CHAPTER 3

PETROLEUM FRACTION DISTILLATION INTERCONVERSIONS

3.0 INTRODUCTION

ASTM and true boiling point (TBP) analytical distillations are used to define the volatility characteristics of petroleum fractions and other complex mixtures. Both are batch distillations which differ mainly in the degree of fractionation obtained during the distillation.

ASTM D86 and D1160 distillations are run in an Engler flask. No packing is employed, and reflux results only from heat losses through the neck of the flask. ASTM distillations are more widely used than TBP distillations because the former are simpler, less expensive, require less sample, and require only approximately one-tenth as much time. ASTM distillations are standardized. TBP distillations vary appreciably in procedure and apparatus.

ASTM distillation methods in use today are:

ASTM Method D86: This method is used for the distillation of motor gasolines, aviation gasolines, aviation turbine fuels, naphthas, kerosines, gas oils, distillate fuel oils, and similar petroleum products. It is carried out at atmospheric pressure. An exposed thermometer is used, and temperatures are reported without stem corrections. **ASTM D86 distillations are plotted in volume percent.**

ASTM Method D1160: This method is used for heavy petroleum products which can be vaporized partially or completely at a maximum liquid temperature of 750 F at absolute pressures down to 1 mm Hg and condensed at the pressures of the test. It is carried out at pressures between 1 mm Hg and 50 mm Hg, absolute. Temperatures are measured with a thermocouple. **ASTM D1160 distillations are plotted in volume percent.**

ASTM Method D2887: Simulated distillation (SD) by gas chromatography appears to be the most simple, reproducible, and consistent method to describe the boiling range of a hydrocarbon fraction unambiguously. This method is applicable to all petroleum fractions with a final boiling point of 1000 F or less at atmospheric pressure. The method is also limited to samples having an initial boiling point of at least 100 F. Figure 3-0.1 shows a typical relation between ASTM D86 and ASTM D2887 distillations for a petroleum fraction. **Simulated distillations are plotted in weight percent.**

ASTM Method D2892: This method is used for distillation of stabilized crude petroleum defined as having a Reid vapor pressure less than 12 psi. It employs a fractionating column of 14-18 theoretical stages operated at a reflux ratio of 5. The method is a form of true boiling point distillation for any petroleum mixture boiling above light naphthas and mixtures with final boiling points below 750 F.

ASTM Method D3710: This method is used to determine the boiling range distribution of gasolines which do not exceed an atmospheric pressure final boiling point of 500 F. It is a gas chromatographic method otherwise similar to D2887.

In ASTM D86, D1160, and D2892 distillations there may be a residue left in the distillation equipment as well as a difference between the volume of the original charge and the sum of the distillate and residue. This difference is usually termed "loss" and is generally thought of as volatile components of the charge which have not been recondensed. For preparation of an ASTM distillation for conversion to a TBP distillation, the percent distilled at the reported temperature is the sum of the distillate collected and the loss.

When heated sufficiently hot, petroleum fractions undergo thermal cracking. Although a function of chemical composition, the amount and severity of thermal cracking increase
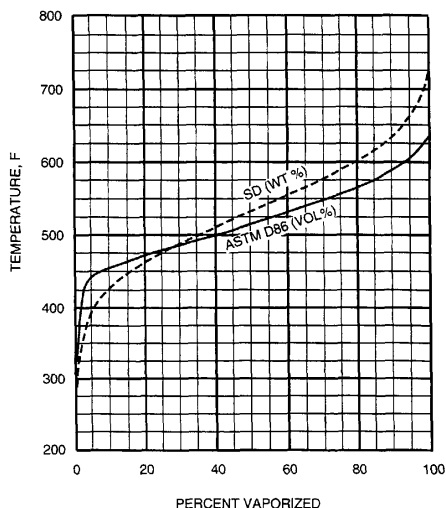
Figure 3-0.1—Typical ASTM D86 and Simulated Distillation Curves for a Petroleum Fraction

API TECHNICAL DATA BOOK

with increasing boiling point, contact time, pressure and temperature. Early editions of this chapter included a correction for cracking for observed ASTM D86 temperatures above 475 F. No correction for cracking is now recommended.

TBP distillations are performed in columns with 15 to 100 theoretical plates at relatively high reflux ratios (i.e., 5 to 1 or greater). The high degree of fractionation in these distillations gives accurate component distributions for mixtures. The lack of use of a standardized apparatus and operational procedure is a disadvantage, but the variations between various laboratories are small because a close approach to perfect separation by boiling point is usually achieved. A TBP curve is also shown in Figure 3-0.2 for comparison with an ASTM D86 distillation.
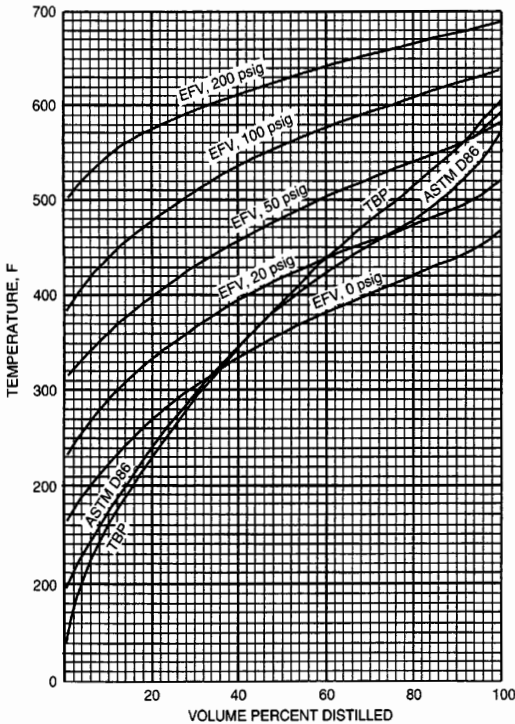
An equilibrium flash vaporization is an experiment carried out at constant pressure to determine the temperature-volume percent distilled relation. The EFV curve is a plot of temperature against percent by volume of liquid distilled, at a constant pressure. Each point on the EFV curve represents a separate equilibrium experiment. The number of equilibrium experiments needed to define all portions of the EFV curve varies with the shape of the curve. Normally, at least five such experiments are required. Figure 3-0.2 also shows the EFV curves of a naphtha-kerosene blend at atmospheric and several superatmospheric pressures compared to ASTM D86 and TBP distillations. The tedious procedures necessary to obtain experimental EFV data have made this type experiment quite rare at this time. Thus, correlations involving EFV have been eliminated from this chapter.

Users are emphatically cautioned against relying heavily on results obtained from these correlations. Because of a lack of standardization and other inherent inadequacies in the methods, the existing ASTM, TBP, and SD data on the same fractions are not sufficiently precise or consistent to develop accurate correlations. Consult the Comments on each Procedure for the accuracy of each method before use.

The correlations of this chapter were developed using data for hydrocarbon stocks and fractions which included many components and exhibited smooth distillation curves. The correlations do not apply to mixtures of few compounds with widely different boiling points.

A schematic diagram of the interconversion procedures is shown in Figure 3-0.3. Correlations are summarized in Table 3-0.4.

Correlations in this chapter are empirical in nature and are arranged according to the various pairs between ASTM, TBP, and SD relations.

Section 3A1	ASTM-TBP	(Atmospheric)
Section 3A2	ASTM-TBP	(Subatmospheric)
Section 3A3	SD-TBP-ASTM	(Atmospheric)
Section 3A4	Interconversions at Subatmospheric Pressures	

Source: Edmister and Pollock, *Chem. Eng. Progr.* **44** 905 (1948)

Figure 3-0.2—ASTM, True Boiling Point, and Equilibrium Flash Vaporization Distillation Curves for a Naphtha-Kerosine Blend

Use of Procedures

Procedures in this chapter are interconnected and are in most respects consistent. In addition, all predicted distiⁱⁱ tion curves are of the correct shape. Careful stu⁻ 3-0.3 and Table 3-0.4 gives the method(ˢ conversion. It should be noted ᵗʰ paths are possible. The ⁻ dures to be usᵉ⁻ ⁱ
Prᵒ⁻

API TECHNICAL DATA BOOK

```
                                          ┌─────────────────────────┐
                                          │   ASTM D2887/D3710      │
                                          │      SIMULATED          │
                                          │     DISTILLATION        │
                                          │                         │
                                          │     (GAS CHROM.)        │
                                          └───────────┬─────────────┘
                                                      │ 4
                                                      ▼
                                          ┌─────────────────────────┐
   Primary Route    3                     │       ASTM D86          │
                                          │                         │
                                          │       760 mm            │
                                          └──────────┬──────────────┘
                                              ▲  1   │
                                              │      ▼
                                          ┌─────────────────────────┐
                                          │         TBP             │
                                          │                         │
                                          │        760 mm           │
                                          └──────────┬──────────────┘
               5                             ▲  5    │
                                             │       ▼
    ┌──────────────────┐          ┌─────────────────────────┐
    │      TBP         │◄─────────│        TBP              │
    │                  │    5     │                         │
    │  Subatmospheric  │─────────►│        10 mm            │
    └──────────────────┘          └──────────┬──────────────┘
                                      ▲  2    │
                                      │       ▼
    ┌──────────────────┐          ┌─────────────────────────┐
    │   ASTM D1160     │◄─────────│     ASTM D1160          │
    │                  │    5     │                         │
    │  Subatmospheric  │─────────►│       10 mm             │
    └──────────────────┘          └─────────────────────────┘
                                             ▲
```
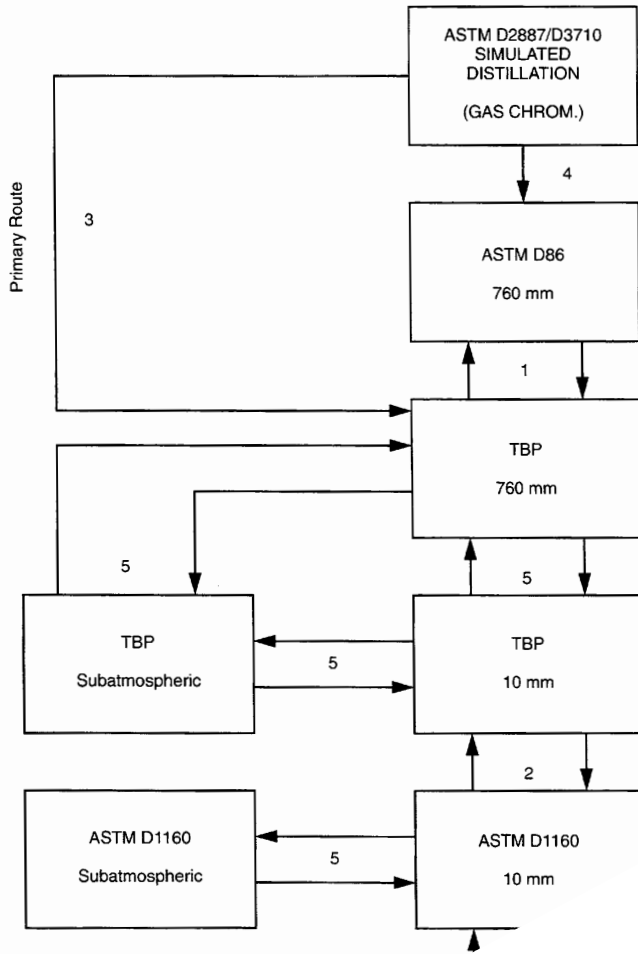
STEP	PROCEDURE
1	3A1.1
2	3A2.1
3	3A3.1
4	3A3.2
5	3A4.1

1994

Procedure 3A3.1 (Step 3) allows direct interconversion of ASTM D2887 (Simulated) and TBP distillations with excellent accuracy as shown in the Comments.

Procedure 3A3.2 (Step 4) relates ASTM D2887 (Simulated) and ASTM D86 distillations with accuracy as given in the Comments. This conversion route should not be used for fractions with D86 distillation temperatures above 600 F.

The conversion of Simulated to TBP distillations can also be carried out in two steps (4 and 1) with little degradation of the prediction. See discussion in Procedure 3A3.1.

Figure 3A2.1 (Step 2) allows conversion of ASTM D1160 to TBP distillations at 10 mm mercury total pressure after which Procedure 3A4.1 (Step 5) can be used to convert the TBP to atmospheric pressure. This method is only rec- ommended for development of a TBP distillation curve if neither an ASTM D86 or simulated distillation are available as the curve, though reasonably shaped, was not able to be verified since insufficient experimental data were available.

Equilibrium flash data, while probably more reproducible than ASTM and TBP data, are obtained using different types of apparatus and many variations in procedure. A computer method for flash calculations and estimation of equilibrium K-Values for petroleum fractions using a modified Soave-Redlich-Kwong (6) equation of state is included in Chapter 8.

NOTE: A report which documents the basis upon which the material in all editions of this chapter was selected has been published by the American Petroleum Institute as *Documentation Reports No. 3-66, No. 2, 3-86,* and *No. 3-93.* All data used for development of prediction methods are referenced in these reports.

TABLE 3-0.4—SUMMARY OF CORRELATIONS FOR CONVERTING DISTILLATION DATA

| Data Available | | Data Desired | | |
Type	Pressure, mm Hg	Type	Pressure, mm Hg	Conversion Method Steps in Fig. 3-0.3
ASTM D2887 (SD)	760	ASTM D86	760	4
ASTM D86	760	TBP	760	1
ASTM D1160	10	TBP	10	2
ASTM D1160	10	TBP	760	2, 5
ASTM D1160	10	ASTM D86	760	2, 5, 1
TBP	10	TBP	760	5
ASTM D2887 (SD)	760	TBP	760	3
ASTM D1160	1	TBP	760	5, 2, 5
ASTM D1160	1	ASTM D86	760	5, 2, 5, 1
ASTM D1160	100	TBP	760	5, 2, 5
ASTM D1160	100	ASTM D86	760	5, 2, 5, 1

Note: All ASTM D86 temperatures at 760 mm Hg are observed values.

PROCEDURE 3A1.1

INTERCONVERSION OF ASTM D86—TBP
DISTILLATIONS AT ATMOSPHERIC PRESSURE

Discussion

The following equation is used to convert an ASTM D86 distillation 50% point temperature to a true boiling point distillation 50% point temperature.

$$TBP\,(50)\ =\ 0.87180\,(ASTM\ D86\,(50)\,)^{1.0258} \qquad (3A1.1\text{-}1)$$

Where:

$TBP\,(50)$ = true boiling point distillation temperature at 50 volume percent distilled, degrees Fahrenheit.

$ASTM\ D86\,(50)$ = observed ASTM D86 distillation temperature at 50 volume percent distilled, degrees Fahrenheit.

To determine the difference between adjacent cut points, use the following equation:

$$Y_i\ =\ A\,X_i^{B} \qquad (3A1.1\text{-}2)$$

Where:

Y_i = difference in true boiling point distillation temperature between two cut points, degrees Fahrenheit.

X_i = observed difference in ASTM D86 distillation temperature between two cut points, degrees Fahrenheit.

A,B = constants varying for cut point ranges, described as follows.

i	Cut Point Range	A	B	Maximum Allowable X_i, (F)
1	100% - 90%	0.11798	1.6606	–
2	90% - 70%	3.0419	0.75497	100
3	70% - 50%	2.5282	0.82002	150
4	50% - 30%	3.0305	0.80076	250
5	30% - 10%	4.9004	0.71644	250
6	10% - 0%	7.4012	0.60244	100

To determine the true boiling point temperature at any percent distilled, add or subtract the proper difference(s) from the predicted 50% true boiling point temperature.

$$
\begin{aligned}
TBP\ \ (0)\ &=\ TBP\,(50) - Y_4 - Y_5 - Y_6 \\
TBP\ (10)\ &=\ TBP\,(50) - Y_4 - Y_5 \\
TBP\ (30)\ &=\ TBP\,(50) - Y_4 \\
TBP\ (70)\ &=\ TBP\,(50) + Y_3 \\
TBP\ (90)\ &=\ TBP\,(50) + Y_3 + Y_2 \\
TBP\,(100)\ &=\ TBP\,(50) + Y_3 + Y_2 + Y_1
\end{aligned}
\qquad (3A1.1\text{-}3)
$$

Procedure

Step 1: Use equation (3A1.1-1) to calculate the TBP distillation temperature at 50% distilled.
Step 2: Use equation (3A1.1-2) to calculate necessary TBP differences.
Step 3: Use equation(s) (3A1.1-3) to calculate desired TBP distillation temperatures.

To determine the ASTM D86 distillation temperatures from the TBP distillation temperatures, reverse the procedure. Thus, equation (3A1.1-1) becomes

$$(ASTM\ D86\,(50)\,)\ =\ \exp\left[\frac{\ln\,(TBP\,(50)\,/\,0.87180)}{1.0258}\right] \qquad (3A1.1\text{-}4)$$

Similarly, all equations (3A1.1-2) can be reversed, and all equations (3A1.1-3) can be modified by changing TBP to ASTM.

3A1.1

COMMENTS ON PROCEDURE 3A1.1

Purpose

The purpose of this procedure is to predict a TBP distillation at atmospheric pressure from an ASTM D86 distillation or the reverse by hand or by computer.

Limitations

Because experimental data on higher boiling fractions are quite scattered, all derivations were carried out on fractions having an ASTM 50% point temperature of 480 F and below. However, the correlation extrapolates well to fractions with ASTM 50% point temperatures up to 600 F. Care should be taken in extrapolating above this point. In addition, initial and final boiling point data are scarce and inaccurate. Thus, values for these points should be taken as rough approximations.

Reliability

Differences between the estimated and experimental TBP values at various volume % distilled points are given below.

| Volume % Distilled | TBP (predicted) — TBP (experimental) | |
	Average	Bias
0	21.9 F	–7.8 F
10	9.0	–1.8
30	5.7	–0.4
50	4.7	–0.1
70	5.6	1.1
90	7.1	2.3
100	4.2	4.0

Seventy-one sets of data were used in development, although fewer points were available at the 0 and 100% points. Average error is defined as the sum of the absolute values of the differences between predicted and experimental temperatures divided by the number of data points, while bias error sums the actual values of the differences.

Special Comment

This method was derived from all data available to the project and was judged to be the most appropriate form for interconversion among the various types of distillations. As additional data become available, the constants in equations (3A1.1-1 and 3A1.1-2) can easily be improved. In addition, users may wish to check the correlation with their proprietary data before using it.

Literature Source

This method was developed by the API Technical Data Book Project at The Pennsylvania State University.

Example

Estimate the atmospheric TBP distillation temperatures for a petroleum fraction having the experimental ASTM D86 distillation temperatures given in the following table. The experimental TBP temperatures are given for comparison with the predicted temperatures.

Volume percent distilled	10	30	50	70	90
ASTM D86 temperature, F	350	380	404	433	469
TBP temperature, F	321	371	409	447	491

Using equation (3A1.1-1)

$$TBP (50) = 0.87180 (404)^{1.0258}$$
$$= 411.2 F$$

Using equation (3A1.1-2) at the 30% point

$$Y_4 = 3.0305 [X_4]^{0.80076}$$

where $X_4 = 404 - 380 = 24 F$

therefore, $Y_4 = 38.6 F$

Using equation (3A1.1-3) at the 30% point

TBP (30) = TBP (50) − Y_4

       = 411.2 − 38.6 = 372.6 F

Similarly, using equations (3A1.1-2) and (3A1.1-3) at the other cut points,

$Y_2 = 45.5, Y_3 = 40.0, Y_5 = 56.0$

TBP (10) = 372.6 − 56.0 = 316.6 F

TBP (70) = 411.2 + 40.0 = 451.2 F

TBP (90) = 451.2 + 45.5 = 496.7 F

The reverse conversion from experimental TBP temperatures to ASTM D86 temperatures is illustrated only for the 50% and 30% points.

(1) Use equation (3A1.1-4) to convert the experimental TBP 50% point temperature.
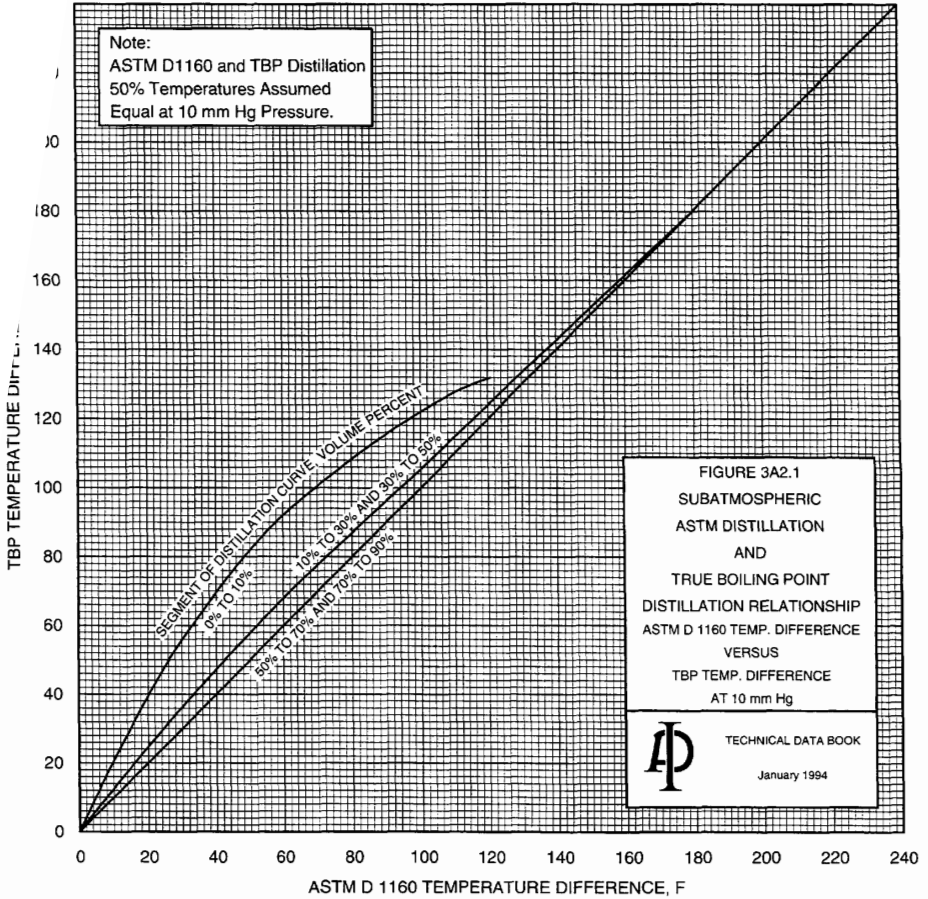
$$\text{ASTM D86 (50)} = \exp\left[\frac{\ln\,(409/0.87180)}{1.0258}\right] = 401.9 \text{ F}$$

(2) Use equation (3A1.1-2) to determine the 50 to 30% ASTM increment.

$$X_4 = \exp\left[\frac{\ln\,(Y_4/3.0305\,)}{.80076}\right] = 23.5 \text{ F}$$

$$\text{where } Y_4 = 409 - 371 = 38$$

(3) ASTM D86 (30) =   ASTM D86 (50) − X_4

               =   401.9 − 23.5

               =   378.4 F

3A2.1

Note:
ASTM D1160 and TBP Distillation
50% Temperatures Assumed
Equal at 10 mm Hg Pressure.

FIGURE 3A2.1

SUBATMOSPHERIC

ASTM DISTILLATION

AND

TRUE BOILING POINT

DISTILLATION RELATIONSHIP

ASTM D 1160 TEMP. DIFFERENCE

VERSUS

TBP TEMP. DIFFERENCE

AT 10 mm Hg

TECHNICAL DATA BOOK

January 1994

ASTM D 1160 TEMPERATURE DIFFERENCE, F

TBP TEMPERATURE DIFFERENCE

1994

3-11

3A2.1

COMMENTS ON FIGURE 3A2.1

Purpose

This figure relates ASTM D 1160 and TBP distillation data at 10 mm Hg absolute pressure.

Reliability

No quantitative evaluation of the correlation could be made because of lack of data. The original reference indicates that temperatures from this method will be within 25 F of the actual values.

Special Comment

The ASTM D 1160 and TBP 50-percent points at 10 mm Hg are assumed to be equal.

Literature Source

Adapted from Edmister and Okamoto, *Petrol. Refiner* **38** [9] 271 (1959); copyrighted in 1959 by Gulf Publishing Company, Houston, Texas.

Example

Estimate the TBP curve at 10 mm Hg for a petroleum fraction having the following ASTM D 1160 distillation temperatures at 10 mm Hg:

Distillation, percent by volume	10	30	50	70	90
Temperature, deg F	300	400	475	550	650

First, from Fig. 3A2.1, find the temperature differences for each segment of the TBP curve at 10 mm Hg:

Segment of Curve (Percent by Volume)	10 mm Hg ASTM D 1160 Temperature Difference (Degrees Fahrenheit)	10 mm Hg TBP Temperature Difference (from Fig. 3A2.1) Degrees Fahrenheit)
10 to 30	100	106
30 to 50	75	82
50 to 70	75	75
70 to 90	100	100

The TBP temperatures are then calculated. The ASTM D 1160 and TBP distillation 50-percent temperatures are assumed to be equal at 10 mm Hg absolute pressure. Here, the 50-percent temperature is 475 F:

30-percent temperature = 475 − 82 = 393 F   70-percent temperature = 475 + 75 = 550 F

10-percent temperature = 393 − 106 = 287 F   90-percent temperature = 550 + 100 = 650 F