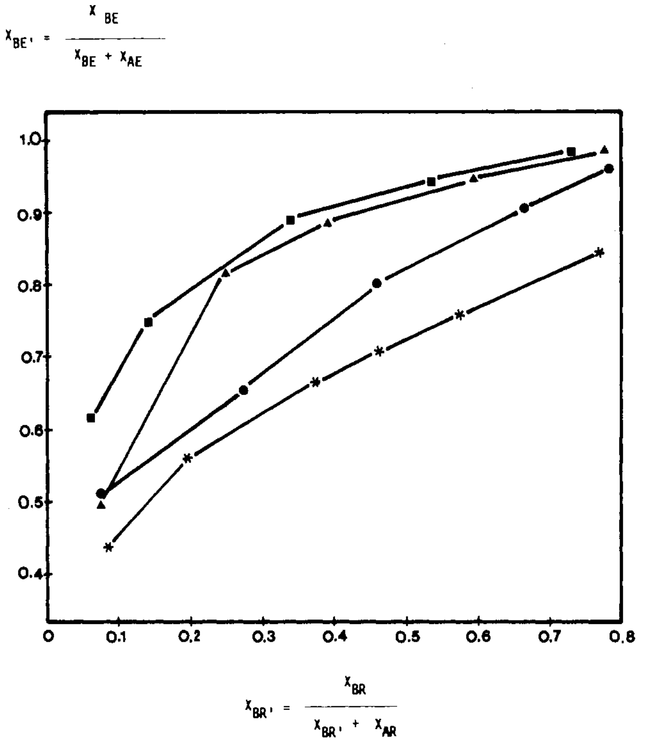

Figure 7. Selectivity diagrams at 20 °C for the system (*) acetonitrile–2-furyloxirane–cyclohexane, (●) acetonitrile–2-furyloxirane–hexane, (▼) acetonitrile–2-furyloxirane–pentane, (■) acetonitrile–2-furyloxirane–isopentane.

These figures show that at room temperature the diagrams are from type II and tend toward type I when the temperature increases.

In Figure 7 one can compare the selectivity diagrams of hexane, isopentane, and pentane relevant to the 2-furyloxirane in acetonitrile at 20 °C. The curve corresponding to cyclohexane is given as a reference.

Results from Figure VII show that the extracting capacity of aliphatic hydrocarbons is practically identical with that of cyclohexane, although they are more selective toward the 2-furyloxirane extraction.

Isopentane is more volatile than pentane but it is also less selective. Therefore pentane seems to be the best hydrocarbon for the 2-furyloxirane extraction in its reactive medium.

Glossary

X_A	weight percent of acetonitrile in one phase
X_B	weight percent of 2-furyloxirane in one phase
X_S	weight percent of a hydrocarbon in one phase
X_{BR}	weight percent of 2-furyloxirane in acetonitrile phase
X_{BE}	weight percent of 2-furyloxirane in hydrocarbon phase
$X_{BR'}$	weight percent of 2-furyloxirane in acetonitrile phase on a hydrocarbon free basis
$X_{BE'}$	weight percent of 2-furyloxirane in hydrocarbon phase on a hydrocarbon free basis

Registry No. 2-Furyloxirane, 2745-17-7; acetonitrile, 75-05-8; isopentane, 78-78-4; pentane, 109-66-0; hexane, 110-54-3.

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Compressed Liquid Propene Densities between 5 and 73 °C at Pressures to 9.6 MPa

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Compressed liquid densities of propene were measured at 11 temperatures between 5 and 73 °C at pressures from near saturation to 9.65 MPa with a vibrating tube densitometer. Comparisons with densities computed using a liquid density correlation, COSTALD, and an existing empirical fit to a BWR equation show that both methods are accurate to better than 0.2% at typical custody-transfer conditions.

Introduction

Since large quantities of propene are bought and sold daily, it is important to know the fluid's density as a function of temperature and pressure for accurate custody transfer. Compressed liquid densities, known to ±0.2% or better, are needed since metering operations occur in the compressed liquid region. Four sets of compressed liquid density data exist in the open literature (*1–4*). Also, there are two correlations (*5*, *6*) for calculating liquid densities of propene. To resolve discrepancies between the sets of data and to evaluate the accuracy of the correlations, we measured the compressed liquid density of propene at 11 temperatures between 5 and 73 °C. Pressures extended from near the vapor pressure to 9.65 MPa.

Experimental Section

Materials. Matheson Research Grade propene with a stated purity of 99.6 mol % minimum purity was used. Gas chromatographic analysis indicated 99.5 mol % with the balance being mostly propane. The propene was frozen with liquid nitrogen and evacuated to remove residual air. To calibrate the densitometer, Phillips Research Grade propane and Linde pure argon, with stated purities of 99.6 and 99.998%, respectively, were used. The propane was evacuated at low temperature to remove any possible air; the argon was used without further purification.

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Table I. Density of Compressed Liquid Propene as a Function of Temperature at Even Increments of Pressure

press., MPa	density, g/cm^3										
	5.0 °C	10.0 °C	15.6 °C	20.0 °C	25.0 °C	30.0 °C	40.0 °C	50.0 °C	60.0 °C	70.0 °C	73.5 °C
1.38	0.5406	0.5326	0.5237	0.5161	0.5073	0.4980					
2.76	0.5437	0.5360	0.5274	0.5202	0.5118	0.5030	0.4841	0.4621	0.4358		
4.14	0.5466	0.5391	0.5309	0.5239	0.5159	0.5076	0.4899	0.4698	0.4470	0.4191	0.4070
5.52	0.5494	0.5421	0.5341	0.5274	0.5198	0.5118	0.4951	0.4765	0.4559	0.4322	0.4226
6.90	0.5520	0.5450	0.5372	0.5308	0.5234	0.5158	0.4998	0.4823	0.4634	0.4423	0.4341
8.27	0.5546	0.5478	0.5402	0.5339	0.5268	0.5195	0.5042	0.4876	0.4700	0.4507	0.4434
9.65	0.5570	0.5504	0.5431	0.5369	0.5301	0.5229	0.5083	0.4924	0.4758	0.4580	0.4512

Table II. Densities of Propene Near the Saturation Boundary

T, °C	P, MPa	d, g/cm^3	T, °C	P, MPa	d, g/cm^3
5.0	0.69_4	0.5390_9		1.20_7	0.5066_7
	0.72_4	0.5391_5		1.24_1	0.5068_0
	0.75_8	0.5392_3		1.27_6	0.5069_2
	0.79_3	0.5393_2		1.31_0	0.5070_3
	0.82_7	0.5393_9		1.34_4	0.5071_5
	0.86_2	0.5394_4	30.0	1.31_0	0.4976_8
	0.89_6	0.5395_5		1.31_6	0.4977_0
	0.96_5	0.5397_2		1.32_4	0.4977_2
	1.03_4	0.5398_7		1.34_4	0.4978_3
10.0	0.79_6	0.5311_4	40.0	1.62_0	0.4787_1
	0.82_7	0.5312_2		1.65_5	0.4788_9
	0.86_2	0.5313_2		1.68_9	0.4790_6
	0.89_6	0.5313_9		1.72_4	0.4792_2
	0.96_5	0.5315_8	50.0	2.06_8	0.4577_4
	1.03_4	0.5317_7	60.0	2.48_2	0.4331_5
	1.10_3	0.5319_3		2.51_7	0.4334_9
	1.24_1	0.5322_8		2.55_5	0.4336_6
15.6	0.91_1	0.5223_7		2.58_6	0.4341_6
	0.93_1	0.5224_2		2.62_0	0.4345_0
	0.94_2	0.5224_8		2.65_4	0.4348_3
	0.96_5	0.5225_3		2.68_9	0.4351_5
	1.00_0	0.5226_2		2.72_3	0.4354_8
	1.03_4	0.5227_3	70.0	3.13_7	0.4058_9
	1.10_3	0.5229_3		3.15_4	0.4059_9
	1.17_2	0.5231_1		3.17_2	0.4063_1
	1.24_1	0.5233_1		3.24_1	0.4073_9
	1.31_0	0.5235_0		3.34_4	0.4089_5
20.0	1.03_4	0.5150_1		3.44_7	0.4104_5
	1.10_3	0.5152_5	73.5	3.30_9	0.3930_5
	1.17_2	0.5154_6		3.31_8	0.3931_8
	1.24_1	0.5156_7		3.34_4	0.3937_8
	1.31_0	0.5158_8		3.37_8	0.3944_6
25.0	1.16_0	0.5065_3		3.41_3	0.3951_4
	1.17_2	0.5065_5		3.44_7	0.3958_2

Apparatus and Procedure. Parrish (*7*) gives complete details of the apparatus and experimental procedure. Measurements were made using a Mettler-Paar DMA 512 vibrating tube densitometer which was immersed in a constant temperature bath. The densitometer was calibrated before and after each run in 1.4 MPa increments using argon and propane. Densities for the calibration fluids were computed from a 32-term BWR equation of state (*7*).

Error Analysis. The estimated total uncertainty (three times the estimated standard deviation plus the estimated systematic error) of the density measurements is ±0.2%. This uncertainty is the same as the estimated uncertainty in the calculated densities of the calibration fluids. Uncertainties in the temperature and pressure are estimated conservatively at ±0.1 °C and ±14 kPa.

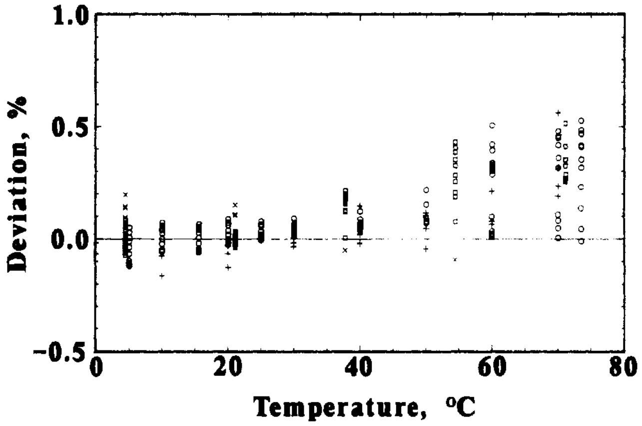

Figure 1. Deviation between calculated and experimental densities of propene. Densities calculated by using COSTALD correlation. The symbols (O), (+), (O), and (X) denote this work and ref *1*, *2*, and *3*, respectively.

Results and Discussion

Tables I and II list the measured densities of propene as a function of temperature and pressure. The only direct comparison of our results with previous work is with portions of the data of Vaughan and Graves (*4*). For the six points at which the temperatures and pressures in the two studies were identical, the discrepancies in measured densities varied between 3.8 and 7.6%. Because of these large differences, we omitted the older work from further comparison.

With the temperature and pressure ranges of the other works differing from each other and from this work, the best means for comparing results is to compare each investigator's work against existing density correlations. We consider two liquid density correlations which currently are used for custody transfer. The first method is COSTALD which is a three-parameter corresponding states method for both pure liquids and liquid mixtures; Thomson et al. (*5*) present details of the correlation. This was used without modification. The data of Dittmar et al. (*1*) were used to obtain the parameters for propene in COSTALD. This method is valid up to a reduced temperature of 0.95.

Table III. Comparison of Experimental Densities with Values Obtained from COSTALD and API

data source	no. of points	error,[a] %			
		COSTALD		API	
		av	max	av	max
this work	142	0.07	0.53	−0.04[b]	−0.38
Farrington and Sage	46	0.13	0.52	0.02	0.25
Dittmar et al.	21	0.05	0.56	−0.10	0.23
Manley and Swift	11	0.57	2.96	0.49	2.70
	9[c]	0.09	0.19	0.04	0.19

[a] Error is defined as calculated density minus experimental density divided by experimental density. [b] Three points not included because of convergence problems. [c] Comparison with values at 140 °F and 600 psia and at 70 °F and 1600 psia omitted.

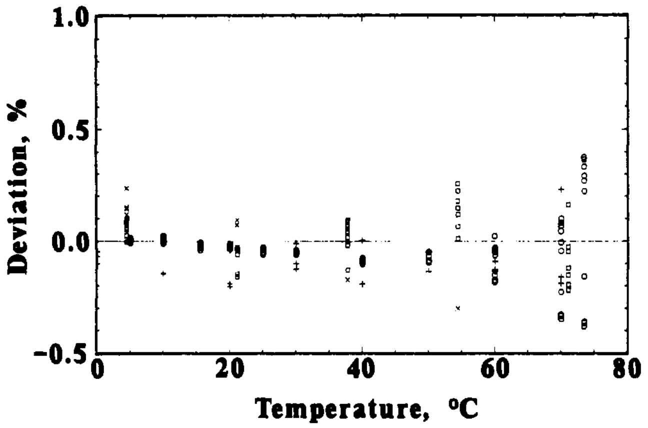

Figure 2. Deviation between calculated and experimental densities of propene. Densities calculated by using API correlation. The meanings of the symbols are the same as given in Figure 1.

The second correlation, denoted here as API, is an empirical fit to the BWR equation. The Appendix gives details of the correlaion which applies between 0 and 74 °C at pressures up to 11 MPa. Hankinson (*8*) used the density data of Farrington and Sage (*2*) and Manley and Swift (*3*) to obtain the equation parameters.

Table III lists the results of a comparison between experimental and calculated densities for propene in the range of this study. Figures 1 and 2 show the deviation between computed and measured densities as a function of temperature for COSTALD and API, respectively. To provide a meaningful comparison, we restricted the range of temperature and pressures to that of the API method. We were unable to obtain convergence when trying to extend API beyond the stated range. Also, we found three cases where the API method did not converge within the stated temperature and pressure limits. However, there were very near the saturation boundary where custody-transfer metering does not take place.

Conclusions

Comparisons of the densities reported here with those given by Farrington and Sage (*2*) and by Dittmar et al. (*1*) indicate an agreement of better than ±0.2% over the range of this study. With the exception of two data points of Manley and Swift (*3*), agreement between this work and their data is well within the ±0.4% uncertinty claimed by them. Both COSTALD and API predict compressed liquid densities to within ±0.2% between 0 and 50 °C. However, both correlations become less accurate at higher temperatures.

Table IV. Coefficients for Eq A-2

a_1	−8.85083	a_5	0.0197889
a_2	0.15326	a_6	2.648021×10^{-4}
a_3	−321914.0	a_7	79510.1
a_4	−0.718199	a_8	0.0146343

Density measurements were made on Phillips Polymer Grade propene. Although the results are not presented here, agreement in density between the Phillips and Matheson propene was better than 0.01% over the range of this study.

Appendix

The correlation, denoted as the API method, for calculating compressed liquid propene densities consists of a vapor pressure equation and a BWR equation of state. Vapor pressures are computed by using

$$\ln P = 9.9107 - 4015.63/(460.068 + t) \qquad \text{(A-1)}$$

where P is the pressure in atm and t is the temperature in °F.

The BWR equation used is

$$P = RTd + (a_1 + a_2RT + a_3/T^2)d^2 + (a_4 + a_5RT)d^3 + a_6d^6 + a_7d^3/T^2(1 + a_8d^2)\exp(-a_8d^2) \qquad \text{(A-2)}$$

where T is in kelvin and d is the density in mol/L. Table IV gives the values of the fitted parameters, a_i. The molecular weight used in this correlation is 42.081.

Acknowledgment

The experimental measurements were taken by J. L. Durm.

Glossary

a_i	coefficients of eq A-2
d	density, mol/L
P	pressure, atm
R	gas constant, 0.08206 atm L mol^{-1} K^{-1}
t	temperature, °F
T	temperature, K

Registry No. Propene, 115-07-1.

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