Example (1): Thermophysical Properties Calculation

Petroleum fraction has the following ASTM D86 Distillation data.

Volume % distilled	0	10	30	50	70	90	95
Temperature (°C)	36.5	54	77	101.5	131	171	186.5

1. Calculate the MeABP of the petroleum fraction. If the API gravity of this fraction is 62,
2. calculate the Watson's characterization factor.
3. Estimate the Watson's characterization factor, molecular weight, aniline point, carbon-to-hydrogen using Winn nomogram.
4. Predict the molecular weight of petroleum fractions by equation developed by Riazi and Daubert $M=1.6607\times10^{-4}\,(MeABP)^{2.1962}\,SG^{-1.0164}$, where MeABP in ^{o}K.
5. Predict the liquid viscosity at atmospheric pressure and temperature 100 ^{o}F and 210 ^{o}F from following equations

   $\log_{v210} = -0.463634-0.166532(API) + 5.13447 \times 10^{-4} (API)^2 - 8.48995 \times 10^{-3} K(API)+[(8.0325 \times 10^{-2} K + 1.24899(API) +0.197680(API)^2) /[API + 26.786 - 2.6296K]$

   $\log v_{100} = 4.39371 -1.94733K + 0.127690K^2 + 3.2629 \times 10^{-4}(API)^2-1.18246 \times 10^{-2} K (API) + [0.17161K^2 + 10.9943(API) + 9.50663 \times 10^{-2}(API)^2 - 0.860218 K (API)] / [API + 50.3642 - 4.78231 K]$

   where $_{v210}$ and v_{100} are the kinematic viscosities at 210 and 100 ^{o}F, in centistokes.
6. Calculate the flash point of petroleum fractions ,

   $FPT= 1/[-0.014568 + (2.84947/T_{10}) + 0.001903 \log (T_{10})]$

   where, FPT = flash point temperature, °R

   T_{10} = ASTM D86 10% temperature (Volume %, °R)
7. Calculate the Pour point of petroleum fractions,

   $Tpp = 234\ 85\ SG^{2\ 970566}\ M^{(0.61235-0.473575\ SG)}\ v_{100}^{(0.310311\ -\ 0.32834\ SG)}$

   where, T_{PP} = pour point of petroleum fraction, in ^{o}R

   v_{100} = kinematic viscosity at 100 F, in cst

   SG= specific gravity at 60 F/ 60 F

   M = molecular weight of petroleum fraction.
8. Calculate the aniline point of petroleum fractions,

   $AP = -1253.7 - 0.139\ MeABP + 107.8\ K + 868.7\ SG$

where, AP = aniline point of petroleum fraction, R

MeABP = mean average boiling point, R

SG = specific gravity at 60 F/ 60 F

K = Watson K factor

9. Calculate the smoke point of petroleum fractions

   $\ln SP = -1.028 + 0.474 K - 0.00168 MeABP$

   where, SP = Smoke point of petroleum fraction, mm

   MeABP = mean average boiling point, R , and K = Watson K factor

10. Calculate the freeze point of petroleum fractions

    $FRP = -2390.42 + 1826 SG + 122.49 K - 0.135 MeABP$

    where, FRP = Freezing point of petroleum fraction, R

    MeABP = mean average boiling point, R

    K = Watson K factor

    SG = specific gravity of petroleum fraction, 60F/60F

11. Calculate the cloud point of petroleum fractions

    $\log CP = -7.41 + 5.49 \log MeABP - 0.712 MeABP^{0\ 315} - 0.133 SG$

    where, CP = Cloud point of petroleum fraction, R.

    MeABP = mean average boiling point, R.

    SG= specific gravity, 60F/60F.

12. Calculate the cetane index of petroleum fractions

    $CI = 415.26 - 7.673 API + 0.186 MeABP + 3.503 API \log MeABP - 193.816 \log MeABP$

    where, CI = cetane index of petroleum fraction.

    API = API gravity.

    MeABP = mean average boiling point, F.

13. Calculate the cetane index CCI of petroleum fractions

    $$CCI = 454.74 - 1641.416 SG + 774.74 SG^2 - 0.5547T_{50} + 97.083(\log_{10} T_{50})^2$$

    where T_{50} is the ASTM D 86 temperature at 50% point in °C.

14. Calculate the diesel index DI of petroleum fractions

    $$DI = (API)(1.8AP + 32)/100$$

    which is a function of API gravity and aniline point in °C.

15. Calculate the refractive index of petroleum fractions

$$n = \left[\frac{1+2I}{1-I}\right]^{1/2}$$

$I = 2.266 X10^{-2} \exp(3\ 905 \times 10^{-4} MeABP + 2.468 SG -5.704 \times 10^{-4} MeABP\ SG)/MeABP^{0\ 0572} SG^{-0720}$

where, n = refractive index at 68F

I = modified Huang characterization parameter at 68F

MeABP = mean average boiling point, D86, R

SG = specific gravity, 60F/60F

16. Calculate the **CH Weight Ratio** of petroleum fractions

$CH = 3.4707 [\exp (1.485 \times 10\text{-}^{2}T_{b} + 16.94 SG -1.2492 \times 10^{-2} T_{b} SG)]T_{b}^{-2.725} SG^{-6.798}$

where Tb is in Kelvin

17. Calculate the **Carbon Residue** of petroleum fractions

$$\%CCR = 148.7 - 86.96 H/C$$

18. Calculate the **asphaltenes%** of petroleum fractions

$$\%Asphahene = a[0.74195 (\%CCR) + 0.01272 (\%CCR)^{2}\ ]$$

where a is 0.385 for atmospheric residue and 0.455 for vacuum residues

19. Calculate the **Viscosity Gravity Constant** of petroleum fractions

a constant. VGC is defined at two reference temperatures of 38°C (100°F) and 99°C (210°F)

$VGC = [10SG - 1.0752 \log_{10}(V_{38} - 38)]/ [10 - \log_{10}(V_{38} - 38)]$

$VGC = [SG - 0.24 - 0.022 \log_{10}(V_{99} - 35.5)]/0.755$

Where V_{38} = viscosity at 38°C (100°F) in SUS (Saybolt Universal Seconds)

V_{99} = Saylbolt viscosity (SUS) at 99°C (210°F)

20. Calculate the ***Reid Vapor Pressure*** of petroleum fractions

$RVP = 3.3922 - 0.02537(T_{5}) - O.070739(T_{10}) + 0.00917(T_{30}) - 0.0393(T_{50}) + 6.8257 \times l0^{-4}(T_{10})^{2}$

where all temperatures are in ^{o}C and RVP is in bar.

21. Calculate the paraffins, naphthenes and aromatic mole fraction , see faham p 53

Solution:

1) The MeABP is calculated using the following equation:

MeABP = VABP -Δ

where -Δ is given by

$\ln \Delta = -0.94402 - 0.00865(VABP - 32)^{06667} + 2.99791 SL^{0\ 333}$

and

SL= [T_{90} — T_{10}]/[90 – 10]

The VABP is obtained from equation :

VABP = (T_{l0} + T_{30} + T_{5}o + T_{70} + T_{90})/5   where all T are in ^{o}F.

The distillation temperatures are converted from (°C to °F , (**F** = 9/5 **C**+32) .

VABP = (129.2 + 170.6 + 214.7 + 267.8 + 339.8)/ 5

=224.4 °F

SL = 2.6325

Δ = 18.279

MeBP = 224.4 - 18.3 = 206.1 °F or 96.7 °C

2) The Watson characterization factor K given by:

K= (MeABP) $^{1/3}$ / SG

From equation API =[141.5/ SG]- 131.5

S G = 141.4/[62 + 131.5] = 0.7313

K= (206.1 + 460)$^{1/3}$ /0.7313 = 11.94

3) from the Winn nomogram by drawing a straight line through input parameters points of (MeABP) =206.1 °F and specific gravity(*SG*)= 0.7313 or API = 62 and extending the line until it cuts to the desired property line. The properties included in the nomogram are API gravity, specific gravity(*SG*), carbon to hydrogen weight ratio (*C/H*), Watson characterization factor (*Kw*), aniline point, molecular weight (*M*), and mean average boiling point (MeABP).

Watson's characterization factor =12

molecular weight =102

aniline point = 120 °F

carbon-to- hydrogen = 5.7

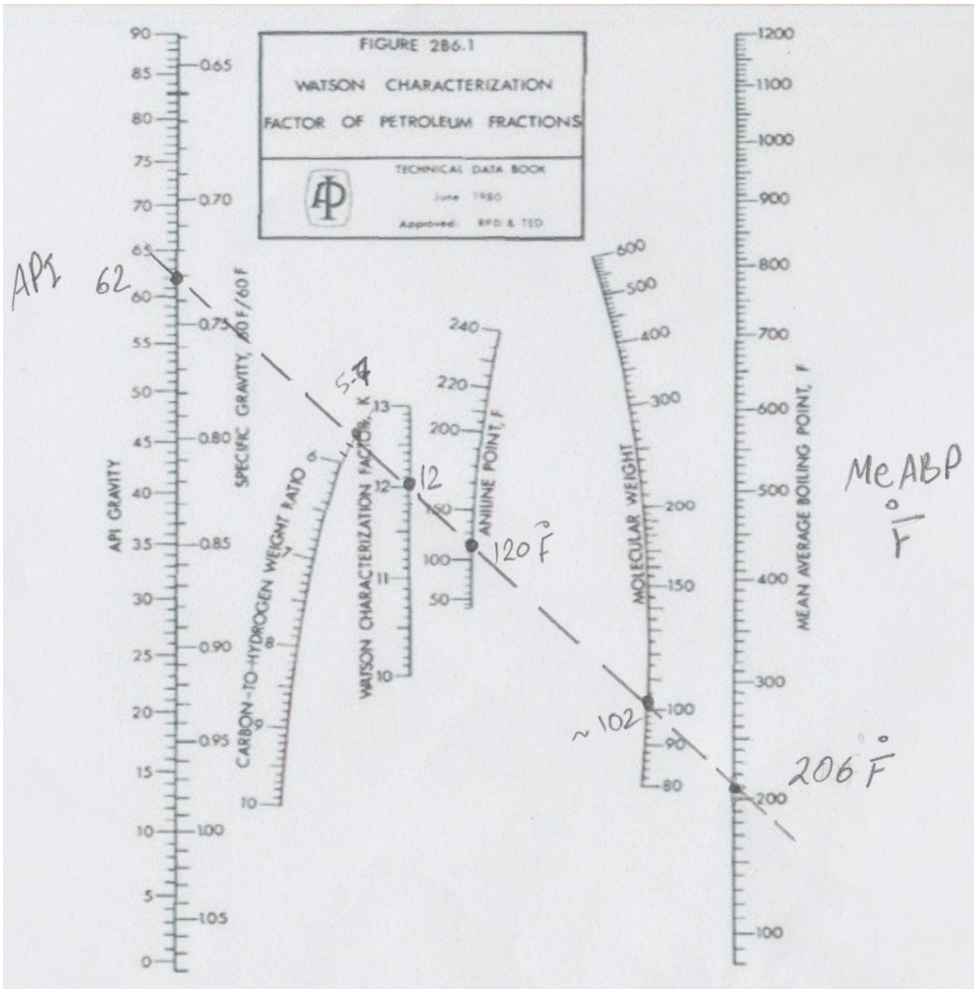

Figure 2.1Winn nomogram for characterization of petroleum fractions. (Daubert T E, 1997)

4) $M = 1.6607 \times 10^{-4} (MeABP)^{2.1962}\ SG^{-1.0164}$

MeABP= 206.1 °F = 96.72 ^oC = 369.7 ^oK

$M = 1.6607 \times 10^{-4} (369.7)^{2.1962}\ (0.7313)^{-1.0164}$

M =99.53

5) for API= 62, K=11.94 , the kinematic viscosities at 210 and 100 ^oF,

$\log_{\nu 210} = -0.463634-0.166532(API) + 5.13447 \times 10^{-4} (API)^2 - 8.48995 \times 10^{-3} K(API)+[(8.0325 \times 10^{-2} K + 1.24899(API) +0.197680(API)^2) /[API + 26.786 - 2.6296K]$

$\log_{\nu 210}$ = , and ν_{210} = cst

$\log \nu_{100} = 4.39371 -1.94733K + 0.127690K^2 + 3.2629 \times 10^{-4}(API)^2-1.18246 \times 10^{-2} K (API) + [0.17161K^2 + 10.9943(API) + 9.50663 \times 10^{-2}(API)^2 - 0.860218 K (API)] / [API + 50.3642 - 4.78231 K]$

$\log \nu_{100}$ = ,and ν_{100} = cst

(1)

Calculate the paraffins, naphthenes and aromatics mole fraction for crude oil having the properties

$API = 34$, $MeABP = 320\ ^\circ C$

Solution

$MeABP = 320\ ^\circ C = 593.15\ K = 1067.7\ ^\circ R$

$\because API = \left(\frac{141.5}{SG} - 131.5\right) = 34 \Rightarrow SG = 0.855$

& $K = (MeABP)^{1/3} / SG =$

$\Rightarrow K = \frac{(1067.7)^{1/3}}{0.855} = 11.95$

from

$$\log \nu_{210} = -0.463634 - 0.166532\,(API) + 5.13447\times10^{-4}(API)^2 - 8.48995\times10^{-3}\,K\,(API) + \frac{8.0325\times10^{-2}\,K + 1.24899\,(API) + 0.197680\,(API)^2}{API + 26.786 - 2.6296\,K}$$

$$\log \nu_{100} = 4.39371 - 1.94733\,K + 0.127690\,K^2 + 3.2629\times10^{-4}(API)^2 - 1.18246\times10^{-2}\,K\,(API) + \frac{0.17161\,K^2 + 10.9943\,(API) + 9.50663\times10^{-2}(API)^2 - 0.860218\,K\,(API)}{API + 50.3642 - 4.78231\,K}$$

where ν_{100} & ν_{210} are the Kinematic viscosities at 100 & 210 °F, in centistockes.

$\Rightarrow \nu_{100} = 5.777$ cSt & $\nu_{210} = 1.906$ cSt

from

$$n = \left(\frac{1+2I}{1-I}\right)^{1/2}$$

values of (I) may be calculated from

$$I = a \exp\left(b \cdot T_b + c \cdot SG + d\ T_b \cdot SG\right) T_b^{e} \cdot SG^{f}$$

where a, b, c, d, e and f are constant varying with molecular weight rang, as following table:

Constant	light fractions	Heavy fractions
Mol. wt. range	70 – 300	300 – 600
Boiling Point range °F	90 – 650	650 – 1000
a	2.266×10^{-2}	2.341×10^{-2}
b	3.905×10^{-4}	6.464×10^{-4}
c	2.468	5.144
d	-5.704×10^{-4}	-3.289×10^{-4}
e	0.0572	−0.407
f	−0.720	−3.333

n is the refractive Index at 20 °C (68 °F)

I is the Huang characterization parameter at 20 °C (68 °F)

T_b is the mean average boiling point, in degree °R

M Molecular weight of petroleum fractions

SG is the specific gravity of petroleum fraction 60°F/60°F

∴

$$M = 42.965\left[\exp\left(2.097\times10^{-4}\,T_b - 7.78712\,SG + 2.08476\times10^{-3}\,T_b\,SG\right)\right] T_b^{1.26007}\ SG^{4.98308}$$

where

③

where M = molecular weight of the petroleum fraction

T_b is the mean average boiling point, in °K

SG is the specific gravity, 60°F / 60°F

$\Rightarrow$ $M = 257.1$ which be considered heavy fraction (see table, above)

& the refractive Index $n = 1.481$

the $R_i = n - \frac{d}{2}$

R_i is the refractivity intercept

n = refractive Index at 20 °C (68 °F) & 1 atm

d is the liquid density at 20 °C (68 °F) & 1 atm in gm/cm³

$\Rightarrow$ $R_i = 1.0535$

$\therefore$ $VGC = \frac{10\ SG - 1.0752 \log(\nu_{100} - 38)}{10 - \log(\nu_{100} - 38)}$

$= 0.8348$

By substituting the constants for heavy fraction, R_i and VGC in

$x_p = a + b\,(R_i) + c\,(VGC)$

$x_n = d + e\,(R_i) + f\,(VGC)$

$x_a = g + h\,(R_i) + i\,(VGC)$

$\Rightarrow$ $x_p = 0.789$ paraffine, $x_n = 0.164$ naphthenes and $X_a = 0.046$ aromatics

not that check $x_p + x_n + x_a = 1.0$

$0.789 + 0.164 + 0.046 = 0.999 \simeq 1.0$