

## Density and Viscosity of Tetralin and *Trans*-Decalin

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New measurements are reported for the density and viscosity of tetralin and *trans*-decalin. The density was determined from room temperature to 60°C for tetralin and to 95°C for *trans*-decalin. The kinematic viscosity was measured up to temperatures slightly above 100°C. Our results improve upon the values recommended by the American Petroleum Institute for these liquids.

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**KEY WORDS:** decalin; density; synfuels; tetralin; viscosity.

### 1. INTRODUCTION

Several studies have documented the demand for reliable thermophysical-property information for coal liquids including density and viscosity [1-5]. To develop methods for calculating these properties experimental data are needed for selected liquid model compounds [5]. In this paper we report new accurate measurements of the density and the viscosity of two such model liquids, namely, tetrahydronaphthalene (tetralin) and *trans*-decahydronaphthalene (*trans*-decalin). The sample liquids employed in this work were prepared by Yesavage and co-workers, who earlier measured the enthalpy of these liquids [6, 7].

### 2. DENSITY OF *TRANS*-DECALIN

The *trans*-decalin used for the measurements was produced from a commercial (*cis* + *trans*) mixture at the Colorado School of Mines as

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described by Robinson et al. [6]. The mole fraction of *trans*-decalin in the final sample was 99.08%, the remaining 0.92% being *cis*-decalin [8]. In contrast to the case of tetralin, discussed later, no repeated check of the purity of the sample was made after the completion of the measurements.

The density of the *trans*-decalin was measured gravimetrically with the aid of a bicapillary pycnometer [9] with a capacity of about 21.7 cm<sup>3</sup> and with precision-bore capillaries with an internal diameter of about 0.9 mm. After weighing the pycnometer with a convenient amount of liquid, the levels  $l_1$  and  $l_2$  of the menisci in the two capillaries were determined, while the pycnometer was in thermal equilibrium in a thermostat whose temperature was controlled to within 2 mK and measured with a calibrated platinum thermometer. The volume  $V$  of the liquid in the pycnometer as a function of the temperature  $t$  in °C was represented by

$$V(t) = V_0(1 + 3\alpha t) + (a + 2\alpha t)l \quad (1)$$

where  $l$  is the average of the heights  $l_1$  and  $l_2$  of the menisci. To determine the constants  $V_0$ ,  $\alpha$ , and  $a$  in Eq. (1) the pycnometer was calibrated with water at seven temperatures between 20 and 65°C, yielding

$$\begin{aligned} V_0 &= (21.72957 \pm 0.00024) \text{ cm}^3 \\ \alpha &= (3.59 \pm 0.08) \times 10^{-6} \text{ }^\circ\text{C}^{-1} \\ a &= (7.707 \pm 0.047) \times 10^{-3} \text{ cm}^2 \end{aligned} \quad (2)$$

The value found for  $\alpha$  is close to the literature value of  $\alpha \approx 3.25 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$  for the thermal expansion coefficient of Pyrex [10]. This calibration was performed with doubly distilled water filtered through a 0.22- $\mu\text{m}$  filter. The density of water was calculated from the equation recommended by the International Association for the Properties of Steam [11–13]. Calibration of the pycnometer with liquid water at temperatures above 65°C turned out to be impractical because of the formation of air bubbles in the pycnometer.

After the pycnometer had been calibrated we measured the density of *trans*-decalin at temperatures from 20 to 95°C. The experimental results are presented in Table I. The measurements between 75 and 95°C involve a slight extrapolation of the working equation (1). The densities were measured with a precision of a few parts in  $10^5$ , while the tolerances of the IAPS equation for water in the temperature range considered is within 1:25,000 [14]. Hence, the accuracy of our density measurements should be within 0.01%.

**Table I.** Density of *trans*-Decalin

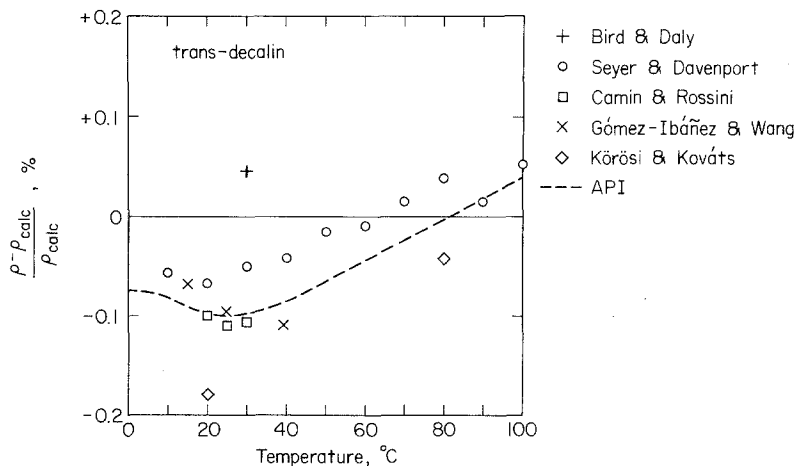
Temperature (°C)	Density (g · cm <sup>-3</sup> )
20.046	0.87055
24.986	0.86686
35.035	0.85934
45.111	0.85185
54.956	0.84443
65.042	0.83670
74.636	0.82942
85.193	0.82137
94.802	0.81398

In the temperature range of our measurements the density  $\rho$  of *trans*-decalin can be represented as a function of the temperature  $t$  by an equation of the form

$$\rho = \rho_0 + \rho_1 t + \rho_2 t^2 \quad (3)$$

with

$$\begin{aligned} \rho_0 &= 0.885358 \text{ g} \cdot \text{cm}^{-3} \\ \rho_1 &= -7.352 \times 10^{-4} \text{ g} \cdot \text{cm}^{-3} \text{ } ^\circ\text{C}^{-1} \\ \rho_2 &= -1.87 \times 10^{-7} \text{ g} \cdot \text{cm}^{-3} \text{ } ^\circ\text{C}^{-2} \end{aligned} \quad (3a)$$



**Fig. 1.** Comparison between the density  $\rho$  of *trans*-decalin reported in the literature and the values calculated from Eq. (3) with Eq. (3a).

This equation reproduces the experimental density data with a standard deviation of 0.003 %.

A comparison between our data and the densities reported by previous investigators [15–19] is shown in Fig. 1. The deviations are of the same order as the differences among the literature data themselves. In Fig. 1 we also include a comparison with the density values recommended by the American Petroleum Institute (API). The values recommended by API differ from our data by amounts up to 0.1 %, which is outside the accuracy of our density measurements.

### 3. VISCOSITY OF *TRANS*-DECALIN

The viscosity of *trans*-decalin was measured with the same Ubbelohde capillary viscometer which was previously employed by us to measure the viscosity of toluene [21]. The capillary viscometer was located in a water bath of about 70 dm<sup>3</sup> whose temperature was controlled to within 2 mK. At temperatures above 95°C the water was replaced with ethyleneglycol. The temperatures were measured with a platinum thermometer or with a quartz thermometer calibrated against the platinum thermometer.

The kinematic viscosity  $\nu$  was deduced from the flow time  $\tau$  by the usual working equation [22]

$$\nu = C\tau - B/\tau \quad (4)$$

The instrument constants  $C$  and  $B$  were determined by calibrating the viscometer again with water at temperatures between 25 and 95°C in intervals of 5°C. The calibration data correspond to flow times ranging from 1500 s at 25°C to 520 s at 95°C. The kinematic viscosity  $\nu = \eta/\rho$  of water was obtained by calculating  $\rho$  from the IAPS Formulation 1984 for the Thermodynamic Properties of Ordinary Water Substance [13] as in Section 2, while the dynamic viscosity  $\eta$  was calculated from the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance [12, 23]. A least-squares analysis of the calibration data yielded

$$\begin{aligned} C &= (5.95549 \pm 0.000087) \times 10^{-4} \text{ mm}^2 \cdot \text{s}^{-1}, \\ B &= (0.531 \pm 0.041) \text{ mm}^2 \end{aligned} \quad (4a)$$

The working equation (4) reproduces the calibration data to within 0.04 %.

The viscosity of *trans*-decalin was measured at temperatures from 25°C to 135°C. The experimental results obtained for the kinematic and dynamic viscosity are presented in Table II. The measurements of the kinematic viscosity correspond to flow times  $\tau$  ranging from 3740 s at 25°C

Table II. Kinematic Viscosity  $\nu$  and Dynamic Viscosity  $\eta$  of *trans*-Decalin

$t$ (°C)	$\nu$ (mm <sup>2</sup> · s <sup>-1</sup> )	$\eta$ (mPa · s)
25.022	2.229	1.932
35.097	1.888	1.622
45.107	1.624	1.383
55.172	1.413	1.193
65.181	1.246	1.043
74.794	1.111	0.9216
85.148	0.9905	0.8136
95.127	0.8934	0.7270
105.081	0.8110	
115.110	0.7407	
125.138	0.6789	
135.116	0.6259	

to 1050 s at 135°C. The kinematic viscosity  $\nu$  was converted into the dynamic viscosity  $\eta$  with the aid of the representative equation (3) for the density of *trans*-decalin.

The values obtained for the kinematic viscosity relative to that of water have an estimated accuracy of 0.1%. The IAPS equation employed for the calibration procedure reproduces the viscosity of water with a tolerance of 0.2%. We expect, therefore, that our viscosity data for *trans*-decalin have an absolute accuracy of about 0.3%.

We found that the viscosity of *trans*-decalin as a function of the absolute temperature  $T$  is best represented by an equation proposed by Vogel [24]:

$$\eta = A \exp[E/(T - T_0)] \quad (5)$$

with

$$A = 0.0258 \text{ mPa} \cdot \text{s}, \quad E = 1037 \text{ K}, \quad T_0 = 57.9 \text{ K} \quad (5a)$$

This equation reproduces the measurements of the viscosity  $\eta$  in the restricted temperature range from 25 to 95°C with a standard deviation of  $1.4 \times 10^{-3}$  mPa · s.

A comparison of the viscosity of *trans*-decalin reported in the literature [15, 25, 26], including the values recommended by API [20], is presented in Fig. 2. The earlier measurements of Seyer and Leslie [25] agree with our results within 0.5%. However, the more recent measurements of Chylinski and Stryjek [26] differ from our results by as much as 1%. The difference between our results and the values recommended by API [20] vary from +0.4% at 20°C to -0.6% at 100°C.

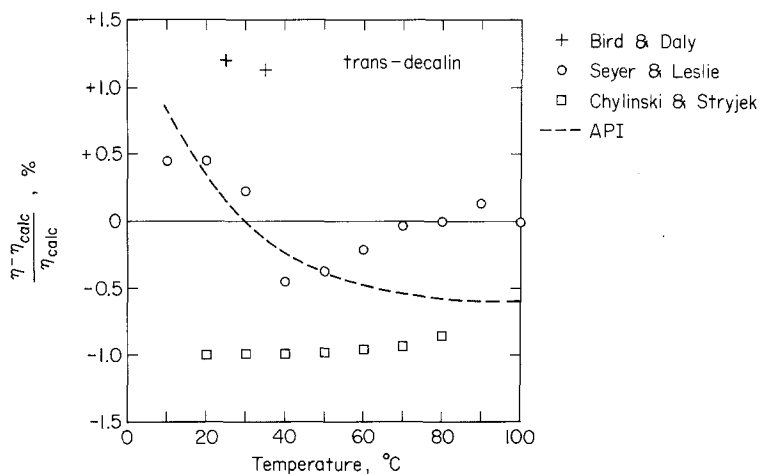


Fig. 2. Comparison between the viscosity  $\eta$  of *trans*-decalin reported in the literature and the values calculated from Eq. (5) with Eq. (5a).

#### 4. DENSITY OF TETRALIN

Originally an attempt was made to measure the density and the viscosity with the same instruments used for *trans*-decalin. However, it was found that the purity of tetralin deteriorated considerably when exposed for extended periods to air. Therefore, it became necessary to arrange for alternative instrumentation so that the tetralin could be kept in a nitrogen atmosphere at all stages of the experiments. These experiments were carried out at Gunma University in Japan.

The measurements were performed with a sample of tetralin triply distilled in a spinning-band distillation column by Yesavage and co-workers [7]. A gas chromatography—mass spectrometry (gc–ms) analysis performed both before and after the experiments indicated a purity better than 99.99 mol%. As independent check of the sample with a Mitsubishi Kasei Model CA02 moisture meter indicated a very small amount of water, within 0.01 wt%.

The density of tetralin was measured in the temperature range from 25 to 55°C with the aid of a Paar densimeter [27]. In this densimeter, the density  $\rho$  of the liquid is related to the period  $\tilde{T}$  of a vibrating  $U$  tube through the working equation

$$\tilde{T}^2 = (a_0 + a_1 t + a_2 t^2)(\rho + \rho') \quad (6)$$

where  $\tilde{T}$  is in ms,  $t$  is in  $^{\circ}\text{C}$ , and  $\rho$  and  $\rho'$  are in  $\text{g}\cdot\text{cm}^{-3}$ , with

$$a_0 = 6.722448, \quad a_1 = -9.316 \times 10^{-4}, \quad a_2 = 2.213 \times 10^{-6}, \quad \rho' = 1.0328 \quad (6a)$$

The constants in the working equation (6) were determined by calibrating the densimeter with distilled water [13] and with dry air [28] in the temperature range from 20 to  $50^{\circ}\text{C}$ . Equation (6) reproduced these density data with a standard deviation of  $1 \times 10^{-5} \text{g}\cdot\text{cm}^{-3}$  in the temperature range from 20 to  $50^{\circ}\text{C}$ . As a test of the accuracy obtainable with the instrument, the density of dilute solutions of 0.05% NaCl in water and of 0.1% NaCl in water was measured at 20 and  $30^{\circ}\text{C}$ . It was found that the measured densities of these solutions agreed with the values calculated from the International Critical Tables [29] to within  $5 \times 10^{-4}\%$ .

We measured the density of tetralin from 25 to  $55^{\circ}\text{C}$  at temperature intervals of  $5^{\circ}\text{C}$ . The results of these measurements are presented in Table III. Taking into account a possible  $0.05^{\circ}\text{C}$  difference between the temperature of the cell of the densimeter and that of the water bath, we estimate our density measurements to have an accuracy within 0.015%.

In the temperature range of our measurements the density  $\rho$  of tetralin can be represented by Eq. (3) with

$$\begin{aligned} \rho_0 &= 0.985305 \text{ g}\cdot\text{cm}^{-3} \\ \rho_1 &= -8.013 \times 10^{-4} \text{ g}\cdot\text{cm}^{-3}\cdot^{\circ}\text{C}^{-1} \\ \rho_2 &= 1.78 \times 10^{-7} \text{ g}\cdot\text{cm}^{-3}\cdot^{\circ}\text{C}^{-2} \end{aligned} \quad (3b)$$

This equation reproduces the data with a standard deviation of  $1.4 \times 10^{-5} \text{g}\cdot\text{cm}^3$ .

In Fig. 3 we show a comparison between our results and some densities reported in the literature [30–35] including the values recommended

Table III. Density of Tetralin

Temperature ( $^{\circ}\text{C}$ )	Density ( $\text{g}\cdot\text{cm}^{-3}$ )
24.951	0.96542
29.948	0.96147
34.949	0.95753
39.952	0.95358
44.948	0.94964
49.949	0.94571
54.950	0.94182

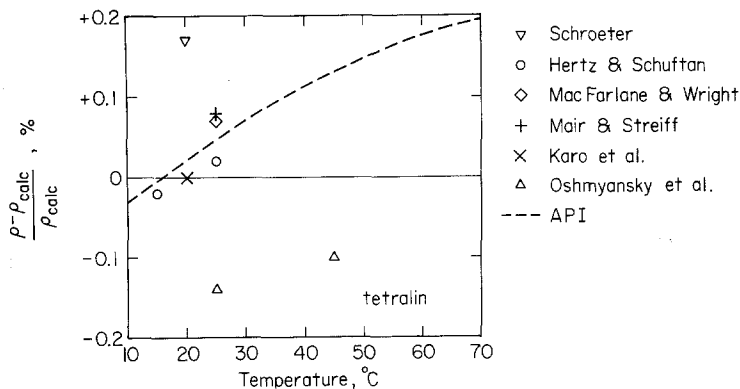


Fig. 3. Comparison between the density  $\rho$  of tetralin reported in the literature and the values calculated from Eq. (3) with Eq. (3b).

by API [36]. The differences between our results and the API values are substantial, becoming as much as 0.16% at 55°C. Because of these sizable differences, we asked Harada of the Hamamatsu College of the Shizuoka Prefectural University in Japan to make an independent check of the density of the same sample of tetralin. In the measurements performed by Harada, two Paar densimeters (DMA 602) were used. To reduce possible effects of any temperature drift and the thermal expansion of the cell in the densimeter, one densimeter was used for the sample liquid and the other for the reference liquid (water). At each temperature the densimeter used for the sample liquid was calibrated with distilled water and dry nitrogen. The temperature was measured with a thermister inside the cell just before and after each density measurement, thus avoiding any effects of a possible self-heating of the thermometer.

Table IV. Comparison Between Two Independent Measurements of the Density of Tetralin

$t$ (°C)	$\rho^a$ (g · cm <sup>-3</sup> )	$\rho^b$ (g · cm <sup>-3</sup> )	Difference (%)
20	0.96935	0.96922	-0.013
25	0.96538	0.96547	+0.009
30	0.96143	0.96151	+0.009
35	0.95748	0.95753	+0.006
40	0.95354	0.95367	+0.014
45	0.94961	0.94973	+0.013

<sup>a</sup> This work.

<sup>b</sup> As measured by Harada [37].



The densities thus measured by Harada at temperatures from 20 to 45°C [37] are compared with our earlier results in Table IV. The two data sets agree within the experimental accuracy of 0.015%. We conclude that our measurements yield a significant improvement over the densities recommended by API.

## 5. VISCOSITY OF TETRALIN

The viscosity of the same sample of tetralin was measured with another Ubbelohde viscometer connected to Teflon and stainless-steel tubing so that the tetralin could be kept in a nitrogen atmosphere at all times. In the usual operation the sample liquid is drawn into a supply bulb by suction [21]. In the present experiments the sample liquid was raised to the supply bulb by applying a pressure with dry nitrogen through an oxy-purge. After decreasing the pressure in the viscometer to atmospheric pressure again through an oxy-purge with a valve to prevent back flow of air, the flow time of a fixed volume of the liquid was measured. The viscometer was located in an oil bath with a temperature stability of 0.01°C. The kinematic viscosity  $\nu$  was related to the flow time  $\tau$  by the working equation (4) with

$$\begin{aligned} C &= (1.09800 \pm 0.00018) \times 10^{-3} \text{ mm}^2 \cdot \text{s}^{-1}, \\ B &= (0.332 \pm 0.032) \text{ mm}^2 \end{aligned} \quad (4b)$$

The instrument constants  $C$  and  $B$  were again obtained by calibrating the viscometer with water at temperatures from 33 to 95°C, corresponding to flow times ranging from 690 to 282 s. The working equation reproduces the calibration data with a standard deviation of 0.05%.

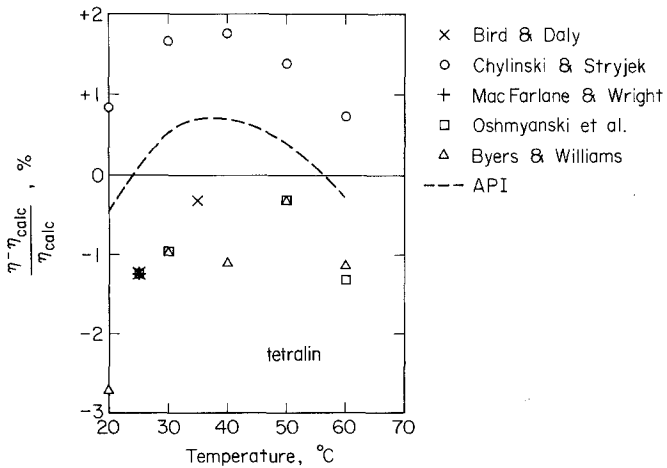
The kinematic viscosity of tetralin was measured at temperatures from 25 to 120°C corresponding to flow times ranging from 1900 s to 590 s. The experimental results are presented in Table V. The accuracy of our viscosity measurements for tetralin is comparable to those for *trans*-decalin as described in Section 3: 0.1% relative to the viscosity of water and 0.3% on an absolute basis.

Since our density measurements for tetralin were restricted to temperatures below 60°C, we converted the experimental values for the kinematic viscosity  $\nu$  into values for the dynamic viscosity  $\eta$  only in the temperature range between 25 and 60°C. In this temperature range the viscosity  $\eta$  can be represented with a standard deviation of  $5 \times 10^{-3} \text{ mPa} \cdot \text{s}$  by the Vogel equation (5) with

$$A = 0.1186 \text{ mPa} \cdot \text{s}, \quad E = 383.9 \text{ K}, \quad T_0 = 162.5 \text{ K} \quad (5b)$$

Table V. Kinematic Viscosity  $\nu$  and Dynamic Viscosity of  $\eta$  of Tetralin

$t$ (°C)	$\nu$ (mm <sup>2</sup> ·s <sup>-1</sup> )	$\eta$ (mPa·s)
24.982	2.088	2.015
29.956	1.884	1.811
34.927	1.729	1.656
39.954	1.595	1.521
44.951	1.476	1.402
49.952	1.371	1.297
54.952	1.279	1.205
59.947	1.197	1.122
64.950	1.123	
69.943	1.057	
74.951	0.9969	
79.969	0.9426	
84.950	0.8922	
89.946	0.8482	
94.949	0.8077	
99.974	0.7695	
104.942	0.7350	
109.968	0.7022	
114.956	0.6725	
119.960	0.6448	

Fig. 4. Comparison between the viscosity  $\eta$  of tetralin reported in the literature and the values calculated from Eq. (5) with Eq. (5b).

In Fig. 4 we show a comparison between our results and values for the viscosity reported in the literature [15, 26, 32, 35, 38] including the values recommended by API [36]. The deviations of the literature values from our measurements vary from  $-2.7$  to  $+1.7\%$ . We think that part of this spread is due to the difficulty of keeping tetralin pure when exposed to air. As described above in our experiments special care was made to avoid contamination of the tetralin. The maximum deviation of the viscosity values recommended by API [36] is  $+0.7\%$  in the temperature range  $25^{\circ}\text{C} < t < 60^{\circ}\text{C}$ , where we are able to give reliable values for the dynamic viscosity  $\eta$ .

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