Physical Properties of Hydrocarbons

Part 15—C_5-C_8 Alkanes

Robert W. Gallant
The Dow Chemical Co., Plaquemine, La.

PARTS OF THE PRODUCT MIX of every refinery are the C_5 to C_8 alkanes (pentane, hexane, heptane, octane). In many cases, they never emerge as a pure product but are upgraded into gasolines or cracked to lower molecular weight hydrocarbons. Although over a billion pounds are produced every year, only a small part of this appears as a purified product for sale. Hexane has achieved a sizeable market as a solvent in polyolefin processes.

Because these compounds are important products in petroleum refining, their physical properties have been extensively studied. Consequently, physical property data are available on all four compounds over a wide temperature range. Sage and co-workers have been the outstanding contributors for the C_5 to C_8 alkanes.

Critical Properties and Vapor Pressure. The critical properties of all four compounds have been experimentally determined. Agreement among various investigators is excellent.[1,2,3]

Experimental data are available on the vapor pressures up to the critical point for pentane,[1,4] hexane,[1,5,7] heptane,[1] and octane.[1,6,8] The American Petroleum Institute has compiled a bibliography of all available literature data on vapor pressures of hydrocarbons.[9] This is an extremely valuable reference work and, hopefully, the forerunner of additional physical property compilations.

Heat of Vaporization. Kozicki and Sage have measured the heat of vaporization of pentane from room temperature to its critical temperature.[10] Data are also available for hexane up to its critical point.[5,11] The experimental data, available up to the boiling point for heptane and octane,[3,6,12] have been extrapolated to the critical point by the Watson equation. Calculated values, when compared with experimental data for pentane and hexane, gave an average error of 1.6 percent. The error increased to 5 percent within 10° of the critical temperature.

Heat Capacity. The vapor heat capacities of all four compounds are very similar, varying only a few percent over the entire temperature range of 0-1,000° C. Kobe[13] has determined the vapor heat capacity of pentane and hexane. Person and Pimental[14] provide data for pentane, hexane, and heptane. A third investigator[15] closely duplicated the data of Kobe and Person for pentane. Hence, it appears the vapor heat capacity data are extremely reliable. The heat capacity of octane was calculated by the method of Rihani and Doraiswamy,[16] with a probable error of less than 2 percent.

The liquid heat capacities are available up to 100° C for hexane,[3,17] heptane,[3,18,19] and octane.[3,17] Pentane data are available only up to 25° C.[2,3] The data for all compounds have been extended to 160° C by the method of Chow and Bright.[20] Above the boiling point, the error averages about 10 percent.

Density. The liquid density of all four compounds has been experimentally determined up to the critical point.[3,7] Additionally, the effect of pressure on the density of hexane,[21] heptane,[22] and octane[8] has been experimentally measured and is presented in Figures 15-6, 15-7 and 15-8.

Viscosity. The vapor viscosities of pentane[15,20] and hexane[20] have been measured up to 300° C. The method of Bromley and Wilke[20] has been used to extend these data to 500° C for pentane and hexane and to cover the 0-500° C range for heptane and octane. Comparison with nine experimental points gave average and maximum errors of 2.0 percent and 5.1 percent, respectively. Above 150° C, the error averages 1 percent.

The liquid viscosities of all four compounds have been studied over a wide temperature range.[3,12,23,24,25] Figure 15-11 presents the effect of pressure on the liquid viscosity of pentane.[26]

Surface Tension. Jasper and Kring[27] have determined the surface tensions of all four compounds up to their boiling point. Jeffries and Derrick[28] have measured the

TABLE 15-1—Physical Properties of the C_5-C_8 Alkanes

	Boiling Point °C	Freezing Point °C	Molecular Weight	Critical Properties °C T_c	Critical Properties PSIA P_c	Critical Properties g/ml d_c
n-pentane	36.1	−129.7	72.15	196.6	489	0.244
n-hexane	68.7	− 95.4	86.17	234.5	440	.234
n-heptane	98.4	− 90.6	100.20	267.0	397	.234
n-octane	125.6	− 56.8	114.22	295.4	362	.235

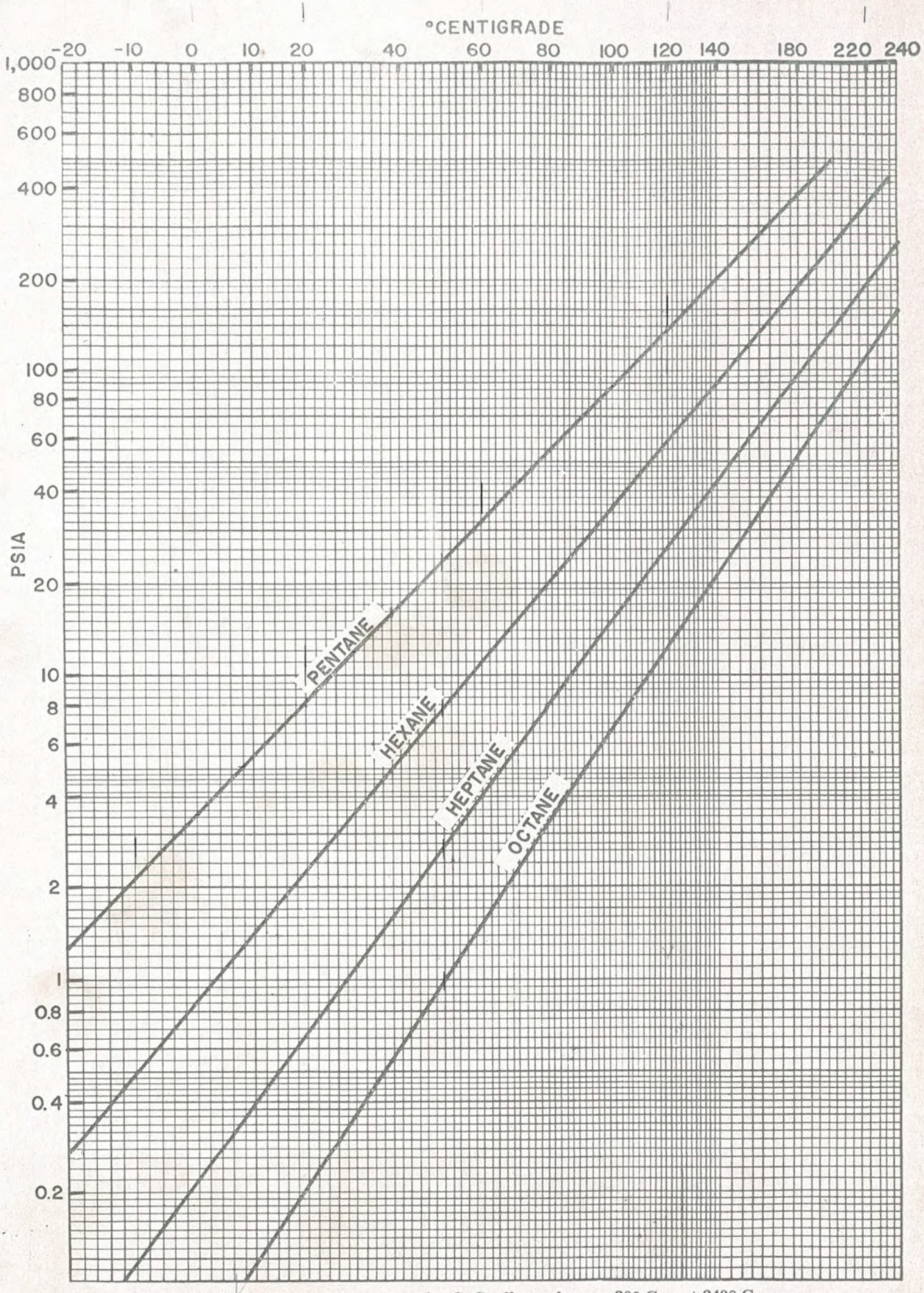

Fig. 15-1—Gives vapor pressure for C_5-C_8 alkanes from −20° C to +240° C.

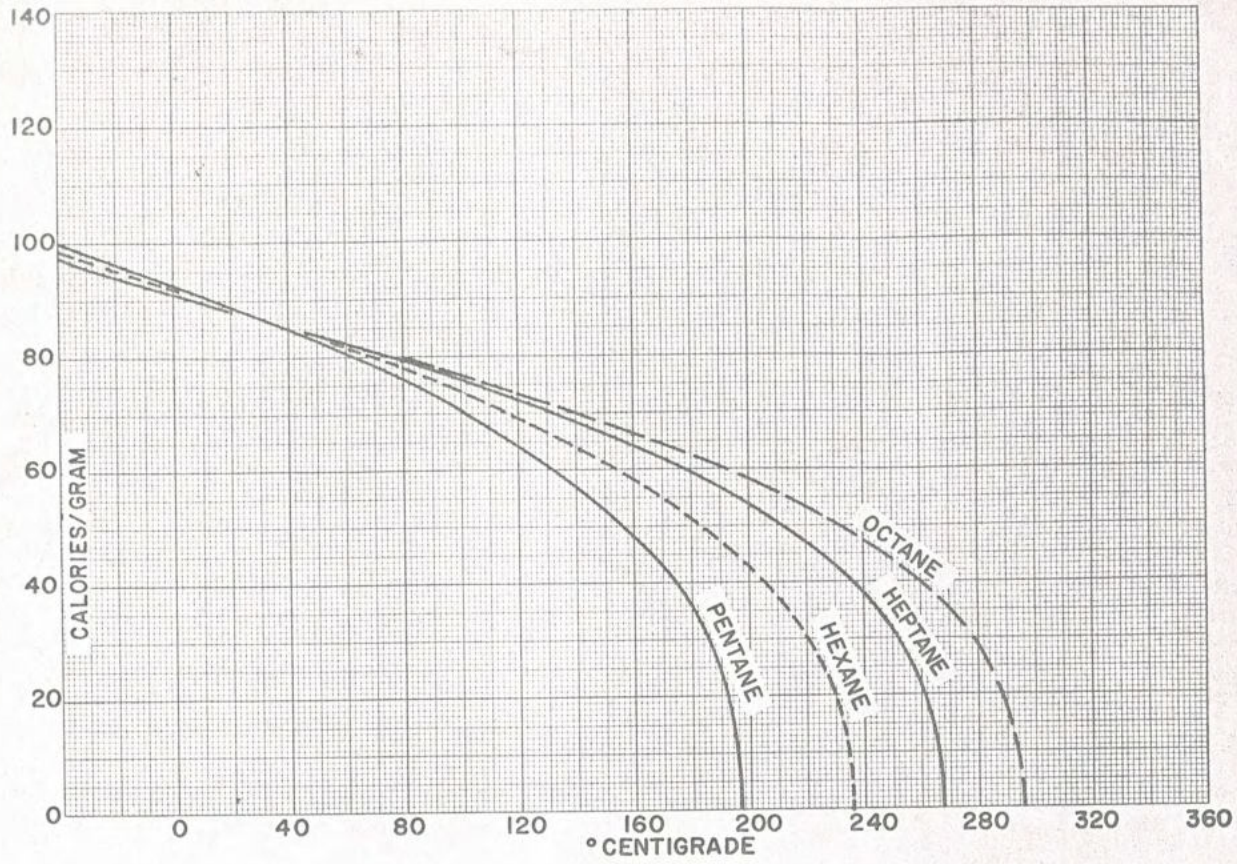

Fig. 15-2—Gives heat of vaporization for C_5-C_8 alkanes from −40° C to +295° C.

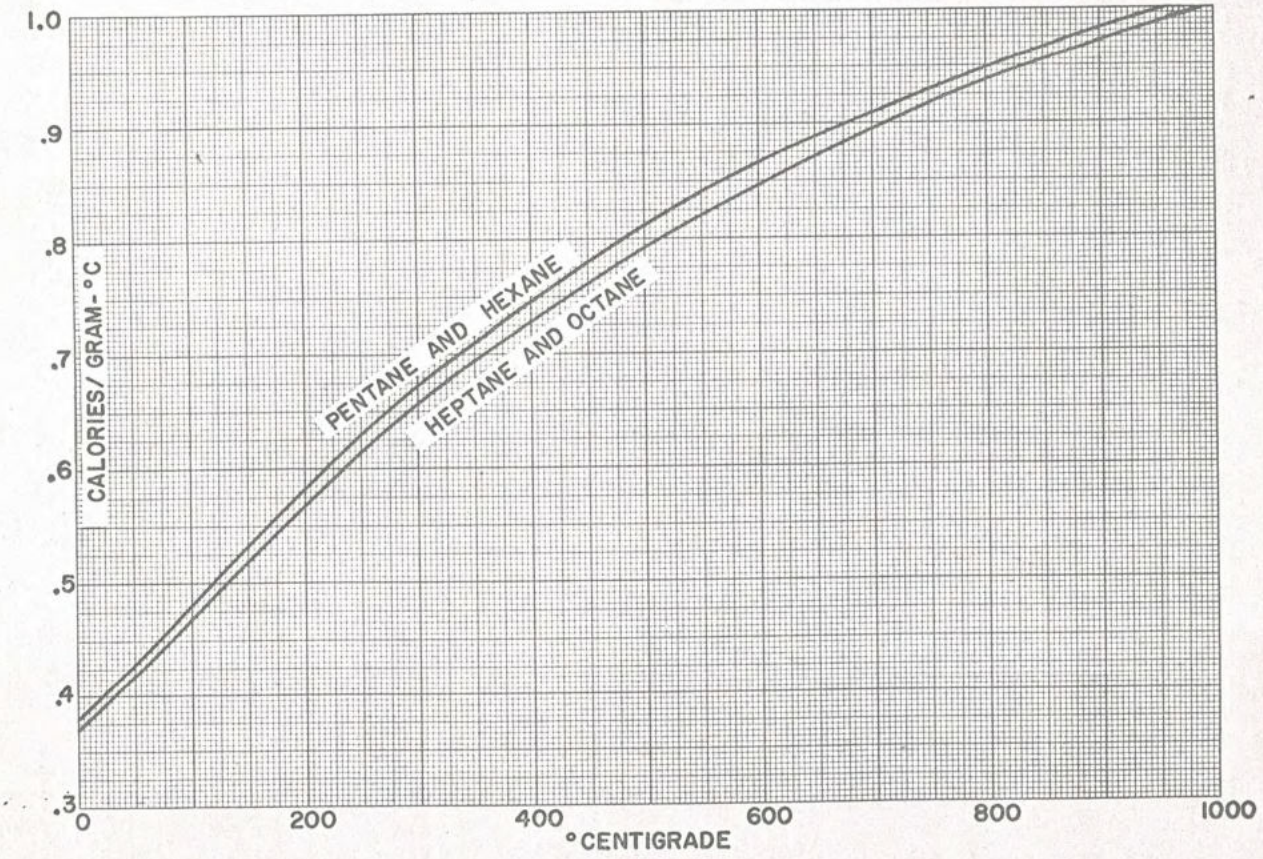

Fig. 15-3—Gives vapor heat capacity for C_5-C_8 alkanes from 0° C to +1,000° C.

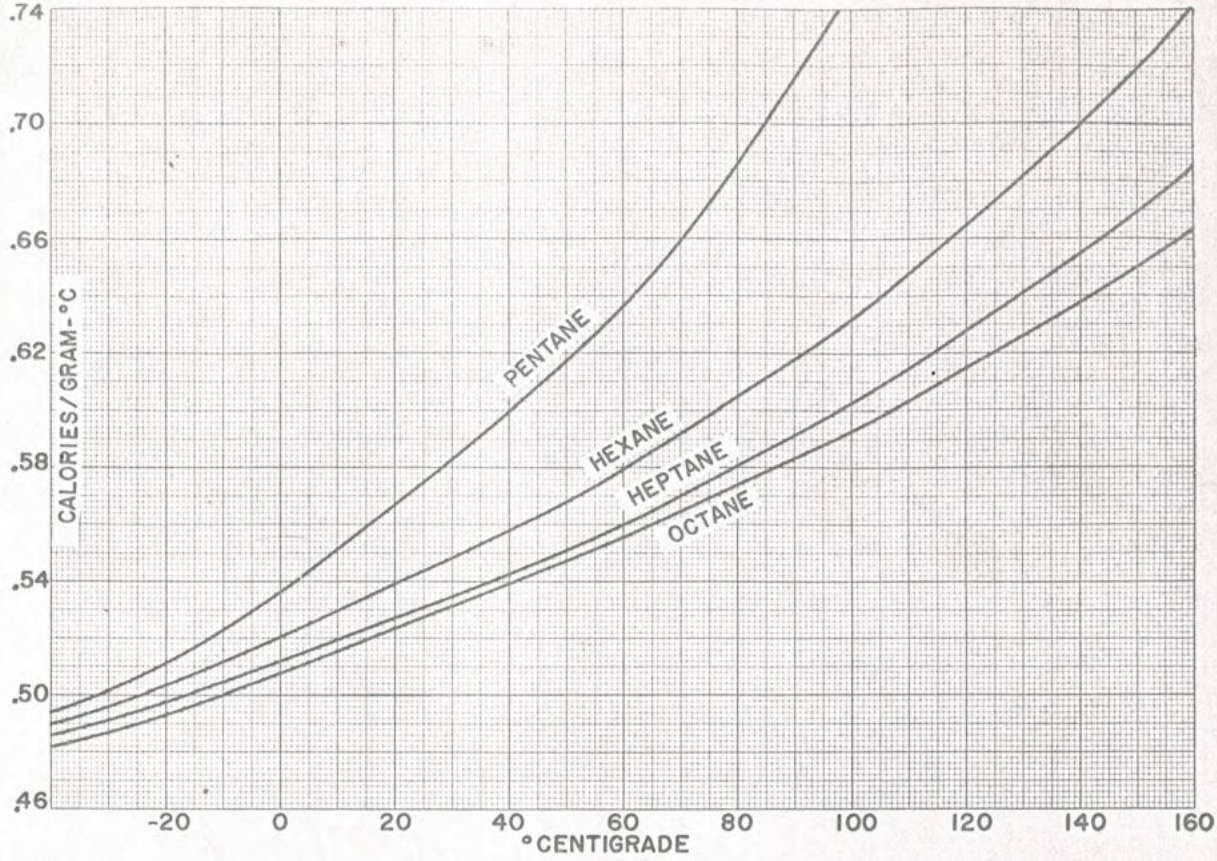

Fig. 15-4—Gives liquid heat capacity for C_5-C_8 alkanes from −40° C to +160° C.

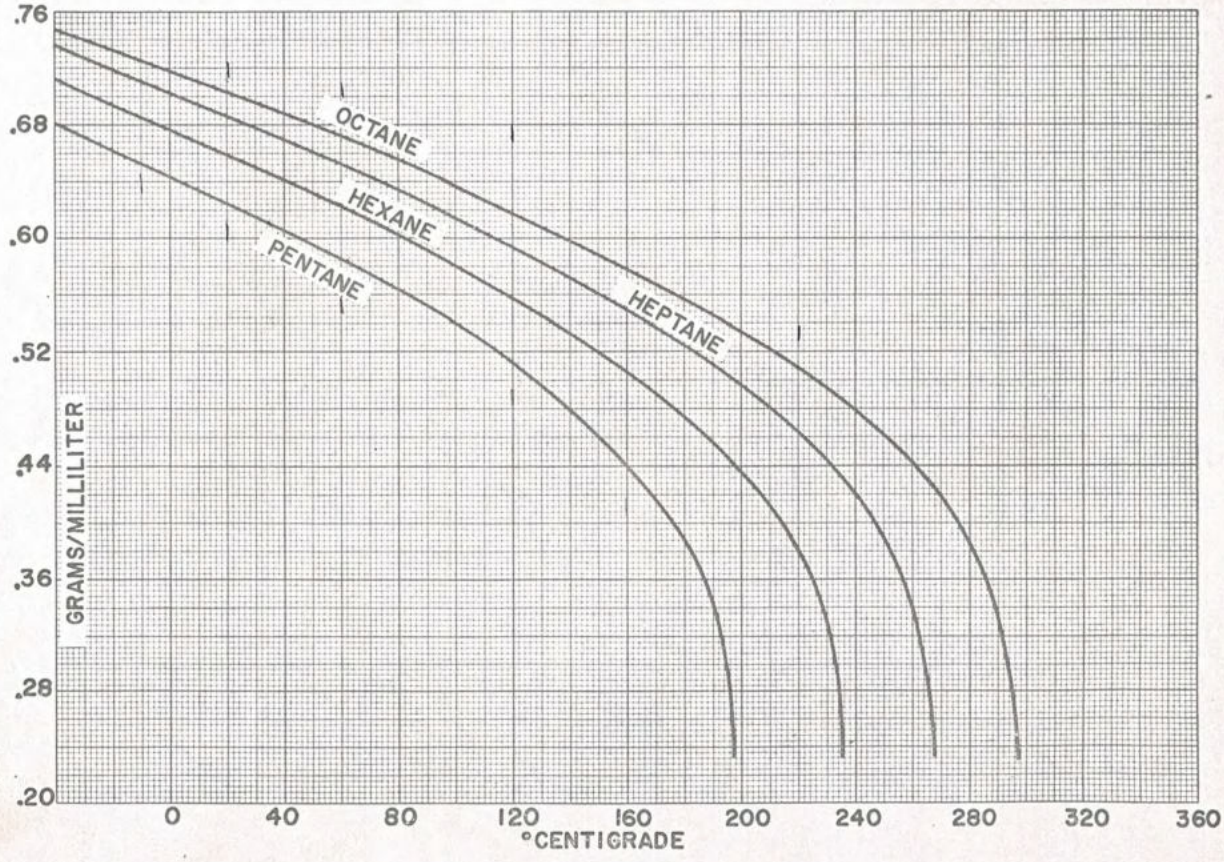

Fig. 15-5—Gives liquid density for C_5-C_8 alkanes from −40° C to +296° C.

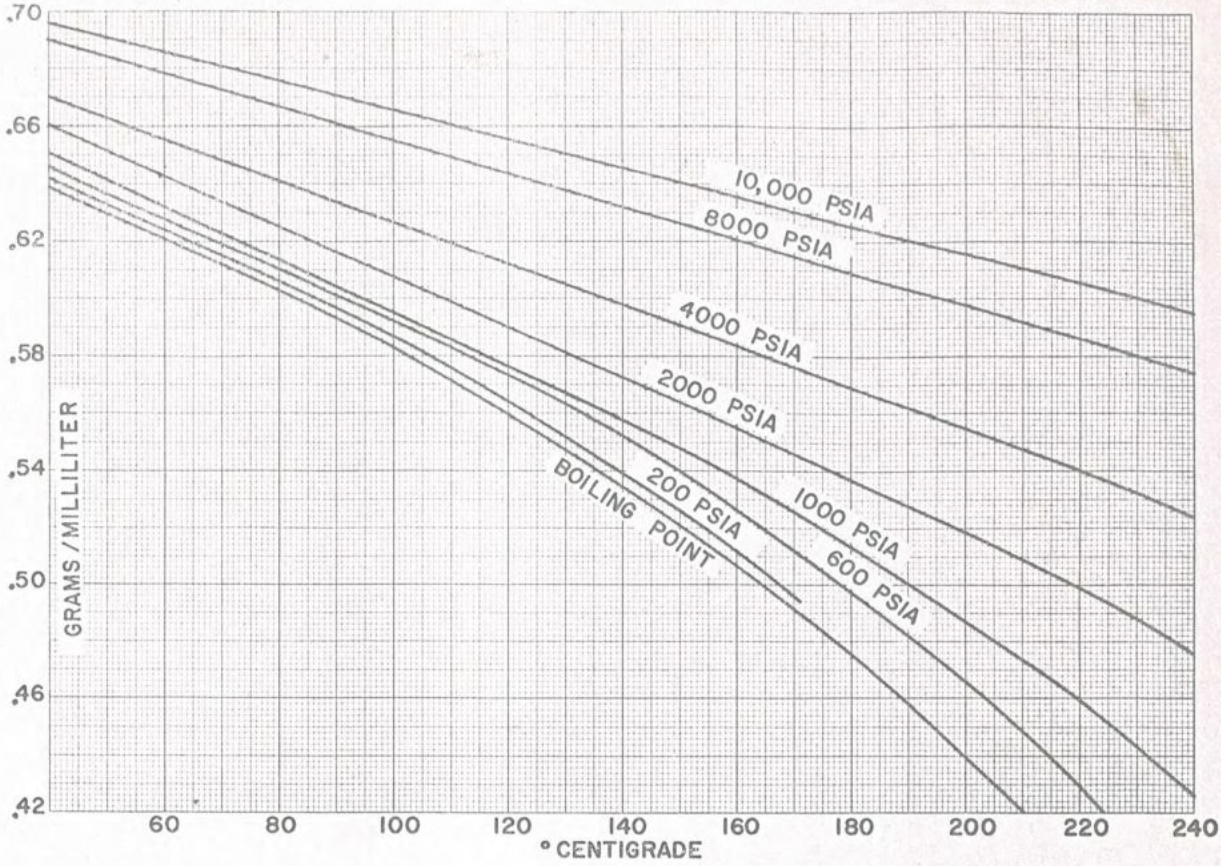

Fig. 15-6—Gives pressure effect on liquid density for hexane up to 10,000 psia and 240° C.

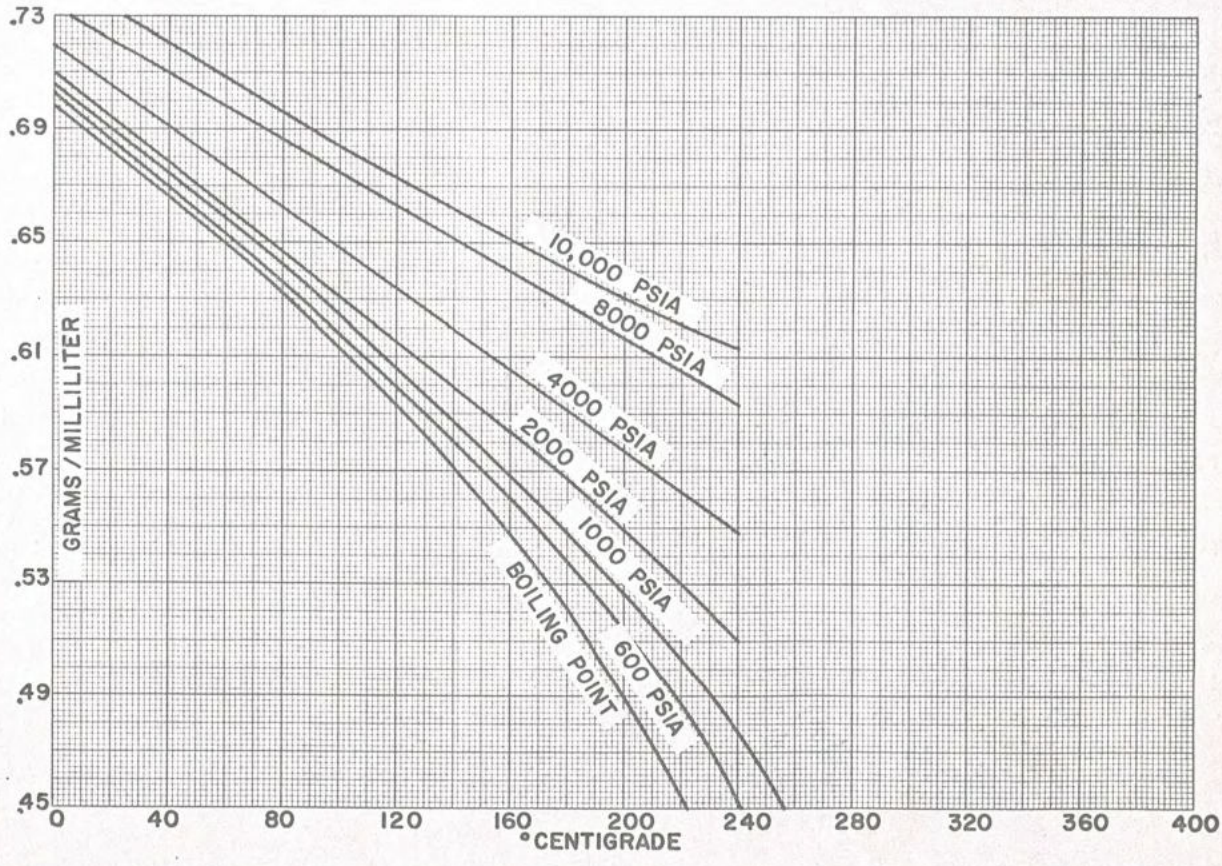

Fig. 15-7—Gives pressure effect on liquid density for heptane up to 10,000 psia and 256° C.

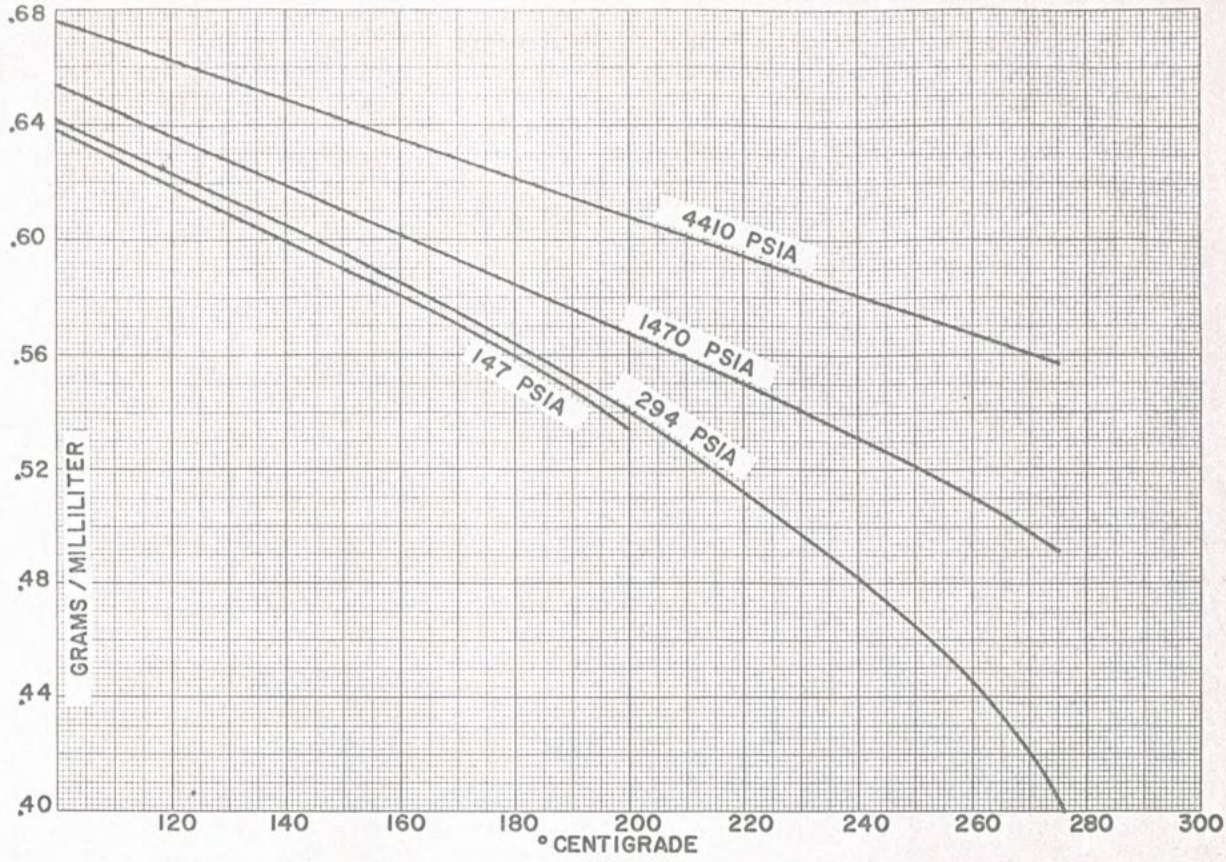

Fig. 15-8—Gives pressure effect on liquid density for octane up to 4,410 psia and 275° C.

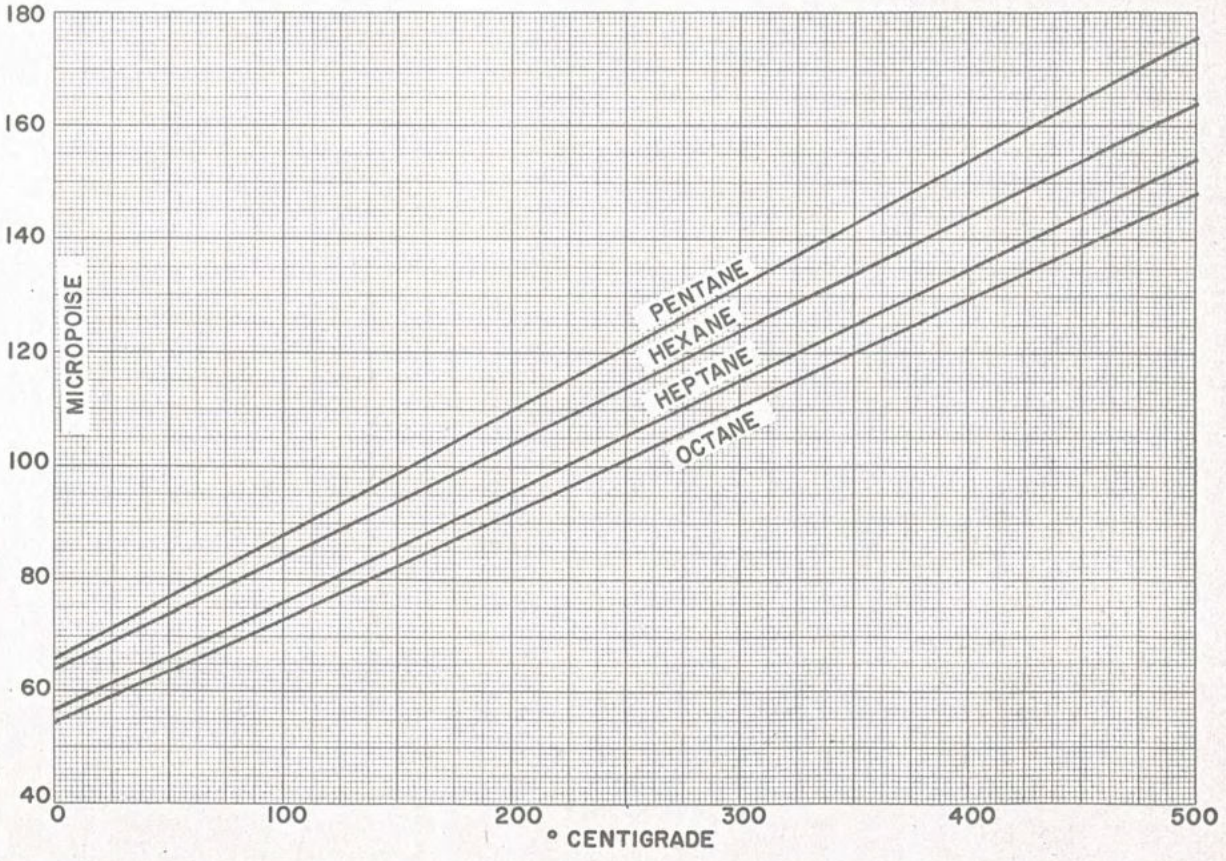

Fig. 15-9—Gives vapor viscosity for C_5-C_8 alkanes from 0° C to +600° C.

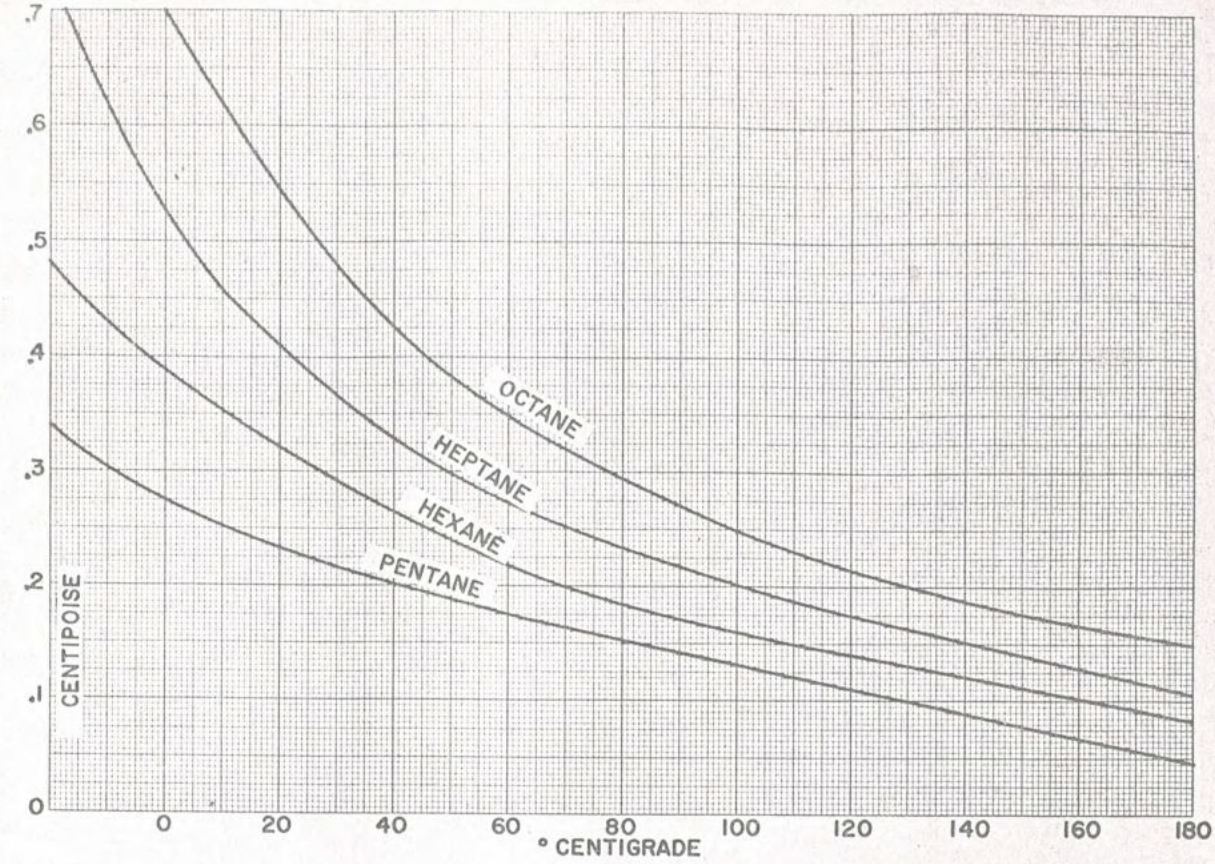

Fig. 15-10—Gives liquid viscosity for C_5-C_8 alkanes from −20° C to +180° C.

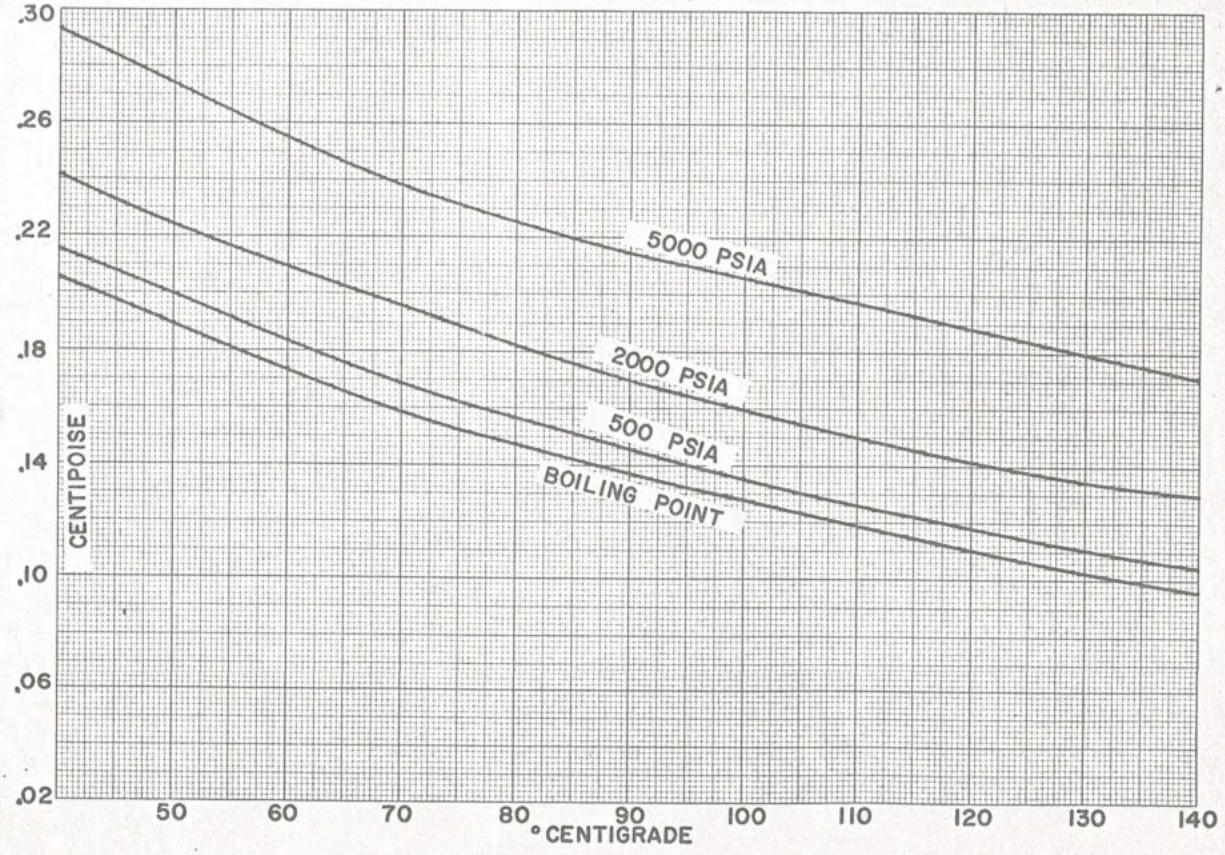

Fig. 15-11—Gives pressure effect on liquid viscosity for pentane up to 5,000 psia and 140° C.

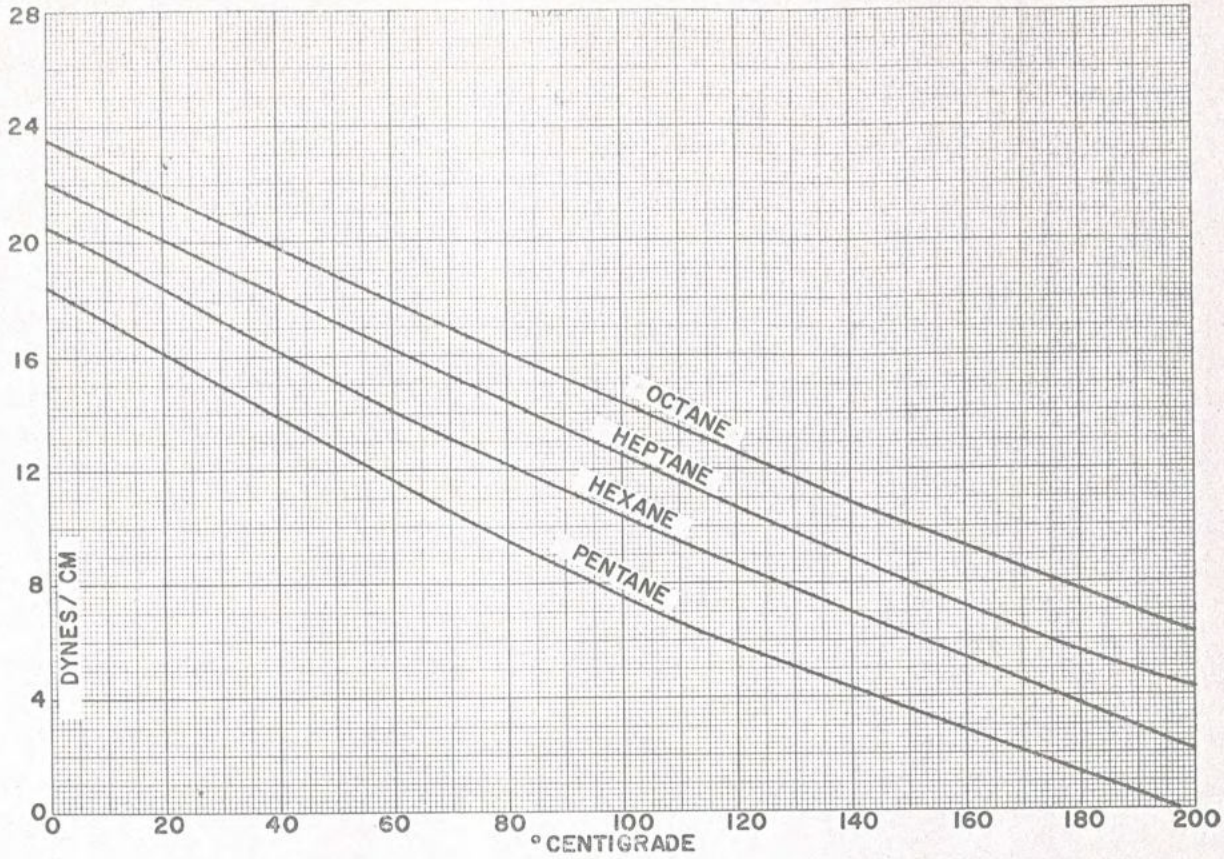

Fig. 15-12—Gives surface tension for C_5-C_8 alkanes from 0° C to +200° C.

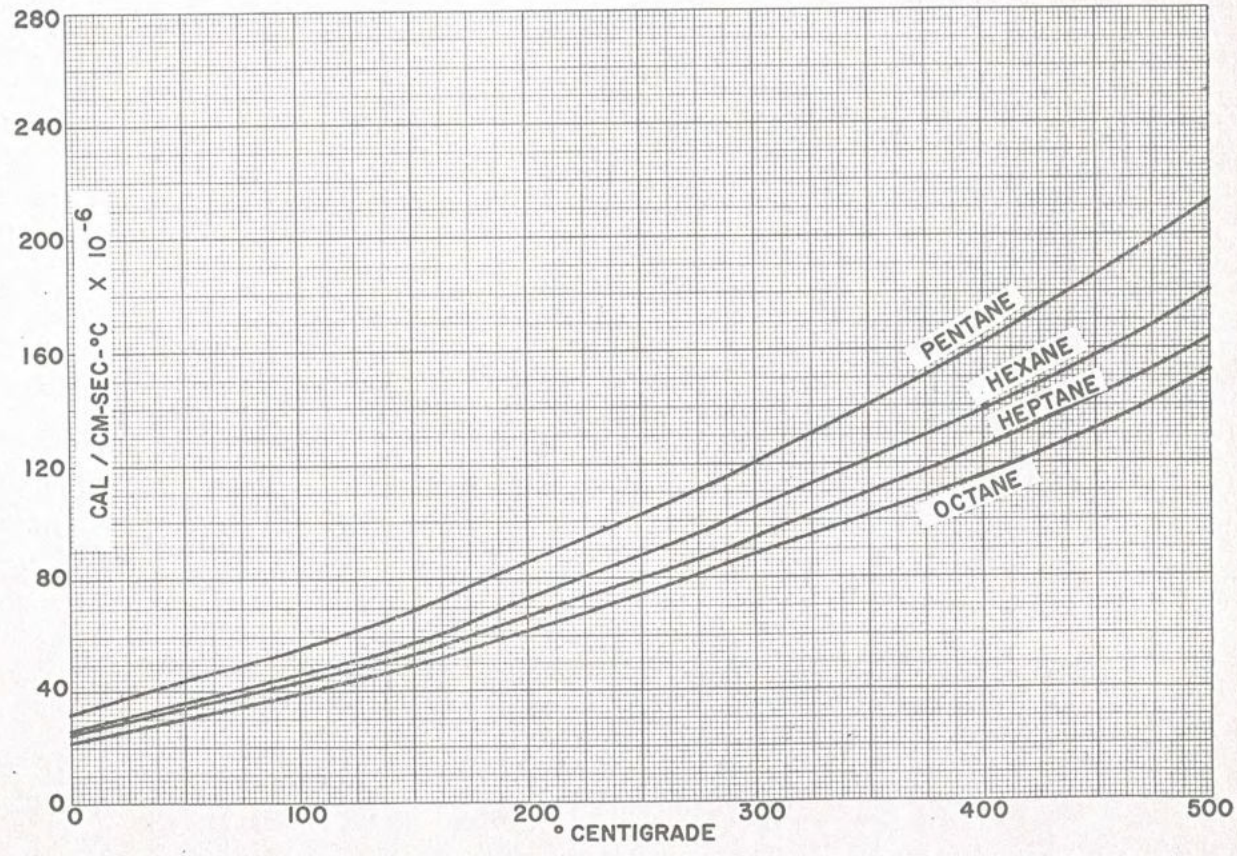

Fig. 15-13—Gives vapor thermal conductivity for C_5-C_8 alkanes from 0° C to +500° C.

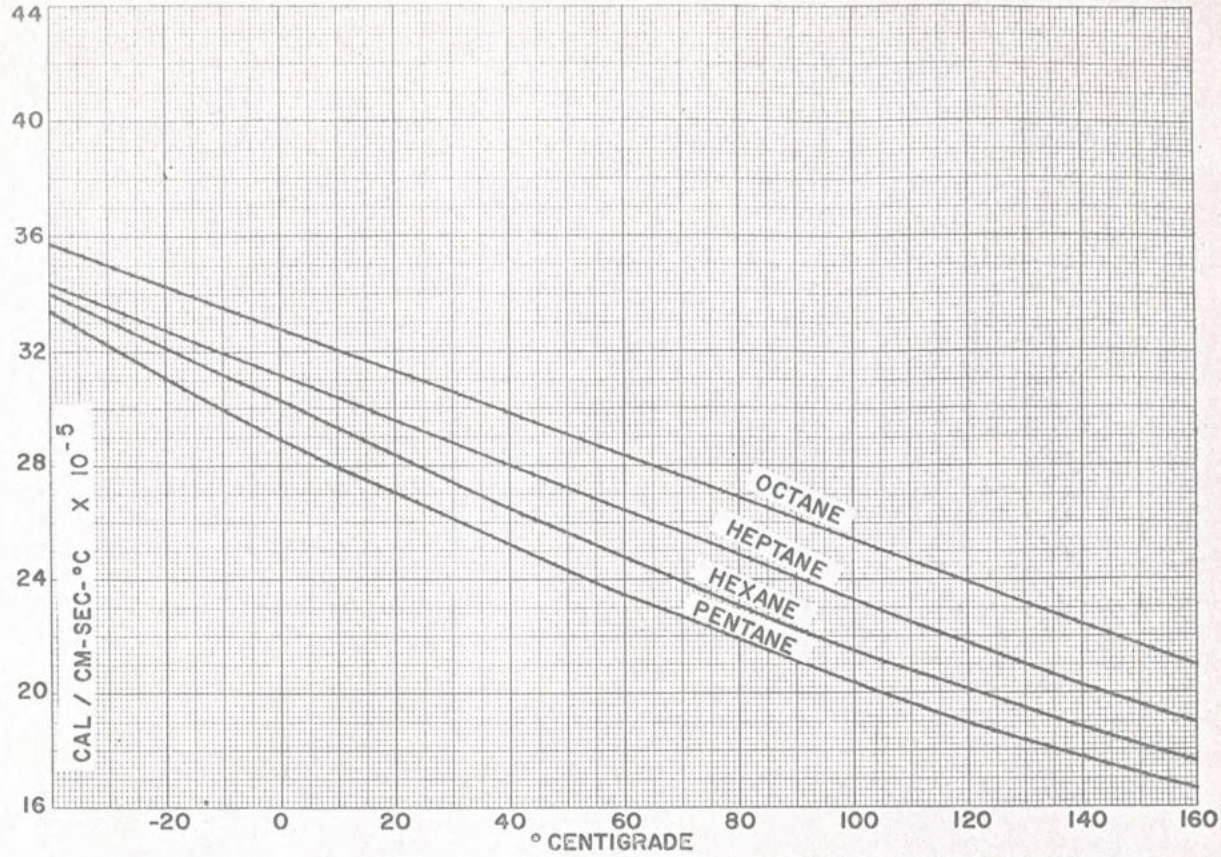

Fig. 15-14—Gives liquid thermal conductivity for C_5-C_8 alkanes from −40° C to +160° C.

surface tension of pentane up to 150° C. These data have been supplemented by other available data[3,11,22] and extended up to 200° C by the nomograph of Kharbanda.[29] The error averaged 3.6 percent when compared with eight experimental values.

Thermal Conductivity. The only extensive vapor thermal conductivity data are that of Wiley[15] for pentane from 50° C to 150° C. The data of Lambert[30] for the vapor thermal conductivity of pentane, hexane, and heptane at 66° C and octane at 82° C have been used to calculate the quasicritical thermal conductivity according to the method of Owens and Thodos.[31] Using their correlation with reduced temperature, the vapor thermal conductivities of the four compounds have been calculated for the 0-500° C temperature range. The error should be less than 3 percent.

Jobst[32] has carried out an extensive study of liquid thermal conductivities over wide temperature ranges. Included are alkanes, alcohols, ketones, and aldehydes. For the alkanes, he has measured the thermal conductivity up to the boiling point. The data have been expanded to 160° C by the method of Robbins and Kingrea.[33] Comparison of calculated values with the experimental data of Jobst gave an average error of 4.4 percent for 19 experimental points. Above 0° C, the average error was 3.5 percent for 11 points.

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Indexing Terms: Computations-4, Heat-7, Heptane-9, Hexane-9, Liquid Phase-5, Octane-9, Pentane-9, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Temperature-6, Vapor Phase-5.

Part 16 "C_5-C_8 Alkenes" will appear in an early issue.