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The Density of Binary Mixtures of N-Octane + N-Dodecane Predictions and Measurements

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Abstract

The knowledge of reservoir fluid's physical properties is crucial in the upstream and downstream processes of the petroleum industry. Cubic equations of state, such as the Soave–Redlich–Kwong (SRK) and the Peng–Robinson (PR) EoS, are still the most used models in PVT modeling of reservoir fluids, and almost the exclusively used models in compositional reservoir simulations. In this e work predication liquid density for binary mixtures of hydrocarbon system (n-Octane + n-Dodecane) using Peneloux introduced a simple method based on the volume translation principles in order to the SRK EOS model at different temperatures from 40 °C up to 120 °C and 100 psig to 4000 psig pressure. The density predicated was calculated using MATLAB software and comparisons with the experimental, The experimental liquid density was measured at different pressures from 100 psig up to 4000 psig, and temperatures from 40°C up to 120 °C The PVT model 3000 GL is supplied with an electrical densimeter measurements have been used to measure the density [1]. The estimated average absolute deviation in percent (AAD%) in densities for binary mixtures We obtained a good result for the deviation if the C12 percentage was lower in the mixture, as the higher the C12 percentage in the mixture, the greater the deviation rate.

Keywords: Density, temperatures, SRK EOS, PVT system

1. Introduction

The first equations widely accepted for calculations of liquid densities were, apparently, the modified Rackett equation (Spencer and Danner, 1972) and the COSTALD model (Hankinson and Thomson, 1979), which can be used to predict liquid densities within approximately 1% of deviation. However, they are typically applicable only in the subcritical range, and as a result, there is a discontinuity in

specific volume calculations when moving from saturated to dense liquid. Later, Peneloux et al. (1982) proposed a constant volume correction (known as "specific volume shift") for the Soave-Redlich-Kwong (SRK) cubic equation of state (EOS) (Soave, 1972) [2]. The correction is particular for each substance and it is independent of temperature. In the paper, they try to generalize the constants used in the correction equation through the Rackett compressibility factor, ZRA. The procedure works reasonably well for hydrocarbons (with deviations below 5%) when the temperature is far from the critical point, in this paper is proposed a correction equation to calculate the specific volume of liquid hydrocarbons, which does not require additional parameters for each substance and can be applied in a wide temperature range.

2. Predict Density

To predict density used Peneloux [5] introduced a simple method based on the volume translation principles in order to the SRK EOS model is defined by:

$$P = \frac{RT}{v-b} - \frac{a_c \propto}{(v)(v+b)} \dots\dots\dots\dots\dots [1]$$

improve the estimation of the liquid molar volume by cubic EOSs.

$$V_{Corr} = V_{SRK} - C_{PEN} \dots\dots\dots\dots [2]$$

Where C_{PEN} is a particular constant for each substance that must be found experimentally but which is generalized as:

$$C_{PEN} = 0.40768(0.29441 - Z_{RA})\frac{RT_C}{P_C} \dots\dots\dots\dots [3]$$

and the Rackett compressibility factor, Z_{RA}, can be calculated as (Reid et al., 1987)

$$Z_{RA} = 0.29056 - 0.0877\omega \dots\dots\dots\dots [4]$$

3. Results and Discussion

The comparisons literature data with the experimental densities of binary mixtures of n-Octane + n-Dodecane have been measured at different temperatures and different pressure ranges between 40 C

up to 120 C &100psig up to 4000 psig. The accuracy of the predictions of the equation of state is represented by the average absolute deviation in percent (AAD%) for the n data points. We notice that as the pressure increases, the temperature increases, and the percentage of C12 increases, the error rate increases

$$AAD(\%) = \frac{100}{n}\sum_{n}\frac{\left|y_{clc.} - y_{\exp.}\right|}{y_{\exp.}} \quad \text{.....(5)}$$

The figures from (1) to (4) show the comparison results of density over wide range of temperature and pressure where the AAD show in table (5) this method yield good predications.

Table (1) Densities(gm/cm^3) for binary mixtures of 20% n- Octane (1) +80% n- Dodecane (2)

T°C / P PSIG	40		60		100		120	
	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.
4000	0.75923	0.74756	0.75072	0.73421	0.73267	0.70407	0.72312	0.68989
3500	0.75662	0.74516	0.74774	0.73179	0.72883	0.70032	0.71880	0.68584
3000	0.75384	0.74276	0.74455	0.72955	0.72469	0.69657	0.71411	0.68179
2500	0.75085	0.74036	0.74111	0.72685	0.72020	0.69282	0.70900	0.67774
2000	0.74764	0.73796	0.73740	0.72391	0.71529	0.68907	0.70339	0.67369
1500	0.74418	0.73556	0.73337	0.72096	0.70991	0.68532	0.69719	0.66964
1000	0.74042	0.73316	0.72898	0.71866	0.70395	0.68157	0.69028	0.66559
500	0.73633	0.73076	0.72416	0.71559	0.69732	0.67782	0.68251	0.66154
250	0.73414	0.72956	0.72157	0.71383	0.69369	0.67594	0.67823	0.65952
100	0.73277	0.72884	0.71995	0.71300	0.69141	0.67482	0.67551	0.65830

Table (2) Densities (gm/cm^3) for binary mixtures of 40% n- Octane (1) +60% n- Dodecane (2)

T°C / P PSIG	40		60		100		120	
	PRED.	EXP.	PRED.	EXP.	PRED.	EXP.	PRED.	EXP.
4000	0.75356	0.74877	0.74455	0.73542	0.72541	0.70145	0.71529	0.68498
3500	0.75082	0.74622	0.74141	0.73247	0.72136	0.69795	0.71072	0.68128
3000	0.74788	0.74367	0.73804	0.72952	0.71698	0.69445	0.70576	0.67758
2500	0.74474	0.74112	0.73441	0.72657	0.71223	0.69095	0.70035	0.67388
2000	0.74136	0.73857	0.73050	0.72362	0.70703	0.68745	0.69439	0.67018
1500	0.73770	0.73602	0.72624	0.72067	0.70132	0.68395	0.68781	0.66648
1000	0.73374	0.73347	0.72160	0.71772	0.69500	0.68045	0.68045	0.66278
500	0.72942	0.73092	0.71650	0.71477	0.68793	0.67695	0.67214	0.65908
250	0.72711	0.72964	0.71375	0.71329	0.68407	0.67520	0.66756	0.65723
100	0.72567	0.72888	0.71203	0.71241	0.68163	0.67415	0.66464	0.65612

Table (3) Densities (gm/cm^3) for binary mixtures of 60% n- Octane (1) +40% n- Dodecane (2)

T°C / P PSIG	40		60		100		120	
	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.
4000	0.74721	0.75468	0.73762	0.73724	0.71726	0.70379	0.70650	0.68125

3500	0.74432	0.75233	0.73431	0.73404	0.71297	0.69984	0.70165	0.67775
3000	0.74122	0.74998	0.73075	0.73084	0.70833	0.69589	0.69639	0.67425
2500	0.73790	0.74763	0.72691	0.72764	0.70329	0.69194	0.69063	0.67075
2000	0.73433	0.74528	0.72277	0.72444	0.69777	0.68799	0.68430	0.66725
1500	0.73047	0.74293	0.71827	0.72124	0.69170	0.68404	0.67728	0.66375
1000	0.72628	0.74058	0.71335	0.71804	0.68496	0.68009	0.66941	0.66025
500	0.72171	0.73823	0.70793	0.71484	0.67741	0.67614	0.66049	0.65675
250	0.71926	0.73705	0.70502	0.71324	0.67327	0.67417	0.65554	0.65500
100	0.71773	0.73635	0.70319	0.71228	0.67065	0.67298	0.65239	0.65395

Table (4) Densities (gm/cm^3) for binary mixtures of 80% n- Octane (1) +20% n- Dodecane (2)

T°C / P PSIG	40		60		100		120	
	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.	Exp.
4000	0.74007	0.74990	0.72982	0.73703	0.70807	0.70324	0.69657	0.68561
3500	0.73701	0.74725	0.72631	0.73398	0.70352	0.69934	0.69142	0.68171
3000	0.73373	0.74460	0.72254	0.73093	0.69859	0.69544	0.68582	0.67781
2500	0.73023	0.74195	0.71849	0.72788	0.69322	0.69154	0.67968	0.67391
2000	0.72645	0.73930	0.71409	0.72483	0.68735	0.68764	0.67292	0.67001
1500	0.72236	0.73665	0.70931	0.72178	0.68086	0.68374	0.66539	0.66611
1000	0.71792	0.73400	0.70408	0.71873	0.67365	0.67984	0.65693	0.66221
500	0.71308	0.73135	0.69832	0.71568	0.66554	0.67594	0.64730	0.65831

250	0.71048	0.73002	0.69521	0.71415	0.66108	0.67399	0.64193	0.65636
100	0.70885	0.72923	0.69326	0.71324	0.65825	0.67282	0.63850	0.65519

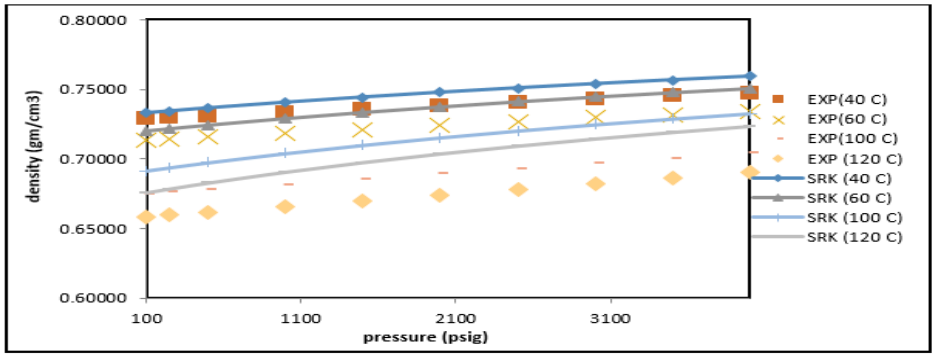

Figure (1) Comparison of density VT SRK EOS with Experimental for binary mixtures of 20% n-Octane (1) + 80% n- Dodecane(2)

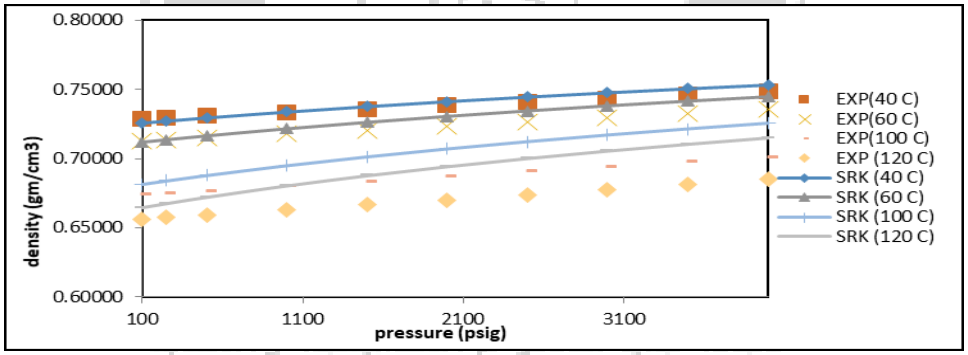

Figure (2) Comparison of density VT SRK EOS with Experimental for binary mixtures of 40% n-Octane (1) + 60% n-Dodecane (2)

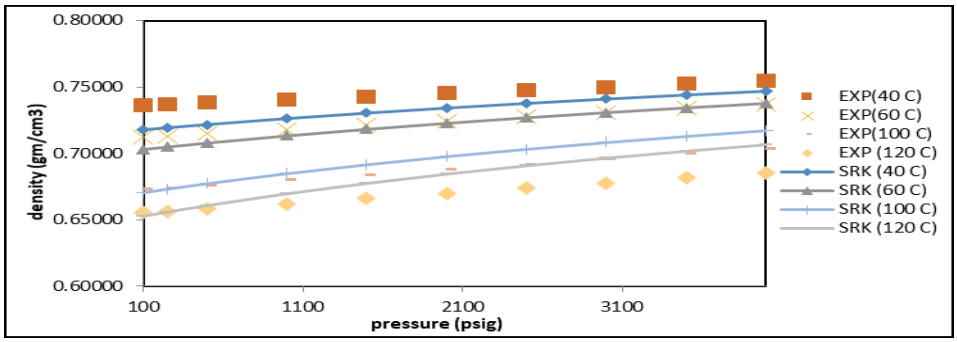

Figure (3) Comparison of density VT SRK EOS with Experimental for binary mixtures of 60% n-Octane (1) + 40% n-Dodecane (2)

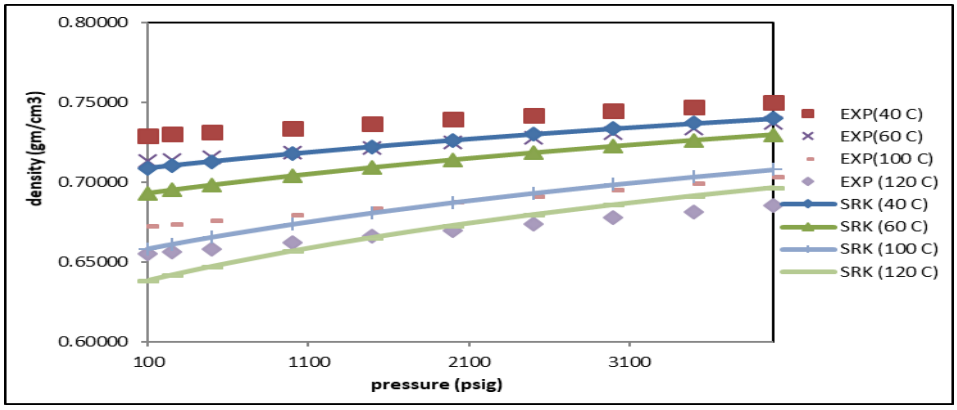

Figure (4) Comparison of density VT SRK EOS with Experimental for binary mixtures of 80% n-Octane (1) + 20% n-Dodecane (2)

Table (5): AAD % of measurement results of binary mixtures with experimental values for densities

Binary mixtures	AAD%
20% n- Dodecane(1) +80% n-Octane (2)	1.4734
40% n- Dodecane(1)+60%n-Octane (2)	1.3290
60%n- Dodecane(1)+40%n-Octane (2)	1.6782
80%n- Dodecane(1)+20%n-Octane (2)	2.5682

4. Conclusions

In this paper is proposed correction equation to calculate the specific volume of liquid hydrocarbons SRK EOS Model is applied to correlate molar volume to predicted density for n-Octane + n-Dodecane The proposed VT- SRK equations of state provide good results with an overall AAD table [5]. The density of binary mixtures n-Octane + n-Dodecane was measured at

temperatures from 40 °C up to 120 °C and pressure from 100 to 4000 psig. The measured density data are in good agreement with the literature data.

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Prediction of hydrocarbon densities at extreme conditions using volume-translated SRK and PR equations of state fit to high temperature, high pressure PVT data

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