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## Field-wide Equation of State Model Development

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### Abstract

The objective of this paper is to present a detailed workflow for developing a field-wide (or basin-wide) “common” equation of state (EOS) model to describe PVT properties<sup>1</sup> of all reservoir fluids and wellstream mixtures at all relevant conditions of pressure and temperature. The presented workflow is a result of having developed many field-wide EOS models in conventional reservoirs around the world, and more recently several basin-wide EOS models for North American unconventional (Eagle Ford, Montney, Bakken, Permian and Scoop/Stack). We address several important considerations in developing a common EOS, as well as when and why a common EOS is needed.

The starting point for developing a common EOS is the use of all measured PVT properties and fluid compositions of surface and reservoir samples. The goal of a common EOS is to provide accurate PVT property estimation of all mixtures found throughout the field/basin – within all reservoir(s), throughout the production system and to final surface products – from discovery to abandonment.

Measured PVT data must be scrutinized for quality using a series of consistency checks that include component and phase material balances, cross plots, and continual comparison with EOS results. Using all PVT data from all samples gives a substantial, statistically significant data set that allows trend analysis and outlier identification.

One key to developing a common EOS model is using a sufficient number of components, and proper characterization of heavy fractions that contain varying proportions of the three hydrocarbon groups (paraffin, naphthene and aromatic compounds – PNA). The heavy fractions single carbon numbers  $C_7$ ,  $C_8$ ,  $C_9$ ... and the remaining “residue”, e.g.  $C_{36+}$  are often given average properties that reflect the relative proportions of PNA compounds – i.e. *relative paraffinicity* (or *relative aromaticity*). The determination

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<sup>1</sup> In this paper we use the term “EOS model” or simply “EOS” to represent a model that predicts phase equilibrium and volumetric behavior. A separate, compositionally-consistent viscosity model is needed in reservoir simulation because near-critical conditions may exist where phase consistency is important. Pipe flow and process calculations often exist far from critical conditions and can, therefore, use independent phase-specific correlations for viscosity (and density) that are more accurate over a wide range of pressures and temperatures.

of single carbon number (SCN) and residue properties is what we refer to as heptanes-plus characterization, and it is this characterization that will differ from field to field, or basin to basin.

Sometimes within a given field or basin, the relative paraffinicity may vary so much that a single, common EOS using SCN description is not possible. Two options remain: developing multiple EOS models, or creating a single EOS with some/all heavy fractions having two subfractions – *paraffinic* and *aromatic* (e.g.  $C_{7P}$  and  $C_{7A}$ ,  $C_{36+P}$  and  $C_{36+A}$ ). In this latter approach, the P-A split must be *estimated*, *correlated* or *measured* for each fluid mixture, making the approach complicated and less common, but necessary in some fluid systems<sup>2</sup>.

Developing a common EOS for a field/basin is necessary because in-situ reservoir fluids may vary spatially, change in composition during depletion and gas injection, and because of fluid mixing throughout the production system – within reservoirs, wells, and topside facilities.

For unconventional basins, only a small number of the thousands of wells have laboratory PVT data available, despite significant well-to-well fluid variations – e.g. gas oil ratio (GOR) ranging from 300 to 300,000 scf/STB in the Eagle Ford and Montney basins. Simple PVT correlations are not applicable over the entire range of fluid compositions. Many wells produce complex retrograde condensates, near-critical fluids, and volatile oils that require an accurate and consistent EOS model for estimating PVT properties required by geologic, engineering, and marketing professionals.

## Introduction

A field-wide EOS<sup>3</sup> is a single EOS that accurately describes the PVT behavior of a wide range of fluid samples, with each sample described by a unique composition. A field-wide EOS is tuned to 10s-100s of PVT samples, and many thousands of PVT data. The methodologies presented in this paper are a result of experience from developing several recent fluid characterization studies in unconventional basins (e.g. Eagle Ford, Montney, Bakken, Permian and SCOOP/STACK), and many field-wide EOS fluid characterizations for conventional reservoirs the past 30 years. **Table 1** gives some of our multi-sample, field-wide and basin-wide EOS model development studies.

## PVT Sample Selection

A robust and accurate field-wide EOS should accurately predict PVT properties & phase behavior for a wide range of fluids with highly varying compositions, and for a relevant range of pressures and temperatures. The following are important considerations:

- Collect and use a large number of fluid samples with PVT data/reports
- Collect and use all production-well samples (surface separator and wireline bottomhole)
- Collect openhole formation testing samples, particularly for fluid initialization/mapping<sup>4</sup>
- Understand differences in methods, equipment and procedures used by commercial PVT laboratories
- Collect samples throughout the reservoir, vertically and laterally

<sup>2</sup> Two examples include (1) vertical compositional gradients showing significant API variation with depth (Schulte 1980) and a saturated gas-oil contact with relatively paraffinic gas cap and relatively aromatic oil zone.

<sup>3</sup> Also called *common EOS*, *multi-sample EOS*, *regional EOS* and *basin-wide EOS*.

<sup>4</sup> Oil-based mud (OBM) contaminated openhole formation test samples in conventional reservoirs are readily decontaminated to yield a good depth-specific composition that can be used in mapping in-situ fluid variations.

- Conduct a wide range of relevant PVT tests – depletion, gas-EOR and crude distillation<sup>5</sup>
- Covering the entire range of known or expected *in situ* gas-oil ratio (GOR) range
- Utilize equilibrium contact samples, when available (Fevang and Whitson 1994)

We define samples into two categories: (1) *Reservoir Representative* and (2) *In-Situ Representative*. A reservoir representative sample is *any* sample collected anywhere in the production system (downhole or surface) with the one constraint that it should not contain significant amounts of temporary, non-reservoir fluids like oil-based mud (OBM). A stock-tank oil (STO) sample is an inexpensive sample that is reservoir representative because it is derived from the reservoir fluids that produced into the well. The EOS is expected to describe the PVT properties of the STO from its composition. Consequently, measured PVT data on a simple STO sample can and should be used in building the EOS model.

Slightly more expensive to collect, but readily available from any well at any time, are separator gas (SPG) and separator oil (SPO) samples. These two samples, taken individually, are reservoir representative because they also are derived from the reservoir fluids that produced into the well. The EOS should be able to predict the separator phase properties (e.g. density and saturation pressure) from separator phase compositions. Consequently, measured PVT data on the separator samples can and should be used in building the EOS model.

A recombined wellstream based on the separator oil and gas samples – recombined at *any* GOR – would also be considered reservoir representative. Again, because the well will produce similar separator samples over a wide range of GORs during depletion. The EOS should be able to predict the PVT properties (e.g. saturation pressure, phase densities, relative volumes and viscosities) of the wellstream at reservoir conditions, in the wellbore, within the tubing, in the separator, and for final products at standard conditions. Consequently, measured PVT data on any recombined wellstream can and should be used in building the EOS model.

Consider a bottomhole sample (BHS) that is later determined to have been collected while the well was coning gas<sup>6</sup>, resulting in an arbitrary mixture of in-situ reservoir gas and in-situ reservoir oil with a GOR that lies somewhere between the solution GOR ( $R_s$ ) of the in-situ reservoir oil and the solution GOR ( $1/r_s$ ) of the in-situ reservoir gas. The BHS does not, as a mixture, represent the in-situ reservoir gas, nor the in-situ reservoir oil. Instead, some arbitrary mixture of the two in-situ reservoir fluids have been collected. The EOS is expected to predict the PVT properties of the coning mixture, and for a wide range of such GOR wellstreams produced in gas-coning wells. Measured PVT data on the samples from coning wells<sup>7</sup> can and should be used in building the EOS model.

Other samples that would normally be considered “*in-situ*” representative can be collected with openhole formation test (OFT) tools, and during DST production tests (e.g. from a limited production interval) with low drawdowns. The compositions from these samples are perhaps the most important

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<sup>5</sup> *Depletion*: CCE (constant composition expansion), CVD (constant volume depletion) or DLE (differential liberation expansion), and multi-stage separator tests | *Gas Injection*: swelling, forward and backward multi-contact, and slintube | *Distillation*: e.g. SCN ASTM D2892.

<sup>6</sup> The sample could just as well have been a separator-recombined wellstream collected during coning.

<sup>7</sup> It has been shown (Fevang and Whitson 1994) that a sample collected during gas coning can provide excellent estimates of the true in-situ reservoir gas and in-situ reservoir oil for an in-situ saturated gas-oil fluid system. This is achieved simply by equilibrating the total sample mixture at initial reservoir conditions based on the equilibrium *contact mixing* (ECM) method. Such a seemingly “bad” sample taken in a coning well creates the opportunity to measure a substantial amount of PVT data for the two in-situ reservoir phases separately, including in-situ compositions of reservoir gas and reservoir oil. These in-situ samples and their PVT data can and should be used in EOS model building – together with all other PVT data collected on reservoir-representative samples.

data for defining in-situ fluid distributions (“fluid initialization”). OFT samples with OBM contamination can often yield accurate estimates of in-situ fluid composition, both for oils and gas condensates, independent of the drawdown during OFT tests (Mott and Whitson 2005).

If PVT data are measured on in-situ representative samples (samples during production or OFT samples without OBM contamination), all such data should also be used in the EOS model building – together with other reservoir representative PVT data. The subset of total samples used in EOS model building that are in-situ representative can range from 0% to a high percentage, but often it is a low percentage. This doesn’t really matter for the ability to build a multi-sample, common EOS for an entire field or basin – the key is having a large set of quality, relevant PVT data for a wide range of fluid samples. Having few *in-situ* samples with measured PVT data is no hinderance for building a reliable and robust common EOS model. In basins like Montney with in-situ fluids being near-saturated or initially saturated two-phase systems, few samples may be in-situ representative, even during the first days of production.

### **EOS Model Development with Oil Based Mud Components**

In the discussion above, we recommend selecting only samples that are *not* OBM contaminated for use in EOS model building. In some situations, however, few or no such uncontaminated samples are available. We have experienced a number of fields that were discovered and delineated without production test sampling, and where OFT samples were all contaminated. Gulf of Mexico and offshore Africa in particular, where permeabilities are high, productivity is a non-issue, and very expensive testing is dropped from the well budget by sampling only with OFT.

In such situations it is required to develop the EOS model using PVT data measured on OBM-contaminated samples, in which case the EOS must include OBM components. OBM components are typically paraffinic in the range  $C_{11}$ - $C_{20}$ . Sometimes a two-component mud is used, but more often a mud with a normal-like distribution of components from  $C_{11}$ - $C_{20}$ , with 5-6 components having significant amounts. Average properties of the OBM are usually reported by the vendor, as well as a mass or molar distribution of the OBM components.<sup>8</sup>

Once the EOS+OBM model is built, including OBM components, all contaminated reservoir-sample compositions should be decontaminated to help in the mapping of in-situ compositions. The decontaminated reservoir compositions are easily found by simply removing the OBM components from the EOS+OBM model. The contaminant-free EOS model will likely be less accurate than an EOS built using uncontaminated sample PVT data. Once the field is put on production and contaminant-free samples can easily be collected, a range of not-contaminated, reservoir-representative samples should be collected and sent to the PVT laboratory for standard testing. These PVT data provide a quality check of the EOS – either confirming its validity, or initiating an EOS model update with the new, not-contaminated PVT data.

### **PVT Data Quality Checks**

It is recommended to use all available PVT samples in EOS development. However, it is also important to evaluate the quality of PVT data for each sample to decide which PVT data should be included in EOS tuning and what weighting factors should be applied to different types of experimental PVT data.

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<sup>8</sup> The vendor-provided OBM properties would be appropriate to use for the first well. Re-use of OBM from one well to the next, results in the need for mud-pit sampling and analysis to determine whether the re-used OBM has a distribution of components that has changed significantly from the original vendor-delivered mud.

Several QC methods are presented in this section using examples from samples collected in the Eagle Ford and Montney basins.

**Compositions.** Reservoir samples (BHS or OFT type) and separator oil sample compositions are measured experimentally using a *Flash-GC-Recombination* procedure. These pressurized samples are brought to 1 atm and a controlled ambient temperature<sup>9</sup>. The resulting flashed oil (FLO) and flashed gas (FLG) are collected, quantified in terms of mass and standard gas volume, respectively. Each flashed phase is fed to an appropriate gas chromatography (GC) system that measures primarily mass amounts of all defined compounds and mass amounts for all single-carbon number fractions, in today's laboratories out to about  $C_{35}$ , with a remaining heavy residue of  $C_{36+}$ . The two flashed mass compositions are recombined to yield the separator oil or recombined reservoir/wellstream mass composition. Mass compositions  $w_i$  are converted to molar compositions using measured  $w_i$  data and assumed molecular weight (MW) values for  $C_{7+}$  fractions<sup>10</sup>. As discussed below, several sources of data uncertainty in the reported mass and molar compositions of reservoir/wellstream mixtures exist and should be considered when developing a multi-sample common EOS model.

Compositional data based on extended gas chromatography analysis can be quality checked by fitting a gamma distribution model (Whitson 1983) to the lab-reported mass amounts of  $C_{n+}$  fractions (see section below on *Gamma molar distribution model*). An example of compositional QC for one of the PVT samples used in the Montney EOS development is shown in **Figure 1**. Doing gamma fitting on many samples will give a good indication of outlier sample analyses, and whether the gamma parameters are similar and/or correlate for a given field/basin.

Compositions are directly measured on stabilized oils and low-pressure (flashed and separator) gas samples using gas chromatography. Measured surface gas compositions are usually accurate because most identified components are library compounds, with only smaller amounts of  $C_{10+}$  plus fractions. We find no reason, in general, to modify reported flashed-gas/separator-gas compositions during the EOS tuning process.

Because oil samples have large amounts of heavy components, laboratories will traditionally (1) add a known mass of some light-heavy hydrocarbon compound (not found in the oil) as an *internal standard*, and (2) use a calibrated baseline “shift” to correctly quantify the mass amounts of the heaviest components. Basically, the GC will “elude” (quantify) only out to some SCN, usually  $C_{35}$  in laboratories today. The internal standard / baseline method ensures (a) the lighter  $C_6$ - $C_{10}$  compounds and SCN components  $C_{11}$ - $C_{35}$  amounts are correctly converted from *response-integrated areas* to mass fractions, and (b) that the non-eluded  $C_{36+}$  amount can be calculated as 1 minus the sum of all mass fractions for components up to  $C_{35}$ .

A typical error seen for the heaviest SCNs (e.g.  $>C_{25}$ ) of a flashed oil is that reported mass fractions are too low (or too high). This is readily seen when comparing reported mass fractions with a gamma distribution model-fit results, as shown in **Figure 2**. The source of this type of error is that the laboratory has not calibrated the baseline adequately. The gamma model can be used to correct some of the heavier mass fractions in a consistent way, and particularly the heaviest fraction  $w_{N+}$ .

<sup>9</sup> Some laboratories offer a cryogenic flash process for gas condensate samples, where the reservoir gas is cooled with liquid nitrogen, followed by a gradual temperature increase with continuous bleeding of gas into a container. When room temperature is reached, the total gas collected represents the “flashed gas” and the remaining liquid is the “flashed oil”; cryogenically-flashed gas and oil samples are not in thermodynamic equilibrium.

<sup>10</sup> “ $C_{7+}$  fractions” or the generic “ $C_{n+}$  fractions” refer to all pure isomer compounds and average single carbon number (SCN) fractions  $i=n, n+1, \dots, N-1$ , and the heaviest plus fraction  $C_{N+}$ , with  $N>30$  usually recommended.

Average MW for a stabilized oil ( $M_{\bar{o}}$ ) *should be* measured by the laboratory to help convert the measured GC mass fractions  $w_i$  to mole fractions  $x_i$  (required by the EOS), where

$$x_i = w_i(M_{\bar{o}}/M_i) \dots\dots\dots (1)$$

for component  $i$  in the stabilized oil. Light components  $C_1$ - $C_6$  and  $C_7$ - $C_{10}$  isomers have *known*  $M_i$ . A challenge is estimating reasonable MWs for the heavier fractions, where:

- a. SCN fractions  $C_7$ - $C_{(N-1)}$  each have an average  $M_i$  that can be represented by  $M_i \approx 14i \pm h_i$  ( $h=2$ : paraffin;  $h=0$ : naphthene,  $h=-6$ : aromatic). Because perfect separation of compounds is not possible with GC or distillation methods, a lab-reported SCN fraction  $C_i$  may in fact contain many lighter (e.g.  $C_{i-1}$  &  $C_{i-2}$ ) and heavier (e.g.  $C_{i+1}$  &  $C_{i+2}$ ) compounds, with a resulting average-SCN average  $M_i$  far removed from the expected value given by  $M_i \approx 14i$ .
- b.  $M_{N+}$  is unknown and must be estimated in a systematic, consistent manner.

Values for  $M_i$  are not known and may vary, so a set of estimates (constant  $h_i$ , or Katz-Firoozabadi  $M_i$  values) are assumed by the laboratory. The measurement uncertainty for  $M_{\bar{o}}$  is up to  $\pm 5$ -10%. The biggest uncertainty is clearly  $M_{N+}$  which cannot be measured, and a back-calculation depends severely on the assumed  $h_i$  values and measured  $M_{\bar{o}}$ .

A consistent estimate of  $M_{N+}$  is found using a tuned gamma distribution model. In the absence of such a model, the following relation applies for an exponential distribution model:  $M_{36+} = M_{7+} + 405$ ; for a gamma distribution shape of 0.7 (quite common) the relationship is  $M_{36+} = 1.28M_{7+} + 385$ , which gives substantially higher (10-70 units)  $M_{36+}$ , as shown in **Figure 3**.

For a multi-sample common EOS model development, it is necessary to use a consistent mass-to-mole conversion for all samples that (1) uses a consistent set of assumed  $M_i$  values, and (2) has the ability to account for measurement uncertainty in the value of stabilized oil  $M_{\bar{o}}$  for each sample.

$M_{\bar{o}}$  is tightly coupled to the  $C_{7+}$  gamma average MW parameter  $M_{7+}$ , because most of the stabilized oil consists of  $C_{7+}$ . Both  $M_{\bar{o}}$  and  $M_{7+}$  are expected to vary considerably from sample to sample in a field, but in a consistent manner. A gamma model fit of each sample gives the ability to identify measurement errors in stabilized oil  $M_{\bar{o}}$  for each sample, based on a relationship between  $M_{\bar{o}}$  and  $M_{7+}$  that can be established using all samples.

An additional uncertainty in molar composition of separator oils (or reservoir fluids) stems from the laboratory flash to standard conditions, where the flash GOR has an uncertainty of about  $\pm 5\%$ . The mathematical recombination of flashed gas and flashed oil (or recombination of separator gas and separator oil) uses the component material balance equation:

$$z_i = y_i F_g + x_i (1 - F_g) \dots\dots\dots (2)$$

where,  $F_g = (1 + \frac{RT_{sc}}{p_{sc}} \frac{\rho_o}{M_o GOR})^{-1}$

and  $\rho_o/M_o$ =molar volume of the oil being used in the recombination (flashed oil or separator oil). This  $F_g$  equation uses consistent SI units, and the recombined molar composition  $z_i$  is either a reservoir fluid  $z_{Ri}$  or a separator oil  $x_{spi}$ .

In summary, there are several well-understood and quantifiable data uncertainties in laboratory molar compositions of flashed oils, separator oils and reservoir fluids determined from the *Flash-GC-Recombination* procedure. The most certain compositional data are flashed and separator gases.

**$C_{7+}$  Molecular Weight and Specific Gravity.** Historically, prior to about 1985, PVT laboratories measured directly the flashed oil MW and specific gravity (SG). Unfortunately, some laboratories no

longer report a measured flashed-oil MW; instead, they compute its value from extended GC data and assumptions about SCN and  $C_{N+}$  MWs. It appears that some laboratories no longer measure  $M_{\bar{o}}$ , while other labs simply don't report the measured value. If  $M_{\bar{o}}$  is measured, it should be used as shown below. So, if a measured  $M_{\bar{o}}$  value is available, ask the lab for its value.

From measured  $M_{\bar{o}}$  and  $\gamma_{\bar{o}}$  we recommend calculating  $M_{7+}$  and  $\rho_{7+}$  from

$$M_{7+} = \frac{w_{7+}}{\frac{1}{M_{\bar{o}}} - \sum \frac{w_{\bar{o}i}}{M_i}} \quad \dots\dots\dots (3)$$

$$\gamma_{7+} = \frac{w_{7+}}{\frac{1}{\gamma_{\bar{o}}} - \sum \frac{w_{\bar{o}i}}{\gamma_i}} \quad \dots\dots\dots (4)$$

In the above equations,  $w_{\bar{o}i}$  = mass fraction of components in the stabilized oil, and  $i = C_6$  and lighter components. These back-calculated  $C_{7+}$  properties are preferred for developing the  $C_{7+}$  characterization.  $M_{7+}$  values are affected only by measurement errors in  $M_{\bar{o}}$ . Back-calculated  $\gamma_{7+}$  from Eq. 4 is not prone to error because  $\gamma_{\bar{o}}$  is highly reliable.

Laboratories often provide “calculated”  $M_{n+}$  and  $\gamma_{n+}$  values ( $n = 7, 10, 15$ , etc.), but these values are *seldom* calculated from the equations above, and they do *not* use the measured flashed-oil properties  $M_{\bar{o}}$  and  $\gamma_{\bar{o}}$ . Instead, lab-calculated  $C_{n+}$  properties are based on extended GC mass fractions  $w_i$ , and *assumed* fraction properties  $M_i$  and  $\gamma_i$  – e.g. Katz and Firoozabadi (1978) or in-house methods. These lab-calculated plus-fraction average properties can be extremely misleading and incorrectly characterize  $C_{n+}$  because assumed fraction properties  $M_i$  and  $\gamma_i$  may not reflect the fluid's relative paraffinicity / aromaticity. Katz-Firoozabadi properties, most commonly used by the laboratories, represent an arbitrary *average* of fluids found in the U. Michigan database when that correlation was developed (Katz and Firoozabadi 1978). Many reservoir fluids are considerably more paraffinic or more aromatic than the fraction properties used by the laboratories.

Accurately measured flashed-oil properties  $M_{\bar{o}}$  and  $\gamma_{\bar{o}}$  should correctly reflect oil relative paraffinicity and be used to characterize  $C_{7+}$ . This is achieved using Eqs. 3 and 4, but we must force the laboratories to measure and report flashed-oil properties  $M_{\bar{o}}$  and  $\gamma_{\bar{o}}$ , and then back-calculate  $C_{7+}$  average properties manually.

**Separator Compositions Equilibrium Check.** To check whether the separator oil samples and separator gas samples are in equilibrium, a “Hoffmann plot” (Hoffman et al. 1953) can be used. In this plot, K-values ( $K_i=y_i/x_i$ ) calculated from separator gas  $y_i$  and separator oil  $x_i$  compositions should fall on a straight line when plotting  $K_i p_{sp}$  versus  $F_i(T_{sp})$ , usually close to the Standing (1979) low-pressure K-value correlation. **Figure 4** shows an example of separator compositions that appear in equilibrium based on the Hoffman plot.

When the Hoffman QC is valid, separator K-values can be used as data in the EOS tuning, as can the separator-recombination GOR. If the Hoffman plot suggests that the two separator samples are *not* in equilibrium, then neither K-values nor separator-recombination GOR should be used in EOS tuning. However, PVT measurements of a mixture  $A$  made up from any two samples – in equilibrium or not – can be used in EOS tuning because the overall mixture  $A$  composition used in the PVT measurements is known.

**Z-factors.** Reported Z-factors can be compared with calculated Z-factors from the Standing-Katz chart (Standing and Katz 1946), e.g. using the Hall and Yarborough BWR EOS fit of this chart (1973). Z-

factors of reservoir gas from CCE and CVD tests can be compared with Standing-Katz Z-factors; produced CVD gases have changing composition that needs to be used. Calculated Z-factors from the Standing-Katz correlation should normally be within  $\pm 1-3\%$  of measured values up to about 10,000 psia. An example Z-factor QC is shown in **Figure 5**.

We do not usually include gas Z-factors as data for EOS tuning because predictions with default component properties – and volume shift factors of lighter components – are accurate without tuning. Seldom do we see EOS gas Z-factors consistently deviating more than 1-3% from Standing-Katz Z-factors for more than a few samples; the occasional sample that shows larger deviations is assumed to reflect data error. If the deviation is consistently significant for all lab Z-factors, then EOS adjustments to volume shift factors may be used, typically changing values only for components with significant mol%<sup>11</sup>.

**Constant Volume Depletion (CVD).** There are two types of material balance checks for CVD experimental data, the commonly-used *forward material balance* (Whitson and Torp 1983) and the less-common *backward material balance* (Whitson and Brule 2000).

The forward material balance starts with an initial composition and moles in the PVT cell, tracking the removed gas component moles, together with reported phase volumes and gas Z-factors, to calculate oil properties and compositions at each stage. Usually the equilibrium oil composition at last depletion stage is reported which can be compared with the calculated final oil composition. K-values are calculated at each stage from reported equilibrium-gas and calculated equilibrium-oil compositions and can be plotted for consistency using  $K_i(p)$  on a log-log paper, or using the Hoffman plot (see Whitson and Torp 1983). The forward material balance is usually accurate for richer gas condensates and volatile oils, but less so for leaner gas condensates (Whitson and Brule 2000). The oil property calculations are very sensitive to reported relative oil volumes ( $V_{ro}$ ) at each stage; higher uncertainty for smaller  $V_{ro}$  values will tend to exaggerate the inaccuracy of calculated oil compositions and properties for leaner systems.

The backward material balance for a CVD test provides a valuable QC for the produced  $C_{6+}$  in the removed gases (proportional to depletion condensate recovery). This material balance uses the final oil composition, final oil volume and its properties, together with produced gas moles and composition at each stage. This allows calculation of the initial fluid composition that can be compared with lab-reported initial composition.

Consider a lab report with 10 mol%  $C_{6+}$  initial fluid, corresponding to an initial oil gas ratio (OGR) of 200 STB/MMscf and an initial condensate in place (ICIP) of 100 million STB. If the backward material balance of the CVD test yields only 9 mol%  $C_{6+}$  initial fluid, this corresponds to “laboratory loss” of ~10 million STB during the depletion test. For an expected 30% condensate recovery, the possibility that the lab has “lost” up to 1/3 of the 30 million STB reserve is unacceptable<sup>12</sup>.

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<sup>11</sup> Changing light pure-compound  $s_i$  values is allowed (because they are not unique measured values), but they should be changed with caution. A good practice is to obtain the light pure-compound densities at reservoir conditions from property tables or special EOS models for the component. The  $s_i$  values can then be adjusted to match these highly-accurate pure-compound densities at relevant reservoir conditions.

<sup>12</sup> The backward material balance error can source from incorrect removed gas compositions and/or incorrect oil volume and properties at the end of the CVD test. If this material balance yields a significant difference in  $C_{6+}$  initial fluid then we make an effort to assess whether that error more likely stems from final oil volume quantification or removed gas  $C_{6+}$  amounts. That assessment usually requires comparison of the lab results and EOS calculations.

An example of forward and backward CVD material balances is shown in **Table 2**. The K-values calculated from forward material balance for a CVD test are shown in **Figure 6**.

**Differential Liberation Expansion (DLE) and Separator Tests.** The DLE QC is also based on a backward material balance, very similar to the backward CVD material balance QC. While the CVD backward material balance deals primarily with a compositional material balance, and particularly for  $C_{6+}$  content, the DLE application concerns mainly a phase material balance where oil density is calculated. Most laboratories don't measure DLE oil densities, they use the backward material balance densities in reporting (Whitson and Brule 2000). Any comparison of reported and material balance calculated oil densities should be very close, as shown in **Figure 7**.

A backward component material balance can be made for DLE compositional data (similar to CVD backward material balance). For volatile and near-critical oils, gas removed  $C_{6+}$  in a DLE test is often less accurate than for CVD tests – unless the DLE test is conducted in a “CVD” PVT cell apparatus, where more attention is given to obtaining accurate  $C_{6+}$  amounts (e.g. using a cryogenic *flash-GC-recombination* method for removed gases).

**High pressure K-values.** Some PVT tests provide direct measurement of K-values at high pressures and reservoir temperature. The data is not always easy to measure, and particularly for heavier components. However, quality high-pressure K-values are invaluable for EOS tuning. The data is usually measured and available in the following PVT lab tests:

- a) *Equilibrium Contact Mixing* (ECM) type measurement (Fevang and Whitson 1994) – A total composition  $z_i$  made up of samples from a saturated gas cap mixed with samples from the underlying oil, flashed to initial reservoir pressure and reservoir temperature. The compositions of equilibrium phases  $y_i$  and  $x_i$  are then measured independently, and the method provides for a rigorous material balance QC.
- b) Multi-contact gas-EOR tests that measure equilibrium phase compositions  $y_i$  and  $x_i$ .
- c) A swelling test that identifies a critical transition (transition from bubblepoint to dewpoint mixture); this brackets the critical point composition where all  $K_i=1$ .

To QC K-value data requires independent knowledge of  $z_i$ ,  $y_i$  and  $x_i$ . A material balance plot (Robinson et al 1978) of  $y_i/z_i$  versus  $x_i/z_i$  should yield a constrained straight line given by Eq. 6:

$$z_i = y_i F_g + x_i (1 - F_g) \quad \dots\dots\dots (5)$$

$$\frac{y_i}{z_i} = \frac{1}{F_g} - \frac{x_i}{z_i} \left( \frac{1}{F_g} - 1 \right) \quad \dots\dots\dots (6)$$

where slope is  $(F_g^{-1} - 1)$  and intercept is  $F_g^{-1}$ .

An equivalent but somewhat more tangible relationship is

$$\frac{z_i}{x_i} = F_g (K_i - 1) + 1 \quad \dots\dots\dots (7)$$

where  $K_i = y_i/x_i$ . Plotting  $z_i/x_i$  versus  $(K_i - 1)$  yields slope= $F_g$  and intercept = 1 at  $(K_i - 1) = 0$  or  $(K_i = 1)$ , with light components having  $(K_i - 1) > 0$ , and heavier components having  $(K_i - 1) < 0$ .

An example of material balance QC for K-values is shown in **Figure 8**, the data showing consistent quality and was very useful developing the Montney basin-wide EOS.

## Heptanes-Plus Characterization

$C_{7+}$  characterization is considered the most important task in developing a reliable EOS. The process includes estimating the component properties for  $C_{7+}$  fractions and establishing component molar/mass amounts in a consistent way. In a field-wide, multi-sample EOS, the component properties will be the same for all samples. The only difference from one sample to another is the composition. Total amount and distribution of  $C_{7+}$  fractions are both independently important. For depletion of a gas condensate, the  $C_{7+}$  amount is critical, while for miscibility and vaporization of an oil, the  $C_{7+}$  distribution is important (Coats 1985), where MMPs are particularly dependent on the heaviest  $C_{N+}$  component amount and properties.

EOS component properties for  $C_{7+}$  fractions are estimated from correlations (e.g. Twu 1984) using known “inspection” (measurable) properties – normal boiling point (NBP) temperature ( $T_b$ ), molecular weight ( $M$ ) and liquid SG ( $\gamma$ ). We first discuss how  $C_{7+}$ ,  $T_{bi}$ ,  $\gamma_i$  and  $M_i$  are estimated, and used to estimate component properties required for EOS calculations ( $T_{ci}$ ,  $p_{ci}$ ,  $\omega_i$ ,  $s_i$ ).

## Gamma Molar Distribution Model

The gamma distribution model can be used to define MWs of  $C_{n+}$  fractions, and both mass and molar quantities of  $C_{n+}$  fractions. Distributions of  $C_{7+}$  and  $C_{11+}$  are commonly used, as are SCN or SCN-range fractions (e.g.  $C_7$  or  $C_7$ - $C_{10}$ ). The gamma model requires three parameters to define the continuous molar distribution function for  $C_{n+}$ :

- Parameter  $\alpha$  defining the *shape* of the distribution ( $\alpha=1$  for exponential distribution)
- Lower bound  $\eta$  defining the minimum MW in  $C_{n+}$
- Average  $M_{n+}$  of the entire  $C_{n+}$  being described by the distribution model

For a field-wide EOS development, the gamma distribution model should be developed for all samples. A single distribution model with common shape and lower bound parameters is often found. Sample-specific average  $M_{n+}$  is expected, where Fahd and Whitson (2018) show that equilibrium phases usually share a common shape  $\alpha$  and lower bound  $\eta$ .

The data that should be used for gamma model development include extended GC compositional data for  $C_{7+}$  fractions of the flashed oil (though separator oil and reservoir fluid compositions can also be used). It is recommended to use lab-reported mass amounts for gamma model development, instead of lab-reported moles. The model can be developed by simultaneously regressing the following gamma model parameters to all samples:

- Lower-bound MWs ( $M_{Li}$ ) for  $C_n$  to  $C_{36+}$  – common for all samples
- Gamma shape  $\alpha$  and lower bound  $\eta$  – usually common for all samples
- Gamma average  $M_{n+}$  – specific for each sample

The common set of  $M_{Li}$  values are determined simultaneously while fitting all samples’ GC mass fraction data.

The resulting gamma distribution model can predict SCN and  $C_{N+}$  amounts for any sample where it is missing (or of bad quality), knowing only  $M_{n+}$  and  $C_{n+}$  mass. The lab reported amount for the heaviest  $C_{n+}$  fraction is often uncertain and may be ignored (weighting factor of zero) during gamma model fitting.

**Figure 9** shows some example results of the  $C_{7+}$  gamma distribution model developed for Montney basin using 150 PVT samples with extended GC data. The model has a common shape, lower-bound and set of  $M_{Li}$  that accurately defines the compositional amounts for the wide range of compositions with  $M_{7+}$  ranging from 130-220.

Many oil-based muds and biodegraded reservoir fluids have a  $C_{7+}$  gamma distribution shape  $\alpha > 5$ .

### Heptanes-Plus Component Properties

**Molecular Weights.** The different sources for defining  $M_i$  for  $C_{7+}$  fractions are:

- a) Single carbon number ASTM distillation D2892 analysis
- b) Correlations such as Twu (1984)
- c) Gamma distribution model tuned to GC and/or distillation data

ASTM D2892 data include measured stabilized oil  $M_{\bar{o}}$  and SCN  $M_i$ . Comparing gamma model MWs for individual components with measured distillation values shows that SCN lower MW bounds are slightly different than found for GC data. This can be seen from **Figure 10**, which shows that the gamma model calculated component  $M_i$  are slightly different compared to ASTM D2892 measured data

The common EOS usually has a single heaviest component with constant  $M_{N+}$  and other properties. As mentioned earlier,  $M_{N+}$  is a linear function of  $M_{n+}$  (based on the gamma model), and a choice must be made about how heavy the  $C_{N+}$  should be. We try to optimize  $M_{N+}$  during the common EOS model development, with the understanding that this introduces a slight material balance error in conversion of lab mass amounts to mole amounts for samples with a wide range of  $M_{n+}$  ( $M_{N+}$ ) values. A field-wide “characterization” gamma model with parameters ( $\bar{M}_{n+}$ ,  $\bar{\alpha}_{n+}$ ,  $\bar{\eta}_{n+}$ ) can be used to yield an optimal  $M_{N+}$ , as well as defining the SCN-average  $M_i$  values in the common EOS<sup>13</sup>.

**Specific Gravities.** The  $\gamma_i(M_i)$  relationship usually reflects an average relative paraffinicity (or aromaticity) that is assumed to be constant for all fractions and for all fluids from a field or basin. It is common to estimate the  $\gamma_i(M_i)$  relationship for individual fractions from surface oil data.<sup>14</sup> Austad et al (1983) and Whitson and Brule (2000) show strong correlations of  $M_{7+}$  and  $\gamma_{7+}$  for a given reservoir. Measured MW of surface oils  $M_{\bar{o}}$  (or  $C_{7+}$ ) may have an uncertainty up to 5-10% for many commercial labs, while specific gravities should be accurate within a fraction of a percent.<sup>15</sup>

The  $M_{7+}(\gamma_{7+})$  correlation is usually somewhat different than the component correlation  $\gamma_i(M_i)$  needed for SCN and  $C_{N+}$  fractions – depending on the mass (molar) distribution of heavy fractions  $w_i$ . This stems from the equations relating individual fractions to average values  $\gamma_{n+}$  and  $M_{n+}$ :

$$\gamma_{n+} = \frac{\sum_{i=n}^{N+} w_i}{\sum_{i=n}^{N+} w_i / \gamma_i} \dots\dots\dots (8)$$

<sup>13</sup> SCN-average  $M_i$  values from gamma model are not sensitive to  $M_{n+}$  (except for the heaviest fraction MW,  $M_{N+}$ )

<sup>14</sup> Historically, Corelab measured and reported  $M_{7+}$  and  $\gamma_{7+}$  by distilling off the  $C_6$ -ends from a flashed or stock tank oil sample. However, in modern PVT reports, measurements are reported for total stabilized oil samples  $M_{\bar{o}}$  and  $\rho_{\bar{o}}$ . In such cases,  $M_{7+}$  and  $\gamma_{7+}$  data should be back-calculated from measured  $\rho_{\bar{o}}$  and  $M_{\bar{o}}$ , as discussed earlier.

<sup>15</sup> Correlating  $\gamma_{7+}(M_{7+})$  data may be difficult for waxy crude oils and some condensates (such as found in Montney). Surface samples may contain an excess of (or be deficient in) wax-forming alkanes when field processing temperatures and/or laboratory handling temperatures drop below the wax appearance temperature.

$$M_{n+} = \frac{\sum_{i=n}^{N+} w_i}{\sum_{i=n}^{N+} w_i/M_i} \dots\dots\dots (9)$$

Only one  $\gamma_i(M_i)$  relationship applies equally to individual fractions  $i$  and  $C_{7+}$  averages  $\gamma_{7+}(M_{7+})$  – when liquid molar volume  $v_L$  at standard conditions is a linear function of MW<sup>16</sup>  $v_{Li}=M_i/\gamma_i=\alpha M_i+\beta$ ; or  $\gamma_i=M_i/(\alpha M_i+\beta)$ . It can be shown that  $v_{Ln+}=M_{n+}/\gamma_{n+}=\alpha M_{n+}+\beta$  for *any* mass distribution  $w_i$  for  $C_{n+}$ .

The best lab data, if available, for developing the  $\gamma_i(M_i)$  correlation is ASTM D2892 distillation. **Figure 10** shows the correlation developed for Montney using available ASTM D2892 data. The Søreide (1989) equation was used to fit these data, changing all four parameters. The  $\gamma_i(M_i)$  relationship is used to estimate all component  $C_{7+}$  gravities, including  $\gamma_{N+}$ , and these values can have a significant effect on the ability of an EOS model to predict oil densities at all conditions. Furthermore, the  $\gamma_i(M_i)$  relationship has a strong impact on estimated EOS component properties ( $T_b$ ,  $T_c$ ,  $p_c$ ,  $\omega$ , and  $s$ ). Striving towards an accurate and representative  $\gamma_i(M_i)$  relationship is one of the most fundamental and important steps in developing a reliable common EOS model for basins and multi-reservoir fields.

**Normal Boiling Point.**  $T_b$  is usually estimated with a correlation based on  $M$  (or carbon number) and  $\gamma$  (e.g. Twu 1984 or Søreide 1989).  $T_b$  represents a point on the vapor pressure curve at “normal” pressure, 1 atm. Ensuring that the EOS model predicts accurately the vapor pressure curve of all components is important because K-values that dictate the efficiency of surface separation and processing (from atmospheric pressure to about 1000 psia) are given by the simple relation  $K \approx p_{vi}(T)/p$ .

An alternative approach to build a field-specific  $T_b(M)$  relationship for  $C_{7+}$  fractions includes two steps (1) a common set of lower MW boundaries ( $M_{Li}$ ) are determined from a field-wide gamma model fit to all the samples with gas chromatography data, and (2) make use of normal-paraffin boiling points ( $T_{bP}$ ) to bound SCN fractions, with carbon number  $i$  containing all compounds that boil in the range<sup>17</sup>  $T_{bLi}=(T_b)_{n-Ci-1} < T_{bi} \leq (T_b)_{n-Ci}$ . The two lower-bound SCN properties ( $M_{Li}$ ) and  $T_{bLi}=(T_b)_{n-Ci-1}$  are then correlated. The  $T_{bL}(M_L)$  relationship for the Montney basin is shown in **Figure 11**. A lower-bound  $T_{bL}(M_L)$  relationship can be used to calculate component-average  $T_{bi}$  knowing average  $M_i$  of SCN fractions (and the heaviest fraction  $C_{N+}$ ).

**Critical Properties.** Critical properties  $T_c$  and  $p_c$  can be estimated using published correlations (e.g. Twu 1984) knowing  $C_{7+}$  component properties  $T_b$  and  $\gamma$ . Acentric factor  $\omega$  can be calculated from a correlation as a function of  $T_b$ ,  $T_c$ , and  $p_c$  (e.g. Lee-Kesler 1976). We recommend that  $\omega$  of  $C_{7+}$  components be chosen such that the vapor pressure (=1 atm) at normal boiling point  $T_b$  be matched exactly by the EOS. This guarantees consistency between  $\omega$  and EOS input ( $T_c, p_c, T_b$ ). Using this approach, the  $C_{7+}$  component properties that should be used in EOS tuning are limited to ( $T_c, p_c, T_b$ ) – not  $\omega$  directly.

$C_{7+}$  component volume shifts  $s_i$  should be calculated such that the component’s (measured or estimated) SG equals the EOS component liquid density at standard conditions (1 atm and 60°F) divided by water density at the same standard conditions. EOS-based PVT packages should “dynamically” update  $s_i$  to always match  $\gamma_i$  for  $C_{7+}$  components during regression – i.e. when other component properties ( $T_c, p_c, T_b$ ) are being modified. In fact, if  $C_{7+}$  volume shifts need modification to improve oil volumetric predictions, it is highly recommended that  $\gamma_i$  values be modified in a systematic and physically-

<sup>16</sup> Robinson and Peng (1978) give constants  $\alpha$  and  $\beta$  for the three hydrocarbon groups: paraffins (P), naphthenes (N), and aromatics (A) –  $\alpha_P=1.163$  and  $\beta_P=28.776$ ;  $\alpha_N=1.1697$  and  $\beta_N=9.622$ ;  $\alpha_A=1.1742$  and  $\beta_A=-2.2862$ , where  $M_i=14i+h$  with  $h_P=2$ ,  $h_N=0$ , and  $h_A=-6$ .

<sup>17</sup> As an example, SCN  $C_7$  contains both six-carbon compounds cyclohexane ( $C_6H_{12}$ ) and benzene ( $C_6H_6$ ).

consistent manner, whereby modified  $s_i$  values are adjusted to ensure that EOS-calculated  $\gamma_i$  values always equal the desired (measured/input/regressed)  $\gamma_i$  values.

## EOS Development

An EOS calculation requires a sample composition and two EOS tables – (1) EOS component properties and (2) binary interaction parameter (BIP) matrix. Component properties are known for pure compounds, while the heavier components properties are estimated based on  $C_{7+}$  characterization methods – with possible adjustments that result from tuning the component properties and BIPs to measured PVT data.

Our workflow for developing a multi-sample EOS model is outlined below:

1. Sample compositional input
2. EOS component slate selection
3. Heptanes-plus pre-tuning characterization
4. EOS tuning strategy – variables selection and weighting factors
5. EOS model validation and consistency check
6. Viscosity model build

## Sample Composition Input

Developing a multi-sample EOS normally requires systematic-but-small modifications for each lab-reported sample composition, simultaneously altered during the global EOS model tuning. Lab-reported compositions always have uncertainty, just like any other measured PVT data. The composition adjustments should be made in a way that (a) replicates lab uncertainties, (b) maintains consistency, and (c) does not alter lab compositional data with the greatest certainty (e.g. separator- / flashed-gas compositions).

A lab characterization is defined as a set of components and MWs reported / used by a laboratory for one specific composition. Gas samples will have fewer components than an oil sample, and the components defined may also differ. Laboratories report mole fractions which have been calculated from measured mass fractions using a set of lab-specific MWs. We use reported mass fractions, if available, else we compute the mass fractions from reported mole fractions and lab-assumed MWs. We generally conserve the total mass and mass fractions of pure compounds, allowing heavier mass fractions to be (a) adjusted in a systematic way, and/or (b) converted to mole fractions using a different set of MWs consistent with the EOS component slate.

Lab reported  $C_{n+}$  mass fractions can be replaced by the well-established field-wide gamma model. Several reasons for replacing lab-reported mass amounts with the gamma model amounts include:

1. Replacing questionable GC data that clearly deviate from trends that the majority of samples follow.
2. Providing a consistent method to adjust uncertainty in reported/measured  $C_{n+}$  MWs.
3. Consistent definition of SCN components, e.g. using a common set of boundary MWs ( $M_L$ ).
4. Consistent definition of mass amount for the common, heaviest fraction, even when the lab PVT reports use varying heaviest fractions, e.g.  $C_{7+}$ ,  $C_{11+}$ ,  $C_{20+}$ ,  $C_{30+}$ ,  $C_{36+}$ .

Compositions of separator oil and gas samples are recombined mathematically using lab-reported recombination gas-oil ratio, either on a molar or mass basis to calculate the total composition using Eq.

10 or 11. The advantage of doing a recombination on mass basis ( $w_i$ ) over a molar basis ( $z_i$ ) is that for mass basis there is no need to know separator oil MW ( $M_{osp}$ ):

$$z_i = y_i F_{gsp} + x_i (1 - F_{gsp}) \quad \dots\dots\dots (10)$$

$$\text{where, } F_{gsp} = \left(1 + \frac{2130 \rho_{osp}}{M_{osp} GOR_{sp}}\right)^{-1}$$

$$w_i = w_{gi} F_{gspw} + w_{oi} (1 - F_{gspw}) \quad \dots\dots\dots (11)$$

$$\text{where, } F_{gspw} = \left(1 + \frac{2130 \rho_{osp}}{M_{gsp} GOR_{sp}}\right)^{-1}$$

$F_{gsp}$  is the gas fraction on molar basis,  $F_{gspw}$  is gas fraction on mass basis,  $\rho_{osp}$  is separator oil density in lbm/ft<sup>3</sup>,  $M_{osp}$  is separator oil MW,  $M_{gsp}$  is separator gas MW and  $GOR_{sp}$  is gas-oil ratio at separator conditions in scf/sep.bbl.

The same equations (10 and 11) are used for single-stage flash (SSF) to ambient conditions, used by laboratories to measure compositions by the *flash-GC-recombination* method for (a) *all* bottomhole samples and (b) separator oil samples. For a SSF, all subscripts above should use “*ssf*” (single stage flash) instead of “*sp*” (separator). Uncertainty in GOR of about  $\pm 5\%$  is expected for separator and SSF recombination.

**Table 4** illustrates the compositional conversions from lab to EOS characterization using the methods discussed above. Comparison of lab-reported molar compositions and calculated molar compositions may differ slightly for two reasons:

1. Component  $M_i$  used in lab characterization for mass to mole conversion are different than in the EOS characterization.
2. Mass amounts of  $C_{7+}$  fractions may have been replaced by the gamma model.

### EOS Component Slate Selection

We always have component amounts for the three non-hydrocarbons  $N_2$ ,  $CO_2$ , and  $H_2S$  and light hydrocarbons  $C_1$ ,  $C_2$ ,  $C_3$ ,  $i-C_4$ ,  $n-C_4$ ,  $i-C_5$ ,  $n-C_5$ , and  $C_6(s)$ . The laboratory component slate for  $C_{7+}$  has changed dramatically during the past 30 years. Prior to  $\sim 1985$  a single  $C_{7+}$  fraction was reported – it’s molar amount, and measured MW  $M_{7+}$  and SG  $\gamma_{7+}$ . By the early 1990s  $C_7$ ,  $C_8$ ,  $C_9$ , and  $C_{10+}$  (or maybe out to  $C_{12+}$ ) became commonplace for lab reporting of the  $C_{7+}$  heavies; however, only measured amounts (moles and/or mass) were reported, with MWs and specific gravities assumed or back-calculated. Gradually, single carbon number amounts up to  $C_{20+}$  and  $C_{30+}$  became common.

An important consideration in defining sample compositions in a common EOS is the  $C_{7+}$  component slate. We typically use SCN from  $C_7$  to  $C_{29}$  with a  $C_{30+}$  heaviest fraction; or SCNs  $C_7$  to  $C_{35}$  with a  $C_{36+}$  heaviest fraction. When isomers are reported by the lab for SCN fractions  $C_7$ ,  $C_8$ ,  $C_9$ , and  $C_{10}$ , we try to include the individual isomers in the detailed EOS model. Some lab samples include  $C_7$ - $C_{10}$  isomers while other lab samples do not. Based on the samples containing isomer information, we develop an average set of split factors that allow conversion from a single SCN amount into isomer amounts for that SCN. With the isomer split-factors we can develop the EOS with isomers<sup>18</sup> (and  $n-C_i$ ) – e.g. SCN “ $C_7$ ” described by  $MC-C_5$ ,  $C-C_6$ , benzene,  $2M-C_6$ ,  $3M-C_6$ , and  $n-C_7$ .

<sup>18</sup> An alternative approach is to develop an EOS model with an average SCN fraction (based on samples with isomer information), *and* isomers of the SCN. Those samples containing isomer information are characterized by

The use of a detailed EOS model with isomers can be important because: (a) the EOS becomes independent of PVT lab reporting, (b) lumped (“child”) PVT models<sup>19</sup> for specific calculations can be consistently developed from the common (“parent”) EOS, and (c) the BTX isomers are often important to process calculations. An example component slate for a basin-wide EOS is shown in **Table 3**.

Our recommendation for building a common EOS is to use the newest samples that include  $C_6$ - $C_{10}$  isomer data to estimate average split factors to estimate isomer amounts from SCN amounts in older samples. Our typical field-wide EOS may have more than 50 components when including non-HCs, light known HCs through  $C_5$ ,  $C_6$ - $C_{10}$  isomers, and SCN fractions out to  $C_{36+}$ .

### Heptanes-Plus Pre-Tuning Characterization

To ensure a starting EOS model that accurately describes the available heavy-ends PVT data (ASTM distillation with SCN cut NBPs, densities and MWs; flashed oil MWs and SGs; and GC component distributions), we conduct a pre-EOS-tuning characterization of the  $C_{7+}$  fractions. This usually involves:

1. Gamma modelling every flashed-oil sample, yielding field-average lower bound  $\eta$  and shape  $\alpha$ , with sample-specific averages  $M_{n+}$ ;
2. Determine an optimal field-wide  $\gamma_i(M_i)$  relationship for  $C_{7+}$  fractions, applicable to all samples; and
3. (a) Use existing NBP correlation for  $C_{7+}$  fractions, e.g. Twu (1984):  $T_{bi}(\gamma_i, M_i)$ ; or (b) develop a field-specific NBP correlation, e.g. correlating lower-boundary gamma MWs  $M_{Li}$  to normal boiling points of normal alkanes  $n$ - $C_{i-1}$ .

Applying consistent methods to build the initial heptanes-plus characterization will ensure a good initial EOS model that normally predicts oil and gas densities accurately ( $\pm 1$ -3%), and provides accurate low-pressure K-values at surface process conditions.

### EOS Tuning Strategy

Tuning an EOS model (Zick 2007) consists of defining an *objective function*  $\chi^2$  as the sum of squares of weighted residuals

$$\chi^2 = \sum_{k=1}^{N_k} (W_k r_k)^2 \quad \dots\dots\dots (12)$$

where  $r_k$  gives the *residual* (mismatch) between measured lab PVT data  $d_{ek}$  and corresponding EOS-calculated result  $d_{ck}$ .  $W_k$  is a user-assigned weighting factor for each residual, and a typical PVT tuning process will have 100s or many 1000s of weighted residuals ( $N_k$ ). The magnitude of data may be orders of magnitude for different data types (e.g. compositions, saturation pressures, and densities), and also for a specific data type (e.g. K-values). The root mean square (RMS) residual  $\bar{r}$  is a good and well-understood metric for such a complex optimization problem,

$$\bar{r} = \sqrt{\frac{\chi^2}{\sum_{k=1}^{N_k} W_k^2}} \quad \dots\dots\dots (13)$$

Defining the residual must be done with care to handle such a wide variety of data and data magnitudes. One recommendation (Zick, 2007) is  $r_k = 100(d_{ck} - d_{ek})/d_{rk}$  where  $d_{rk}$  is a reference value for data  $k$ . For an

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the isomers, while lab compositions with SCN amounts only are assigned to the average-SCN ( $C_i$ ) – e.g. *methylcyclo-pentane*, *benzene*, *cyclo-hexane*, *n-C<sub>7</sub>*, and  $C_7$ .

<sup>19</sup> For example, highly-lump EOS for reservoir simulation; SCN EOS model for process calculations.

isolated measurement, such as the saturation pressure of an experiment, the reference value might be the experimental data,  $d_{rk}=d_{ek}$ . For a series of measurements of a given data type in an experiment – for example oil relative volume in a CVD test – the maximum experimental value could be used for  $d_{rk}$ .

If the standard deviation ( $\sigma_k$ ) is known for each measurement error ( $d_{ck}-d_{ek}$ ) then the weighting factor could be defined as  $W_k=d_{rk}/(100\sigma_k)$ . A more-heuristic approach to assigning weighting factors is normally used, taking into account lab data uncertainty, number of data of a specific type, and the relative importance of key data (e.g. saturation pressure and type).

EOS-calculated results ( $d_{ck}$ ) depend on the following “variables”: (1)  $N_c$  component EOS parameters ( $M_i, T_{ci}, p_{ci}, \omega_i, s_i, k_{ij}$ ), and (2)  $N_c-1$  molar amounts of the mixture  $z_i$  whose properties are being calculated (times total number of PVT samples  $N_s$ ). Changing any of the EOS parameters and/or  $N_c-1$  mixture component mol% values may impact some or all calculated results ( $d_{ck}$ ). For a 20-component EOS model and a single PVT sample ( $N_s=1$ ), the number of “variables” that can be altered to minimize the objective function is theoretically<sup>20</sup>  $N_v=309=(5N_c)+((N_c^2-N_c)/2)+(N_c-1)$ . If we disallow changes in the 10 pure-compound EOS properties ( $M_i, T_{ci}, p_{ci}, \omega_i$ ), the number of variables drops to  $N_v=269$ . The number of PVT data measurements for a single sample might range from 50 to 500.

If we have  $N_s=20$  samples, each with  $N_k$  measured PVT data, and no changes in 10 pure-compound EOS properties are allowed, the total variables would increase to  $240+N_s(N_c-1)=620$ . Such a multi-sample EOS tuning study might easily have several thousands of PVT data measurements. Still, a major goal of reducing the complexity of the EOS tuning challenge is to reduce the number of variables used, retaining those variables that (a) are most uncertain and (b) have a significant impact on calculated results ( $d_{ck}$ ). This is achieved by (1) using only 1-2 variables per mixture composition, and (2) searching for which of the many  $C_{7+}$  properties have the greatest impact on predictions for the entire PVT database, and particularly key PVT such as near-critical phase behavior, saturation pressures, compositions (K-values), and two-phase relative volumes.

As an example, the Montney basin-wide EOS model had  $N_s=56$  sample mixtures,  $N_k\approx 2000$  PVT data, and total components  $N_c=56$ , the total number of variables used was  $N_v=118$  (4 component-property-related, 11 BIPs-related, and 103 composition-related).

**Variable Selection.** Two variable types have been mentioned – (1) EOS parameters and (2) compositions of the samples used for PVT measurements. Reducing the vast number of potential variables to a smaller subset is an important task.

Each variable must be assigned an initial value, a lower bound, and an upper bound. These three quantities can have a strong influence on the search for an optimal solution. The solution found may be a *local* minimum of the objective function; if unsure, try searching again with different initial values (without changing anything else). If all searches initiated with different starting variable values result in the same set of optimal variable values, one can assume that the global minimum has been located.

**EOS Parameter Variables.** Default EOS component properties ( $M_i, T_{ci}, p_{ci}, \omega_i, s_i$ ) and binary interaction parameters ( $k_{ij}$ ) depend on the PVT software and its method(s) of  $C_{7+}$  characterization, use of laboratory compositional data (e.g. SCN versus individual isomers for  $C_7, C_8, C_9$ , and  $C_{10}$ ), and preferences for assigning BIPs. For pure compounds the properties ( $M_i, T_{ci}, p_{ci}, \omega_i$ ) are known and should not be altered during the tuning process; volume shift  $s_i$  and BIPs involving pure compounds

<sup>20</sup>  $5N_c$  = total number of EOS component properties variables;  $(N_c^2-N_c)/2$  = total number of BIPs variables; and  $N_s(N_c-1)$  = total number of composition-related variables.

may, however, be modified during EOS tuning when accurate, adequate, and appropriate data (e.g. K-values) are available for the pure compounds<sup>22</sup>.

For  $C_{7+}$  SCNs, lumped SCN groups, and the heaviest  $C_{N+}$  fraction, adjustments can be made to the default properties ( $M_i$ ,  $T_{ci}$ ,  $p_{ci}$ ,  $\omega_i$ ,  $s_i$ ) and BIPs involving these fractions. We usually limit the changes in the EOS parameters to  $\pm 5\%$  except for the  $C_{N+}$  fraction, where changes up to 10% may be allowed. BIPs amongst the hydrocarbon (HC) pairs are often limited to changes of  $\pm 0.02$ - $0.05$  except for  $C_{N+}$  fraction, where BIPs may reach a magnitude of  $\pm 0.1$ - $0.2$  (usually positive).

One approach to limiting the number of variables being used to modify  $C_{7+}$  EOS component properties is to use a *ramping* method, whereby the change in a property such as  $T_c$  for  $C_7$ - $C_{(N-1)}$  changes in magnitude with increasing MW, smallest (no) change for  $C_7$  and maximum change for the heaviest fraction  $C_{N-1}$ . The slope of this ramping is a single variable that changes many  $C_{7+}$  fraction properties in a consistent (monotonic) manner. The property changes for  $C_{N+}$  are not usually linked with the direction and magnitude of changes to lighter  $C_{7+}$  fractions, mainly because so little information is available for  $C_{N+}$ .

*HC-HC* BIPs are often calculated from the Chueh-Prausnitz (Chueh 1968) correlation

$$k_{ij} = 1 - \left[ \frac{2\sqrt{D_i D_j}}{D_i + D_j} \right]^6 \dots\dots\dots (14)$$

where  $D_i = \hat{v}_{ci}^{1/3}$ , and  $\hat{v}_{ci}$  = molar critical volume of component  $i$  used specifically for estimating BIPs from the Chueh-Prausnitz correlation; its value is *not* equal to the EOS-defined molar critical volume<sup>23</sup>  $v_{ci}^{EOS} = \left( \frac{RT_{ci}}{p_{ci}} \right) Z_c^{EOS} - s_i b_i$ . A user-input value of  $\hat{v}_{ci}$  (or  $\hat{Z}_{ci}$ ) must be input as an additional component property. This can be estimated from correlations e.g. Twu (1984), similar to other critical properties such as  $T_c$  and  $p_c$ .

BIPs for component pairs with non-HCs such as  $CO_2$ ,  $N_2$ , and  $H_2S$  can be adjusted from default values when PVT measurements are available for mixtures containing significant amounts of non-HC components.

As previously mentioned, hundreds of potential EOS parameter variables exist. The selection process is time-consuming and tedious. A comprehensive search of the many combinations of EOS variables – or trying all variables simultaneously – might give us guidance about which subset of EOS variables should be used. Currently we do not have a fully-automated variable search method. For a given EOS model development, we will try tens if not hundreds of different EOS variable combinations, searching for the one(s) that provide accurate PVT properties for all samples, but also show smaller required changes in EOS parameters from their initial values. During this variable selection process, we may turn off composition variables discussed below (to speed up the variable search process).

**Composition Variables.** Composition changes to the mixture mol% amounts reported by the laboratory can be justified by experimental uncertainties related to (1) GC mass amounts, (2)  $C_{7+}$  average and individual-fraction MWs, and (3) GORs used in recombining separator and SSF samples. A

<sup>22</sup> Katz and Firoozabadi (1978) showed that accurate component K-values can be calculated with Peng-Robinson (1978) EOS using positive BIPs between  $C_i$  and  $C_{7+}$  components, increasing with MW from  $\sim 0.01$ - $0.1$ . PR EOS models almost always require non-zero (often positive  $C_i$ - $C_{7+}$ ) BIPs, while default all HC-HC default BIPs for SRK are usually set to 0.

<sup>23</sup>  $Z_c^{EOS} = 1/3$  for RK or SRK EOS, and  $Z_c^{EOS} = 0.307$  for PR EOS.

composition variable should, ideally, attempt to correct these laboratory uncertainties in a consistent manner for all components.

Our approach to compositional variables may include any of the following three variables: (1) recombination GOR adjustment, typically limited to  $\pm 5\%$  of the lab-reported value; (2) gamma model average  $M_{n+}$  (usually  $C_{7+}$ , sometimes  $C_{11+}$  or  $C_{10+}$ ) with a maximum adjustment  $\pm 5\text{-}10\%$ , resulting in the re-calculation of mass and molar amounts for some or all of the  $C_{n+}$  fractions; and, seldom, (3) independent adjustment of only the  $C_{N+}$  amount, maximum  $\pm 25\%$  of the gamma-model  $C_{N+}$  amount.

Compositional variables are specific for each sample, and they will impact *only* the EOS-calculated results for a particular sample. Thus, for  $N_s$  samples, the number of composition variables can range from 0 to  $3N_s$ , typically  $2N_s$ .

Any compositional adjustment is constrained by the limitation of improving most PVT calculations for a particular sample, and certainly the key PVT data (given higher weighting factors). As a rule, we find that the maximum mol% change is in methane (and total  $C_{7+}$ ), usually  $<1$  mol% from lab-reported, but sometimes up to a maximum change of 2 mol%.

The recombination-GOR composition variable has a strong impact on oil sample bubblepoint pressure, multi-stage separator and DLE GORs. The sample-specific gamma average  $M_{n+}$  variable has a direct impact on surface oil densities, and an indirect impact on gas sample dewpoints. The EOS base characterization gamma average  $M_{n+}$  variable mainly influences the heaviness of  $C_{N+}$ , thereby impacting all samples somewhat, and significantly gas condensate dewpoints and oil sample gas-injection tests like slimtube MMP and vaporization. The adjustment of  $C_{N+}$  amount can have a pronounced impact on dewpoints and liquid dropout behavior.

**Table 6** shows the comparison of initial and final Montney EOS predictions of different PVT data for one sample. The initial EOS has no compositional adjustment while in the final EOS, the sample composition is adjusted with maximum 1 mol% change in methane content, together with adjustments made by EOS component variables. **Table 5** shows an example from Montney basin-wide EOS development, where a sample composition is compared before and after EOS tuning. It can be seen in the table that the composition was modified by maximum 0.7 mol% (methane) compared to the lab-reported composition.

**Weighting Factors Adjustments.** Throughout the EOS tuning process, it is necessary to re-evaluate the weighting factors (initially set to 1). As mentioned earlier, the weighting factors should take into consideration relative data uncertainty, number of data of a given type, and the relative importance of key data. The process of changing weighting factors is subjective, and correlates strongly with an engineer's experience and patience. Our general approach increases the weighting factor of saturation pressures because these data represent an important phase equilibrium state, and because there are far fewer saturation pressures than, for example, other types of data such as densities and relative oil volumes.

Each time the weighting factors are changed, the entire shape of the objective function changes – emphasizing, de-emphasizing, creating or removing minima and maxima compared with the previous optimization (using different weighting factors). With thousands of data making up the objective function, and each data with its own weighting factor, it is obvious that any optimal solution found is non-unique. The decision of which PVT data to include, the weighting factor used, the set of variables chosen, the setting of initial and bounding values for each variable – all of these user decisions result in

the optimal solution found. Even if a global optimum is found, the set of final EOS tuning variables are “your creation” – not mine, and not your colleague’s.

Many assessments of the final EOS model can be made – e.g. plots and tables of measured versus calculated data, statistical quantities like RMS %-error and average %-bias for the entire data set, specific PVT types, specific samples, etc. Establishing whether an EOS model is sufficiently accurate is in “the eyes of the beholder” (not least their understanding of how PVT properties impact the applications using the EOS model). It is impossible to establish a unique “best” tuned EOS model.

EOS prediction results for different Montney samples from our basin-wide, tuned EOS model are summarized in **Figure 12** through **Figure 15** and **Table 7**. This Montney basin-wide EOS predicts PVT data accurately for all samples, with a wide range of compositions, and for relevant temperatures and pressures from reservoir to surface conditions. **Figure 16** shows  $C_1$  and  $C_{7+}$  content versus recombination GOR for the different samples used in Montney EOS model development. The accuracy demonstrated over such a large p-T-z space lends confidence to the EOS model’s ability to predict accurate PVT properties for new samples – samples that most likely fall within the range of fluids used in building the EOS – and for samples that may be outside the range of tuned samples, e.g. injection gases differing from those used in developing the EOS model.

### Viscosity Modeling

After the EOS model has been tuned to satisfaction, the viscosity model can be developed. The Lohrenz-Bray-Clark (LBC) correlation (Lohrenz et al. 1964) is often used for gas and oil viscosity calculations when compositional consistency is required (e.g. when a critical condition is approached and the gas-oil phase properties approach the same value). The original correlation is attributed to Jossi et al. (1962), where viscosity is given as a fourth degree polynomial in reduced density ( $\rho_r = \rho/\rho_c$ ). Critical density ( $\rho_c$ ) is calculated using component critical volumes (or critical Z-factors) and a simple mixing rule. Lohrenz et al. (1964) provide a correlation for  $C_{7+}$  critical density ( $\rho_{c7+}$ ) as a function of  $M_{7+}$  and  $\gamma_{7+}$ , together with the recommendation to use a compositionally-consistent density relationship – that of Alani and Kennedy (1960) based on van der Waals cubic EOS applied to petroleum mixtures.

The LBC model has a bad reputation for oil and high-pressure gas viscosity *predictions* – i.e. without tuning to measured oil and gas viscosity data. This is likely attributed to inappropriate estimates of  $C_{7+}$  critical volumes<sup>24</sup>  $v_{ci}$  ( $\rho_{ci} = 1/v_{ci}$ ). Our preferred method to estimate  $C_{7+}$  fraction  $v_{ci}$  values is summarized by Yang et al. (2007). The idea is to establish  $v_{ci}$  for each  $C_{7+}$  fraction such that the LBC correlation matches exactly a liquid viscosity at 1 atm and reservoir temperature  $\mu_{Li}(p_{sc}, T_R)$ . An appropriate correlation for  $\mu_{Li}$  is the Orrick and Erbar (1973) group contribution technique. If all  $C_{7+}$  fraction values of  $v_{ci}$  are estimated in this manner, we find that predicted oil and high-pressure gas viscosities are usually predicted with 5-15% (close to measurement accuracy). This approach should yield accurate viscosities whether  $C_{7+}$  fractions are described by average SCNs, or each SCN fraction is split into PNA sub-fractions.

If the LBC viscosities still do not predict measured viscosities with sufficient accuracy – even with tuning of the  $C_{7+}$  fraction  $v_{ci}$  values – then some of the original five Jossi polynomial coefficients may be slightly altered along the lines discussed by Lee and Thodos (Lee and Thodos 1990). Our experience with altering the Jossi coefficients is that only the coefficients for higher-order terms  $a_2$ ,  $a_3$  and  $a_4$  ( $\dots + a_2\rho_r^2 + a_3\rho_r^3 + a_4\rho_r^4$ ) should be modified, but it is important to include both gas and oil viscosities

<sup>24</sup> Interestingly, no one seems to use the Lohrenz et al. correlation  $\rho_{c7+}(M_{7+}, \gamma_{7+})$  developed from a large database of reservoir oil viscosities.

when tuning the LBC coefficients. Also, one must always check that tuned coefficients yield a monotonic and physical behavior of the Jossi equation right-hand side,  $\sum_{i=0}^4 a_i \rho_r^i$ , e.g. following guidelines by (Lee and Thodos 1990).

An example of lab oil viscosity data match with the Montney basin wide EOS model using LBC correlation is shown in **Figure 17**.

### Validating an EOS Model

Several consistency checks can and should be made on any EOS model:

1. The software creating an EOS model should always provide three tables with units specified:
  - (a) Component names and properties ( $Name_i, M_i, T_{ci}, p_{ci}, \omega_i, s_i$ ).
  - (b) All non-zero BIPs ( $k_{ij}$ ), with clearly-labeled  $i$ - $j$  values/names for each pair.
  - (c) Example composition in mol% for the component slate given in (a).

Also, the software should clearly state the EOS<sup>25</sup> used.

2. The software creating an EOS model should, at minimum, always calculate a saturation pressure at some relevant temperature for the example composition (above), reporting: saturation pressure and type, and equilibrium phase properties (compositions, K-values, densities, MWs, and viscosities). Additionally, an ambient flash – e.g. one atmosphere and 60°F, with the same calculated properties reported.

All calculated results should be verified in any other software making use of the same EOS model and example composition. *All* calculated results should yield the same as from the original software with 3-5 significant digits. Larger deviations must be reconciled and understood before continued use.

3. Plot of EOS saturation-pressure K-values ( $K_i$ ) versus (a) EOS-calculated NBP ( $T_{bi}^{EOS}$ ) or (b) EOS K-values from an ambient-condition flash, e.g.  $K_i(T_{SC}, p_{SC})$ . Either plot should yield a monotonic trend (at least for *HCS* of the same family<sup>26</sup>); *CO*<sub>2</sub> and *H*<sub>2</sub>*S* may show non-monotonicity without this indicating an inconsistency.

Hydrocarbon component monotonicity shown in this plot should guarantee that K-values do not “cross” in the pressure range from 1 atm to saturation pressure. Crossing K-values would suggest that neighboring components change their relative preference to partition into the gas and oil phases as a function of pressure. When we identify K-values crossing from an EOS model, careful study usually shows that the BIPs were modified inconsistently for neighboring components; BIPs have only a minor role on K-values at low pressures, while BIPs can have a dominant role for higher pressures.

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<sup>25</sup> The original SRK (Soave 1972) is almost always used, but SRK variations are found and sometimes used as the default instead of the original equation. The Peng-Robinson EOS is found in two forms, as originally published in 1976 (Peng and Robinson 1976) and the modification of the  $m$  correlation for hydrocarbons with  $\omega > 0.4$  given by Robinson and Peng in 1978 (Robinson and Peng 1978). Furthermore, some EOS software requires an extra keyword to engage the use of the volume shift correction by Peneloux et al. (1982).

<sup>26</sup> Non-monotonic K-value behavior can be seen for individual isomers in a single carbon number fraction.

4. The check given in step (3) above is the most important consistency check for consistency of *phase behavior* for individual components. An additional check is that atmospheric liquid densities of all  $C_{7+}$  fractions at standard conditions (i.e. specific gravities) – calculated from the EOS model,  $\gamma_i^{EOS} = \rho_{Li}^{EOS}(T_{sc}, p_{sc}) / \rho_w(T_{sc}, p_{sc})$  – follow the observed trends of ASTM distillation data and/or the  $\gamma_i(M_i)$  relationship used to develop the  $C_{7+}$  characterization.

During EOS tuning,  $C_{7+}$  component properties  $(T_{ci}, p_{ci}, \omega_i)$  may be modified to improve phase behavior predictions of lab PVT data. If the corresponding volume shifts  $s_i$  are held constant – and *not* adjusted dynamically to re-fit the desired component specific gravity – then  $(T_{ci}, p_{ci}, \omega_i)$  changes can result in unphysical liquid densities of  $C_{7+}$  fractions from the EOS model. Consistent, dynamic updating of the  $C_{7+}$  fractions will provide more-robust EOS tuning performance by ensuring better oil density predictions.

5. A similar check for individual  $C_{7+}$  fraction liquid viscosities should also be made at a relevant  $(p, T)$  condition – we normally use 1 atm and reservoir temperature. As mentioned in (4) above,  $C_{7+}$  component properties  $(T_{ci}, p_{ci}, \omega_i, s_i)$  may be modified to improve phase and volumetric behavior predictions of lab PVT data. One result of the EOS tuning is that individual  $C_{7+}$  fraction liquid viscosities may be unphysical (e.g. highly non-monotonic). The procedure given by Yang et al. (Yang, 2007) should ensure that individual  $C_{7+}$  fraction liquid viscosities maintain physical consistency.

**Figure 18** and **Figure 19** show some example QC plots of our Montney basin-wide EOS.

## Conclusions

Some key conclusions about developing a common field-wide/basin-wide EOS are summarized below:

1. Incorporate a large number of fluid samples spread throughout the field/basin, with a comprehensive set of PVT tests (depletion, EOR and crude distillation data), spanning a large range of fluid types (GORs).
2. All samples can and should be used in the EOS model development. Uncontaminated sample PVT are preferred for tuning the EOS model, and will in general lead to a more reliable EOS model.
3. Openhole formation testing samples can be very useful in mapping initial fluid variations. OBM-contaminated samples must be mathematically decontaminated, but this is a reliable process that should result in excellent composition estimates at the point of sampling.
4. Quality checks should be performed on lab PVT data as a guide towards (a) whether the data should be included in the EOS tuning process, and (b) setting weighting factors of individual data.
5. The tuned EOS model should contain complete compositional information, including isomers for  $C_7$ - $C_{10}$  fractions (when reported for a sufficient number of samples), extended single-carbon number fractions out to  $C_{29}$  or  $C_{35}$ , with a remaining heaviest fraction  $C_{30+}$  or  $C_{36+}$ .
6. Detailed and thorough heptanes-plus characterization based on TBP crude distillation data and extended compositional analysis from gas chromatography (GC) is an essential starting point for any multi-sample EOS model development.
7. EOS model tuning is a multi-stage process that must effectively reduce hundreds of potential uncertain EOS and compositional parameters down to a manageable set of (e.g.) less than ten variables that change the EOS parameters directly, and 1-2 variables per sample that represent

the uncertainty in laboratory reported compositions well known for the *flash-GC-recombination* method.

8. In addition to defining which variables to use, their initial values, lower- and upper bounds, each PVT data may be assigned a non-default weighting factor to (a) emphasize key PVT data, (b) emphasize a key data type (like saturation pressure) that has many fewer measurements than data (like density), and (c) de-emphasize data of low quality and/or of little importance.
9. The tuned, detailed EOS will provide a “parent” EOS model that forms the basis for creating “child” EOS models designed for specific applications – e.g. gas EOR reservoir simulation, flow assurance, surface processing, and generating black-oil tables.
10. The examples of methods presented in this paper are given for the Montney basin that contains a wide range of reservoir fluids from dry gas to near-critical mixtures to low-moderate oils (similar to other shale basins like Eagle Ford). Similar multi-sample field-wide EOS models have been developed during the past 35 years for many conventional reservoirs around the world.
11. A basin-wide EOS model has a particular advantage because (a) many thousands of wells in a basin may have only 50-100 PVT reports while (b) the gas-oil ratio variation from one well to the next can vary by orders of magnitude. Furthermore, lab PVT studies of liquid-rich fluids (with GORs in the range 1,000-10,000 scf/STB) do *not* provide directly the PVT data required by many disciplines, and correlations are not applicable.

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## Nomenclature

$\bar{r}$	Root mean square (RMS)
$\mu_L$	Liquid viscosity, <i>cp</i>
$d_c$	EOS calculated data
$d_e$	Input data to PVT regression
$F_g$	Gas fraction on molar basis
$F_{gw}$	Gas fraction on weight basis
$K$	Equilibrium ratio (K-values)
$k_{ij}$	Binary interaction parameter between component <i>i</i> and component <i>j</i>
$M$	Molecular weight
$N$	Number of PVT data points
$N_c$	Number of EOS components for EOS regression
$N_s$	Number of PVT samples
$N_v$	Number of total variables for EOS regression
$p_c$	Component average critical pressure, <i>psia or kPa</i>
$p_{sc}$	Standard pressure, <i>psia or kPa</i>
$R$	Universal gas constant, $J.mol^{-1}.K^{-1}$
$r$	Residual
$R_s$	Surface gas volume from reservoir oil phase per unit surface oil volume from reservoir oil phase, <i>scf/bbl or Sm<sup>3</sup>/m<sup>3</sup></i>
$r_s$	Surface oil volume from reservoir gas phase per unit surface gas volume from reservoir gas phase, <i>bbl/MMscf or m<sup>3</sup>/Sm<sup>3</sup></i>
$s$	Component dimensionless volume-shift factors

$T_b$	Component average normal boiling point temperature, °R or K
$T_c$	Component average critical temperature, °R or K
$T_{sc}$	Standard temperature, °R or K
$v_c$	Component critical molar volume, $ft^3/lbmol$ or $m^3/kmol$
$w$	Component mass fraction
$W$	Weight factor
$x$	Component mole fraction in oil phase
$y$	Component mole fraction in gas phase
$z$	Component mole fraction in overall mixture
$Z_c$	Component critical Z-factors
$\rho$	Density, $lbm/ft^3$ or $kg/m^3$
$\rho_r$	Reduced density
$\sigma$	Standard deviation
$\omega$	Component acentric factors
$\gamma$	Specific gravity

### Subscripts

6-	Components lighter than hexane
6+	Hexane and heavier components
7+	Heptane and heavier components
A	Aromatic
g	Gas phase
gsp	Gas phase at separator conditions
i	Component index
k	PVT data index
L	Lower-bound
N+	Component index of the heaviest fraction in EOS characterization
n+	$C_n$ and heavier components where 'n' being usually 7 or 11
o	Oil phase
$\bar{o}$	Stabilized surface crude (oil and condensate)
osp	Oil phase at separator conditions
P	Paraffinic

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TABLE 1 – WHITSON FIELD/BASIN WIDE EOS DEVELOPMENT PROJECTS IN THE PAST 35 YEARS.		
Region	Country	Fields / Basins
Europe	Denmark	South Arne
	Italy	Tempa Rossa
	Italy	Val D'agri
	Norway	Asgard (Smorbuk, Smorbuk South, etc.)
	Norway	Dagny
	Norway	Fram
	Norway	Greater Ekofisk Area
	Norway	Gullfaks South
	Norway	Oseberg, Oseberg East and Oseberg South
	Norway	Troll
	Norway	Gjoa, Grane, Sleipner, Vale and Visund
	Romania	Independenta
South America	UK	Jade
	Colombia	Foothills Area (Cusiana, Cupiagua, Pauto Complex)
North America	Venezuela	Orocual
	Canada	Amauligak (Beaufort Sea)
	Canada	Weyburn
	Canada	Montney
	USA	Bakken
	USA	Eagle Ford
	USA	Permian
	USA	SCOOP/STACK/MERGE
	USA	GOM - Magnolia, Ursa, Macondo & Baldpate
	USA	Several West Texas CO2 EOR fields (Slaughter, Postae, Welch, Mallet, Salt Creek)
Middle East	Iran	South Pars
	Iraq	Shaikan
	Iraq	Sheikh Adi
	Oman	Barik
	Qatar	Dukhan
	Qatar	North Field
	Saudi Arabia	10 largest oil fields, 10 gas condensate fields
	UAE	Asab
	UAE	Bab
	UAE	Bunduq
	UAE	Lower Zakum
Africa	UAE	Ghasha, Hair Dalma, Rumaitha and Shuwaihat
	Algeria	MLNW and Ohanet
	Angola	Chissonga
	Equatorial Guinea	Belinda
	Ghana	Jubilee
	Ghana	Tweneboa
	Libya	El Mehari
	Libya	Gullebi
	Libya	Bu Attifel, Faregh and Nakhla
	Nigeria	Assa-North and Ohaji South
	South Africa	E-CE
	Tanzania	Songo Songo
	Tunisia	Hassdrubal, Ashtart, El Franig and Miskar
	Asia	Indonesia
Indonesia		Natuna Sea and Kido
Kazakhstan		Karachaganak
Pakistan		Ratana
Philippines		Malampaya
Vietnam		Ca Rong Do
Vietnam		Rang Dong
Vietnam		Su Tu Trang
Vietnam		CLJOC, HLJOC and Minh Hai

} Unconventional Basins

TABLE 2 – EXAMPLE OF CVD MATERIAL BALANCE QC FOR A MONTNEY SAMPLE. (Forward MB: Final Oil Composition    Backward MB: Initial Reservoir Composition)					
Forward Material Balance			Backward Material Balance		
Component	Measured mol%	Calculated mol%	Component	Measured mol%	Calculated mol%
N <sub>2</sub>	0.000	-0.059	N <sub>2</sub>	0.170	0.180
CO <sub>2</sub>	0.100	0.005	CO <sub>2</sub>	0.200	0.216
H <sub>2</sub> S	0.000	0.000	H <sub>2</sub> S	0.000	0.000
C <sub>1</sub>	8.790	7.728	C <sub>1</sub>	65.830	65.976
C <sub>2</sub>	7.110	7.361	C <sub>2</sub>	10.750	10.705
C <sub>3</sub>	8.070	7.998	C <sub>3</sub>	5.750	5.763
i-C <sub>4</sub>	2.840	2.309	i-C <sub>4</sub>	1.160	1.250
n-C <sub>4</sub>	5.630	5.492	n-C <sub>4</sub>	2.320	2.345
i-C <sub>5</sub>	3.590	3.383	i-C <sub>5</sub>	0.990	1.027
n-C <sub>5</sub>	3.940	3.903	n-C <sub>5</sub>	1.060	1.068
C <sub>6</sub>	5.660	5.943	C <sub>6</sub>	1.370	1.325
C <sub>7</sub>	7.070	7.689	C <sub>7</sub>	1.610	1.509
C <sub>8</sub>	9.360	10.294	C <sub>8</sub>	1.990	1.837
C <sub>9</sub>	6.920	7.382	C <sub>9</sub>	1.360	1.286
C <sub>10</sub>	5.330	5.326	C <sub>10</sub>	0.970	0.973
C <sub>11+</sub>	25.590	25.250	C <sub>11+</sub>	4.470	4.540
Total	100	100	Total	100	100

TABLE 3 – COMPONENT SLATE FOR MONTNEY BASIN WIDE DETAILED EOS CHARACTERIZATION <sup>27</sup> .						
N <sub>2</sub>	C-C <sub>5</sub>	C <sub>8</sub> -SCN	C <sub>11</sub>	C <sub>21</sub>	C <sub>31</sub>	
CO <sub>2</sub>	C <sub>6</sub> -SCN	C <sub>8</sub> *	C <sub>12</sub>	C <sub>22</sub>	C <sub>32</sub>	
H <sub>2</sub> S	C <sub>6</sub> *	E-Benzene	C <sub>13</sub>	C <sub>23</sub>	C <sub>33</sub>	
C <sub>1</sub>	MC-C <sub>5</sub>	m-xylene	C <sub>14</sub>	C <sub>24</sub>	C <sub>34</sub>	
C <sub>2</sub>	C-C <sub>6</sub>	o-xylene	C <sub>15</sub>	C <sub>25</sub>	C <sub>35</sub>	
C <sub>3</sub>	Benzene	C <sub>9</sub> -SCN	C <sub>16</sub>	C <sub>26</sub>	C <sub>36p</sub>	
i-C <sub>4</sub>	C <sub>7</sub> -SCN	C <sub>9</sub> *	C <sub>17</sub>	C <sub>27</sub>		
n-C <sub>4</sub>	C <sub>7</sub> *	124TM-BEN	C <sub>18</sub>	C <sub>28</sub>		
i-C <sub>5</sub>	MC-C <sub>6</sub>	C <sub>10</sub> -SCN	C <sub>19</sub>	C <sub>29</sub>		
n-C <sub>5</sub>	Toluene	C <sub>10</sub> *	C <sub>20</sub>	C <sub>30</sub>		

<sup>27</sup> Component  $C_i^*$  ( $i=6$  to  $10$ ) is defined as the single carbon number component which is devoid of its respective lab reported isomers. These components are generally reported as normal paraffins by the PVT labs when they report isomers in their GC analysis. However, we have found that these components are not exactly normal paraffins but more paraffinic than the total SCN fractions  $C_i$  (mentioned as  $C_i$ -SCN in the table). The properties ( $M$ ,  $\gamma$ ,  $T_b$ ) of such fractions can be calculated by having (a) extended GC analysis of a stock tank oil sample with isomers and (b) measured properties of total SCN fractions i.e.  $C_i$ -SCN of the same sample. One source of getting measured properties of SCN fractions is ASTM D2892 analysis. In the absence of such analysis,  $C_i^*$  can be approximated as  $n-C_i$ .

**TABLE 4 – WORKFLOW FOR DEFINING SAMPLE COMPOSITIONS IN THE EOS CHARACTERIZATION.**

Lab Characterization 01		Lab Characterization 02			EOS Characterization			
Comp	SPG mol%	Comp	SPO mol%	REC mol%	Comp	SPG <sup>1</sup> mol%	SPO <sup>2</sup> mol%	REC <sup>3</sup> mol%
N <sub>2</sub>	0.49	N <sub>2</sub>	0.03	0.37	N <sub>2</sub>	0.49	0.05	0.37
CO <sub>2</sub>	0.61	CO <sub>2</sub>	0.11	0.48	CO <sub>2</sub>	0.61	0.13	0.48
H <sub>2</sub> S	0.00	H <sub>2</sub> S	0.00	0.00	H <sub>2</sub> S	0.00	0.00	0.00
C <sub>1</sub>	81.85	C <sub>1</sub>	7.60	62.07	C <sub>1</sub>	81.85	7.72	62.10
C <sub>2</sub>	9.69	C <sub>2</sub>	4.26	8.24	C <sub>2</sub>	9.69	4.31	8.25
C <sub>3</sub>	4.79	C <sub>3</sub>	6.60	5.27	C <sub>3</sub>	4.79	6.67	5.29
i-C <sub>4</sub>	0.65	i-C <sub>4</sub>	1.76	0.95	i-C <sub>4</sub>	0.65	1.79	0.95
n-C <sub>4</sub>	1.25	n-C <sub>4</sub>	4.98	2.24	n-C <sub>4</sub>	1.25	5.04	2.26
i-C <sub>5</sub>	0.26	i-C <sub>5</sub>	2.77	0.93	i-C <sub>5</sub>	0.26	2.81	0.94
n-C <sub>5</sub>	0.24	n-C <sub>5</sub>	3.58	1.13	n-C <sub>5</sub>	0.24	3.63	1.14
C <sub>6</sub> *	0.11	C-C <sub>5</sub>	0.41	0.11	C-C <sub>5</sub>	0.00	0.42	0.11
C <sub>7</sub> *	0.04	C <sub>6</sub> *	6.49	1.81	C <sub>6</sub> *	0.11	6.56	1.83
C <sub>8</sub> *	0.01	MC-C <sub>5</sub>	1.08	0.29	MC-C <sub>5</sub>	0.00	1.07	0.29
C <sub>9</sub> *	0.01	C-C <sub>6</sub>	1.10	0.29	C-C <sub>6</sub>	0.00	1.07	0.29
C <sub>10</sub> *	0.00	Benzene	0.47	0.13	Benzene	0.00	0.46	0.12
C <sub>11</sub>	0.00	C <sub>7</sub> *	5.44	1.48	C <sub>7</sub> *	0.04	5.35	1.46
C <sub>12</sub>	0.00	MC-C <sub>6</sub>	1.71	0.46	MC-C <sub>6</sub>	0.00	1.90	0.51
		Toluene	1.24	0.33	Toluene	0.00	1.37	0.37
		C <sub>8</sub> *	5.63	1.51	C <sub>8</sub> *	0.01	6.29	1.68
		E-Benzene	0.98	0.26	E-Benzene	0.00	0.99	0.26
		o-xylene	0.42	0.11	o-xylene	0.00	0.42	0.11
		C <sub>9</sub> *	5.61	1.50	C <sub>9</sub> *	0.01	5.52	1.48
		124TM-BEN	1.29	0.34	124TM-BEN	0.00	1.18	0.31
		C <sub>10</sub> *	4.56	1.21	C <sub>10</sub> *	0.00	4.26	1.14
		C <sub>11</sub>	4.12	1.10	C <sub>11</sub>	0.00	3.85	1.03
		C <sub>12</sub>	3.26	0.87	C <sub>12</sub>	0.00	3.02	0.81
		C <sub>13</sub>	3.31	0.88	C <sub>13</sub>	0.00	3.07	0.82
		C <sub>14</sub>	2.63	0.70	C <sub>14</sub>	0.00	2.45	0.65
		C <sub>15</sub>	1.97	0.53	C <sub>15</sub>	0.00	2.01	0.54
		C <sub>16</sub>	1.65	0.44	C <sub>16</sub>	0.00	1.59	0.42
		C <sub>17</sub>	1.42	0.38	C <sub>17</sub>	0.00	1.47	0.39
		C <sub>18</sub>	1.42	0.38	C <sub>18</sub>	0.00	1.44	0.38
		C <sub>19</sub>	1.31	0.35	C <sub>19</sub>	0.00	1.29	0.34
		C <sub>20</sub>	1.01	0.27	C <sub>20</sub>	0.00	1.01	0.27
		C <sub>21</sub>	0.94	0.25	C <sub>21</sub>	0.00	0.92	0.24
		C <sub>22</sub>	0.80	0.21	C <sub>22</sub>	0.00	0.82	0.22
		C <sub>23</sub>	0.73	0.19	C <sub>23</sub>	0.00	0.73	0.20
		C <sub>24</sub>	0.65	0.17	C <sub>24</sub>	0.00	0.66	0.18
		C <sub>25</sub>	0.61	0.16	C <sub>25</sub>	0.00	0.63	0.17
		C <sub>26</sub>	0.53	0.14	C <sub>26</sub>	0.00	0.52	0.14
		C <sub>27</sub>	0.48	0.13	C <sub>27</sub>	0.00	0.48	0.13
		C <sub>28</sub>	0.42	0.11	C <sub>28</sub>	0.00	0.43	0.12
		C <sub>29</sub>	0.38	0.10	C <sub>29</sub>	0.00	0.39	0.10
		C <sub>30p</sub>	4.24	1.13	C <sub>30p</sub>	0.00	4.20	1.12

<sup>1</sup>SPG composition is brought from lab characterization by conserving lab reported mass amounts and converted to moles using EOS components molecular weights

<sup>2</sup>SPO composition is brought from lab characterization by conserving lab reported mass amounts and converted to moles using EOS component molecular weights and also replacing lab reported C<sub>7</sub> fractions mass amounts with the gamma model

<sup>3</sup>Mathematical recombined composition calculated from SPO and SPG compositions defined in the EOS characterization and using lab reported F<sub>g</sub>

TABLE 5 – EXAMPLE OF A SAMPLE COMPOSITION BEFORE AND AFTER EOS TUNING.

Comp	Lab Reported	After Tuning	Comp	Lab Reported	After Tuning
	mol%	mol%		mol%	mol%
N <sub>2</sub>	0.22	0.30	C <sub>16</sub>	0.78	0.72
CO <sub>2</sub>	0.07	0.07	C <sub>17</sub>	0.69	0.66
H <sub>2</sub> S	0.00	0.00	C <sub>18</sub>	0.66	0.64
C <sub>1</sub>	39.61	40.31	C <sub>19</sub>	0.59	0.57
C <sub>2</sub>	10.10	10.41	C <sub>20</sub>	0.45	0.45
C <sub>3</sub>	8.77	8.56	C <sub>21</sub>	0.41	0.40
i-C <sub>4</sub>	1.34	1.52	C <sub>22</sub>	0.36	0.36
n-C <sub>4</sub>	4.13	4.21	C <sub>23</sub>	0.32	0.32
i-C <sub>5</sub>	1.52	1.38	C <sub>24</sub>	0.28	0.28
n-C <sub>5</sub>	2.42	2.23	C <sub>25</sub>	0.28	0.27
C-C <sub>5</sub>	0.26	0.17	C <sub>26</sub>	0.21	0.22
C <sub>6</sub> *	2.86	2.68	C <sub>27</sub>	0.22	0.20
MC-C <sub>5</sub>	0.70	0.57	C <sub>28</sub>	0.20	0.18
C-C <sub>6</sub>	0.74	0.62	C <sub>29</sub>	0.17	0.16
Benzene	0.12	0.10	C <sub>30p</sub>	1.79	1.64
C <sub>7</sub> *	2.74	2.92			
MC-C <sub>6</sub>	1.22	1.10			
Toluene	0.32	0.32			
C <sub>8</sub> *	2.85	3.06			
E-Benzene	0.60	0.58			
o-xylene	0.17	0.14			
C <sub>9</sub> *	2.46	2.55			
124TM-BEN	0.28	0.26			
C <sub>10</sub> *	2.11	2.23			
C <sub>11</sub>	1.86	1.79			
C <sub>12</sub>	1.48	1.39			
C <sub>13</sub>	1.47	1.41			
C <sub>14</sub>	1.12	1.12			
C <sub>15</sub>	1.05	0.91			

TABLE 6 – COMPARISON OF LAB PVT DATA CALCULATIONS WITH INITIAL EOS (NO COMPOSITIONAL ADJUSTMENT) AND FINAL EOS (WITH COMPOSITIONAL ADJUSTMENT).							
Pres	Single Phase Oil Density (g/cc)						
	psia	Lab Data	Initial EOS <sup>1</sup>	Tuned EOS <sup>2</sup>			
	7015	0.540	0.562	0.548			
	6015	0.529	0.550	0.535			
	5515	0.523	0.543	0.528			
	5015	0.516	0.536	0.520			
	4715	0.512	0.531	0.515			
	4571	0.509	0.529	0.513			
	4415	0.506	0.526	0.510			
	4320	0.504	0.528	0.508			
Pres	CVD Oil Saturation (%)			CVD Gas Z-factors			
	psia	Lab Data	Initial EOS	Tuned EOS	Lab Data	Initial EOS	Tuned EOS
	4320	100	97	100	-	0.895	0.899
	3715	66	81	78	0.839	0.811	0.819
	3115	60	73	70	0.801	0.775	0.791
	2515	56	67	64	0.795	0.767	0.788
	1915	52	61	58	0.814	0.783	0.803
	1315	48	56	52	0.851	0.822	0.837
	715	43	51	47	0.905	0.880	0.889
Pres	Temp	Solution Gas Oil Ratio (scf/STB)					
		psia	°F	Lab Data	Initial EOS	Tuned EOS	
		4320	153	2885	2681	2795	
		67	75	39	25	24	
		15	60	0	0	0	
<sup>1</sup> EOS model without any tuning to component properties and no compositional adjustment							
<sup>2</sup> EOS model with tuned component properties and sample composition							

TABLE 7 – EXAMPLE OF SEPARATOR TEST PVT RESULTS WITH THE MONTNEY COMMON EOS MODEL.						
PVT Samples	Total GOR		Oil Density at $p_s(T_R)$		STO Density	
	Lab Data	EOS Calc	Lab Data	EOS Calc	Lab Data	EOS Calc
Sample 1	2706	2685	0.510	0.506	0.778	0.776
Sample 2	2375	2337	0.515	0.518	0.776	0.777
Sample 3	1671	1663	0.577	0.588	0.798	0.795
Sample 4	1252	1240	0.601	0.619	0.794	0.794

$p_s(T_R)$  is the saturation pressure of the sample at reservoir temperature

Figures

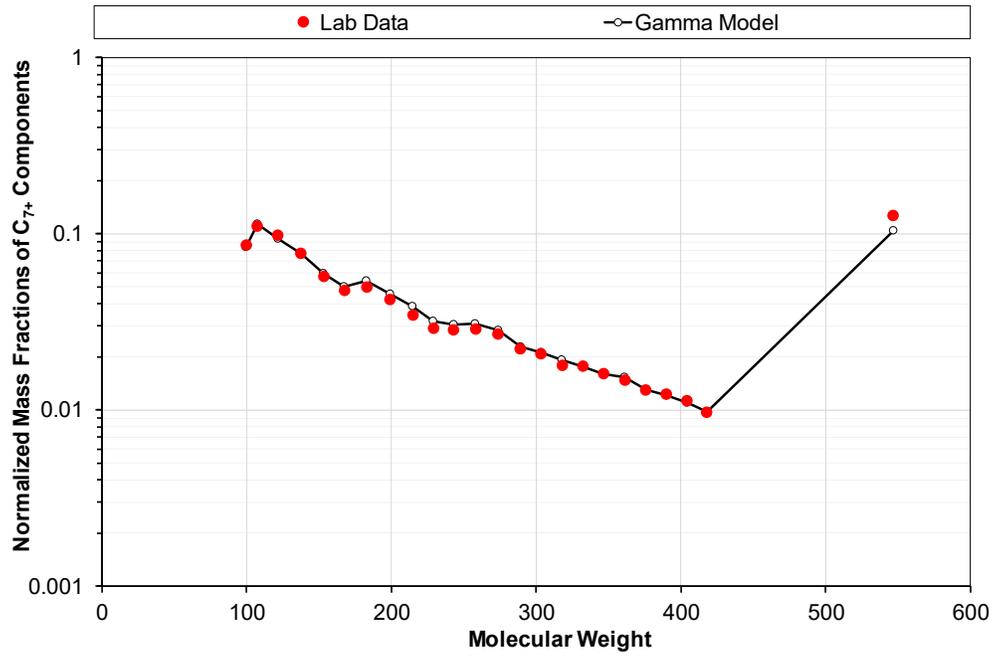


Figure 1. Example of using the gamma distribution model to quality check the sample composition.

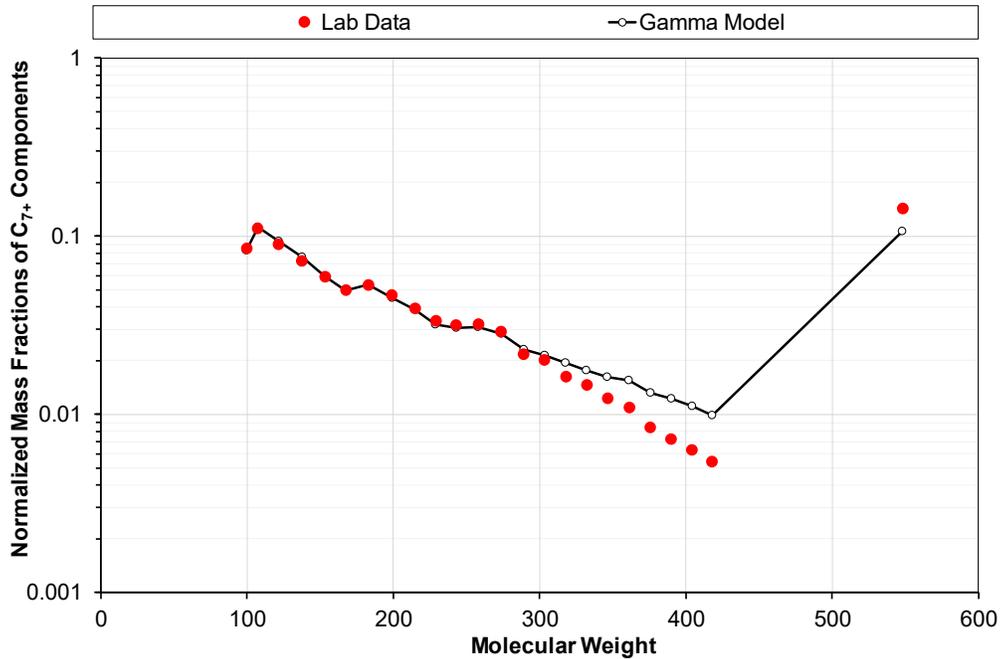


Figure 2. Example showing bad quality gas chromatography data for C<sub>20+</sub> fractions which can be corrected using the gamma distribution model.

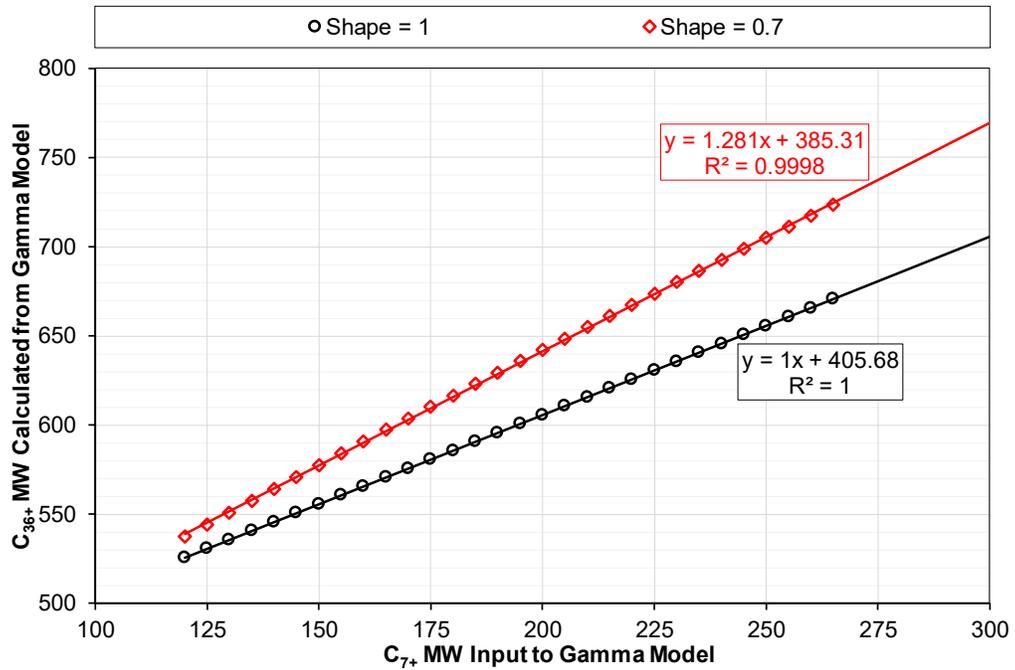


Figure 3. Calculations of sample  $C_{36+}$  molecular weight as a function of sample  $C_{7+}$  MW with a gamma distribution model with shape = 1 (exponential) and shape = 0.7.

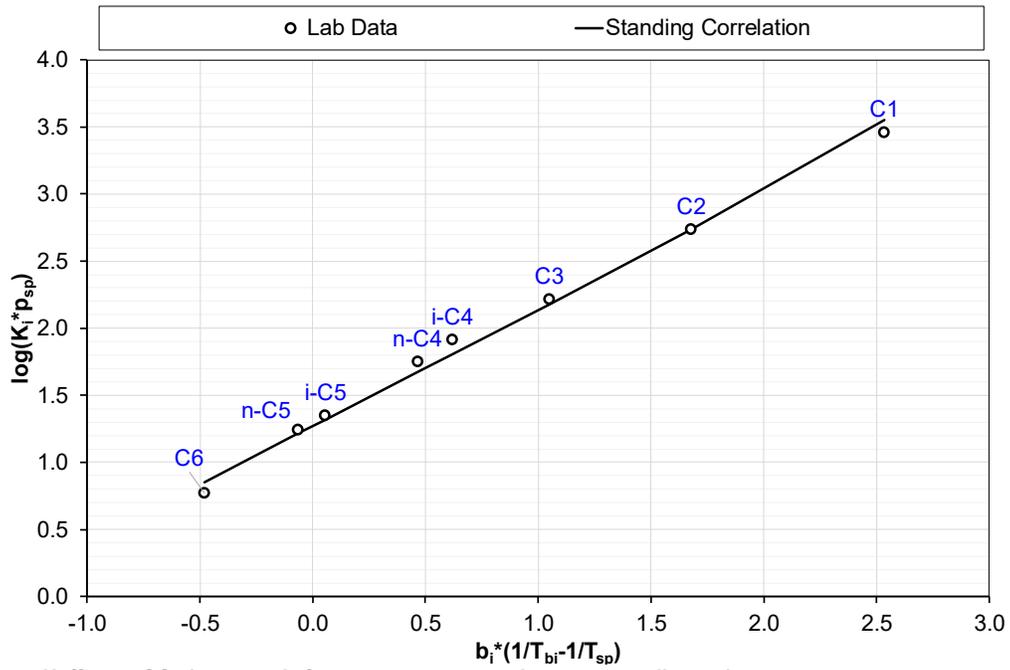


Figure 4. Hoffmann QC plot example for a separator gas and a separator oil sample.

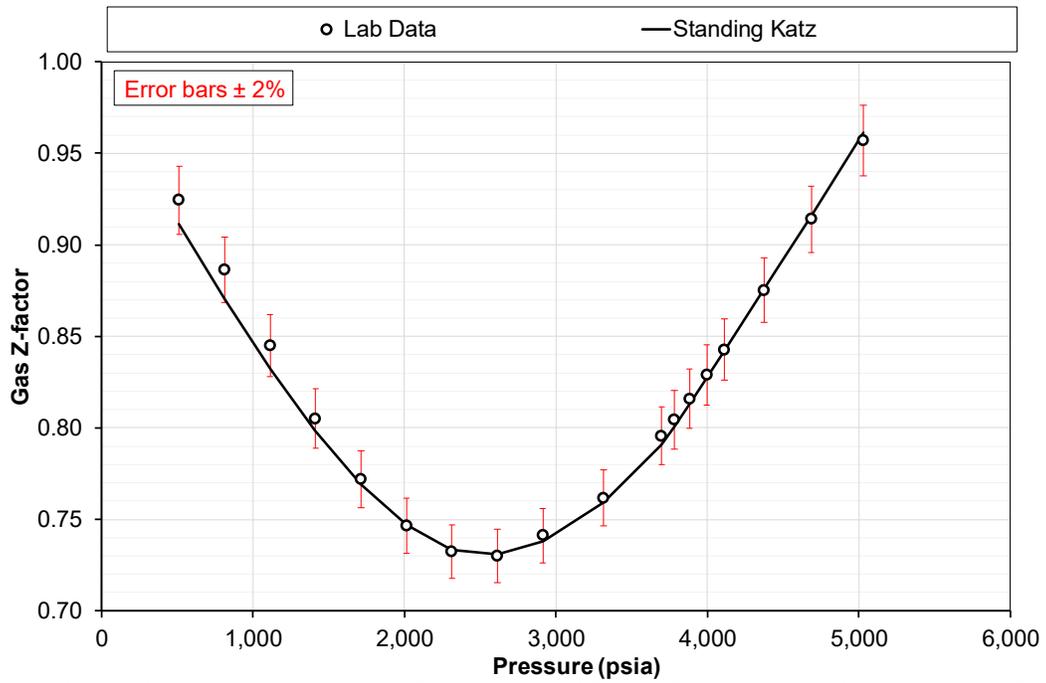


Figure 5. Quality check of the lab reported gas Z-factors from CCE and CVD experiments using Standing Katz Z-factor chart.

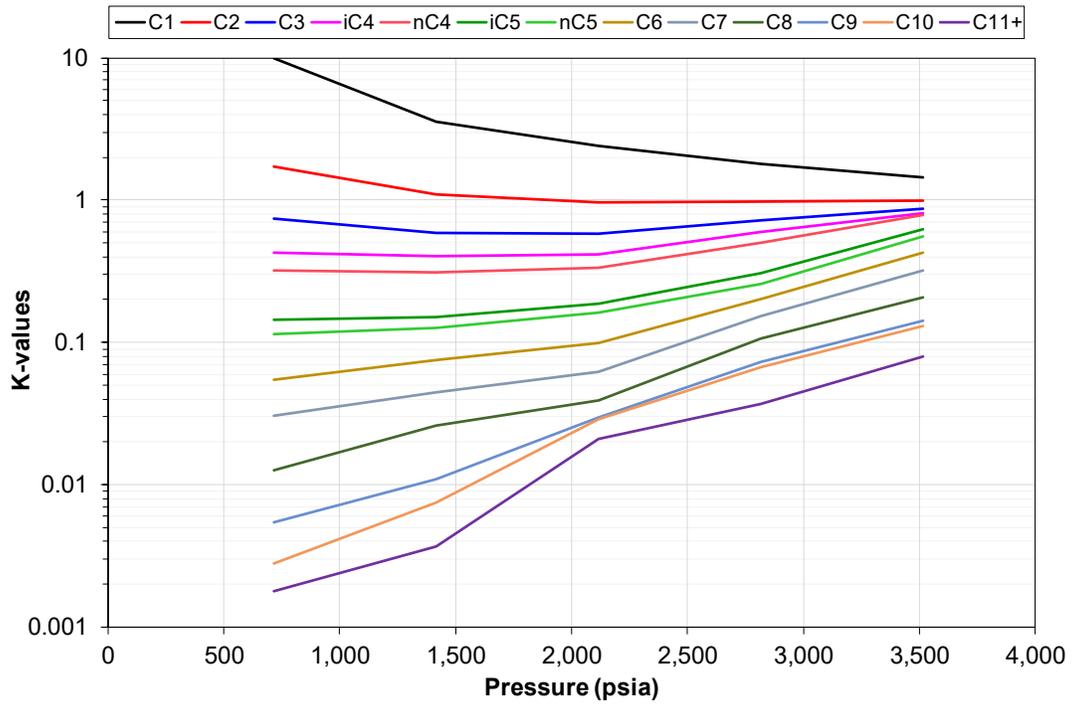


Figure 6. CVD data QC by plotting K-values calculated from lab reported gas compositions and forward material balance calculated equilibrium oil compositions at each pressure stage of the experiment.

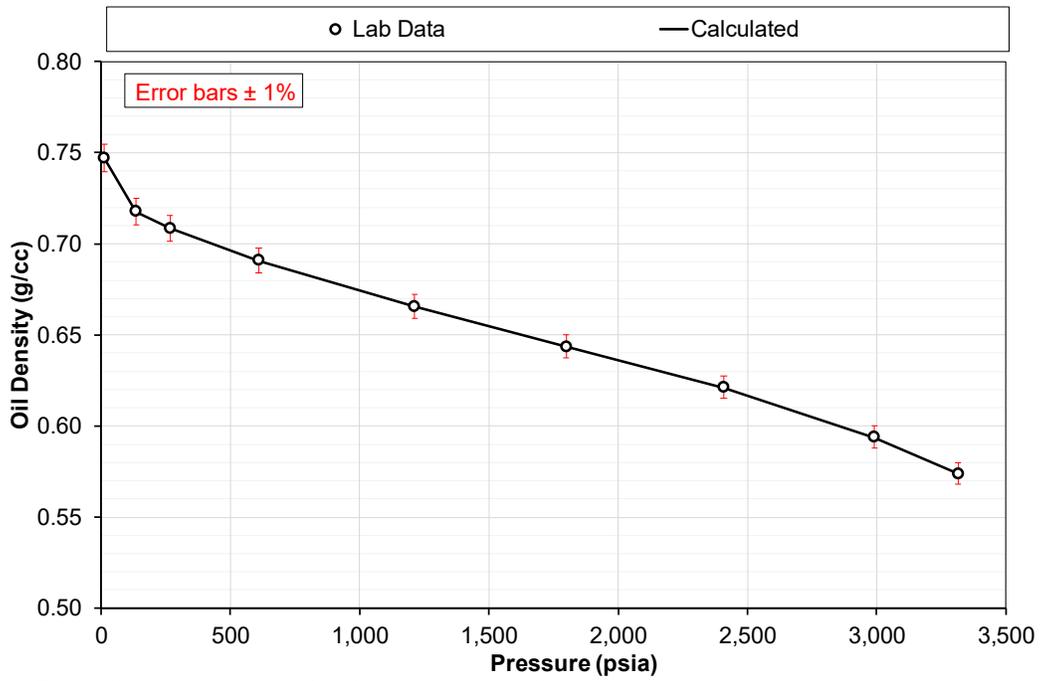


Figure 7. Quality checking lab reported DLE oil densities with material balance calculations.

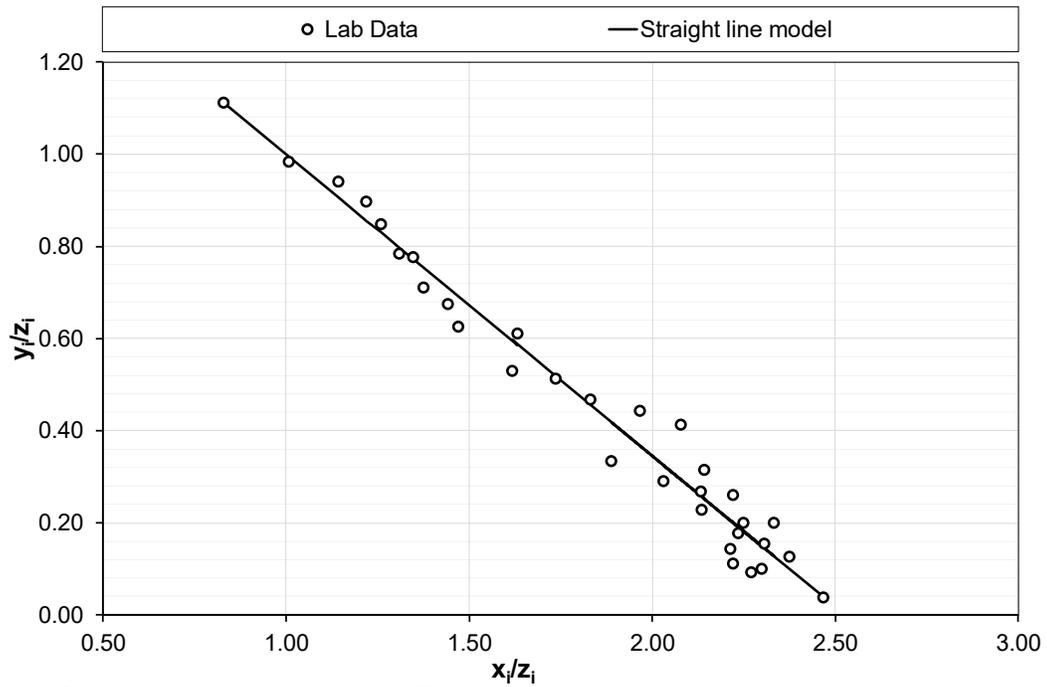


Figure 8. Quality checking the lab reported equilibrium compositions ( $y_i$  and  $x_i$ ) at reservoir pressure and temperature with material balance calculations knowing the total composition  $z_i$ .

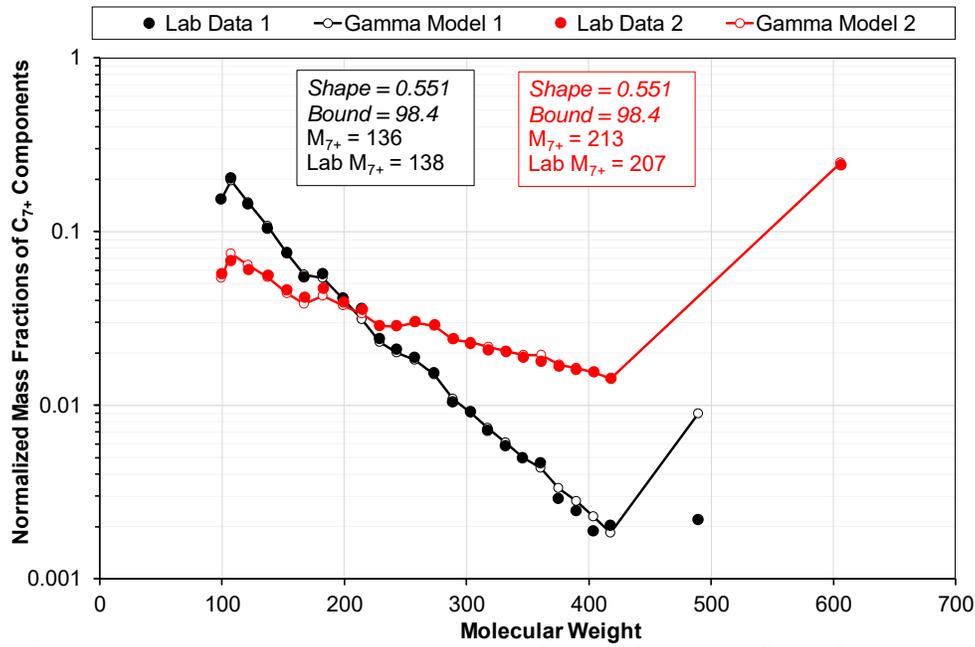


Figure 9. Example showing Montney basin-wide gamma model fit results for the two different (C<sub>7+</sub>, MW) samples.

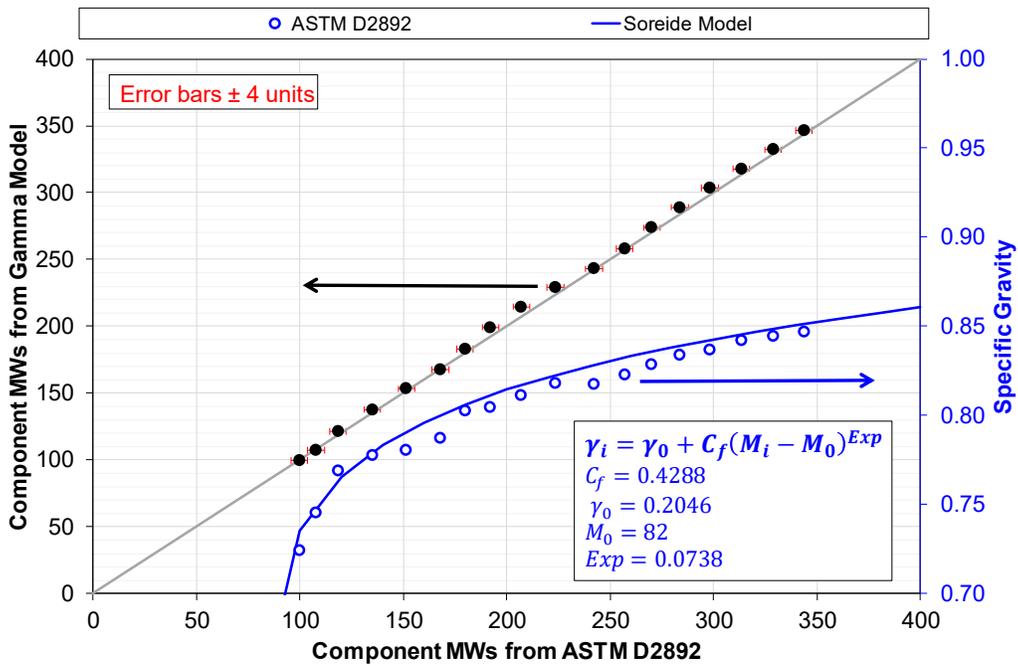


Figure 10. Comparison of gamma model calculated component molecular weights versus ASTM D2892 measured data for the Montney basin (in black). Sørense correlation developed for Montney using ASTM D2892 measured data (in blue).

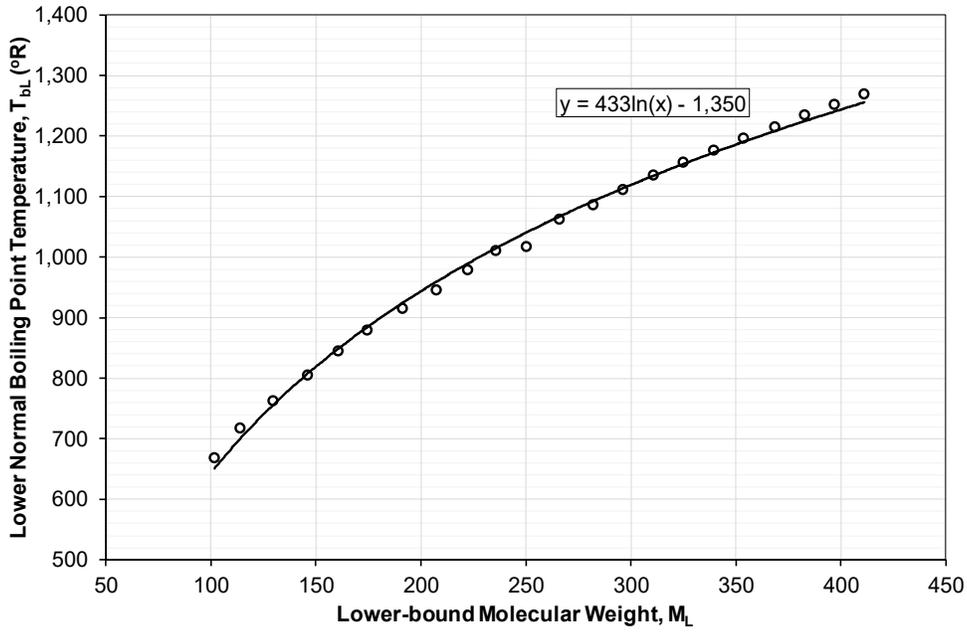


Figure 11. Lower normal boiling point temperature versus (gamma model) lower-bound molecular weight correlation developed for the Montney basin.

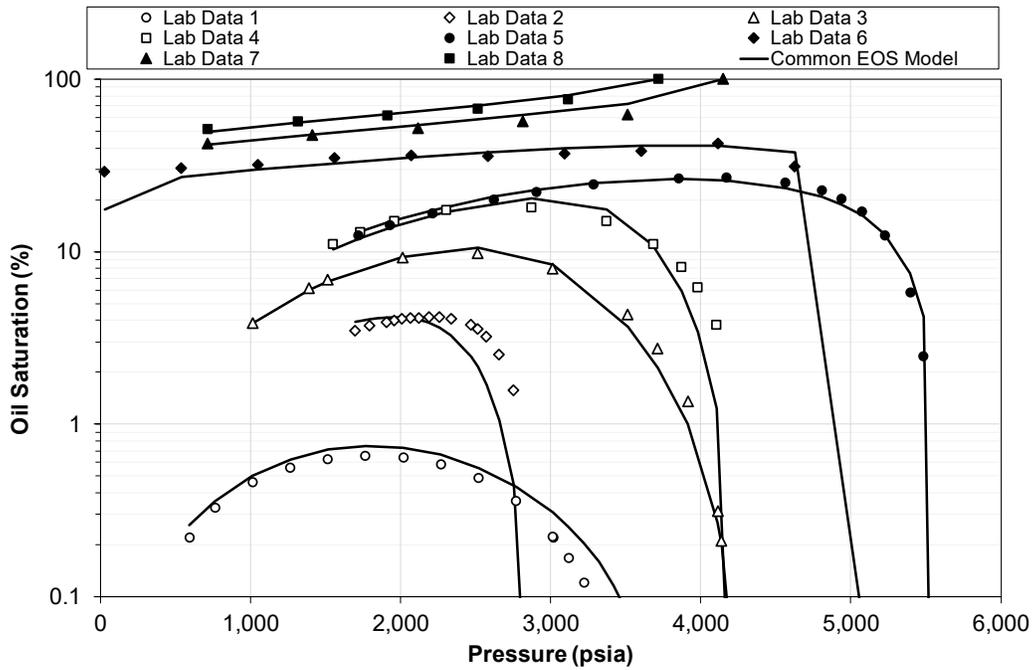


Figure 12. Oil saturations calculated by a common Montney EOS model for the different Montney samples used in the EOS model development, ranging from lean gas condensate (maximum liquid drop out less than 1%) to black oils.

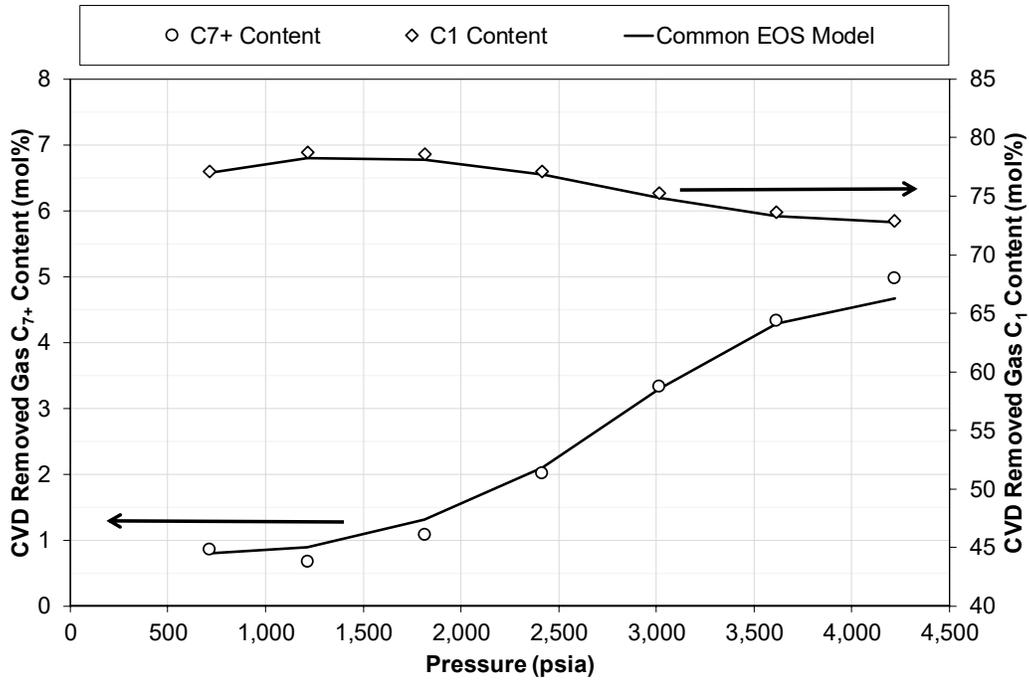


Figure 13. CVD removed gas compositions calculated by the common EOS model for one of the PVT samples used in the EOS model development.

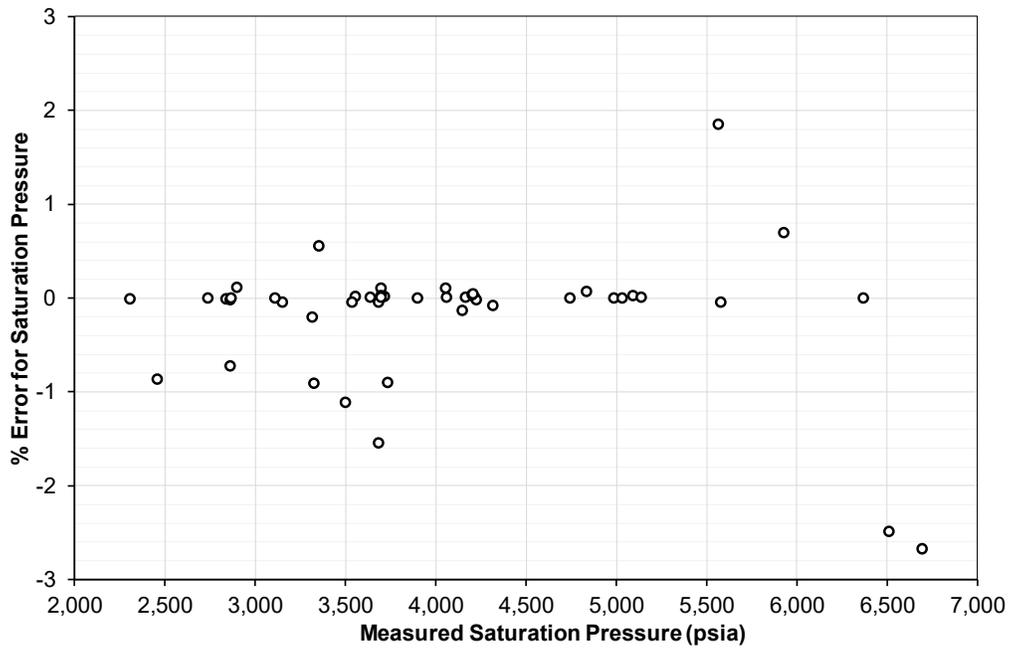


Figure 14. Saturation pressure deviations with the common Montney EOS model for the different PVT samples used in the EOS model tuning.

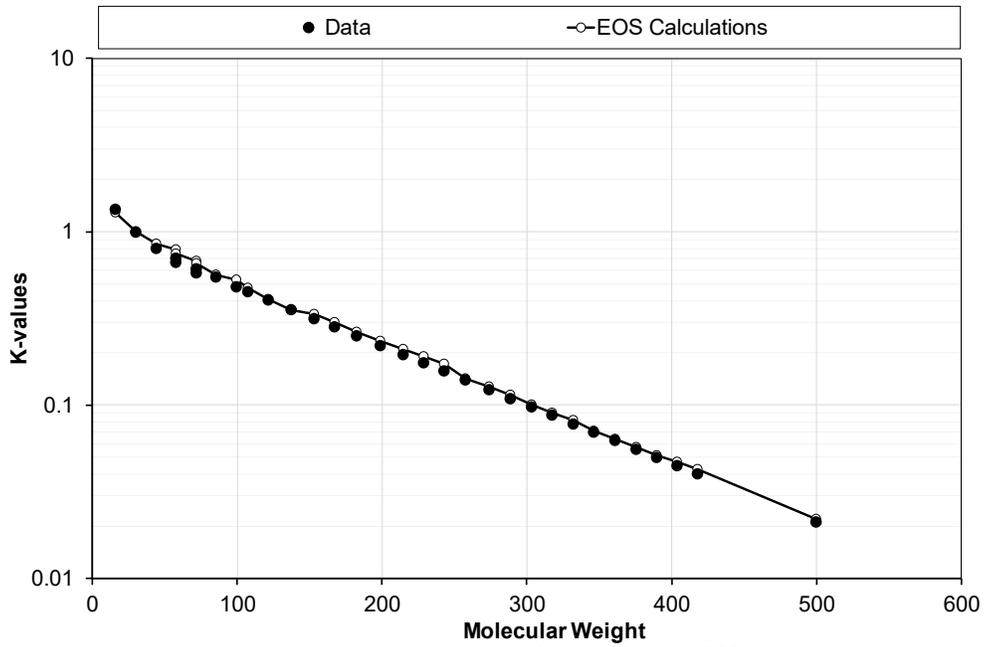


Figure 15. High pressure (and temperature) K-values calculated by the Montney EOS model against the input data used for the EOS tuning.

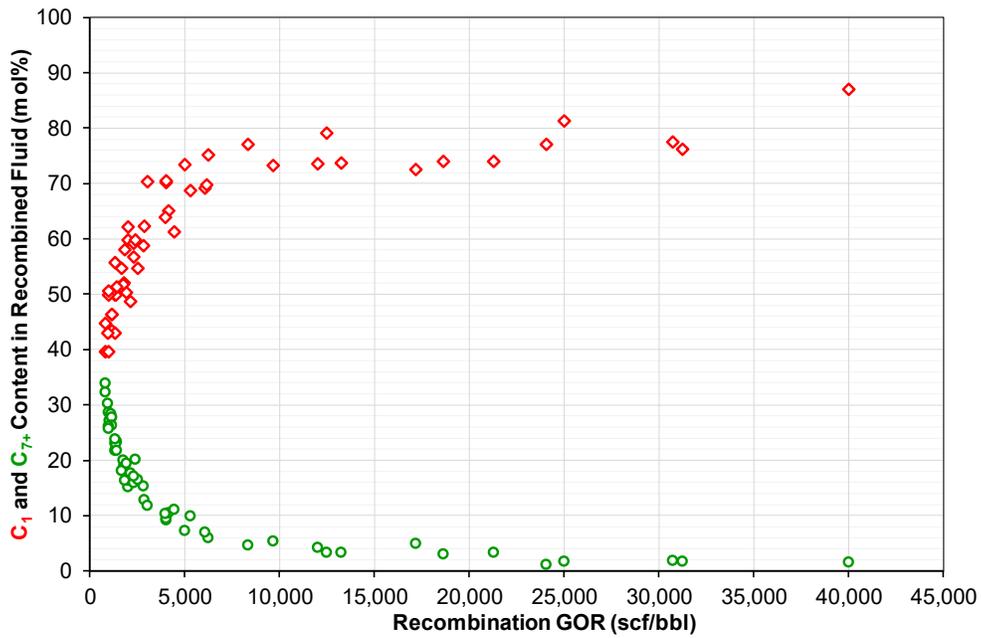


Figure 16.  $C_1$  and  $C_{7+}$  contents in recombined fluid versus recombination GOR for the different samples used in the Montney basin-wide EOS model development.

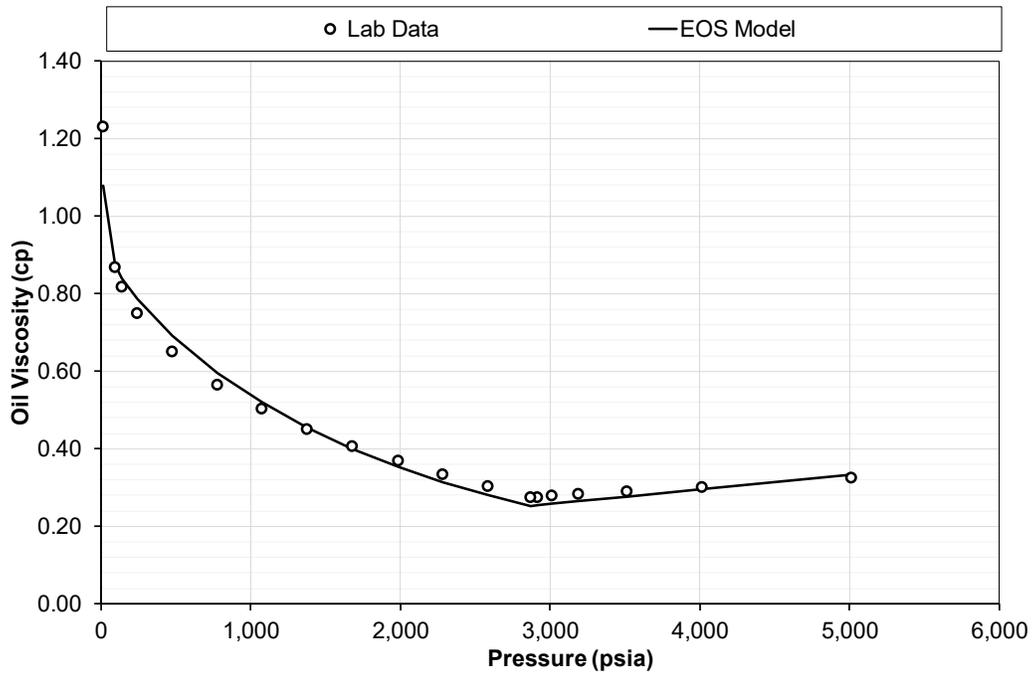


Figure 17. Oil viscosities calculated by the common Montney EOS model for one of the oil samples used in the EOS model development.

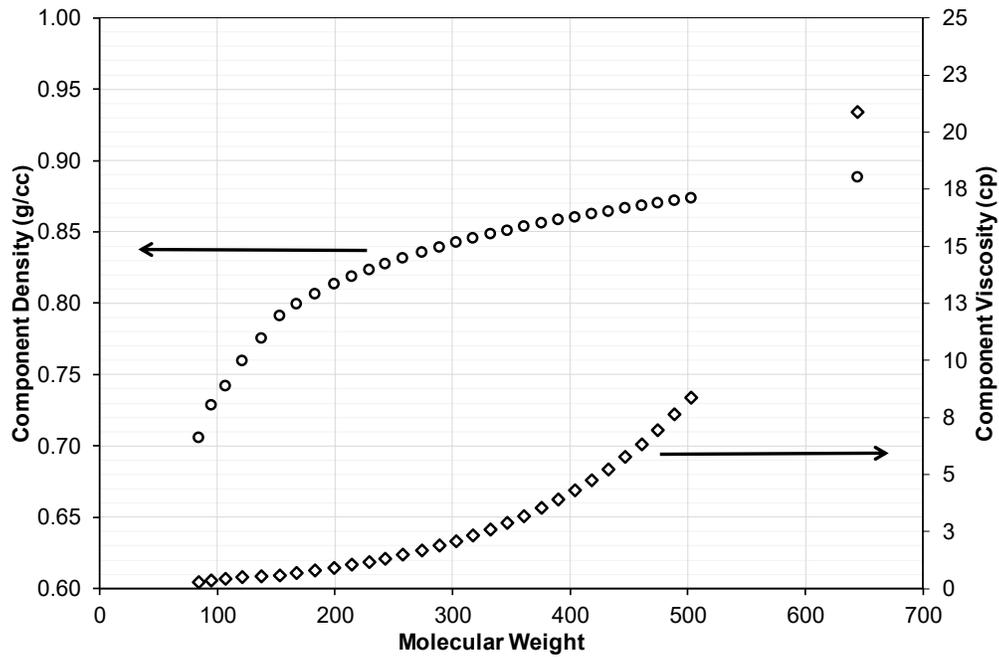


Figure 18. Monotonicity check of the components' density and viscosity versus molecular weight for the final (common) Montney EOS model.

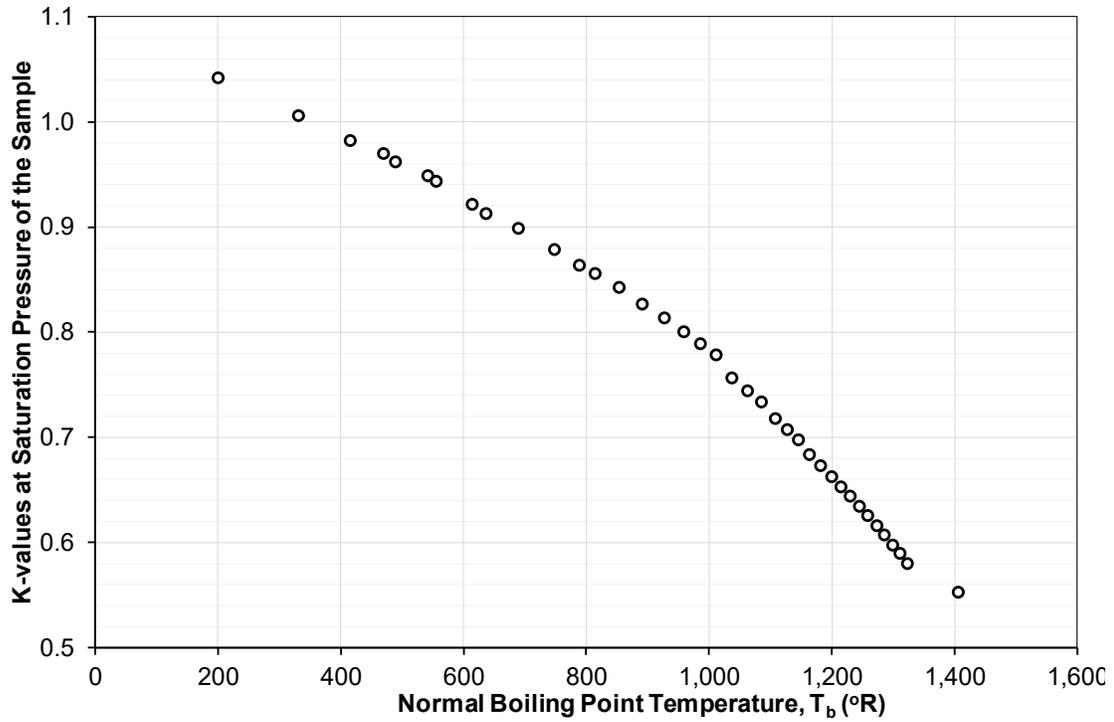


Figure 19. Monotonicity check of component K-values versus normal boiling point temperatures for final Montney EOS model at saturation pressure of one of the PVT samples used in the Montney EOS model development.