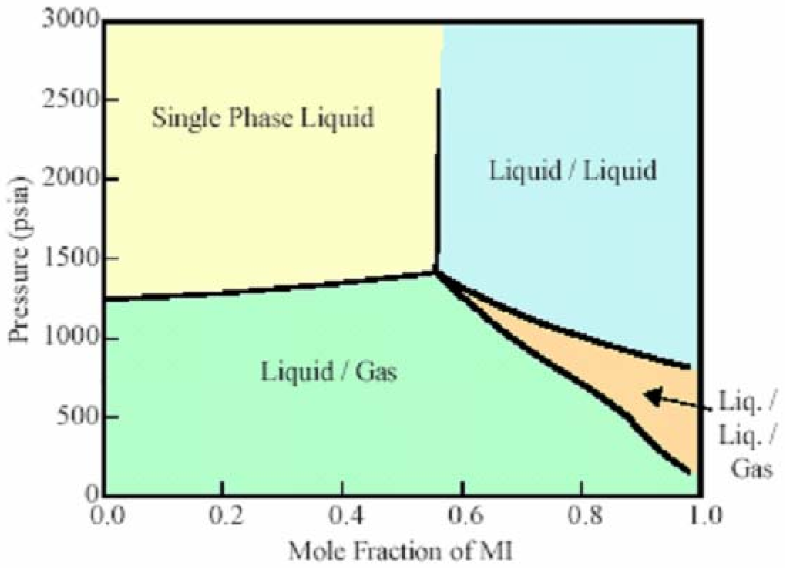


Fig. 1—Phase diagram for Schrader Bluff fluids.

The stability of each phase present in a multiphase regime can be tested with the Michelsen analysis, as for the two phase case, using the Gibbs energy tangent plane distance criterion. However, the initial estimates for phases that will be split off are not limited to the vapor/liquid equilibrium phases characterised by the Wilson K-values: additional estimates are chosen from the following phases:

- Each inorganic component
- Lightest hydrocarbon
- Heaviest hydrocarbon
- Ideal gas
- Arithmetic mean of existing phases.
- Wax-prediction of cloud point[29]

The solution method used for Michelsen stability criterion is a Successive substitution with GDEM (general dominant eigenvalue method) follow by BFGS if that does not work. These trial phases are tested in turn until one indicates instability, in which case the whole system is unstable, and the algorithm proceeds to split of that phase, provided that phase does not already exist. If none of the trial phase indicates instability, the state is assumed to be stable.

Difficulties in Flash

- **Large CPU Requirement:**
- **Many Flash calculations per iteration**
- **Large number of components**
- **Number of phase changes**

- **Convergence Problems:**
- **Near critical point - equations singular**
- **Near phase boundary - oscillation may occur**

- **Other:**
- **EOS may NOT accurately represent the system**
- **Limited PVT data means EOS must extrapolate behavior into phase space.**

---

[29] For more information see SPE 27629

Summary of Flash

The complete solution procedure is therefore:

guess K_i

solve the Rachford-Rice equation to get V

from V get L, x_i and y_i

from x_i and y_i and the EoS, calculate f_{iL}, f_{iV}

Test for convergence:

- either converged
- or recalculate K_i and start again.

15. Demo of Gas Injection into an Oil

Statement of problem

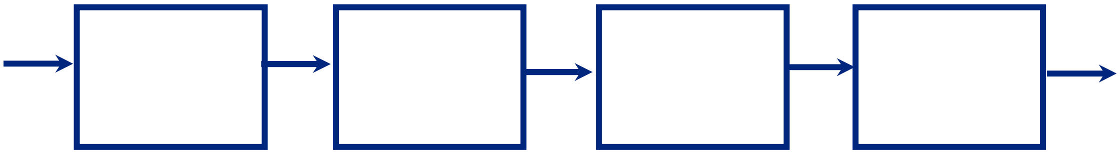
Assume we have a reservoir full of oil, with no water and no free gas. The oil is made up of 3 pure components:

C1 - 60%   C3 - 25%   C10 - 15%

The initial reservoir temperature = 100°C

The initial reservoir Pressure 260 Barsa

For this simple exercise we shall model a small part of the reservoir with 4 horizontal grid blocks, each having a pore volume = 2.5rm^3.



The total volume for our simulation is therefore = 10 rm3

We inject gas into the first grid block. The Injection gas is 100% C1. The gas injection rate is 3.0 rm^3/day. One PV injected every 3.33 days.

Production is on RESV control of 3.0 rm3/day.

Three time steps of 0.3, 0.3 and 0.4 days were chosen.

(Output written at 0, 0.3, 0.6 and 1.0 days).

OBSERVE THE CHANGES IN

oil (liquid) saturation

gas (vapor) saturation

mole fractions in the oil phase (XMF)

mole fractions in the gas phase (YMF)

vapor mole fraction (VMF)

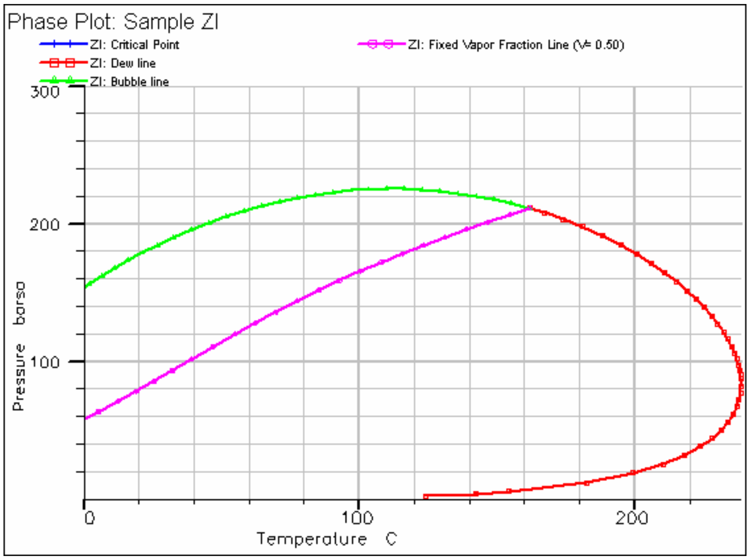
saturation pressure (PSAT)

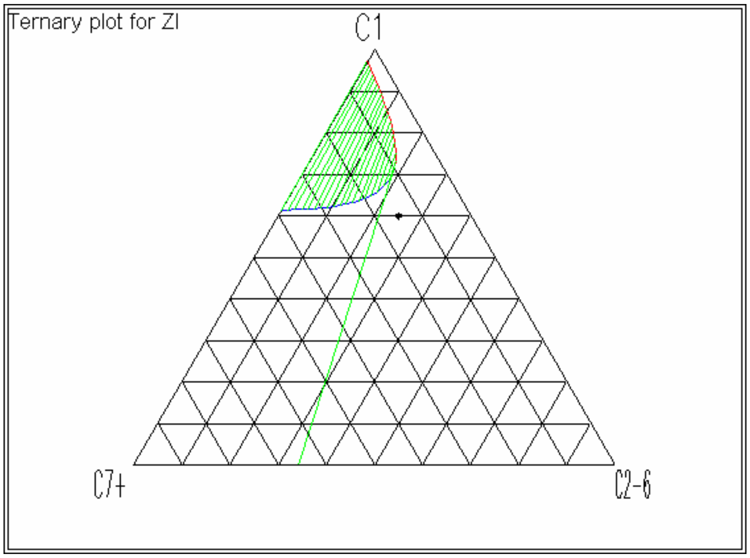
viscosity of the oil phase (VOIL), and

viscosity of the gas phase (VGAS)

Solution of problem

First plot the phase diagram of the initial reservoir fluid and the ternary diagram at the initial conditions:





Use PVTi to create a PVO file to include in our ECLIPSE 300 model.

Examine the initial conditions in the reservoir model.

Initial Pressure = 260.0 Barsa

Sat Oil	1.0	1.0	1.0	1.0
Sat gas	0.0	0.0	0.0	0.0
XMF				
C1	0.6	0.6	0.6	0.6
C3	0.25	0.25	0.25	0.25
C10	0.15	0.15	0.15	0.15
YMF				
C1	---	---	---	---
C3	---	---	---	---
C10	---	---	---	---
VMF	0.0	0.0	0.0	0.0
PSAT	225.2	225.2	225.2	225.2
VOIL	0.056	0.056	0.056	0.056
VGAS	---	---	---	---

After 1 time step at 0.3 days (Pressure = 250.6 Barsa)

Sat Oil	0.57318	1.0	1.0	1.0
Sat gas	0.42682	0.0	0.0	0.0
XMF				
C1	0.6506	0.62456	0.60627	0.60164
C3	0.20117	0.23519	0.24622	0.24901
C10	0.14822	0.14025	0.14751	0.14935
YMF				
C1	0.74841	---	---	---
C3	0.17940	---	---	---
C10	0.072191	---	---	---
VMF	0.41824	0.0	0.0	0.0

PSAT	250.6	234.5	227.6	228.8
VOIL	0.051	0.052	0.054	0.055
VGAS	0.034	---	---	---

Although we are injecting 100% C1, the gas composition in the first grid block is now 75% C1, 18% C3 and 7% C10. The concentration of the intermediate component C3 in the oil has decreased from 25% to 23.5%. Mass transfer of intermediates from the oil phase to the gas phase has therefore enriched the dry injection gas.

After 2 time steps at 0.6 days (Pressure = 247.2 Barsa)

Sat Oil	0.30364	0.85563	1.0	1.0
Sat gas	0.69636	0.14437	0.0	0.0
XMF				
C1	0.61390	0.66208	0.62320	0.60745
C3	0.17476	0.22170	0.23687	0.24577
C10	0.21134	0.12522	0.13993	0.14678
YMF				
C1	0.81167	0.71628	---	---
C3	0.13868	0.19972	---	---
C10	0.049656	0.08399	---	---
VMF	0.68243	0.14173	0.0	0.0
PSAT	247.2	247.0	233.3	227.9
VOIL	0.067	0.046	0.051	0.05554
VGAS	0.028	0.037	---	---

The gas composition at the leading edge of the gas front has now risen from 18% C3 to 20% C3 and the C3 concentration of the oil in block 2 has decreased. The gas at the leading edge has enriched more.

After 3 time steps at 1.0 days (Pressure = 244.5 Barsa)

Sat Oil		0.19183	0.36832	0.86377	1.0
Sat gas		0.80817	0.63168	0.13623	0.0
XMF					
	C1	0.59609	0.62144	0.65588	0.62553
	C3	0.13716	0.19982	0.21807	0.23621
	C10	0.26676	0.17874	0.12605	0.13826
YMF					
	C1	0.86059	0.77470	0.71375	---
	C3	0.100641	0.16727	0.20396	---
	C10	0.049656	0.05802	0.08229	---
VMF		0.79595	0.61814	0.13342	0.0
PSAT		244.5	244.4	244.2	233.9
VOIL		0.082	0.056	0.046	0.050
VGAS		0.025	0.031	0.036	---

The gas composition at the leading edge of the gas front is now over 20% and is very close to the concentration of C3 in the oil (20.4% compared with 21.8%). Concentration of C10 in the two phases is getting closer (8.2% in the gas and 12.6% in the oil) so the two phases are getting more and more similar. This is supported by the viscosity of the two phases becoming similar: oil initially had a viscosity of 0.056 cp but the oil viscosity in block 3 is now 0.046 cp, close the gas viscosity of 0.036 cp. We are close to miscibility.

16. Composition Variation with Depth

This section will examine how gravity affects the distribution of hydrocarbon components in a fluid column.

Effect of gravity on composition

- Theory: heavier molecules will, given enough time, tend to migrate towards the bottom of an oil column
- Gross assumptions in PVT experiment:
- Assumes that the system is in gravitational and diffusive equilibrium and that there is no thermal gradient in the column

Heavier molecules will, given enough time, tend to migrate towards the bottom of column. Many investigations have been made of compositional gradients and several authors have defined simulation procedures to estimate the component distributions with depth. Generally, these estimates have not measured up to known distributions. A study by Montel, Caltagirone and Pebayle has attempted to analyse the discrepancies by looking at times for fluid columns to come into equilibrium under gravitational, thermal and diffusive gradients. They estimate that equilibrium times may be the order of millions of years!

The composition with depth experiment in PVTi makes some gross assumptions with respect to the work of the French group above; however, it may be useful in predicting trends. The experiment assumes that the system is in gravitational and diffusive equilibrium and that there is no thermal gradient in the column.

The change in Gibbs free energy of a component can be related to a change in the log of that component's fugacity, i.e.:

$$dG_i = RTd(\ln f_i) \qquad (i = 1,2,\ldots,N)$$

The change in Gibbs energy can also be related to mole weights:

$$dG_i = M_i g dh \qquad (i = 1,2,\ldots,N)$$

where g is the gravitational constant and dh is the change in height from a specified reference which will subsequently be denoted with the superscript 0.

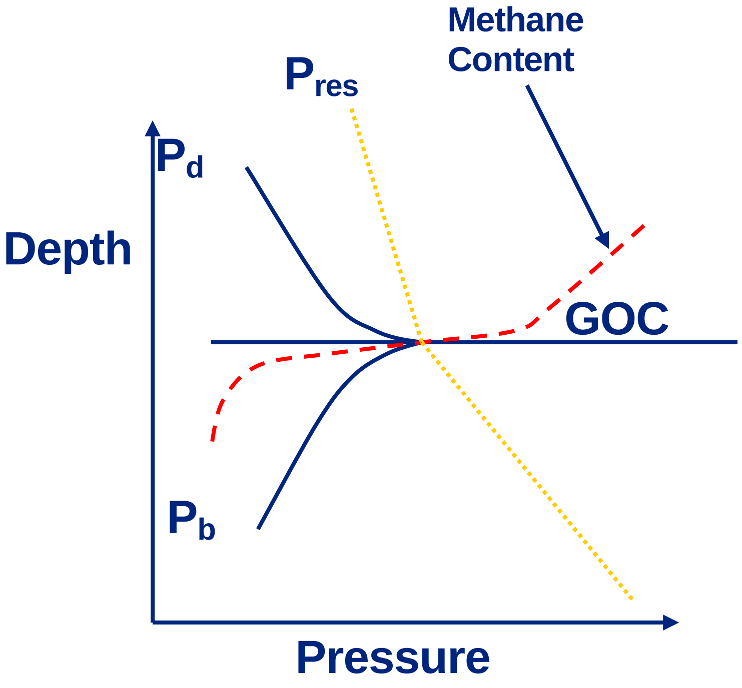
Equating and integrating gives:

$$\ln f_i = \ln f_i^0 + \frac{M_i g}{RT}(h - h^0)$$

Thus knowing the composition, $\{z_i^0\}$ and pressure P^0 at the reference height h^0 allows us to calculate the composition and pressure at other heights from these N equations and a mole constraint on the new composition, $\{z_i(h)\}$.

Starting from an oil and moving up a column, the fluid will become lighter and tend towards a gas (condensate). Two types of grading are possible.

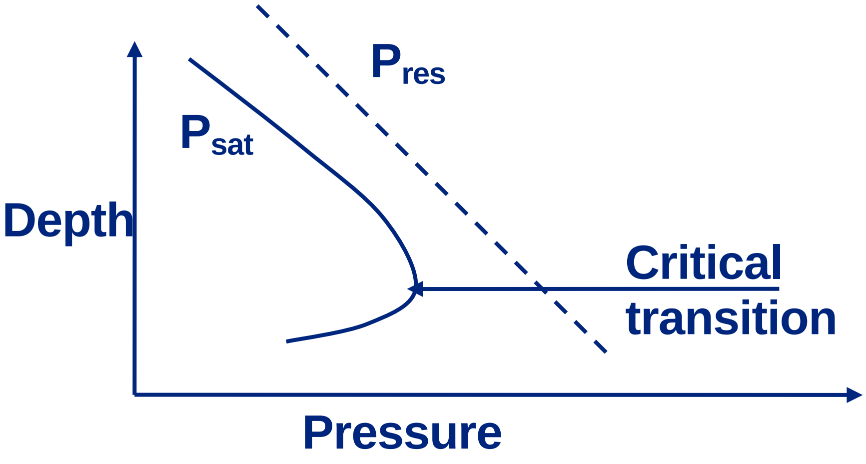
The traditional picture[30] is of the fluid going from an oil to a gas with a distinct gas-oil contact (goc) at some unique depth. At the goc the dew-point gas is in equilibrium with the bubble-point oil, and the fluids have a different composition. If this situation occurs it will be predicted by PVTi and a goc should be entered in the SOLUTION section ECLIPSE.

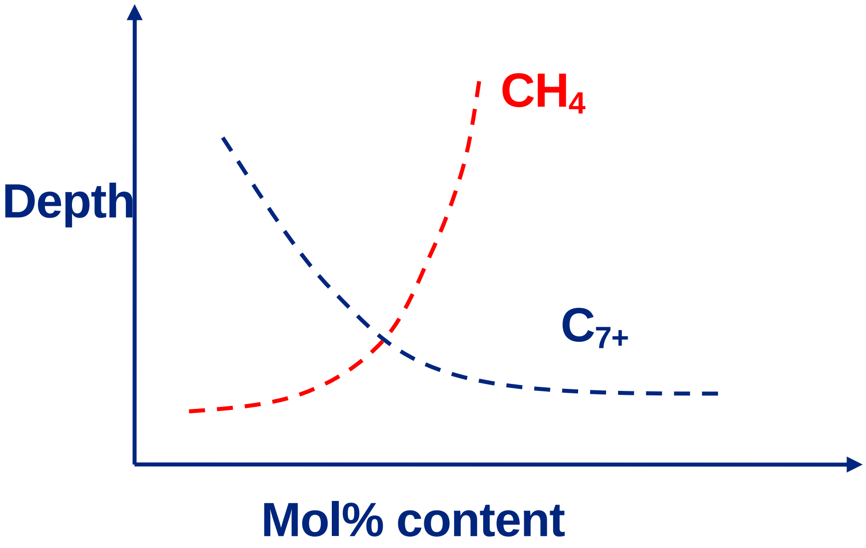


---

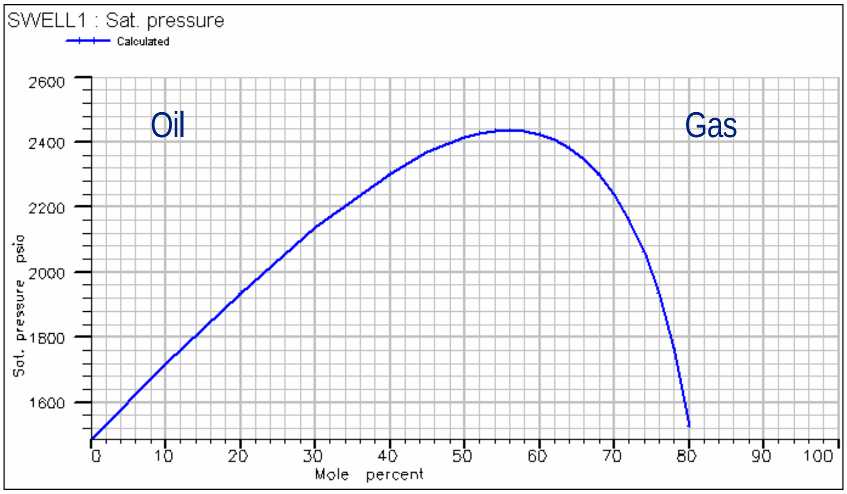
[30] Note depth is increasing downwards in all these picture.

The other possibility is of the fluid grading from an oil to a gas without a contact. This case corresponds to the critical temperature of a particular composition equaling the reservoir temperature. There is a smooth transition from oil to gas through a “critical” composition and the fluid is said to be “super-critical”. If this process occurs, it too will be predicted by PVTi and can be defined in ECLIPSE.

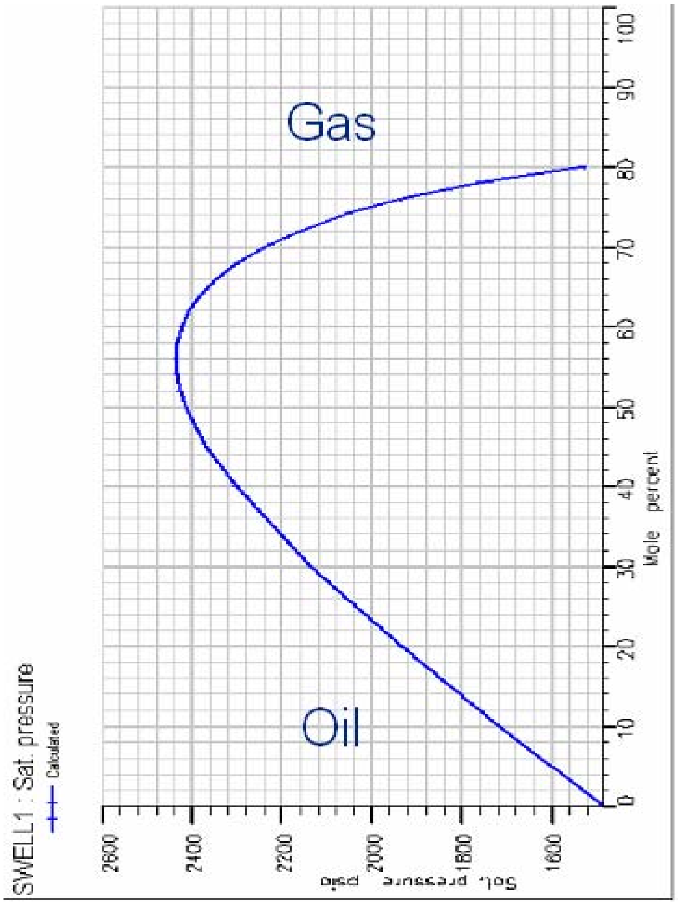




An alternative way of looking at this transition from oil to gas with no goc is to recall the diagram we saw earlier in the description of the miscible process:

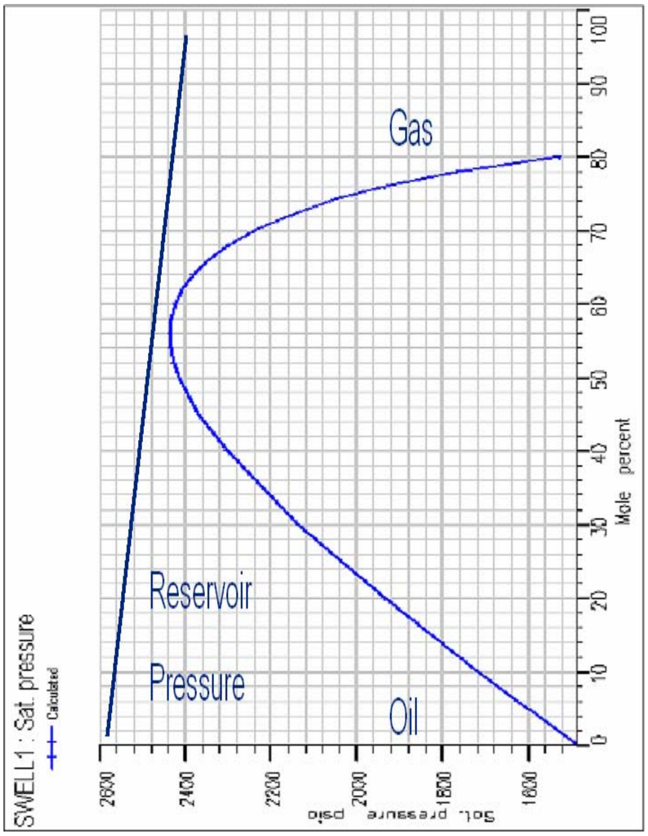


Recall that we were injecting gas into an oil, with the x axis representing the percentage of injected gas. Ignore the numerical values on the x-axis and rotate the picture by 90 degrees, we get:



This shows the saturation pressure for a fluid that has more light components at the top and more heavy components at the bottom. If we now add a line showing the reservoir pressure as a function of depth:

Error!



we can see that the reservoir pressure is greater than the saturation pressure at all depths, and therefore that the reservoir is single-phase at all depths.

Summary of composition vs. depth

Heavier molecules will, given enough time, tend to migrate towards the bottom of column. If composition varies with depth, there are two possibilities:

1. There could be a gas-oil contact (goc) with a gas composition just above the goc that is in equilibrium with the oil composition just below the goc.
2. There could be smooth transition from an oil at the bottom of the oil column to a gas at the top of the column, without a clear goc.

PVTi will predict the variation of composition with depth and ECLIPSE will model either of the two types of transition. This will be discussed in detail in the section on equilibration.

17. From ECLIPSE 100 to ECLIPSE 300

In this section you will understand the main differences between ECLIPSE 100 and ECLIPSE 300, find out the main ECLIPSE 300-specific keywords, and learn how to set up and run ECLIPSE 300 models.

Introduction to running ECLIPSE 300

Running ECLIPSE 300 is similar to running ECLIPSE 100, but not identical.

We will highlight similarities and differences.

We start by comparing the equations that we solve in black-oil and in compositional simulation.

Similar combination of:

- Continuity Equation
  - (Black Oil: Conservation of Mass)
  - (Compositional: Conservation of moles)
  - (Compositional: EoS to determine phases)
- Fluid Flow Equation

In both black-oil and in compositional simulation we start with a continuity equation. A continuity equation is a conservation equation.

In the black-oil case, we are conserving the mass of each phase:

> the total mass of oil at the beginning of a time step is equal to the total mass of oil at the end of the time step,
>
> the total mass of gas at the beginning of a time step is equal to the total mass of gas at the end of the time step,
>
> the total mass of water at the beginning of a time step is equal to the total mass of water at the end of the time step.

For instance for the oil phase we require that the mass of oil in a grid block at the end of a time steps must equal the total mass at the beginning of the time step plus any mass that entered the block minus any mass that left the grid block.

In the compositional case, as we have already discussed, we consider the behavior of the components that make up the phases. Therefore **the total mass of oil does not have to be conserved**. Similarly, the total mass of gas does not to be conserved. What is conserved is the total mass of each component.

- For instance if the hydrocarbon in a grid block changes state from 100% oil to 100% gas then clearly the total mass of oil is not conserved, but the total mass of methane is conserved, whichever phase the methane happens to be in.
- Another example is the case of two wells, one well producing X bpd of oil, and some gas, the other well producing Y bpd of oil and some gas. If the composition of the hydrocarbon produced from each well is different, then the total produced from both wells will be X+Y. Again, the total mass of methane produced will be the sum of the methane produced from each well[31].

In the compositional case, we need one extra step. Having decided what components are in a grid block, and what the pressure and temperature of that grid block is, then we have to solve the flash equation to calculate the amount and properties of each phase in the grid block. Once we know what phases are present, we are in exactly the same position as the black oil case. So in both black-oil and in compositional simulation we solve the fluid flow equations in the same way.

We distinguish between black-oil and compositional techniques because ECLIPSE 300 can be used for both black-oil and in compositional simulation.

ECLIPSE 100

- **Black oil**

ECLIPSE 300

- **Black oil**
- **K-Value compositional**
- **EoS compositional**
- **Thermal**

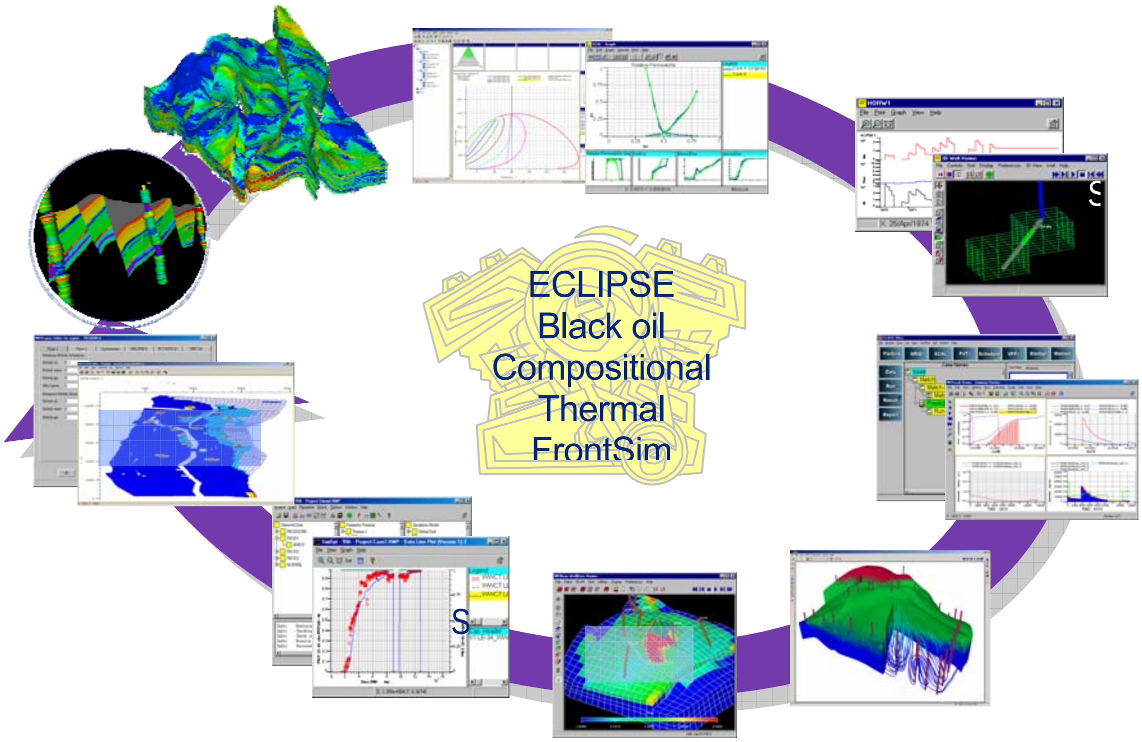
---

[31] In general, the difference should be small. For example if one well is producing 2694.3 bpd of oil and the other well is producing 2668.4 bpd then the sum of the oil produced from both wells could be 5368.0 bpd instead of 2694.3+2668.4 = 5362.7 bpd.

ECLIPSE 300 can also be run in Thermal mode to model steam injection. In this case, we have to again be careful to distinguish between a component and a phase. Thermal simulations allow the water component H2O to be present in both the water phase and the gas phase. The gas phase can therefore consist of a mix hydrocarbon components and the water component.

ECLIPSE 300 is run in the same way as ECLIPSE 100.

- **ECLIPSE 300 is a batch orientated program taking input from a standard data file. Other input files of the same type can be referenced by the INCLUDE keyword**
- **All pre-processor output (i.e. from PVTi, VFPi, FILL, GRID, FloGrid, SCAL, SCHEDULE, Petrel RE) go through the ECLIPSE 300 data file (normally via the INCLUDE keyword)**
- **ECLIPSE 300 models can be set up, run and monitored by ECLIPSE Office or Petrel RE.**



As in ECLIPSE 100, if the data file submitted to ECLIPSE 300 is called BASE.DATA, then the following files can be created by the run:

`PRINT` file	Main printer output	(`RPT...` keywords)
`DEBUG` file	Debug output	(`DEBUG` keyword)
`MSG` file	Message output (XML format)	(`MSGFILE` keyword)
`GRID` file	Grid geometry file	(`NOGGF` and `GRIDFILE` keyword)
`EGRID` file	Compact Grid geometry file	(`NOGGF` and `GRIDFILE` keyword)
`SAVE` file	Data for fast restarts	(`SAVE` keyword)
`INITIAL` file	Initialization file	(`PSEUDOS` keyword and `INIT` keyword)
`INSPEC` file	Initial index file	(`INSPEC` keyword in `RUNSPEC` section)
`RESTART` file	Restart runs / grid graphics file	(`RPTSCHED` keyword)
`SMSPEC` file	Specifications for summary file	(`SUMMARY` section)
`SUMMARY` file	Line graphics file	(`SUMMARY` section)
`RSM` file	Run summary file	(`SEPARATE/LOTUS` keywords)
`RFT` file	RFT and PLT graphics file	(`WRFTPLT` keyword)
`RSSPEC` file	Restart index file	(`RSSPEC` keyword in `RUNSPEC` section)
`HMD` file	Gradients file for SimOpt	(`HMDIMS` in `RUNSPEC` section)
`GRFT` file	RFT gradients for SimOpt	(`GRADRFT` in `SCHEDULE` section)

The production of all of these files, except for the main printer output, is controlled by the keywords indicated. The contents and hence the size of the printer output file are controlled using the `RPTGRID`, `RPTPROPS`, `RPTREGS`, `RPTSCHED`, `RPTSMRY`, `RPTSOL`, `OUTSOL` and `RPTRST` keywords.

In addition, you can choose whether input and output files are to be formatted or unformatted, (`RUNSPEC` section keywords `FMTIN`, `FMTOUT` and `FMTSAVE`), and whether `RESTART` and `SUMMARY` files are to be unified (see the `RUNSPEC` section keywords `UNIFIN`, `UNIFOUT` and `UNIFSAVE`).

Formatted files are standard 80 character card image files, and can be examined with any text editor. They may be straightforwardly transferred between different computers, although this can usually also be done for unformatted files. All the files generated by the ECLIPSE programs can be converted from formatted to unformatted files or vice-versa using the utility program Convert – on a PC you can run this utility with $convert and on a Unix or Linux system with @convert.

In general, unformatted non-unified files should be used. They can allow you to make efficient use of disk space and on some systems make it possible for you to examine output as the simulation progresses. They also reduce the time to read the starting solution in a restart run. Unified files should be used if the number of files being produced is a problem. Unified files also reduce the size of your catalog considerably (but not the amount of disk space used).

Data File Sections

An ECLIPSE 300 data file contains the same sections[32] as ECLIPSE 100:

RUNSPEC	Dimensions and Options
GRID	Shape and Volume
EDIT (opt)	Modify Rock Properties
PROPS	Fluid Properties, Rock Fluid and Fluid-Fluid Interactions
REGIONS (opt)	Reservoir Subdivision
SOLUTION	Initial State
SUMMARY (opt)	Output Required
SCHEDULE	Well Data and Production Schedule

The content of many of these sections is similar in both case, but is not always identical. The PVT data and some of the SCHEDULE keywords for example are very different.

---

[32] ECLIPSE 300 also contains an OPTIMIZE section that is not available in ECLIPSE 100. This section defines the components of an optimisation loop and is described in the Optimization section of the technical description manual.

RUNSPEC	Similar
GRID	Similar
EDIT (opt)	Same
PROPS	Fluid Properties: different Rock-Fluid and Fluid-Fluid: similar
REGIONS (opt)	Similar
SOLUTION	Similar
SUMMARY (opt)	Similar
SCHEDULE	Different

As a reminder for those not totally familiar with the details of each section, the ECLIPSE Reference manual chapter “Data File Overview” provides a complete description. The following table is reproduced from that chapter, with the text in ***bold italics*** showing the extra compositional information.

`RUNSPEC`	Title, problem dimensions, switches, phases present, ***components***
`GRID`	Geometry of grid (location of grid block corners), and rock properties (porosity, absolute permeability, etc.) in each grid block.
`EDIT`	Modifications to calculated pore volumes, grid block centre depths and transmissibilities.
`PROPS`	Tables of properties of reservoir rock and fluids as functions of fluid pressures, saturations (density, viscosity, relative permeability, capillary pressure, etc.) ***and compositions. The equation of state description in compositional runs.***
`REGIONS`	Splits computational grid into regions for calculation of • PVT properties • Saturation properties • Initial conditions • Fluids in-place • ***EOS regions***

`SOLUTION`	Specification of initial conditions in reservoir - may be: • Calculated using fluid contact depths to give equilibrium • Read from a restart file set up by an earlier run • Specified by the user for every grid block (Not recommended for general use)
`SUMMARY`	Data to be written to the Summary file after each time step. Necessary if certain types of graphical output (for example water-cut as a function of time) are to be generated after the run has finished. ***Molar rates an quantities can be requested.*** If this section is omitted no Summary files are created.
`SCHEDULE`	Specifies the operations to be simulated (production and injection controls and constraints) and the times at which output reports are required. Vertical flow performance curves and simulator tuning parameters may also be specified. ***Separator conditions and injection gas composition are also defined here.***
`OPTIMIZE`	Specifies a reservoir optimization problem (objective function, control parameters, constraints).

RUNSPEC Section

The RUNSPEC section is similar to that of ECLIPSE 100. To run in compositional mode, one extra keyword is required. COMPS must be used to define the number of components used in the model.

DIMENS

number of grid cells in each direction

UNITS

Units (FIELD, METRIC, LAB, PVTM)

OIL

WATER

GAS

COMPS

Number of components

WELLDIMS

Maximum number of wells and connections

Everything else can be defaulted

Example of a RUNSPEC section:

```
--  Comments can be inserted before the RUNSPEC Keyword
RUNSPEC
--  Request FIELD units
FIELD
--  Oil water and gas phases are present
WATER
OIL
GAS
--  Nine components in study (plus water)
COMPS
9 /
--  Grid is 19 by 19 by 4 cells
DIMENS
19 19 4 /
--  One saturation and pressure table region, up to 40 rows in each
TABDIMS
1 1 40 40 /
--  Maximum of 2 wells, each with a maximum of 2 completions
WELLDIMS
2 2 /
GRID      (start of Grid section)
```

Solution Methods

ECLIPSE 100 and ECLIPSE 300 contain options for both the fully implicit (FULLIMP) and IMPES (IMplicit Pressure Explicit Saturation) solution procedures. The fully implicit method is stable and may be used to solve ‘difficult’ problems such as coning studies. Although IMPES is potentially unstable, it is less dispersive and sometimes faster than the fully implicit method, and may be used on ‘easy’ problems such as history matching applications if the timesteps are small and the solution is not changing much. ECLIPSE 300 also has options for AIM (Adaptive Implicit Method) and IMPSAT (Implicit Pressure and SATuration). The AIM method for compositional studies is a compromise between fully implicit and IMPES methods, allowing cells in ‘difficult’ regions to remain fully implicit while employing the advantage of an IMPES description in ‘easy’ regions.

The default solution procedure is `AIM` for most compositional runs and is `FULLIMP` for all black oil runs. For dual porosity problems and for radial models, the default is `FULLIMP`. The default solution procedure may be changed by using one of the keywords `AIM`, `FULLIMP`, `IMPSAT` or `IMPES` in the RUNSPEC section.

We assume that the flow is constant over the time step. The pressures in the flow equations are always those at the end of the time step. The main difference between the methods is that the mobilities may be taken either at the start or at the end of the time step. If any of the terms in the transmissibility calculation are pressure-dependent (for instance transmissibility multipliers) then they too may be taken either at the start or at the end of the time step.

FULLIMP

The fully implicit method is the default for black oil runs in both ECLIPSE 100 and ECLIPSE 300. It is not recommended for most compositional runs where there are often too many components to be able to use the fully implicit method efficiently.

Newton’s method is used to solve the non-linear residual equations R(X) = 0. Several iterations may be required to reduce the residuals to a ‘sufficiently small’ value. In ECLIPSE 300, the main measure used to define the meaning of ‘sufficiently small’ is that the solution change over a non-linear iteration should be small.

IMPES

The IMPES residual is similar to the fully implicit residual except that all flow and well terms are computed using molar densities at the beginning of each timestep.

The linear equations arising from Newton's method are also much easier to solve in the IMPES case because derivatives of flows with respect to saturations are zero. The linear equations are solved sequentially, first for pressure and subsequently for saturation changes. This contrasts with the fully implicit method where the linear equations must be solved simultaneously.

The IMPES method is unstable for large time steps, as the flows will not react to the change in composition and saturation over the time step. In extreme cases, all of a phase might flow out of a cell but IMPES will assume that the flow will continue even if there is none of that phase left. This may lead to an unrealistically low amount of that phase in that cell. At the next step, none of the phase will flow out, but a large amount could flow in. This leads to the IMPES instability.

In ECLIPSE 300, the IMPES (IMplicit Pressures Explicit Saturations) formulation is in reality an IMPEM (IMplicit Pressure Explicit Mobility) method. The mass terms are evaluated using both pressures and molar densities at the end of the timestep. The flow terms between cells are evaluated assuming that the saturations, generalized mobilities and reservoir density terms are all fixed at the previous timestep

AIM

AIM is a compromise between the fully implicit and IMPES procedures. Cells with a high throughput ratio are chosen to be implicit for stability and to obtain large timesteps, while the majority of cells can still be treated as IMPES where the solution may be changing little. All completions are treated implicitly. The target fraction of implicit cells in a compositional run is 1%, but this can be altered by the `AIMFRAC` keyword.

IMPSAT

This treats pressure and phase saturations implicitly, but phase compositions explicitly. This method is ideal for runs involving large capillary pressures, which would cause instability in `IMPES` or `AIM` methods. In the `IMPSAT` mode we add three extra primary solution variables which represent the phase saturations.

GRID Section

The GRID section is the same in ECLIPSE 100 and ECLIPSE 300, and in black-oil and in compositional runs.

EDIT Section

The EDIT section is the same in ECLIPSE 100 and ECLIPSE 300, and in black-oil and in compositional runs.

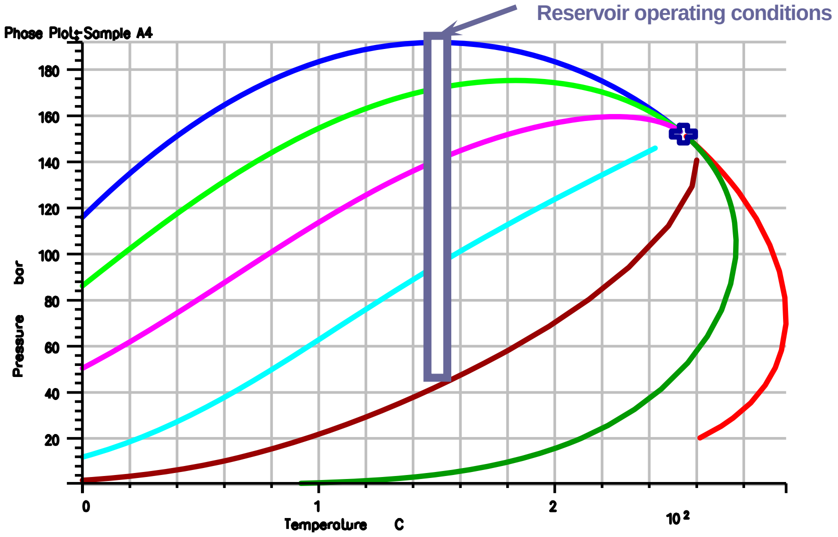
PROPS Section

The props section contains both SCAL data and PVT data. The SCAL data is the same in ECLIPSE 100 and ECLIPSE 300, and in black-oil and in compositional runs. The PVT data is completely different. The PVT data is usually contained in a separate file such as the .PVO file generated by PVTi, and is INCLUDEd in the PROPS section.

If the composition is varying with depth, then this variation can be entered in this section with the ZMFVD keyword.

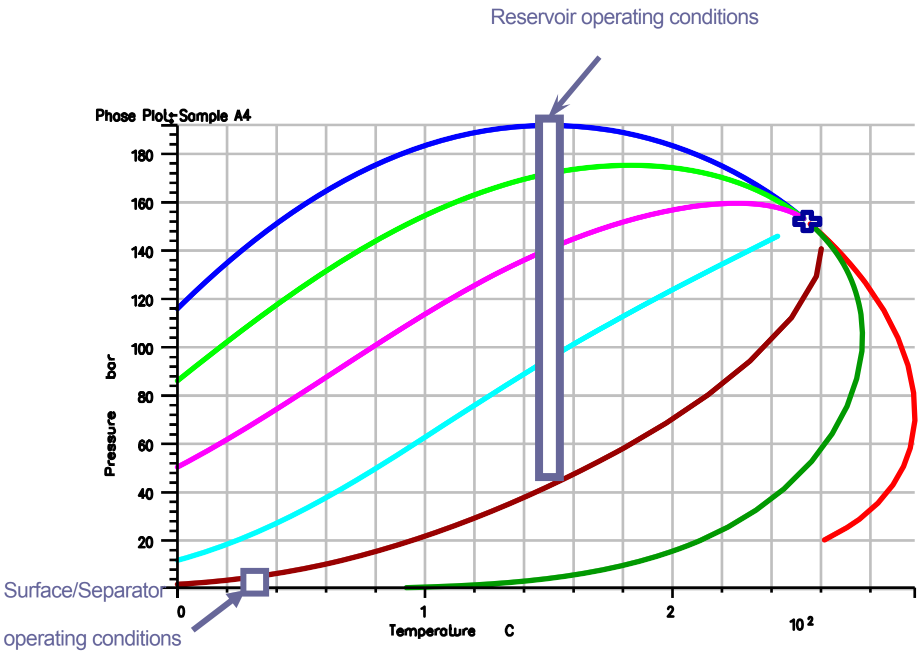
Surface EoS

For a reservoir with no temperature variation, the Pressure-Temperature range within the reservoir during its lifetime can be represented by the box below:


Reservoir operating conditions

Fluid A4: 50% C1, 30% C4, 20% C12 - $T_c = 254\ ^oC$

The reservoir fluids will be produced through the wells and separators and will eventually end up at surface or separator conditions. These will typically be as shown:



As we discussed in the section on PVT analysis, the CVD or DL experiments are considered to represent what happens within the reservoir but the CCE experiments represent behavior in the separators.

Ideally we would match all experiments using the same set of EoS parameters, so that the same EoS matched the fluid at reservoir conditions, at separator or surface conditions, and at all pressures and temperatures in between. This is usually the case and we would normally expect each fluid to be described by one EoS. In some cases however you may not be able to regress to both CCE and CVD/DL experiments in the limited time that you will have available to perform the PVT analysis. You may find that you can either match the CCE observations or the CVD/DL observations, but not both with the same EoS parameters. If this is the case then ECLIPSE 300 will allow you to provide surface EoS values that are different from the reservoir EoS values, the surface values coming from a regression to CCE experiments and the reservoir values from a match to the CVD or DL experiments. We do not recommend using this option unless absolutely necessary.

There must be the same number of surface equations of state as reservoir equations of state. The properties of each surface EoS default to those of the corresponding reservoir equation of state, but any or all of these may be over-written using the following keywords[33]:

EOSS	
TCRITS	
PCRITS	
VCRITS or ZCRITS	
MWS	
ACFS	
OMEGAAS	
OMEGABS	
SSHIFTS	
TBOILS	(Zudkevitch-Joffe EoS only)
TREFS	(Zudkevitch-Joffe EoS or Thermal)
DREFS or GREFS	(Zudkevitch-Joffe EoS or Thermal)
PREFS	(Thermal only)
BICS	

Items in these keywords default to the reservoir equation of state values. For example, to modify just the last two `TCRIT` values you can enter

```
TCRITS
   7* 1078.0 1345.0 /
```

When performing separator calculations, a choice of surface equation of state must be made. By default, the flash calculations for a well use the EoS number corresponding to the cells in which that well is completed. For example, a well completed in cells in reservoir EoS region 2 will use surface EoS2. If a well is completed in cells in more than one reservoir EoS region, a warning is issued, and the first value encountered used.

It is possible to over-ride this choice of surface EoS using the keywords `FIELDSEP` and `SEPCOND`. The eighth argument of `FIELDSEP` and the tenth argument of `SEPCOND` may be used to specify a non-default EoS number to be used in separator fluid-in-place and surface rate calculations, respectively.

By default, `FIELDSEP` obtains separator volumes in place for the whole field and for fluid-in-place regions using the equation of state specified for the cell, as specified with `EOSNUM`.

---

[33] `RTEMP`, parachors and viscosity values are not used in surface calculations.

Multiple EoS regions

If there is more than one EoS region then each keyword will expect the data for region 1, followed by the data for region 2, etc. This means that you will have to merge a number of PVO files into one large PVO file. For instance suppose you have two EoS regions. If the first PVO file contains:

```
-- Critical temperatures Deg R
 TCRIT
  5.484599855E+02  2.271599940E+02  3.430799909E+02  6.656399824E+02
  1.126799970E+03  1.303199965E+03          /
 -- Critical pressures PSIA
 PCRIT
  1.071331110E+03  4.923126500E+02  6.677816960E+02  6.186973900E+02
           3.509380920E+02  2.552677830E+02 /
```

and the second PVO file contains:

```
-- Critical temperatures Deg R
 TCRIT
  5.484599855E+02  2.271599940E+02  3.430799909E+02  6.656399824E+02
  1.126799970E+03  1.353199965E+03            /
 -- Critical pressures PSIA
 PCRIT
  1.071331110E+03  4.923126500E+02  6.677816960E+02  6.186973900E+02
           3.509380920E+02  2.592677830E+02    /
```

then ECLIPSE 300 will expect one file containing:

```
-- Critical temperatures Deg R
 TCRIT
  5.484599855E+02  2.271599940E+02  3.430799909E+02  6.656399824E+02
  1.126799970E+03  1.303199965E+03          /
  5.484599855E+02  2.271599940E+02  3.430799909E+02  6.656399824E+02
  1.126799970E+03  1.353199965E+03            /
 -- Critical pressures PSIA
 PCRIT
  1.071331110E+03  4.923126500E+02  6.677816960E+02  6.186973900E+02
           3.509380920E+02  2.552677830E+02 /

  1.071331110E+03  4.923126500E+02  6.677816960E+02  6.186973900E+02
           3.509380920E+02  2.592677830E+02    /
```

Pressure Tables

When running ECLIPSE 300 in black-oil mode, PVT tables of oil and gas properties as a function of pressure have to be defined in that same way as in ECLIPSE 100, using keywords such as `PVDO` or `PVTO` and `PVTG` or `PVTG`.

When running in compositional mode, the density or gravity of the oil and gas phase are calculated by the program from the composition of each phase. Any values for oil and/or gas given in the `DENSITY` or `GRAVITY` keyword are ignored, although the values for water are still used.

Saturation tables consistency

For both black-oil and compositional runs, the SCAL data is the same. Either family of keywords can be used, {`SWFN`, `SGFN` and `SOF2`/`SOF3`} or {`SWOF` and `SGOF`/`SLGOF`}.

The oil, water and gas saturation tables, for each particular saturation table number region, must obey certain consistency requirements. These are:

1. S_{gmax} must not exceed 1- S_{wco}

If this condition is violated then the gas saturation in the gas cap will be re-set to 1- S_{wco}, to prevent a negative oil saturation.

Normally, if there is no oil in the gas cap, S_{gmax} = 1- S_{wco}.

2. S_{gco} must not exceed 1- S_{wmax}

If this condition is violated, the gas saturation in the water zone will be re-set to 1- S_{wmax}, to prevent a negative oil saturation.

Normally, there is no initial free gas below the gas cap and the water zone is fully saturated with water, thus S_{gco} = 0 and 1- S_{wmax} = 0.

3. S_{omax} must equal 1- S_{wco}

4 $k_{row}(S_{omax})$ must equal $k_{rog}(S_{omax})$

5. $k_{rw}(S_w=0) = k_{rg}(S_g=0) = k_{rog}(S_0=0) = k_{row}(S_0=0) = 0$.

Otherwise, phases can be mobile even at zero saturation and there is nothing to stop saturations going negative.

In oil-wet system modeling, in order to apply correctly the Killough wetting phase model on the oil phase (option 7, Item 2 of `EHYSTR` keyword), the consistency requirements are slightly modified

1. S_{gmax} must equal 1- S_{oco}

3. S_{omax} is normally = 1

6. $\underline{S_{wmax}}$ must equal 1- $\underline{S_{oco}}$

Small relative permeabilities

Normally, the critical water saturation $\underline{S_{wcr}}$ is set to the value $\underline{S_w}$ of in the last table entry (in `SWOF` or `SWFN`) for k_{rw} for which $k_{rw} < 10^{-6}$ in ECLIPSE 100 and for which $k_{rw} < 10^{-20}$ in ECLIPSE 300. This is just a convenient way of finding the last zero relative permeability value while accounting for machine zero. You can override this by entering a value in the `TOLCRIT` keyword so that the critical saturation is the value of $\underline{S_w}$ in the last table entry where k_{rw} < TOLCRIT.

The same applies to the critical values for oil and gas saturations.

This ability to override the default critical saturations may be of use

- in pathological cases involving end point scaling (keyword `ENDSCALE` in `RUNSPEC`)
- in cases where SCAL tables have been generated automatically and may contain small non-measurable values that you wish to ignore
- for comparison with certain other simulators that use a different tolerance.

REGION Section

As well as the existing regions available for black-oil models, compositional models can also have different EoS regions. The most common application of this study is a study containing two or more disconnected reservoirs, coupled through the productive system.

If cells with different EOS region numbers are in the same equilibration region, the initial state will not generally be in hydrostatic equilibrium, as the EOS determines the phase densities. The program will issue a warning if this occurs.

SOLUTION Section

The initial reservoir conditions can be defined in one of three ways:

1. They can be calculated by the equilibration facility using the `EQUIL` keyword.
2. They can be set directly in each grid block, using the keywords `PRESSURE` or `PRVD`, `SWAT`, `SGAS`. For a black-oil run you will also

need `RS` or `PBUB`, and `RV` or `PDEW`. For a compositional run you will also need `XMF` and `YMF`.

3. They can be read from a `RESTART` file or a `SAVE` file generated by an earlier run (see keyword `RESTART` or `LOAD`) or from an ECLIPSE 100 run (see keyword `GETSOL`)

The equilibration facility is a means of calculating the initial conditions on the basis of hydrostatic equilibrium

Equilibrium Initialisation

If you are using `EQUIL`, then for each equilibration region you should specify the pressure at a given datum depth, the positions of the gas-oil and water-oil contacts, and the value of the capillary pressure at each contact.

The EQUIL keyword

1. **Datum depth**
2. **Pressure at this datum depth**
3. **Depth of OWC (or GWC in gas-water problems)**
4. **P*cow* at OWC (or GWC gas-water problems)**
5. **Depth of GOC**
6. **P*cog* at GOC**

If there is no gas cap, the gas-oil contact should be placed above the top of the reservoir; if there is no mobile water, the water-oil contact should be placed far enough below the bottom of the reservoir to exclude any transition zone.

In gas-water models, instead of a gas-oil contact and a water-oil contact there is a gas-water contact. There is no need to enter any data concerning the non-existent oil phase. But it is also possible to have a gas-water contact in a three-phase model: for a gas condensates where all the oil is initially vaporized in the gas phase. In this case the water-oil contact and the gas-oil contact should both be placed at the gas-water contact. In problems containing a gas-water contact, the gas-water capillary pressure should be supplied in the water saturation tables (keyword `SWFN`). For consistency, the capillary pressure data in the gas saturation tables should be set to zero.

Within each equilibration region, the calculation is performed in two stages.

1. The first stage sets up an internal table of phase pressures and other properties against depth.
2. The second stage interpolates this table to obtain the fluid conditions in each grid block in the region.

The internal table stores the values of the phase pressures (Po, Pw, Pg) at a number of equally-spaced depths within the equilibration region. The number of depth points in this table is set using the keyword `EQLDIMS` in the `RUNSPEC` section. The value should be increased when finer definition is required, for example in problems where the oil or gas zones only occupy a small fraction of the overall reservoir thickness.

Between each pair of depth points in the table, the pressure gradient of each phase is calculated iteratively using a density consistent with the average pressure within the depth step. If the datum depth lies in the oil zone, the oil pressure values are calculated first, stepping from the datum depth up to the top and down to the bottom of the equilibration region. The water pressure on the oil-water contact can now be obtained, and the water pressure values are calculated. Similarly the gas pressure values are calculated starting from the gas-oil contact.

The internal pressure table is then used to obtain the local fluid conditions at each depth. The water saturation is determined by inverse look-up of the water capillary pressure table (entered with keyword `SWFN` or `SWOF`) for the grid block, such that

$P_{cow}(Sw) = Po - Pw$

If Po - Pw exceeds the highest capillary pressure value in the SWFN/SWOF table (corresponding to the lowest saturation value Sw_{min}), the water saturation is set equal to Sw_{min}.

If Po – Pw is less than the lowest capillary pressure in the table (corresponding to the highest saturation value Sw_{max}), the water saturation is set equal to Sw_{max} and the oil pressure is adjusted to follow the water pressure gradient.

The gas saturation is similarly determined by inverse look-up of the gas capillary pressure table (keyword `SGFN`, `SGOF` or `SLGOF`) for the grid block, such that

$P_{cog}(Sg) = Pg - Po$

If Pg – Po is less than the lowest capillary pressure value in the table (corresponding to the lowest gas saturation value Sg_{min}), the gas saturation is set equal to Sg_{min}.

If P_{cog} exceeds the highest capillary pressure in the table (corresponding to the highest gas saturation value Sg_{max}), the gas saturation is set equal to Sg_{max} and the oil pressure is adjusted to follow the gas pressure gradient.

Since the water and gas saturations outside the transition zones are set to the respective end-point values in the saturation function tables, the end-points of the two tables must be consistent. Normally the lowest gas saturation in the `SGFN` or `SGOF` table should be zero (so that Sg = 0 below the gas transition zone), and the highest gas saturation in this table should be 1 - Sw_{min} (so that So = 0 above the gas transition zone). The lowest water saturation value in the `SWFN` or `SWOF` table should be the connate value (so that Sw = Sw_{co} above the water transition zone), and the highest water saturation in this table should be 1.0 (so that Sw = 1.0 below the water transition zone).

In cases where the water-oil and gas-oil transition zones closely overlap, the treatment outlined above may produce negative oil saturations. For example, where the water-oil transition zone extends above the gas-oil transition zone, the water saturation ($Sw > Sw_{min}$) and the gas saturation ($Sg = Sg_{max}$) add to more than 1.0. If this occurs, the water and gas saturations are recalculated from the gas-water capillary pressure, which is taken as the sum of the water-oil and gas-oil capillary pressures

$P_{cow}(Sw) + P_{cog}(Sg=1-Sw) = Pg – Pw$

The EQUIL keyword

9. Accuracy option 0 or 1 = centre point equilibrium. N = fine grid equilibrium

Default= 0

In the second stage of the equilibration calculation, the local fluid conditions are determined in each grid block in the equilibration region. The internal table is interpolated to obtain the pressures and saturations at the grid block center depth, or at the depths determined by the 9th argument of the `EQUIL` keyword.

Given the fluid densities, the equilibration procedure sets up saturation against depth curves such that, in the transition zone when two phases are mobile, the hydrostatic pressure variation is balanced by the capillary pressure between the phases. This can be done on a finer grid than that used for the simulation, the resulting saturations being integrated over the cell volumes at the end of the equilibration to provide a starting point for the simulation.

In general, the use of a fine grid equilibration will yield a more accurate fluid in place, but may lead to some fluid movement upon starting the simulation.

Thermodynamic equilibrium

In ECLIPSE 300 compositional mode, an extra complication exists: as well as ensuring that the initial saturations are in equilibrium, the thermodynamic equilibrium between phases must be considered. Three methods exist of setting up the initial composition variation, which is usually with depth:

1. No gas-oil phase contact exists within the reservoir.

   This option should be used for single hydrocarbon phase initial states, such as condensates above the dew point, or oils above the bubble point. This option should also be used for "supercritical" reservoirs in which a smooth transition exists between oil and gas, the saturation pressure being less than the fluid pressure throughout the depth range.

   Use `ZMFVD` to specify the initial composition with respect to depth. The gas-oil contact should be set above the reservoir if the single phase hydrocarbon is an oil or below the reservoir for a gas. In the supercritical case the gas-oil contact depth may be set to a point within the reservoir. The simulator sets the phase identification method to produce a phase change at this depth.

   As mentioned above, for a condensate field you should set the oil-gas contact depth to the oil-water contact depth. This identifies the study as a condensate to the simulator.

2. For cases in which there is a gas-oil contact within the reservoir, and the vapor composition is known.

   Use `ZMFVD` to specify the initial vapor composition. A retrograde dew point pressure calculation is performed for the vapor and the pressure is set to this at the contact. The composition of the liquid in equilibrium with the saturated vapor is used below the contact. As pressure increases with depth this oil is undersaturated.

   Alternatively, `COMPVD` may be used to specify a compositional variation in the liquid as well as in the vapor. However, the composition specified at the gas-oil contact must be that of a gas.

3. For cases in which there is a gas-oil contact within the reservoir, and the liquid composition is known.

   Use `ZMFVD` to specify the initial oil composition. A bubble point pressure calculation is performed for the liquid and the pressure is set to this at the contact. The composition of the vapor in equilibrium with the saturated liquid is used above the contact. As pressure decreases above the contact this may yield an oil phase upon flashing. If so, the dropped-out oil is removed and only the vapor is used, so that saturated vapor only exists above the contact.

Alternatively, `COMPVD` may be used to specify a compositional variation in the vapor as well as in the liquid. However, the composition specified at the gas-oil contact must be that of an oil.

The EQUIL keyword

10. Compositional option.

- **1 = Single hydrocarbon phase.**
- **2 = GOC in field – gas composition specified**
- **3 = GOC in field – oil composition specified**

Default = 1

Choosing the wrong value is one of the most common mistakes in using ECLIPSE 300

You should carefully choose the right option the tenth argument of the `EQUIL` keyword.

- **If EQUIL(10) = 2 or 3**
  then datum depth must be = gas-oil contact
- **If EQUIL(10) = 2 then Psat = dew-point pressure is calculated**
- **If EQUIL(10) = 3 then Psat = bubble-point pressure is calculated**
- **Psat should = Pdatum = datum pressure EQUIL(2)**
- **If Psat is not close to Pdatum, Pdatum is reset = Psat.**
- **Setting EQUIL(11) = 1 prevents the resetting.**

If there is a gas-oil contact within the reservoir so that you are using EQUIL(10)= 2 or 3 then the datum depth must be set to the gas-oil contact.

ECLIPSE 300 will calculate the appropriate saturation pressure P_{sat} and compare it with the datum pressure P_{datum}. If

$|P_{sat} – P_{datum}| > 1$ atm

then P_{datum} will be reset to P_{sat}. If the difference is large then you will get a warning message, and should review your PVT data.

The 11th argument of `EQUIL` may be set to 1 to suppress the setting of P_{datum} will be reset to P_{sat} in options 2 and 3. This is not recommended as it yields a system that is not in initial equilibrium, but honors the specified pressure.

Output of initial solution

A wide range of solution and property values can be output either to the PRT file or to restart files.

1 To output to the PRT file, use

RPTSOL

PR SWAT SOIL VOIL PSAT XMF YMF SOLVD /

2 You can use in RPTRST[34] to specify which solutions are to be written to the restart files so that they can be visualised in 3D.

RPTRST

PRES SWAT SOIL VOIL PSAT XMF YMF ZMF /

If specified in the SOLUTION section, these mnemonics will continue to be used in the simulation schedule.

Note that PSAT is not used in the simulation and is therefore not normally calculated. Some extra computing is therefore needed to work out Psat and you should therefore not automatically ask for Psat unless you need it. The extra work however is small compared to the total computing involved in the simulation.

---

[34] The old OUTSOL keyword does the same thing as RPTRST, but is not recommended.

The output from SOLVD can sometimes provide very useful debugging information if inconsistent data has been specified. Add SOLVD to the RPTSOL keyword and look for SOLVD in the PRT file. The output is a table of pressures, densities and saturations as a function of depth:

```
Equilibration region 1 ( Representative Saturation table 1 )

 Depth   Poil    Pwat    Pgas    Deno    Denw   Deng    Soil    Swat   Sgas
 Metres  Barsa   Barsa   Barsa   Kg/M3   Kg/M3  Kg/M3
 ------  ------  ------- ------   -----  -----  -----   -----   ------  -----
 500.00  99.881  100.000  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 500.20  99.882  100.001  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 500.41  99.883  100.003  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 500.61  99.884  100.004  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 500.82  99.885  100.005  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 501.02  99.886  100.006  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 501.22  99.887  100.008  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 501.43  99.888  100.009  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 501.63  99.890  100.010  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 501.84  99.891  100.012  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 502.04  99.892  100.013  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 502.24  99.893  100.014  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 502.45  99.894  100.015  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 502.65  99.895  100.017  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 502.86  99.896  100.018  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 503.06  99.897  100.019  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 503.27  99.898  100.021  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 503.47  99.899  100.022  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
 503.67  99.900  100.023  98.354 51.905  64.019 0.0054  0.1100  0.8900  0.00
```

etc

Non-equilibrium Initialisation

Equilibration methods such as those described above are the normal method of initializing a simulation. The aim is to set up a static initial configuration: one in which phases present are in equilibrium and in which initial inter-block flows are zero.

In some cases, however, you may want to start a study from a point in existing production. An example might be initialization of a compositional study from the status of a black oil model at some stage in its history. As flow patterns have developed, this cannot be done by equilibration, and you must specify the initial pressures and saturations. In such a non-equilibrium initialization, a sufficient set of data is required to define the initial state. Pressures and saturations are defined using the `PRESSURE`, `SGAS` and `SWAT` keywords. Alternatively, these may be taken from an ECLIPSE 100 `RESTART` file using the `GETSOL` keyword.

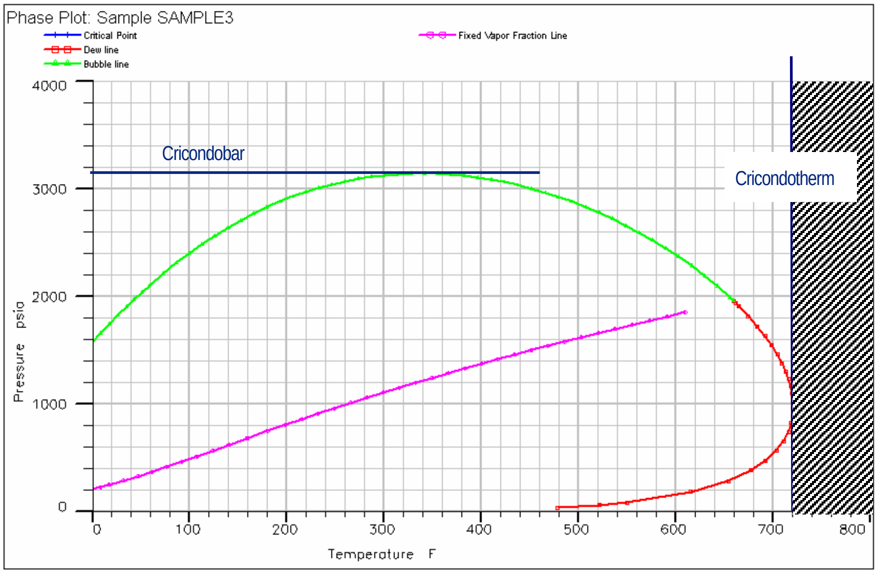
In the compositional case the liquid and vapor compositions must also be specified. Two possibilities exist:

1. Specify the liquid and vapor compositions explicitly using the `XMF` and `YMF` keywords.

2. Enter tables of composition with respect to pressure using the `XMFVP` and `YMFVP` keywords. These tables can be generated by the PVT*i* package from constant volume depletion or differential liberation experiments to ensure that the chosen liquid and vapor are close to inter-phase equilibrium.

State Transitions

A cell in a compositional run may be water-filled, or in a one or two phase hydrocarbon state. The one phase states may possess a saturation pressure - this is a pressure, usually lower than the current phase, at which a second hydrocarbon phase will appear.



For temperatures above the cricondentherm, however, such a pressure will not exist, and the cell composition will lead to a single hydrocarbon phase at all pressures.

Detecting the appearance of a two phase state in the latter case is performed using the Michelsen stability test. This is carried out at each timestep. ECLIPSE 300 uses the stability test for all cells, avoiding saturation pressure tracking. The Michelsen stability test involves the minimization of a function G* as a function of a trial phase composition Y, starting from both liquid - and vapour-like initial estimates. If a non-trivial minimum can be found with G*<0, the hydrocarbon mixture is unstable, and a flash calculation is performed to establish the phase split.

Restarts

Restarts are used for instance at the end of a history match to investigate a number of possible forecasting runs, or generally to avoid having to redo a simulation that has already been done. You may for instance have already performed a simulation from the year 2000 to the year 2020, but now want to re-run the period 2010 to 2020 with different well controls. There are two ways of restarting:

1. Using RESTART
2. Using LOAD
3. Using GETSOL

We have already mentioned how to generate restart files, and the use of restarts in ECLIPSE 300 is similar to that in ECLIPSE 100. The advantage of restart files is they are compatible across different versions of ECLIPSE. The main disadvantage is that ECLIPSE needs to re-read all the data file up to the SCHEDULE section and recalculate transmissibilities, etc. A feature that is both an advantage and a disadvantage is the ability to change some of this data for a restart run, so that the base run and the restart run are working with incompatible data.

To use the much faster LOAD option, we need some SAVE files. These are written at time 0 (just after Initialisation) and can be written at any report step. The steps at which they are written can be controlled with the SAVE, MULTSAVE, AUTOSAVE and ENDSAVE keywords. Restarts using the SAVE/LOAD facility are known as “fast” restarts. The main disadvantage is that they cannot be used across different versions of ECLIPSE.

To perform a “fast” restart:

1. The initial status is taken from the SAVE file.

2. To restart from run BASE at step 5:

3. Think a new file name root, BASE_R1

4. If the SAVE option has been used in BASE then BASE_R1. DATA need only contain:

```
LOAD
'BASE' 5 /
SCHEDULE
```

-- Continue schedule data from step 5;

END

Note that MULTIN, UNIFIN, FMTIN can go before LOAD to specify multiple/unified and formatted/unformatted cases.

The use of GETSOL to restart a run is usually for the special case of restarting a compositional run from a black-oil run. In this case the composition in each grid block also has to be specified.

SUMMARY Section

The summary section is similar to that for ECLIPSE 100. Extra keywords are available to output compositional quantities such as molar production rates and totals.

SCHEDULE Section

This section is similar to that in ECLIPSE 100. The SCHEDULE section drives the simulation by:

- Defining, opening and closing wells
- Specifying times during the simulation at which output reports are to be produced, restart files written etc.
- Modifying the default time stepping controls, convergence criteria etc., if required.

The simulation moves through a series of user defined report steps. To perform a report step, the simulator may take one or more time steps.

In the SCHEDULE section each keyword is processed as it is read, and ordering can be important.

To define a well and its mode of operation, the following keywords must be used:

WELSPECS ***(WELLSPEC)***	**Sets general specification data.** **Can be linked to DRILLING the well.**
COMPDAT ***(WELLCOMP)***	**Defines the position and properties of the well completions. Akin to PERFORATING the well.**
WCONPROD ***(WELLPROD)***	**Defines production well targets and limits. Similar to OPERATING the well.**
WCONINJE ***(WELLINJE)***	**Defines injection well targets and limits. Similar to OPERATING the well.**

The keywords in brackets and in italics refer to original ECLIPSE 300 keywords. We recommend using the keywords common to both ECLIPSE 100 and ECLIPSE 300. The compatible keywords are WELSPECS, COMPDAT, WCONPROD, WCONINJE.

Two extra well keywords may be needed in compositional runs:

1. We may need WSEPCOND to provide non-default separator conditions with WCONPROD
2. More importantly, we probably need WINJGAS to provide injection gas details with WCONINJE

Remember that if we are not injecting any gas then we can probably model our reservoir with a black-oil model. The main difference in the SCHEDULE section between black-oil and compositional runs is as follows:

- In a **black-oil** run, we need to specify how much gas we are injecting.
- In a **compositional** run we not only have to specify how much gas we are injecting but we also have to specify the composition of that gas.

As with ECLIPSE 100, `WCONINJE` sets operating controls and limits for injection wells. When gas is injected it needs to be used in conjunction with `WINJGAS`

WCONINJE

1. Well name

2. Injector fluid type WATER, GAS

3. Open shut flag for well OPEN, STOP, SHUT, AUTO

4. Method used to control well:
RATE, RESV, BHP, THP, GRUP

5. Surface flow rate target or upper limit

6. Reservoir Fluid volumetric rate target or upper limit

7. BHP target or upper limit - 10000 ATM

8. THP target or upper limit

9. THP target or limit – Default, no limit

10. Injection well VFP number

Injection Gas Composition

- The gas may be a wellstream with a defined composition (WELLSTRE).
- The gas may be provided by a named group. Gas used for fuel (GRUPFUEL) and sales (GRUPSALE) is by default subtracted first.
- The gas may be provided by the production stream of a named well.
- Advance gas (GADVANCE) will be used for re-injection prior to the gas produced by this group from the reservoir.
- The injected gas may be a mixture from a number of sources (WINJMIX). Alternatively gas from a set of sources may be taken in a specified order (WINJORD).

The injected gas composition may be provided in the following ways:

- The gas may be designated as a named wellstream, whose composition is defined explicitly in keyword `WELLSTRE`.
- The gas may be provided by the production stream of a named group. Gas used for fuel (`GRUPFUEL`) and sales (`GRUPSALE`) is by default subtracted from a source group’s available gas supply for re-injection, but the keyword `WTAKEGAS` may be used to alter the priorities for re-

injection, fuel and sales. The injection gas supply from the source group may be augmented by advance gas defined in keyword `GADVANCE`. The advance gas will be used for re-injection prior to the gas produced by this group from the reservoir.

- The gas may be provided by the production stream of a named well. The gas supply from the source well may be augmented by advance gas defined in keyword `WADVANCE`. The advance gas will be used for re-injection prior to the gas produced by this group from the reservoir.
- The injected gas may be a mixture from a number of sources. The mixture may be specified by the fractional contribution from each source (keyword `WINJMIX`). Alternatively the gas from a set of sources may be taken in a specified order (keyword `WINJORD`).

Groups with gas injection targets should have the nature of their injected gas defined in one of the above ways with the keyword `GINJGAS`. If there is not enough available gas from the source to fulfill the group's injection requirement, an additional type of gas import named "make-up gas" may be defined for the injecting group. This comes from a named wellstream, which has an infinite supply and will make up the extra requirement to fulfill the group's injection target.

In general, therefore, the composition of the injected gas can vary with the injection rate and the supply of available gas from the sources. When the gas comes from a limited source (namely a group or well production stream), the injection gas is taken from the following supplies in the stated order:

1. The source's advance gas stream (if defined), up to its specified maximum rate.
2. The source's production stream, minus the specified fuel usage and the gas reserved for sale if the source is a group (unless the priorities are re-ordered by `WTAKEGAS`).
3. The injecting group's make-up gas stream.

- By default, a group will inject produced gas at the required rate even if that rate is greater than the gas production rate.
- The WAVAILIM keyword limits the available gas supply.
- If a limited source of gas is shared between two or more injection groups, the injection calculation may have to be iterated to re-allocate any unused but available gas.

If the injecting group does not have a make-up gas stream defined, there may possibly be a shortfall between its injection requirement and the injection gas supply. By default, the group will continue to fulfill its injection requirement and the shortfall between supply and injection rate will show up as a negative excess in the gas accounting tables. However, if the `WAVAILIM` keyword is entered the injection rate will be limited by the available gas supply. A shortfall between supply and injection demand will cause the group to reduce its injection rate to match the available gas supply; the group will then be under availability control for gas injection.

When the injected gas composition can vary with the injection rate (when there is make-up or advance gas, or when the injection stream is defined by `WINJORD`), the injection calculation may be iterated a number of times until the estimated injection rate (from which the composition is determined) and the actual injection rate converges. Similarly, when the `WAVAILIM` keyword is entered and a limited source of gas is shared between two or more injection groups, the injection calculation may have to be iterated a number of times to ensure that, if any groups inject less than their allocated share of available gas, their unused share of available gas is re-allocated to other groups. The maximum number of these iterations, and their convergence tolerance, is controlled by items 3 and 4 of keyword `GCONTOL`

WINJGAS

1. Well name

2. Injector fluid type GAS, STREAM, MIX, WV, GV

3. Name of well or mixture for injection fluid

4. Name of Make-up well or stream

5. Separator stage

The WELLINJE keyword specifies both what the well is injecting and the injection rate. Note that we recommend using the combination of WCONINJE and WINJGAS instead of WELLINJE, for compatibility with ECLIPSE 100.

WELLINJE

1. Well name

2. Injector fluid type WAT, GAS, STREAM, MIX, WV, GV

3. Addition description for injection fluid

4. Method used to control rate:
WAT, GAS, BHP, THP, RV, WG, RE, TM, CW, GR

5. Oil flow rate target or upper limit

6. Water flow rate target or upper limit

7. Gas flow rate target or upper limit

8. BHP target or limit - 10000 ATM

9. THP target or limit - 10000 ATM

10. Reservoir volume rate target or limit

11. Wet gas rate target or limit

12. Re-injection target fraction (or voidage) - 1

13. Re-injection target type WELL, GROUP

14. Name of well or group on item 13

15. Sales Gas rate (better to use GCONSALE, GRUPSALE)

16. VFP index for well

17. Make-up gas name

18. Surface or reservoir re-injection - S

19. Stage used to define separator injection, 0 = ALL

20. Target molar rate

22… 24 (steam)

Some other additional well keywords are available in ECLIPSE 300 that are not available in ECLIPSE 100, for instance WELLWAG.

WELLWAG

1. **Well Name**
2. **Type of cycle: T (time in days), M (months) Y (years)**
3. **First fluid to be injected: W or G**
4. **Injection Period for first fluid**
5. **Second fluid to be injected: default**
6. **Injection Period for second fluid**

- **If injection rates are re-specified using WELLINJE (or WCONINJE), then WELLWAG has also to be re-specified.**
- **OK with WELLTARG.**

Another keyword only available in ECLIPSE 300 is WECONMF, which set economic limits on the production of individual components. It can for instance be used to limit the mole fraction of nitrogen or carbon dioxide in the production wells. If the limit that you set is exceeded, then the actions are similar to those for the WECON keyword:

- The worst-offending connection in the well is closed.
- The worst-offending connection and all connections below it in the well are closed. Here, “below” is interpreted as “further from the wellhead according to the connection ordering”. The connection ordering may be specified in the `COMPORD` keyword.
- The well itself is closed.

Well lists and Actions

In all these well keywords, the first field is a well name, or a list of well names. A well name root, enclosed in quotes and ending with an asterisk (*), can be used to refer to several wells in one record. Alternatively a well list name, enclosed in quotes and beginning with an asterisk (*), may be used. Well lists are constructed with the keyword `WLIST`. The options in well keywords that expect well names are therefore:

- A name of a single well,	e.g. ‘WELL_AB_5’
- a well name root,	e.g. ‘WELL*’
- a well list,	e.g. ‘*EAST’

where we have already defined (for example)

```
WLIST
‘*EAST’  NEW    ‘WELL_AD_3’  ‘B5’ ‘WELL_FX8’  ‘INJ2’ /
/
```

In the example above, we have created a new well list called ‘*EAST’ that contains 4 wells called ‘WELL_AD_3’, ‘B5’, ‘WELL_FX8’ and ‘INJ2’. Wells can be added to or deleted from the list, and can be moved from one list to another.

Well lists can be dynamic as well as static, so that can be reset automatically at the beginning of each time step. For example, the list might be made up of all the wells in a particular group that have a water cut greater than 0.7. Another example is

```
WLISTDYN
  '*HIGHGOR'   1* WGOR > 100 /
/
```

which will create a list of all the wells whose GOR is greater than 100. The wells in this list can change from time step to time step, as the GOR of each well changes. The automatic updating of a dynamic well list at the end of every time step may be disabled by setting item 2 of this keyword to 'OFF ' and leaving items 3 to 5 blank. The contents of this well list then become static. To reverse this action, set item 2 to 'ON' (and leave items 3 to 5 blank).

ACTION keywords

Another way of controlling wells is using the family of ACTION keywords.

The ACTION keyword marks the start of a set of SCHEDULE section keywords that are to be stored for later processing when a specified condition is satisfied. The idea behind action is:

IF

(condition)

THEN

(actions).

The ACTION keyword specifies a field condition for triggering an action. The `ACTIONG`, `ACTIONR`, `ACTIONW` and `ACTIONS` keywords offer greater flexibility, and specify actions triggered by group, region, well and segment conditions respectively. The `ACTIONX` keyword discussed below is even more general. The set of keywords must be terminated with the `ENDACTIO`[35] keyword. The keywords between the `ACTION` and `ENDACTIO` keywords are processed when the condition defined in the `ACTION` keyword is satisfied.

Any keyword specifying data for wells, groups or separators may be placed between `ACTION` and `ENDACTION`. Each action initiated with the ACTION keyword is executed only once[36], at the end of the timestep during which its

---

[35] As ECLIPSE only reads the first 8 characters of a keyword, it is usual and acceptable to type `ENDACTION` instead of `ENDACTIO`.

[36] If you use the `ACTIONX` keyword, you can specify how many times you want the action to be performed.

triggering condition is first satisfied. However, any number of action keyword sets may be declared, each with its own triggering condition; the maximum number being limited to MAXACT in `ACTDIMS` item 1. Each action keyword set must be bracketed by a pair of `ACTION(G,R,W,S)` and `ENDACTIO` keywords, and is distinguished by its action name defined in item 1 of the keyword. If an `ACTION` family keyword is re-entered with the same action name as a previously declared action, the action keyword set is overwritten by the new information.

It is possible to nest actions by including the definition of the inner action within the keyword set of the ‘outer’ action (that is before its `ENDACTIO` keyword). This offers you great flexibility, but care should be exercised

The example below shows two action keyword sets. The first action (named ACT1) will open well PROD5 when the field gas oil ratio is greater than 3.0 and change the well oil production rate limits to 2000. The second action (named ACT2) will end the run when the average pressure in the field falls below 3000 psi

```
ACTION
    ACT1 FGOR > 3.0 /
WELOPEN
    PROD5 OPEN /
 /
WELTARG
    'P*' ORAT 2000 /
 /
ENDACTIO

ACTION
    ACT2 FPR < 3000.0 /
END
ENDACTIO
```

ACTIONX

The idea behind ACTIONX is:

IF

(condition1 AND condition2 OR condition3 …)

THEN

(actions).

In the `ACTION(G,R,W,S)` type keywords the single triggering condition compares the current value of a quantity against a constant value defined in the keyword. For example, in `ACTIONW` the condition might be that a well's GOR is greater than 3.0. In addition to this, the `ACTIONX` keyword also allows a comparison against the current value of another quantity. For example, a condition might be that a well's GOR is greater than the current value of its controlling group's GOR or than the average field GOR.

Multiple triggering conditions may be combined in the `ACTIONX` keyword using Boolean AND and OR operators to form the condition set. Conditions on quantities associated with well connections, well segments, wells, groups and regions may thus be combined in a single `ACTIONX` keyword.

Conditions may be set on the combined properties of a static (see `WLIST` keyword) or dynamic (see `WLISTDYN` keyword, ECLIPSE 300 only) list of wells. Grouping wells together using lists for the purposes of defining controlling conditions in an `ACTIONX` keyword offers more flexibility than conventional well groups. For example, a well in ECLIPSE 300 may belong to more than one list (see also `WELLDIMS` keyword item 11).

Conditions may be set on the day, month and year that the simulation has reached. Such a condition may be used to model the seasonal availability of workover and drilling rigs or to prevent the `ACTION` being triggered before or after a specific date.

Please note that:

- The order of the items in the quantities is similar to the way summary mnemonics are defined, i.e. the mnemonic is the first item and it is then followed by a well or group name, etc. This is to be contrasted with the order of these items in the `ACTION(G,R,W, S)` type keywords.
- A condition consisting of constant quantities on the left and right hand sides is not permitted. A condition may however consist of a constant quantity on the left hand side and a variable quantity on the right hand side.
- No checks are in place on the type of quantities that are compared in a condition. So for example, a (meaningless) condition on a region's pressure being less than a connection's water cut would be allowed.
- If sufficient conditions are met for the `ACTIONX` keyword to trigger the processing of its set of SCHEDULE section keywords, then details of those conditions that are true will be written to the print file.
- Combined rates, totals and ratios for all the wells in a well list may be written to the summary file using an appropriate group summary mnemonic (see the table in the ECLIPSE Reference Manual entry for `ACTIONX`) followed by the well list name.
- If a well keyword (for example `WELTARG`) is placed between `ACTIONX` and `ENDACTIO`, instead of entering the name of a specific well in the keyword you may enter a question mark (?). ECLIPSE then applies

the keyword data to whichever well (or wells) are involved in triggering the action.

- If there is more than one condition in the action that concerns wells, different sets of wells may trigger different conditions. These set of triggering wells are combined logically in the same manner as the conditions themselves. The question mark in the well keywords will then apply to this combined set of wells. Note that if conditions are combined with logical AND operators, there may be no wells that trigger every condition and thus the well keywords will not have any effect, even though the overall action has been triggered.
- Full checking of the keywords entered with an action keyword cannot be performed until the action is actually implemented, since it is possible to use wildcards in many of the keywords. However, before a simulation run is attempted the data can be run in `NOSIM` mode. This then does whatever checks it can on the keywords within any action keyword blocks that have been defined. All the most common types of ‘grammatical’ and typographical errors will be found, but problems resulting from wildcards feeding inappropriate well/group names to keywords are not found.
- An action may be triggered on a grid block quantity by defining a region to consist of one grid block (keyword `FIPNUM`) and selecting a region quantity in a condition

Examples

Example 1

The action named ACT1 reduces the liquid rate target by 20% of all wells starting with ‘PR’ whose GOR exceeds that of the FIELD when the gas production rate of the FIELD exceeds 50,000 Mscf/day. The action will be repeated at the end of each time step whilst the condition set is true.

```
ACTIONX
    ACT1 100000 /
    GGPR FIELD > 50000 AND  /
    WGOR 'PR*' > GGOR FIELD /
/
WTMULT
    '?' LRAT 0.8 /
 /
ENDACTIO
```

Example 2

The action named ACT2 opens well PR-A5 when the combined water cut of all the wells in list *LIST1 exceeds 0.7 and when the water production rate of list *LIST1 exceeds the water production rate of either list *LIST2 or *LIST3. Action ACT2 is performed once only.

```
ACTIONX
    ACT2 1 /
    GWCT ‘*LIST1’ > 0.7           AND   /
    ( GWPR ‘*LIST1’ > GWPR ‘*LIST2’ OR    /
    GWPR ‘*LIST1’ > GWPR ‘*LIST3’     ) /
/
WELOPEN
    PR-A5 OPEN /
 /
ENDACTIO
```

Example 3

The dynamic well list *HIGHWCT contains all wells that have a water cut exceeding 0.8. In any year between March and October, the action WORKOVER will be triggered if the list *HIGHWCT contains more than 4 wells. This action will set an economic limit on the wells in the *HIGHWCT list such that they will be worked over. The WORKOVER action also contains a nested action WECONOFF that is triggered when the simulation advances past October. WECONOFF stops any further workovers in the winter by re-specifying the WECON keyword with a high water cut limit.

```
WLISTDYN
    '*HIGHWCT' '*' WWCT > 0.8 /
/
ACTIONX
    WORKOVER 10000 /
    MNTH  .GE. MAR  AND /
    MNTH  .LE. OCT  AND /
    GMWL '*HIGHWCT' .GE. 4 /
/
```

```
WECON
    '*HIGHWCT' 2* 0.75 2* CON /
/
ACTIONX
    WECONOFF 1 /
    MNTH .GT. OCT /
/
WECON
    '*' 2* 1.0 2* CON /
/
ENDACTIO
ENDACTIO
```

Example 4

The action named DELAY opens well PR-A5 when the simulation has advanced past the 1st June 2021 and the FIELD’s water cut exceeds 0.8.

```
ACTIONX
    DELAY 1 /
    GWCT ‘FIELD’ > 0.8  AND /
    DAY  > 1         AND /
    MNTH > JUN        AND /
    YEAR > 2021          /
/
WELOPEN
    PR-A5 OPEN /
 /
ENDACTIO
```

Separators

Separators are in general designed to separate three phases: oil, water and gas. In ECLIPSE 300 we assume that the water has already been removed and that we are only separating oil and gas. The composition of the feed is known, as is the temperature and pressure of each separator stage.

If no separator is specified, then the default is a single-stage separator to standard conditions. However a single-stage separator is not usually optimal and oil recovery can be improved by having more stages[37].

In ECLIPSE 300, you can have a field separator that is used to report total field production, and test separators attached to individual wells or to groups of wells.

To define a separator for a well, use WSEPCOND, specify the name of the well (or the group of wells) and the name of the separator associated with the well. This separator name must have been previously entered with `SEPCOND`. If a well is defined in `WSEPCOND` as having its own separator, then that separator is used for that well.

- If WSEPCOND is not used, and the well can trace its parentage to a group which has a default separator specified (see SEPCOND), then this is used. If this is not the case, the separator conditions specified with FIELDSEP is used. If FIELDSEP was not entered, a single flash to standard conditions is used.

The SEPCOND keyword

SEPCOND defines separator conditions.

1. **Separator name**
2. **Group for which separator is default**
3. **Stage index**
4. **Stage temperature**
5. **Stage pressure**
6. **Liquid output destination - FEED OF NEXT STAGE**
7. **Vapor output destination - CONVERT TO GAS VOLUME**
8. **K-value table number (If K - values to be used)**

---

[37] As oil is worth more than gas, separators are usually designed to optimise oil and not gas recovery.

9. Gas-plant number (if gas plant to be used)

10. Surface equation of state number

11. Temperature for NGL evaluation

12. **Pressure for NGL evaluation**

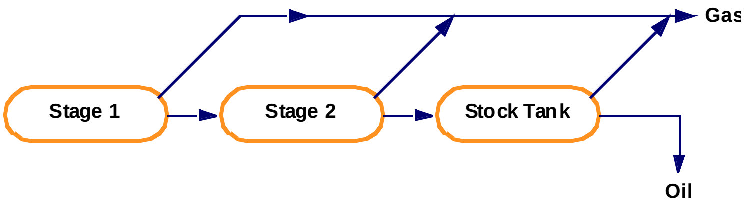
SEPCOND can be used to define the separator stages for a well or for a group of wells.

- Each line of SEPCOND data introduces a new stage, specifies the name of the separator condition, and sets the temperature and pressure. Several lines may be used to build up a multi-stage separator condition. Any number of stages can be specified, although the default limit is 5. The default limit on the number of stages per separator is 5. This may be increased using the 5th argument of the WELLDIMS keyword. The default limit on the number of separators (including the FIELDSEP separator) is 4. This may be increased using the 8th argument of the WELLDIMS keyword.
- After the stage temperature and pressure, the next argument defines the destination of the liquid output from the separator. For all but the last stage in a separator, this is to a later stage, usually the next stage. The default destination is 0, which implies the next stage for all except the last stage, and the stock tank for the last stage.
- The following argument defines the destination stage of the vapor output from the field separator. This is usually accumulated with the stock tank or field separator vapor, the volume rate being taken by conversion to a volume at standard conditions. This is done when the destination stage is set to 0, which is the default.

Example:

```
SEPCOND
SepA  G   1   80 815 /
SepA  G   2   60 14.7 /
/
```

The following picture describes a three stage separator, with the stock tank as the third stage



and the keyword required for this separator might be:

```
SEPCOND
SEP ' ' 1   80 815  /
SEP ' ' 2   80  65  /
SEP ' ' 3   60 14.7 /
/
```

If neither WSEPCOND not SEPCOND is used, the all wells will use the separator defined by FIELDSEP. Several lines of `FIELDSEP` data may be used to build up a multi-stage separator. As with SEPCOND, each line defines the stage index, the stage pressure and temperature, the destination of the liquid (usually the next stage) and the destination of the vapor (usually stock tank)

At each stage in SEPCOND or FIELDSEP, a K-value table rather than an equation of state can be used to perform the flash to the stage temperature and pressure. If multiple equations of state are available in the model, then you can choose which one should be used for this stage. The equation of state can be defaulted, in which case the fluid from a well is flashed using the equation of state for the cells in which the well is completed. If an equation of state index is specified, this forces the use of a given surface equation of state.

- **The rates and compositions for the oil and gas of up to 9 stages can be output in the SUMMARY section.**
- **The gas from any stage of a separator can be used as a source of re-injection fluid - see GINJGAS, WINJGAS, GRUPINJE, WELLINJE, WINJMIX, and WINJORD.**

Gas Plants

- **A gas plant may be used instead of a separator stage - item 9 of keyword SEPCOND, item 7 in FIELDSEP**
- **Keyword**

  GPTABLE - for Oil recoveries

  GPTABLEN - for Oil and NGL recoveries

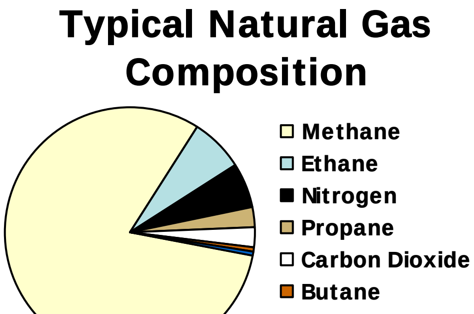
  GPTABLE3 - for Oil, NGL and Gas recoveries

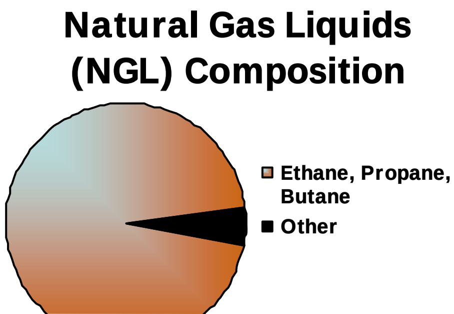
A gas plant table may be used instead of a flash calculation for a separator stage (see item 9 of keyword `SEPCOND`). In almost all cases, a single stage only will be required. Gas plant tables are defined with keyword `GPTABLE`, `GPTABLEN` or `GPTABLE3`. The table defined with `GPTABLE` specifies the oil recovery fraction (the number of moles of liquid output per mole of feed) for each component as a function of the 'heavy' mole fraction of the feed. The components that comprise the heavy fraction are also defined in the table.

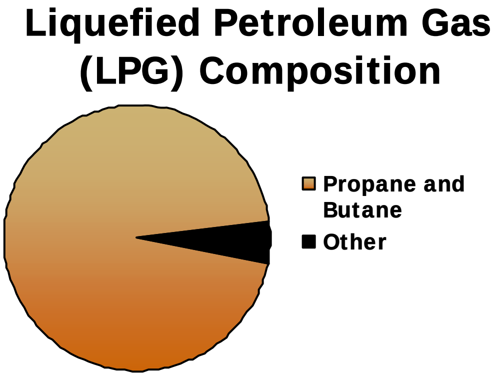
The `GPTABLEN` keyword should be used instead of `GPTABLE` if NGL (natural gas liquid) output is also required. The table defined with `GPTABLEN` specifies both the oil recovery fractions and the NGL recovery fractions for each component as a function of the heavy mole fraction of the feed. The `DNGL` keyword should also be used to set the partial densities in the NGL stream.

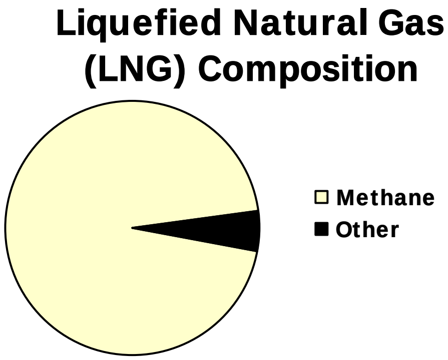
The `GPTABLE3` keyword should be used instead of `GPTABLE` or `GPTABLEN` if you want to specify recovery factors for oil, gas and NGL and you don't want these recovery factors to add up to 1. You can use this keyword to reduce or exclude one or more components in the post separator oil, NGL or gas streams. This might arise if for instance you are removing all the H2S or N2 from the production stream, in which case you would use `GPTABLE3` and define the recovery factor for that component to be zero in all phases. The `DNGL` keyword should also be used to set the partial densities in the NGL stream.

The following pie charts show the composition of a typical natural gas, of NGL, and of LPGs and LNGs. Other liquefied gases are Compressed Natural Gas (CNG) and Gas-to-Liquid (GTL).






Liquefied Petroleum Gas (LPG) Composition


Liquefied Natural Gas (LNG) Composition

Recovery Plant

- The recovery plant option takes all the gas produced from the field and processes this into NGL and remaining gas.
- RECOVERY keyword

The Recovery Plant option takes all the gas exported from the field and processes this into NGLs and remaining gas. All other field quantities, such as GOR and gas-injection are reported prior to this processing. The aim of this facility is to model processing of the gas produced by the reservoir through facilities such as coolers, which can extract additional liquids from the stock tank gas.

Recovery plant calculations are turned on if the `RECOVERY` keyword is encountered. The recovery plant table may be specified in the SOLUTION or SCHEDULE sections, and may be re-specified during the SCHEDULE section.

The `RECOVERY` keyword has two arguments, followed by a table of one or more rows of data.

The first argument specifies the lower component index used to define the ‘heavy’ fraction. This defaults to the last component.

The second argument specifies the upper component index used to define the ‘heavy’ fraction. This defaults to the last component.

The first column of the table is a list of possible concentrations of the heavy fraction. There other columns (one for each component) list the NGL recovery fractions of that component as a function of the ‘heavy’ mole fraction. The recovery fraction is the number of moles of NGL per mole of feed for each component.

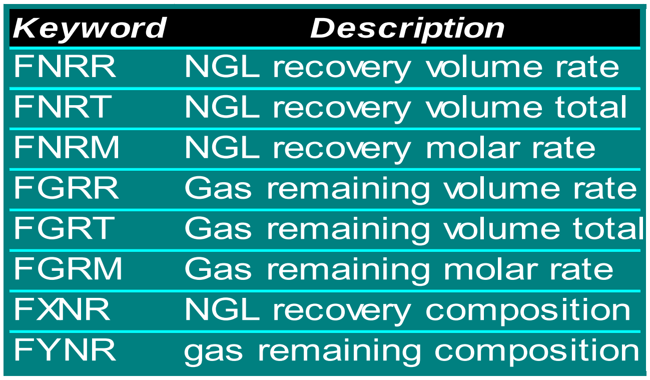
The defaults for items 1 and 2 imply that the recovery plant table is normally of recovery fractions against the mole fraction of the last component in the feed.

```
RECOVERY
7 9
-- heavy  CO2   N2    c1  c2  c3 c4-6 cz7 cz8 cz9
   0.0    0.0  .002 .001 .45 .65  .98   1    1   1
   0.2    0.0  .002 .001 .48 .68  .99   1    1   1
/
```

The feed used by the recovery table is the export gas from the field, which is the total gas production minus gas used for fuel and for re-injection.

The volume of NGL produced is obtained using Amagat’s law, adding partial molar volumes. The molar density used is that entered with DNGL.

The rate of production of recovered NGLs and of the remaining gas is reported in the printed output, and may be obtained from the SUMMARY section using the following keywords:



Keyword	***Description***
FNRR	NGL recovery volume rate
FNRT	NGL recovery volume total
FNRM	NGL recovery molar rate
FGRR	Gas remaining volume rate
FGRT	Gas remaining volume total
FGRM	Gas remaining molar rate
FXNR	NGL recovery composition
FYNR	gas remaining composition

Group Controls

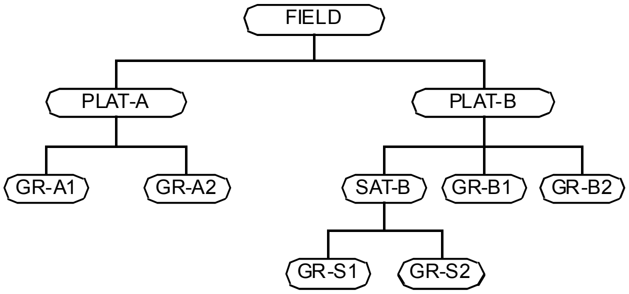
The multi-level grouping hierarchy

- **Each WELSPECS specifies a group name,**
- **FIELD is default name and always exists as the first group.**
- **Other groups are children of this group.**
- **A simple case has one layer of groups, but GRUPTREE will set up a more complex hierarchy.**

Each well must belong to a particular group, which is named when the well is first declared with keyword `WELSPECS`. Rate targets and limits, and economic limits, can be applied to each group and to the whole field. This provides a standard three-level (well - group - field) control hierarchy, where controls and limits can be specified independently at each level.

If controls or limits are required on more than three levels, a highly flexible multi-level hierarchy can be built up using the keyword `GRUPTREE`. This keyword declares additional groups that do not contain wells, but instead act as 'parents' to other groups at a lower level.

An example of a five-level hierarchy is shown below:



The field occupies the highest level, level 0. PLAT-A and PLAT-B are node-groups at level 1. The groups at level 2 are all well-groups except for SAT-B which is a level-2 node-group. Groups GR-S1 and GR-S2 are level-3 well-groups subordinate to SAT-B. GR-A1 and GR-A2, and their respective wells, are subordinate to PLAT-A. GR-B1 and GR-B2, and their respective wells, are subordinate to PLAT-B. GR-S1 and GR-S2, and their respective wells, are subordinate to both SAT-B and PLAT-B. When the wells are included (below levels 3 and 4), the hierarchy has five levels in total

Group production control

- **Groups can be used to impose collective controls and limits.**
- **The overall oil, water, gas or liquid production rate of a group or field meets a specified target.**
- **The individual wells produce in proportion to a specified GUIDE RATE or their PRODUCTION POTENTIAL subject to obeying their own flow and pressure limits.**
- **Group name roots can be used for all group keywords except for GRUPTREE**

Selected groups at any level in the hierarchy (including the field) can be made to produce at a target value of any one of the following quantities

- Oil production rate
- Water production rate
- Gas production rate
- Liquid (oil + water) production rate
- Reservoir fluid volume rate
- Wet gas rate (which is the volume that the hydrocarbon mixture would occupy at standard conditions if it were an ideal gas)
- Production balancing fraction (which limits the group's reservoir fluid volume production rate to the specified fraction of its reservoir fluid volume injection rate).
- Calorific value rate.

- **The target or upper limit is specified as oil rate, water rate, gas rate, and liquid rate.**

- **The target Rate is apportioned between individual wells so that each well (and group) produces in proportion to the guide rate or potential, subject to its individual flow and pressure limits.**

The control target is set using keyword `GCONPROD`. The group's target rate is apportioned between the individual wells in proportion to each well's specified guide rate. A guide rate can optionally be defined for any phase; oil, water, gas, liquid or reservoir fluid, using keyword `WGRUPCON`. If the phase differs from the phase under group control, the guide rate is translated into a guide rate for the controlled phase using the well's production ratio for the previous time step. Thus, for example, the target oil production rate of a group can be apportioned among its subordinate wells such that each well produces similar amounts of liquid. This can be done by giving each well the same guide rate for the liquid phase.

If a well's guide rate has not been specified, it is set at the beginning of each time step to a value that depends on the well's production potential. The production potential is defined as the instantaneous production rate that the well would initially have in the absence of any constraints on flow rate, at the current grid block conditions. By default, the well's guide rate is set equal to its production potential of the phase under group control. This enables, for example, a group's target oil production rate to be apportioned among the individual wells such that the wells produce in proportion to their potentials. Alternatively, the keyword `GUIDERAT` can be used to specify the coefficients of a general formula for well guide rates as a function of their oil, water and gas production potentials. This can enable, for example, wells with high water cut to be given a progressively smaller guide rate as they water out.

- **When there is enough production potential the group target will be met.**
- **If not, the group is passive, and targets become limits.**
- **When a group's rate is exceeded, group production is imposed at the limiting rate.**

The individual wells can be subject to their own flow and pressure constraints. For example, if a well would violate its bottom hole pressure limit when producing its full share of the group's production target, the well will operate at its bottom hole pressure limit. The production rates of the other wells will increase in proportion to their guide rates (or potentials) to meet the group's target, as long as they do not violate any of their own flow or pressure limits. A well that is producing its full share of the group's production target is said to be under group control, while a well constrained by its own flow or pressure limits is said to be under individual control.

You can prevent certain wells from coming under group control. These wells will continue to operate according to their individual flow or pressure constraints, regardless of any group flow target.

- **When there is enough production potential the group target will be met.**
- **If not, the group is passive, and targets become limits.**
- **When a group's rate is exceeded, group production is imposed at the limiting rate.**

Drilling queues

QDRILL defines a drilling queue for wells. If a group cannot meet its target, the first well in the drilling queue subordinate to that group will be opened.

The drilling queue can be either

- **sequential, from which wells are opened in the order in which they were placed in the queue,**
- **or prioritized, from which wells are opened in decreasing order of their drilling priority.(WDRILPRI or DRILPRI).**

WDRILTIM defines the time to drill a well

At some stage in the simulation, it may happen that all the group-controlled wells in the group have hit one of their constraints and have either dropped out of group control or have been closed. The group can then no longer meet its flow target, and its production rate will decline. This situation can be postponed by placing additional wells in a drilling queue, using either keyword `QDRILL` or keyword `WDRILPRI`. When a group can no longer meet its production target, the simulator will scan the drilling queue and open a suitable well. The well must be subordinate to the group that is unable to meet its target, but not subordinate to any lower level group that is operating at its own production target or limit for the same phase.

The drilling queue may either be a sequential queue, from which wells are opened in the sequence in which they were placed in the queue, or a prioritized queue from which wells are opened in decreasing order of their drilling priority. Well drilling priorities may be set manually in keyword `WDRILPRI` or calculated from their current potentials according to a function defined with keyword `DRILPRI`.

The rate of opening new wells from the drilling queue can be limited by specifying the time taken to drill each well with keyword `WDRILTIM` and allocating drilling rigs to groups with keyword `GRUPRIG`.

Fuel and Sales Gas

By default, all the production of a well, separator or group is available for re-injection.

If GRUPSALE or GRUPFUEL specified, this is removed first.

Remainder is available for re-injection.

If this is insufficient to meet injection requirement, a make-up or imported gas may be added.

Fuel and sales gas may be specified as a rate, a fraction or a combination.

Summary of Group keywords

- **GRUPFUEL** - Specifies the fuel rates of the gas produced from a group.
- **GRUPGR** - Specifies the user guide rates for a group.
- **GCONINJE** - Specifies the injection control data for a group. Both the nature of the fluid to be injected and the target and limiting rates at which injection is to occur are defined.
- **GRUPLIM** - Specifies group economic limits, alias for GECON.
- **GCONPROD** - Specifies the production targets and limits for a group.

- **GRUPSALE** - Specifies the sales rate for the gas produced from a group.
- **GRUPTREE** - Sets up a grouping hierarchy, and introduces a new group if necessary - specifies the names of the ‘son’ and ‘father’ groups.
- **GSATCOMP -** Specifies the composition of the oil or gas to be injected or produced by a satellite group.
- **GSATINJE** - Specifies the rate at which oil or gas is to be injected by a satellite group.
- **GSATPROD** - Specifies the production rates for a satellite group.
- **GECON -** Specifies the economic limits for a group.
- **GCONPRI -** Sets the production rate limits for groups using the Prioritization Option.
- **GTADD** – Add or subtract from group target limits

Example data sets

A number of example data sets are provided with every release of a new version of ECLIPSE 300. These can be found in the directory on your system in which the software is installed[38]. Within this directory, look for …./ecl/2006.1/e300/data. This will contain at least the following files:

CASE1.DATA	SPE3 condensate problem
CASE2.DATA	Restart from CASE1
CASE3.DATA	Chappelear and Nolen SPE black-oil coning study
CASE4.DATA	SPE5 volatile oil problem
CASE5.DATA	Kazemi et al dual porosity system
CASE6.DATA	Faults, grid file, initial GOC
CASE6G.DATA	INCLUDE file for CASE6
CASE7.DATA	10m slimtube using LAB units
CASE8.DATA	Gas Plants
CASE9.DATA	Gas diffusion
CASE10.DATA	Black-oil using PVTi-generated tables
CASE11.DATA	Group controls
CASE12.DATA	more complex model, with more wells
CASE13.DATA	Odeh's SPE1 problem
CASE14.DATA	SPE6 problem
CASE15.DATA	Carter-Tracy aquifer and volatile oil
CASE16.DATA	Numerical aquifer and volatile oil
CASE17.DATA	Use of K-values
CASE18.DATA	Gas-Water option
CASE19.DATA	Multiple EoS regions
CASE20.DATA	Gas field
CASE21.DATA	Use of tracers
CASE25.DATA	Velocity-dependent relative permeabilities

Most of the new releases of ECLIPSE 300 since 2001 also have a separate subdirectory (2001a,2002a, 2004a, 2005a, 2006.1) that contains datasets that demonstrate some of the new facilities in that release.

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[38] If you don't know where that directory is, ask whoever installed our software on your machine, or on a Unix or Linux system type "which @e300" and you should get …../ecl/macros/@e300.exe.

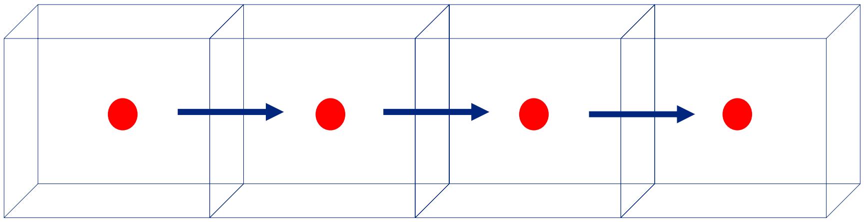
18. ECLIPSE 300 Advanced Topics

In this section we will review a number of specialized topics and see how they are modeled in ECLIPSE 300. The topics we shall review are:

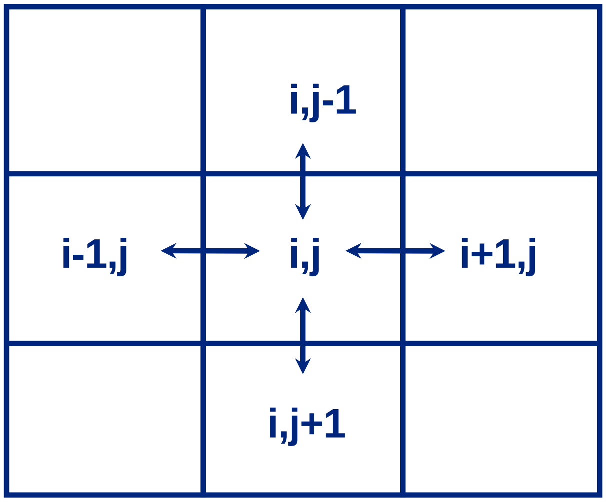
- **Grid Orientation, 9-point and MPFA**
- **Numerical Dispersion**
- **Near-Critical Oil and Gas Relative Permeabilities**
- **Convergence Reports**
- **ECLIPSE 100/200 Miscibility Model**
- **Diffusion**
- **Components in water**
  - **CO2 Solution in water**
  - **CO2 Sequestration**
  - **Gas-Water Systems**
    - **Calorific values**
  - **Multi-component water**
- **Tracers**
- **Transport Coefficients**
- **Gas flow near wells**
  - **Non-Darcy flow**
  - **Gas pseudo-pressure**
  - **Velocity-dependent rel perms**
- **Multi-Phase Flash**
- **Solids**

19. Grid Orientation, 9-point and MPFA

The basic assumption in finite difference simulation is that flow is from the center of one cell to the center of the next cell. The transmissibility between the two cells is calculated across the face joining the two cells.



The default discretization uses a five-point discretization in two dimensions or a seven point discretization in three dimensions.



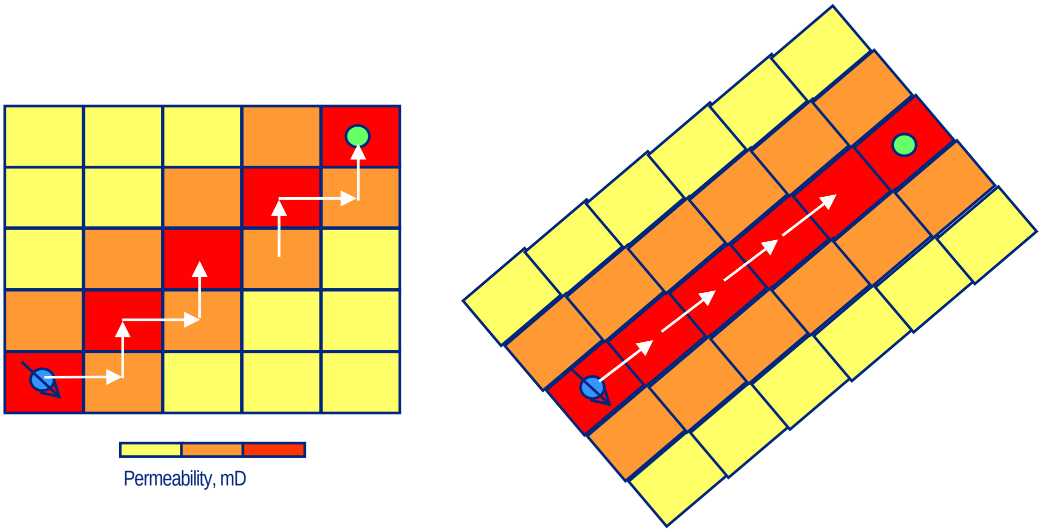
However when the grid is non-orthogonal, or the flow is not aligned with the principal directions of the grid, then the solution accuracy may be compromised by this discretization.

There are two independent schemes in ECLIPSE that address grid non-orthogonality and grid orientation effects only. The two schemes should not be used together.

1. The `NINEPOIN` scheme reduces the effect of grid orientation effects for flows not aligned with the principal grid directions, but does not account for non-orthogonality.
2. The Multi Point Flux Approximation (MPFA) scheme is a rigorous treatment of grid non-orthogonality and tensor permeability. The MPFA nine-point scheme is activated by the `MPFA` keyword.

9-point Scheme

The flow between cells only goes though cell faces, there is no flow across corners between cells. Consider two possible simulation grids linking an injector and a producer. Assume the permeability is favorable for flow between the injector and the producer.



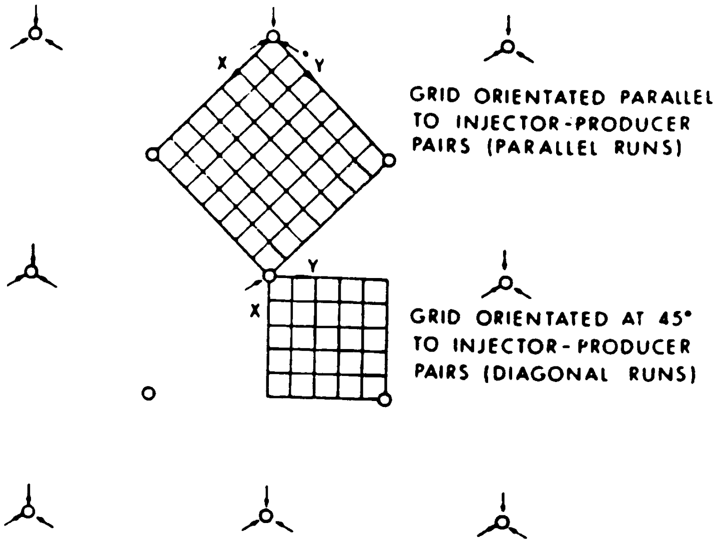
- In the left-hand case above, the injected water will need 8 steps to reach the producer, and will sweep more of the reservoir.
- In the right-hand case the injected water will need 5 steps to reach the producer, and will sweep less of the reservoir

Grid Orientation definition:

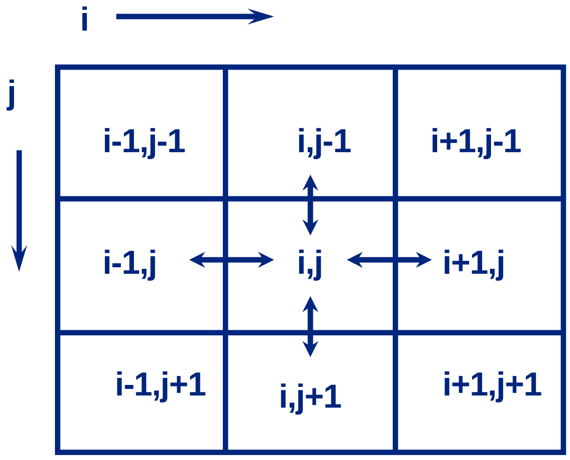
“Where the orientation of the grid relative to the flow affects the results.”

Refinement in the grid do not converge the results to one solution

Consider two different grid orientations that could be used to simulate fluid displacements in 5-Spot symmetry elements



In the first (upper) case, the grid is orientated parallel to injector-producer pairs. We will call this a "parallel grid"[39]. The second (lower) grid is oriented at 45 degrees to the injector-producer pairs. We will call this a "diagonal grid". In both grids the distance between the injector and the producer is the same. Remember however that fluids only usually flow between neighbouring cells[40].



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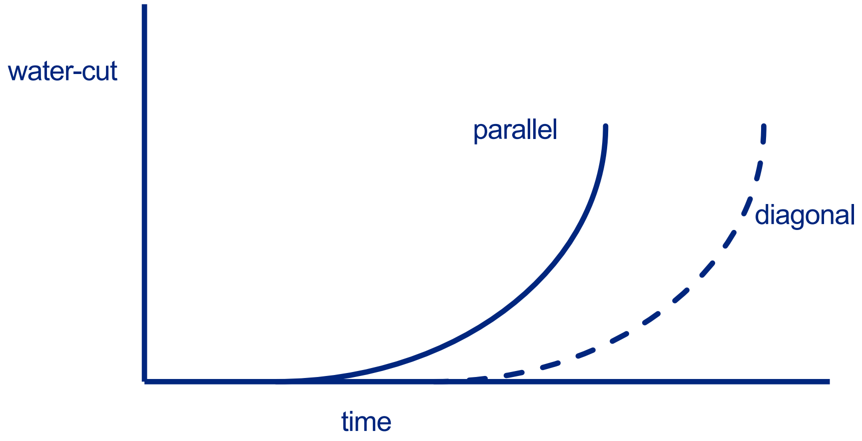
[39] The word "parallel" in this section is not related to running the simulator in parallel across different processors or different computers.

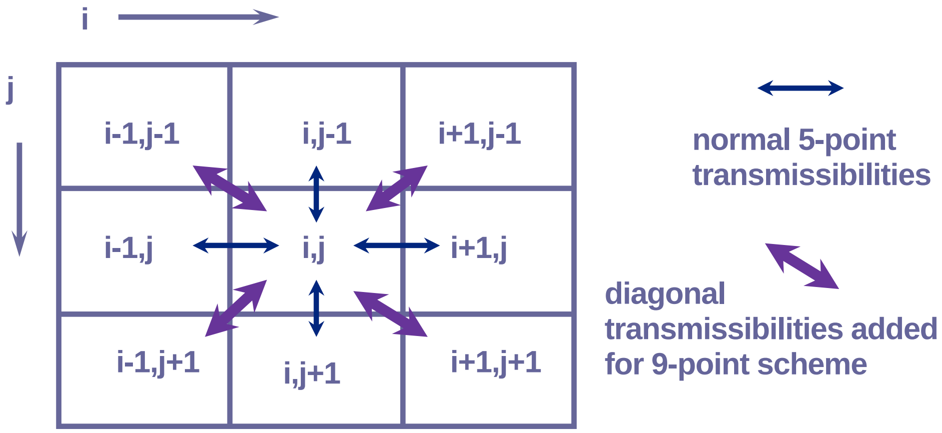
[40] One exception that you already know is the case of non-neighbour connections, for instance in LGRs.

We would therefore expect fluids to flow faster from cell (i,j) to cell (i+1,j) than from cell (i,j) to (i+1,j+1). If we run a simulation with each grid and plot the breakthrough time at the production well, then as expected the diagonal grid will have fluid breakthrough at a later time than the parallel grid. The diagonal grid will also recover more oil than the parallel grid model as it will sweep a greater volume of the reservoir.



The `NINEPOIN` keyword in the `RUNSPEC` section activates a nine-point scheme based on adding diagonal transmissibilities in the areal (XY) direction in order to reduce grid orientation effects when the flow is not aligned with the grid. Additional non-neighbor connections are added between diagonal neighbors. The flows between each cell and its eight neighboring cells (in the areal dimension) are computed using a two-point approximation to the pressure gradient. The standard five-point transmissibilities are first obtained from data entered in the `GRID` and `EDIT` sections, and these are then modified to obtain the nine-point transmissibilities.

- **ECLIPSE 300 uses a modified version of the 9-point algorithm by Yanosik and McCracken to reduce grid orientation effects in high mobility ratio displacements.**



- **Latest versions follow Shiralkar and Stephenson.**

- **NINEPOINT keyword**
- **Adds diagonal transmissibilities in the XY plane as non-neighbour connections.**
- **Total x- and y- transmissibilities are preserved.**
- **Flow computed using 2-point pressure gradient approximation**

Within the code, transmissibilities that fall outside the normal pattern are stored as non-neighbor connections. There is an extra computing cost associated with these terms, and the nine-point option is best used only for injection of highly adverse mobility fluids where the grid orientation effect is a problem. The run time will be increased due to the large number of additional NNCs created between diagonal neighbors.

The option is invoked by using the `NINEPOIN` keyword in the RUNSPEC section. The nine-point transmissibilities will then by default be calculated across the entire grid. However, by using the `NINENUM` keyword in the GRID section, you can choose to apply the scheme only in nominated regions of the reservoir.

- NINEXZ keyword in XZ plane
- NINEYZ keyword in YZ plane

You can choose to apply the `NINEPOIN` scheme in the XZ or YZ planes with the `NINEXZ` and `NINEYZ` keywords. By default the 9-point scheme is applied in the XY plane. You may want to apply the scheme in a cross-section if for instance you want to more accurately model the flow orthogonal to a horizontal well.

This option is specifically designed to account for grid orientation effects and is not designed to deal with discretization errors arising from grid non-orthogonality

9-point Example

Quarter 5-Spot Pattern

Water injector and liquid rate producer
Well to well distance is 1866.7619 feet

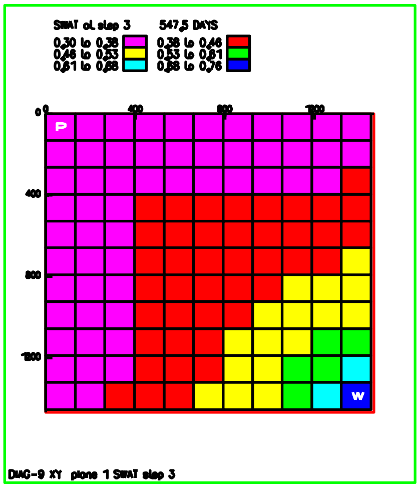
11 x 11 grid in both Diagonal and Parallel

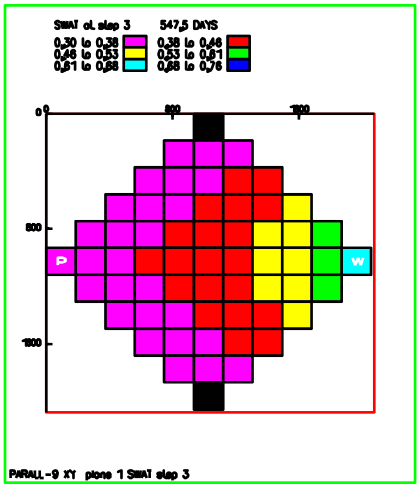
Run both Diagonal and Parallel with both 5-point and 9-point

Examine the ECLIPSE 300 data sets
- Diag-5.data
- Diag-9.data
- Parall-5.data
- Parall-9.data

Run the 4 data sets with ECLIPSE 100

Plot and evaluate the results with ECLIPSE Office using files:
- LINE.GRF – Line plots
- PARALL.GRF – 2D grid plots



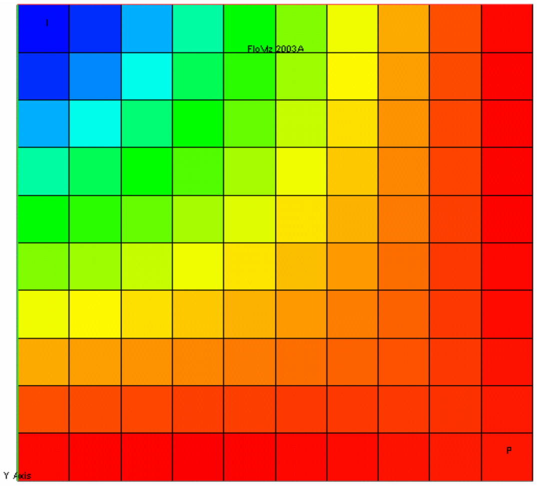


A second example also shows grid orientation effects:

Diagonal Grid:

- 1200 x 1200 x 30 foot reservoir
- ∆x = ∆y = 120 feet
- x 10 x1 grid
- Water injector in corner 1,1
- Liquid rate producer in corner 10,10

Water saturation display:

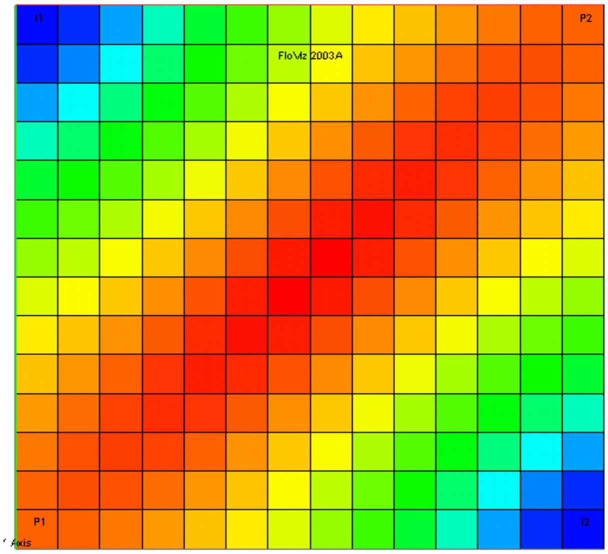


Parallel Grid:

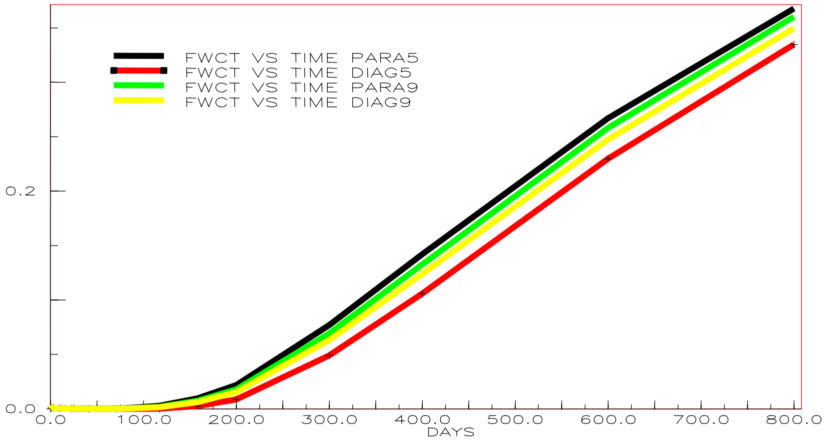
- 1680 x 1680 x 30 foot reservoir

- $\Delta x = \Delta y$ = 120 feet
- 14 x 14 x1 grid
- Water injector in corners 1,1 and 14,14
- Liquid rate producer in corners 1,14 and 14,1

Water saturation display:



Running both models with and without the NINEPOINT keyword gives the following results for water cut:



GRID ORIENTATION EFFECTS, FIG. 1, WATER CUTS

As you can see, using the nine-point scheme does not completely eliminate grid orientation effects, but makes the results from parallel and diagonal grid much closer.

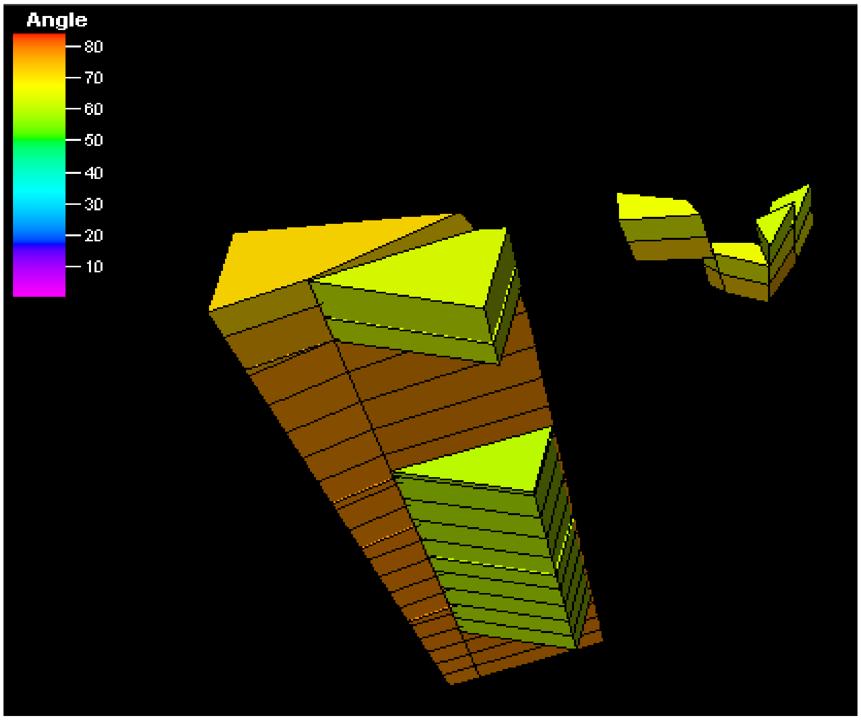
Multi Point Flux

Transmissibility equations assume the cells are near orthogonal, and flow equations assume that flow is orthogonal to the face between cells. It is possible to create models in which these assumptions are not valid:

1. The cells may not be orthogonal
2. The flow pattern may not be the same as the grid pattern

Non-orthogonality

Some common causes of non orthogonal cells are that the grid model is created either using faults as I & J trends or in cases of complex horizon and fault intersections.



Tensor permeabilities

Full tensor permeabilities are sometimes required to describe complex reservoirs.

- Tensor permeabilities:
  Upscaling of geological models to reduce the number of gridblocks to reasonable values can produce tensor permeabilities.

Tensor permeabilities also arise in complex cross-bedded systems as the dip direction is often not along the axis system.

- Conventional reservoir simulation ignores the tensor permeabilities and approximates using a diagonal tensor with principal axes along the grid axes.

Given a detailed heterogeneous reservoir description at the geological scale, upscaling is normally carried out to reduce the model size to one suitable for reservoir simulation. These upscaling procedures will generally create full tensor permeabilities, even if the permeabilities in the fine geological grid are not represented as tensors.

Example showing small grid blocks with scalar permeabilities that have to be upscaled into one large grid block with tensor permeability.

```
10. 10. 10. 10. 10. 10. 10.   100. 100. 100. 100. 100. 100. 100.
10. 10. 10. 10. 10. 10.   100. 100. 100. 100. 100. 100. 100.
10. 10. 10. 10. 10.   100. 100. 100. 100. 100. 100. 100. 10.
10. 10. 10. 10.   100. 100. 100. 100. 100. 100. 100.  10. 10.
10. 10. 10. 10.100. 100. 100. 100. 100. 100. 100.  10. 10. 10.
10. 10. 10.100. 100. 100. 100. 100. 100. 100.  10. 10. 10. 10.
10. 10.100. 100. 100. 100. 100. 100. 100.  10. 10. 10. 10. 10.
10. 100. 100. 100. 100. 100. 100. 100.  10. 10. 10. 10. 10. 10.
100. 100. 100. 100. 100. 100. 100. 10. 10. 10. 10. 10. 10. 10.
100. 100. 100. 100. 100. 100.   10. 10. 10. 10. 10. 10. 10.100
100. 100. 100. 100. 100.   10. 10. 10. 10. 10. 10. 10.   100.
100. 100. 100. 100. 100.10. 10. 10. 10. 10. 10. 10.   100. 100.
100. 100. 100. 100.  10. 10. 10. 10. 10. 10. 10.  100. 100. 100.
100. 100. 100.10. 10. 10. 10. 10. 10. 10.   100. 100. 100. 100.
100. 100.10. 10. 10. 10. 10. 10. 10.  100. 100. 100. 100. 100.
100.  10. 10. 10. 10. 10. 10. 10. 100. 100. 100. 100. 100. 100.
```

Full tensor permeabilities also arise in complex cross-bedded systems where the dip directions will not in general coincide with a local coordinate direction. A further case for full tensor permeabilities is in the modeling of fractured systems.

Conventionally, reservoir simulators ignore the full tensor nature of the absolute permeability and assume the permeability can be represented by a diagonal tensor whose principal axes coincide with the local coordinate axes. This allows the construction of the usual 5 point discretization in 2D or 7 point in 3D which can be solved efficiently in the simulator. Introducing a full tensor permeability extends the stencil of the discretization scheme to 9 points in 2D and either 19 or 27 points in 3D.

- **Full Tensor permeabilities can be used in the Multi-point Flux Approximation (MPFA)**

- **Control volume discretisation of Aavatsmark *et al.***
- **No flow between diagonal neighbours as in NINEPOINT**

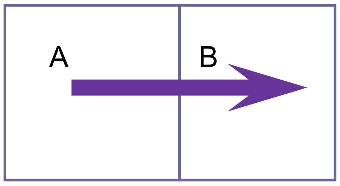
- **Keywords PERMXX, PERMYY, PERMZZ : diagonal**
- **Keywords PERMXY, PERMYZ, PERMZX : off-diagonal**

- **Limitation : only 2-point connections are made across faults**

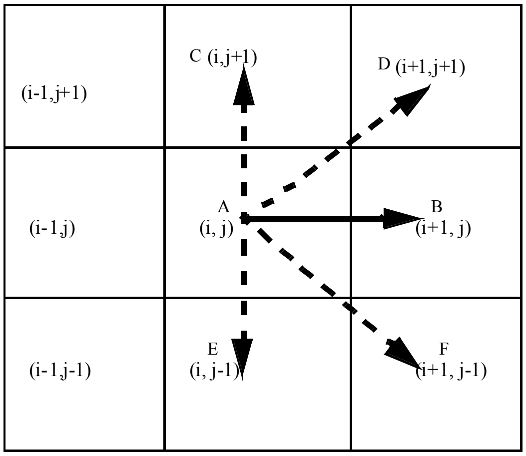
ECLIPSE 300 allows a full tensor description of the absolute permeability. The permeability tensor may either be supplied by a pre-processor by upscaling the properties on the geological model, or else it may be entered by keywords `PERMXX`, `PERMYY`, `PERMZZ` (which describe the diagonal components) and `PERMXY`, `PERMYZ`, `PERMZX` to describe the off-diagonal components.

The flow equations arising from the permeability tensor description are constructed using a Multipoint Flux Approximation (MPFA). The transmissibilities are calculated by the control volume discretization due to Aavatsmark et al. The MPFA can only be used in corner point geometry, not block centered geometry.

The standard two-point flow between cells A = (i, j) and B = (i + 1, j)



is generalized when using MPFA to also depend on steering terms from the neighboring cells C, D, E and F.



Similarly in 3D, the flow between any two cells may depend on up to 16 steering transmissibilities and this leads to a 19 or 27 point scheme.

Note that the flows between adjacent cells depend on steering terms from adjacent cells, but there are no flows created between cells which are diagonal neighbors as in the `NINEPOIN` scheme.

The discretization scheme is selected by the `MPFA` keyword. The MPFA is a rigorous treatment of both cell non-orthogonality and tensor permeability. Even for a diagonal isotropic tensor, the MPFA will generally lead to a 9 point discretization in 2D in order to remove the bias of grid non-orthogonality and grid orientation effects.

- MPFA is expensive in cpu time and should only be used in regions of the reservoir where it is needed. The keyword MPFANUM defined those cells for which it will be used.
- Multipoint transmissibilities can be imported instead from the unstructured grid module in FloGrid using the MPFNNC keyword.
- MPFA discretization reduces to 5- or 7-points when both
-     - the grid system is orthogonal and
-     - the permeability tensor is diagonal

The MPFA discretization is applied by default across the entire grid. The MPFA or nine point discretization reduces to a standard two point flux scheme (that is, a five-point scheme in 2D or a seven-point scheme in 3D) if the grid is sufficiently orthogonal.

For example, the MPFA discretization reduces to 5- or 7-points when both

- the grid system is orthogonal and
- the permeability tensor is diagonal

In general, when the grid is either non-orthogonal or is a full tensor then a 9-point (2D) or 27 point (3D) discretization results. It is possible to control the application of the MPFA scheme based on a cell non-orthogonality indicator. Essentially for grids which are nearly orthogonal we want to apply the MPFA discretization only in regions of high non-orthogonality to reduce the CPU time. You can apply the MPFA in selected regions by using the `MPFANUM` keyword. The MPFA is only applied where the `MPFANUM` array equals 1. Further control may be achieved by applying the discretization only within nominated local grids using the `MPFA` keyword within a `CARFIN` and `ENDFIN` pair.

You can also use the MPFA on unstructured grids generated by a pre-processor such as FloGrid. The multipoint flux non-neighbor connections are exported to ECLIPSE through the `MPFNNC` keyword.

Restrictions

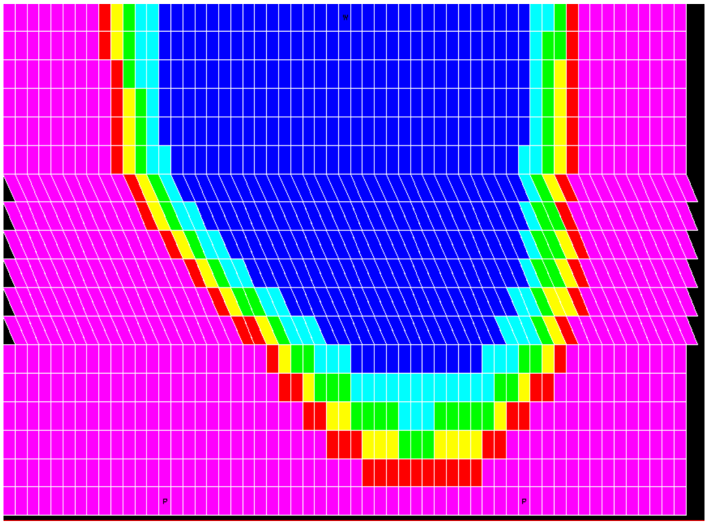
The MPFA discretizations cannot at present be used with:

- The parallel option (keyword `PARALLEL`)
- Velocity dependent relative permeabilities (keyword `VELDEP`)
- Cell coarsening (keyword `COARSEN`)
- The Diffusion option (keyword `DIFFUSE`)
- The Thermal option (keyword `THERMAL`)
- Radial geometry (keyword `RADIAL`)

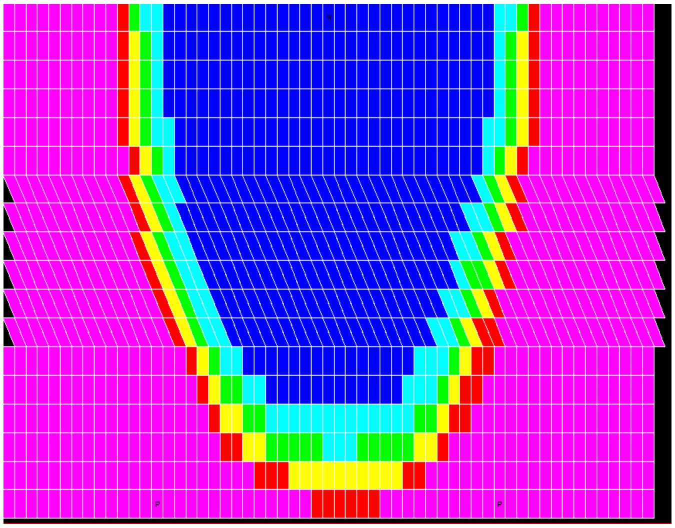
MPFA Example

The effect of using `MPFA` can be seen in the example below. This is an areal view of a reservoir with a water injector in the center of the top row and two oil producers symmetrically placed in the bottom row. The field is homogeneous: all physical properties the same in each block.

We would expect the water front to move symmetrically towards the producers. However as we can see from the first picture the water tends to follow the orientation of the grid blocks. As the grid blocks move to the right then the water moves to the right.

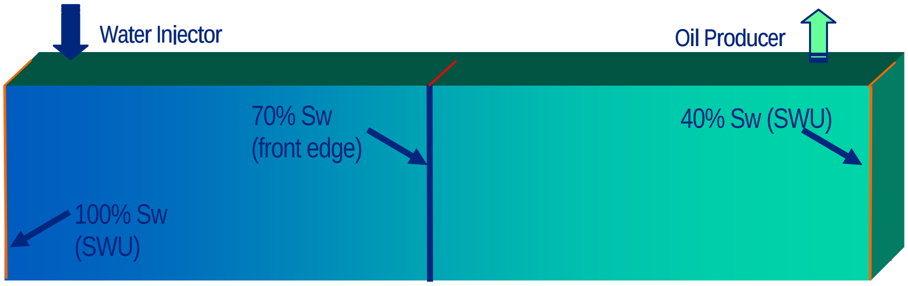


In the second picture we have used MPFA to correct the non-orthogonality of the grid. The flow of water is now much more symmetric.



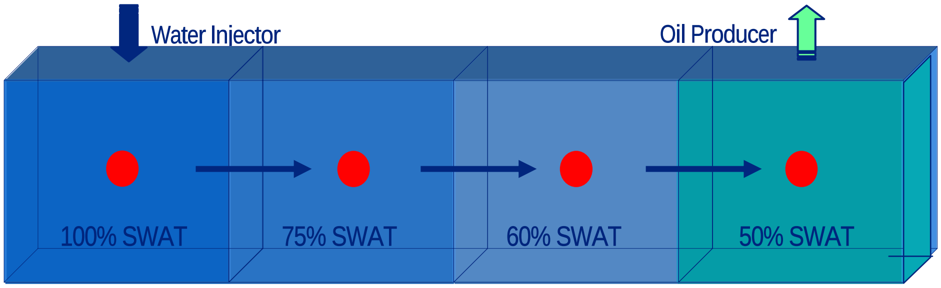
20. Numerical Dispersion

To understand numerical dispersion we first look at a simple case of water injection into a homogeneous reservoir.



Suppose the water saturation at the water injector is 100% and the water saturation at the producer is 40%. Midway between them the front edge of the injected water is at 70% saturation.

Now compare this with a simulator model of the same process[41].



Because we are dealing with grid block and with a single saturation within each grid block, we can only have an average saturation within a grid block. In this case the simulator is calculating for instance that the grid block containing the oil producer has 50% water instead of the 40% in the reservoir. The general result of this averaging over the block volume is numerical dispersion.

Numerical dispersion occurs both in black-oil and in compositional simulation, but the effects can be more severe in compositional simulation.

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[41] Note that the well is in a slightly different position in the two cases. This does not affect the discussion.

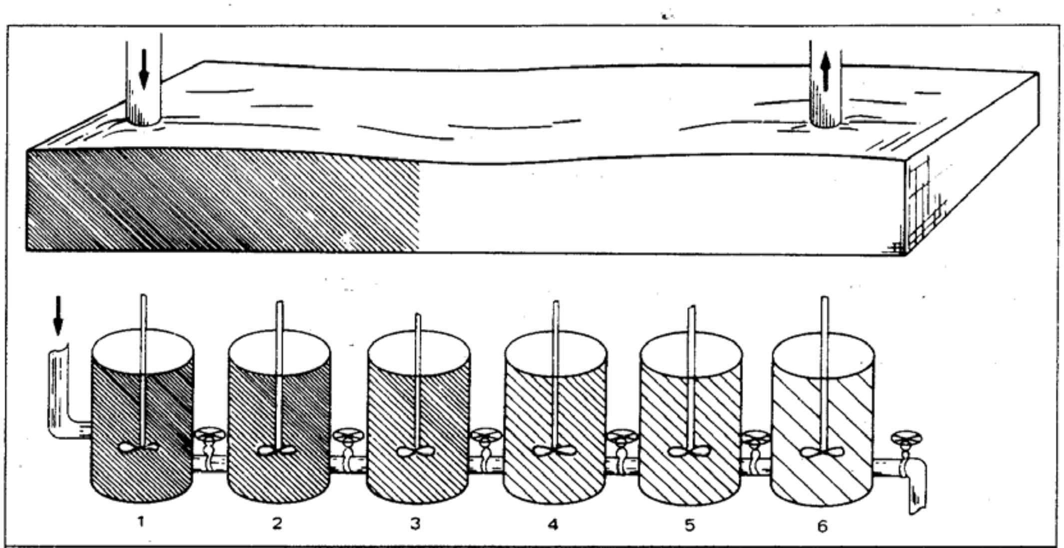
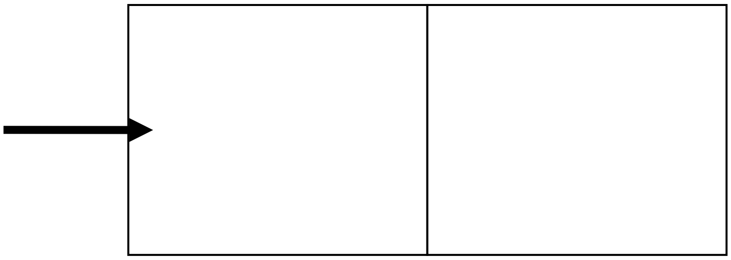


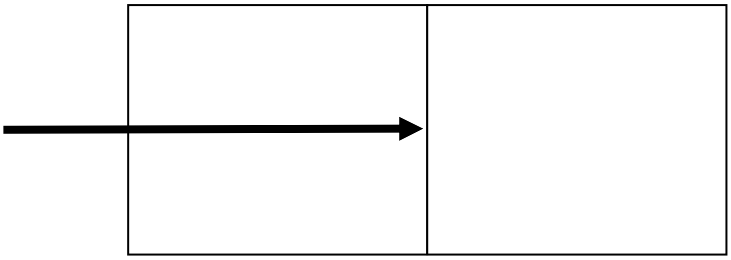
Fig. 2.1—A well-stirred tank analog of a simulator grid system.

Creating a model of the reservoir by dividing it into grid blocks of finite size creates dispersion. The cause of dispersion is that fluid entering one side of a grid block is instantly available at the other end of the grid block, so that oil, water and gas move infinitely fast within a grid block. If the saturation of the fluid in that block is greater than its critical saturation, the fluid will move into the next gridblock downstream. As soon as the fluid is in the downstream block, it will move infinitely fast within that block.

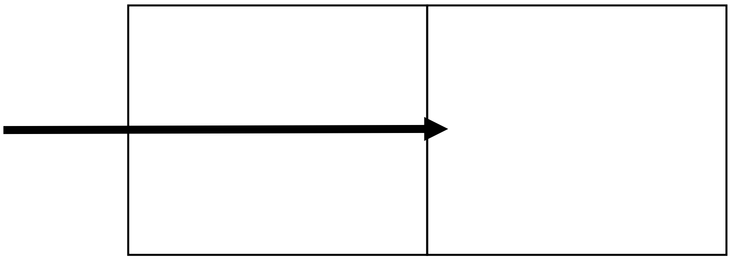
1) Water enters one side of a grid block



2) Water instantly available at the other side



3) Water available for flow into the next block



The bigger the grid blocks, the bigger the dispersion.

In compositional simulation, dispersion of components can have an important effect on the resulting properties of fluids within the grid blocks, as compositional effects often depend crucially on the relative concentration of components.

- In the field or laboratory - dynamic miscibility achieved over “small” distance.
- In simulator, injected solvent must travel through several (or a few) grid blocks to mix with oil to achieve dynamic miscibility. But the size of each grid block may be 100’s of feet/meters.
- One-dimensional condensing-gas drive (Coats) needed 40 to 80 blocks between wells for results to stabilize.

The following pictures show the results of simulating CO2 injection into an oil. The models all cover the same area of a quarter of a five-spot. The gas injector is in the top right-hand corner and the producer is in the bottom left-hand corner[42]. The solution displays are of gas saturations, and all results are at the same simulation time.

The solutions are for grid of varying dimension: 3x3, 10x10, 20x20, 40x40 and 100x100.

The 3x3 grid shows that (at that time step) in the grid block containing the producer gas saturation has reached almost 50%. The injection grid block has a gas saturation of about 75%, whereas in all other models the injection grid block has a gas saturation of almost 85%. Lowest gas saturation is 50% in the other diagonal corners. Mean gas saturation is 58%.

The 10x10 grid also has almost 50% gas saturation in the producer grid block. Lowest gas saturation is 36% in the other diagonal corners. Mean gas saturation is 61%.

The 20x20 grid also has almost 45% gas saturation in the producer grid block. Lowest gas saturation is 11% in the other diagonal corners. Mean gas saturation is 61%.

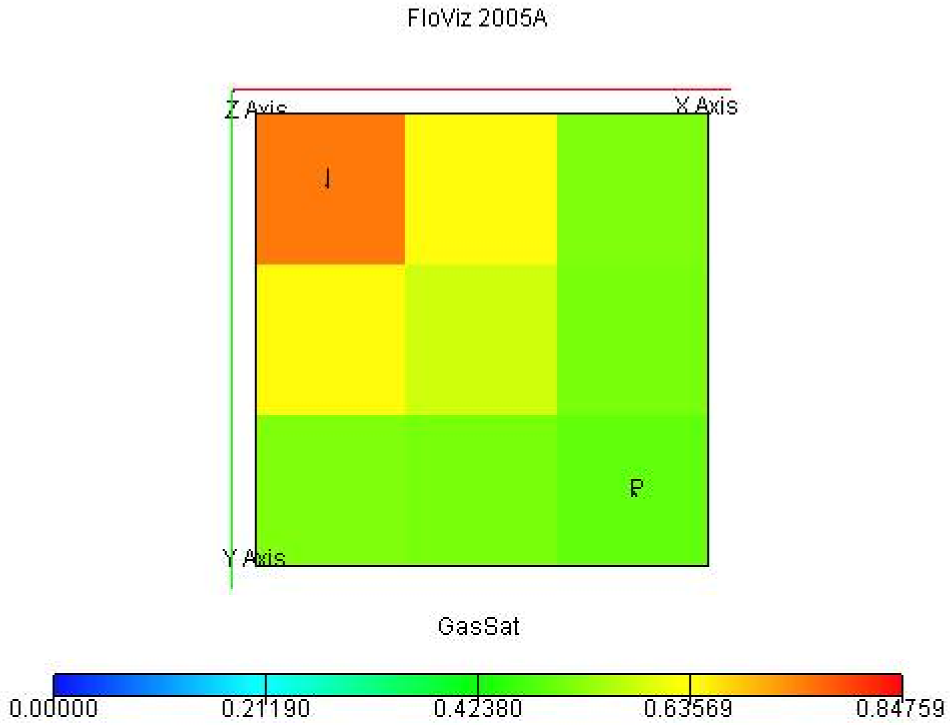
The 40x40 grid also has about 40% gas saturation in the producer grid block. Lowest gas saturation is 7%. Mean gas saturation is 58%.

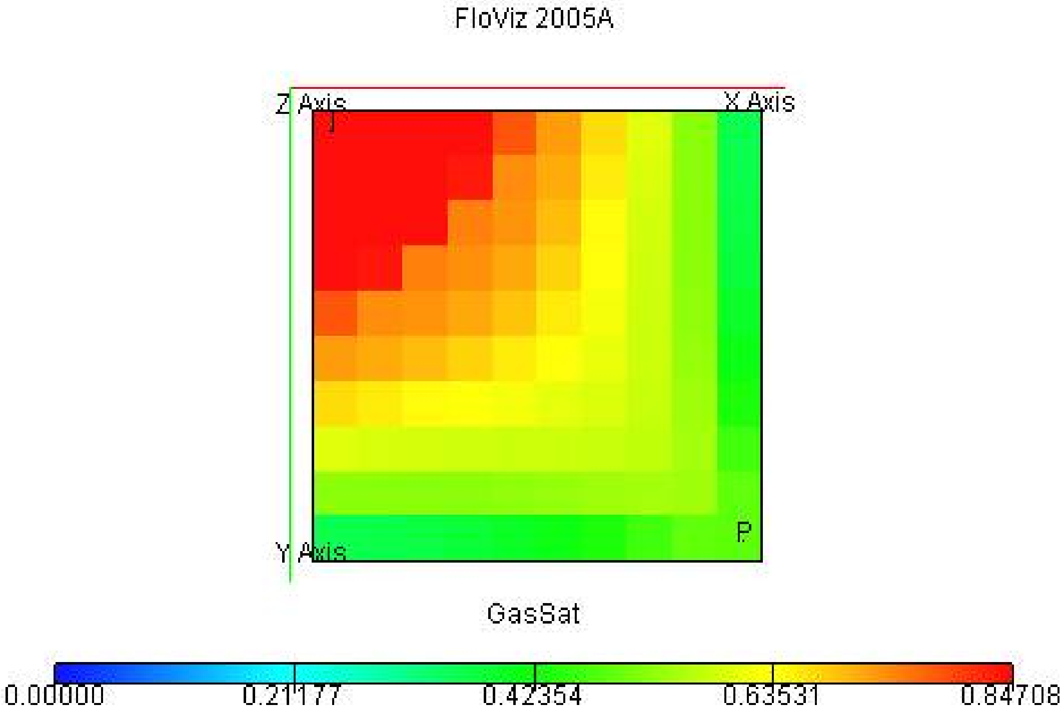
The 40x40 grid also has about 40% gas saturation in the producer grid block. Lowest gas saturation is 7%. Mean gas saturation is 46%.

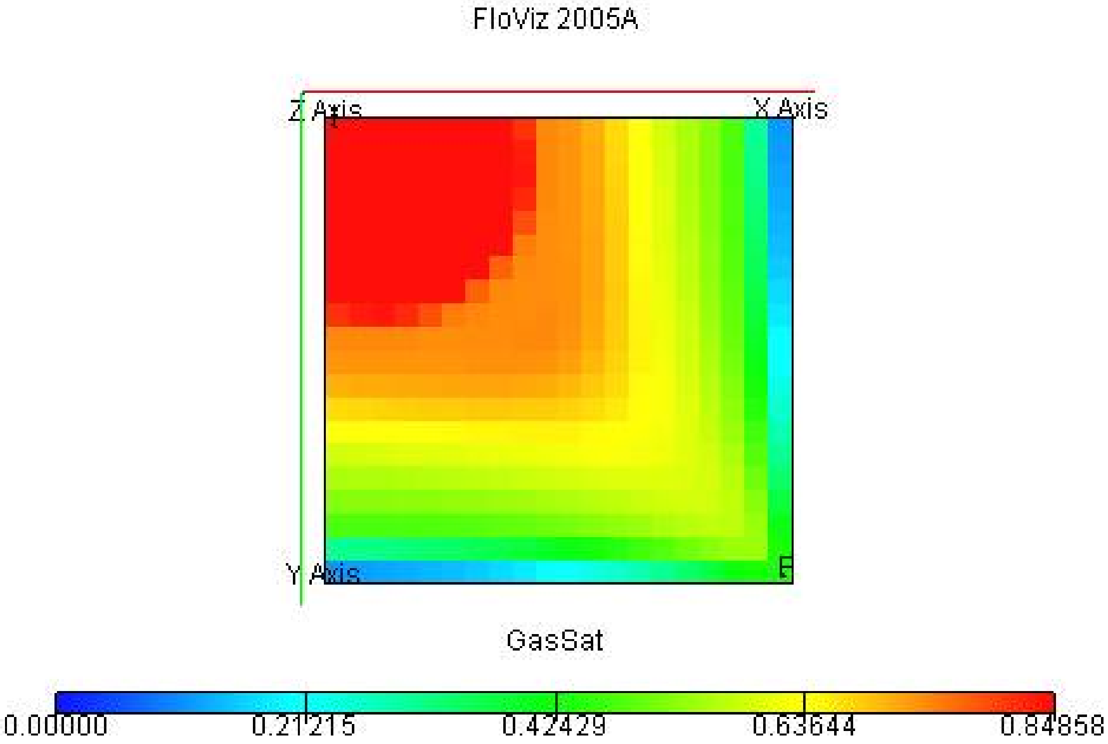
As a result, gas breakthrough times, total oil recovery and other observables all vary from model to model.

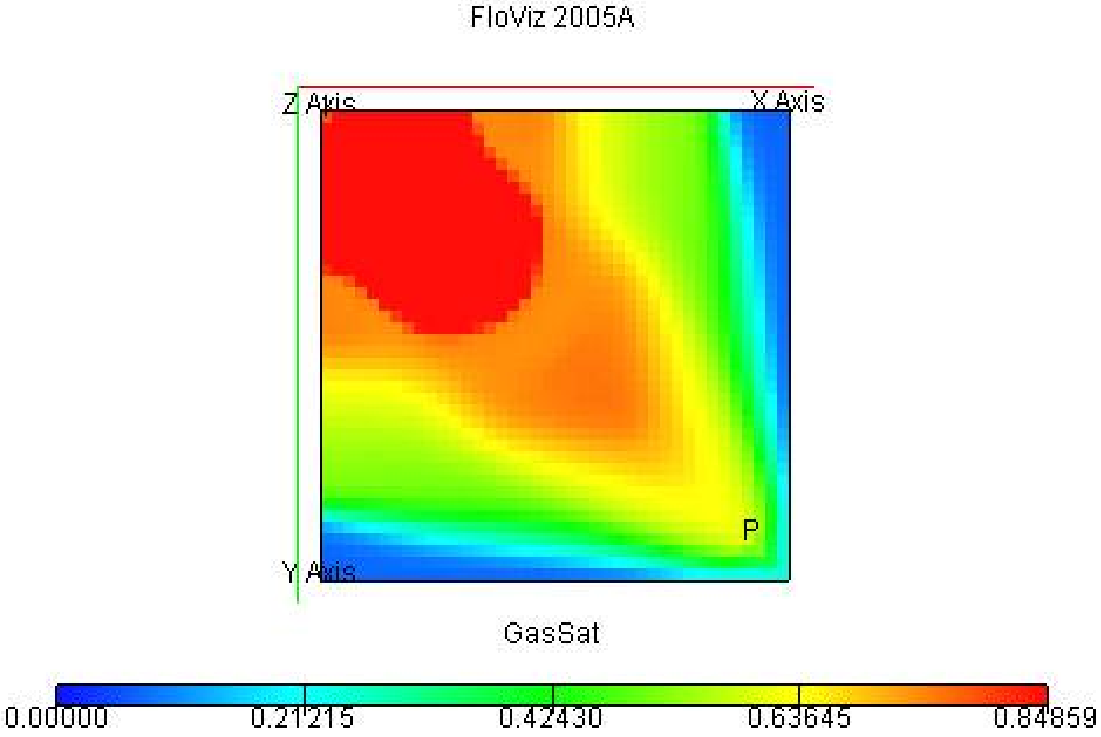
---

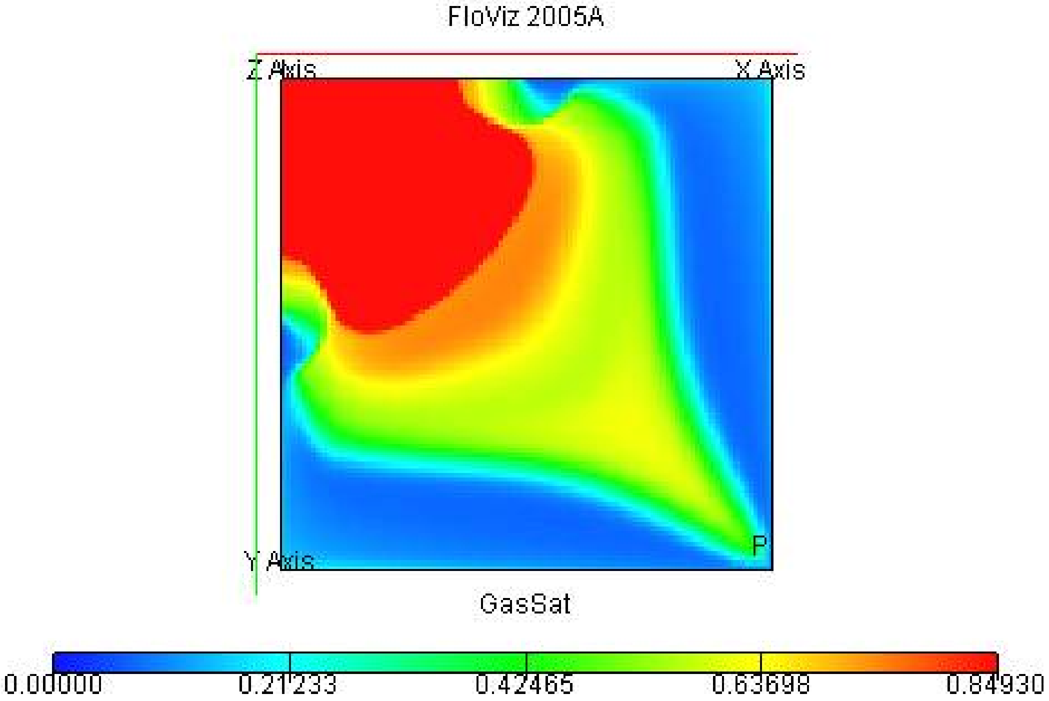
[42] Because the well is in the center of the grid block and the size of the grid blocks is changing, the exact coordinate of the well is slightly different for each model.


FloViz 2005A
Z Axis
X Axis
I
P
Y Axis
GasSat
0.00000
0.21190
0.42380
0.63569
0.84759


FloViz 2005A
Z Axis
X Axis
I
P
Y Axis
GasSat
0.00000
0.21177
0.42354
0.63531
0.84708


FloViz 2005A
Z Axis
X Axis
Y Axis
E
GasSat
0.00000
0.21215
0.42429
0.63644
0.84858


FloViz 2005A
Z Axis
X Axis
P
Y Axis
GasSat
0.00000
0.21215
0.42430
0.63645
0.84859


FloViz 2005A
Z Axis
X Axis
Y Axis
P
GasSat
0.00000
0.21233
0.42465
0.63698
0.84930

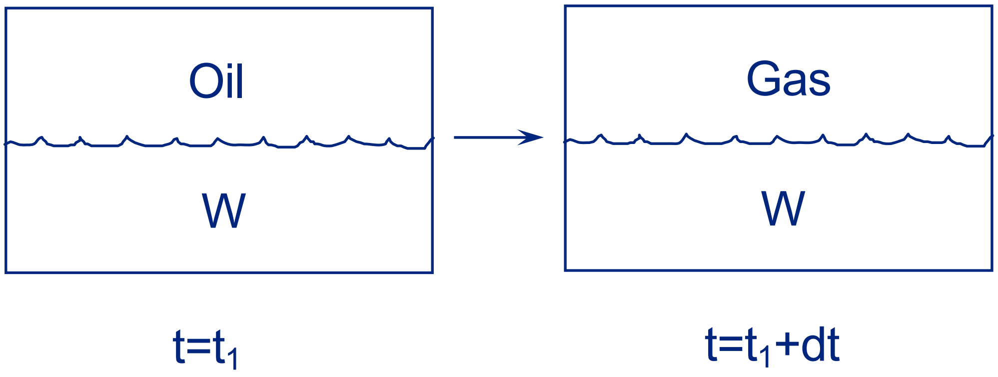
21. Interpolation of Relative Permeabilities

Near Critical Oil and Gas Relative Permeabilities

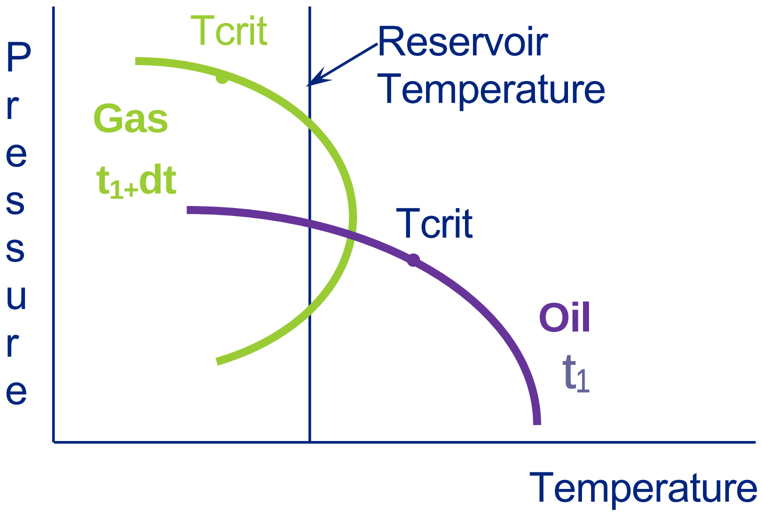
We have suggested earlier that in compositional simulation the important question is whether the hydrocarbon fluid is single-phase or two-phase. If the fluid is single-phase, we can calculate its properties without having to worry about whether we should call this fluid “oil” or “gas”.

This is correct so far as static properties of the fluid such as density, compressibility, etc. One property for which the name and the identification of the single-phase fluid is important is the relative permeability. If the fluid is an oil then we use oil relative permeability curves. . If the fluid is a gas then we use gas relative permeability curves. In general the two curves are not the same.

Another difficulty in compositional simulation is that a cell can be full of oil at one timestep and full of gas at the next timestep.



For this to happen, we just need a slight increase in the C1 concentration in the grid block, or a slight decrease in the concentration of the heavier components. This change in concentration would be enough to move the phase envelope slightly up and to the left; the critical point then moves from the right of the reservoir temperature (which defines an oil) and goes to the left of the reservoir temperature (which defines a gas). This can happen without any change in pressure in the grid block.



Question: What should hydrocarbon relative permeability be?

At time t1, if we have an oil we would normally use kro. At time t1+dt we should then use krg as we have a gas.

$$t_1 : \quad K_{ro} \ and \ K_{rw}$$
$$t_1 + \Delta t : K_{rg} \ and \ K_{rw}$$

The relative permeability curves for oil and gas are usually very different, and this change from oil to gas would therefore cause a discontinuous change in the mobility of the fluid. This is clearly not physical, as (for instance) adding a few molecules of gas should not discontinuously change the mobility.[43]

Answer - There must be continuity between hydrocarbon relative permeability Kro when system is an oil, Krg when system is a gas.

This should always be the case when we have a single-phase hydrocarbon, whatever the value of the water saturation

Solution - Define a water-hydrocarbon relative permeability Krh when have single phase HC system.

---

[43] SCAL experiments are usually only performed on the original reservoir oil, and perhaps on one gas composition. In the case of gas injection into an oil, when the fluid mixture goes thorough the critical point, we would ideally like to have experimental measurements of the relative permeability of a number of fluid mixtures as the fluid moves from 100% original oil to 100% injected gas.

When Tc of the fluid is a long way to the right the reservoir temperature Tres, then Krh becomes Kro. When Tc is a long way to the left of Tres then Krh becomes krg. To set up the interpolation between kro and krg, we first define a pseudo-critical temperature Tcrit[44]

$$T^{crit} = \frac{\sum_{comp} T_c V_c z_c}{\sum_{comp} V_c z_c}$$

.

We then measure how far away Tcrit is from the reservoir temperature by defining a factor f:

Define: f = Tcrit/Tres

f = 1 crit.temp = reservoir temp.

f > 1 for oil Tcrit > Tres

f < 1 for gas Tcrit < Tres

System completely oil when: f = 1.25

completely gas when: f = 0.75

We can see that if Tcrit > Tres then we have an oil and f > 1. Similarly if Tcrit < Tres then we have a gas and f < 1. We arbitrarily choose to interpolate the hydrocarbon relative permeabilities when the value of f is between[45] 1.25 and 0.75.

- If f>1.25 the we use kro
- If f<0.75 then we use krg
- If f is between 1.25 and 0.75 then we interpolate between kro and krg.

We define interpolating function E:

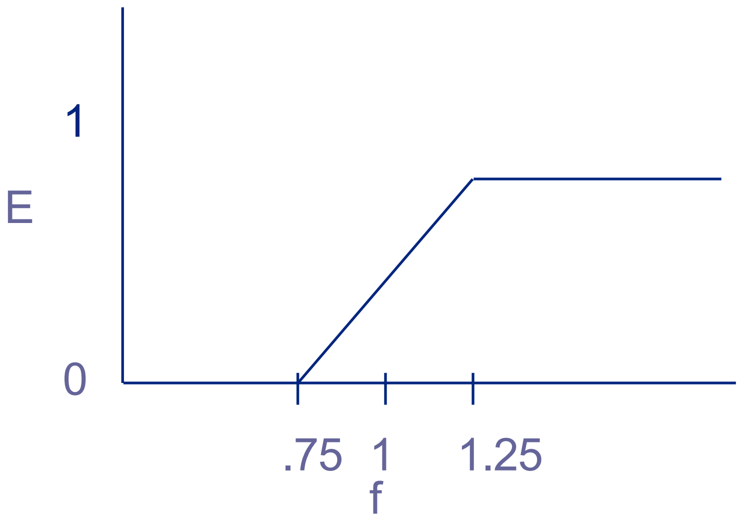
E = (f-fg)/(fo-fg) in the region 0.75 < f < 1.25

---

[44] This is the Li correlation

[45] These limits can be modified with the keyword LILIM.

E = 0 or 1 outside range



Our hydrocarbon-water relative permeability is then defined as:

$$K_{rhw} = E \bullet K_{row} + (1 - E) K_{rgw}$$

These values for single-phase hydrocarbon to water relative permeabilities are used by default whenever the value of the factor f is between 0.75 and 1.25. If you want, you can prevent the interpolation in one of two ways:

- **NOMIX prevents any interpolation**
- **ISGAS also prevents interpolation by saying that all single-phase grid blocks are gas and not oil.**

We do not recommend the use of these keywords in general, as they can have unexpected consequences. For instance NOMIX can lead to sudden discontinuous flows if oil does change to gas (or vice versa). ISGAS will call all single-phase cells gas, even if they are clearly oil-filled.

If all three phases are present, then the oil and gas relative permeabilities for the default ECLIPSE method is calculated from:

$$K_{ro} = gK_{rhw}(S_w) + (1-g)K_{rog}(S_o)$$

$$\text{where} \quad g = (S_w - S_{wc})/(S_w - S_{wc} + S_g)$$

$$K_{rg} = hK_{rhw}(S_w) + (1-h)K_{rgo}(S_g)$$

$$\text{where} \quad h = (S_w - S_{wc})/(S_w - S_{wc} + S_o)$$

Near Miscible Oil-Gas Relative Permeabilities

We have discussed how we interpolate between oil-water and oil-gas relative permeabilities as the oil and gas composition get close to each other.

What about oil-gas relative permeabilities?

Under normal conditions, oil & gas reservoir fluids form distinct, immiscible phases

Immiscible phases are separated by an interface

- **associated with inter-facial tension (IFT)**
- **when IFT=0, fluids mix => miscibility**

residual oil saturation to gas (and water) directly proportional to IFT

- **For the "normal" immiscible case, we use rock curves.**
- **With miscibility, we have straight line (0,0) to (1,1) rel perm curves.**

How do we interpolate between miscible and immiscible relative permeability curves?

Use keyword MISCIBLE in RUNSPEC section, and supply parachors.

The interpolation between the immiscible oil-gas relative permeability curve and the miscible straight-line relative permeability curve is not done by default. You have to use the MISCIBLE keyword in the RUNSPEC section and also provide extra information to calculate the surface tension.

Note that the MISCIBLE keyword has different effect in ECLIPSE 100.

***MacLeod & Sugden*:**

- **The molecular weight of a liquid**
  *** the fourth root of its surface tension**
  / by the difference between the density of the liquid and the density of the vapor in equilibrium with it
  is essentially constant over wide ranges of temperature

$$\sigma^{1/4} = \frac{P(\rho_L - \rho_V)}{M}$$

- **This defines the parachor P**
- **P can be visualized as a comparative volume between two liquids and is reasonably independent of temperature**
- **http://www.pirika.com/chem/TCPEE/ST/MS.htm**

- **Given the parachors P, surface tension is calculated from the Macleod-Sugden correlation**

$$\sigma = \left[\sum P_i (md_l.x_i - md_v.y_i)\right]^4$$

- **This expression will go to zero as the compositions become equal – there is no surface tension for a one-phase state!**
- **We can therefore use sigma to interpolate between miscible and non-miscible cases.**

$$F = \left(\frac{\sigma}{\sigma_0}\right)^N$$

- **We define an interpolation factor**

where σ_0 **is a reference surface tension, taken by default as the field average. This can be set with the MISCSTR keyword. N can be set using MISCEXP.**

- **The interpolation factor is then used to interpolate between miscible and immiscible curves:**

$$K_{ro} = FK_{ro}^{imm} + (1 - F)K_{ro}^{misc}$$

- **The scaling first calculates scaled critical saturations, then scales the rel perms themselves.**

You can specify an immiscible rel perm curve using the MISCNUM keyword. This may for instance have a non-zero critical value.

Alternatively, you can provide two tables:

- **A table of surface tension as a function of pressure (STVP)**
- **A table of F as a function of surface tension (FVST)**

Interpolation is also done for capillary pressures, as these must also go to zero as the surface tension vanishes.

Summary of rel perm interpolation

1. **For one hydrocarbon phase and water, what happens as Tc => Tres?**

We interpolate between oil-water rel perms and oil-gas rel perms.

This is the default.

2. For oil and gas phase, what happens as the oil and gas composition get close to each other?

We interpolate between the oil-gas rock curves and a straight line.

This is not the default. Use MISCIBLE and supply parachors.

22. Convergence

1. Introduction

This document describes how to improve the convergence and the speed of the Eclipse simulators by simple changes to the data file.

The data chosen to model the reservoir may be such that the simulator can only solve the model by taking extremely short timesteps or excessive amounts of cpu time. Modifying existing keywords or adding new keywords can sometimes lead to dramatic improvements in the speed of the simulation without changing the results to engineering accuracy. We will show which keywords can speed up the run in this way.

If the data cannot be changed, convergence criteria can sometimes be chosen to improve simulator performance. Results of a run can depend on the convergence criteria and how they are applied, so in some cases there is a trade-off between accuracy and speed. We will show how to detect these cases and how to choose suitable convergence criteria.

Most of the advice and suggestions apply equally to all the simulators. When there are differences in the detailed treatment between Eclipse 100, 300 and 500 we will highlight these differences and explain how the data for each simulator can be tuned to improve performance. When we use the word 'Eclipse' without specifying 100, 300 or 500 then we are referring to all the simulators.

A case study

- **We received an ECLIPSE model from a client**
- **The model was “chopping” timesteps**
- **Run times were many hours**

- **We were asked if we could make it run faster.**

We looked at the evidence

- The main suspect was one of the production wells.
- We looked at the data in detail:

```
-- WELL SPECIFICATION DATA
--
--    WELL        GROUP   LOCATION       BHP     PI
--    NAME        NAME       I   J      DEPTH   DEFN
WELSPECS
   'PRODUCER'   'G'        10   10        8400   'OIL'  /
/
```

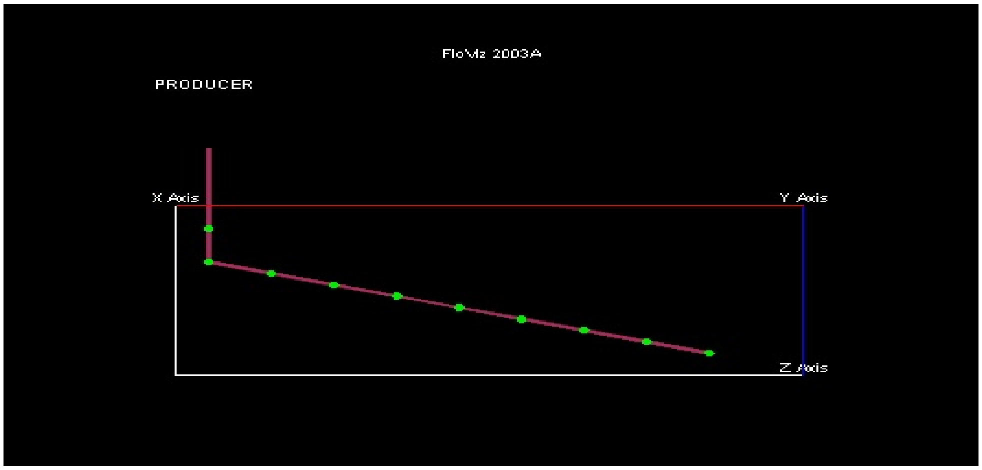
The main suspect

```
-- COMPLETION SPECIFICATION DATA
--
--    WELL       LOCATION- OPEN/  SAT   CONN  WELL
--    NAME         I  J K1 K2  SHUT    TAB   FACT  DIAM
COMPDAT
   'PRODUCER'   10 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    9 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    8 10 3  3  'OPEN'       0    -   1         0.5  /
   'PRODUCER'    7 10 3  3  'OPEN'       0    -   1         0.5  /
   'PRODUCER'    6 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    5 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    4 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    3 10 3  3  'OPEN'       0        -1        0.5  /
   'PRODUCER'    2 10 3  3  'OPEN'       0        -1        0.5  /
/
```

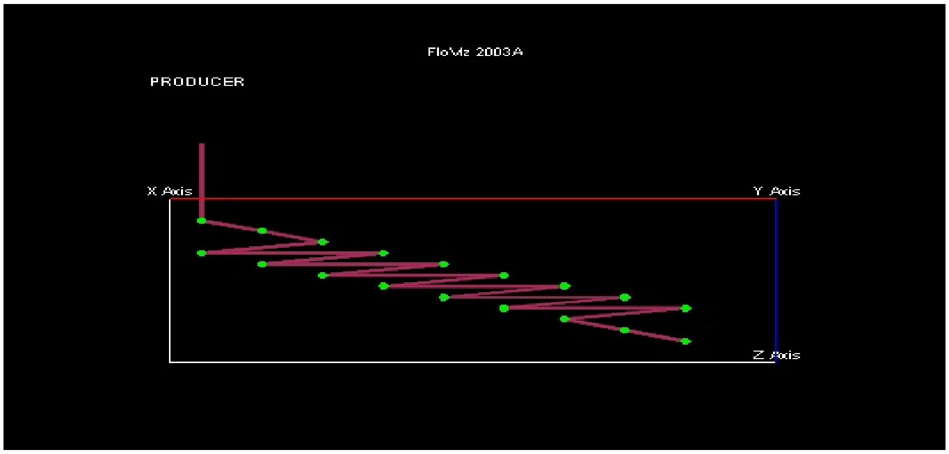
New evidence

- **The well specification data looked OK**
- **Completion data looked OK**
- **The well production controls also looked OK**

- **We looked at the “photographic” evidence**
- **We expected to see:**



- We saw:



The explanation

- **The run was a Restart run.**
- **The base run had the well completed in a higher layer.**
- **The restart had the well completed in a lower layer.**

- **The well now had completions in both layers**
- **COMPORD was used to depth-order the wells so the display joined the completions in that order – note the default well model in ECLIPSE does not assume any order.**

What made us suspect the wells?

- If a run is misbehaving, how do we find clues that will point us towards the guilty?
- More generally, how do we speed up an ECLIPSE run?
- What runs can be speeded-up?

ALL runs can be speeded-up. If a model has difficulty converging or even if it running very efficiently the computing time can still be reduced by running it on a faster computer, or by reducing the number of grid blocks or the number of variables. If the model is suitable, parallel computing can also reduce computing time.

The rest of this section however will look at the cases where we are having convergence problems or cases of unusually slow runs, and will discuss how to identify the data issues that are causing these difficulties.

Data-independent solutions

- **Buy a faster machine!**
- **Reduce the number of grid blocks**
- **Run in parallel**

Identify data issues

- **Time-stepping**
- **Convergence problems**

We will explain

- **How to get more information**
- **What the details of the output mean**
- **What to look for in the data**
- **How to fix some of the problems**

2. Background to timesteps and iterations

An Eclipse simulation	is made up of one or more report steps.
A report step	is made up of one or more time steps.
A time step	is made up of one or more non-linear iterations.
A non-linear iteration	is made up of one or more linear iterations.

When you set up the data model to run Eclipse, you are asked to specify the report steps that you want. You therefore have direct control of the number of report steps and the time gap between them. Reducing the number of report steps can sometimes reduce the cpu time.

- **Default values control how many timesteps will be used to reach the next report. These default values will work well in most cases.**

- **You may need to adjust some of the defaults such as the timestep limit. In easy cases, fewer time steps will lead to less cpu time. In difficult cases, reducing the maximum timestep may help.**

- **TSCRIT or TUNING keyword to adjust the maximum timestep.**

Eclipse has default values that control how many timesteps will be used to reach the next report that you have asked for. These default values will work well in most cases, but there are times when you may need to adjust some of the defaults so that the simulation takes fewer timesteps. In many (but not all) cases, fewer time steps will lead to less cpu time. In some difficult cases, reducing the maximum timestep may speed up the run.

Different default values also control how many non-linear iterations will be used to solve each timestep. These values should normally be left unchanged. In a few cases, adjustments to the convergence criteria can improve the performance of the simulator. In most cases however the greatest improvements in performance are obtained by identifying the cause of the non-linear problem and changing the data model to reduce the non-linearity. The major part of this document will explain how to avoid problems of this type, and how to find and fix the problems if they do occur.

By the time problems occur in the linear iterations, it is usually too late to fix them by adjusting the linear convergence control. Some controls can be changed in extreme circumstances, but the best advice is to avoid such problems by controlling the timestepping and the non-linear iterations.

2.1 Reports of timesteps and iterations

The number of report steps, time steps and non-linear iterations can be found in both the PRT file and the LOG file - the shorter form of output which appears on the screen (for interactive runs) or is sent to a log file (for batch or background runs). On UNIX systems, you can use the grep command to find all the necessary information; on PCs you may need to use your favorite editor and find the information one line at a time. Details are reported in a different way in Eclipse 100 on the one hand and Eclipse 300 and 500 on the other.

For a UNIX system and an Eclipse 100 log file called BASE.LOG, the command

```
grep TSTEP BASE.LOG >BASE.STEPS
```

will create a file BASE.STEPS that will contain one line for each timestep. Each line will be of the form:

```
STEP   15  TIME=  400.00 DAYS ( +30.0 DAYS REPT  3 ITS)  (4-FEB-2003)
```

"STEP 15"	means this is the 15th timestep.
"TIME= 400.00 DAYS"	means there have been 400 simulated days since the beginning of the simulation.
"+30.0 DAYS"	shows that the latest timestep was of 30 days.
"REPT"	is a mnemonic explaining why 30 days were chosen. "REPT" means that a report step has been reached.
"3 ITS"	means 3 non-linear iterations were needed to solve the 30 day timestep.
"(4-FEB-2003)"	is the current simulation date.

For a UNIX system and an Eclipse 300 log file called BASE.LOG, the command

```
grep ";" BASE.LOG >BASE.STEPS
```

will create a file BASE.STEPS that will contain one line for each timestep of the form:

```
Rep ;  400.0 30.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.6 .00000 1.3E06 3
```

"Rep"	is the mnemonic that shows that a report step has been reached,
"30.0"	shows that the latest timestep was of 30 days,

the next 8 numbers show the GOR, water cut, oil/gas/water production rates, average field pressure, and gas and water injection rates,

"3"	at the end of the line means that 3 non-linear iterations were needed to solve the 30-day timestep.

If the AIM option is used then the line will have and extra number at the end,

```
Rep ;  400.0 30.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.6 .00000 1.3E06 3 2%
```

2% shows the percentage of the cells that was solved fully implicitly.

3. Report Steps

The number of report steps and the time between report steps will depend on the type of model that you are simulating:

- For a prediction or forecasting run lasting for instance 30 years you may for instance ask for monthly reports for the first year, quarterly reports for the next 5 years, and yearly reports for the rest of the simulation.
- For history matching you may ask for weekly reports for the first year and for monthly reports for remainder of the history match, to test the validity of your model on a finer time scale.
- For slim-tube experiments, reporting intervals are likely to be minutes and hours

Computing time may be reduced by changing the requested reports if the following three conditions apply:

1. You are asking for more reports than you actually need
2. Each report step is being reached in just a single timestep
3. Each time step is being solved in a small number of non-linear iterations. By small we ideally mean one, but savings could also be made if the timestep is taking 2 or 3 iterations.

If you have created a file BASE.STEPS and find that it mainly contains lines of the form:

```
STEP  40  TIME= 400.00 DAYS ( +10.0 DAYS REPT  1 ITS)   (4-FEB-2003)
STEP  41  TIME= 410.00 DAYS ( +10.0 DAYS REPT  1 ITS)  (14-FEB-2003)
STEP  42  TIME= 420.00 DAYS ( +10.0 DAYS REPT  1 ITS)  (24-FEB-2003)
STEP  43  TIME= 430.00 DAYS ( +10.0 DAYS REPT  1 ITS)   (6-MAR-2003)
```

so that each timestep is a report step, and each timestep is solved in one iteration, then the run may go 2 or 3 times faster if you allow the simulator to produce report steps once a month instead of once every 10 days.

The example above was for an Eclipse 100 run. The same applies for an Eclipse 300 run with:

```
Rep ; 400.0 10.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.6 .00000 1.3E06  1
Rep ; 410.0 10.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.5 .00000 1.3E06  1
Rep ; 420.0 10.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.4 .00000 1.3E06  1
Rep ; 430.0 10.0 8.7838 .19498 1.4E05 32884. 1.2E06 4843.3 .00000 1.3E06  1
```

4. Timesteps

Having reached one report step, Eclipse will decide what timestep to take next according to:

- how easy or difficult the previous timestep was
- how the convergence of the previous time step compared with the convergence targets
- how much simulation time is left until the next report step
- whether either you or the default limits forced it to take a particular time step

You can set the timestep limits by using the TUNING keyword in any of the Eclipse simulators, or by using the TSCRIT keyword in Eclipse 300.

4.1 Maximum Timestep

The first example of how a run can be speeded-up is similar to the report step example already given. If you have created a file BASE.STEPS and find that it mainly contains lines of the form:

```
STEP   40  TIME=  400.00 DAYS ( +10.0 DAYS MAXS  1 ITS)    (4-FEB-2003)
STEP   41  TIME=  410.00 DAYS ( +10.0 DAYS MAXS  1 ITS)   (14-FEB-2003)
```

```
STEP   42  TIME=  420.00 DAYS ( +10.0 DAYS MAXS  1 ITS)   (24-FEB-2003)
STEP   43  TIME=  430.00 DAYS ( +10.0 DAYS MAXS  1 ITS)    (6-MAR-2003)
```

The mnemonic MAXS means that this timestep is the maximum allowed according to the TUNING keyword. Again we see that each timestep is a report step, and each timestep is solved in one iteration, and the run may go 2 or 3 times faster if you allow the simulator to produce report steps once a month instead of once every 10 days. For Eclipse 300 the mnemonic is "Max", and you can set the maximum timestep either using the TUNING or the TSCRIT keyword.

The syntax to set the maximum timestep to 30 days using the TUNING keyword is:

```
TUNING
1* 30 /
/
/
```

and using TSCRIT:

```
TSCRIT
2* 30 /
```

Note that the default maximum timestep in Eclipse 100 is 365 days and in Eclipse 300 is 50 days. The limit will only be 10 days if it has been set to 10 in a TUNING or TSCRIT keyword.

The maximum timestep should be compatible with the report step interval. If you are asking for a report at the beginning of each month and have a timestep limit of 30 days, then those months with 31 days will need at least two timesteps. Increasing the timestep limit to 31 days would allow every month to be covered in one timestep if there were no other limitations. If you are asking for reports every 3 months, the maximum timestep should be at least 92 days.

You may sometimes help the non-linear solver by setting a lower value for the maximum timestep size. If the simulator is frequently chopping timesteps and you cannot find the cause as described in section 5 below, then reducing the maximum timestep can speed up the run.   You can always allow the timesteps to increase later in the simulation, after a difficult modeling problem has been overcome.

4.2 Maximum Timestep after a well change

A similar inefficiency can arise with the maximum step after a well change. There is a default limit of how big a timestep can be taken immediately after any well keyword has been used. The default value for Eclipse 300 is 20 days, and the default for Eclipse 100 is “unlimited”. If you are history matching and setting new well rates at the beginning of each month, then Eclipse 300 will be unable to take any timestep greater than 20 days. Rather than simulate January for example with a 20-day timestep followed by an 11-day timestep, Eclipse will even-out the timesteps by having two 15.5-day timesteps. The mnemonic for this choice of timestep is 'HALF' in Eclipse 100 and 'HRep' in Eclipse 300 and 500. The timestep summary will then be:

```
STEP   1  TIME=  15.50 DAYS ( +15.5 DAYS HALF  1 ITS)    (15-JAN-2002)
STEP   2  TIME=  15.50 DAYS ( +15.5 DAYS REPT  1 ITS)    ( 1-FEB-2002)
STEP   3  TIME=  14.00 DAYS ( +14.0 DAYS HALF  1 ITS)    (14-FEB-2002)
STEP   4  TIME=  14.00 DAYS ( +14.0 DAYS REPT  1 ITS)    ( 1-MAR-2002)
STEP   5  TIME=  15.50 DAYS ( +15.5 DAYS HALF  1 ITS)    (15-MAR-2002)
STEP   6  TIME=  15.50 DAYS ( +15.5 DAYS REPT  1 ITS)    ( 1-APR-2002)
STEP   7  TIME=  15.00 DAYS ( +15.0 DAYS HALF  1 ITS)    (15-APR-2002)
```

Increasing the maximum step after a well change to be more than 31 days could improve the timestepping to be:

```
STEP   1  TIME=  31.00 DAYS ( +31.0 DAYS REPT  1 ITS)    ( 1-FEB-2002)
STEP   2  TIME=  28.00 DAYS ( +28.0 DAYS REPT  1 ITS)    ( 1-MAR-2002)
STEP   3  TIME=  31.00 DAYS ( +31.0 DAYS REPT  1 ITS)    ( 1-APR-2002)
```

You may need to reduce the maximum timestep after a well change. If for instance you expect a major change in reservoir behavior every time you change the well controls, then you can save cpu time by setting this value to for instance 1 day, using

```
TUNING
9* 1 /
/
```

/

or

TSCRIT

10 1 /*

4.3 Timestep Reason

Some of the more common reasons for timestep selection are:

Mnemonic		**Explanation**
E100	**E300**	
INIT	Init	first timestep
MAXF	MIF	maximum increase factor
REPT	Rep	report step
HREP	Hrep	half step to report
CHOP	Redu	timestep chopped
DIFF		follows CHOP
TRNC	TTE	TTE limit
	SCT	Solution Change
	TPT	Throughput Limit

5. Non-Linear Convergence Criteria

The equations that the simulators are trying to solve are non-linear. By non-linear we mean that for instance doubling the tubing-head pressure of a water injector will not usually double the amount of water injected, and doubling the oil saturation in a grid block will not usually double the oil mobility in that grid block.

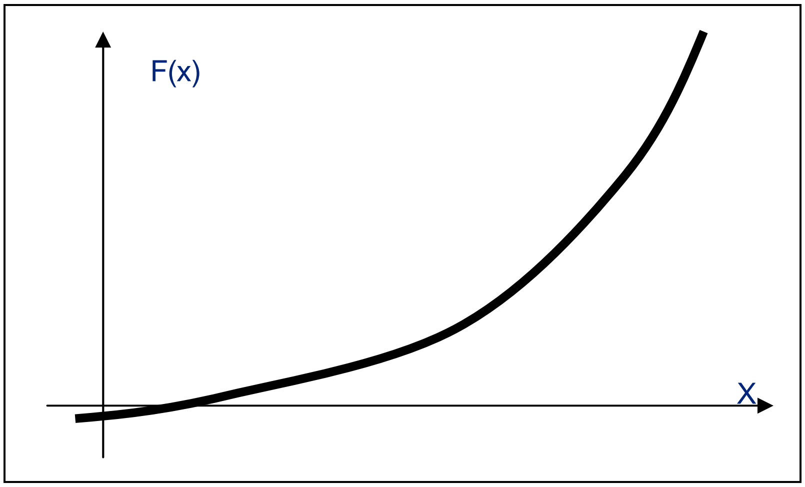
The simulators use an iterative process based on Newton's method to solve these non-linear equations:

1. We linearise the equations

2. We solve the linear equations

3. We check if this linear solution gives us a “good enough”[46] non-linear solution.

If it does then we move to the next timestep. If not we calculate the change needed to improve the solution, then go back to step 1.



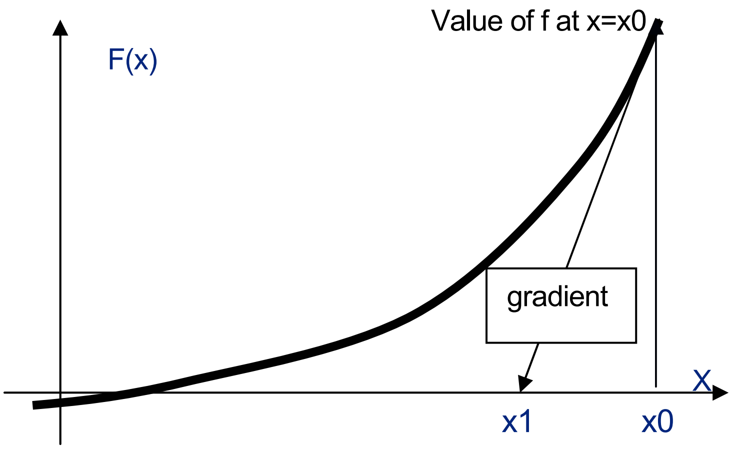
Consider the above curve. “f” is a one-dimensional function of x. We want to find the value x_{sol} that gives us $f(x_{sol})=0$, and we have an initial guess that x_{sol} = x0. We calculate the value of f with x=x0 and see that we are a long way from the solution, so we can start iterating.

<u>First Iteration:</u>

- Assume that f is a linear function instead of a non-linear function.
- Step 1: To linearise f in this case all we have to do is to calculate the gradient of f at x=x0.
- Step 2: We now solve this linear function and get a new estimate for the solution. Our new estimate is x1.

---

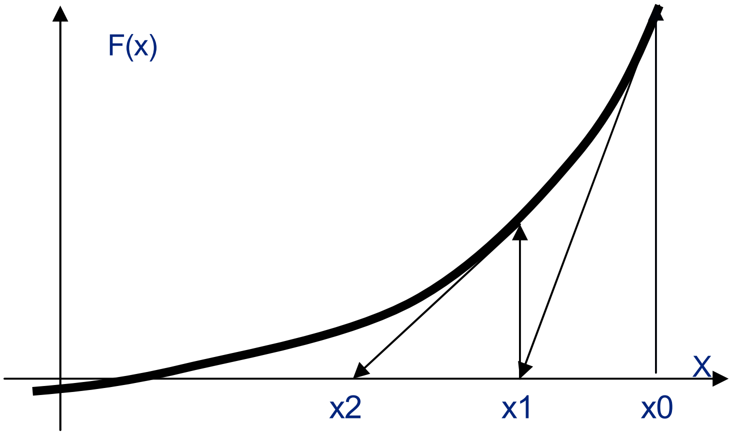
[46] We shall explain later what we mean by “good enough”.



- Step 3: Check whether x1 is a good enough solution by calculating f at x=x1. We decide that we don't yet have a good enough solution so we continue.

<u>Second Iteration:</u>

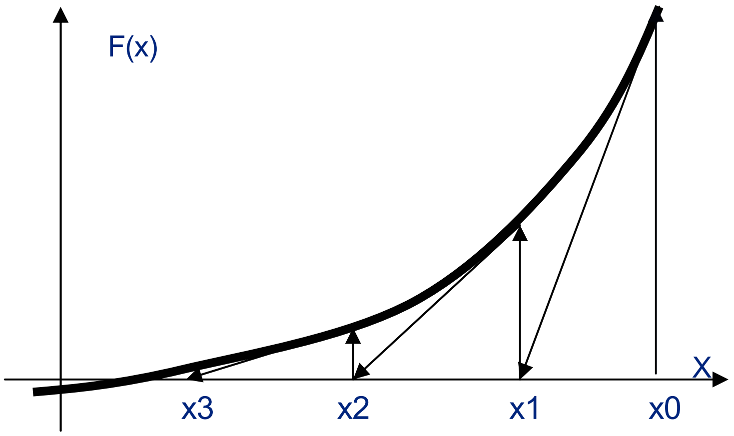
- Assume again that f is a linear function instead of a non-linear function.
- Linearise f by calculating the gradient of f at x=x1.
- Solve this linear function and get a new estimate for the solution. Because we are solving a linear equation in one variable, we can solve the linear problem easily and we do not need to iterate. Our new estimate is x2.



- Check whether x2 is a good enough solution by calculating f at x=x2. We decide that we don't yet have a good enough solution so we continue.

Third Iteration:

- Linearise f by calculating the gradient of f at x=x2.
- Solve this linear function and get a new estimate for the solution. Our new estimate is x3. We check whether x3 is a good enough solution by calculating f at x=x3.



- We decide that it is good enough solution so we stop with a solution of x3. We have solved the problem in three non-linear iterations.

If we had been solving for a large number of variables, for instance 1 million variables[47], then we cannot solve the linear equations directly and we will need to perform a number of linear iterations for each non-linear iteration.

5.1 Definition of non-linear iterations

Each time the simulator goes through steps 1 to 3, it performs one non-linear iteration. The total number of times the simulator goes through these steps for each timestep is the number of non-linear iterations for that timestep. There is a limit to the number of non-linear iterations that the simulators will try before giving up and trying with a smaller timestep. This limit depends on the simulator and on the solution method, and is set using either the TUNING or the CVCRIT keyword.

---

[47] A 100,000 grid-block compositional model with 8 hydrocarbon components and water will have one million variables to solve at every timestep.

You can check on how well the model is converging to a solution by looking at the number of non-linear iterations for each timestep, as described in section 2.1:

1	non-linear per timestep means the step was very easy to converge
2 to 3	non-linears per timestep means the step was easy to converge
4 to 9	non-linears per timestep shows an increasingly difficult problem
> 10	non-linears per timestep can mean a problem with the model

5.2 Definition of convergence

We need a test to decide when we can stop the iterations and carry on to the next timestep, i.e. to decide when the solution that we have is 'good enough'. A test of convergence can be based on a small residual or a small change in solution. The residual can be thought of as a measure of how close we are to solving the non-linear problem. Eclipse 300 uses the change of solution as its basic convergence test. This is in contrast to Eclipse 100 where the default is to use the residual for the primary test. In the case of Dual Porosity Eclipse 100 runs, the TUNINGDP keyword will cause iterations to converge if either the residual or the solution change is small enough.

Solution Change Check

The maximum solution changes over all cells for all primary variables, pressure and molar densities are calculated and compared to two limits, one for pressure and one for saturation.

SCONVP	Set by 1st data item in CVCRIT	default 0.1 atm
SCONVS	Set by 7th data item in CVCRIT	default 0.01

The variables used by Eclipse 300 and 500 are pressure and molar densities. The pressure change is compared directly, while molar density changes are converted to effective saturation changes.

The maximum solutions change over all cells and all solution variables is converted to an "actual-over-target" (aot) which is a ratio of the current maximum divided by the target. When the value of aot falls below 1, then the timestep is converged.

If the 8th data item in the DEBUG3 keyword is set greater than 0, then the program will output a line of debug which shows the convergence details. The

UNIX grep command can be used to produce smaller summaries of the output:

e.g.grep ";|aot" ROOT.DBG will produce something like:

```
NLStep= 0 lin= 23 aot=   97.21 Rmax= .7162E-01 Rsum= .9919E-05 egain=-.1000E+01
NLStep= 1 lin= 19 aot=  17.55 Rmax= .1762E+00 Rsum= .1329E-06 egain=-.1000E+01
NLStep= 2 lin= 21 aot=    2.94 Rmax= .1421E-01 Rsum= .6285E-06 egain=-.1000E+01
NLStep= 3 lin= 12 aot=     .77 Rmax= .7252E-02 Rsum= .7476E-08 egain=-.1000E+01
 Rep ;  8901.0 1.00 8.7838 .19498 1.4E05 32884. 1.2E06 4843.6 .00000 1.3E06 4 2%
NLStep= 0 lin= 27 aot= 137.50 Rmax= .7587E-01 Rsum= .2011E-04 egain= .1805E+00
NLStep= 1 lin= 26 aot=   79.23 Rmax= .7589E-01 Rsum= .1743E-04 egain= .1676E+00
NLStep= 2 lin= 26 aot=   76.18 Rmax= .7279E-01 Rsum= .1676E-04 egain= .2621E+00
NLStep= 3 lin= 24 aot=    9.30 Rmax= .9062E-01 Rsum= .8301E-06 egain=-.1000E+01
NLStep= 4 lin= 24 aot=    9.00 Rmax= .8764E-01 Rsum= .8028E-06 egain=-.1000E+01
NLStep= 5 lin= 13 aot=     .08 Rmax= .9509E-01 Rsum= .9853E-09 egain=-.1000E+01
 MIF ;  8903.0 2.00 8.7860 .19501 1.4E05 32880. 1.2E06 4844.2 .00000 1.3E06 6 2%
```

This shows two time steps:

1. Non-linear iterations start with iteration 0, which is a first guess at the new solution. The first 4 lines above show iterations 0 to 3. Iteration 3 has an aot of 0.77, which is less than 1. The worst residual is now less than the target, so the iterations have converged. The simulator provides a timestep report which starts “Rep” meaning a report has been reached, and a “4” near the end of that line means that 4 non-linears were needed to converge.

2. The second timestep needs a total of 6 iterations. In this step we see that the aot at the last non-linear iteration drops from 9.00 to 0.08. This is a sign of “quadratic convergence” which will occur when the simulator is very close to the solution and reduces the aot by two or more orders by magnitude at each non-linear iteration.

Details

1. If you wish to tighten (reduce) the convergence criteria, there are minimum values below which SCONVP and SCONVS cannot be set. The pressure

minimum is 0.01 and the effective saturation minimum 0.005. The pressure minimum can be ignored by setting the data item (1st in CVCRIT) negative. This behavior is not documented, and may be changed in future releases.

2. The convergence tolerances are relaxed slightly at each non-linear iteration, to make convergence easier as the number of iterations increases. The hope is that this will allow a difficult timestep, without significantly affecting the results. The factor used is:

Factor = 1.0 + “iteration number”/”maximum iterations”

3. An additional check is made that the sum of the residuals, which is a measure of total material balance error, is not excessive. This is a safety measure that can prevent convergence but rarely gets invoked in production cases.

4. Even if the solution change is too great and aot>1, the maximum residual may be small enough for the timestep to be converged. The criterion used is the variable SNLRMX set using the 11th data item in CVCRIT. The residual considered is the residual calculated using the previous iteration and is not the new residual resulting from the solution change. Because of this the test tends not to be effective very often.

Gain Option

The details above tend not to have a significant impact in the majority of cases. However there is an option that can sometimes significantly effect performance. The idea is to speed the code up by not taking an extra non-linear iteration if that iteration is likely to generate a very small solution change. We predict the behavior of the next iteration based on the history of previous timesteps. We calculate a gain factor from previous timesteps and rather than using the aot we use:

EAOT=MIN(2.0*AOT*EGAIN,AOT)

Where EAOT - Effective aot
AOT - Is the aot as calculated above
EGAIN - A measure of the expected improvement at the next step

The gain value is printed out with the non-linear debug. See the example above.

The gain option can be switched on by setting the 68th switch of the OPTIONS3 keyword to 1. If OPTIONS3(68)=1 then the option can be tuned using the 19th switch of the OPTIONS3 keyword. If OPTIONS3(19)=1, the gain will not be used if any cell has changed state during the iteration. In this case you might expect the previous history to be less valid.

We have seen some examples where this option is combined with small changes in the problem and leads to dramatic changes in iteration sequence. In cases such as these it may be preferable to increase speed simply by loosening the convergence criterion (1st item in CVCRIT) rather than relying on the gain option.

5.3 Tracking the source of the problem

- A single cell can cause non-convergence. As we increase the number of cells in a simulation, we increase the odds that a cell will cause non-convergence.

If the are only one or two cells in the reservoir model that are causing problems, we can identify the cells and check if there is any engineering or data reason which could explain why they are causing problems. For example the cells may be at or near well completions, in which case well control could be modified, or could be cells with very small pore volumes in which case the MINPV keyword could be used.

5.3.1 Eclipse 100

In Eclipse 100, you will get non-linear debug if you set “NEWTON=2” in RPTSCHED.

This will produce output of the form:

```
IT= 0   CNV      CELL     MAT BAL   DPRESS    DSWAT    DSGAS
OIL 1.00424   ( 28, 45,  3)  5.3D-03     0.00  0.00000  0.00000
WAT-0.00288(   9,   3,  3) -1.3D-07     0.00  0.00000  0.00000
GAS********   (   5, 45,  1) -1.3D-02     0.00  0.00000  0.00000
```

```
    LINIT= 5 NSCHP=    6 NCHOP=    0 NSTAT1,2,3=    50  5400    0 NTRAN=  321
IT= 1   CNV      CELL     MAT BAL   DPRESS    DSWAT    DSGAS
OIL-1.99144    (  5, 45,  1)  4.3D-02   -24.89  0.00026 -0.20000
WAT-0.16316 (  2,   4,  4) -3.7D-06   -14.02  0.00490  0.00000
GAS********    (  5, 45,  1) -3.1D-02   -24.89  0.00026 -0.20000

    LINIT= 3 NSCHP=  195 NCHOP=    0 NSTAT1,2,3=    50  5370   30 NTRAN=   30
IT= 2   CNV      CELL     MAT BAL   DPRESS    DSWAT    DSGAS
OIL-0.62319   (   5, 45,  1)  1.7D-02   -21.15  0.00081 -0.01843
WAT-0.04162 ( 28,  5,  3) -1.3D-04   -30.47  0.00139  0.04000
GAS********    (  5, 45,  1) -2.2D-02   -21.15  0.00081 -0.01843

    LINIT= 3 NSCHP=   44 NCHOP=    3 NSTAT1,2,3=    50  5367   33 NTRAN=   25
IT= 3   CNV      CELL     MAT BAL   DPRESS    DSWAT    DSGAS
OIL-0.30993    (  5, 45,  1) -8.9D-05   -26.44  0.00088 -0.21134
WAT-0.04591 ( 28,  4,  3) -4.0D-05   -19.80  0.00666  0.11687
GAS********   (  5, 45,  1) -1.4D-02   -26.44  0.00088 -0.21134
```

This shows the first 4 non-linear iterations (IT=0, IT=1, IT=2, IT=3) in a case that has convergence problems.

The first line shows IT=0, the first iteration, and CNV etc are column headers for the next 3 lines.

The columns are:

CNV	The worst residual for the OIL, WATer and GAS phases
CELL	The cell that has the worst residual
MAT BAL	That cell's material balance, a measure of mass accuracy
DPRESS	The change in pressure in that cell since the last iteration
DSWAT	The change in water saturation since the last iteration
DSGAS	The change in gas saturation since the last iteration

The residual for gas in all 4 iterations is shown as ******* which means that it is greater than the maximum printable value. It has a very high residual at each iteration for cell (5,45,1), so that is the cell that is causing problems.

After each iteration report above, the line starting LINIT= provides more information on what is happening within the model.

LINIT = number of iterations required to solve the linearise equations.

NSCHP = number of saturation changes that were altered to suppress possible oscillations.

NCHOP = number of times the changes in P, Rs, or Rv were reduced to increase stability.

NSTAT1,2,3 is the number of cells in solution state 1,2,3
Solution state 1 means no oil is present in the cell
Solution state 2 means both oil and gas are present in the cell
Solution state 3 means no gas is present in the cell

NTRAN is the number of state transitions since the last non-linear iteration.

Any non-zero value of NSCHP or NCHOP increases material balance errors for the subsequent non-linear iteration and therefore reduces the chances of convergence. Some saturation chops can be avoided by adjusting relative permeability curves in such a way that the critical saturation is not the same as the lowest saturation value in the table. For instance, instead of

```
SWFN
  0.2  0     7
  0.3  0.07  4
  0.4  0.15  3
  0.5  0.24  2.5
  0.6  0.33  2
  0.8  0.65  1
  0.9  0.83  0.5
  1    1     0    /
```

try using

```
SWFN
```

```
  0.2   0      7
  0.21  0       1*
  0.3   0.07   4
  0.4   0.15   3
  0.5   0.24   2.5
  0.6   0.33   2
  0.8   0.65   1
  0.9   0.83   0.5
  1    1      0     /
```

The new saturation value at 0.21 may help convergence. It will not affect the initial fluids-in-place but will unfortunately slightly reduce the water mobility for water saturations between 0.2 and 0.3. This may not be important to engineering accuracy.

Look for oscillations in the CNV for a phase. If one iteration has a positive value, the next iteration has a negative value, then the next is positive, then negative, etc. then there is a non-linearity in the system. These are sometimes associated with sudden changes in the slope of the relative permeability curves. If you have access to the SCAL program, you can plot these slopes and look for discontinuities. If you have access to a spreadsheet program then you can numerically calculate and plot the slopes. Remember that Eclipse will use all the values of saturation and relative permeability that you give in the table without any smoothing. You should therefore try to avoid tables such as

```
SWFN
  0.2       0       7
  0.21       0      1*
  0.3        0.07   4
  0.301     0.07    4
  0.398     0.14    3
  0.4       0.15    3
  0.401     0.17    3
  0.402     0.19    3
  0.5       0.24    2.5
  0.6       0.33    2
```

```
  0.8     0.65   1
  0.9     0.83   0.5
  1       1      0    /
```

The table above has saturation values that are too close to each other and the slopes of the relative permeabilities shows severe changes. You should also try to avoid tables such as

```
SWFN
  0.2     0      7
  0.3     0.     4
  0.5     0.01   2.5
  0.51    0.60   2
  0.8     0.68   1
  0.9     0.83   0.5
  1       1      0    /
```

The table above has a very sudden krw change from krw=0.01 at Sw=0.5 to krw=0.60 at Sw=0.51 and will certainly cause convergence problems.

5.3.2 Eclipse 300

In Eclipse 300, you can have either a visual display of the grid blocks causing convergence problems or you can look at numerical output in the same way as for ECLIPSE 100.

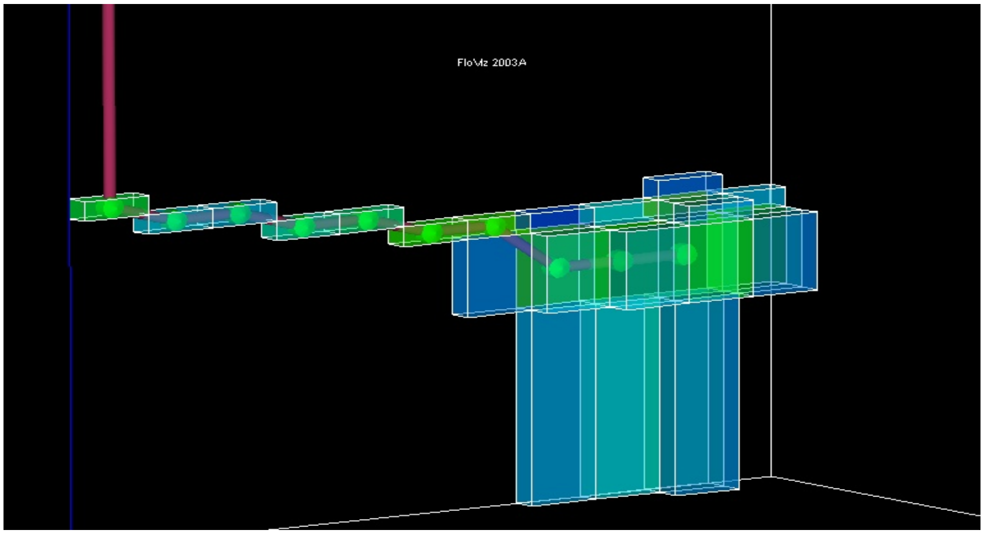
Visual option in RPTRST – ask for CONV

- Output of cells which are causing convergence problems. By default, CONV=10 is set so that the worst 10 cells will be output

Output

- CONV_VBR: Worst cells based on volume balanced residual
- CONV_PRU: Worst cells based on pressure updates

Adding CONV to the RPTRST keyword will send two new outputs to the restart files. Each cell will have two new variables that will be used to count the number of times that cell has been one of the most difficult cells to converge. At the beginning of the simulation each cell will have its counter set to zero. At every timestep, the 10 most difficult cells will have their counter increased by 1. At the end of the run you can display the cells with the most problems.



In the example above we have used the threshold option to remove all cells that have had less than a few cases of difficult convergence. The cells that are highlighted are the most difficult cells, and are clearly associated with one of the wells.

Alternatively, you will get non-linear debug if the 8th data item in the DEBUG3 keyword is set greater than 0. Some of the debug information has already been described in section 5.2 above. Typical output is of the form:

```
Iteration        0 linears req        7
DX Pressure  0    -40.075969 25 32  4   F    1.469590
DX    Comp  1     -0.000375 25 32  1   T   0.010000
DX    Comp  2     -0.000980 25 32  1   T   0.010000
DX    Comp  3     -0.025419 25 32  1   F   0.010000
DX    Comp  4     -0.002318 25 32  1   T   0.010000
DX    Comp  5     -0.000318 25 32  3   T   0.010000
DX    Comp  6      0.009711 25 32  1   T   0.010000
DX    Comp  7      0.008562 25 32  1   T   0.010000
```

```
DX    Comp  8      0.004396 25 32  1   T    0.010000
DX    Comp  9      0.001465 25 32  1   T    0.010000
DX    Comp 10      0.000907 25 32  4   T    0.010000
NLStep= 0 lin= 7 aot=  27.27 Rmax=0.8514E+00 Rsum=0.2739E-03 egain=0.2624E-01
 Iteration          1 linears req          5
DX Pressure  0     -0.563835 25 32  1   T    1.592056
DX    Comp  1      0.000035 25 32  1   T    0.010833
DX    Comp  2      0.000063 25 32  1   T    0.010833
DX    Comp  3      0.001887 25 32  1   T    0.010833
DX    Comp  4      0.000242 25 32  1   T    0.010833
DX    Comp  5      0.000111 25 32  1   T    0.010833
DX    Comp  6      0.000270 26 32  1   T    0.010833
DX    Comp  7      0.000238 26 32  1   T    0.010833
DX    Comp  8      0.000127 26 32  1   T    0.010833
DX    Comp  9      0.000044 26 32  1   T    0.010833
DX    Comp 10     -0.000317 25 32  2   T    0.010833
NLStep= 1 lin=  5 aot=    0.38 Rmax=0.1921E-01 Rsum=0.1448E-04 egain=0.3165E-01
 Max changes:          pres       40.6      25 32  4             temp      0.00      0  0  0
                       oil satn  0.516E-01  17  7  1           gas satn -0.178E-01  17  8  1
                       wat satn -0.939E-03  25 32  4           eng dens   0.00      0  0  0
 Throughput ratio:avrg    0.404E-01 max    0.192              26  32   2
 MIF ;   103.0 9.00 6.9094 .01725 8973.3 157.46 62000. 3531.4    0.0 60500. 2 2%
```

This output shows two non-linear iterations leading to a timestep report.

The first line:

```
Iteration          0 linears req          7
```

shows that the iteration 0 (the initial estimate) needed 7 linear iterations to solve the linear problem.

The next 11 lines consist of one line for each of the solution variables showing the largest change in that variable in any cell during this iteration. The solution variables for each grid block are the pressure in the grid block and the molar density of each hydrocarbon component, and a water term. This model has 9 hydrocarbon components. Water is written as component 10.

```
DX Pressure  0    -40.075969 25 32  4   F    1.469590
DX    Comp  1     -0.000375 25 32  1   T    0.010000
DX    Comp  2     -0.000980 25 32  1   T    0.010000
DX    Comp  3     -0.025419 25 32  1   F    0.010000
DX    Comp  4     -0.002318 25 32  1   T    0.010000
DX    Comp  5     -0.000318 25 32  3   T    0.010000
DX    Comp  6      0.009711 25 32  1   T    0.010000
DX    Comp  7      0.008562 25 32  1   T    0.010000
DX    Comp  8      0.004396 25 32  1   T    0.010000
DX    Comp  9      0.001465 25 32  1   T    0.010000
DX    Comp 10      0.000907 25 32  4   T    0.010000
```

In each of these lines, DX means the solution change. The first line is the Pressure change. The largest pressure change was an increase of 40.075969 psi in cell (25,32,4), which happen to contain an injecting completion. The "F" on that line means "False", in that the pressure variable has not converged, as the pressure change is greater than 1.469590, which is the maximum pressure change, allowed for convergence.

The second DX line shows the largest change in the molar density, expressed as a saturation equivalent, for component 1. This increase of 0.000375 was in cell (25,32,1) and is less than the convergence maximum of 0.01, so that the component 1 variable is considered to be converged. In fact all the components have converged except for component 3.

The non-linear iteration however has not converged since two of the variables (pressure and component 3) are not yet converged.

The next line is a summary of the first iteration (iteration 0) and has already been discussed in section 5.2 above.

```
NLStep= 0 lin= 7 aot=  27.27 Rmax=0.8514E+00 Rsum=0.2739E-03 egain=0.2624E-01
```

NLStep=0	states that this in non-linear step 0
Lin=7	says that 7 linear iterations were needed to solve it
Rmax=	0.8514E+00 is the worst (maximum) residual at the beginning of this iteration
Rsum=	0.2739E-03 is the sum of all the residuals at the beginning of this iteration

egain=0.2624E-01 is the gain discussed in section 5.2

The next line

```
Iteration        1 linears req        5
```

is the start of the report on the second non-linear iteration, Iteration 1, which needed 5 linear iterations.

The net 11 lines are the solution changes. They are similar to the reported changes for the first non-linear iteration except that now both the pressure and component 3 have changed by less than the new convergence criteria. The non-linear iterations have now converged.

```
NLStep= 1 lin=  5 aot=   0.38 Rmax=0.1921E-01 Rsum=0.1448E-04 egain=0.3165E-01
```

Is the report for that converged iteration showing that the maximum residual at the beginning of that iteration was down to 0.1921E-01 and the sum of residuals was down to Rsum=0.1448E-04.

There then follows a report on the changes during that timestep.

```
 Max changes:     pres      40.6      25 32  4          temp      0.00      0  0  0
                  oil satn  0.516E-01  17  7  1         gas satn -0.178E-01  17  8  1
                  wat satn -0.939E-03  25 32  4         eng dens  0.00      0  0  0
```

The maximum pressure and saturation changes are reported, as well as the cells in which this change occurred. In the case of thermal runs, the maximum temperature and energy density changes are also reported.

The maximum throughput is reported next. Throughput is defined as the volume flowing through a cell divided by the pore volume of the cell. If the throughput is too high it could cause convergence problems, and the pore volume of the cell that has the high throughput should be examined.

```
Throughput ratio:avrg   0.404E-01 max   0.192            26  32   2
```

The last of these lines is the report of production, etc. for the timestep. These report steps have been described in section 3.

```
 MIF ;   103.0 9.00 6.9094 .01725 8973.3 157.46 62000. 3531.4    0.0 60500. 2 2%
```

SUMMARY:

- **To get more information for ECLIPSE 300,** add ‘CONV’ to RPTRST

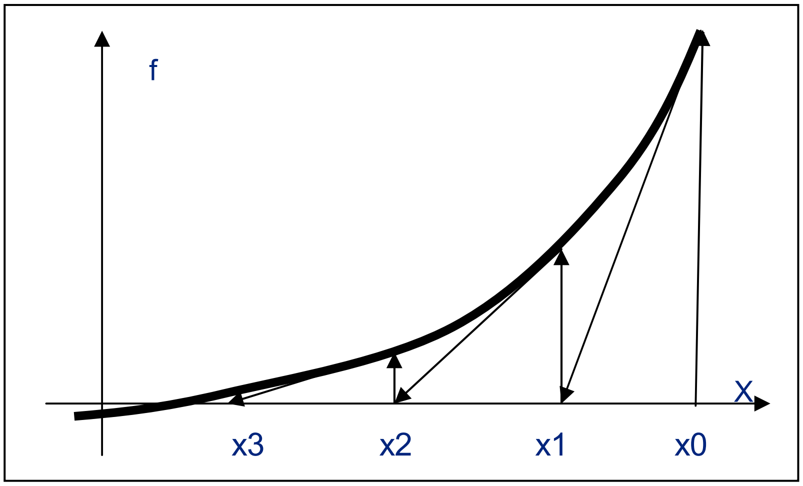
```
or use
    DEBUG3
      7* 1 /
```

6. Discussion on Non-Linearity

6.1 Slope instability

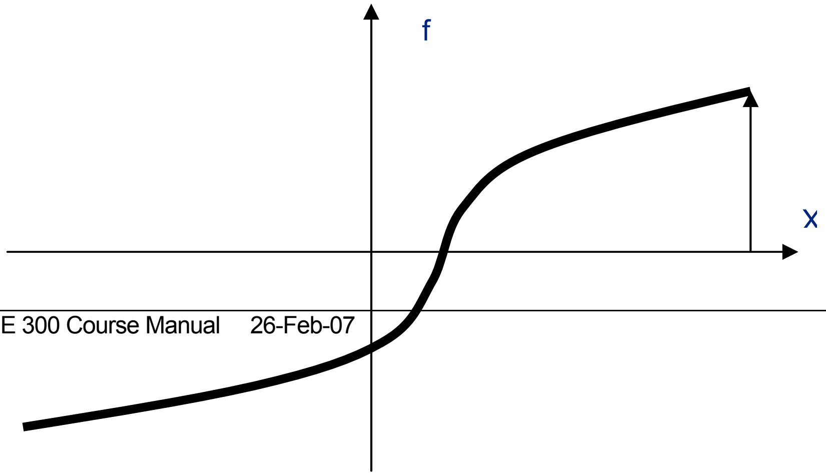
The most common cause of a convergence failure of the non-linear equations is probably data that causes steep changes in slope in the equations.

We have already seen how a well-behaved non-linear equation can be solved in a few iterations by an iterative technique. Each iteration brings us closer to the solution, and in principle we can get as close to the solution as we want.

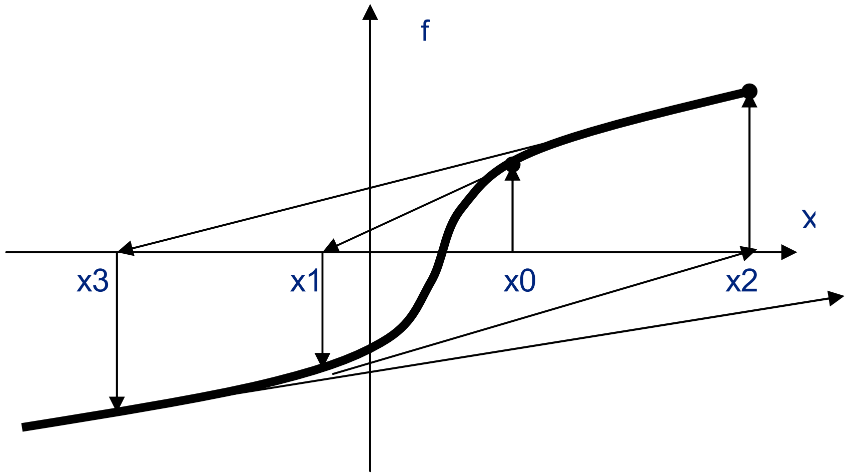


Newton-Raphson convergence

Suppose however that the data that has been provided to ECLIPSE is very discontinuous. For example the relative permeability curves could be very steep over a small range of saturations. In this case the function that we are trying to solve could look like this:



This type of function cannot easily be solved iteratively unless we start very close to the solution.



Divergent Newton-Raphson iteration process

Suppose our first estimate is x0. Following our normal iterative procedure, the next estimate will be at x1, the next at x2, then x3. Each iteration takes us further and further away from the solution.

If this situation arises, the iterations will not converge. They will continue until the limit on the number of iterations is reached, then the timestep will be chopped. This will continue until the timestep is small enough that so little has changed during the timestep that we start on the linear part of the curve very close to the solution.

6.2 IMPES instability

A different kind of instability is associated with explicit schemes. Once some kind of instability occurs (via throughput or capillary pressure say), the manifestation is often in the form of poor convergence. A few general problems are worth noting:

1. In explicit cells it is possible to attempt to extract more fluid than is present. This physical inconsistency leads to a residual that can't be driven to zero. The only course of action is to reduce the timestep. Preventing timestep chops for this reason is difficult, as the timestep predictor is based on the old solution, not the one we're about to walk into. It's possible that AIM could be used to ease these situations by making potential cells implicit.

2. Flow reversal. An IMPES simulation running without instability appears at first sight a linear (or very near linear) problem in particular in formulations with masses as variables. However, flow reversals are a major non-linearity, and as the number of cells in a model increases the odds of having a flow reversal between Newton iterations becomes high, resulting in iteration counts of 3 or 4. In this case the attraction of an AIM solver increases, because we're already doing 3 or 4 iterations hence why not attempt to increase the allowable timestep by making a small fraction of cells implicit.

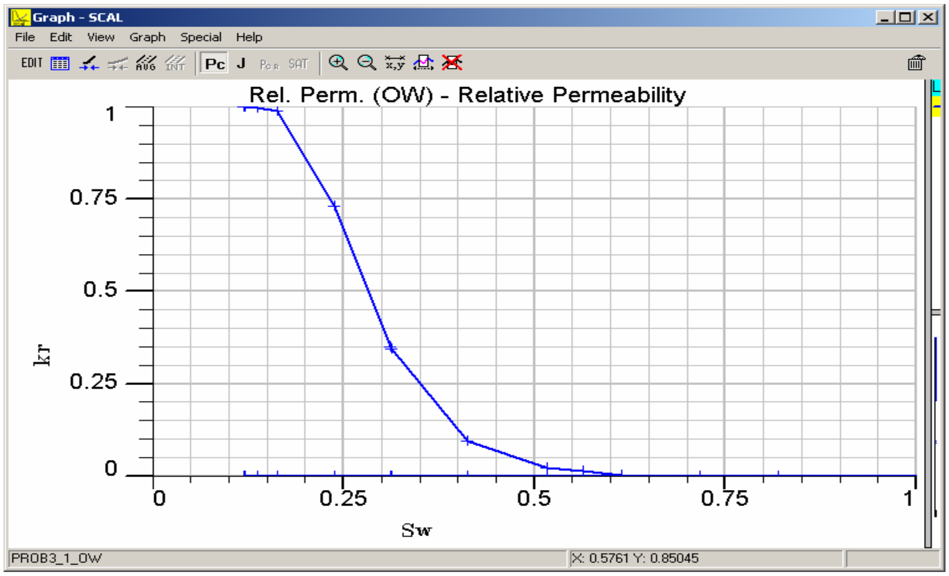
3. The group control algorithm needs to be used and checked with some care as it can produce well rate instabilities, which cause violent swings in the field leading to poor convergence.

4. Non-monotonic VFP tables can cause convergence problems. VFP tables are checked by default in Eclipse 300 and can be switched on in Eclipse 100 by the EXTRAPMS keyword. Always check all warnings relating to VFP tables.

7. Another Example

We noticed in another case of poor convergence that the grid blocks that were having convergence problems were all using the same saturation table number (SATNUM). Grid blocks using other saturation table numbers had no problems.

The plot of the relative permeabilities looked OK:



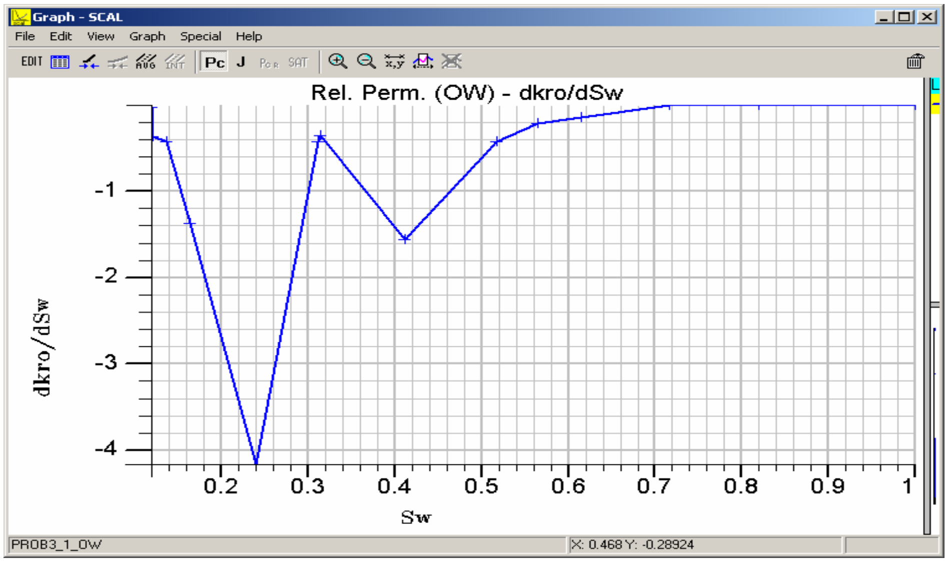
and the table itself looked fine:

```
-- SOIL   KROW    KROG
SOF3
   0       0       0
   0.181   0       0
   0.283   0.0001  0.0001
   0.385   0.0015  0.0015
   0.436   0.0124  0.0124
   0.483   0.0217  0.0217
   0.588   0.0939  0.0939
   0.686   0.3499  0.3499
   0.689   0.3501  0.3501
   0.761   0.7323  0.7323
   0.837   0.9887  0.9887
   0.863   0.9978  0.9978
   0.879   1       1
   0.880   1       1   /
```

We only found the problem when we plotted the derivatives of Kro using the SCAL program[48]:

---

[48] You can also do this using a spreadsheet.



There was clearly something unusual happening around 30% oil saturation, equivalent to about 70% water saturation.

```
--  SOIL     KROW     KROG
SOF3
    0         0         0
    0.181     0         0
    0.283     0.0001    0.0001
    0.385     0.0015    0.0015
    0.436     0.0124    0.0124
    0.483     0.0217    0.0217
    0.588     0.0939    0.0939
    0.686     0.3499    0.3499
    0.689     0.3501    0.3501
    0.761     0.7323    0.7323
    0.837     0.9887    0.9887
    0.863     0.9978    0.9978
    0.879     1         1
    0.880     1         1   /
```

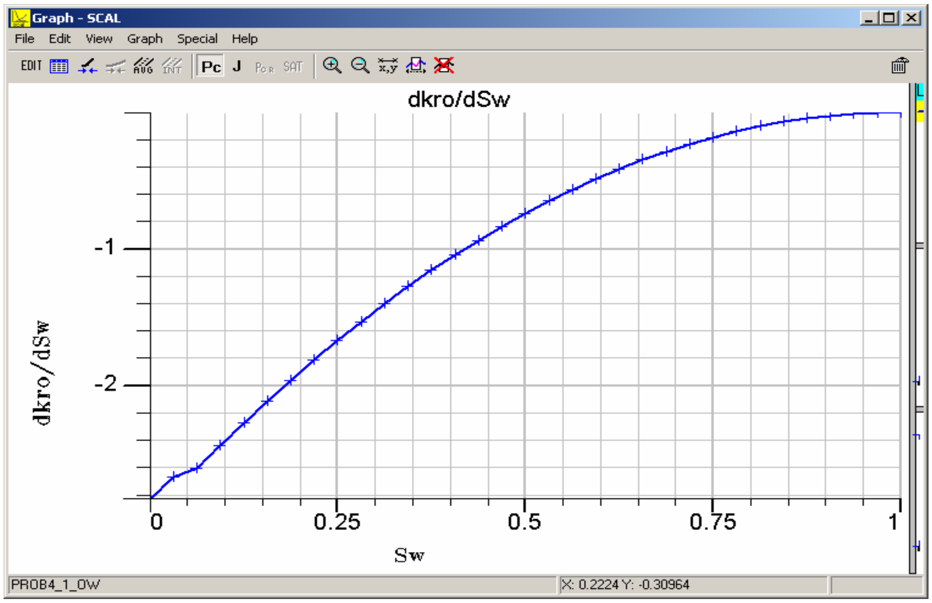
The table had been generated automatically, combining two other tables, and had two saturation values that were very close together. The precision meant that the slopes around those values changed rapidly whenever the grid block saturation was around 30% oil, and this was the cause of the convergence problem. Remember that ECLIPSE honors whatever data you put in, so ECLIPSE will not adjust any of the relative permeabilities, however discontinuous.

The fix was simple. Removing either of the two lines did not change the flow behavior of the fluids, and made the simulator run much faster:

```
-- SOIL   KROW    KROG
SOF3
   0      0       0
   0.181  0       0
   0.283  0.0001  0.0001
   0.385  0.0015  0.0015
   0.436  0.0124  0.0124
   0.483  0.0217  0.0217
   0.588  0.0939  0.0939
   0.689  0.3501  0.3501
   0.761  0.7323  0.7323
   0.837  0.9887  0.9887
   0.863  0.9978  0.9978
   0.879  1       1
   0.880  1       1   /
```

Another small change was also suggested for the engineer to consider. Relative permeability values close to zero and close to 1 are probably not experimentally measured but are probably calculated from a correlation. It may be worth reviewing whether values such as 0.0001 or less should be in fact zero, and whether values greater than 0.999 should be set to 1.

The final derivative slope after all the changes was very smooth:


Graph - SCAL
File
Edit
View
Graph
Special
Help
EDIT
AVG
INT
Pc
J
Pc R
SAT
dkro/dSw
-1
-2
dkro/dSw
0
0.25
0.5
0.75
1
Sw
PROB4_1_OW
X: 0.2224 Y: -0.30964

8. Convergence problem Checklist

- **Check all problem and warning messages.**

- Does the model run better with no tuning keywords?
  Remove TUNING or TSCRIT or CVCRIT keywords and try to run.

- Grid data
  Check whether you need to set a minimum pore volume

- PVT and VFP data
  Use EXTRAPMS in Eclipse 100. In all simulators, avoid PVT or VFP extrapolations
- SCAL data
  Check the slopes of all relative permeability tables.

- Radial runs:
  Is the inner radius too small?
- Dual porosity runs:
  Is sigma too large
- LGRs
  Are the cells too small?

23. ECLIPSE 100 pseudo-compositional

A number of attempts have been made to model compositional effects using black-oil simulation. These effects are best modeled using a compositional simulator such as ECLIPSE 300, but facilities exist in ECLIPSE 100 to approximate compositional effects by extending the black-oil model.

We shall discuss two pseudo-compositional effects:

1. a GI model of the preferential stripping of light components from oil by a gas drive
2. a black-oil miscibility model

ECLIPSE 100 GI model

One inadequacy with the black-oil approach is with the treatment of gas injection above the saturation pressure, where the black-oil model cannot describe the stripping of liquid components in inverse proportion to their molecular weights[49].

The standard black oil model assumes that the saturated hydrocarbon fluid properties are functions of pressure only and disregards any compositional dependence in the saturated fluid PVT properties. As a consequence, when dry gas is injected the gas continues to re-vaporize liquid at a rate governed only by the local pressure. The vapor saturates over a zone whose thickness is of the order of one grid block - in particular all the liquid in the vicinity of the injectors evaporates rapidly. Results obtained with fully compositional simulation models suggest that liquid saturation profiles would vary more slowly.

A number of extensions of the black oil model to treat compositional effects during gas injection have been reported in the literature, and all methods hinge on extending the fluid property treatment so that the saturated fluid properties depend not only on pressure but also on an additional parameter which characterizes compositional changes in the reservoir liquid and vapor phases at constant pressure.

The model described here is based on the method proposed by Cook, Jacoby and Ramesh. The extra parameter introduced into the model to represent the light-end stripping effects is a cumulative injection gas flow parameter (Gi) and is analogous to tracking the flow of the dry injection gas around the reservoir grid. We track the cumulative amount of dry injection gas (Gi), which has contacted the oil in each grid cell, and this is the correlating parameter used to

---

[49] We discussed this effect earlier when we explained the vaporising gas drive process in the chapter on miscibility.

determine the fluid property changes at constant pressure. An extra variable has therefore to be stored in each grid cell corresponding to the Gi variable.

- **Black-Oil model assumes properties are a function of P only**
- **So when dry gas is injected over a condensate below Pdew, the gas will continue to revapourise at a rate dependent only on P.**

- **Pseudo-compositional approach is to add one more parameter**
- **GI model is to keep track of how much gas has passed over the oil.**
- **The more gas has passed, the less oil is picked up.**

The saturated hydrocarbon PVT properties should now contain a dependence on both pressure and Gi. In practice, it is usually the variation of Rs*sat* and Rv*sat* with Gi that is the most significant. For example, it is likely that Rv*sat* could be reduced by an order of magnitude before complete vaporization of the liquid in a cell finally occurred.

Using the Gi model

The keyword `GIMODEL` in the `RUNSPEC` section is used to activate the option. Gas condensate and live oil must also be declared active phases using keywords `VAPOIL` and `DISGAS` in the `RUNSPEC` section. The `IMPES` solution method should not be used when the Gi model is active.

The oil and gas PVT properties are specified using the `PVTO` and `PVTG` keywords in the usual way. When the Gi model is active, the data specified using the `PVTG` and `PVTO` keywords refer to fluid conditions at GI=0. A two-dimensional variation of saturated fluid properties is required for the option to specify the full (P, Gi) dependence of Rs*sat*, Rv*sat*, Bo*sat* and Bg*sat*.

Use either the keywords `RVGI`, `RSGI`, `BGGI`, `BOGI` or the single keyword `GIALL` to specify these variations, and these should be defined in the `PROPS` section. Note that the function values entered under these keywords refer to **multiplier** values on the saturated data contained in the `PVTO` and `PVTG` keywords (that is, at Gi=0). The corresponding Gi-nodal values are specified using the `GINODE` keyword in the `PROPS` section.

The PVT properties specific to the Gi model can be echoed using the ‘`GINODE`' mnemonic in the `RPTPROPS` keyword. Output of the values of Gi in each cell at each report time can be produced using the ‘`GI`' mnemonic in the `RPTSCHED` keyword. Debug from the option can be produced using integer 30 of the `DEBUG` keyword.

In RUNSPEC

- **GIMODEL**
- **VAPOIL**
- **DISGAS**

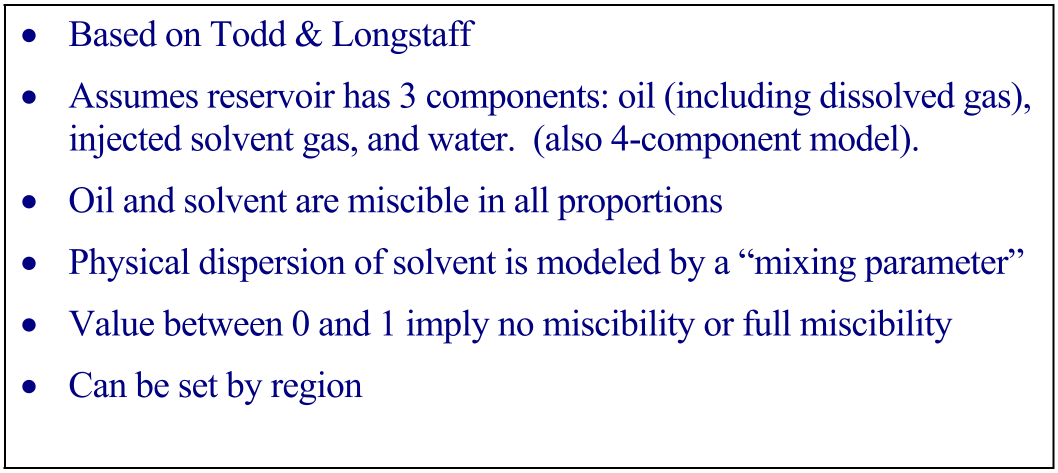
In PROPS

- **RVGI, RSGI, BGGI, BOGI**
- **or GIALL**
- **and GINODE**

If you are using the enumeration option to specify the initial solution (instead of EQUIL) then you will need to use the keyword GI in the solution section to define the initial GI values in each grid block.

ECLIPSE 100 Miscibility model

The Miscible Flood model is an implementation of the empirical treatment suggested by M. Todd and W. Longstaff.



- Based on Todd & Longstaff
- Assumes reservoir has 3 components: oil (including dissolved gas), injected solvent gas, and water. (also 4-component model).
- Oil and solvent are miscible in all proportions
- Physical dispersion of solvent is modeled by a “mixing parameter”
- Value between 0 and 1 imply no miscibility or full miscibility
- Can be set by region

The Todd-Longstaff model is an empirical treatment of the effects of physical dispersion between the miscible components in the hydrocarbon phase. The model introduces an empirical parameter, ω, whose value lies between 0 and 1, to represent the size of the dispersed zone in each grid cell. The value of ω thus controls the degree of fluid mixing within each grid cell. A value of $\omega=1$ models the case when the size of the dispersed zone is much greater than a typical grid cell size and the hydrocarbon components can be considered to be fully mixed in each cell. In this case the miscible components have the same value for the viscosity and density, as given by the appropriate mixing rule formulae. A value of $\omega=0$ models the effect of a negligibly thin dispersed zone between the gas and oil components, and the miscible components should then have the viscosity and density values of the pure components. In practical applications an intermediate value of ω would be needed to model incomplete mixing of the miscible components.

A value of $\omega=1$ results in a piston-like displacement of oil by the injected solvent. If $\omega=0$ the displacement is similar to an immiscible displacement (except for the treatment of relative permeability). An intermediate value results in a continuous solvent saturation increase behind the solvent front. Todd and Longstaff accounted for the effects of viscous fingering in 2D studies by setting $\omega=2/3$ independently of mobility ratio. For field scale simulations they suggested setting $\omega=1/3$. However, in general history matching applications, the mixing parameter may be regarded as a useful history matching variable to account for any reservoir process inadequately modeled.

Miscibility and Pressure

As we have already discussed, gas is only miscible with the reservoir oil at higher pressures. We model the transition between miscibility and immiscibility as a function of pressure by using the `PMISC` keyword. The `PMISC` function interpolates between the immiscible and miscible values of the PVT properties, relative permeability data and capillary pressure data. This keyword is optional; if it is not present then miscibility is assumed at all pressures.

Using the Miscibility model

The keyword `MISCIBLE` in the `RUNSPEC` section activates the model.

The keyword `MISCNUM` should be used in the `REGIONS` section to define the miscibility region to which each grid cell belongs. This keyword is optional, and a default region number of 1 is assumed. The maximum region number that can be defined (`NTMISC`) must be entered in item 1 of the keyword `MISCIBLE` in the `RUNSPEC` section. You can override the miscible flow calculation of the gas and oil properties in certain cells in the grid. If a cell is allocated a `MISCNUM` region number of zero, then the gas and oil will be assumed to be immiscible under all conditions in the cell.

- **Assumes straight-line relative permeability curves**
- **Mixing parameter TLMIXPAR**
- **Uses mixing rules for viscosity and density**

- **pressure-dependent miscibility factor**

```
PMISC
-- pressure  miscibility (M)
    1000      0.0
     4000     0.0
     4100     1.0
     9000     1.0   /
```

The mixing parameter, ω, should be input in the `PROPS` section under the keyword `TLMIXPAR`. A single real number in the range 0 to 1 must be supplied for each miscible region. If a different mixing parameter is required for the effective densities, a second mixing parameter can be supplied for each miscible region. If the grid contains any cells whose `MISCNUM` region is zero, the mixing parameter is automatically set to zero in those cells.

For gas-oil runs, the keywords `SGFN` and `SOF2` should only be entered if there is at least one cell which has a `MISCNUM` region number of zero. For those cells that are allocated a positive `MISCNUM` region number, ECLIPSE assumes that the gas-oil capillary pressure is zero and the relative permeabilities are equal to their respective saturations.

In oil-water-gas runs the keywords `SOF2` and `SWFN` are obligatory. In the miscible regions, the `SWFN` data defines the water relative permeability and water-hydrocarbon capillary pressure in the usual way. The `SOF2` keyword represents the relative permeability of the hydrocarbon phase with respect to hydrocarbon phase saturation. If there are any immiscible regions in the grid, the `SOF3` and `SGFN` keywords must be used to enter the immiscible gas-oil relative permeabilities.

The **hysteresis** model is available in both the miscible and the immiscible zones. In the miscible zones, a two phase treatment (water/hydrocarbon) of the hysteresis effect is invoked on the water-hydrocarbon capillary pressures and relative permeabilities.

The **Saturation Table Rescaling** option is also available in both the miscible and immiscible zones of the grid. In the miscible regions, the saturation table endpoints for the hydrocarbon phase should be entered as oil-in-water data using the appropriate scaling keywords. Data entered for gas end-points will be ignored in the miscible zones.

The miscible residual oil saturation and critical gas saturation versus water saturation tables can be defined in the `PROPS` section using the keywords `SORWMIS` (and `SGCWMIS` when the Solvent model is used). A maximum of `NTMISC` tables, each with a maximum of `NSMISC` rows of data, are allowed. The `SORWMIS`/`SGCWMIS` keywords are not obligatory and an effective residual oil saturation of 0.0 and critical gas value of 0.0 will be assumed if the appropriate keyword is omitted. The miscible solvent-oil relative permeability curves can be modified using the `MSFN` keyword. If the `MSFN` keyword is omitted, straight line relative permeability curves are used.

The surface densities of the stock-tank oil, water and solution gas components should be defined using the existing `DENSITY` or `GRAVITY` keyword. The surface density of the injection gas must be entered using the `SDENSITY` keyword in the `PROPS` section. In the immiscible zones, the injection gas surface density is taken from the `DENSITY` or `GRAVITY` keyword to equal that of the solution gas.

Specification of pressure function data for the pure components is unaltered from the usual data requirements of ECLIPSE. If the oil is defined as dead (no `DISGAS` keyword in `RUNSPEC`) then the initial solution gas is omitted from the GOR reports in the results file and the GOR refers to the solvent-oil ratio. It is possible to include the initial solution gas in the GOR reports by defining the oil component to be live (keyword `DISGAS` in `RUNSPEC`). In either case, the reported saturation values for oil and solvent refer to the relative volume occupied by each component as if they were not mixed.

As already mentioned, the pressure dependence of miscibility can optionally be controlled by using the `PMISC` keyword.

- **PMISC is used to interpolate between miscible and immiscible relative permeability curves**

- **First scale the endpoints**

  Sor = Sorm*M + Sori*(1-M)

- **then scale kr**

  kr = krm*M + kri*(1-M)

If `DISGAS` has been specified in the `RUNSPEC` section, the value of `DRSDT` refers to any immiscible zones in the grid. Its default value in these regions will be infinity. In the miscible zones, the value of `DRSDT` is always zero.

Residual oil in miscible case

A feature of miscible gas injection processes that may also be modeled is the screening effect of high water saturation on the contact between the miscible gas and the in-place oil in each grid cell. The effective residual oil saturation to a miscible gas drive is found to increase with increasing water saturation and correct modeling of the effect is important since it may reduce the efficiency of the miscible displacement.

Extra option: Water blocking

- The effective residual oil saturation to a miscible gas drive can increase with increasing water saturation
- At high water saturations, water may prevent access to oil in some of the smaller pores.
- SORWMIS

```
--  Sw  Sormis
    0.0  0.0
    0.2  0.07
    0.8  0.11 /
```

- also for gas

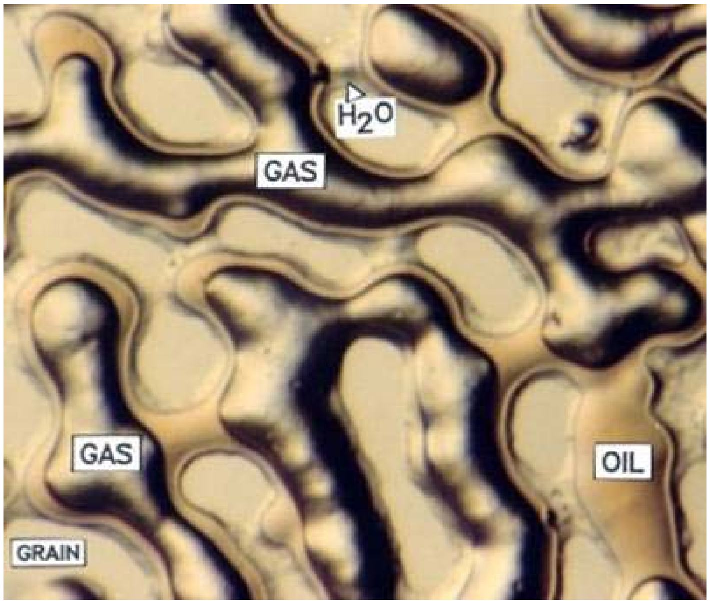
The process is modeled by introducing an effective residual oil saturation, Sor, which depends on the water saturation. Mobile oil saturation is then calculated by

$So^* = Max(So-Sor, 0.0)$

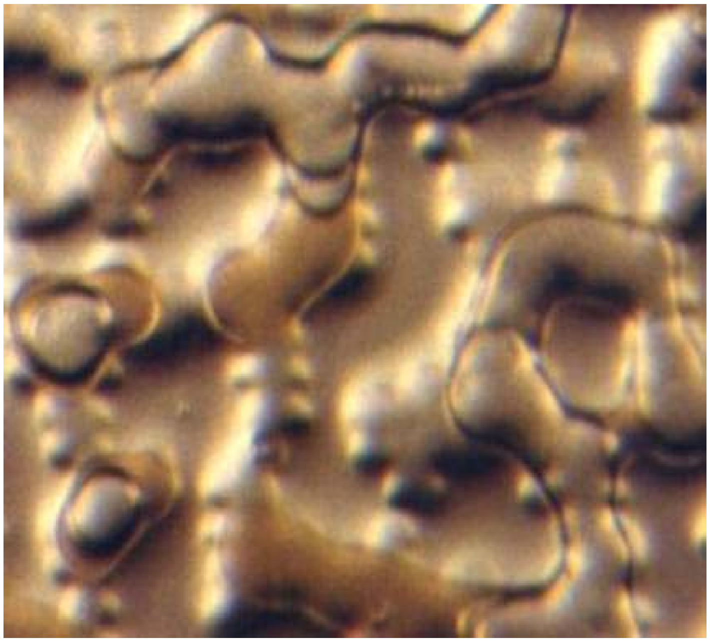
The mobile oil saturation So^* is then used to determine the relative permeabilities of miscible components and the effective gas and oil viscosities and densities in each grid cell. The keyword `SORWMIS` sets the effective residual saturation.

We can see the effective residual oil in the following pictures from :
http://www.mktechsolutions.com/Miscble%20Gas.htm

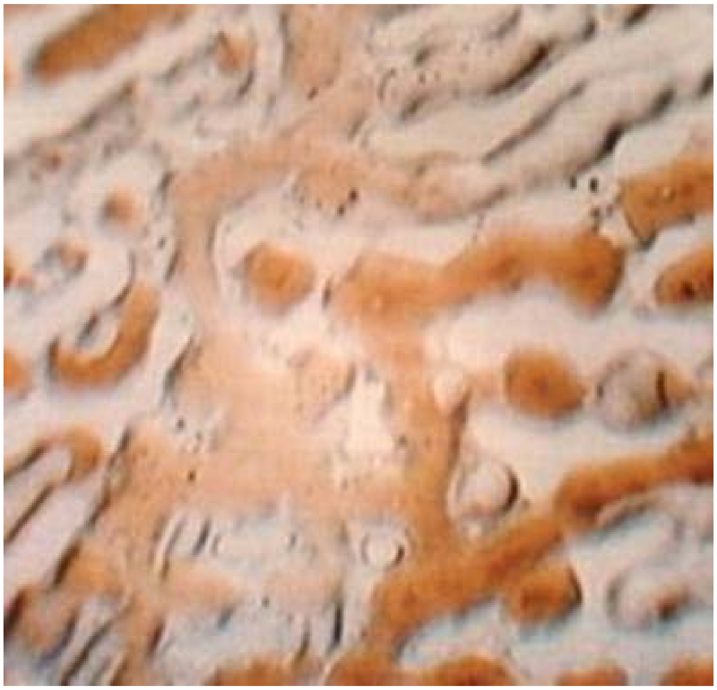
The first picture shows the oil, water and gas distribution in rock at a pressure of 1000 psig, below the miscible pressure. There is a clear interface between the phases.



At a higher pressure of 1500 psig, we are close to miscibility.



At 2500 psig, we have miscibility between the oil and gas phases, but there is still some oil left in parts of the rock that have not been reached by the gas.



ECLIPSE 100 Solvent model

This ECLIPSE 100 solvent model is a 4-component extension of the Todd and Longstaff model. The four components are water, oil, reservoir gas and an injected solvent.

Using the Solvent model

RUNSPEC data

SOLVENT Activates the Separate Solvent component

MISCIBLE Initiates the mixing calculation

If `SOLVENT` is specified, then the 4-component model is used. `SOLVENT` should only be used with all the other 3 phases (Water, Oil, Gas) present.

If `MISCIBLE` is specified, then the mixing calculations are used, employing the 3-component model if `SOLVENT` is **not** specified and the 4-component model when `SOLVENT` is specified.

PVT data

In the 4-component model, PVT data needs to be supplied for the Solvent. This consists of the `PVDS` and `SDENSITY` keywords:

SDENSITY Surface density of the Solvent

PVDS Pressure dependent data for each PVT region, analogous to `PVDG`.

Relative Permeability data

`SSFN` defines the solvent relative permeability.

In 4-component cases the miscibility function needs to be defined to control the transition from miscible to immiscible relative permeabilities. This is done using the `MISC` keyword and the optional `PMISC` keyword in the `PROPS` section.

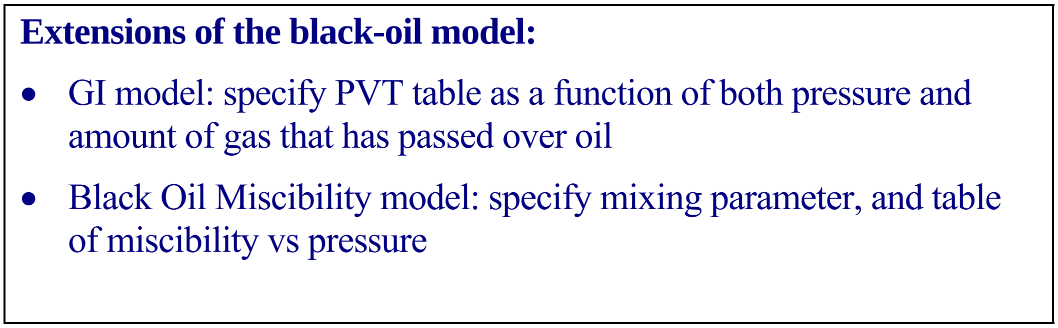
The miscible solvent-oil relative permeability curves can modified using the `MSFN` keyword. If the `MSFN` keyword is omitted, straight line relative permeability curves will be used.

Injecting solvent into the reservoir

Solvent can be injected by specifying a gas injection well. A separate keyword `WSOLVENT` can then be used to specify a fraction of the gas flow as solvent.

It is also possible to initialize the model by enumeration and to include a Solvent saturation. This is achieved using the `SSOL` keyword in the `SOLUTION` section.

Summary: Pseudo-compositional Models



Extensions of the black-oil model:

- GI model: specify PVT table as a function of both pressure and amount of gas that has passed over oil
- Black Oil Miscibility model: specify mixing parameter, and table of miscibility vs pressure

24. Diffusion in oil and gas

There are two diffusion models in ECLIPSE 300.

1. In the first model diffusion is driven by the concentration gradient.

$$J_i = -cD_i\left(\frac{\partial x_i}{\partial d}\right)$$

where

Ji	is the molar flux of component i per unit area
c	is the total molar concentration given by c = 1/V^m
V^m	is the molar volume of the mixture
Di	is the diffusion coefficient of component i
$\left(\frac{\partial x_i}{\partial d}\right)$	Is the mole fraction gradient

2. In the second model diffusion is driven by the gradient of the chemical potential:

$$J_i = -c\left(D_i^a \frac{\partial \ln f_i}{\partial \ln x_i}\right)\bullet\frac{\partial x_i}{\partial d}$$

where

Di^a	is the activity-corrected diffusion coefficient of component i
xi	is the mole fraction
fi	is the component fugacity

- **At high pressures, concentration gradient is not most accurate predictor for diffusion.**
- **Component chemical potential should be used. Can then include effect of gravity.**

$$\mu = \mu_0 + RT \ln f_i - M_i g\left(h - h_0\right)$$

- **M = Molecular Weight**
- **G = Gravity Constant**

- **h = Elevation**
- **For isothermal, horizontal flow and using** , m/RT, **let Di^a be defined by**

$$J_i = -cD_i^a x_i \frac{\partial \ln f_i}{\partial d}$$

Expanding

$$\frac{\partial \ln f_i}{\partial d} = \frac{\partial \ln f_i}{\partial \ln x_i} \frac{1}{x_i} \frac{\partial x_i}{\partial d}$$

So that

$$J_i = -c\left(D_i^a \frac{\partial \ln f_i}{\partial \ln x_i} \right) \bullet \frac{\partial x_i}{\partial d}$$

Comparing with

$$J_i = -cD_i \left(\frac{\partial x_i}{\partial d} \right)$$

We find that

$$D_i^a = \frac{D_i}{\partial \ln f_i / (\partial \ln x_i)}$$

Thermal diffusion and hydrostatic equilibrium

The term “thermal diffusion” is used here to describe the diffusion of components caused by a temperature gradient, and should not be confused with diffusion in a thermal simulation. The thermal diffusion term is usually small, but has been included for simulating the initial conditions in a reservoir where there is a temperature gradient. In the absence of any wells and aquifers, a simulation run reaches a steady state when there is no diffusive flow.

The thermal diffusive flow will be zero when

$$\frac{\partial}{\partial d}\left[\mu_i - M_i gh + M_i D_i^T \ln(T)\right] = 0$$

for each phase. The second term in this equation drives the heavy components to the bottom of the reservoir. The third term drives those components with a low enthalpy / high entropy to the hottest parts of the reservoir. When this last term is included the reservoir will not be in thermodynamic equilibrium (since energy is flowing) but it is in hydrostatic equilibrium. The reservoir temperature can be set with either the `TEMPVD` keyword or the `TEMPI` keyword.

The steady state solution is independent of the diffusion coefficients. However, these coefficients control the time it takes the reservoir to reach a steady state. Large timesteps can be used if the simulation is run using the full implicit method `FULLIMP`.

Summary of Diffusion

Three possibilities exist in ECLIPSE 300:

1. **Use normal diffusion coefficients and mole fractions as the driving force. Normal diffusion coefficients are entered using DIFFCOIL and DIFFCGAS.**

2. **Use activity corrected diffusion coefficients and chemical potential as the driving force. Activity corrected diffusion coefficients are entered using DIFFAOIL and DIFFAGAS.**

At low pressures, the two coefficients are equal, as fi -> xiP

3. **The diffusion of components because of a temperature gradient can be simulated with DIFFTGAS and/or DIFFTOIL.**

   These keywords can only be used with DIFFAGAS and/or DIFFAOIL and in non-isothermal runs using TEMPVD or TEMPI.

   Oil diffusive flow is usually much less than gas diffusive flow.

25. Components in Water

There are several facilities in ECLIPSE 300 to model the interaction of gaseous components with water. Depending on what you are trying to model, you can choose to:

- Add CO2 solubility to an existing 3-phase model
- Describe the detailed effects of CO2 sequestration
- Allow all components in a gas-water study to be in both phases

You can also provide salinity information that will more accurately describe some of these effects, and also model more than one type of water.

CO2 solution in water

CO2 Sequestration (2006.1)

Gas -Water Systems

Salinity

Multi-Component water

Given the current technology, it would be impractical to solve equations allowing all possible components to be in all phases.

In the standard compositional models:

The oil phase can have C1,..,Cn, CO2, N2 and H2S

The gas phase can have C1,..,Cn, CO2, N2 and H2S

The water phase can have H2O

Note no H2O in the oil or gas phase

Only H2O in the water phase

The three options below show what is currently possible.

CO2SOL: any gas, any oil, CO2 in all three phases, salinity

CO2SEQ: CO2 + water, salts + salting out

GASWAT: any gas + water, constant salinity

CO2SOL, CO2SEQ and GASWAT all estimate the fluid properties differently. Only one of these can be used in any one simulation run.

CO2 in the water phase

CO2SOLis a three-phase compositional option for simulating CO_2 flooding in oil reservoirs (EOR, storage in oil depleted reservoirs). Water is not allowed to dissolve in the gas or oil phases, CO_2 can be present in the three phases, and other components in the oil and gas phases.

When CO2 is injected into an oil reservoir a significant amount of the CO2 will dissolve into the water.

In a WAG injection the solution of the CO2 can be a very important factor.

The CO_2 solution algorithm allows carbon dioxide to dissolve in the aqueous phase.

CO2SOL:

The oil phase can have C1,..,Cn, CO2, N2 and H2S

The gas phase can have C1,..,Cn, CO2, N2 and H2S

The water phase can have H2O, CO2

Note no H2O in the gas phase

Features of CO2SOL

- EOR or depleted oil/gas reservoir storage
- Solubility dependent on salt concentration - tracer solution
- Any number of hydrocarbon components
- Possible to change parameters for:

- PVT description of fluid by EOS, phase partitioning and density
- Table input solubility,viscosity

Limitations of CO2SOL

- No H2O in the gas phase and therefore no salting out effect. However when using SOLUBILI the salting-out effect is taken into account by correcting solubility in pure water with the Chang et al. correlation for brine
- Salt concentration evaluated explicitly (from tracer solution)
- Solubility for a fixed temperature
- Salt crystalisation is not possible since the salt is represented as a tracer

The phase equilibrium between the aqueous CO_2 and the hydrocarbon phases is then defined by the conditions that the fugacity values are equal.

- To model CO2 in water, fugacities for the CO2 in all three phases must be calculated for the 3 phase flash.
- The fugacity for aqueous CO2 is constructed to match solubility data in the form:

$$f_{CO_2}{}^{A} = P \cdot a_{CO_2} \cdot \phi(P)$$

- The function $\phi(P)$ is constructed by considering a pure CO2/aqueous mixture
- The gas phase fugacity is obtained from EOS.
- Phase equilibrium between aqueous CO2 and hydrocarbon phases is defined by the conditions that fugacity values are equal.

This option is switched on using the `CO2SOL` keyword in the `RUNSPEC` section.

The initial dissolved CO_2 solubility as a function of depth may be specified using the `RSWVD` keyword or the `RSW` keyword. This initial solution honors this value unless it exceeds the saturated CO_2 concentration in which case the saturated value is used. Note that the initial CO_2 concentration may not be in exact equilibrium with the hydrocarbon phases and initial flash modifies the input values slightly.

CO2SOL turns on the option.

The initial dissolved CO2 as a function of depth can be specified with RSWVD keyword.

The initial dissolved CO2 as a function of depth can be specified with RSWVD keyword. The initial saturation honors this value unless it exceeds the saturated CO2 concentration, in which case the saturated value is used.

The program has default values for the solubility data. The default aqueous properties are from Chang, Coats and Nolen (SPE 35164, 1996).

Alternatively, the SOLUBILITY keyword allows the input of non-default properties.

The first line of the solubility table represents water at standard condition, when the dissolved CO2 is at a minimum. ECLIPSE does not assume that this minimum is zero – it uses the value in the first line of the solubility table.

Details of the solubility properties used are obtained by using SOLU in the RPTPROPS keyword.

The solubility data may be entered using the `SOLUBILI` keyword. Alternatively, a default set of data is provided by the program. The default aqueous phase properties follow the correlations given by Chang, Coats and

Nolen. All or any of these properties may be overwritten; see the `SOLUBILI` keyword for details.

```
SOLUBILITY

-- Pressure      Rs(CO2)    Bwater  Viscosity  Compressibility  Saturated
-- Psia          Mscf/stb    RB/Mscf     CP          1/Psi      mole fraction

    14.6959    0.0021    1.02802    0.30000  0.00000272  0.00028895
   787.3909    0.0836    1.04759    0.30000  0.00000272  0.01120103
  1560.0858    0.1268    1.05784    0.30000  0.00000272  0.01689270
  2332.7808    0.1511    1.06357    0.30000  0.00000272  0.02006145
  3105.4757    0.1656    1.06700    0.30000  0.00000272  0.02195732
  3878.1707    0.1752    1.06923    0.30000  0.00000272  0.02318996
  4650.8656    0.1820    1.07083    0.30000  0.00000272  0.02407221
  5423.5606    0.1874    1.07210    0.30000  0.00000272  0.02477146
  6196.2555    0.1921    1.07320    0.30000  0.00000272  0.02538009
  6968.9505    0.1967    1.07426    0.30000  0.00000272  0.02596283
  7741.6454    0.2012    1.07532    0.30000  0.00000272  0.02654488
  8514.3404    0.2057    1.07637    0.30000  0.00000272  0.02712623
  9287.0353    0.2103    1.07743    0.30000  0.00000272  0.02770689
 10059.7303    0.2148    1.07848    0.30000  0.00000272  0.02828686
 10832.4252    0.2193    1.07953    0.30000  0.00000272  0.02886613
 11605.1202    0.2238    1.08058    0.30000  0.00000272  0.02944471
 12377.8151    0.2284    1.08164    0.30000  0.00000272  0.03002261
 13150.5101    0.2329    1.08269    0.30000  0.00000272  0.03059981
 13923.2050    0.2374    1.08374    0.30000  0.00000272  0.03117633
 14695.9000    0.2420    1.08478    0.30000  0.00000272  0.03175217
/
```

Using CO2SOL

RUNSPEC section

This option is switched on using the CO2SOL keyword. Unlike in the CO2SEQ option, water is not defined as a component in COMPS and CNAMES as it is absent in the oil and gas phase.

The DIFFUSE keyword allows for the molecular diffusion of gases.

PROPS section

The initial dissolved CO_2 may be specified as a function of depth using the RSWVD keyword.

THE SOLUBILI keyword allows the user to enter a solubility data set as a function of reservoir pressure. This table will be automatically corrected for the salinity effect if the SALINITY keyword has been used. The SOLUBILS keyword is similar to the SOLUBILI keyword but lets you enter a salt concentration dependent table. In such a case, the salt concentration is taken from the brine tracer if the BRINE keyword is specified.

If neither SOLUBILI or SOLUBILS is used then the solubility data is defaulted to the values of Chang et al.

The coefficients for molecular diffusion must be set with DIFFCGAS if the DiFFUSE option is used.

Initial state constructed by equilibration

If an initial oil-gas contact exists within the reservoir you may specify either the vapor or the liquid phase composition at the contact, either ZMFVD or COMPVD can be used.

If only a single phase is present the composition may be entered using ZI or with respect to depth using ZMFVD.

SOLUTION section

Water content in CO_2 can be defined by RSW or RSWVD.

SCHEDULE section

The composition of the injected gas can be specified using the keyword WINJGAS

Mole fraction xCO_2 can be output by asking for AMF in RPTSCHED.

Summary of CO2SOL

CO2SOL turns on the option.

The program has default values for the solubility data. Alternatively, the SOLUBILITY keyword allows the input of non-default properties.

Details of the solubility properties used are obtained by using SOLU in the RPTPROPS keyword.

The initial dissolved CO2 as a function of depth can be specified with RSWVD keyword.

CO2 Sequestration

CO2SEQ:

No oil phase

The gas phase can have CO2, H2O,NACL,CACL2

The water phase can have CO2, H2O,NACL,CACL2

Note no C1,..,Cn in the gas phase

This option models the injection and sequestration of CO2 into aquifers.

In the CO2 sequestration option only two phases are considered, a CO2-rich phase and an H2O-rich phase. The CO2-rich phase is labeled the gas phase and the H2O-rich phase is labeled the water (liquid) phase. Components are specified as usual with the COMPS keyword. Allowed components name are currently CO2, H2O, NACL and CACL2.

Saline aquifer storage

Two phases ,H2O rich phase, CO2 rich phase

Components: CO2, H2O,NACL,CACL2

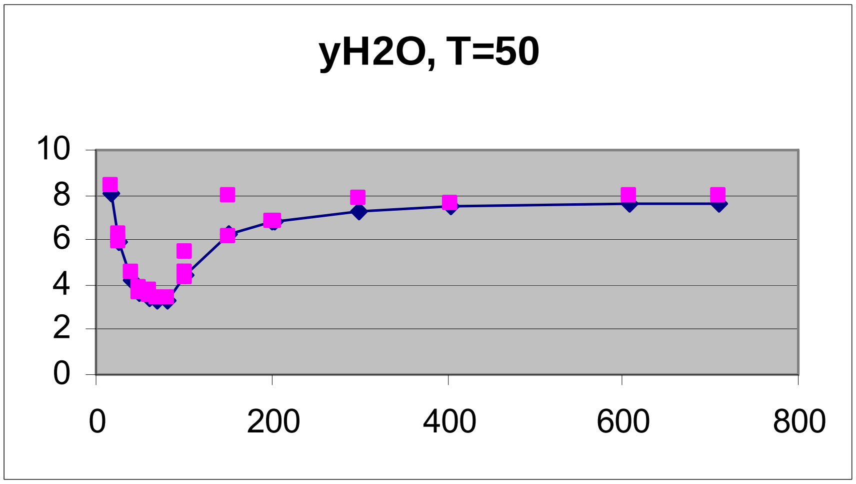
Fluid properties based on a combined gas-eos/water activity model, P 1-600 Bar, T 12-100, Salt concentrations 0-5 molal

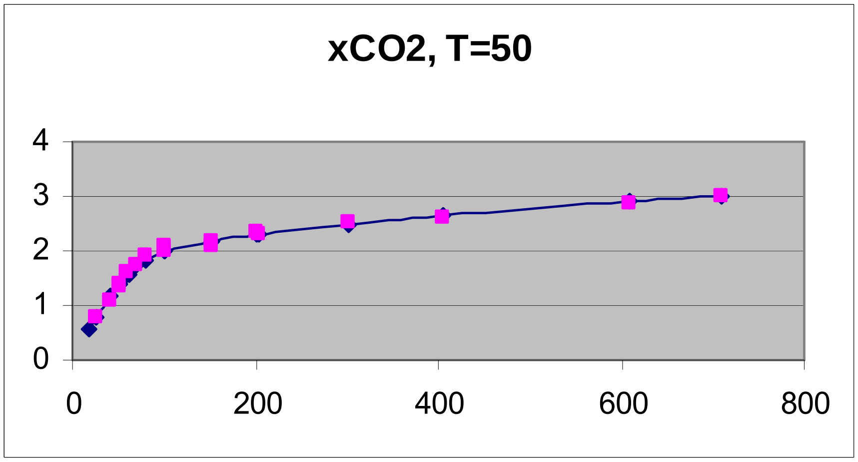
Salting out effect

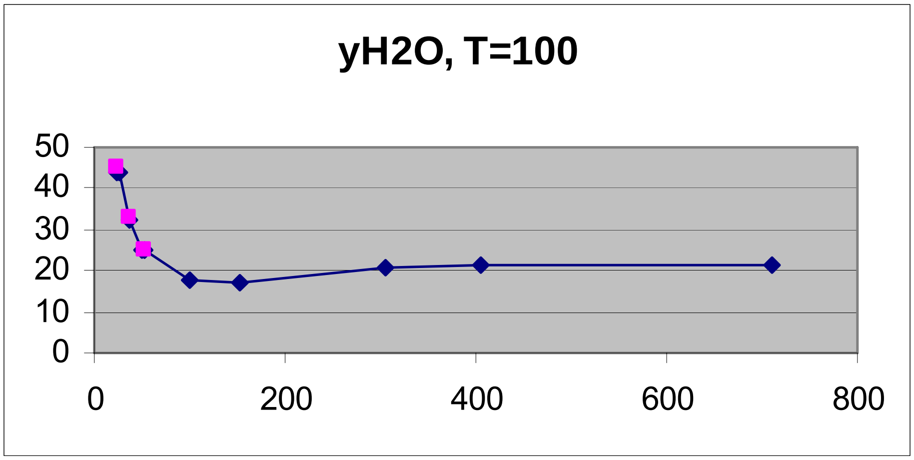
Temperature fixed but can vary on a cell by cell basis

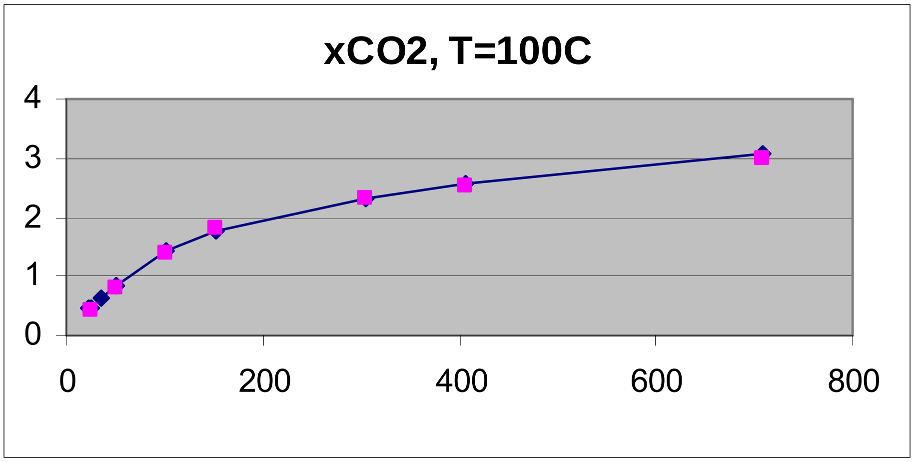
The mutual solubilities of CO_2 and H_2O are calculated to match experimental data for typical CO_2 sequestration conditions: typically 12-100 degrees C and up to 600 bars. They are calculated following the procedure given by Spycher and Pruess (2005), based on fugacity equilibration between water and a CO_2-phase. Water fugacity is obtained by Henry's law, while CO_2 fugacity is calculated using a modified Redlich-Kwong equation of state.

The mole fractions predicted by CO2SEQ have been compared with the values from Spycher and Pruess over a range of pressures and temperatures, and show good agreement allowing for the spread in experimental values. The following graphs show xCO2 and yH2O calculated with CO2SEQ as solid lines. Experimental data from Spycher et al. 2003 are shown as square symbols. The temperature is in degrees C and the x-axis shows pressures in bars.









Using CO2SEQ

RUNSPEC section

The option switched on using the CO2SEQ keyword. The number of components is specified by the COMPS keyword. Four components are currently allowed: CO_2, H_2O, NaCl and $CaCl_2$.

PROPS section

Fluid component properties are assigned internally based on the names given in the CNAMES keyword (labeled 'CO2', 'H2O', 'NACL', 'CACL2').

The water relative permeability is input using the WSF keyword, while the gas relative permeability and the gas-water capillary pressure are entered using the GSF keyword.

The initial state is constructed by equilibration. If an initial gas-water contact exists within the reservoir you may specify either the vapor or the aqueous phase composition at the contact; either ZMFVD or COMPVD can be used.

If only a single phase is present the composition may be entered using ZI or with respect to depth using ZMFVD.

SOLUTION section

The EQUIL keyword is used for initial state equilibration.

Initial state set by enumeration

Liquid, gas and total compositions are specified explicitly with keywords XMF, YMF and ZMF respectively.

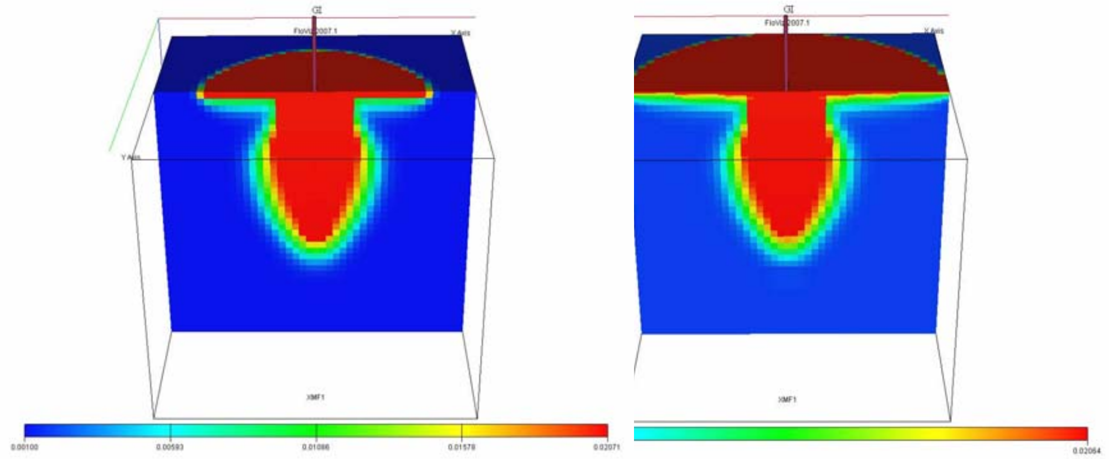
SCHEDULE section

The composition of the injected gas can be specified using the keyword WINJGAS.

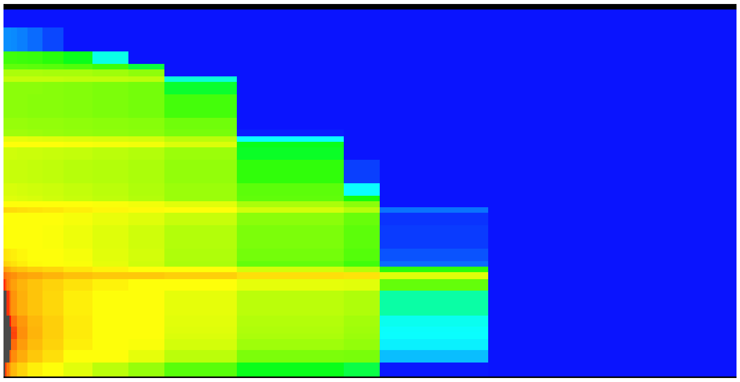
Mole fractions xCO_2 and yH_2O are output by writing XMF and YMF in RPTS

ECLIPSE functionality compatible with CO2 sequestration:

- **Advanced well modelling (Horizontal, multi segmented wells etc.)**
- **Integrated geomechanics and flow model**
- **Parallel, LGR's**



CO2 evolving towards the cap rock



Injection into a reservoir with shale layers

Summary of CO2SEQ

- CO2SEQ switches on the option.
- Water relative permeabilities are entered using the WSF keyword, and gas relative permeabilities and gas-water capillary pressures using the GSF keyword.
- WINJGAS defines the injection composition.

Gas-water systems

For modeling gas phase/aqueous phase equilibrium using an EoS

Main application is **Gas reservoirs**, or **Depleted gas reservoirs**

The gas-water option in ECLIPSE 300 provides a method of modeling gas phase/aqueous phase equilibria using an equation of state. The Peng Robinson equation of state is modified following the suggestions of Soreide and Whitson to obtain accurate gas solubilities in the aqueous phase.

GASWAT:

No oil phase

The gas phase can have C1,..,Cn, CO2, N2, H2S and H2O

The water phase can have C1,..,Cn, CO2, N2, H2S and H2O

GASWAT allows a multi-component gas phase and models CO_2, N_2, H_2S and H_2 solubilities in water.

Features

- EOS for gas water system
- Can handle different gas species as H2S, N2
- Constant salinity on a regional basis (SALINITY keyword).
- Temperature on a cell by cell basis, or temperature may vary with depth
- Gas calorific values can be defined and reported, and gas quality production controls are available.

The temperature of the reservoir may vary with depth, and this is reflected in the equation of state treatment, in which temperature coefficients are stored to be combined with the temperature of each cell. A global salinity value may be entered to correct the default equation of state modifications for brine concentration. The modified equation of state coefficients may also be over-ridden by the engineer.

- Water relative permeabilities are entered using the WSF keyword, and gas-water relative permeabilities and gas-water capillary pressures using the GSF keyword.
- These correspond to the SOF2 and SGFN keywords.
- Saturation tables can be output using the WSF and GSF keywords in the RPTPROPS keyword.
- DENSITY values are not used. Water and gas densities are calculating from the EoS.

Molecular diffusion between gases can be modeled using the DIFFUSE option.

Limitations

- No salting out effect (constant salinity)
- Prediction of H2O in the gas phase not so accurate as CO2SEQ (for typical CO2 sequestration conditions)

Peng Robinson EOS is modified following paper of Soreide and Whitson to obtain accurate gas solubility in the aqueous phase.

In ECLIPSE 100, internally, aqueous/gas two phase system is treated like a two phase oil/gas system.

In the Peng-Robinson EOS recall that

$$\alpha^{1/2} = 1 + f(\omega)(1 - T_r^{1/2})$$

This has the general form:

$$\alpha^{1/2} = p + qT^{1/2} + rT + sT^{-3}$$

Soreide and Whitson proposed two changes.

Change 1:

For the water component the above expression for $\alpha^{1/2}$ is replaced by

$$\alpha^{1/2} = 1 + aq_1(1 - aq_2 T_r) + aq_3(T_r^{-3} - 1)$$

with default values:

aq1 = 0.4530

aq2 = 1.0 - 0.0103Cs 1.1

aq3 = 0.0034

where cs = brine concentration

Change2:

Different binary interaction coefficients are used for the gas and aqueous phases.

Temperature dependence of aqueous phase binary interaction coefficient

$$k_{jw}^{a} = bq_1 + bq_2 T_{rj} + bq_3 T_{rj}^2$$

with default values

bq1 = Ao(1+Socs)

$bq2 = A1(1+S1cs)$

$bq3 = A2(1+S2cs)$

where

$Ao = 1.112 - 1.7369\ wj^{-0.1}$

$A1 = 1.1001 + 0.836\ wj$

$A2 = -0.15742 - 1.0988\ wj$

$So = 0.017407$

$S1 = 0.033516$

$S2 = 0.011478$

Special BIC are used between N2, CO2, and H2S and the aqueous phase

$$k^a_{N2w} = -\ 1.70235\ (1 + 0.025587cs^{0.75}) + 0.44338(1+0.08126cs^{0.7505})T_{rN2}$$

with similar expressions for kaCO2w and kaH2Sw

Using GASWAT for CO_2 storage

RUNSPEC section

This option is switched on using the GASWAT keyword. The number of components is specified by the COMPS keyword. Water has to be defined as a component; salts are not components. The WATER keyword should not be present, as H_2O is a component specified in COMPS.

The DIFFUSE keyword allows for molecular diffusion of gases.

PROPS section

The water relative permeability is input using the WSF keyword, while the gas relative permeability and the gas-water capillary pressure are entered using the GSF keyword.

Salinity can be set up by the SALINITY keyword or on a regional basis with the SALINITR keyword

The coefficients for molecular diffusion must be set with DIFFCGAS if the diffusion option is used.

Initial state constructed by equilibration:

- If an initial gas-water contact exists within the reservoir you may specify either the vapor or the aqueous phase composition at the contact, either ZMFVD or COMPVD can be used.
- If only a single phase is present the composition may be entered using ZI or with respect to depth using ZMFVD.

SOLUTION section

The EQUIL keyword is used for initial state equilibration.

Initial state set by enumeration:

- Liquid phase composition can be set with XMF, the gas phase composition with YMF and the total composition with ZMF.

SCHEDULE section

The composition of the gas injected can be specified using the keyword WINJGAS.

Mole fractions xCO_2 and yH_2O can be output by writing mnemonics XMF and YMF in RPTSCHED.

Calorific values

- Molar calorific values can be entered using the CALVAL keyword. Gas qualities, calorific production rates and totals are calculated and reported.
- A group can be given a quality target (GQUALITY keyword).

The `GASWAT` option also allows molar calorific values to be entered under the `CALVAL` keyword. Gas qualities, calorific production rates and calorific production totals for wells and groups are calculated and reported.

Specifying group production quality

Where a group target is set - for example a required group gas production rate - the group distributes this target amongst the wells in the group using guide rates. By modifying these guide rates we can weight the production between low and high quality wells so that a required group quality is obtained. This required quality can be set using the `GQUALITY` keyword.

This option applies only if:

1. The group has more than one son under group control
2. At least one of the group controlled sons has a quality better than the required target and at least one has a quality worse than the required target.

Generally a point is ultimately reached when the required calorific value can no longer be met (for example if all the wells in the group are producing gas of too low a quality). The quality does not then honor the required target.

If you are using more than one EoS region:

The keyword CALVALR can be used to define different calorific values for components in each EoS regions

This allows ECLIPSE to calculate the calorific production rate from a well completed in different EoS regions.

Units

These are entered in the PROPS section under the `CALVAL` keyword. The metric units are kJ/kg-mol. For conversion purposes 1 M3=0.04165935 kg-mol at normal standard conditions. Well and group quality is reported in kJ/kg-mol. Calorific rates and totals are in kJ/D and kJ respectively. The equivalent field units are BTU/lb-mol etc.

Calorific well and group production rates and totals are reported in the PRT file under the REPORT, FIELD and WELLS headers. The gas quality is also reported - this is the mixture calorific value per mole.

Summary of GASWAT

In ECLIPSE 100 - RUNSPEC use “GASWAT”

Component ‘H2O’ must be present

Additional Keywords

SALINITY, AQCOEF, BICAQ1, BICAQ2, BACAQ3

Gas Quality keywords

CALVAL, GQUALITY

Note on conversions for salinity units

As the various CO_2 options use different frameworks within ECLIPSE, units for salinity input differ.

Salt concentrations in XMF and YMF must be entered in mole fraction. The SALINITY keyword unit is molality (mol/kg of pure water). Salinity in SOLUBILS must be expressed in kg/m^3 of brine.

Conversions between these different units are described below.

Molality to mole fraction

Mole fraction of x = (molality/ 55.50683) * mole fraction of H20

So if mole fraction of H_2O = 1 - x

Mole fraction of x = (molality/ 55.50683) / [1+(molality/ 55.50683)]

Molality to mass per volume unity (kg/m^3)

Mass per volume unity = (d/B) * (molality*0.058440)/[1+(molality*0.058440)]

where

d = surface brine density

B = brine volume factor

Summary of CO2SOL, CO2SEQ and GASWAT

The most suitable option to choose depends on the conditions that need to be modeled.

1. Geological Storage in Aquifers

   Using CO2SEQ option, two phases are considered: a CO_2-rich phase (labeled gas phase), and an H_2O-rich phase (labeled liquid phase).
   This option gives accurate mutual solubilities of CO_2 in water (xCO_2) and water in the CO_2-rich phase (yH_2O). Salts are described as components of the liquid phase.

   The GASWAT option provides a gas/aqueous phase equilibrium method. The liquid mole fraction $x\ CO_2$ is accurately predicted; however, the gas phase mole fraction yH_2O is less accurate. The gas composition is not restricted to CO_2/H_2O, as other gases and their solubility in water can be included.
2. Geological Storage in Oil Depleted Reservoirs and EOR (Enhanced oil recovery)

   The option best suited for this case is CO2SOL. Water is not considered in the oil or gas phase, but the solubility of CO_2 in the water phase is accounted for. The gas/oil composition is not restricted to CO_2 but only CO_2 is considered soluble in water.
3. Geological Storage in Gas Depleted Reservoirs

   This case can be modeled using the GASWAT option by adding gas components, such as CH_4 and H_2S for example.
4. ECBM

   The COAL option provides a diffusive flow and sorption model for enhanced coal bed methane recovery (ECBM). A full description of this option is provided in the ECLIPSE Technical Description Manual.

Modeling Water

We shall discuss three ways of modeling the water phase and water components in reservoir simulation:

1. Traditionally
2. The Brine option
3. Multi-component water

Traditional Modeling of Water

- PVTW

Ref. Press Bw Cw Muw Muww /

- DENSITY

oil water gas /

Or

- GRAVITY

oilapi water gas /

The BRINE option

- **What if Water Salinity (and consequently density and viscosity) vary with depth?**
- **What if the salinity of injected water is different from that of formation water?**

The BRINE keyword is used to model salt in water. Salinity is modelled as a tracer. PVT properties of salt water are specified using the PVTWSALT keyword, and BDENSITY can optionally be given as a function of salt.

The initial distribution of salt as a function of depth is defined by SALTVD. The salt concentration in the injected water (if any) can be defined using WSALT.

- BRINE Keyword in RUNSPEC
- Salinity is modelled as a tracer
- PVTWSALT instead of PVTW
- BDENSITY function of salt – optional
- SALTVD
- WSALT – default zero!

Because salt is modeled as a tracer, the flow of brine is solved explicitly. The distribution of salt may not be modeled as accurately with large timesteps if high salinity values lead to large density or viscosity differences.

Multi-Component water

Instead of the BRINE option, water of varying salinity can be modelled by having one “component” for salt water and one “component” for fresh/sweet water

- **Oil and gas modelled as before**
- **Water can have more than one component, but these are only allowed in the water phase**

- **Improved modelling for salt in water**
- **Can also model other components in water (bacteria, solids, …)**

- **Allows more than one type of ‘water’ to be defined. (Analogous to Oils with different APIs).**
- **They are allowed to have different:**
  - **i) Molecular Weights**
  - **ii) Densities**

iii) Viscosities

iv) Compressibilities

- **They are of course allowed to mix**

The water density is calculated by:

$$b_w = 1/V_w$$

$$Vw = \sum_c w_c \times \frac{M_{wc}}{\rho_{ref_c} \times \left(1 + X_c + X_c^2\right)}$$

$$Xc = c_{P_c} \times \left(P - P_{ref\,c}\right)$$

and the viscosity by:

$$\mu_w = \sum_c w_c \times \frac{\mu_{ref_c}}{(1 + Y_c + Y_c^2)}$$

$$Y_c = -c_{V_c} \times \left(P - P_{ref\,c}\right)$$

Using Multi-Component water

RUNSPEC

COMPW: how many water components

PROPS

properties of water components:

CREFW, DREFW, MWW, PREFW, VREFW, WNAMES

(note these are now by EoS region, not PVT region)

SOLUTION

WMFVD – similar to XMFVD – water mole fraction vs. depth

Also WI or WMF

SCHEDULE

WELLSTRW – similar to WELLSTREAM – defines possible water streams

WINJW – similar to WINJGAS – defines composition of injected water

Converting PVTW to water component data

- In standard simulations, water is modeled as a single component, with properties specified by the PVTW and DENSITY keywords. We can also model this using the multiple component water option with a single water component
- Note however, that PVTW and DENSITY data are specified for each PVT region, while water component data is specified for each EOS region. The two models can produce different answers if the regions do not match
-

Keyword	Value
MWW	**18.015**
PREFW	**PVTW(1)**
DREFW	**DENSITY(2)/PVTW(2)**
CREFW	**PVTW(3)**
VREFW	**PVTW(4) and PVTW(5)**

Applications and Limitations

- Model Fresh Water injection in a brine-reservoir or vice-versa.
- Model Reservoir souring (when used with SOLID and REACTIONS)
- Model scale deposition (when used with SOLID and REACTIONS)

- Model cold water injection with decay of injected water viscosity (when used with REACTIONS)
- Model Brine and fresh water in Multi-segment wells

The multi-component water model can be used in place of the single component water model in most standard simulations (black oil, EoS or K-value). However, it can not be used at present in certain cases where water has special properties. Therefore, options that **cannot** be used with the multi-component water model include:

- GASWAT or CO2SOL
- THERMAL
- FLUX
- GSATPROD
- IMPSAT

In addition, there are currently some limitations when specifying water source terms:

- The water entering / leaving the reservoir from an aquifer is made up entirely of the last water component
- The water entering / leaving a multi-segment well using the source / sink term is made up entirely of the last water component

Examples:

The following data sets come with the ECLIPSE installation:

- **MCW0.DATA Brine model using tracers**
- **MCW1.DATA Brine model**
- **MCW2.DATA MSW Brine model**
- **MCW3.DATA Brine+Solids+Reaction**

- **MCW.GRF GRF to compare results**

Reservoir Souring Example

- **When the nutrient rich water is injected in a reservoir containing bacteria, H2S is generated according to the reaction:**

0.00662 SOLID+WAT1 →0.1H2S+WAT2

- **The reaction rate is given by:**

$$Rr = V_b . A_r . \exp\left(-E_r / \left(RT\right)\right) . \Pi c_{ri}^{\ n_{ri}}$$

The following data are needed to model this reaction:

In RUNSPEC:

```
-- Eight hydrocarbon components
COMPS
        8 /
-- Two water components
COMPW
        2 /
-- One reaction
REACTION
        1 0 0 0 /
```

In PROPS:

```
-- We call the solid component “SOLID”
CNAMES
```

```
 H2S  C1   C3   C6   C10  C15  C20  SOLID /

-- Component volatility
CVTYPE
 LIVE LIVE LIVE LIVE LIVE LIVE LIVE SOLID /

-- Remember the Reaction is  0.00662 SOLID+WAT1 →0.1 H2S+WAT2
STOREAC
-- H2S   C1    C3    C6   C10   C15   C20   SOLID  WAT1 WAT2
   0.0  0.0   0.0   0.0   0.0   0.0   0.0  6.62E-3  1.0 0.0 /
STOPROD
-- H2S   C1    C3    C6   C10   C15   C20   SOLID  WAT1 WAT2
   0.1  0.0   0.0   0.0   0.0   0.0   0.0     0.0   0.0 1.0 /
REACCORD
-- H2S   C1    C3    C6   C10   C15   C20   SOLID  WAT1 WAT2
   0.0  0.0   0.0   0.0   0.0   0.0   0.0     1.0   1.0 0.0 /
REACRATE
  1.0  /
```

In SOLUTION:

```
-- Initial water concentration with depth
WMFVD
-- depth  WAT1  WAT2
    1000   0.0   1.0
   10000   0.0   1.0  /

-- Initial solid saturation and MF
SSOLID
  400*6.62E-3  /
SMF
  2800*0.00
   400*1.00  /
```

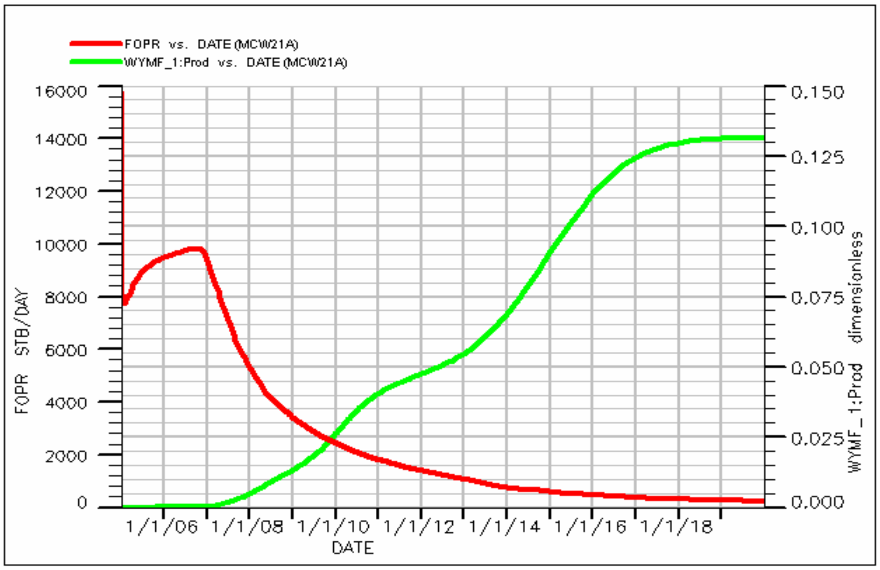
In SCHEDULE:

```
WELLSTRW
'Brine' 1.0 0.0 /
```

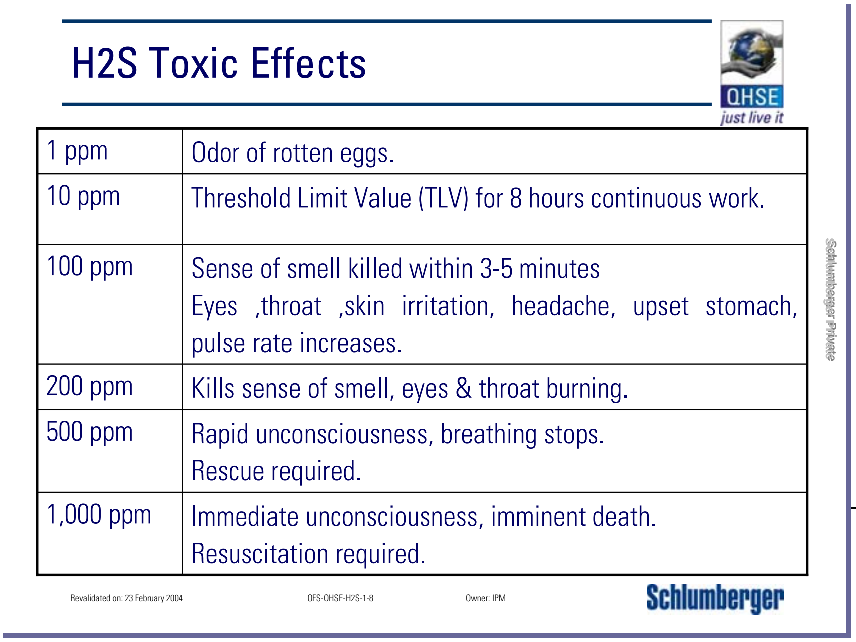
```
/

WINJW
'Inje' STREAM 'Brine'/
/
```

Souring Example: RESULTS

The following graph shows the decline of oil production over time as the amount of H2S generated and produced increases.



Note that the toxic concentration of H2S is very low:

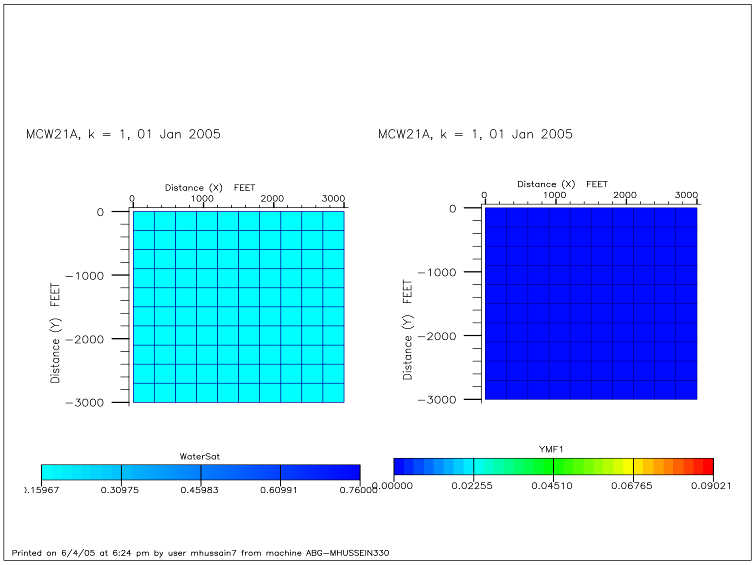


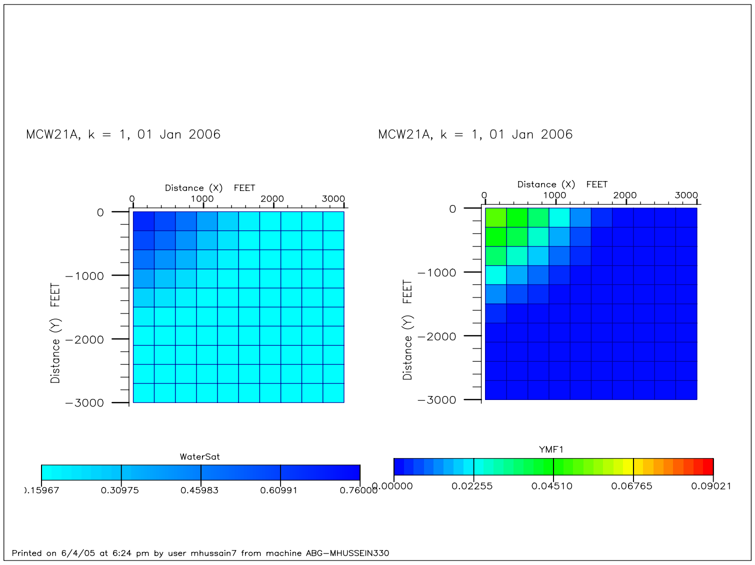
H2S Toxic Effects

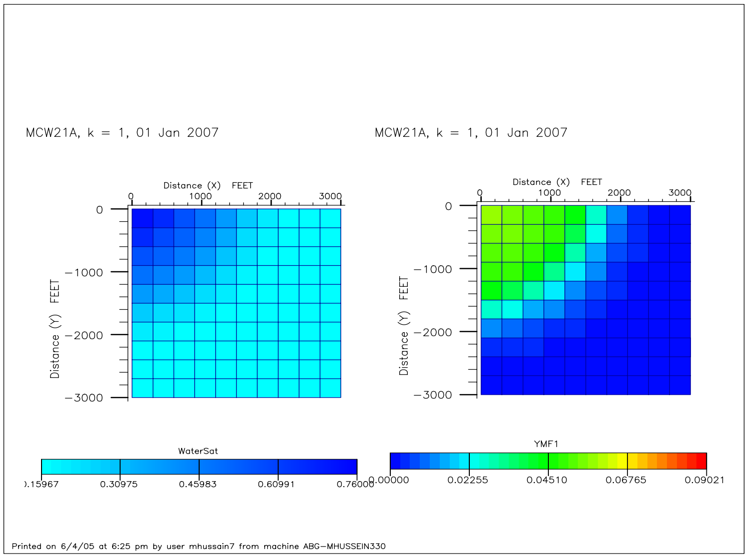
1 ppm	Odor of rotten eggs.
10 ppm	Threshold Limit Value (TLV) for 8 hours continuous work.
100 ppm	Sense of smell killed within 3-5 minutes Eyes ,throat ,skin irritation, headache, upset stomach, pulse rate increases.
200 ppm	Kills sense of smell, eyes & throat burning.
500 ppm	Rapid unconsciousness, breathing stops. Rescue required.
1,000 ppm	Immediate unconsciousness, imminent death. Resuscitation required.

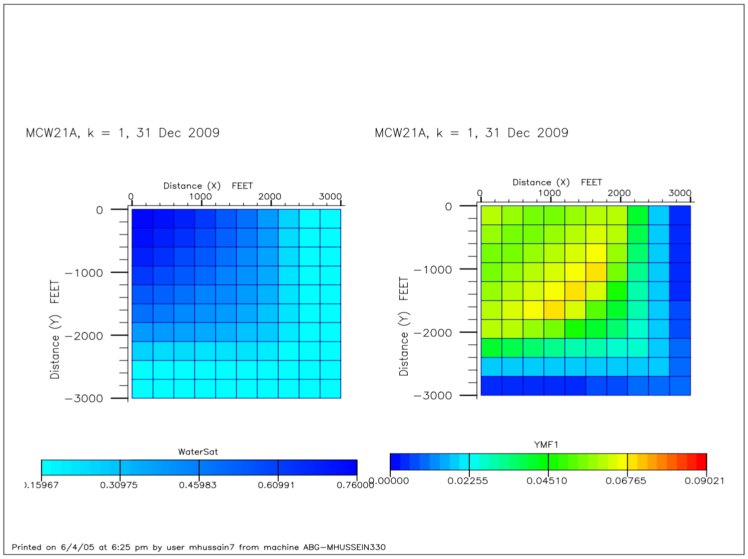
Revalidated on: 23 February 2004 OFS-QHSE-H2S-1-8 Owner: IPM

The next few pictures show the water saturation and H2S concentration is the reservoir at different times. Initially there is no H2S in the reservoir, but as the nutrient-rich containing bacteria water is injected then more and more H2S is generated.









Summary of Multi-Component water

- **Oil and gas modelled as before**
- **Water can have more than one component, but these are only allowed in the water phase**

- **Improved modelling for salt in water**
- **Modelling of other components in water (bacteria, solids, …)**
- **Can be used with REACTIONS and SOLIDS**

26. Coal-bed methane, and CO2 in coal

- **Based on dual porosity model**
  Gas only or Gas-water system
  Flow equations are solved in fractures only.
  The coal matrix only contains coal and gas.
  Only gas diffusion (concentration gradient) in the matrix is tracked
- **Primary Recovery**
  Pressure depletion

Coal is full of fractures, called “cleats” by the coal industry.

Horizontal fractures are called Face cleats and vertical fractures are called Butt cleats.

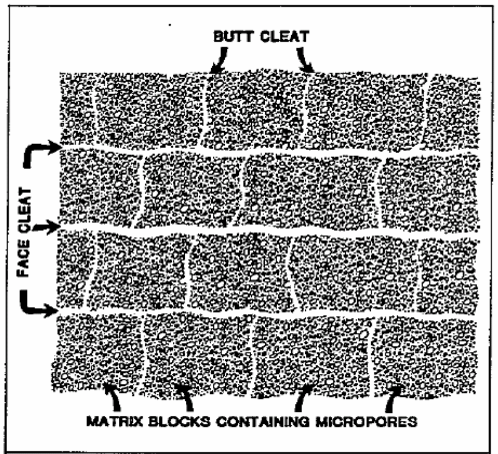


Fig. 2—Plan view of the dual-porosity nature of coal.

Adsorbed methane concentration is a function of pressure given by Langmuir isotherm

$$Fg = DIFFMF\ .\ Dc\ .\ (GCb - GCs)$$

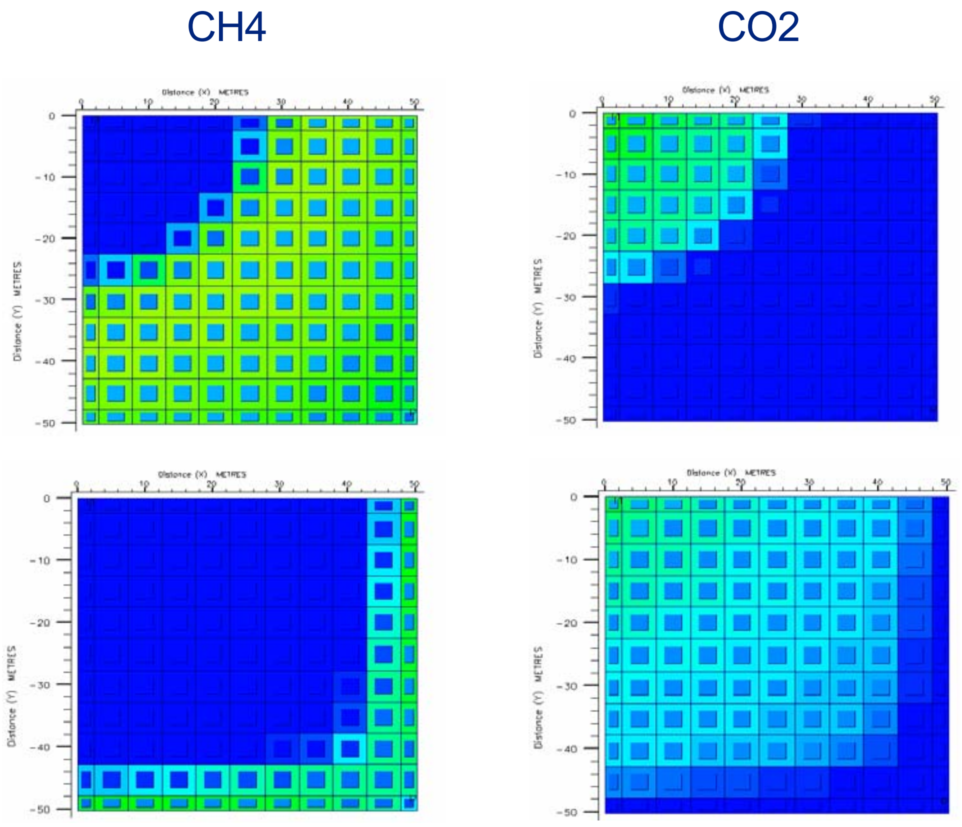
Extended Coalbed Methane

CO2 adsorbs on coal far more strongly than CH4 or N2.

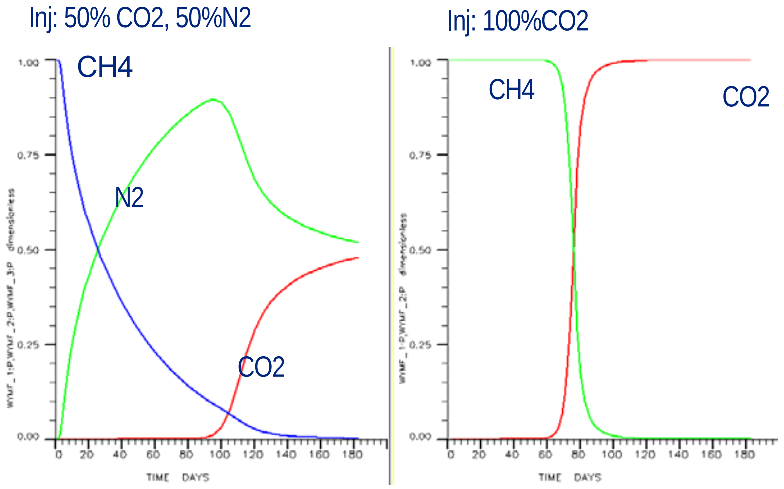
Injected CO2 flows through coal fractures, adsorbs into coal matrix displacing CH4

- **We can have any number of components, CH4,CO2,N2...**
- **Extended Langmuir isotherms**
- **Coal shrinkage & swelling**
  Palmer & Mansoori
- **Dual porosity**
- **Time dependent sorption**
- **Coal regions**
  Define different isotherms
  No coal in some regions
- **CO2 solubility in water**
- **Compatible with Parallel**

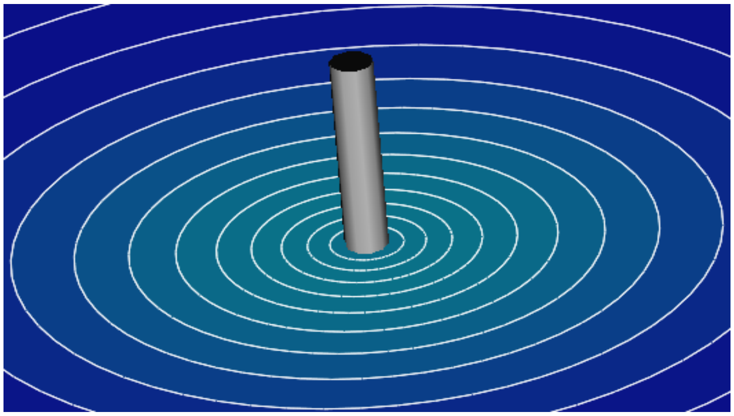
The following picture shows the results of a simulation in which we injected CO2 to displace methane in the coal matrix. The picture is the usual dual-porosity display of both matrix and fracture block mole fractions, and shows how the CO2 displaces more and more methane as time goes on.



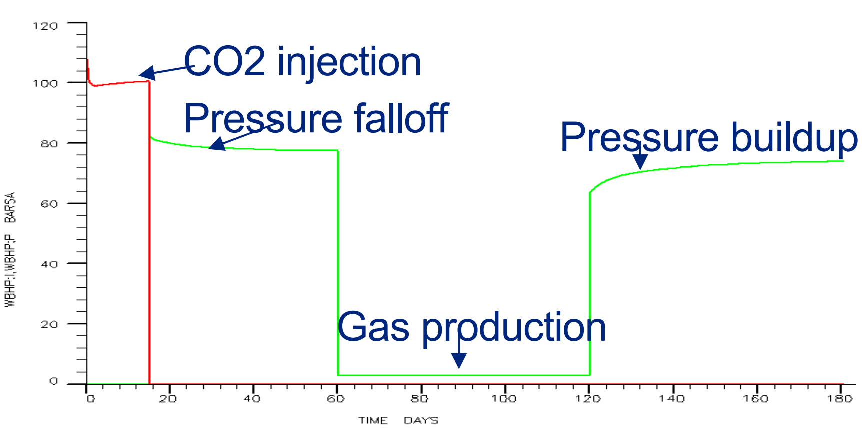
This is also shown in the following line graphs of the composition of the produced gas. The right-hand plot is for a case where we inject a 100% CO2; the CO2 is adsorbed onto the coal matrix in preference to CH4. The left-hand plot is for a case where we inject a mixture of 50% CO2 and 50% N2; the CO2 is adsorbed onto the coal matrix in preference to CH4 and N2.

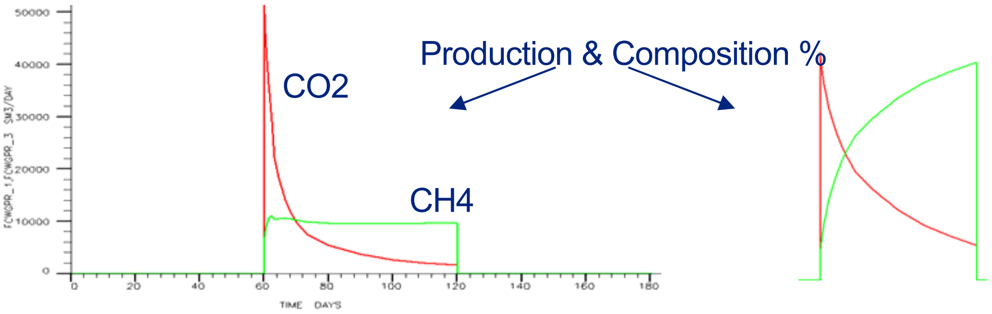


This extended coal-bed methane (ECBM) has been validated on one of the SPE benchmarks, “Numerical Comparison Study for ECBM, SPE 75669”. This simple model is a radial 29*1*1 grid, and simulates the injection of CO2.

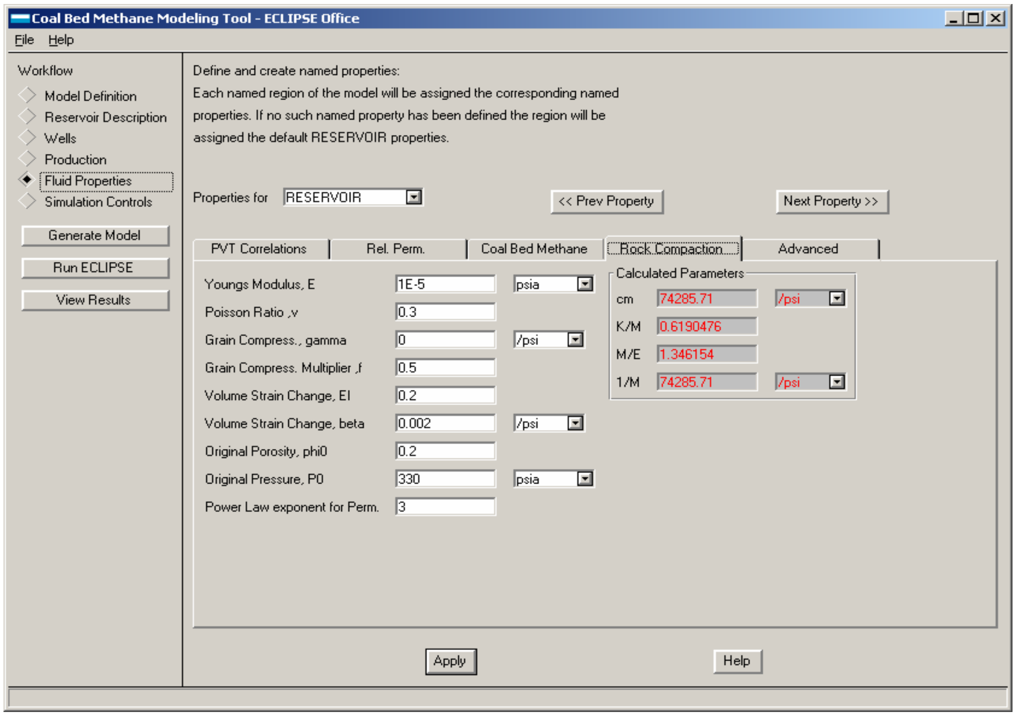


Results of the ECLIPSE ECBM simulation are shown in the next two plots. All the published results from other simulators were very similar.





To help with the creation and running of coal-bed methane models, ECLIPSE Office has a CBM template that provides a simple panel interface to input all the necessary data.



Define and create named properties:
Each named region of the model will be assigned the corresponding named properties. If no such named property has been defined the region will be assigned the default RESERVOIR properties.

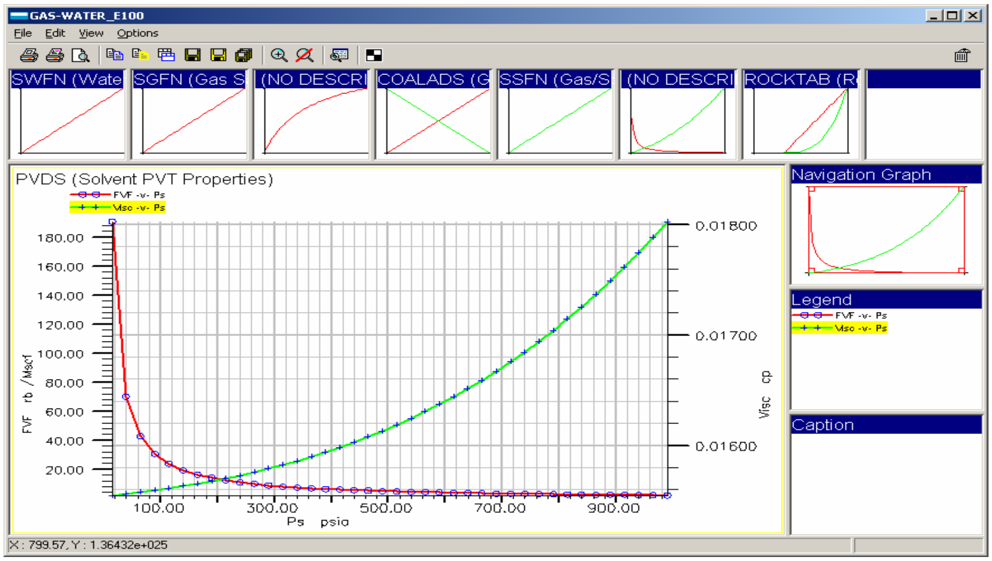
Properties for RESERVOIR

Youngs Modulus, E	1E-5	psia
Poisson Ratio ,v	0.3	
Grain Compress., gamma	0	/psi
Grain Compress. Multiplier ,f	0.5	
Volume Strain Change, El	0.2	
Volume Strain Change, beta	0.002	/psi
Original Porosity, phi0	0.2	
Original Pressure, P0	330	psia
Power Law exponent for Perm.	3	

Calculated Parameters

cm	74285.71	/psi
K/M	0.6190476	
M/E	1.346154	
1/M	74285.71	/psi

Results can then be viewed in the normal way:



X : 799.57, Y : 1.36432e+025

27. Tracers and De-lumping

Tracers in ECLIPSE 300 are attached to components and not to phases.. There are three tracer options in ECLIPSE 300. Tracers are also used to “lump” components to approximately predict detailed fluid compositions using fewer number of components.

- Passive Tracers
- TRACK option
- Environmental Tracers

- Lumping and de-lumping

Passive tracers

- The Tracer Tracking option is a general facility to follow the movement of marked fluid elements during a simulation.
- For instance a tracer in the water phase can track the movement of injected water, or other chemical properties of the water.
- Tracers can model variations of salinity in water, but ECLIPSE also has a special BRINE tracking option.

The ECLIPSE Tracer Tracking option is a general facility to follow the movement of ‘marked’ fluid elements during a simulation run.

The Tracer Tracking option has a wide variety of reservoir modeling applications. In the case of tracers defined to exist in the water phase, it may be used, for example, to determine the movement within the reservoir of water injected into any number of injection wells or to predict concentration of chemicals in the water produced from the reservoir. Tracers can also model the variations in salinity although ECLIPSE has a special `BRINE` option to model salinity.

- Initial tracer concentration can be set for each region as a function of depth.
- Initial tracer concentration can of course be zero.
- Tracers can be defined in injection wells
- Tracers in this case are “passive” tracers, in that they do not affect the physical properties of the phase that is carrying them.
- Passive tracers do not degrade with time.

The initial tracer concentrations may be supplied in one of two ways. The most direct method is enumeration using the keyword `TBLK` in the SOLUTION section of the input data. An alternative method is to define a series of tracer concentration versus depth tables in the `SOLUTION` section, together with the associated region numbers in the `REGIONS` section of the input data. The data is entered by means of the keywords `TVDP` and `TNUM` respectively, and control of the depth table and region data output is achieved using the `RPTSOL` and `RPTREGS` keywords. This depth method of data input is especially suited to tracking fluid which initially exists within a particular region of the reservoir. In the case of gas condensate reservoirs, it is thus possible to track the oil which initially exists in the vapor phase in separate regions of the reservoir and to determine its subsequent movement through the reservoir grid. The Tracer option could also be used to predict the concentration of chemical impurity species (such as the sulphur content of the oil) in the hydrocarbon production streams.

By default ECLIPSE Tracer Tracking option assumes that the presence of tracers does not affect the PVT properties of the phases in which they are embedded. The tracers are thus to be regarded as passive. The tracer concentrations are updated fully-implicitly at the end of each time-step after the oil, water and gas flows have been computed

- **ECLIPSE 300 does not require the TRACERS keyword in the RUNSPEC section, unlike ECLIPSE 100. It needs the TRACER keyword in the PROPS section.**

The Tracer Tracking facility in ECLIPSE 300 does not require the keyword `TRACERS` in the `RUNSPEC` section; it is activated by entering the `TRACER` keyword in the PROPS section of the input data. The names of each tracer and their associated stock tank phases are defined using the `TRACER` keyword.

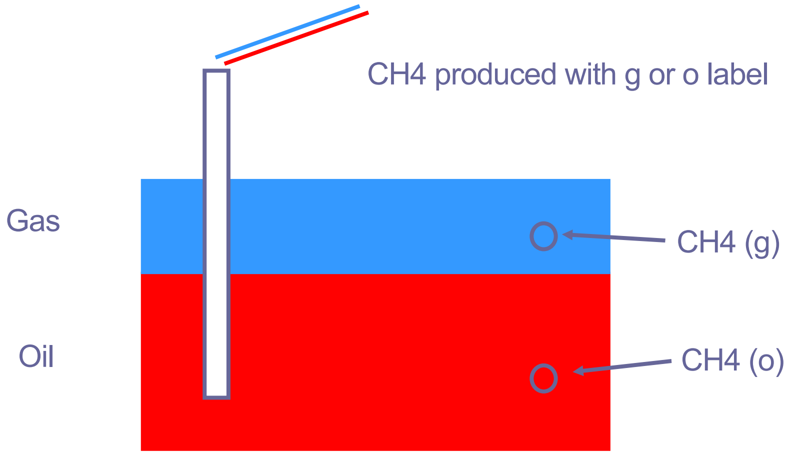
You may specify the initial concentration of a water phase tracer in each of the analytic aquifers in a simulation run. This can be achieved using the `AQANTRC` keyword in the `SOLUTION` section of the input data. Output of the status of each water tracer for each analytic aquifer is obtained at each report time using the mnemonic `AQUCT` or `AQUFET` in the `RPTSCHED` keyword

Tracer injection control is achieved by means of the `WTRACER` keyword in the `SCHEDULE` section. This keyword allows the specification of the concentration of a particular tracer in the injection stream for each well. A default injection concentration value of zero is assumed for tracers not defined under the `WTRACER` keyword. The `WTRACER` keyword optionally allows the injected tracer concentration to be a function of the total cumulative fluid injected, which can be useful for modeling H2S generating processes.

The TRACK option

- The TRACK option allows a division of hydrocarbons in the reservoir to be tracked through into recovered surface volumes.

`The TRACK` option allows you to track a division of hydrocarbons in the original reservoir through into recovered surface volumes. The option is enabled by entering the `TRACK` keyword in the `RUNSPEC` section.



Formulation

Suppose we divide the hydrocarbons in a reservoir into those lying above the GOC (gas-oil contact) and those lying below it. As the reservoir is produced these components will flow through the field to the production wells. Generally, each component will move along a different path. For example, the light components such as methane will fraction into the reservoir vapor, and tend to rise to the top of the reservoir. The heavy components will tend to remain in the oil and stay at the bottom of the reservoir.

At a given producer, each component will have a fraction from below the GOC and a fraction from above it. We can thus define two streams, one of components originating from below the GOC and one from above. If these are run separately through the separator system we can obtain stock tank oil and stock tank gas volumes attributable to each of these streams.

With the enhanced Tracking option it is possible to divide the reservoir in any way the user desires.

Usage

The Tracking option is turned on using the `TRACK` keyword. This allows the initial fluid to be split at the GOC or at a given depth. The following text discusses splitting at the GOC; splitting at a specified depth is analogous.

In the tracking model, production volume rates originating from hydrocarbons above and below the GOC are reported separately in the `PRINT` file and when using `SUMMARY` section mnemonics.

- SUMMARY keywords:

  As well as WOPR, we have WOPRA and WOPRB
  As well as WOPT, we have WOPTA and WOPTB
  Similarly WGPRA, WGPRB, WGPTA, WGPTB

- and for groups and field.

Summary items are as follows:

- For wells:

  The `SUMMARY` mnemonic for the oil surface volume production rate of a given well is `WOPR`. The oil surface volume production rates from above and below the GOC are `WOPRA` and `WOPRB` respectively.

These are totaled over time separately, so that the total production from the well is `WOPT` and the totals from above and below the GOC are `WOPTA` and `WOPTB`.

`WGPRA`, `WGPRB`, `WGPTA` and `WGPTB` are similar items for well gas rates and totals.

- For groups:

  The well contributions are summed over the group structure.

  `GOPRA` and `GOPRB` are the group rates from above and below the GOC. These are totaled over time, so that `GOPTA` and `GOPTB` are the group totals from above and below the `GOC`. `GGPRA`, `GGPRB`, `GGPTA` and `GGPTB` are similar items for group gas rates and totals.

- For the field:

  The field items follow those of the well and groups.

  `FOPRA` and `FOPRB` are the field rates from above and below the GOC; `FOPTA` and `FOPTB` are the field totals from above and below the GOC.

  `FGPRA`, `FGPRB`, `FGPTA` and `FGPTB` are similar items for field gas rates and totals.

Enhanced TRACKing

To enable enhanced tracking you need to use the `REGDIMS` keyword in the `RUNSPEC` section to define the maximum number of user defined regions. It is strongly recommended that this maximum does not exceed the actual maximum as it can represent a considerable unnecessary overhead. An additional option in the `TRACK` keyword is the ‘`REGONLY`’ keyword that can be used in place of ‘`GOC'` or ‘`DEPTH`’ if region tracking is the only facility required.

To define the regions the `TRACKREG` keyword in the `REGIONS` section must be used.

Fluid in place reports

When the fluid in place in the reservoir at surface conditions is reported, the track option includes extra reports for the surface volumes obtained from the fluid in the reservoir which originated above and below the gas oil contact. These volumes may be obtained for the entire reservoir or by fluid in place reporting region.

The normalization option

When the fluid in place or the production from a well is obtained the tracers are used to define a stream from above the GOC and a stream from below the contact. These are then flashed separately so that the volumes from above and below can be reported separately. The sum of these two volumes will not generally be exactly equal to the total volume produced by the well, for three reasons:

1. Injection gas, which is not from original reservoir components.
2. The separator flash is not linear, so the volume of oil and gas resulting from a mixture is not the same as the sum of the volumes of two sub-mixtures.
3. The tracer solution will disperse like any numerical solution, so that the sum of the A and B tracer concentrations will not generally equal exactly one.

The `NORM` option is provided so that you can request that the volumes be normalized to equal the total rate of the well.

Alternative production reporting

An alternative method for calculating the production from above and below the GOC is to directly split a well's volumetric flow rate according to the tracer concentrations above and below the contact. This method is known as the molar volumetric split and the resulting field, group and well rates and totals are calculated in addition to the standard TRACK option production quantities.

The molar volumetric split quantities may be reported using the following SUMMARY section mnemonics:

- For wells:

  W(O,G)P(R,T)1 gives the oil and gas surface volume production rates and totals from fluids above the GOC
  W(O,G)P(R,T)2 gives the oil and gas surface volume production rates and totals from fluids below the GOC

- For groups:

  G(O,G)P(R,T)1 gives the oil and gas surface volume production rates and totals from fluids above the GOC
  G(O,G)P(R,T)2 gives the oil and gas surface volume production rates and totals from fluids below the GOC

- For the field:

  F(O,G)P(R,T)1 gives the oil and gas surface volume production rates and totals from fluids above the GOC
  F(O,G)P(R,T)2 gives the oil and gas surface volume production rates and totals from fluids below the GOC

Summary of TRACK option

- Components above and below the GOC (or a specific depth) can be tracked separately.

- You can find out how many of the produced molecules came from the gas cap or the oil column.

Environmental Tracers

Account for:

- **Adsorption of tracer onto to rock**
- **Decay of the tracer over time**
- **Molecular diffusion over time**

- **For more information see the Technical Description manual.**

Lumping and Delumping

We can run a detailed compositional simulation using tracers to model individual components that have been grouped into pseudo-components,

De-Lumping…..WHY?

- **Reservoir description using 5-10 components**
  Adequate for phase behavior
  CPU constrained

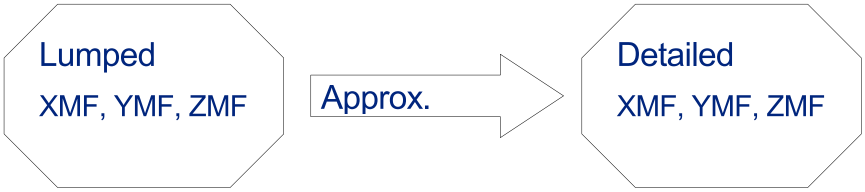
- **Surface facilities using 16-30 components**
  Less CPU bound
  wide range of P and T
  need detailed specifications

- **We want to run our simulations with 5-10 components**
- **We want to report production of 16-30 components**

This is an implementation of paper SPE 49068 by Leibovici *et al*. The idea is to do a full simulation with as small a number of components as possible and then to use multiple tracers carried on each of these ‘lumped’ components to represent the detailed composition of that component.

- **Reservoir model uses LUMPED composition**
- **Simulation reports on DETAILED composition**
- **For example,**
  5 lumped components for history match, prediction, etc...
  Add de-lumping to report production of 27 detailed components at a fraction of the cost of full 27 component run
- **SPE-49068 (Leibovici, Barker, Wache)**

- **Can do a “flash” calculation for regular LUMPED simulation run (i.e. ZMF => XMF, YMF)**
  Need liquid/vapor DETAILED composition
- **Flow the detailed components in the reservoir**
  Tracer for each detailed component


Lumped
XMF, YMF, ZMF

Approx.

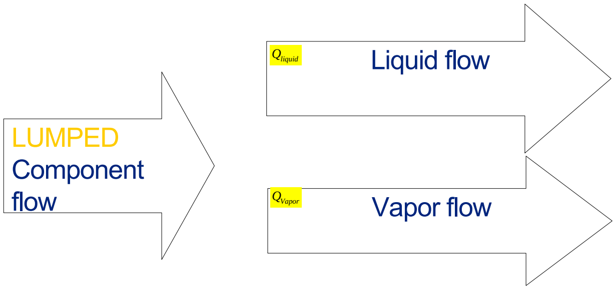
Detailed
XMF, YMF, ZMF

The rationale and details of the approach are explained in the above paper.

- For LUMPED, ignore BICs
- use regression to calculate C_o, C_1, C_2 in

$$\ln(k_i) = C_o + C_1\sqrt{a_i} + C_2 b_i$$

- **plug in detailed EOS**
- **Use above to calculate detailed K-values**
- **Use LUMPED V and L to calculate detailed values of** X_i, Y_i

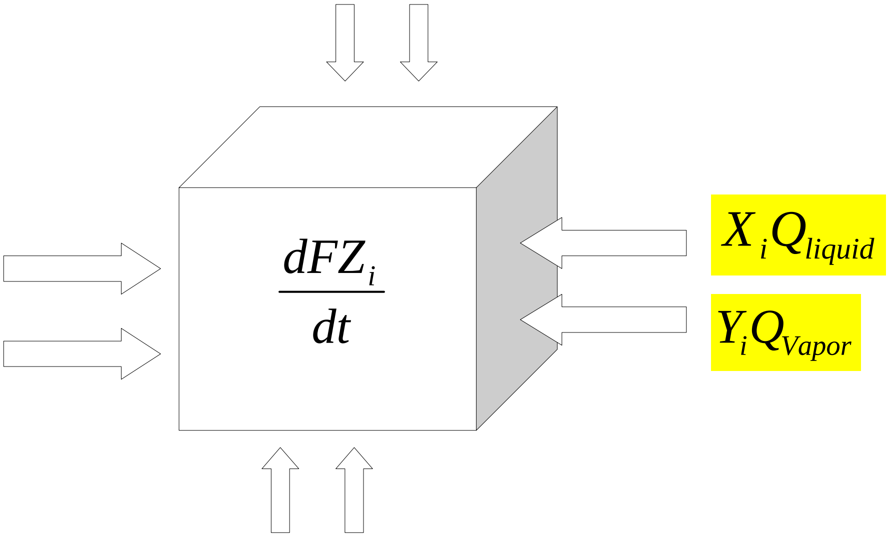


LUMPED Component flow

Q_{liquid} Liquid flow

Q_{Vapor} Vapor flow

Component balance uses the detailed components



$$\frac{dFZ_i}{dt}$$

X_iQ_{liquid}

Y_iQ_{Vapor}

Here we will concentrate on how to apply this procedure.

How to use Lumping/De-lumping

- **RUNSPEC**
  LUMPDIMS
- **PROPS**
  Detailed composition DETAILMF or DETAILVD
  ACFDET, MWDETAIL, TCRITDET, PCRITDET,
  OMEGAADE, OMEGABDE
- **SCHEDULE**
  WINJEDET

The facility is switched on with the `LUMPDIMS` keyword in the `RUNSPEC` section. This gives the number of lumped components (not necessarily as many as the number of components in the 'lumped' simulation) and a maximum for the number of detailed components.

The detailed composition of the fluid is described in the `PROPS` section. The `LUMPING` keyword assigns the number of detailed components to each lumped hydrocarbon component and also allows names to be attached to them. **The order in which the detailed components are entered is important as it will be assumed by later keywords.** The initial detailed state of the reservoir is specified with the `DETAILMF` or `DETAILVD` keyword, which determines the proportion of the detailed components making up the lumped components. This can vary with depth.

Various physical properties of the detailed components can also be specified in the `PROPS` section with the `ACFDET`, `MWDETAIL`, `TCRITDET`, `PCRITDET`, `OMEGAADE`, and `OMEGABDE` keywords. These are identical in nature to their 'normal' simulation counterparts, though as in a normal simulation, not all the *`CRITDET` keywords are needed in a given simulation.

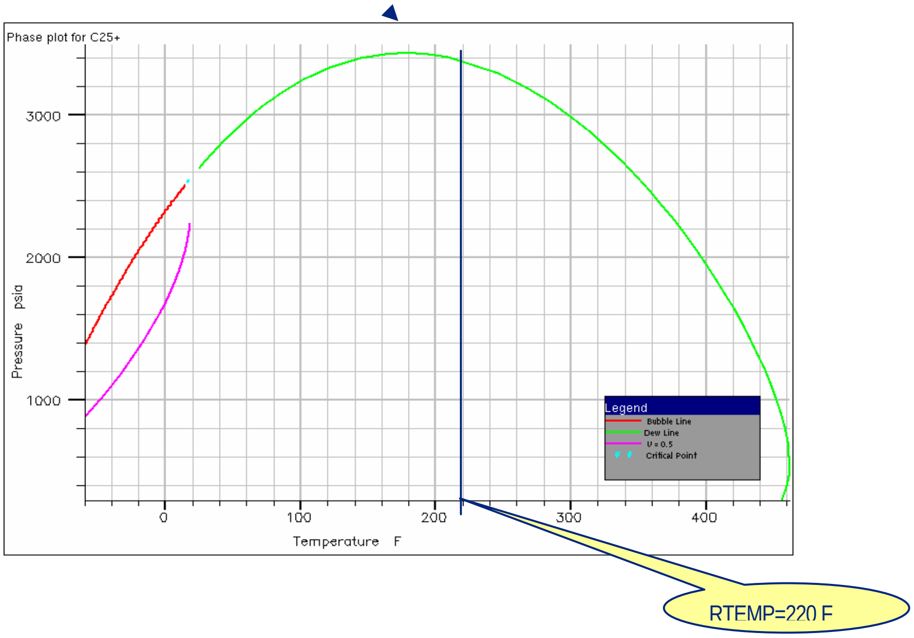
The detailed composition of an injected fluid is given by using the `WINJEDET` keyword in the `SCHEDULE` section. This must be given for each injection well. For a given well the make-up of the detailed fluid is described in an analogous way to the `DETAILVD` keyword.

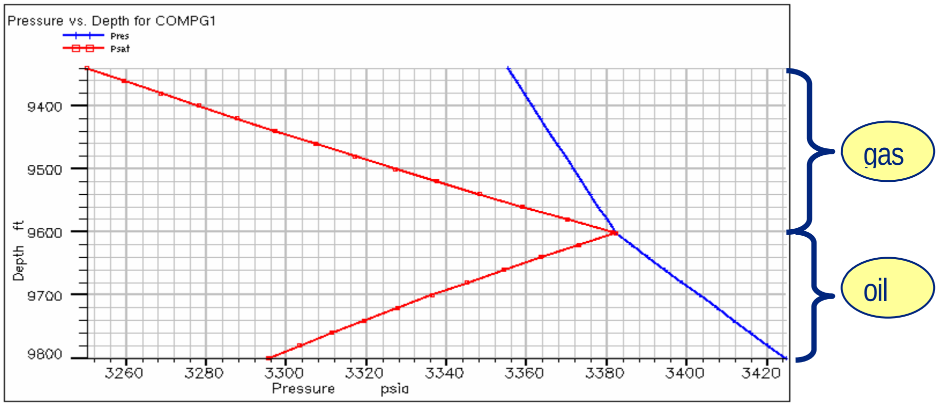
Output relies on the standard tracer output with the well, group and field tracer concentration (summary keywords `WTPC`, `GTPC` and `FTPC`) now representing the mole fraction of that detailed component within the overall fluid from that well, with the names of the tracers being those given in the `LUMPING` keyword. No other summary output is available.

Case Study of Lumping/De-lumping

- DETAILED fluid has 27 components
- LUMP these 27 components down to 5,7,13 components
- Compare LUMPED with DETAILED on sector model
- Compare LUMPED with DETAILED on full field model

We first regress the 27-component model to the experimental observations, then look at the properties of the 27-component characterisation. The fluid is a condensate at the reservoir temperature.

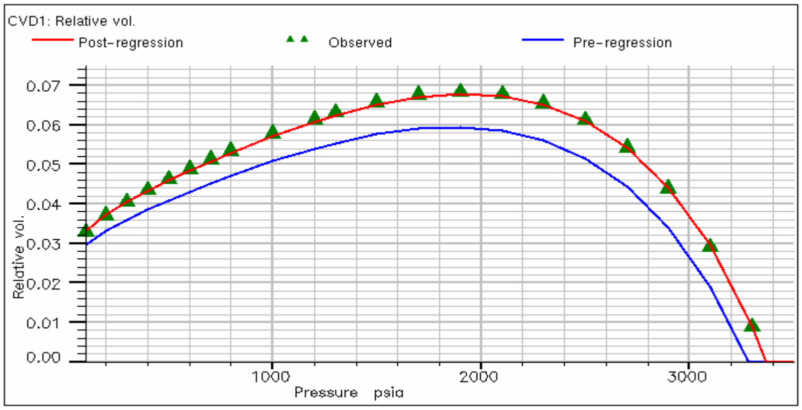




These 27 components are now lumped[50] to 5, 7 and 13 component descriptions. We look in detail at the 7 component case. The methane is left as a separate component, the other 26 components are lumped into 6:

- **Lump => Detailed**
- C1 => C1
- C2+ => C2 C3 IC4 NC4
- C5+ => IC5 NC5 C6 C7
- C8+ => C8 C9 C10 C11
- C12+ => C12 C13 C14 C15
- C16+ => C16 C17 C18 C19
- C20+ => C20 C21 C22 C23 C24 C25+

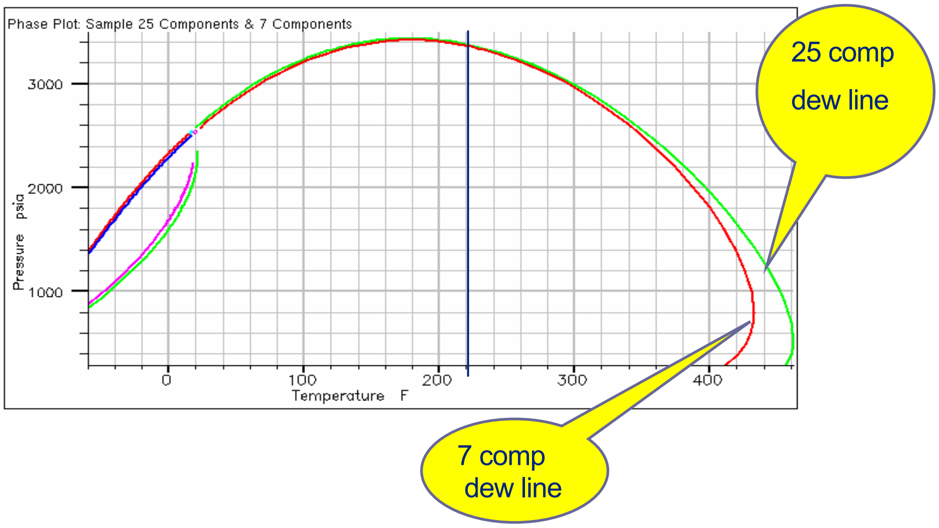
The 7-component model is then regressed, showing a good fit to the observations:

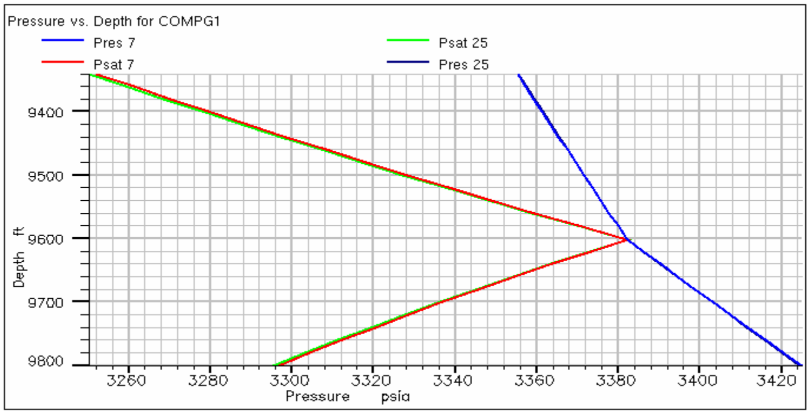


The phase plot for the 7-component model matches the 27-component phase plot in the region of interest, and the pressure vs. depth curves also agree:

---

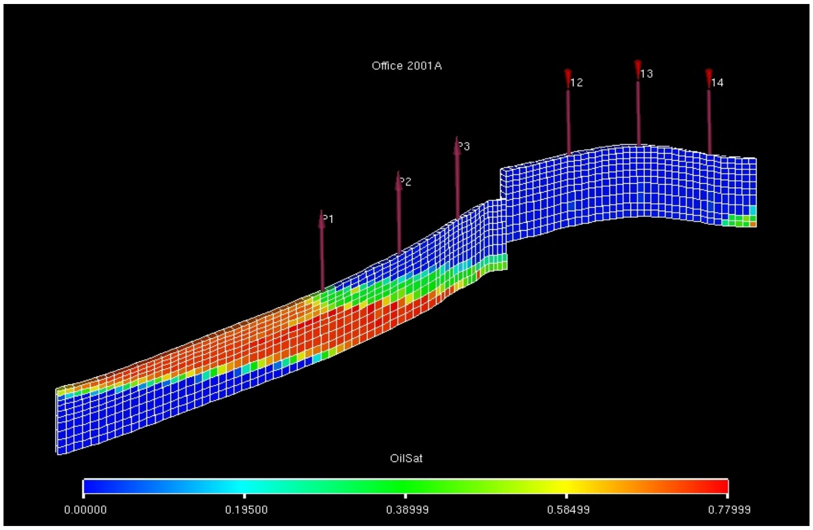
[50] We called this “grouping” in the first part of this course.





Similar results could be shown for the 5 and 13 component models.

We now apply these fluid models, one at a time, to a sector model.

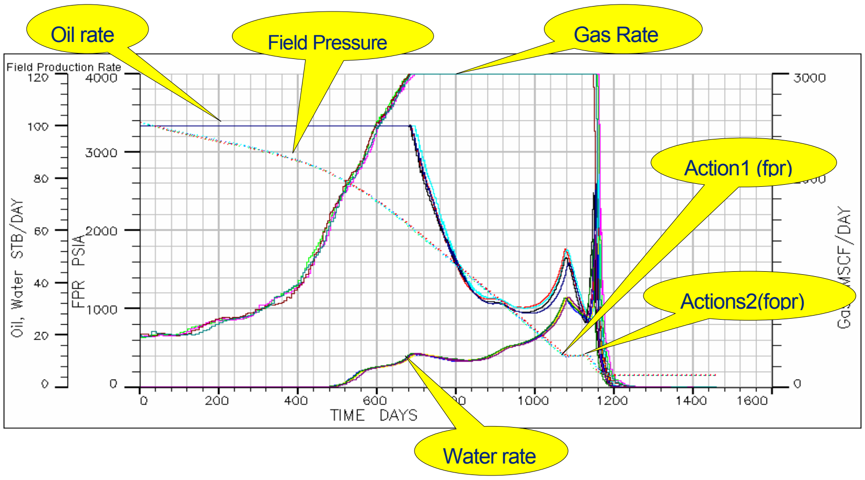


The model has 3 producers (P1, P2, P3), and they start on oil-rate control, with a limited by Gas-rate.   We are injecting methane and the injectors are on voidage replacement with a fraction (vrf)= 0.45.

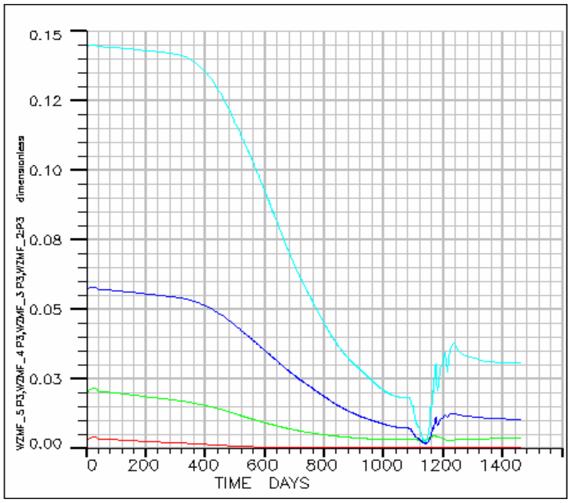
There are two ACTION keywords.

- ACTION1 FPR<400 => vrf=1.0
    - initiates ACTION2 (shut in if FOPR<5000)

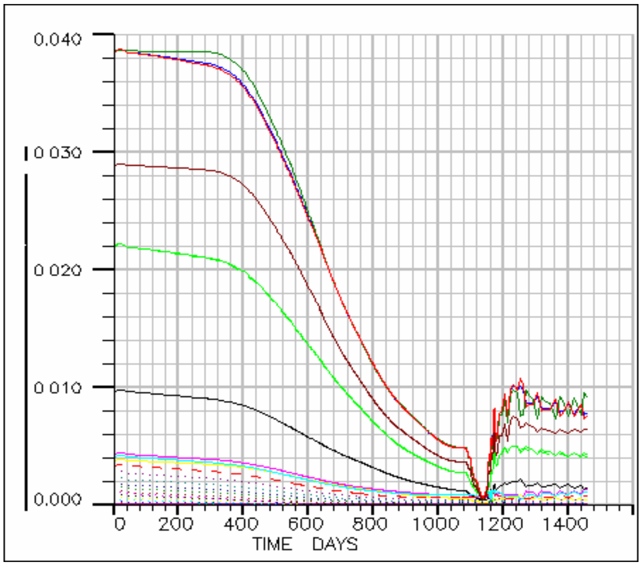
The results show very similar behaviour of all the usual observed quantities such as oil rate, water rate, gas rate, and average field pressure. This is not surprising and confirms that the 5, 7, and 13-component models do indeed represent the behaviour of the detailed 27-component model.



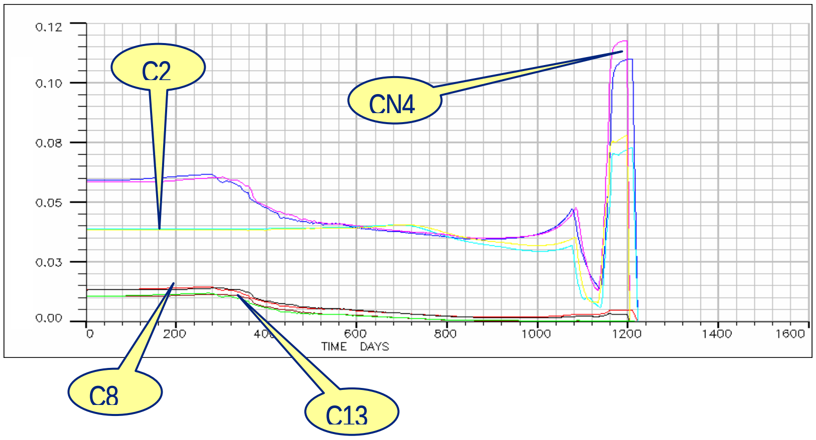
We will now examine the composition of the fluid coming out of each well for the 5-component model. The next picture shows a plot of the mole fraction of each of the 5 components for the producer P3, as a function of time.



Because we are using the LUMPING option and have provided data to ECLIPSE of both the lumped and the de-lumped compositions and properties, we can also calculate the de-lumped mole fractions being produced from P3. This gives us a 27-component prediction based on a 5-component simulation.

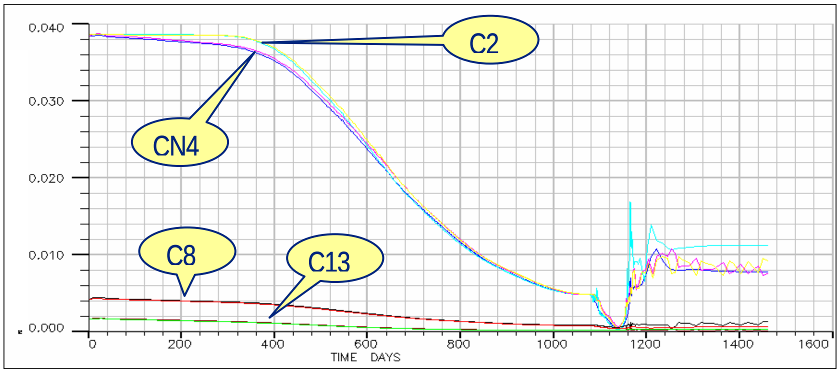


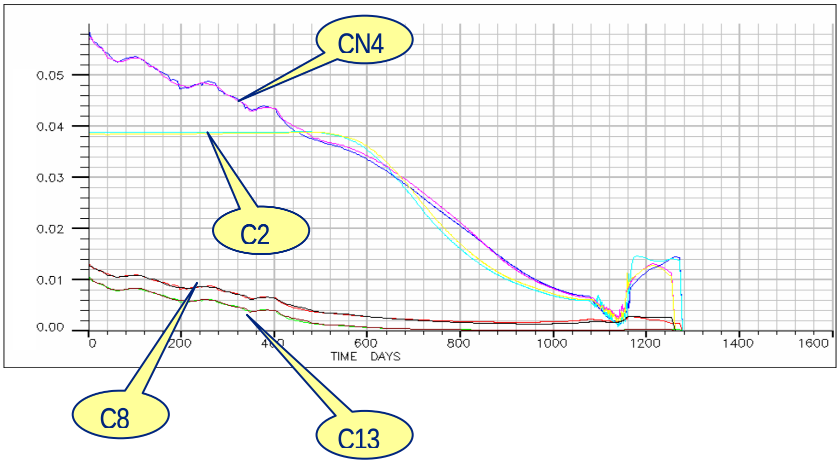
We can then compare the results of the de-lumped 5-component simulation with the results of the detailed 27-component simulation. We do this for each well in turn, for a selection of components. The first plot compares the C2, CN4, C8 and C13 mole fractions produced by well P1:



The agreement is generally good, and is also good for the components that have not been plotted (as the picture would become too complex).

Results for wells P2 and P3 also show good agreement between the de-lumped 5-component simulation and the detailed 27-component simulation:





Summary of Lumping/De-Lumping

- Easy to set up, given detailed PVT data
- Good agreement between De-Lumped and detailed solutions
- De-lumping significantly faster than full detailed run

28. Transport coefficients

The component mobilities can be modified in ECLIPSE 300 by including transport coefficients, based on the work by John Barker and John Fayers. The transport coefficients alpha act as multipliers to the mobility.

- **Can boost or hold back the flow of a given component**
- **Can be used to model fingering that occurs with adverse mobility ratios**
- **Also modelling gas injection into gas**

- **TRCOEFF in RUNSPEC section**
- **ALPHA in props section**
- **different coefficients for transport in the oil phase and the gas phase**

Example of ALPHA table:

```
ALPHA
--  Oil Coefficients   Gas Coefficients
 .4   1 1 1 1 1 1       1.5  1.4  1.0  0.91  0.80
 .6   1 1 1 1 1 1       1.3  1.2  1.0  0.93  0.85
 .8   1 1 1 1 1 1       1.1  1.1  1.0  0.97  0.9
 .9   1 1 1 1 1 1       1.0  1.0  1.0  1.0   1.0  /
```

29. Gas flow near a well

The next three topics are closely related and refer to models of the detailed flow around a producing well.

Non-Darcy Flow

Generalized Pseudo Pressure

Velocity Dependent Relative Permeabilities

Non-Darcy Flow: turbulence increases pressure drop near well

Generalized Pseudo Pressure [GPP]: condensate blocks well inflow

Velocity Dependent Relative Permeabilities: low Interfacial Tension at high velocities increases gas and oil relative permeability

For Non-Darcy Flow we use the Forcheimer model of Holditch and Morse.

The Generalized Pseudo Pressure [GPP] follows Whitson and Fevang.

Velocity Dependent Relative Permeabilities is based on the work of various authors at the Department of Petroleum Engineering of Heriot-Watt University.

Non-Darcy Flow

The non-Darcy feature we consider here is the Forcheimer correction; which takes into account the inertia effects due to high velocity that may occur for instance around gas producers or in high permeability regions such as fractures. Turbulent flow is modeled by adding a velocity-dependent term to the pressure drop.

Deriving the equations

Darcy flow is given by:

$$q = \left(\frac{KA}{\mu}\right)\frac{dP}{dx}$$

$$or$$

$$\frac{dP}{dx} = \left(\frac{\mu}{KA}\right)q$$

where

q = volumetric flow rate (cm3/s)

K = permeability (Darcys)

A = area for flow (cm2)

μ= viscosity (cP)

dP/dx = pressure gradient (Atm/cm)

In the Holditch and Morse model for non-Darcy flow, we add a velocity-dependent term for turbulent flow:

$$\frac{dP}{dx} = \left(\frac{\mu}{KA}\right)q + \beta\rho\left(\frac{q}{A}\right)^2$$

where

ρ = fluid mass density

q/A = fluid velocity

and β is the user input non-Darcy flow coefficient or Forcheimer parameter in units of $Atm.s^2g^{-1}$ = 1 F (Forcheimer). Typical values of β =107 - 109 at K = 60mD, which gives 9.86 F.

We can rewrite the equation as

$$\frac{dP}{dx} = \left(\frac{\mu}{KA}\right) q \left(1 + \frac{\beta \rho q K}{A\mu}\right)$$

then

$$q = \left(\frac{KA}{\mu}\right)\left(\frac{dP}{dx}\right) / \left(1 + \frac{\beta \rho q K}{A\mu}\right) = \left(\frac{KA}{\mu}\right)\left(\frac{dP}{dx}\right) F_{ND}$$

with the non - Darcy flow factor given by :

$$F_{ND} = \frac{1}{\left(1 + \frac{\beta \rho q K}{A\mu}\right)}$$

The flow velocity is a function of F_{ND} and F_{ND} is a function of the flow velocity, so we have two coupled equations to solve for phase p. Thus we have a quadratic equation for F_{ND} whose solution is:

$$F_{ND} = \frac{-1 + \sqrt{(1 + 4B)}}{2B}$$

where

$$B = \left(\frac{C_2 \beta T K}{A}\right)\left(\Delta \phi_p\right)\left(\frac{\rho_p K_{rp}{}^2}{\mu_p{}^2}\right)$$

C_2 is a unit conversion constant. You can output the values of F_{ND} and $B/\Delta\Phi$ using the mnemonics FFORG and BFORG in the `RPTSOL` or `RPTSCHED` keywords.

Example

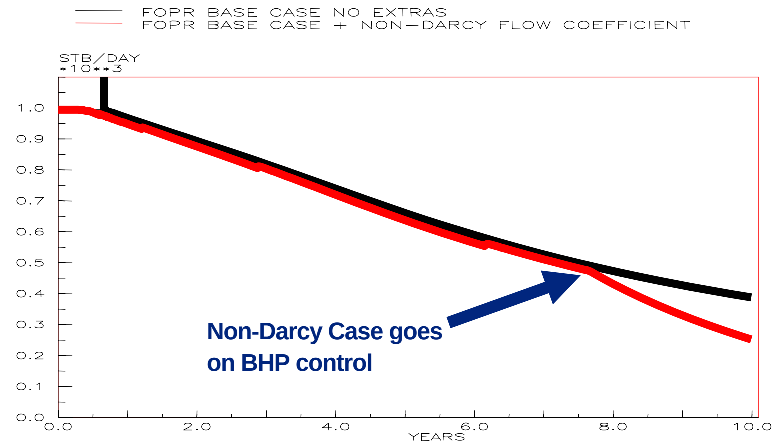
We show the effect of non-Darcy flow on the simulation of a gas condensate.

- **9 Component PR3 Fluid Description**
- **C7+ C12+ C22+**
- **Field Units, Fully Implicit Solution**
- **1-D Radial Grids - thickness = 100 feet**
- **Permeability = 100 mD, unless noted**
- **Initial Pressure = 7000 psia**
- **Dew Point Pressure = 6578 psia**
- **Reservoir Temperature = 320^o F**

Well controls:

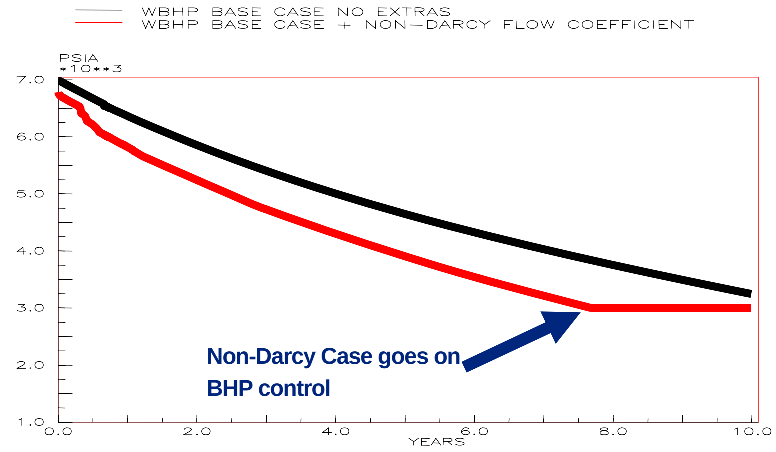
- Constant Gas Production Rate = 5000 Mscf/day
- BHP = 3000 psi
- Compare
  Oil Production Rate
  Well BHP
  Gas Production Rate

Results from the simulation show that if we don't take into account non-Darcy flow we will overestimate the oil production. The non-Darcy flow case has a lower BHP compared to the Darcy flow model, and goes on to BHP control while the Darcy flow model continues producing at its target gas rate.



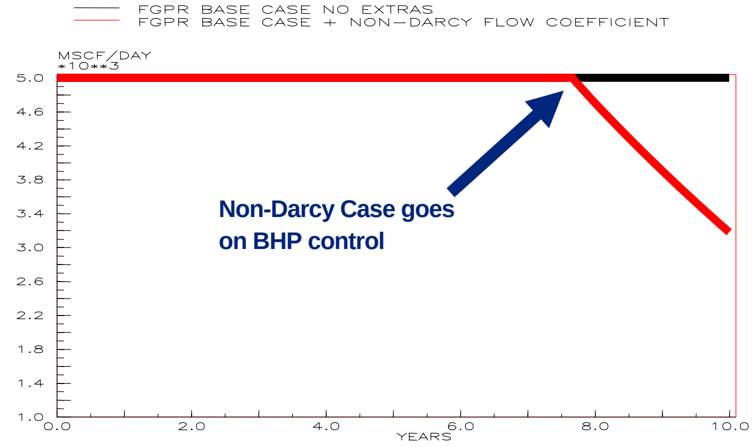
Non-Darcy Case goes on BHP control

COMPARISON OF STANDARD ECLIPSE RESULTS WITH NON-DARCY MODEL



Non-Darcy Case goes on BHP control

COMPARISON OF STANDARD ECLIPSE RESULTS WITH NON-DARCY MODEL



Non-Darcy Case goes on BHP control

COMPARISON OF STANDARD ECLIPSE RESULTS WITH NON-DARCY MODEL

Using Non-Darcy Flow

- You can input the Forcheimer parameter with the keyword VDFLOW in the PROPS section
- You can use the VDFLOWR keyword to set different Forcheimer parameters for different regions.
- ECLIPSE will calculate the Forcheimer parameter if velocity-dependent relative permeabilities are used – see later.

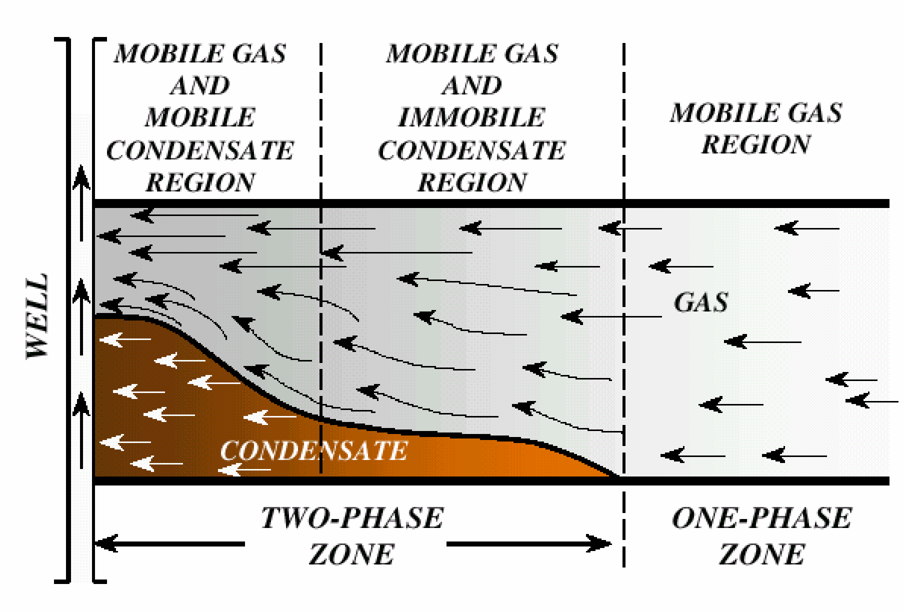
Summary

Turbulence reduces production at high gas flow rates.

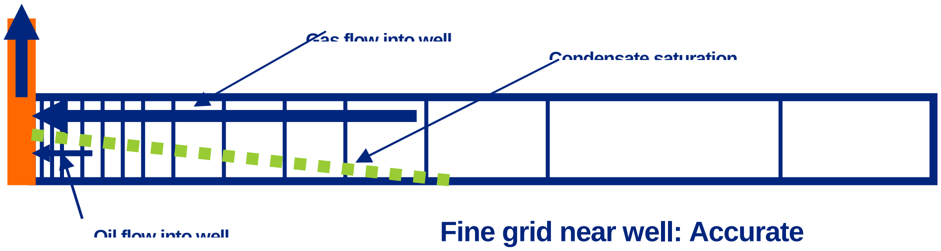
Generalised pseudo-pressure

- As pressure in and around gas condensate well falls below dew point - condensate blocking reduce well deliverability
- GPP allows more accurate description of well inflow in coarse grid

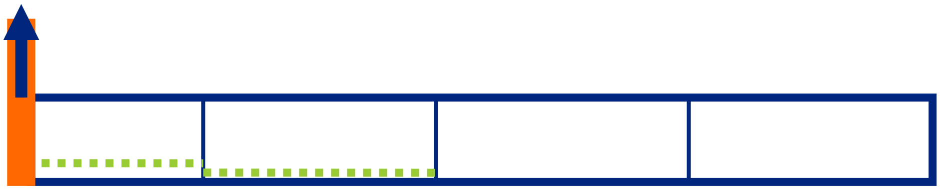
In a gas condensate reservoir, if the pressure around a producing well drops below the dew point, then condensate will drop out and form a condensate bank around the well bore.



The picture above shows the hydrocarbon behavior at a particular time, after the pressure has dropped has dropped below the dew point. If the size of a grid block containing the well connection is less than the size of the two-phase hydrocarbon zone (shown) above) then our simulation model will also show some condensate drop out.



Fine grid near well: Accurate saturations, pressures and flow

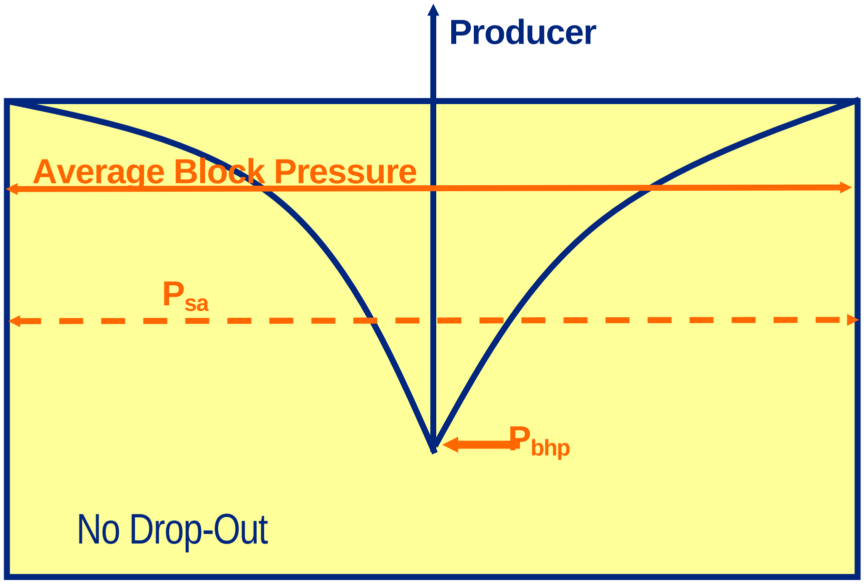


Coarse grid near well: Inaccurate saturations, pressures and flow blocking

To accurately model any mobile condensate, the grid block should be smaller than the mobile condensate region shown above, although the size of this region will of course change with time.

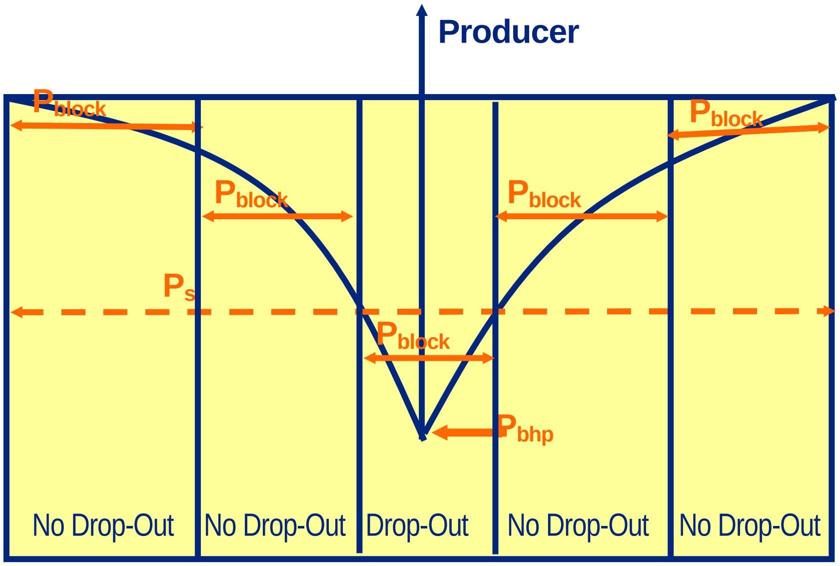
- **In a grid block containing a producer, the average block pressure will be higher than the pressure at the well.**
- **Suppose the dew point has a value between the block pressure and the well pressure.**
- **If we use the average block pressure in our calculations, we will predict no condensate drop out.**
- **If we refine the grid block with an LGR, we will find that there is some drop-out around the well bore.**

Consider however the situation when the grid block is much greater than the two-phase region. The average pressure in that grid block can be above the dew point, in which case the model will predict no condensate drop out for that well.



Pressures within a grid block: $P_{block} > P_{sat} > P_{bhp}$

Smaller grid blocks, or maybe an LGR around the well, would predict more accurately the formation of the condensate bank.



Pressures within a refined grid block

As an alternative, you can use the generalized pseudo-pressure (GPP) method of Whitson and Fevang.

- **Condensate drop-out will affect the mobility in the grid block**

- **GPP tries to account for condensate drop-out**
- **GPP alters the total mobility in a well grid block**

- **Based on Whitson and Fevang**
  Generalised Pseudopressure Well treatment in Reservoir Simulation, Optimisation of Gas Condensates, Aberdeen, June 1997

GPP tries to account for the decreased mobility around the well caused by the condensate drop out.

The generalized pseudo-pressure method of Whitson and Fevang [Ref. 73] is also available in ECLIPSE 300. The option can be requested for all wells with the `PSEUPRES` keyword, which should be entered early in the `SCHEDULE` section before any well operations or time stepping keywords are specified. Alternatively this option can be activated for individual wells by entering GPP in item 8 of keyword `WELSPECS` Calculation controls are set with keyword `PICOND`. The calculation and its implementation are described below.

Consider the flow of phase j = (oil, gas), in a radial homogenous media of height h and permeability K. Darcy's law describes the velocity of the fluid at radius r in the equation:

$$v_j = \frac{Q_j}{2\pi rh} = \frac{KK_{rj}}{\mu_j}\frac{dP}{dr}$$

where Q_j is the in-situ volumetric flow rate, K_{rj} and μ_j are the phase relative permeability and viscosity and

$$dP / dr$$

is the pressure gradient. The phase volumetric flow rate Q_j is related to phase molar flow rate nj by:

$$Q_j = n_j V_{mj}$$

where V_{mj} is phase molar volume. Combining and re- arranging gives:

$$n_j \frac{dr}{r} = 2\pi Kh \frac{K_{rj} b_j}{\mu_j} dp$$

where the phase molar density

$$b_j = 1 / V_{mj}$$

For component *i*, the component phase molar rate will be:

$$n_{ij} \frac{dr}{r} = 2\pi Kh x_{ij} \frac{K_{rj} b_j}{\mu_j} dp$$

where x_{ij} is the mole fraction of the ith component in the jth phase.

Integrating between the Peaceman pressure equivalent radius r_B and the well radius r_W gives

$$n_{ij} \int_{r_W}^{r_B} \frac{dr}{r} = 2\pi Kh \int_{p_W}^{p_B} x_{ij} \frac{K_{rj} b_j}{\mu_j} dp$$

Summing component phase molar rates in the oil and gas phases for component *i*:

$$(n_{io} + n_{ig}) \left[\ln\left(\frac{r_B}{r_W} \right) + S \right] = 2\pi Kh \int_{p_W}^{p_B} \left[x_i \frac{K_{ro} b_o}{\mu_o} + y_i \frac{K_{rg} b_g}{\mu_g} \right] dp$$

or:

$$n_i = T \int_{p_W}^{p_B} M_i(p) dp$$

- **Basic assumption for all flow is that**

  Flow = Mobility * Transmissibility * dP

- **For well inflow, Mobility is taken as**

  Inflow = MobilityPblock*Transmissibility*(Pblock - Pbhp)

The well connection factor, *T*, including the skin factor, *S*, is given by:

$$T = \frac{2\pi Kh}{\ln\left(\frac{r_B}{r_W}\right) + S}$$

and the Component Generalized Molar Mobility (CGMM) is given by:

$$M_i = x_i\frac{K_{ro}b_o}{\mu_o} + y_i\frac{K_{rg}b_g}{\mu_g}$$

Normally, we do not consider the pressure dependency in the integral. Instead, we compute the CGMM at the block pressure:

$$\int_{p_W}^{p_B} M_i(p)dp \to M_i(p_B)[p_B - p_W]$$

However we have already discussed that the block pressure can be a poor approximation for a gas condensate where, although the block pressure may be well above the dew point and hence the gas relative permeability is high, the well pressure may be well below the dew point in which case the gas relative permeability can be substantially reduced. In this case, we want perform the integral in more detail.

To prevent accumulation of moles in the completion cell, the ratio of CGMM for component *i* to the Total Generalized Molar Mobility (TGMM) must be a constant:

$$z_{pi} = \frac{M_i}{M_T}$$

where:

$$M_T = \sum_i M_i$$

Therefore, we can write:

$$n_i = Tz_{pi}\int_{p_W}^{p_B} M_T(p)dp$$

where:

$$M_T = \frac{K_{ro}b_o}{\mu_o} + \frac{K_{rg}b_g}{\mu_g}$$

If the block pressure *pB* exceeds the dew point pressure, the production composition *zpi* is simply the total hydrocarbon composition in the block. If the block pressure is less than the dew point pressure, the production composition is computed from CGMM for oil and gas.

When the Generalized Pseudo-Pressure (GPP) model is applied in ECLIPSE 300, rather than re-writing the appropriate parts of the well model, we simply modify the conventional well inflow equation through the addition of the component dimensionless flow blocking factor, *FBi*, to give:

$$n_i = TF_{Bi}M_i(p)[p_B - p_W]$$

where:

$$F_{Bi} = \frac{1}{M_i(p_B)}\frac{1}{(p_B - p_W)}z_{pi}\int_{p_W}^{p_B} M_T(p)dp$$

We can write:

$$M_i(p_B) = z_{pi}M_T(p_B)$$

therefore we define the total dimensionless flow blocking factor, *FB*

$$F_B = \frac{1}{M_T(p_B)}\frac{1}{(p_B - p_W)}\int_{p_W}^{p_B} M_T(p)dp$$

and hence the modified inflow equation becomes:

$$n_i = TF_BM_i(p)[p_B - p_W]$$

This final form of the GPP inflow equation differs only from the normal inflow equation by the additional multiplication factor *FB*.

Define blocking factor F_B

$$F_B = \frac{\int_{P_{bhp}}^{P_{block}} M_T dP}{M_T\left(P_{block} - P_{bhp}\right)}$$

then instead of
Inflow = MobilityPblock*Transmissibility*(Pblock - Pbhp)

we use
Inflow = F_B*MobilityPblock*Transmissibility*(Pblock - Pbhp)

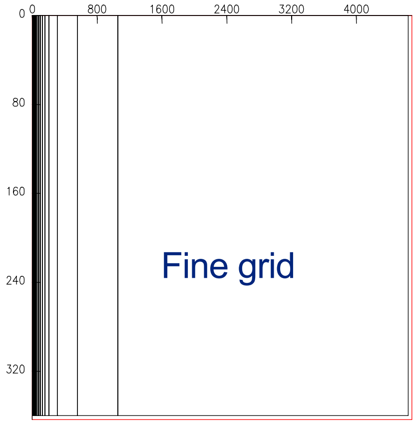
The integral is constructed by trapezium rule, following the suggestions made by Whitson and Fevang. In practice the integral is constructed at the beginning of each timestep, assuming the block conditions have changed significantly.

- Explicit
- … so may not be accurate when time steps are so large that pressures are changing significantly during the time step

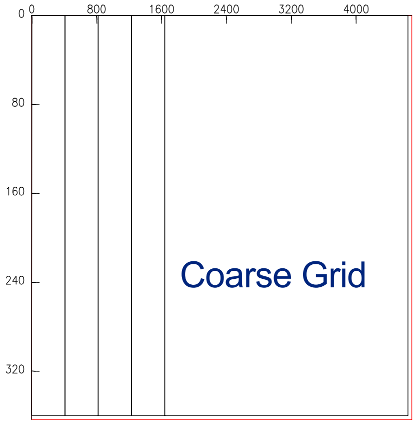
Example of GPP

We compare two different simulation grids:

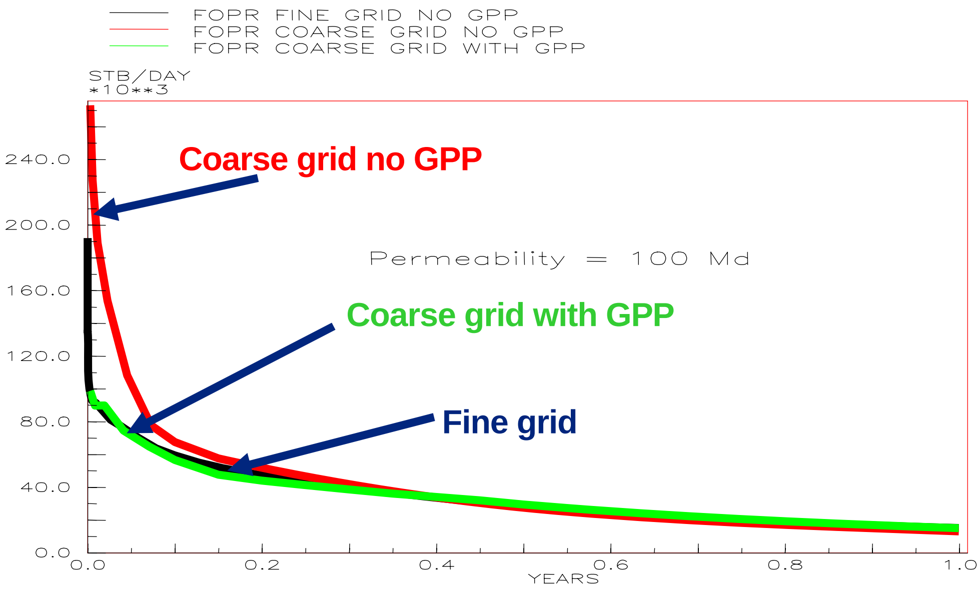
Δr = 1 2 3 4 5 6 7 8 9 10 12 15 20 25 50 100 250 500 3583



Δr = 410 410 410 410 3000

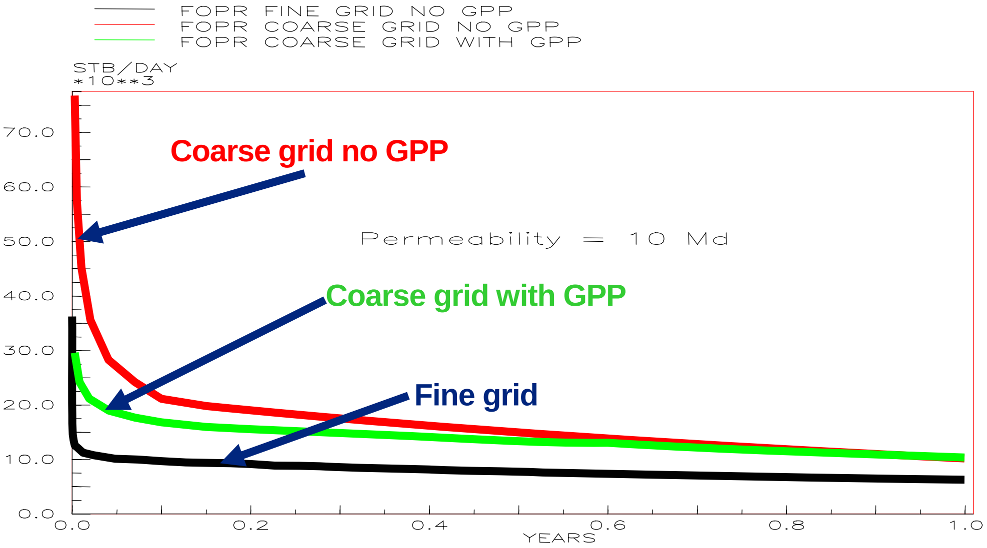


- BHP = 1000 psi
- Compare
  Oil Production Rate
  Gas Production Rate
  Oil Saturation near well



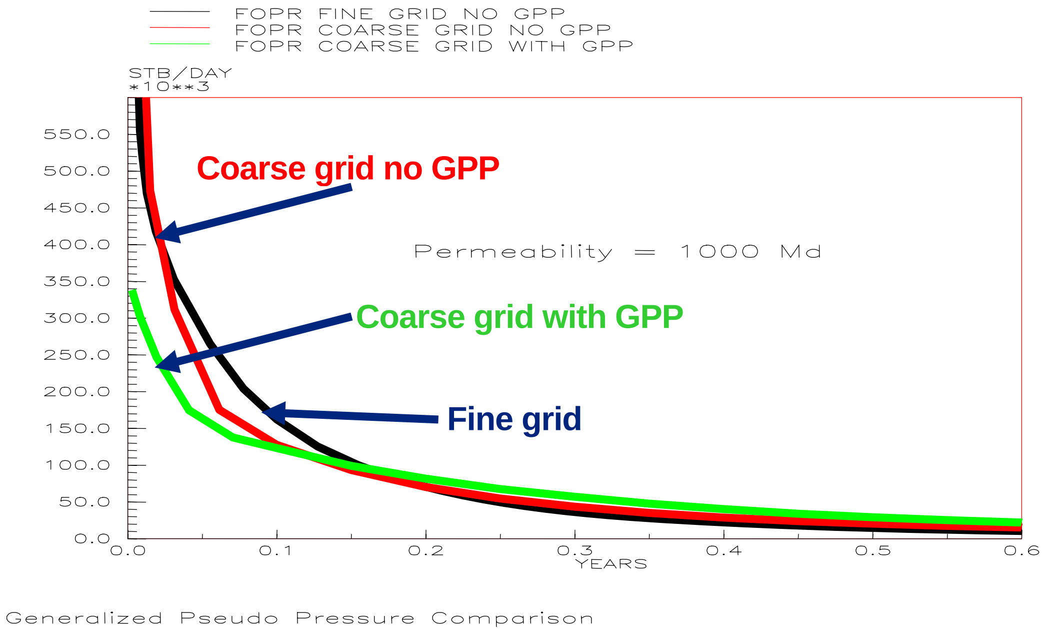
Generalized Pseudo Pressure Comparison

For this case, if the permeability is 100 mD then the coarse grid with GPP gives very similar results to the fine grid.



Generalized Pseudo Pressure Comparison

For a lower permeability, the coarse grid with GPP is a better approximation to the fine grid.



For a higher permeability, there is no clear advantage in using GPP. In this case the pressure distribution will be less sharp around the well, the pressure drop will extend for a longer distance and drop-out will occur further from the well, so there is relatively less need for the GPP model.

Using Generalised Pseudo Pressure

- ECLIPSE 100 and ECLIPSE 300:
  To choose GPP for a well,
  WELSPECS(8) = GPP
- ECLIPSE 300:
  To set GPP for all wells,
  PSEUPRES keyword in SCHEDULE section

You can ask for this option for all wells with the `PSEUPRES` keyword, which should be entered early in the `SCHEDULE` section before any well operation or time stepping keywords are specified. Alternatively this option can be activated for individual wells by entering GPP in item 8 of keyword `WELSPECS`. Calculation controls are set with keyword `PICOND`.

Summary of GPP

- If permeability is low and gas production is high then the grid block size will affect production.
- A coarse grid block will overestimate production of both gas and condensate.
- GPP corrects this overestimate

Velocity-Dependent Relative Permeabilities

At high gas velocities, in addition to the Forcheimer correction we can also take into account more complex effects by introducing a velocity dependence of the relative permeabilities. The model may make the oil and gas relative permeabilities functions of Capillary Number (CN) and/or the Forcheimer parameter, depending on the switches you set using the `VELDEP` keyword in the `RUNSPEC` section. Properties of the velocity-dependent relative permeabilities for the oil and gas are set with the keywords `VDKRO`, `VDKRG` and `VDKRGC`.

- Intended for gas condensate systems

We expect a reduction of the PI (Productivity Index) when a well BHP drops below the dew point

This does not occur in practice (field)

These models are intended for gas condensate systems where the expected reduction in Productivity Index (PI) when a well bottom hole pressure drops below the fluid dew point pressure has not been observed in practice. Several theories have been suggested as to why the gas relative permeability in particular remains relatively high but the current consensus seems to imply that a combination of low InterFacial Tensions (IFTs) at reservoir conditions and high velocities as flow converges towards a producer are the main driving forces.

- **Theory: why does gas relative permeability remains relatively high?**
- Combination of low Inter-Facial Tensions (IFTs) at reservoir conditions
- Created by high velocities as flow converges towards a producer
- **For ECLIPSE 100 combine IFT and velocity into Capillary Number**

Normal engineering practice is to combine IFT and velocity through the so-called Capillary Number: several alternative definitions are possible and three are shown below. Of course, where flow velocities are high, turbulence effects as predicted by the Forcheimer model become significant and a model for this effect has been developed as part of this overall scheme.

- **Model makes gas and oil relative permeability function of Capillary Number (CN)**
- **Add Forcheimer model when turbulence effects become significant**

Capillary number model

- **The CN model has two effects on the gas and oil relative permeability as CN increases:**

1. **Residual saturation reduces**
2. **Relative permeability curve changes from user-specified (immiscible) to miscible curve (internally generated)**

The CN model has two effects on the gas and oil relative permeabilities, namely as the CN increases:

1. It reduces the residual saturations
2. It changes the relative permeability from the user-specified (immiscible) saturation curves towards an internally-generated miscible curve.

The CN is calculated from one of three alternate models[51]. For phase j = (oil, gas)

---

[51] Note that Capillary Number Model 1 for the oil and gas phases depends only on the gas velocity and gas viscosity. This apparent discrepancy has been verified by experiment.

$$N_{cj} = \frac{v_g \mu_g}{\sigma}$$

or

$$N_{cj} = \frac{KK_{rvj} \Delta P_j}{\sigma L}$$

or

$$N_{cj} = \left(2\phi S_j KK_{rvj}\right)^{1/2} \frac{\Delta P_j}{\sigma}$$

where σ is the gas-oil surface tension.

- **Once the phase CN has been calculated**
- **Calculate Normalized Capillary Number (NCN)**

$$N_{cnj} = \frac{N_{cbj}}{N_{cj}}$$

- **N_{cbj} is Base Capillary Number (BCN) = lower threshold value below which the CN has no effect of the phase relative permeabilities.**
- **BCN should be determined experimentally/ECLIPSE 100 will estimate**

Once the phase CN has been calculated, we can calculate the Normalized Capillary Number (NCN)

$$N_{cnj} = \frac{N_{cbj}}{N_{cj}}$$

where N_{cbj} is the phase Base Capillary Number (BCN). The phase BCN is a lower threshold value below which the CN has no effect on the phase relative permeabilities. As with all the parameters in this and the Forcheimer models, the phase BCN should be determined experimentally for the reservoir and fluid of interest. If this data is not available, it may be estimated using the following procedure.

Base capillary number estimation

Generally, the rock or base relative permeability curves used to describe the flow of gas and oil within the reservoir will have been generated at or near ambient conditions. Ideally, the phase CNs will have been measured from these laboratory analyses and are reported to you; in practice, this is rarely the case. At ambient conditions, the reservoir gas and condensate are as different in composition as it is possible to get; therefore, the gas-oil surface tension is likely to be its maximum. In addition, the low pressure gas viscosity is likely to be at its minimum.

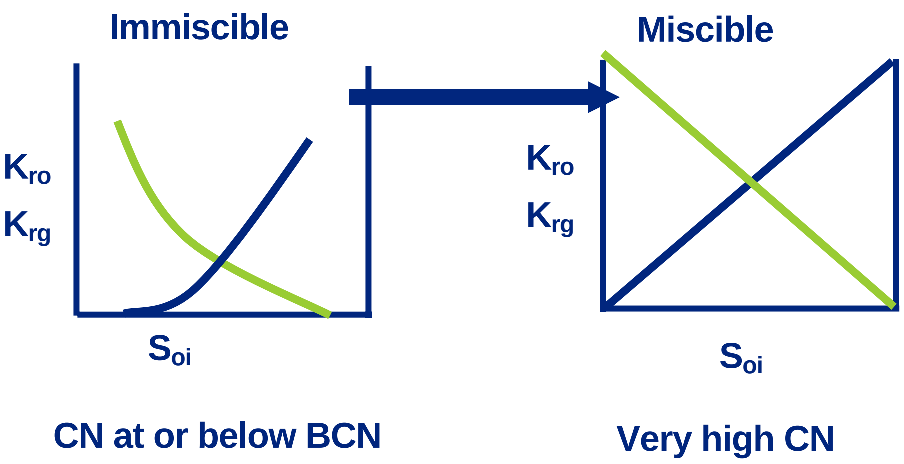
Using PVTi, it should be possible to perform a Constant Volume Depletion (CVD) experiment on the reservoir fluid, starting from the dew point and ending at the likely abandonment pressure. The values of the gas-oil surface tension and gas viscosity can then be taken from this final stage pressure.

Away from the wells, fluid velocities rarely exceed 10 ft/day [~ 3.5x10-5 m/s]. This value for gas velocity along with the low pressure gas-oil surface tension and gas viscosity can be used to estimate the oil and gas BCN in the absence of experimental data.

The effect of CN

CN can have two effects on the relative permeability curves:

1. The input relative permeability curves are modifies and tend towards straight-line miscible relative permeability curves
2. Experimental evidence suggests that as the CN rises above the BCN, the residual saturation is reduced.



Given a phase residual saturation S_{rbp} determined from routine Special Core AnaLysis (SCAL), the effect of the CN dependency is to change the residual saturation to

$$S_{rbj} \rightarrow X_j S_{rbj}$$

$$where$$

$$X_j = 1 - e^{\left(-m_j N_{cnj}\right)}$$

X_j is the saturation scaling parameter and m_j **must** be experimentally determined.

- **As CN rises above the BCN, the residual saturation is reduced**
- **Use saturation scaling parameter X_j**
- **Must know from Special Core Analysis: a phase residual saturation S_{rbj} and parameter m_j (determined experimentally)**

$$S_{rbj} \rightarrow X_j S_{rbj}$$

$$where$$

$$X_j = 1 - e^{\left(-m_j N_{cnj}\right)}$$

If m_j is set to zero phase residual saturation is zero and independent of CN.

Example

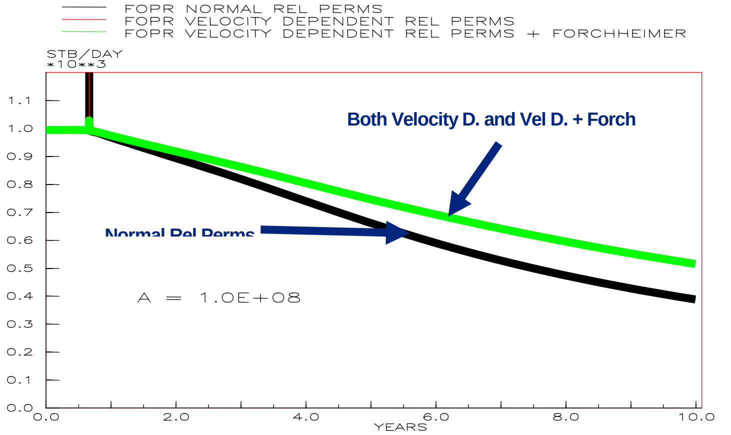
In this example we will use the CN calculated from the first of the capillary models:

$$\beta_j = \frac{a_j}{\phi^{b_j} s_j^{\ c_j} \left(KK_{rvj}\right)^{d_j}}$$

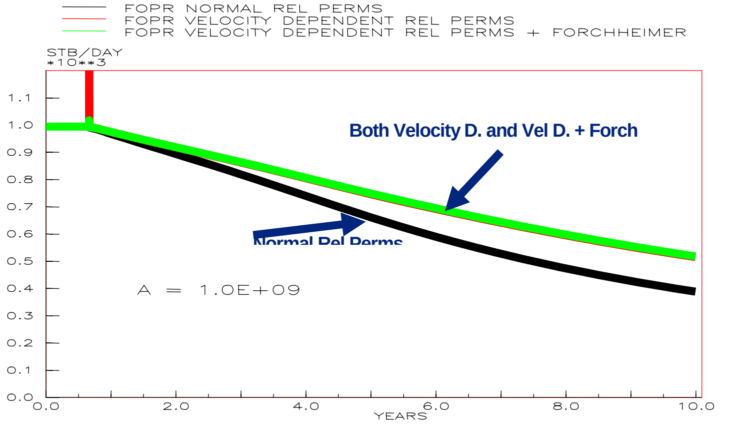
We will use a form independent of saturation and porosity by setting b=c=0. D=0.5 and we will vary “a” between 10**8 and 10**11.

- Constant Gas Production Rate = 5000 Mscf/day
- BHP = 3000 psi
- Compare
  Oil Production Rate
  Oil Saturation near well
  Oil Relative Permeability
- The grid is radial, with
- dr = 1.75 2.32 5.01 10.84 23.39 50.55 109.21 235.92 509.68 1101.33 feet

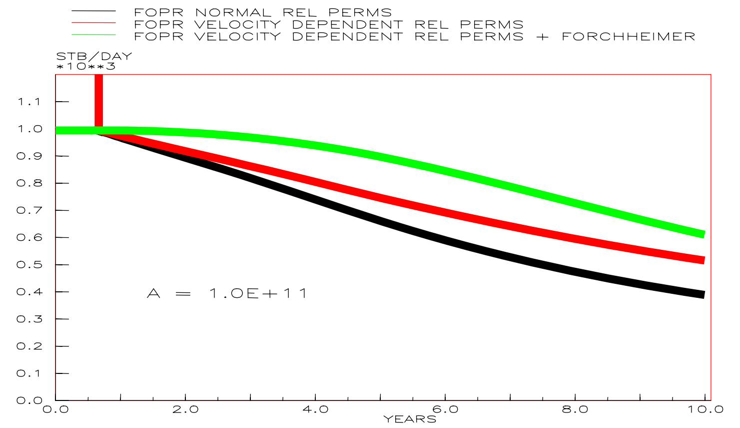
The next slides show the oil production rate for varying values of parameter a:



Comparison of Normal, Velocity Dependent Rel Perms w-w/o Forchheimer



Comparison of Normal, Velocity Dependent Rel Perms w-w/o Forchheimer



Comparison of Normal, Velocity Dependent Rel Perms w-w/o Forchheimer

As you can see:

- for a=10**8, using velocity dependent rel perms increases oil production. Applying the Forcheimer model does not lead to any further increase in production.
- for a=10**11, using velocity dependent rel perms also increases oil production but now applying the Forcheimer model gives us a further increase in production.

Alternative model

An alternative model for CN effects in gas relative permeability has been implemented following some of the ideas introduced in the work of Whitson, Fevang and Saevareid. This model is designed for near wellbore flows exhibiting condensate 'blockage' type behavior in a gas condensate reservoir. It may be activated via item 5 of the `VELDEP` keyword in the `RUNSPEC` section.

This model is more straightforward than the above in that:

- Only the gas relative permeability is modified
- There is no effect on residual saturations
- There is no lower threshold or base capillary number value. (Below which the CN has no effect on the gas relative permeabilities.)
- It depends on only two parameters, both of which have default values.
-

- VDKRGC **keyword to set Fevang and Whitson VDRP model parameters**

- **Only 2 parameters needed by the user**

In the implementation in ECLIPSE 300, the CN-modified gas relative permeability is a mixture of a straight-line miscible relative permeability and the input immiscible, rock relative permeability; this mixture is controlled by a CN dependent transition function that depends on the gas capillary number.

- **Velocity dependence is taken in account through the capillary number (Nc):**

$$N_c = \frac{v_g \mu_g}{\sigma}$$

- **"Immiscible" curve (user-specified) is linked with "miscible" curve through a transition function**

$$f_I(N_c) = \frac{1}{(\alpha \cdot N_c)^n + 1}$$

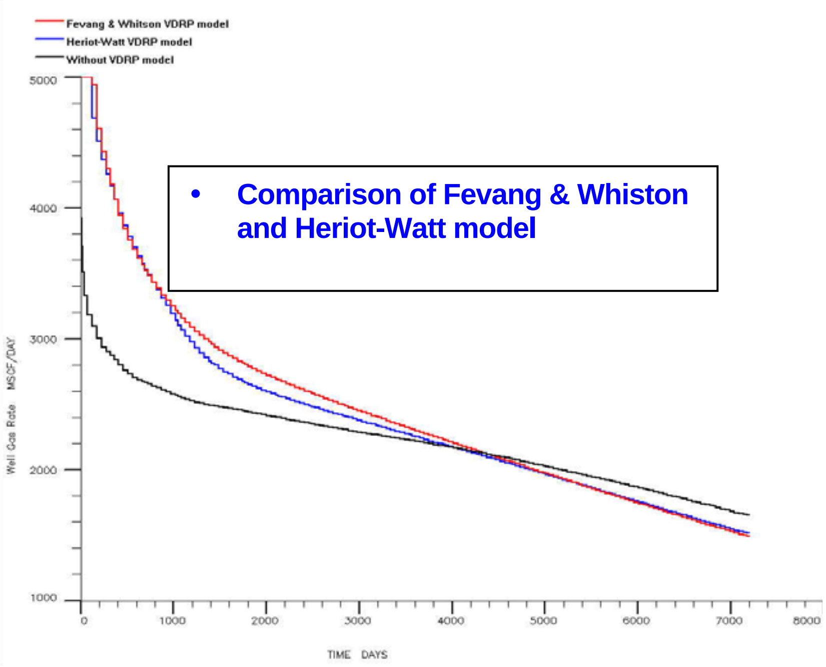
where

$$\alpha = \frac{\alpha^0}{\bar{k}_{rg}} \; ; \; \alpha^0 = \frac{C}{\sqrt{K\Phi}}$$

This model depends on two parameters. These parameters are defaulted to 0.65 and 1.0E4 respectively, with the keyword `VDKRGC` permitting you to override these values.

Item	Parameter
1	*N (0.65)*
2	*C (104)*

This alternative model for CN effects in gas flows cannot of course be used at the same time as the original CN model for gas flows. It can, however, be used in conjunction with the original model for CN effects in oil flows and the Forcheimer model for inertial effects in oil and gas flows. The selection of models is controlled by the `VELDEP` keyword.



- **Comparison of Fevang & Whiston and Heriot-Watt model**

Both CN and Forcheimer effects may be including in the generalized pseudo pressure option that calculates a blocking factor due to near well condensate drop-out. This is controlled by the `PICOND` keyword.

Recommendations

- Understand the difference between the models
- **What happened in your field?**
- **What happened in other fields with similar situations?**
- Create 1-D grids to evaluate effect of models on your near well flow
- **Compare fine and coarse grid results in 1-D**
- Permeability and PVT (condensate richness) will be important

- **Use the GPP model for cases with low gas velocity**
- **Use the GPP model with coarse grid only**
- **Be careful with GPP model for high and low permeability cases**
- **Use Non-Darcy (Forcheimer) model do increase pressure drop at high gas velocities**

- **For average 3-D field case**
  - **Use coarse grid and GPP if condensate blockage is dominant (low velocities)**
  - **Use VDRP and Forcheimer in fine grid (LGR near well) if velocities are high**
  - **If your simulations have stability problems at high velocities turn GPP off**

30. Multi-Phase Flash

- There are several situations where there are more than 2 hydrocarbon phases
- For a flash to detect all the phases present a special Multi-Phase Flash (MFLASH) is available

Multi-Phase systems appear when

- Wax or Asphaltenes are present in the oil
- Have high CO2 concentration at low temperatures

- We will look at both systems

Asphaltenes

The simulator can be used to predict when asphaltene precipitation first occurs. At the end of each time step a multi-phase flash is performed to determine whether a stable asphaltene phase exists. The multi-phase flash first determines whether one or more liquid phases are stable. A liquid phase is then identified as an asphaltene phase if:

the heaviest hydrocarbon is an aromatic (see the `HYDRO` keyword), and

the heaviest hydrocarbon represents more than a third[52] of the phase (by weight).

The saturation, density and molar density of the asphaltene phase are stored in the simulator as solid properties.

- **ECLIPSE 300 predicts when asphaltene precipitation first occurs.**

---

[52] The factor of a third is chosen to make sure that we correctly identify the heaviest phase. Suppose the flash says there are 4 stable phases and gives us the component splits for each phase. The flash has to decide which component split is oil, gas, wax and asphaltene. Light components identify a gas, heavy components an oil, if there are a lot of paraffins then it is wax, and if there is a lot of heavy aromatic then it is asphaltene.

- **At the end of each timestep, determines if we can have more than one liquid phase.**
- **If so, then assumes it is asphaltene if the heaviest component is aromatic (keyword HYDRO) and is more than 1/3 of the phase.**

At present the asphaltene phase is ignored in the flow calculations, so this model should only be used as an indicator of whether asphaltene precipitation occurs in the reservoir.

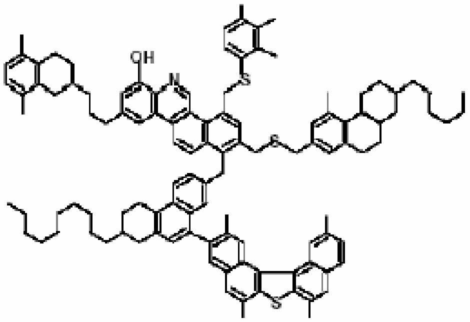
Asphaltene prediction is carried out in compositional runs using an Equation of State, if the `SOLID` keyword is used, and if the heaviest hydrocarbon is an aromatic (see the `HYDRO` keyword).

- Heavy oil components can be subdivided into
- Paraffin components
- Naphthalene components, and
- Aromatic components
- These PNA[53] components under certain conditions will form Wax and Asphaltene phases

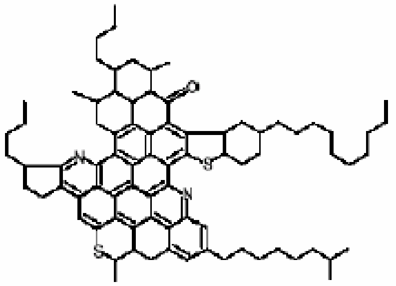
According to Seight (1992), Cimino *et al* (1995) the asphaltenes molecules look like:

---

[53] An alternative classification is the four fractions SARA. Amongst the four SARA fractions, only the Saturates are distinguishable from the others as a chemical class. The Aromatics, Resins and Asphaltenes constitute a compositional continuum with respect to molar mass and polarity. The ratio of resins to asphaltenes is more important than the absolute asphaltene content in controlling asphaltene precipitation.



(a)

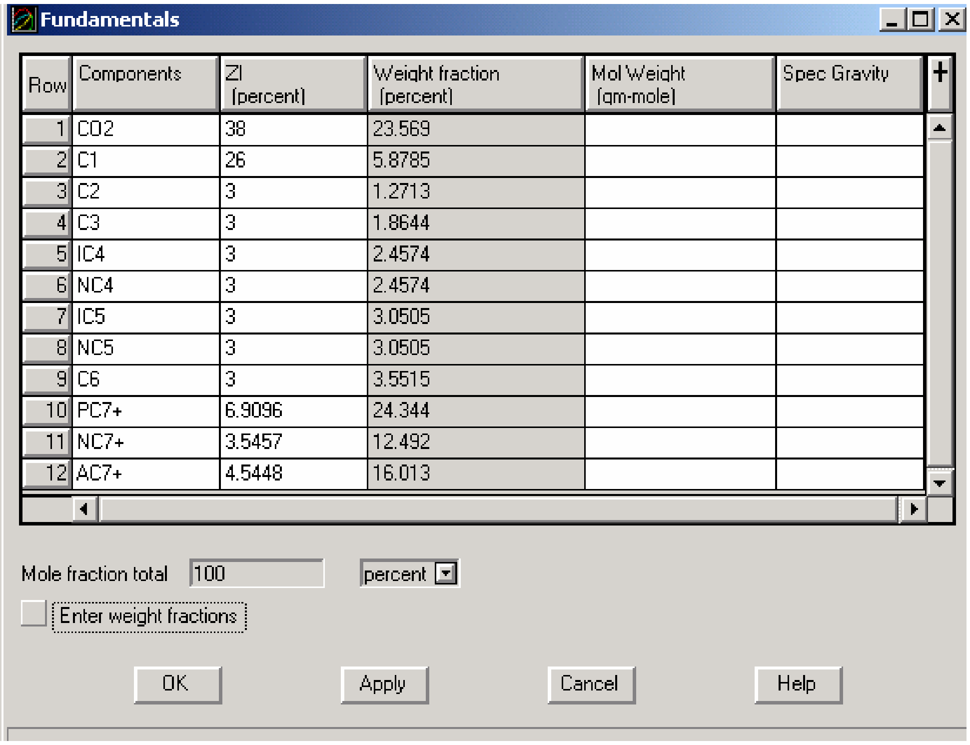


(b)

Asphaltene deposition causes different problems to different people:

- Reservoir engineer
  - Formation damage and in-situ plugging
- Production engineer,
  - Near well formation damage and production engineer, near well formation damage and subsurface and surface equipment plugging and malfunctions;
- Refining engineer,
  - Distillation column and equipment pluggage and tankage capacity loss, as well as catalyst deactivation
- Transportation engineer,
  - Pipeline pluggage and capacity loss; and finally, for the
- For the asphalt production specialist,
  - blending and asphalt quality headaches

The detailed properties of the different phases can be obtained from PVTi by performing a multiphase flash (MFLASH).



Row	Components	ZI (percent)	Weight fraction (percent)	Mol Weight (gm-mole)	Spec Gravity
1	CO2	38	23.569		
2	C1	26	5.8785		
3	C2	3	1.2713		
4	C3	3	1.8644		
5	IC4	3	2.4574		
6	NC4	3	2.4574		
7	IC5	3	3.0505		
8	NC5	3	3.0505		
9	C6	3	3.5515		
10	PC7+	6.9096	24.344		
11	NC7+	3.5457	12.492		
12	AC7+	4.5448	16.013		

Mole fraction total: 100 percent

☐ Enter weight fractions

When we characterize the plus component, we can define this plus component in PVTi as being made up of different percentages of Paraffin, Naphthalene, and Aromatic (PNA) components if this PNA split is available in the PVT laboratory report. A flash of this fluid in PVTi can predict more than the usual two hydrocarbon phases.

```
Expt MFLASH4  :  Multiphase Flash Calculation


 Peng-Robinson       (3-Parm)  on ZI      with PR corr.
 Lohrenz-Bray-Clark Viscosity Correlation


 4 phase state


 Specified temperature  Deg F        50.0000
 Specified pressure    PSIA       1000.0000


 ------------------------------------------------------------------
                     Fluid properties
 ------------------------------------------------------------------
```

```
Property            Liquid      Wax         Asp. Liq.   Vapor
------------------  ----------  ----------  ----------  ----------
Phase fraction      0.67759     0.07475     0.08841     0.15926
Mole Weight         49.25286    250.00000   162.15558   28.63906
Z-factor            0.23006     1.17974     0.67757     0.66993
Viscosity           0.09988     0.09204     0.26461     0.01577
Density LB/FT3      39.14254    38.74467    43.75600    7.81608
Molar Vol LB/FT3    1.25829     6.45250     3.70590     3.66412
-------------------------------------------------------------------
```

Using Asphaltenes

- Use SOLID in RUNSPEC
- Solid saturation can be plotted with SSOLID

Example of Asphaltene deposition

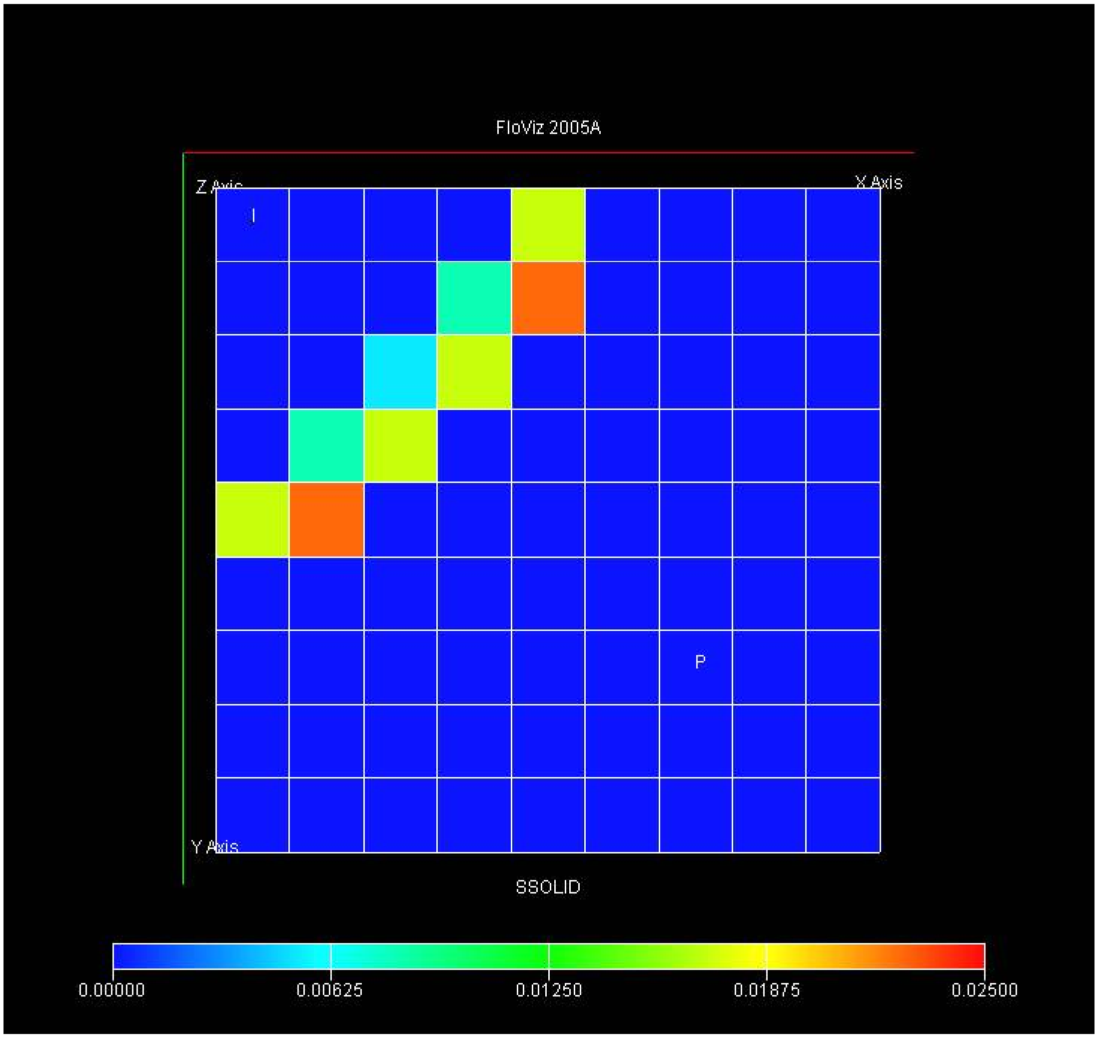
- **Copy CASE1.DATA to CASE1ASP.DATA**
- **Add MULTIPHASE in RUNSPEC**
- **In PROPS, component C7+3 is defined as Asphaltene:**

```
HYDRO
   N N H H H H H H A   /
```

- **In SCHEDULE, ask for solid output as well as oil and gas**

```
RPTRST
   SOIL SGAS SSOLID   /
```

The SSOLID display below shows those grid blocks where asphaltenes precipitation would occur at a certain timesteps.



CO2 Rich Systems

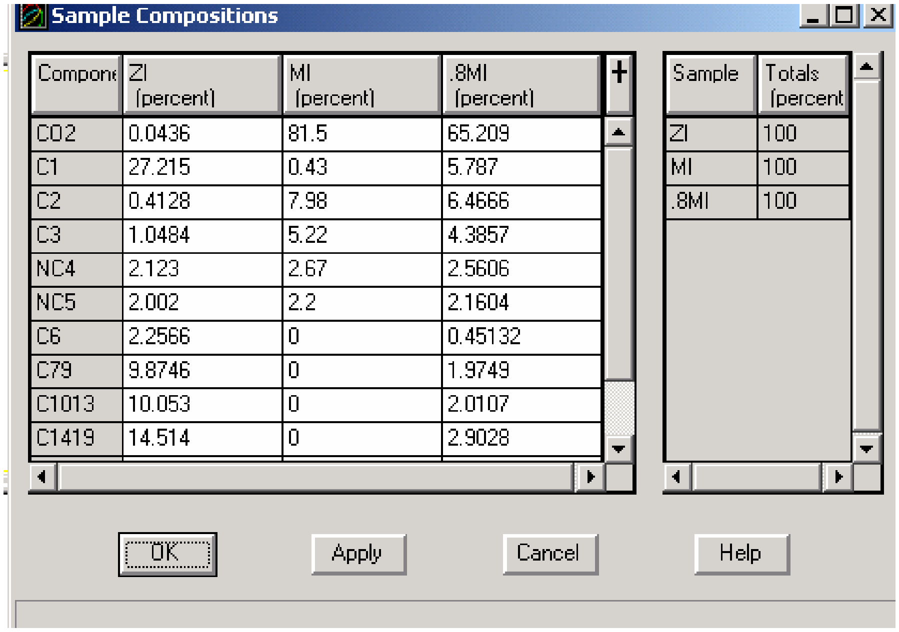
As we have already seen, injecting CO2 into a suitable oil can lead to miscibility and increased recovery. There are however some possible disadvantages in injecting CO2. The presence of CO2 can for instance encourage the formation of asphaltenes.

Another disadvantage is that high concentrations of CO2 can lead to the formation of two hydrocarbon fluid phases. Although ECLIPSE 300 uses the same flash package as PVTi, the current version of the simulator does not model the flow of two liquid phases, so you should use PVTi to predict whether your fluid mixture can form two hydrocarbon fluid phases.

- Fluid mixtures of oil and CO2 can exhibit multi-phases at low temperatures
- The MFLASH in PVTi can determine the phases present – this flash calculation is accurate but very slow in terms of CPU time
- BUT ECLIPSE 300 does a 2-phase flash – which is very fast.
- Difficulties can arise when there are 3 hydrocarbon phases present
- We (may) have seen this in the slim tube displacements when CO2 is injected at low temperatures and pressures

Example:

- SPE 71485 “Three- and Four Phase Flow Compositional Simulations of CO2/NGL EOR”
- Gives fluid compositions and a multi-phase diagram
- We can put these compositions into PVTi and see MFLASH results



Compone	ZI (percent)	MI (percent)	.8MI (percent)
CO2	0.0436	81.5	65.209
C1	27.215	0.43	5.787
C2	0.4128	7.98	6.4666
C3	1.0484	5.22	4.3857
NC4	2.123	2.67	2.5606
NC5	2.002	2.2	2.1604
C6	2.2566	0	0.45132
C79	9.8746	0	1.9749
C1013	10.053	0	2.0107
C1419	14.514	0	2.9028

Sample	Totals (percent
ZI	100
MI	100
.8MI	100

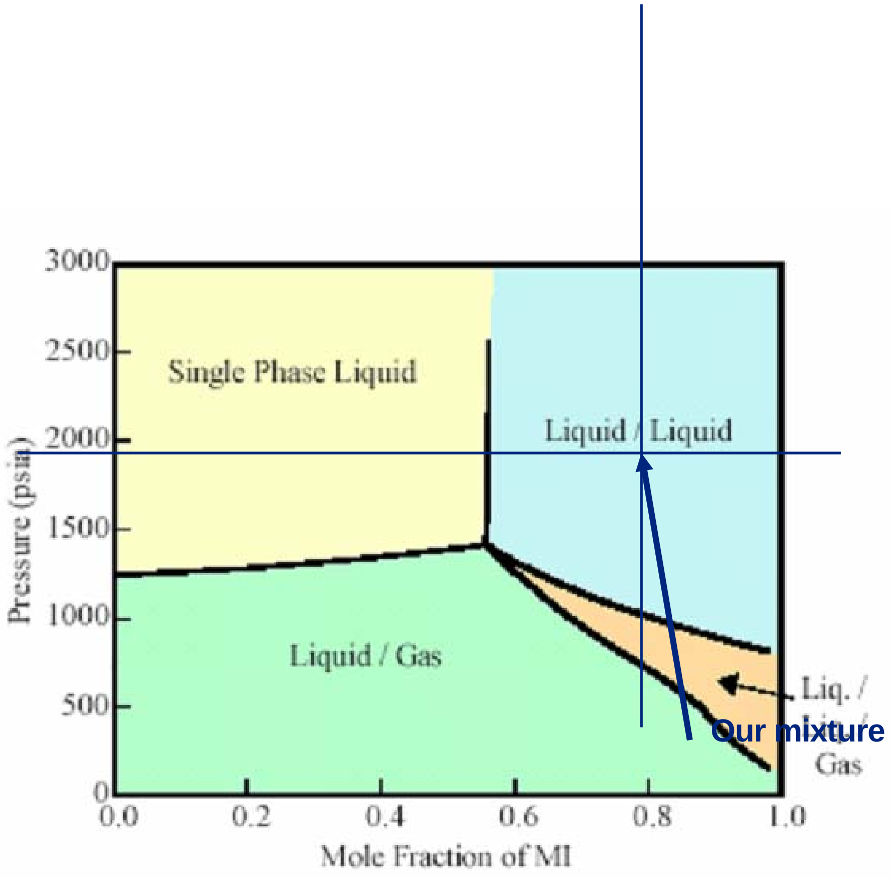
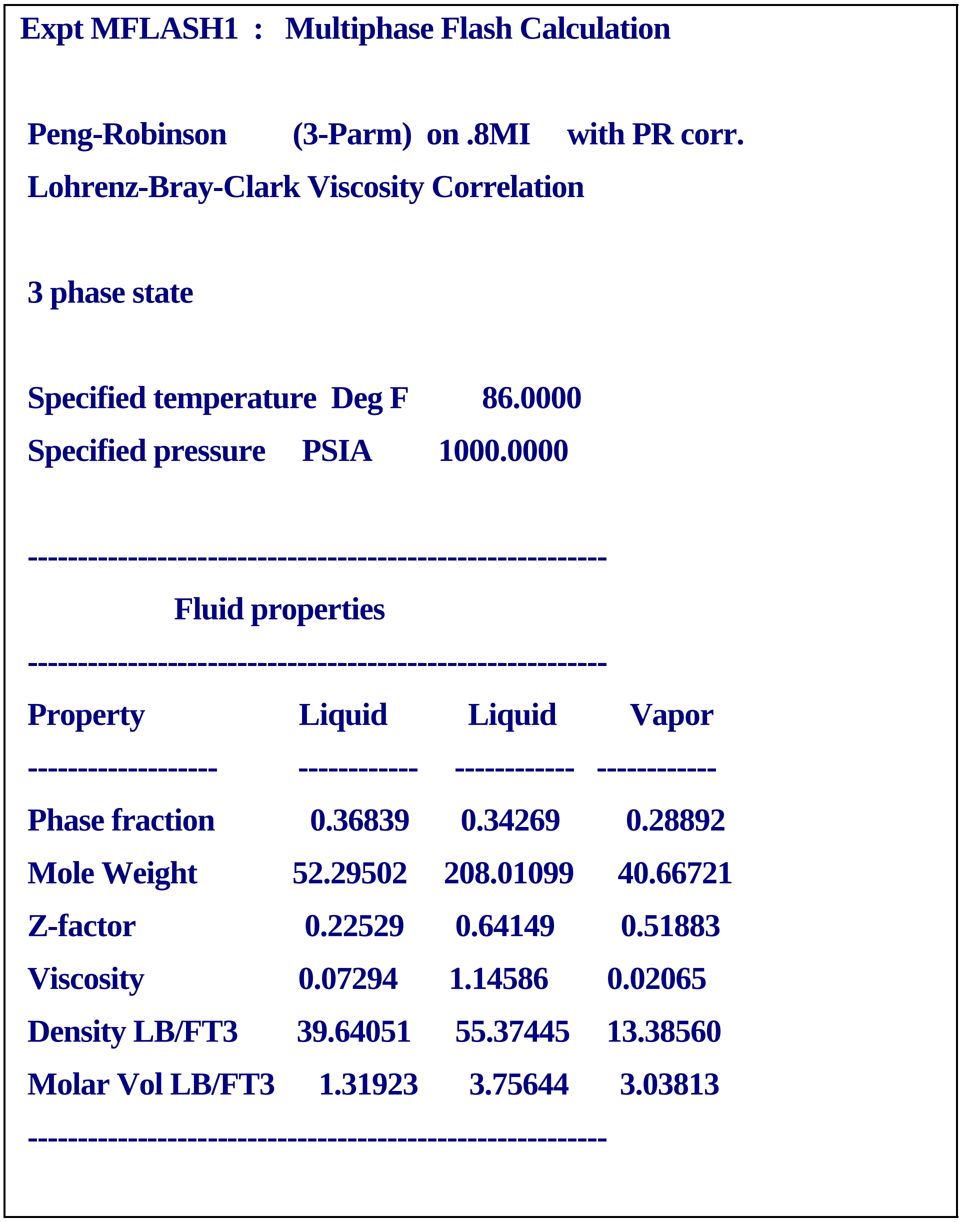


Fig. 1—Phase diagram for Schrader Bluff fluids.

The results of the multiple flash in PVTi shows the presence of two hydrocarbon liquid phases, in other words of two oils, one light and one heavy



```
Expt MFLASH1  :   Multiphase Flash Calculation


 Peng-Robinson        (3-Parm)  on .8MI     with PR corr.
 Lohrenz-Bray-Clark Viscosity Correlation


 3 phase state


 Specified temperature  Deg F         86.0000
 Specified pressure     PSIA        1000.0000


 -------------------------------------------------------
                 Fluid properties
 -------------------------------------------------------
 Property              Liquid        Liquid       Vapor
 ------------------    ------------  ------------ ------------
 Phase fraction          0.36839      0.34269       0.28892
 Mole Weight           52.29502    208.01099     40.66721
 Z-factor                0.22529      0.64149       0.51883
 Viscosity              0.07294     1.14586      0.02065
 Density LB/FT3         39.64051     55.37445    13.38560
 Molar Vol LB/FT3       1.31923      3.75644      3.03813
 -------------------------------------------------------
```

Using Multi-Phase

The `SOLID` keyword must be used in the `RUNSPEC` section if multi-phase components are present.

The `HYDRO` keyword in the `PROPS` section defines multi-phase components.

You can output solid saturations with `SSOL` and display them in the same way as (for instance) oil saturation with `SOIL`.

31. Solids

Solid components can be used with the Black-Oil, Equation of State (EoS), K-value, or Thermal options. Within the reservoir, these components remain in the solid phase throughout the simulation. However, solid components can be converted to fluid components through a chemical reaction. A solid component could be used, for example, to simulate production and take up of coke during combustion.

Solid components can be used in ECLIPSE 300 in black-oil compositional or thermal mode.

- **Within the reservoir, solids remain in the solid phase during the simulation UNLESS they are converted during a chemical reaction.**

Solids are either:

- **Suspended in the oil phase, and move with the oil, or**
- **adsorped onto the rock, reducing the pore volume available for flow**

Solids can be either suspended in the oil phase, or adsorbed on to the formation. Adsorption isotherms can be defined which determine the fraction of solids in suspension.

Suspended solids are transported with the flow.

Solids that adsorb to the formation reduce the pore volume available for flow. Permeability multipliers can be used to model this effect.

- The CVTYPE keyword is used to specify solid components.
- Properties for solid-only components are defined using special keywords
- The solid components are ignored by the flash. They are not part of either the liquid (oil) or the vapour (gas) phases.

The `SOLID` keyword must be used if solid components are present.

The `CVTYPE` keyword can be used to specify solid phase components. The `CVTYPES` keyword can be used to specify solid phase components at surface conditions.

These solid components are ignored by the flash - they cannot enter the liquid or gas phase. The only way they can change is through a chemical reaction, when they can become a different component.

Asphaltenes are a special type of solid and have been discussed in the previous section.

Using Solids

- Use SOLID in RUNSPEC
- CVTYPE defines solid-phase components
- SOLIDADS is the solid adsorption table
- SMF is the initial solid mole fraction
- Solid saturation can be a with SSOLID

32. Aziz's Ten Golden Rules

From Professor Khalid Aziz, Stanford University – "Ten Golden Rules for Simulation Engineers", *JPT* – November 1989, 1157

1. Understand Your Problem and Define Your Objectives

Before you do any simulation:

- Understand characteristics of reservoir
- Understand fluids
- Objective of study clearly stated on paper
- Ask yourself if the objective are realistic

2. Keep it Simple

Start and end with simplest model

Consistent with

- the nature of the reservoir
- Objective of study
- Availability of data

Most sophisticated model available – may not serve your needs

Understand model limitations and capabilities

3. Understand Interaction Between Different Parts

Reservoir not an isolated entity

Connected to

- Aquifers
- Surface facilities

Separation into different components

- may be inappropriate – neglects interactions
- when appropriate – can lead to substantial savings

4. Don't Assume Bigger is Always Better

- Always question size of a study that is limited by the computer resources and/or budget
- Greater number of blocks and components do not automatically translate into greater accuracy and reliability (reverse sometimes true)

5. Know Your Limitations and Trust Your Judgments

- Remember simulation is not an exact science – more of an art
- Trust your judgment – based on analysis of the field or lab observations
- Do simple material balance to check simulation results

6. Be Reasonable in Your Expectations

- Don't try to get from the simulator what it is incapable of producing
- Remember – if you exclude a mechanism during model development – cannot study its effect with that model

7. Question Data Adjustments for History Matching

- Remember HM process does not have a unique solution
- A good HM with inappropriate adjustments to the data will lead to poor predictions
- Pay close attention to physical and geological reasonableness

8. Don't Smooth Extremes

- Pay attention to extremes in permeability (barriers and channels)
- Be careful in the process of averaging
- Never average out extremes

9. Pay Attention to the Measurement and Use Scales

Measurement values at the core scale may not directly apply at larger block scale – do influence values at other scales

- Permeability may be a scalar at some small scale – and a tensor at larger scale
- Dispersive terms in our equations are a result of process of averaging

10. Don't Skimp on Necessary Laboratory Work

Models do not replace lab experiments

- designed to understand the nature of the process
- Or measure essential parameters of the equations being solved

Plan lab work with its end use in mind

Appendix 1: Flash exercise

Z1=0.8, Z2=0.3, Z3=0.1

K1=11, K2=1, K3=0.1

$$g(V)=\sum_{i=1}^{nc}\frac{z_i\left(K_i-1\right)}{1+V\left(K_i-1\right)}=0$$

How many phases?

What is V? L? xi, yi?

Solution:

$$g(V)=\frac{Z_1\left(K_1-1\right)}{1+V\left(K_1-1\right)}+\frac{Z_2\left(K_2-1\right)}{1+V(K_2-1)}+\frac{Z_3(K_3-1)}{1+V\left(K_3-1\right)}=0$$

$$\frac{0.8(11-1)}{1+V(11-1)}+\frac{0.1(1-1)}{1+V(1-1)}+\frac{0.1(0.1-1)}{1+V(0.1-1)}=0$$

$$g(V)=\frac{8}{1+10V}+\frac{-0.09}{1-0.9V}$$

Step 1 - Check to see if Case 1 (root in [0,1])

or Case 2 (root <0) {no need to solve for V here}

or Case 3 (root > 1) - {no need to solve for V here}

$$g(V)=\frac{8}{1+10V}+\frac{-0.09}{1-0.9V}$$

$$g(0)=\frac{8}{1}-\frac{0.09}{1}=7.91$$

$$\mathrm{g}(1)=\frac{8}{1+10}-\frac{0.09}{1(-0.09)}=\frac{8}{11}-\frac{0.09}{0.1}=0.72727-0.9=-0.17273$$

So g(0) > 0 and g(1) < 1, and so we know there is a solution for V between 0 .and 1

$$g(V)=\frac{8}{1+10V}-\frac{0.09}{1-0.9V}=0$$

$$\frac{8}{1+10V}=\frac{0.09}{1-0.9V}$$

$$8(1-0.9V)=(1+10V)0.09$$

$$8-7.2V=0.09+0.9V$$

$$7.91=8.1V$$

So we can solve for V and then for L:

$$V = \frac{7.91}{8.1} = 0.97654 \quad 97.65\% \text{ vapor}$$

$$L = 1 - V = 0.02346 \quad 2.34\% \text{ Liquid}$$

We now develop equations for xi and yi

$$(1 - V)x_i + Vy_i = Z_i$$

$$also \quad K_i = \frac{y_i}{x_i}$$

$$therefore \qquad x_i = \frac{Z_i}{1 + V(K_i - 1)}$$

$$and \quad y_i = \frac{K_i Z_i}{1 + V(K_i - 1)}$$

then solve for C1, C3, and C10 mole fractions in the liquid and vapor.

$$for \ C_1 : x_1 = \frac{0.8}{1 + 0.9765(10)} = 0.0743$$

$$y_1 = \frac{11(0.8)}{1 + 0.9765(10)} = 0.817$$

$$for \ C_3 : x_2 = \frac{0.1}{1 + 0.9765(1 - 1)} = 0.1$$

$$y_2 = K_1 x_1 = 1(0.1) = 0.1$$

$$C_{10}: x_3 = 1 - x_1 - x_2 = 1 - 0.743 - 0.1 = 0.823$$

$$y_3 = 1 - y_1 - y_2 = 1 - 0.817 - 0.1 = 0.083$$

Glossary of Terms

Acentric Factors

The Acentric factor of a given component is a log function of the component liquid pressure at a reduced temperature of 0.7:

$$\omega = -\log_{10} P_{vp} - 1$$

Originally formulated by Pitzer (*J. Am. Chem. Soc*., **77**, p.3427, 1955) it is a measure of the non-sphericity of the component molecule, and hence an indicator of the degree of non-ideal behaviour to be expected from the component.

Alani-Kennedy Correlation

Correlation used to predict the density of hydrocarbon liquids.

Amagat’s Law

The partial volume of a gas in a mixture of gases is defined as that volume which the gas would occupy if it alone were present at the same temperature and pressure as the mixture of the gases. (For an ideal gas this follows directly from Dalton’s Law of partial pressures).

Aliphatic

Aliphatic organic compounds are based on paraffin hydrocarbons, and include compounds such as ethylene and acetylene (and related compounds) that have multiple carbon bonds. Excluded from this definition are all cyclic compounds based on the benzene ring.

API Gravity

Liquid density measurement-degrees API.

`EQ. 1`

$$\gamma = \frac{141.5}{(API + 131.5)}$$

Aromatic

Aromatic organic compounds are based on, or contain, at least one benzene ring.

Avagadro's Hypothesis

Equal volumes of gas at the same conditions of temperature and pressure contain the same number of molecules.

BIP

Binary Interaction Parameter. Sometimes referred to as Binary interaction Coefficient (BIC). Physically, they can be interpreted as describing any polar (electrical) forces between molecules.

Boyle's Law

For a fixed mass of gas at constant temperature, the product of its pressure and volume is a constant. (i.e. pV = constant, and therefore a plot of p vs. 1/V will be a straight line).

Btu

British thermal unit. The quantity of heat required to raise the temperature of pound of water by one Fahrenheit degree. Btu/SCF is the common field unit for the calorific value of hydrocarbon gases.

Carr, Kobayashi and Burrows

Co-authors of a correlation for the calculation of gas viscosity.

CCE

Constant Composition Expansion. Along with the constant volume depletion, the (CVD) forms the two most informative experiments performed on gas-Condensates. Expansion proceeds in stages, from above the saturation pressure, without any of the PVT cell contents being drawn off. The absolute volume occupied by the fluid and the proportion of condensed liquid are measured.

Charles' Law

For a fixed mass of gas at constant pressure, its volume is directly proportional to the absolute temperature.

Clausius Clapeyron Equation

An equation which relates the vapour pressure of a component to the latent heat of vaporization, and the ratio of absolute temperature to the component's normal boiling point.

Convergence Pressure

The pressure at which the K-values of components in a binary mixture become unity. At the critical temperature, this is equivalent to the critical pressure.

Condensate

Liquid hydrocarbons recovered from a gaseous well stream by simple separation.

Corresponding States: The Law of

Systems are in corresponding states if two of their reduced variables are equal.

Critical Point

The point at which the intensive properties of the liquid and vapour in a system become equal

Critical Pressure

The pressure prevailing at the critical point.

Critical Temperature

The temperature prevailing at the critical point. Above this temperature liquefaction cannot occur by isothermal compression.

Critical Volume

The volume occupied by one mole of substance at its critical point.

CVD

Constant Volume Depletion. One of the most important laboratory experiments performed on gas-Condensates and volatile oil systems.

Dalton’s Law of Partial Pressures

The partial pressure of a gas in a mixture of gases is defined as that pressure which the gas would exert if it alone were present at the same temperature and pressure as the mixture of the gases.

Dew Point

The pressure at which a liquid phase first appears during the isothermal decompression of a vapour.

Enthalpy

A thermodynamic energy term.

Entropy

The entropy of a system relates the heat content of the system to its absolute temperature.

Equilibrium

A system can be considered to be in equilibrium with its surrounding when the net transfers of mass and energy between them have ceased.

Extensive Properties

Extensive properties of a system are those properties whose value is dependent on the amount of substance in the system, e.g. Heat content, volume internal energy.

Fugacity

A real gas function analogous to pressure in an ideal gas.

GC

Gas Chromatography

Gibbs Free Energy

Thermodynamic energy.

GPM

Gallons per Thousand (M). An expression usually applied to Propane, Butanes and Pentanes to quantify the expected yields of these intermediate components from a given process and gas stream. The gallons are U.S. gallons and the thousands refer to thousands of standard cubic feet of gas. Coefficients for calculating GPM values for gas mixtures are included.

Graham's Law

The rate at which a gas diffuses through a porous partition is inversely proportional to square root of the gas density.

Helmholtz Free Energy

Thermodynamic energy function.

Hoffman Crump Hocott Analysis

A graphical method for checking the validity of reported separator gas and oil compositions, by computing the implied equilibrium constants (K-values) and the relationship to the measured separator conditions.

Ideal Gas

A gas that obeys the ideal gas laws, and therefore fulfils the conditions implied by these laws. (i.e. the molecules of the gas are vanishingly small, and there are no intermolecular forces). However many real gases do behave ideally over certain limited ranges of conditions.

Intensive Properties

Intensive properties are those properties of a system that are independent of the quantity of substance(s) in the system, e.g. specific heat, viscosity, refractive index, density.

Isothermal

An isothermal process takes place at constant temperature.

Isobaric

Isobaric processes occur under conditions of constant pressure.

Isentropic

Describes a process or system change that takes place at constant entropy.

Isenthalpic

Describes a process or system change that takes place at constant enthalpy.

Kay's Mixing Rule

For certain purposes, a mixture of gases can be considered as a single gas having properties which are the sum of the mole fraction weighted properties of the individual gas components. The most common application of this rule is the computation of pseudo-reduced temperatures and pressures for a gas mixture in order to calculate Z-factors: i.e.

$$T_{pr} = \sum_{i=1}^{N} zi \frac{T}{T_{ci}}$$

Latent Heat

The heat transfer accompanying a change of state at constant pressure.

Le Chatelier's Principle

When a system in equilibrium is subjected to a perturbation or change, it will react in such a way as to minimize the effects of the change.

MCN

Multiple Carbon Number. Multiple carbon number groups are groupings of hydrocarbon components that are considered as one substance for equation of state matching purposes.

Mole

A mass of substance (pure component or mixture) equal to its molecular weight in pounds, grams, kilograms, or any other pre-specified mass units. For example the mole weight of ethane 30.068. A pound mole is therefore 30.068 pounds of ethane; a gram mole would be 30.068 grams.

Natural Gas Liquids (NGLs)

Liquids obtained from a gas stream by processes other than simple separation, (i.e. significant chilling accomplished either by refrigeration or via the use of a turbo expander).

Normal Conditions

Alternative reference conditions for gas measurements, usually with metric systems of measurement, e.g. Nm^3 (normal cubic meters). The conditions are: Temperature 0°C, Pressure 1.01325 Bar.

PNA

Paraffins, Naphthenes and Aromatics.

Phase

A phase is a system, or part of a system, which is homogeneous and has definite boundaries.

Phase Rule

The number of intensive degrees of freedom available to system is limited by the number of components and the number of phases comprising the system. Mathematically $F+P=C+2$, where F is the number of degrees of freedom, P the number of phases, and C the number of components. (e.g. water and water vapour forming a system: there are two phases but only one component, and therefore one degree of freedom exist. Only one intensive property can be varied independently, hence varying pressure will fix the temperature and vice-versa. This is consistent with the fact that the vapour-liquid equilibrium of a pure component is defined by a line on the phase diagram.

Reduced Pressure

Prevailing gas pressure expressed as a multiple of the critical pressure of the gas. (Used only for pure components. For gas mixtures it is the pseudo-reduced pressure).

Reduced Temperature

As above, but referred to critical temperature.

Reid Vapour Pressure

Vapour pressure of liquid products, usually used in a transportation/shipping context. Liquids with a Reid vapour pressure above atmospheric will need to be transported under pressure (e.g. by pipeline).

SCN

Single Carbon Number. Grouping of components which, if all paraffins, would have the same number of carbon atoms, and hence all the isomers of the same formula. However, the criterion for inclusion within a given group is normally that the component in question has a normal boiling point within the range defined by the paraffins having that carbon number. In this way, non-paraffins will often be included in SCN groups to which they do not strictly (e.g. Benzene will be included in the C_7 group, despite having only 6 carbon atoms).

Standing Chart

Chart of Z-factor vs. pseudo-reduced pressure, for a range of values of pseudo-reduced temperature. (After M. B. Standing, 1942).

TBP

True Boiling Point

Vapour

A gas below its critical temperature.

VLE

Vapour Liquid Equilibrium.

Watson Characterization Factor

The cube root of the average normal boiling point of a liquid hydrocarbon mixture divided by its specific gravity at 60°F. It is often denoted at K (not to be confused with equilibrium K-factors) and is a measure of the aromaticity of the mixture. Highly paraffinic mixtures will have a value approaching 13, whereas highly aromatic mixtures will have a characterization factor of 10.

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