

## SUPPORTING INFORMATION

### Extending the Modified Regular Solution Model to Predict Component Partitioning to the Asphaltene-Rich Phase

F. Ramos-Pallares and H.W. Yarranton

#### *n*-Paraffin Precipitant Density

The effective densities of the *n*-paraffin precipitants with carbon numbers lower or equal than seven were calculated from the following correlation<sup>1</sup>:

$$\rho = (a_1 + a_2T) + [(b_1 + b_2T)P] \quad (S1)$$

where  $a_1$ ,  $a_2$ ,  $b_1$  and  $b_2$  are fluid-specific parameters,  $T$  is the absolute temperature in K, and  $P$  is the pressure in MPa. Fluid-specific parameters in Eq. S1 are summarized in Table S1.

**Table S1.** Parameters for the effective liquid density correlation for *n*-paraffins.

component	$a_1$ (kg m <sup>-3</sup> )	$a_2$ (kg m <sup>-3</sup> K <sup>-1</sup> )	$b_1$ (kg m <sup>-3</sup> MPa <sup>-1</sup> K <sup>-1</sup> )	$b_2$ (kg m <sup>-3</sup> MPa <sup>-1</sup> K <sup>-1</sup> )
Methane	532.157	-0.69737	0.42606	0.001143
Ethane	704.900	-0.82749	0.21442	0.002012
Propane	793.847	-0.85489	0.05305	0.002440
<i>n</i> -Butane	846.443	-0.85024	-0.05448	0.002648
<i>n</i> -Pentane	878.006	-0.82817	-0.09229	0.002648
<i>n</i> -Hexane	901.512	-0.80985	-0.14176	0.002685
<i>n</i> -Heptane	918.603	-0.79155	-0.17738	0.002692

The density of *n*-paraffins with carbon numbers higher than seven was predicted from the Tait-COSTALD correlation<sup>2</sup>:

$$\rho_{T,P} = \rho_{T,P_0} \left[ 1 - C \ln \left( \frac{B+P}{B+P_0} \right) \right]^{-1} \quad (S2)$$

where  $\rho_{T,P}$  is the density of the fluid at a temperature,  $T$ , and pressure,  $P$ , and  $\rho_{T,P_0}$  is the density at  $T$  and atmospheric pressure,  $P_0$ . The density at atmospheric pressure can be calculated from the component molar volume and molecular weight ( $\rho = MW/v$ ). The molar volume can be calculated from the modified Rackett correlation<sup>3</sup>:

$$v_s = \frac{RT_c}{P_c} Z_{RA} \left[ 1 + (1 - T/T_c)^{2/7} \right] \quad (S2)$$

where  $v_s$  is the molar volume of the saturated liquid at temperature  $T$ ,  $T_c$  is the critical temperature,

$P_c$  is the critical pressure, and  $Z_{RA}$  is the Rackett compressibility factor. The Rackett compressibility factor is calculated by fitting the modified Rackett correlation to match the component specific gravity. The density of the component at atmospheric pressure was assumed equal to that of the saturated liquid because the compression correction between the saturation and atmospheric pressure is very small<sup>4</sup>. The parameters  $C$  and  $B$  in Eq. S2 are given by:

$$C = 0.0861488 + 0.0344483\omega \quad (S3)$$

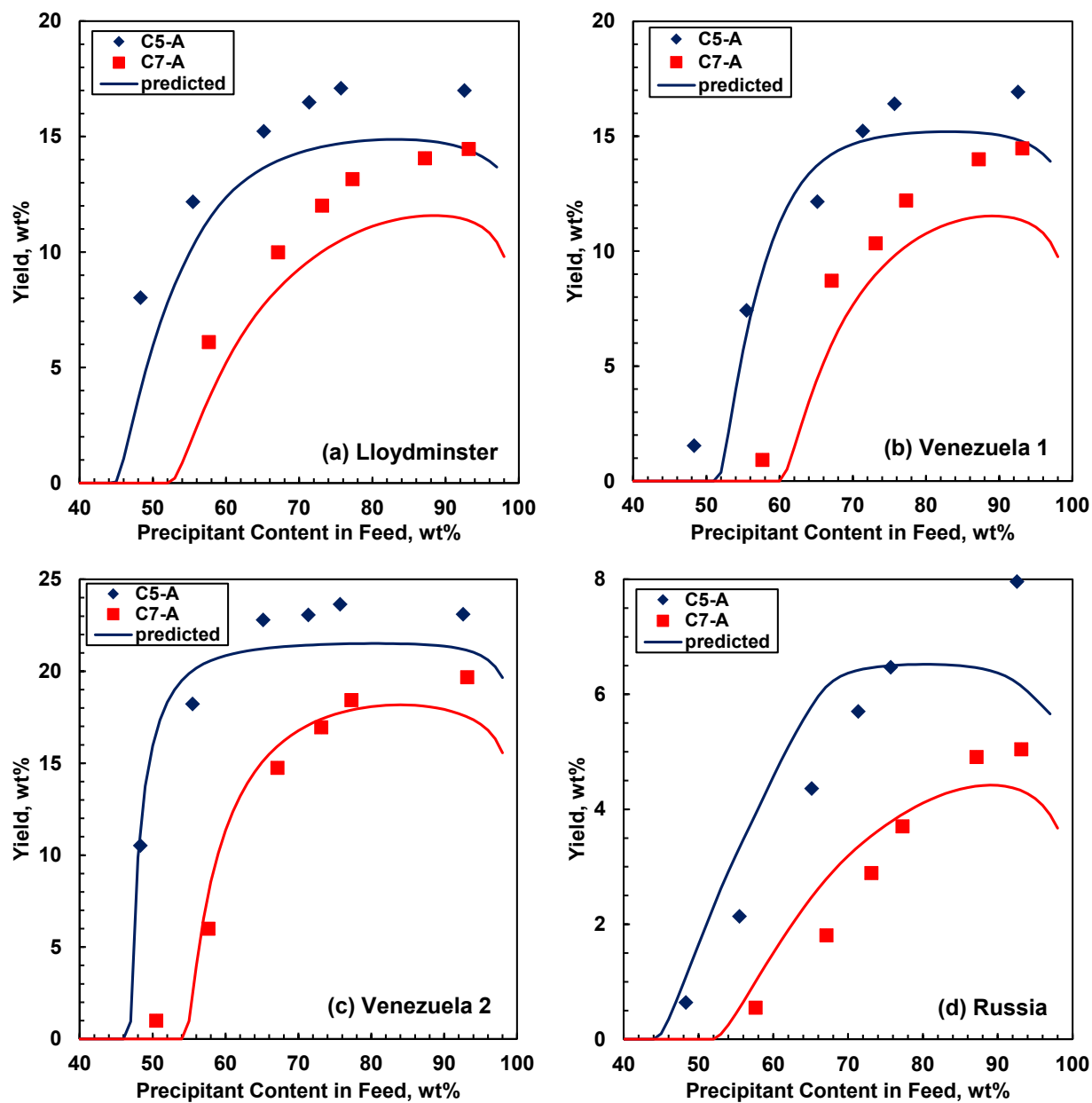
$$\frac{B}{P_c} = -1 - 9.0702A^{1/3} + 62.45326A^{2/3} - 135.1102A + eA^{4/3} \quad (S4)$$

$$A = 1 - T_r \quad (S5)$$

$$e = \exp(4.79594 + 0.250047\omega + 1.14188\omega^2) \quad (S6)$$

where  $\omega$ , and  $T_r$  are the acentric factor and reduced temperature.

**Test Dataset 3: Additional Yield data at 0°C.**



**Figure S1.** Measured and predicted yields at 0°C and 0.1 MPa with *n*-pentane (C5) and *n*-heptane (C7) for: a) Lloydminster (Western Canada) heavy oil; b) Venezuela 1 heavy oil; c) Venezuela 1 heavy oil; d) Russia heavy oil.

## References

- (1) Saryazdi, F.; Motahhari, H.; Schoeggl, F.F.; Satyro, M.A.; Yarranton, H.W. Density of Hydrocarbon Mixtures and Bitumen Diluted with Solvents and Dissolved Gases. *Energy Fuels* **2013**, 27, 666–3678.
- (2) Thomson, G. H.; Brobst, K. R.; Hankinson, R. W. An Improved Correlation for Densities of Compressed Liquids and Liquid Mixtures. *AIChE J.* **1982**, 28, 671-676.
- (3) Spencer, C. F.; Danner, R. P. Improved Equation for Prediction of Saturated Liquid Density. *J. Chem. Eng. Data*, **1972**, 17, 236-241.
- (4) Motahhari, H.; Satyro, M. A.; Taylor, S. D.; Yarranton, H. W. Extension of the Expanded Fluid Viscosity Model to Characterized Oils. *Energy Fuels* **2013**, 27, 1881-1898.