An aerial photograph of an oil field at sunset. The scene shows a drilling rig, several storage tanks, and various pieces of equipment on a reddish-brown dirt pad. The background features rolling hills and a clear sky with a warm orange glow from the setting sun. In the foreground, there are several white modular buildings and a line of vehicles. The overall atmosphere is industrial and serene.

# ASTM D2892 in EOS Development

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## **ASTM D2892 Data for Better C7+ Characterization in EOS Modelling**

**Curtis Hays Whitson  
Bilal Younus  
Mathias Carlsen**

Prepared for:  
**General Public**

May 13, 2018

# ASTM D2892 Data for Better C<sub>7+</sub> Characterization in EOS Modelling

## Summary

An EOS model requires five properties for each component in a mixture: critical pressure ( $p_c$ ), critical temperature ( $T_c$ ), acentric factor ( $\omega$ ), molecular weight ( $M$ ) and volume shift ( $s$ ). The three first properties define the vapor pressure curve of the component, and the last two properties (parameter) ensures accurate prediction of liquid density for that component. The five properties are readily available for pure compounds.

The component properties of heavier constituents – often defined as *single carbon number* (SCN) fractions, containing many unknown isomers – must be estimated. Gas chromatography measures the mass amount for SCNs, but without information about the SCN properties. The SCN fraction estimation procedure relies on an M-T<sub>b</sub>- $\gamma$  relationship between molecular weight, normal boiling point ( $T_b$ ), and liquid density at standard conditions (i.e. specific gravity,  $\gamma$ ). That relationship will vary from one reservoir fluid system to another, and is primarily determined by the relative amounts of paraffins, naphthenes, and aromatics in each SCN. Experimental TBP distillation data from ASTM 2892 provides data to establish the M-T<sub>b</sub>- $\gamma$  relationship for SCNs from C<sub>6</sub> to about C<sub>20+</sub> (sometimes C<sub>25+</sub>). This relationship is specific for the reservoir fluid system being characterized.

Without ASTM 2892 data, assumptions and generalized (e.g. Katz-Firoozabadi) correlations must be used for the M-T<sub>b</sub>- $\gamma$  relationship, resulting in greater uncertainty in the prediction of EOS component properties and their mixtures.

In summary,

- C<sub>7+</sub> component properties are not well defined and are normally different from one reservoir/field/basin to another depending on the relative “paraffinicity” or “aromaticity” of the fluid system.
- ASTM D2892 data provides a basis for generating the M-T<sub>b</sub>- $\gamma$  relationship based on actual, measured data from the field, resulting in a more robust and accurate characterization of the C<sub>7+</sub> fractions used in the EOS.
- In the absence of ASTM D2892 data, the only data readily available for C<sub>7+</sub> characterization is the measured average  $\gamma$  and MW of stock-tank or ambient-pressure flashed oils. This type of data has many limitations and drawbacks, not least being that the M-T<sub>b</sub>- $\gamma$  relationship is no longer unique to the fluid system being modelled.

Any reliable EOS calculation results require two sets of data (a) sample composition and (b) representative component properties. In any EOS characterization, there are always two types of components: (a) pure (library) components (e.g. CH<sub>4</sub>, CO<sub>2</sub> etc.) and (b) C<sub>7+</sub> hydrocarbon fractions which are mixtures of many pure components often grouped as single carbon number (e.g. C<sub>10</sub>, C<sub>11</sub> etc.). The EOS properties of pure components are well known. However, for hydrocarbon fractions, properties depend on hydrocarbon type (aromatic, paraffinic, etc.) and the amount of different types of components present in each fraction.

As an example, the single carbon number C<sub>7</sub> can have different proportions of benzene and normal heptane in crudes collected from different parts of the world. Benzene is an aromatic

compound (MW=78.11 and  $\gamma = 0.88$ ) and normal heptane is normal paraffin (MW=100 and  $\gamma = 0.687$ ). Therefore, properties of C<sub>7</sub> fraction depends on how much of benzene and normal heptane are present in the crude oil sample.

The ASTM D2892 data provide a basis for generating  $\gamma$  -MW and MW-T<sub>b</sub> relationships based on actual, measured data from the field, which result in a more robust and accurate characterization of the C<sub>7+</sub> fractions. One example is shown in Figure 1 taken from the classical SPE paper by Katz and Firoozabadi (1978). From Figure 1, it can be seen that the data measured in the field deviates from that of normal paraffins, indicating the aromatic character of the crude oils used in this particular study.

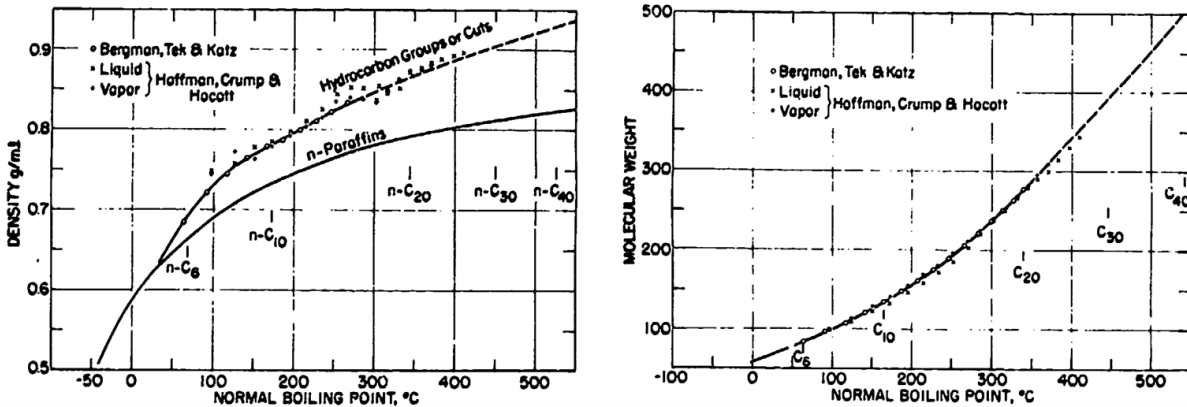


Figure 1: Developing  $\gamma$  -T<sub>b</sub> and MW-T<sub>b</sub> relationship for C<sub>7+</sub> characterization for EOS modeling (Katz & Firoozabadi, 1978)

In the absence of ASTM D2892 data, the only data readily available for C<sub>7+</sub> characterization is measured average  $\gamma$  and MW of C<sub>7+</sub> fractions of stock tank oil or separator oil. This data can be used to develop MW- $\gamma$  relationship and to estimate the degree of aromaticity and paraffinicity in crude oils from a specific field/reservoir/basin. However, such type of data has many limitations and drawbacks:

- 1) There is no information on measured boiling points of different hydrocarbon fractions.
- 2) The average C<sub>7+</sub> MW and  $\gamma$  data covers usually a small range. C<sub>7+</sub> MWs of stock tank condensates are usually in the range of 130-150 and for stock tank oils is 180-220. However, the C<sub>7</sub> and heavier fractions MWs in EOS characterization usually range from 96 to 500. Therefore, this limited data range leaves high uncertainty in characterizing many EOS components for which the properties do not fall in the range of measured data.
- 3) Sometimes the labs do not measure the average molecular weights and just calculate those using arbitrary molecular weights (e.g. Katz Firoozabadi 1978) for different fractions and sample composition. Such data is not representative of the true “character” (aromaticity/paraffinicity) of the sample collected and should not be used for C<sub>7+</sub> characterization

## References

- [1] Whitson, C.H. and Brule, M.R.: "Phase Behavior", SPE monograph (2000), chapter 5 and Appendix C.
- [2] Katz, D.L. and Firoozabadi A.: "Predicting Phase Behavior of Condensate/Crude-Oil Systems Using Methane Interaction Coefficients", SPE 6721 (1978)

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### **Whitson AS**

Skonnertveien 7.  
Trondheim, Norway  
curtishays@whitson.com

### **Whitson USA LLC**

3410 W Dallas St.  
Houston, TX 77019, US  
carlsen@whitson.com

**[www.whitson.com](http://www.whitson.com)**

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