



A Honeywell Company

Calculation of UOP Characterization Factor and Estimation of Molecular Weight of Petroleum Oils

UOP Method 375-07

Scope

This method is for calculating the UOP Characterization Factor of petroleum oils from API gravity and distillation or viscosity data. Average molecular weight of petroleum oils is estimated from API gravity and distillation data. The UOP Characterization Factor, commonly called K, is indicative of the general origin and nature of a petroleum stock. Values of 12.5 or higher indicate a material predominantly paraffinic in nature. Highly aromatic materials have characterization factors of 10.0 or less.

References

- ASTM Method D 86, "Distillation of Petroleum Products at Atmospheric Pressure," www.astm.org
- ASTM Method D 88, "Saybolt Viscosity," www.astm.org
- ASTM Method D 445, "Kinematic Viscosity of Transparent and Opaque Liquids (and the Calculation of Dynamic Viscosity)," www.astm.org
- ASTM Method D 1160, "Distillation of Petroleum Products at Reduced Pressure," www.astm.org
- ASTM Method D 1250, "Guide for the Use of Petroleum Measurement Tables," www.astm.org
- ASTM Method D 1298, "Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method," www.astm.org
- ASTM Method D 2161, "Practice for Conversion of Kinematic Viscosity to Saybolt Universal Viscosity or Saybolt Furol Viscosity," www.astm.org
- Smith, R. L., and Watson, K. M., *Ind. Eng. Chem.*, **29**, 1408 (1937)
- Watson, K. M., Nelson E. F., and Murphy, G. B., *Ind. Eng. Chem.*, **27**, 1460 (1935)

Outline of Method

The UOP Characterization Factor, K, can be calculated using either distillation or viscosity data. The distillation data procedure calculates the K factor using data obtained from ASTM D 1298, "Density,

IT IS THE USER'S RESPONSIBILITY TO ESTABLISH APPROPRIATE PRECAUTIONARY PRACTICES AND TO DETERMINE THE APPLICABILITY OF REGULATORY LIMITATIONS PRIOR TO USE. EFFECTIVE HEALTH AND SAFETY PRACTICES ARE TO BE FOLLOWED WHEN UTILIZING THIS PROCEDURE. FAILURE TO UTILIZE THIS PROCEDURE IN THE MANNER PRESCRIBED HEREIN CAN BE HAZARDOUS. MATERIAL SAFETY DATA SHEETS (MSDS) OR EXPERIMENTAL MATERIAL SAFETY DATA SHEETS (EMSDS) FOR ALL OF THE MATERIALS USED IN THIS PROCEDURE SHOULD BE REVIEWED FOR SELECTION OF THE APPROPRIATE PERSONAL PROTECTION EQUIPMENT (PPE).

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Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method,” in combination with either ASTM D 86, “Distillation of Petroleum Products AT Atmospheric Pressure,” or ASTM D 1160, “Distillation of Petroleum Products at Reduced Pressure,” dependent on the sample, and the nomographs or engineering charts incorporated in the method. The viscosity data procedure calculates the K factor using data obtained from ASTM D 1298 in combination with either ASTM D 445, “Kinematic Viscosity of Transparent and Opaque Liquids (or the calculation of Dynamic Viscosity),” or ASTM D 88, “Saybolt Viscosity” and the nomographs incorporated in the method.

The Average molecular Weight is estimated using the same data as for the K factor distillation data procedure, but with a different set of nomographs.

The Appendix describes a procedure to calculate the K factor and the molecular weight using the relative density and ASTM Distillation data and equations that were derived from curve fits of the nomographs.

If the sample is beyond the scopes of these methods, other standard methods may be substituted. In some cases, this may involve additional calculations to convert the observed data to the appropriate units.

Definitions

Cubic average boiling point is the cube of the sum of the products of the volume fraction multiplied by the cube root of the boiling point of each component expressed in degrees Rankine.

Mean average boiling point is the arithmetic average of the true molal boiling point and the cubic average boiling point expressed in degrees Fahrenheit.

Molecular weight, as employed herein, is that average molecular weight of a petroleum fraction and not that of a single, pure compound.

True molal average boiling point is the sum of the products of the mol fraction multiplied by the boiling point of each component.

UOP Characterization Factor, K, of a petroleum oil is defined as the cube root of its cubic average boiling point, in degrees Rankine, divided by its relative density at 60°F (15.56°C).

Volumetric average boiling point is the arithmetic average boiling point over the range of 10% to 90% of the ASTM distillation.

Apparatus

No additional apparatus is required beyond the apparatus listed in the above methods.

Procedure

Determine the API gravity or relative density at 60°F of the sample according to ASTM D 1298.

Perform an ASTM distillation by either ASTM D 86 or D 1160, as appropriate for the sample. Correct the data to 760 mm Hg and for material loss as specified in these methods. Convert temperatures recorded in degrees Celsius to degrees Fahrenheit.

Characterization factor may also be estimated using kinematic viscosity at 100, 122 or 210°F (38, 50 or 99°C). Kinematic viscosity is determined directly from ASTM D 445. Saybolt viscosity, determined by ASTM D 88, can be converted to kinematic viscosity using ASTM D 2161.

Calculations

UOP K Factor from API Gravity and ASTM Distillation

Volumetric Average Boiling Point

Calculate the volumetric average boiling point as the average of the 10, 30, 50, 70 and 90 vol-% temperatures. Calculate the slope as °F per percent (°F/%) by subtracting the 10 vol-% temperature from the 90 vol-% temperature, and dividing the difference by 80 vol-%.

Cubic Average Boiling Point

Obtain the value of the correction to be applied to the volumetric average boiling point using Figure 1. Using the value of the slope calculated above, go to the bottom of the chart, then proceed vertically to the curve which represents the value of the volumetric average boiling point. Interpolate between curves as needed. Read the value of the vertical scale on the left side corresponding to this point to obtain the value of the correction term. *Subtract* this term from the volumetric average boiling point to calculate the cubic average boiling point.

UOP Characterization Factor, K

Determine the UOP Characterization Factor, K, using the cubic average boiling point and API gravity. Locate the cubic average boiling point on the horizontal scale at the bottom of Figure 2. Locate the API gravity on the vertical scale at the left of the graph. Find the intersection of the vertical and horizontal lines from these points. Read the number of the curve nearest to this point. This number, corrected by interpolation for the distance of the point from the nearest curve, is the characterization factor, K.

Example:

Calculate the characterization factor for a gas oil of 28.7° API at 60°F having the following distillation properties:

ASTM Distillation (Corrected to 760 mm Hg Pressure)

Volume-%	10	30	50	70	90
Temp., °F	598	700	755	802	874

$$\text{Volumetric average boiling point} = \frac{598 + 700 + 755 + 802 + 874}{5} = 746$$

$$\text{Slope} = \frac{874 - 598}{80} = 3.45^\circ\text{F/volume-\%}$$

$$\text{Correction term} = 5^\circ\text{F from Figure 1}$$

$$\text{Cubic average boiling point} = 746 - 5 = 741^\circ\text{F}$$

$$\text{Characterization factor, K} = 12.03 \text{ from Figure 2}$$

UOP K Factor from API Gravity and Kinematic Viscosity

Viscosities measured at high temperatures yield more reliable values for characterization factors than viscosities measured at low temperatures. Viscosity at low temperatures is influenced by the width of boiling range as well as by relative density and characterization factor. For samples that do not yield a

full distillation range by ASTM Method D 1160, the use of viscosities measured at 210°F (99°C) is preferred, where practical. Nomographs based on viscosities measured at 100°F (38°C) and 122°F (50°C) are also included for convenience.

The UOP Characterization Factor, K , is determined from Figures 3, 4 or 5, respectively, by entering with the API gravity and kinematic viscosity at 100, 122 or 210°F (38, 50 or 99°C). Locate the API gravity on the horizontal scale at the bottom of the chart. Locate the kinematic viscosity on the vertical scale at the left of the chart. Find the intersection of the vertical and horizontal lines from these points. Read the number of the curve nearest to this point. This number, corrected by interpolation for the distance of the point from this curve, is the characterization factor, K .

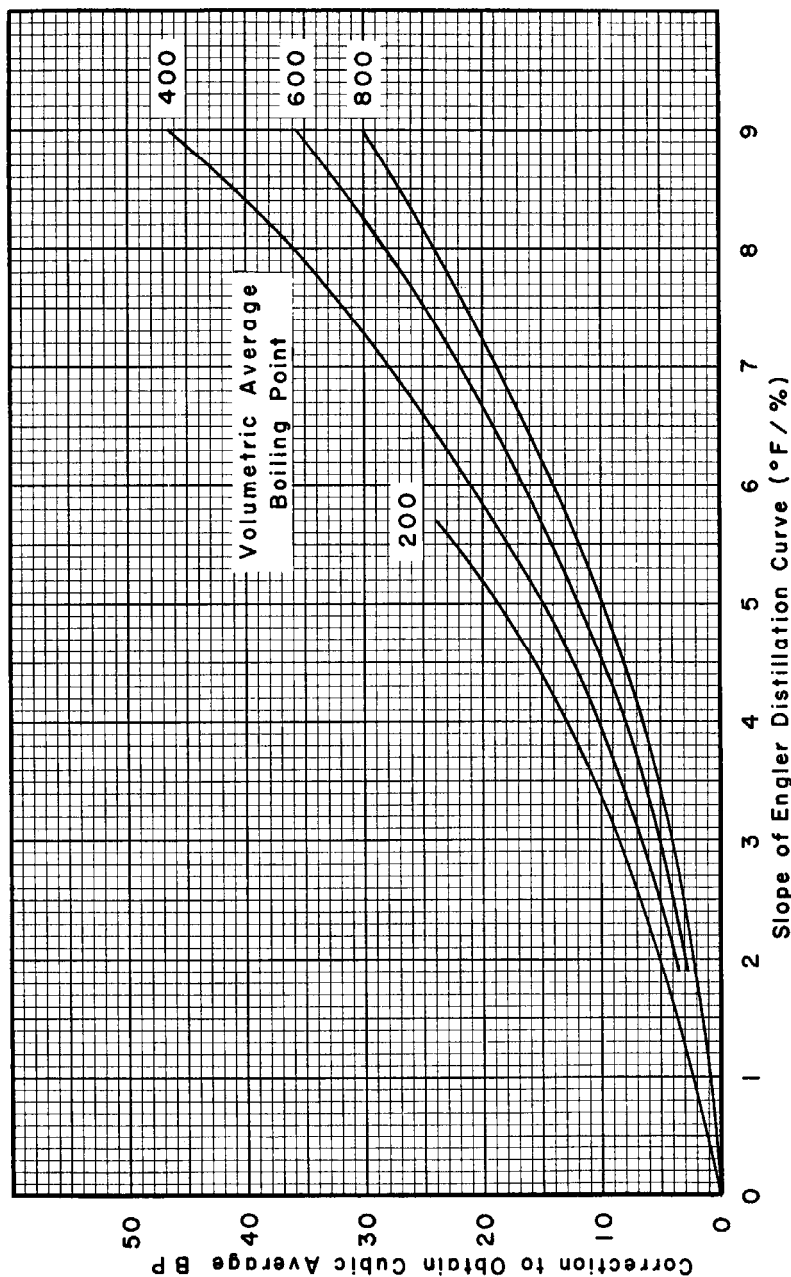


Figure 1
Cubic Average Boiling Point from Volumetric Average Boiling Point
and Distillation (Engler) Slope

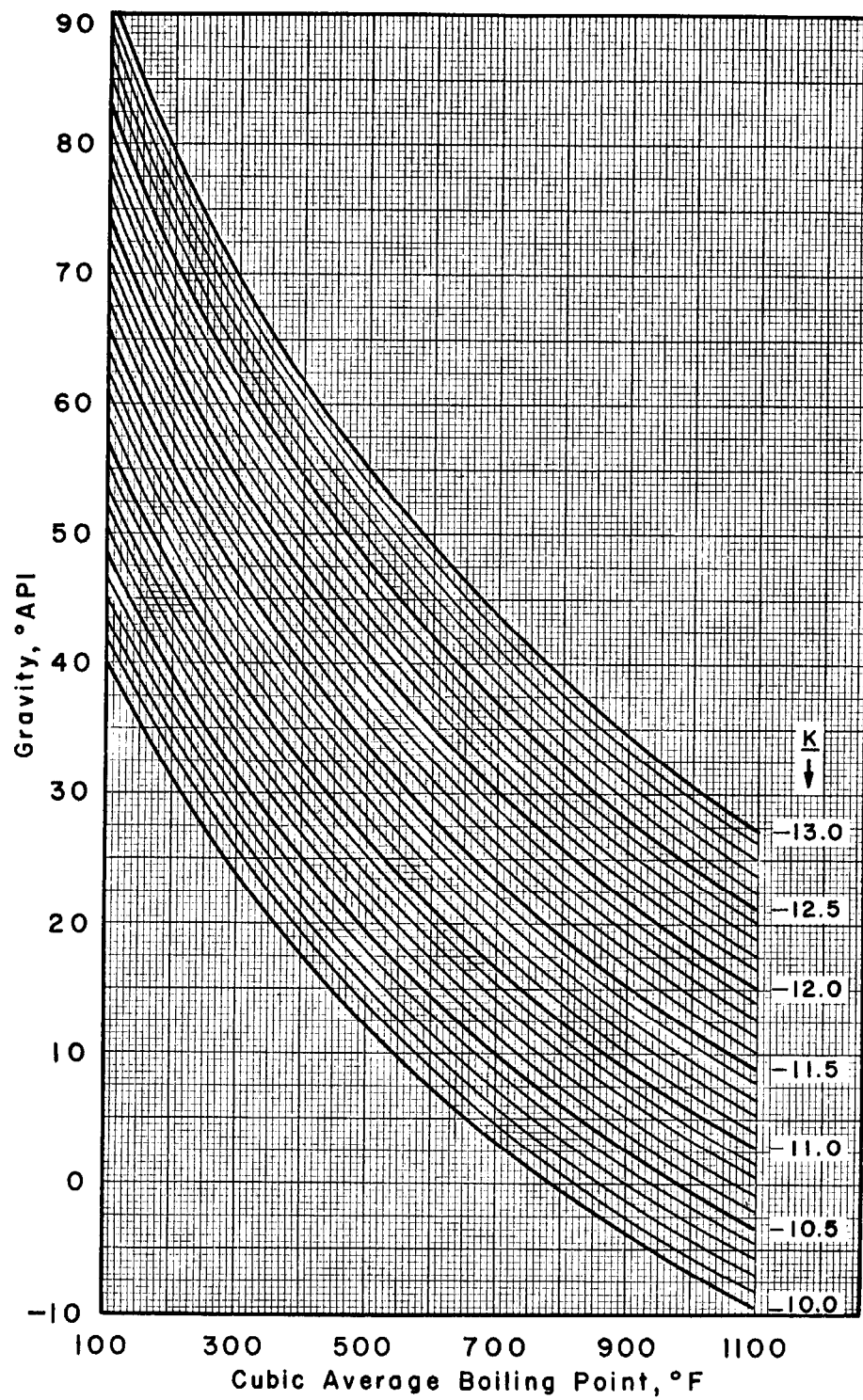


Figure 2
UOP Characterization Factor K ,
from API Gravity and Cubic Average Boiling Point

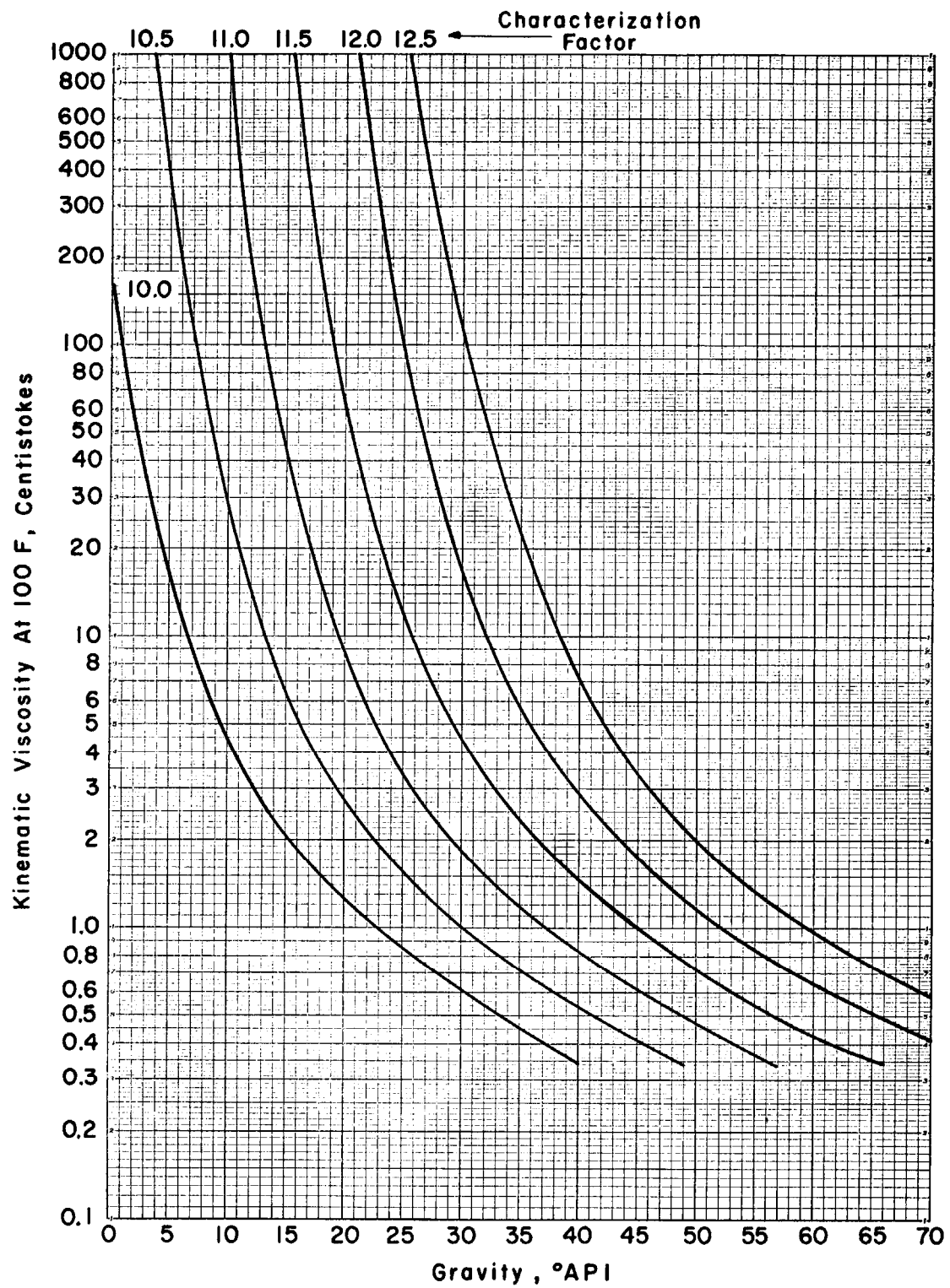


Figure 3
Characterization Factor from Viscosity at 100 F and °API

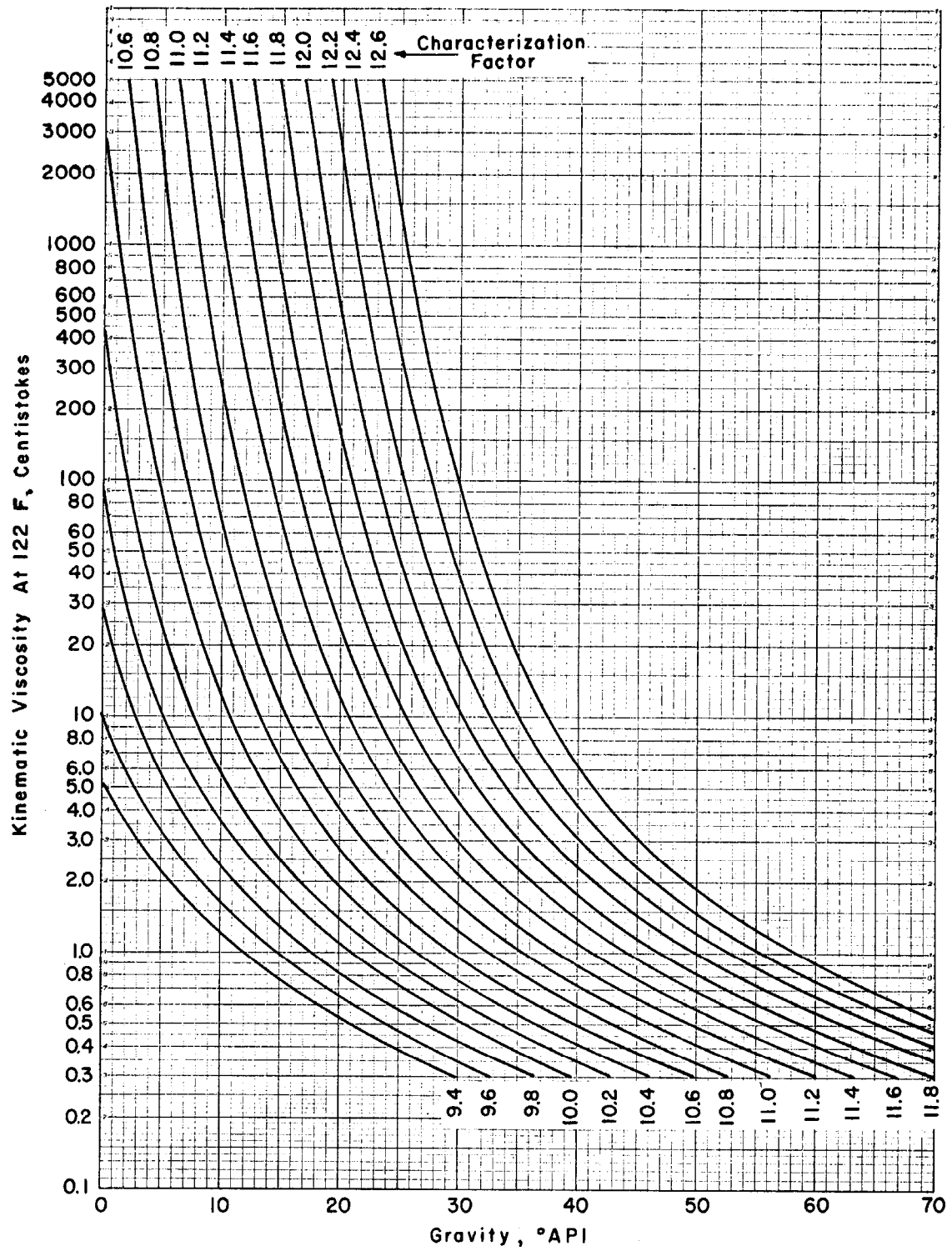


Figure 4
Characterization Factor from Viscosity at 122 F and °API

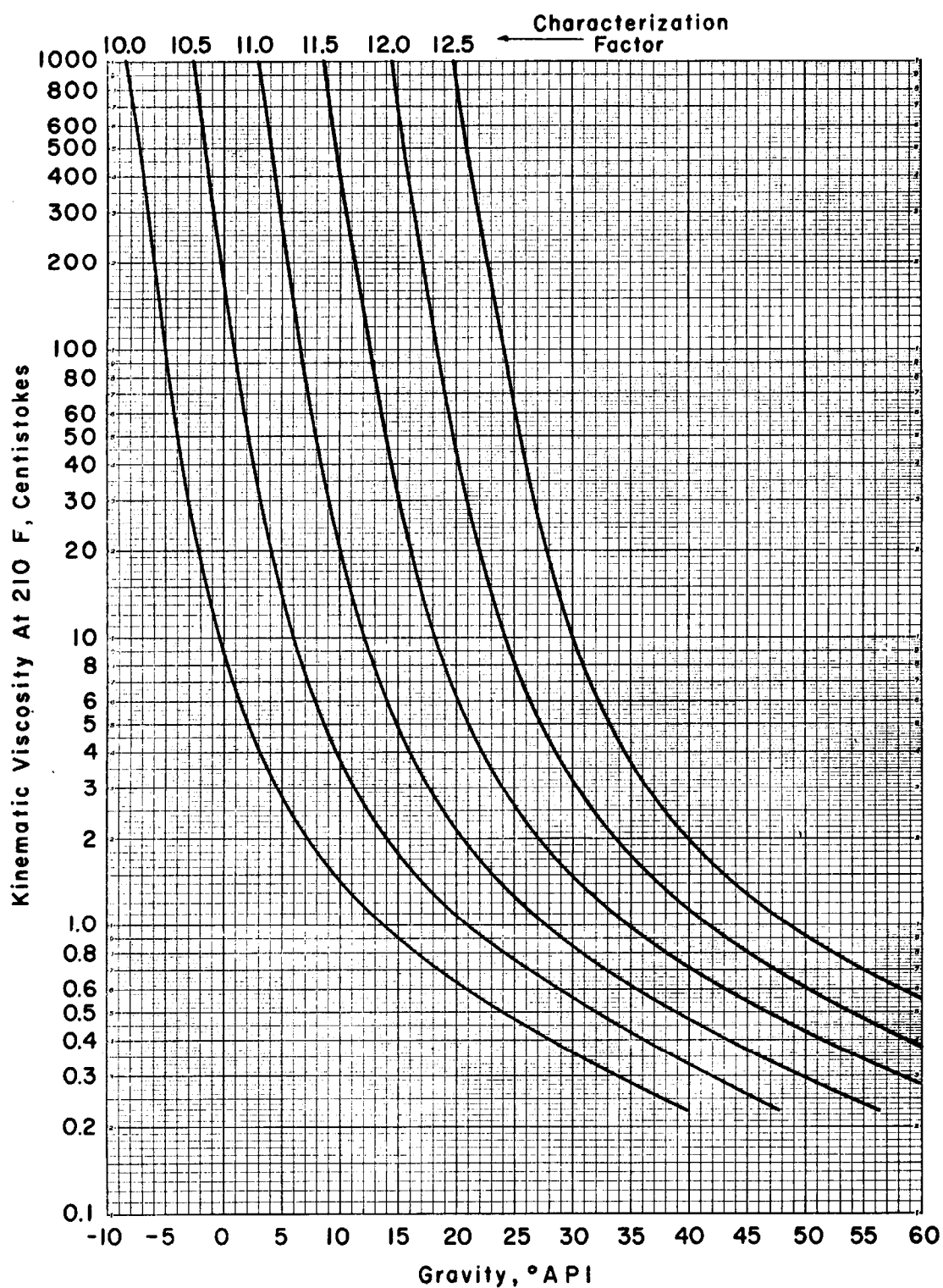


Figure 5
Characterization Factor from Viscosity at 210 F and °API

Example:

Calculate the characterization factor for the gas oil of the previous example from API gravity and viscosity measured at 210°F.

From ASTM D 88:	39.7 Saybolt Universal Seconds
From ASTM D 2161:	4.1 centistokes
From ASTM D 1298:	28.7 °API
From Fig. 5:	K = 12.0

Molecular Weight from API Gravity and ASTM Distillation

The molecular weight of typical petroleum fractions may be estimated by this method. It should not be applied to estimating the molecular weight of a pure hydrocarbon compound.

Calculate the volumetric average boiling point and slope from the distillation data as in the previous section. Using Figure 6, obtain the correction to be applied to the volumetric average boiling point. Enter Figure 6 on the horizontal scale at the value of the slope and proceed vertically to the curve which represents the value of the volumetric average boiling point, interpolating between curves if necessary. Read the value of the vertical scale on the left which corresponds to this point to obtain the value of the correction term. *Subtract* this term from the volumetric average boiling point to obtain the mean average boiling point.

Determine the molecular weight using Figure 7. Locate the mean average boiling point on the horizontal scale at the bottom of the chart. Locate the API gravity on the vertical scale at the left of the chart. Find the intersection of the vertical and horizontal lines from these points. Read the number of the diagonal curve nearest this point. This number, corrected by interpolation for the distance of the point from this curve, is the molecular weight.

Example:

Volumetric average boiling point	= 746
Slope	= 3.45 °F/volume-%
From Figure 6: Correction term	= 17 F
Mean average boiling point	= 746 – 17 = 729°F
From Figure 7: Molecular weight	= 345

Precision

An estimated standard deviation is not reported because insufficient data are available at present to permit this calculation with at least 4 degrees of freedom. The precision and accuracy of this method is dependent upon the precision and accuracy of the methods used to obtain the experimental data upon which the calculations are based. Precision is also dependent upon interpolation of the nomograph.

Time for Analysis

The elapsed time and labor requirement for one calculation are identical, 0.2 hour.

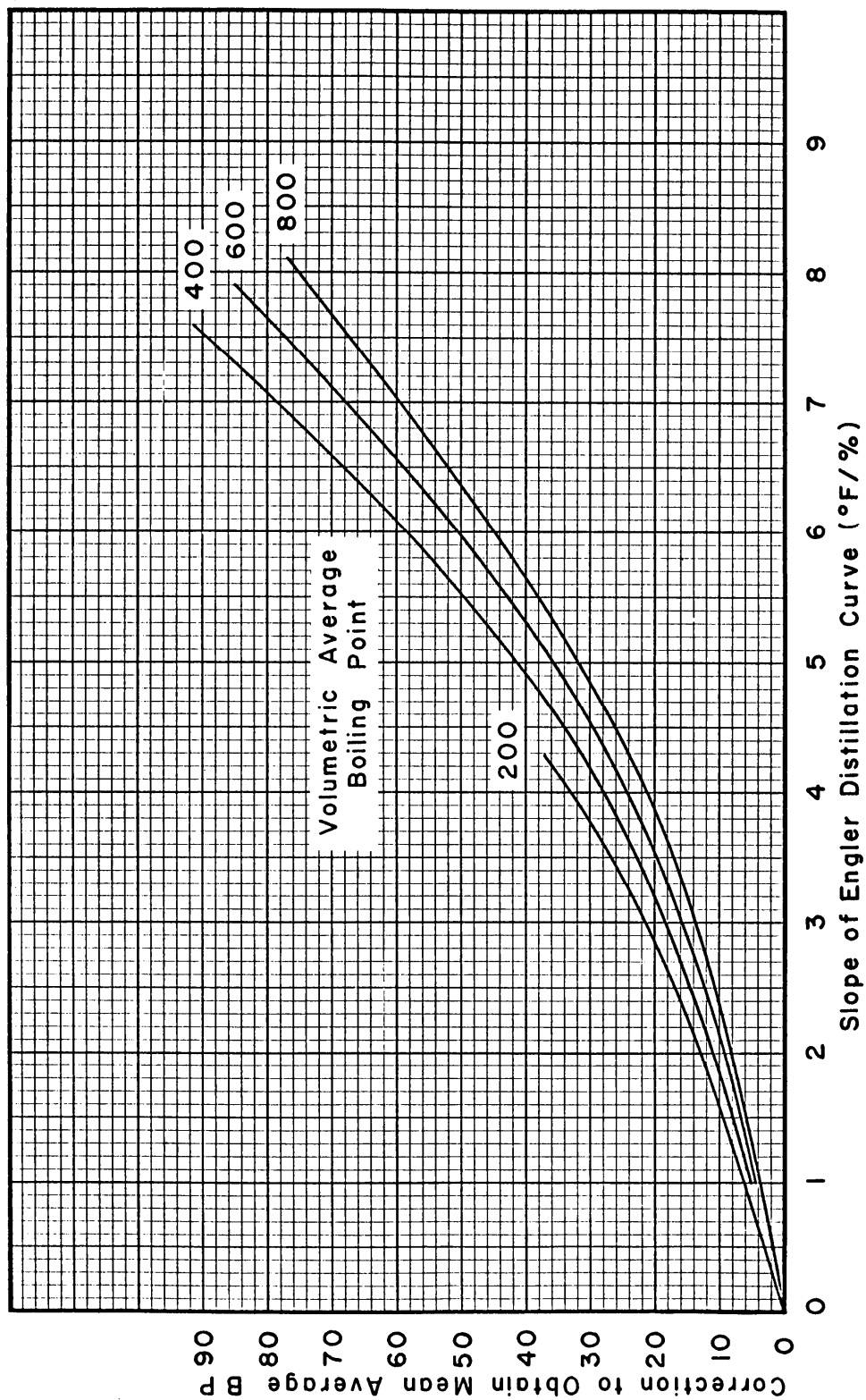


Figure 6
Mean Average Boiling Point from Volumetric Average Boiling Point
and Distillation (Engler) Slope

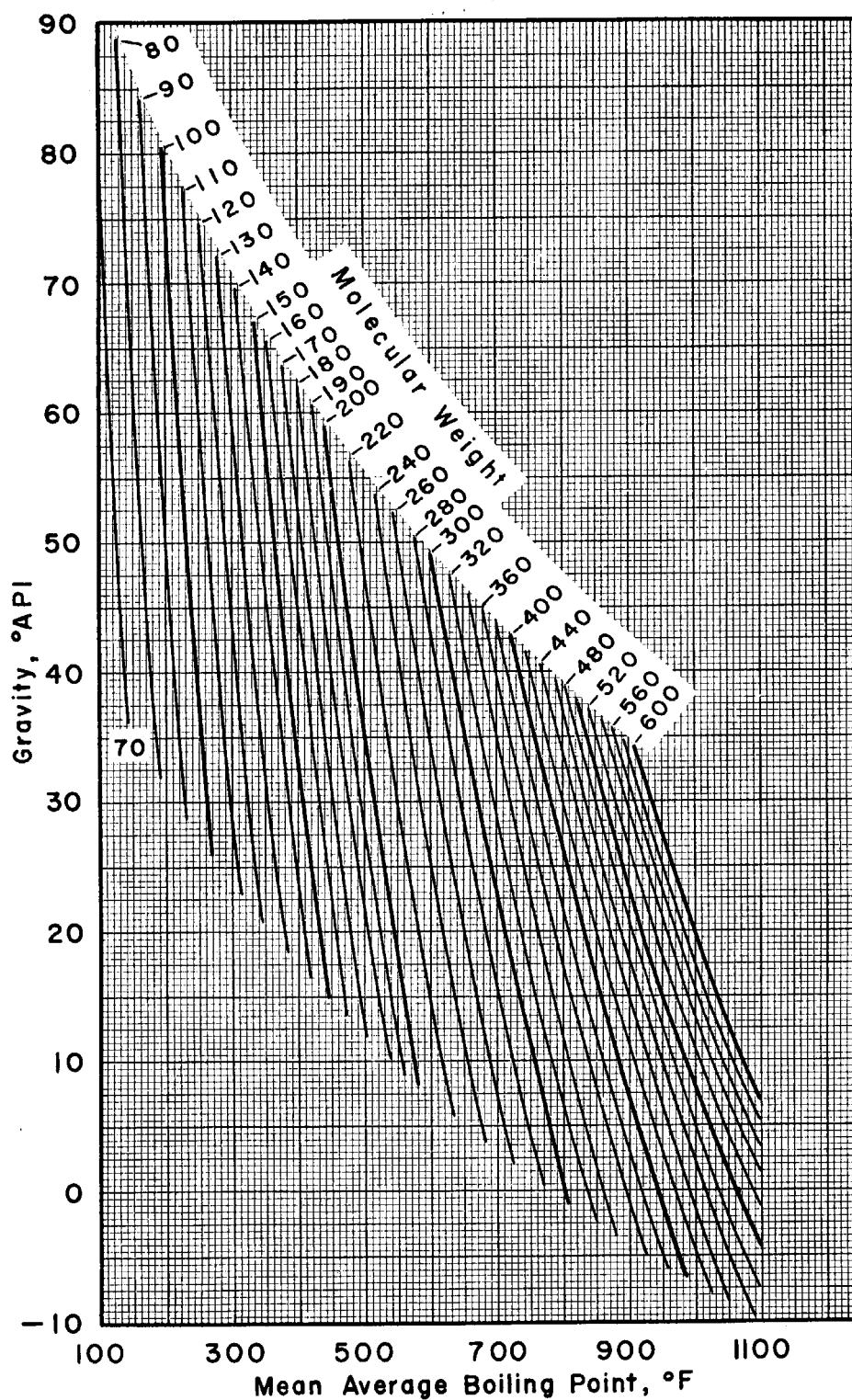


Figure 7
Molecular Weight from Mean Average Boiling Point and API Gravity

Appendix

If desired, computation by a computer or programmable calculator may be substituted for the nomographs using the equations given below. Except for Equations A1, A2, A6, and A7, these relationships were derived from curve fits of Engineering Charts which, in turn, were derived from empirical data. Consequently, any attempt to use these equations to extrapolate beyond the limit of the nomographs will produce results that, at least, must be viewed with suspicion.

UOP K Factor from API Gravity and ASTM Distillation

Calculate the volumetric average boiling point, °F, as follows:

$$V = \frac{B_{10} + B_{30} + B_{50} + B_{70} + B_{90}}{5} \quad (A1)$$

where:

B_{10} = temperature of ASTM distillation, 10% over, °F
 B_{30} = temperature of ASTM distillation, 30% over, °F
 B_{50} = temperature of ASTM distillation, 50% over, °F
 B_{70} = temperature of ASTM distillation, 70% over, °F
 B_{90} = temperature of ASTM distillation, 90% over, °F
 V = volumetric average boiling point, °F
 5 = constant for averaging

Calculate the slope of distillation, °F/volume-%, as follows:

$$S = \frac{B_{90} - B_{10}}{80} \quad (A2)$$

where:

B_{10} , B_{90} = previously defined
 S = slope of distillation, °F/volume-%
 80 = constant, volume-% (90-10 volume-%)

Calculate the cubic average boiling point, °F, as follows:

$$C = A + VE \quad (A3)$$

where:

A = defined by Equation A4
 C = cubic average boiling point, °F
 E = defined by Equation A5
 V = volumetric average boiling point (Equation A1), °F

$$A = -0.581 S^2 - 1.339 S \quad (A4)$$

where:

A = correction factor
 S = slope of the distillation (Equation A2)
 -0.581 = constant derived from curve fit of the nomograph
 1.339 = constant derived from curve fit of the nomograph

$$E = 0.000297 S^2 + 0.001438 S + 1 \quad (A5)$$

where:

E = correction factor
 S = previously defined
 0.000297 = curve fitting constant
 0.001438 = curve fitting constant

Calculate the relative density at 60°F, g/mL, as follows:

$$D = \frac{141.5}{131.5 + G} \quad (A6)$$

where:

D = relative density at 60°F, g/mL

G = API gravity, °API

131.5 = constants, from ASTM D 1298

141.5 = constants, from ASTM D 1298

Relative density can be determined directly, thus eliminating the need for this conversion.

Calculate UOP Characterization Factor, K, as follows:

$$K = \frac{(C + 459.7)^{1/3}}{D} \quad (A7)$$

where:

C = cubic average boiling point (Equation A3)

D = relative density (Equation A6)

K = UOP Characterization Factor

459.7 = constant to convert degrees Fahrenheit to degrees Rankine

Molecular Weight from Relative Density and ASTM Distillation

Calculate the mean average boiling point, °F, as follows:

$$M = \frac{C + F + VH}{2} \quad (A8)$$

where:

C = previously defined (Equation A3)

F = defined by Equation A9

H = defined by Equation A10

M = mean average boiling point, °F

V = volumetric average boiling point (Equation A1)

$$F = -1.901 S^2 - 7.498 S \quad (A9)$$

where:

F = correction factor

S = slope of the distillation (Equation A2)

-1.901 = curve fitting constant

7.498 = curve fitting constant

$$H = 0.000328 S^2 + 0.006081 S + 1 \quad (A10)$$

where:

H = correction factor

S = slope of the distillation (Equation A2)

0.000328 = curve fitting constant

0.006081 = curve fitting constant

Calculate the average molecular weight as follows:

$$W = \text{antilog}[IM + J + (L/M)] \quad (A11)$$

where:

I = defined by Equation A12
J = defined by Equation A13
L = defined by Equation A14
M = mean average boiling point (Equation A8)
W = average molecular weight

$$I = -0.000067214393 D^2 - 0.0013189667 D + 0.0023229745 \quad (A12)$$

where:

D = relative density (Equation A6)
I = correction factor
-0.000067214393 = curve fitting constant
0.0013189667 = curve fitting constant
0.0023229745 = curve fitting constant

$$J = 1.496307 D^2 - 2.4028499 D + 2.7013135 \quad (A13)$$

where:

D = previously defined (Equation A6)
J = correction factor
1.496307 = curve fitting constant
2.4028499 = curve fitting constant
2.7013135 = curve fitting constant

$$L = -92.008149 + 240.43988 D - 166.84095 D^2 \quad (A14)$$

where:

D = previously defined (Equation A6)
L = correction factor
-92.008149 = curve fitting constant
166.84095 = curve fitting constant
240.43988 = curve fitting constant

Curve-fitting equations using the viscosity data have not been determined.

Example:

Calculate the characterization factor for a gas oil of 28.7° API at 60°F having the following distillation properties:

ASTM Distillation (Corrected to 760 mm Hg Pressure)

Volume-%	10	30	50	70	90
Temp., °F	598	700	755	802	874

$$\text{Volumetric average boiling point} = \frac{598 + 700 + 755 + 802 + 874}{5} = 746$$

$$\text{Slope} = \frac{874 - 598}{80} = 3.45^\circ\text{F/volume-\%}$$

$$\text{Cubic average boiling point (C)} = (-0.581(3.45)^2 - 1.339(3.45)) + 746(0.000297(3.45)^2 + 0.0014389(3.45) + 1) = 740.8$$

$$\text{Relative density} = 141.5 / (131.5 + 28.7) = 0.8833$$

$$\text{Characterization factor, K} = (740.8 + 459.7)^{1/3} / 0.8833 = 12.03$$