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EVALUATION OF THE APPLICATION OF SOME GAS CHROMATOGRAPHIC METHODS FOR THE DETERMINATION OF PROPERTIES OF SYNTHETIC FUELS

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EVALUATION OF THE APPLICATION OF SOME GAS
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PROPERTIES OF SYNTHETIC FUELS
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ABSTRACT

The purpose of the investigation was to evaluate the applicability, to some synthetic fuels, of some gas chromatographic methods now under development for use with petroleum based fuels. Thirty-two (32) jet and diesel fuel samples which were prepared from oil shale and coal syncrudes were examined. The boiling range distribution of each was determined by gas chromatography, and from that data distillation properties were calculated. The calculated results gave sufficient agreement with the measured values that the equations could be useable in their present form. Bulk fuel properties (°API, flash point, viscosity) were calculated for the sixteen (16) JP-5 and Diesel No. 2 type fuels. The results show that the equations would not give useable results. Capillary column gas chromatography was used to determine the n-alkane content of the eight (8) JP-5 type samples and the results related to the observed freezing points. The results show that the concentrations of the long straight chain molecules in the fuels exert influence on the freezing point but are not the complete controlling factor.

SUMMARY

Increasingly, attempts are being made to use gas chromatography to provide fuel composition and distillation data for a variety of petroleum fuels. A recent reference describes attempts to obtain a correlation between ASTM Test Method D86, Test for Distillation of Petroleum Products, and ASTM Test Method D2887, Test for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography. Equations were obtained for calculating D86 data points from D2887 data. Equations were also obtained for calculating some bulk fuel properties from the gas chromatography data, and others for substituting D2887 data for D86 data in some correlative equations for estimating the heat of combustion and the hydrogen content. The purpose of this investigation was to evaluate the application of these methods to some synthetic fuels. The equations were applied to 32 fuels, of varying properties, derived from oil shale and coal syncrudes. Volatility correlations and bulk fuel properties were determined. The results show that some of the methods would be applicable in their present form. The equations for obtaining D86 data points from D2887 data, and those using
D2887 data in the correlative equations for estimating heat of combustion and hydrogen content can be applied in their present forms. The use of the other equations to obtain bulk fuel properties (°API, flash point, and viscosity) was not successful.

In another part of the investigation capillary gas chromatography was used to determine the concentrations of the n-alkanes in some of the fuels. Those concentrations were examined for relationships with freezing points, as noted for petroleum fuels. The results show that the concentrations of the long straight chain molecules in the fuels exert influence on the freezing point but are not the complete controlling factor.

INTRODUCTION

Methods of measuring chemical and physical properties of petroleum products, and also correlating them to fuel quality and combustion performance, are constantly being modified, changed and improved. Recently, the use of gas chromatography was introduced to provide fuel composition and distillation data for a variety of fuels. For gasolines, for example, gas chromatographic data has been used to calculate vapor pressure, aniline point, pour point, and octane rating. Presently, though, ASTM Test Method D86, Test for Distillation of Petroleum Products (ref. 1) is used for measuring and controlling the distillation characteristics of many petroleum products. This test is equivalent to a one-plate distillation and only provides a general idea about the true distillation properties of a fuel. The use of gas chromatography, though, shows promise for providing far more information in a much simpler fashion. An ASTM Test Method, D2887, Test for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography (ref. 2) is increasingly being used but has not yet been approved for use in aircraft turbine fuel specifications. The D2887 test method is equivalent to a distillation with over 100 theoretical plates. One restriction in its use has been the lack of a suitable correlation between the D86 and the D2887 tests. Recently, (ref. 3), an attempt has been made to obtain a correlation between D86 and D2887 for jet fuels and obtain D86 data points from D2887 measurements. In addition, equations were generated for calculating bulk fuel properties from the gas chromatography data and the substitution of D2887 data for D86 data in some correlations was examined.

The purpose of this report is to examine the applicability of the gas chromatography methods derived for petroleum fuels to some fuels derived from oil shale and coal syncrudes. These fuels approximated JP-4, JP-5, diesel #2, and broad-specification fuels. The regression equations computed in reference 3 can be used to estimate D86 distillation values from D2887 measurements for both wide-cut and kerosine type aircraft turbine fuels, and appear to have sufficient precision for most purposes. These equations were applied to all of the synthetic fuels. For calculating physical properties, only those equations that gave reasonable accuracy with petroleum fuels were used, namely, flash point, viscosity and API.
gravity for kerosine fuels. The equations suggested for use in substituting D2887 data for D86 data in some new correlative methods for estimating the net heat of combustion and the hydrogen content were applied to all of the fuels.

One other use of gas chromatography for determining a physical property was examined in this report. Specifically, for the JP-5 type fuels only, the n-alkane content of... as determined by capillary gas chromatography, and that content related to the freezing point of the fuel.

FUELS

The fuels examined in this work were those prepared from TOSCO shale oil, H-Coal and COED coal syncrudes by the Atlantic-Richfield Company under an NASA contract (ref. 4). Thirty-two jet fuel samples of varying properties were produced by processes commonly in use in petroleum processing — distillation, hydrogenation and catalytic hydrocracking. The processing conditions were those required to meet two levels of specifications regarding aromatic, hydrogen, sulfur and nitrogen contents at two yield levels. Each process stream was split by distillation to give four distillation ranges. The volatility specifications of the fuels produced were approximately those found in the following: (1) JP-4 (Jet B) with a 561K (550°F) end point and 20.7 x 10³ N/m² (3 psi) maximum Reid vapor pressure, (2) JP-5 (Jet A) with a 561K (550°F) end point and a 311K (100°F) minimum flash point, (3) a broad specification fuel incorporating the volatility of a JP-4, 20.7 x 10³ N/m² (3 psi RVP) and the end point of a diesel No. 2, 616K (650°F), (4) Diesel No. 2 with a 616K (650°F) end point and a 311K (100°F) minimum flash point. All the physical and chemical tests required for aircraft turbine fuels were reported by ARCO for the 32 fuels using standard ASTM methods. Sixteen of these fuels were from a TOSCO shale oil syncrude, 8 from an H-Coal syncrude, and 8 from a COED (coal-derived) syncrude. The properties of the fuels obtained are given in Table I. The distillation data, obtained by ASTM D86 are given in Table II. In this method a 100-ml sample is distilled under prescribed conditions, and systematic observations of thermometer readings and volumes of condensate are made. The initial boiling point (IBP) is defined as the thermometer reading that is observed at the instant that the first drop of condensate falls from the lower end of the condenser tube. The percent recovered is the volume in milliliters of condensate observed in the receiving graduate, in connection with a simultaneous thermometer reading. The end point (EP) or final boiling point (FBP) is defined as the maximum thermometer reading obtained during the test.

METHODS FOR DETERMINING JET FUEL PROPERTIES

ASTM D2887 Data

ASTM Test Method D2887, Test for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography, was used to obtain the gas chromatographic data. The data was obtained from the Quality Control Laboratory, AFAPL,
Wright-Patterson Air Force Base. A Perkin-Elmer 900 gas chromatograph with a flame ionization detector was used. SE-30 column packing (3% loading) was used in an 1/8" x 15' column, with the temperature programmed at 8° per minute from 233 to 573K (-40 to 572°F). In this method a sample is introduced to the gas chromatographic column, which separates hydrocarbons in boiling point order. The area under the chromatogram is recorded throughout the run. Boiling temperatures are assigned to the time axis from a calibration curve obtained under the same conditions by running a known mixture of hydrocarbons covering the boiling range expected in the sample. From these data the boiling range distribution is obtained. The data is tabulated as percent recovered at each selected interval and the boiling temperature assigned to that interval from the calibration curve. The results obtained for 31 of the 32 fuels are given in Table III. The initial boiling point (IBP) is defined as the point at which a cumulative area count equal to 0.5 percent of the total area under the chromatogram is obtained. The final boiling point (FBP) is the point at which a cumulative area count equal to 99.5 percent of the total area under the chromatogram is obtained.

EQUATIONS FOR ESTIMATING D86 DATA POINTS (REF. 3)

The equations were generated using a step-wise regression analysis method to obtain the greatest reduction in the error sum of squares. The method determines the optimum independent parameters (i.e., D2887 data points) to calculate the dependent parameter (a preselected D86 data point). In the course of the study, equations were determined for wide-cut fuels only (JP-4 and Jet B), kerosine type fuels only (JP-5 and Jet A), and for both wide-cut and kerosine fuels together. The equations used in this report were those considered by the author of reference 3 to be the most reliable, and preferred for estimating D86 properties from measured D2887 values for any fuel ranging from a wide-cut JP-4 to a narrow-cut kerosine such as JP-5. The equations are shown in Table IV. In order to calculate the initial boiling point (IBP) and final boiling point (FBP), D2887 percent recovered points other than those given in Table III are needed. The temperatures at those points (2%, 97%, and 98%) were obtained by interpolation from a plot of temperature against percent recovered. A typical plot is shown in figure 1. In making such plots the initial boiling point is plotted at 0 and the final boiling point at 100 percent recovered.

EQUATIONS FOR ESTIMATING BULK PROPERTIES OF KEROSINE FUELS (REF. 3)

°API

The equation used to calculate °API values is given in Table V. The values needed are readily obtained from the D2887 data. As noted before, °API is readily measured, but using this equation might have some value since the degree of correlation is high and the standard error of estimate is less than 1 °API.
Flash Point

The flash point equation is also given in Table V. For this equation, D2887 data including IBP and FBP are needed. Also needed is the °API value. This value was calculated from the specific gravity value given in Table I.

Viscosity

The viscosity equation is also shown in Table V. For this one also the °API value is needed in addition to the distillation values.

SUBSTITUTION OF D2887 DATA FOR D86 DATA IN CORRELATIONS

Recently two correlative methods for estimating fuel properties were published by ASTM. They are D3338 for estimating the net heat of combustion and D3343 for estimating the hydrogen content. Both of these new standards need the average D86 distillation temperature (10%, 50%, and 90% recovered) as input data. To use ASTM D2887 in place of the D86 distillation method, a D2887 average distillation temperature which is numerically identical to the D86 average distillation temperature is needed. Statistical methods were used to determine the optimum three or five D2887 distillation data points whose average would best correlate with the 10%, 50%, and 90% recovered average temperature using the D86 distillation method. The use of the following equations was recommended in reference 3:

\[
\frac{(10\% + 50\% + 90\%)}{3} \text{D}_86 = \frac{(10\% + 50\% + 95\%)}{3} \text{D}_2887
\]

for JP-4, Jet B fuels,

\[
\frac{(10\% + 50\% + 90\%)}{3} \text{D}_86 = \frac{(10\% + 50\% + 95\%)}{3} \text{D}_2887 - 2K(3.6^\circ F)
\]


For JP-4 fuels no correction factor was needed and the average distillation temperature calculated from the three D2887 data points was within 5.6K (10°F) of the D86 average 95% of the time. For kerosine fuels, a 2K (3.6°F) correction factor was required, and agreement to within 3.3K(6°F) 95% of the time was found.

N-ALKANE CONTENT OF JP-5 TYPE FUELS BY CAPILLARY GAS CHROMATOGRAPHY

The n-alkane content data were obtained from the Naval Research Laboratory, Washington, D.C. Ten-gram fuel samples were fractionated by absorption on activated silica gel. The saturated fraction was eluted from the silica gel with n-pentane which was then evaporated to a volume of 50 ml. One gram of an internal standard was then added for quantitation.
of the gas chromatographic analysis. The latter was carried out on an all
glass Perkin-Elmer 3920B chromatograph. The 300 ft. glass capillary
column had an OV-101 wall coating. A 1.5 microliter sample was split
80:1 in the GC inlet. A standard comprised of n-alkanes was run each
day to obtain retention time comparisons.

Four of the saturate fractions were also examined by gas chromatography/
mass spectrometry. The presence of a parent peak in this analysis con-
firmed the identity of peaks thought to be n-alkanes based on GC retention
times. The results are given in Table VI.

RESULTS AND DISCUSSION

Comparison of Measured and Calculated D86 Data Points

The D86 distillation test method is equivalent to a one-plate dis-
tillation, and as such cannot give accurate data in regard to the effective
distribution of the boiling points of the sample. For a more accurate
determination a laboratory fractionating distillation, commonly called
"true boiling point" is used. There is no standard procedure, and columns
with considerably different efficiencies (from 20 to 100 theoretical plates)
have been used. This method determines the distribution more accurately
but yet has difficulty in establishing the initial and final boiling
points. In looking at the data from the two methods, there is usually
agreement somewhere around the midpoint of the range. The D2887 method
is equivalent to a distillation with over 100 theoretical plates, and
agrees very well with the "true boiling point" distillation method. And,
again, in comparing data from D86 and D2887, agreement occurs somewhere
about the mid-range with the GC data giving lower IBP and higher FBP. A
typical set of curves for the two methods is shown in figure 2. There
is still concern over the fairly wide spread in values at the initial and
the final boiling points, though it is recognized that a good bit of the
difference may lie in the fact that the initial and final boiling points
are defined differently in the two methods. It is not surprising then that
the standard errors of estimate in the estimating equations are largest
at the initial and final boiling points.

The data from the equations in Table IV are given in Table VII and
plotted against the measured values in figures 3-10. The error bar for
one standard error of estimate is included. The data used to generate
these equations were from JP-4 and JP-5 fuels, but in this report they are
applied to all the fuels, JP-4 JP-5, Diesel No. 2, and broad-specification.
The data for the JP-4 type samples prepared from shale are shown in
figure 3, and it can be seen that in three of the four instances, both the
initial and the final boiling points are within one standard error of
estimate. Further, with the exception of one sample practically all of the
other values are within one standard error of estimate. For the two fuels
prepared from H-Coal (fig. 4), the results are similar. The initial
boiling points are within a standard error of estimate, while the final boiling points are well without. The latter is also true for the 90 percent points. For the other points, they are mostly just outside of one standard error of estimate. The results for the fuels prepared from the COED crude are not unlike those from the H-Coal source, though in this case the agreement is quite a bit better. The initial boiling points are just beyond one standard error of estimate, and the final boiling points are also without. In contrast, the 90 percent points are within the estimate and the remaining points are mostly within. In contrast, the 90 percent points are within the estimate and the remaining points are mostly within.

In figure 5 the results for the JP-5 type fuels prepared from shale are shown. For all four fuels the initial and the final boiling points are within one standard error of estimate. This is also true of the 90 percent points. Three of the four 50 percent points are within one standard error, while three of the four ten percent points are without. All of the 20 percent points are outside of the standard error. The results for the coal-derived fuels, shown in figure 6, are somewhat more varied. The initial boiling points are within one standard error of estimate, but one of the final boiling points does not meet that criterion. For the COED samples, the 90 percent points are within the error, but for the H-Coal samples they are not. For the remaining points, in most instances the measured values are close to but not within one standard error of estimate, with the most serious error occurring at the 10 percent points. No clear distinction can be seen between the shale and coal samples, and the results indicate that the method should be useful with these JP-5 type samples.

In figure 7 are plotted the results for the Diesel #2 type fuels prepared from oil shale syncrude. It was noted before that the equations being used were not generated from any #2 fuels but would be applied to them nevertheless. It is perhaps not surprising then that the final boiling points are close to but not within one standard error. There is good agreement at the 90, 50, and 20 percent points for two of the three samples, with one showing a large error at the 20 percent point, and all showing large errors at the 10 percent points. By contrast, though, the initial boiling points were in good agreement with the measured values. Some of the results for the coal samples shown in figure 8 are abbreviated because of the foaming encountered with the D86 measurement. For the H-Coal sample, the initial boiling point is within the error criterion, but the other points are not. For the similar COED sample, all of the points are within one standard error of estimate. For the full range COED sample, only the initial and 50 percent points are within the error.

In figure 9 are the results for the broad-specification type fuels prepared from oil shale. For three of the four fuels the initial boiling point is within one standard error of estimate, while the reverse is true for the final boiling points. For the 90 percent points two are within and two are outside of the error. A similar pattern holds for the remaining points for these fuels. In figure 10 it is immediately apparent that the agreement for the final boiling point with both H-Coal samples is not good. The 90 percent point for both is also outside of one standard
error of estimate, while for the remaining points some are within and some are not. It can be seen in figure 10, also, that the large error at the final boiling point is not repeated for the COED samples. The 90 percent points are both outside but close to one standard error, and for the most part the agreement of the other points are good.

The differences between the calculated and measured values for the D86 data points are shown in figure 11. For the JP-4 type fuels, it can be seen that more of the points for shale fell within one standard error of estimate than did those for coal. And for the shale results most of the points that were without were from one fuel. More work with the JP-4 type fuels derived from shale would show whether the method is generally useful, as is indicated, or whether we would see more points outside of the one standard error of estimate. For the JP-5 type fuels no clear distinction can be seen between the shale and coal samples, and the results indicate that the method should be useful with these JP-5 type samples. The differences found for the diesel #2 and the broad-specification fuels are also plotted in figure 11, and it can be judged that this method can be applied to fuels other than the JP-4 and JP-5 types even using the equations in their present form. It would be preferable of course to modify them as necessary as input data from higher boiling fuels becomes available. Further, new calibration standards that would include compounds more prevalent in the coal syncrudes should be examined.

Calculation of Bulk Fuel Properties

Bulk properties of Diesel #2 fuels were also calculated together with the JP-5 fuels. The *API data, measured and calculated are shown in Table VIII and plotted in figure 12. The agreement between the two is not good. Further, a clear separation between the shale and coal samples is observed, with the shale fuels showing calculated values lower than the measured and the coal derived fuels showing values higher than the measured ones. The reasons for the results are not clear. It appears that the volatility of the coal samples are comparable to those from shale, but the densities of the coal samples are much higher than those of similar petroleum products. There may be effects of components in the fuel that are volatile but attract enough in the liquid to give high densities. In determining the reasons for the results, attention would have to be given to the calibration curves used for the D2887 data, and consider the possibility of having a separate set for shale, coal and petroleum fuels. The results from the calculation of the flash points of the Jet A type samples are given in Table VIII, and plotted in figure 13 against the measured values. It can be seen that in all instances that the calculated values are all much higher than the measured values. The equation obviously could not be applied in its present form to give meaningful results. The input to the equation involves the TBP, FBP, 5 percent off, 25 percent off, and density, and it is not obvious where modifications should be made. In Table VIII also are the results for the diesel #2 type fuels also, and the plot also in figure 13. As noted before, the
equations were generated from kerosine fuels, but nevertheless were applied to the diesel type, and in this instance the agreement appears to be no worse than it is with the Jet A samples. The values for the COED samples are in least agreement, the values for the shale samples are somewhat close in some instances, and those for the H-Coal samples somewhere in between.

The results for the calculation of viscosity from the equation in Table V are shown in Table VIII, and plotted against the measured values in figure 14. The measured values for the four Jet A type fuels from shale are not much different from each other and the calculated values are in good agreement, close to or within one standard error of estimate. The values for the coal-derived fuels are more varied. It should be noted, though, that the measured values for the COED samples are not far apart. One value for an H-Coal sample may be suspect. It appears, then, that the equation is not useful with the coal samples, though some samples fall not far outside one standard error of estimate. The results for the calculation of Diesel #2 fuels were not included since a number of the measured values were reported as being solid at 239K(-30°F).

Substitution of D2887 Data for D86 Data in Correlations

The two recently published standards for estimating the net heat of combustion and for estimating the hydrogen content are anticipated to be widely used in aircraft turbine fuel specifications. It was of particular interest then to test the applicability of substituting the D2887 data for the D86 using the synthetic derived fuels. Again the method was applied to all of the fuels not limiting the application to just the JP-4 and JP-5 fuels. The data derived is given in Table IX and plotted in figure 15. The dotted lines show an interval of 5.6K(10°F) for the JP-4 and broad-specification fuels, and a 3.3K(6°F) interval for the JP-5 and Diesel #2 type fuels. For the JP-4 fuels, with one exception, all of the values were within the 5.6K(10°F), 95% of the time expectation. For the broad-specification fuels, three of the values are outside of the 5.6K(10°F) expectation. It should be noted however, that the results can be viewed as a shifting of the data to the left as a result of shifting to the higher final boiling point. The coal samples which had low D2887 values when compared to the D86 shifted to values about comparable, while the shale samples which were more comparable shifted to D2887 values which were higher than the D86 values. The relative positions of the coal and shale samples did not change. A similar pattern is noted for the JP-5 and Diesel #2 fuels, though fewer points are available for comparison. For the JP-5 fuels, most of the shale values are within the 3.3K(6°F) expectation, while most of the coal values are not. In going to the higher temperatures in the No. 2 fuels, the shale values are shifted and, perhaps fortuitously, the D2887 values agree very well with the D86 values. The lone coal value is now close to being within expectation, where with the JP-5 samples those coal values were not within expectation. The results suggest that the D2887 substitution would be acceptable for shale samples of either.
JP-4 or JP-5. There would be some question in regard to the use with coal samples of JP-5, though it seems that the substitution would be useful with coal samples of JP-4. The results are also favorable for considering the use of the method with fuels of higher boiling point and broadened specification.

N-Alkane Content-Freezing Point Relationships

The n-alkane content of the JP-5 type fuels was determined as described and the results of that determination are given in Table VI. One of the methods suggested for estimating freezing points of jet fuel fractions is based on a linear relationship between the experimental freezing points and the total content of the last three members of the n-paraffin series in the fuel (ref. 5). A plot of the sum of the C_{14} to C_{17} n-alkanes concentration against freezing points is shown in figure 16. A 'reasonable' straight line can be fitted to the data for the shale and the COED fuels. No attempt was made to establish a fit, but just to show that some points readily fit and some do not. Other work has found that the saturate fraction of fuels exerted the greatest influence on freezing point, but that the aromatic fraction was also important. That statement would seem to accurately describe the results found here. In a recent report on properties and composition of jet fuels derived from alternate energy sources (ref. 6), it was reported that the total n-alkane concentration did not afford a significant relationship with freezing point. The freezing point did show some dependence on the amount of the larger hydrocarbons present. That dependence was tested against a model which equates the dissolution of a solid in a liquid to form an ideal solution with the melting of pure solute at the lowered temperature where solution is taking place. It was found that a plot of the logarithm of the C_{16} concentration (log[X_{C_{16}}]) of those jet fuels against the reciprocal of the temperature of the freezing point gave a reasonable adherence to a solubility plot. This was in agreement with previous work with model fuel systems which showed that the largest n-alkane present had a marked control over the freezing point of a fuel. In figure 17 the solid line is the plot of the mole % [C_{16}] against freezing point in a commercial kerosine type solvent. The solid squares are from JP-5 samples, described in reference 5, from oil shale, tar sands, and coal. The samples derived under the program in this report exhibit a similar trend but are displaced to lower freezing points. The results could be described as anomalous, and join other anomalous freezing point behavior found in other studies, or it could be concluded that n-alkanes exert control over the freezing point of jet fuels, but that the relationship between composition and freezing point is not completely defined by the concentration of the largest n-alkane in these samples.
CONCLUDING REMARKS

It was the purpose of this report to test the applicability of some gas chromatographic methods for measuring volatility and other properties of petroleum fuels to fuels from other sources. The results show that for a variety of fuels from two primarily different sources that some of the methods would be applicable in their present form. It should be remembered, though, that the equations used appeared to have sufficient precision for most purposes, but that the author of reference 3 believed that additional data was needed to increase the statistical validity of the equations. Nevertheless, those equations dealing solely with volatility, i.e., getting $D_{65}$ data from $D_{2887}$ data, and using $D_{2887}$ data in the correlative equations, can be applied in their present forms. In general, also, the shale-derived fuels fit somewhat better than the coal-derived fuels. By contrast, the attempt to determine bulk fuel properties from the suggested equations was not successful. Modification of the equations or changes in the underlying calibration curves are needed.

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Naval Research Laboratory, Chemistry Division, Fuels Section, Washington, D.C. - N-Alkane Content - Capillary Gas Chromatography.

REFERENCES


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### Shale

- IBP - 561 K (250-550°F)
- 5% - 425 K °F
- 10 - 423 K °F
- 15 - 425 K °F
- 20 - 425 K °F
- 30 - 425 K °F
- 40 - 425 K °F
- 50 - 425 K °F
- 60 - 425 K °F

### Coal

- IBP - 561 K (250-550°F)
- 5% - 424 K °F
- 10 - 424 K °F
- 15 - 424 K °F
- 20 - 424 K °F
- 30 - 424 K °F
- 40 - 424 K °F
- 50 - 424 K °F
- 60 - 424 K °F
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Shale
394 - 616 K
(250 - 650°F)

Coal
394 - 616 K
(250 - 650°F)

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TABLE III. - BOILING RANGE DISTRIBUTION BY GAS CHROMATOGRAPHY (ASTM D 2887) DATA FOR SOME SYNTHETIC JET FUELS

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394 - 561 K (250 - 550°F)

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- H-Coal

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TABLE IV. - EQUATIONS FOR ESTIMATING D86 DATA FOR BOTH JP-4 AND KEROSENE FUELS (REF. 3)

Equations - Independent Variables are D2887 Percent Recovered Points (D86 Calculated Points in K, D2887 Percent Points in K)

<table>
<thead>
<tr>
<th>Percent Recovered</th>
<th>Equation</th>
<th>Std. error of coeff.</th>
<th>Correl. est., K(°F)</th>
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</table>
| IBP<sub>D86</sub> | 15.04 + 0.816[1.8(2%) - 459.72] + 0.378[1.8(10%)
- 459.72] - 0.182[1.8(65%) - 459.72] + 0.089[1.8(98%) - 459.72] | 0.996                 | 4.6(8.31)            |
| 10%<sub>D86</sub> | 61.03 + 0.154[1.8(5%) - 459.72] + 0.675[1.8(10%)
- 459.72] - 0.082[1.8(15%) - 459.72] + 0.316[1.8(35%) - 459.72] | 0.997                 | 3.2(5.72)            |
| 20%<sub>D86</sub> | 37.48 + 0.251[1.8(10%) - 459.72] + 0.210[1.8(20%)
- 459.72] + 0.572[1.8(35%) - 459.72] - 0.081[1.8(90%) - 459.72] | 0.998                 | 2.3(4.13)            |
| 50%<sub>D86</sub> | 17.56 - 0.064[1.8(5%) - 459.72] + 0.182[1.8(35%)
- 459.72] + 0.625[1.8(50%) - 459.72] + 0.209[1.8(65%) - 459.72] + 0.046[1.8(FBF) - 459.72] | 0.997                 | 2.2(3.94)            |
| 90%<sub>D86</sub> | -12.36 - 0.077[1.8(25%) - 459.72] + 0.457[1.8(75%)
- 459.72] - 0.624[1.8(85%) - 459.72] + 0.890[1.8(90%) - 459.72] + 0.319[1.8(95%) - 459.72] | 0.992                 | 3.3(6.00)            |
| FBP<sub>D86</sub> | 106.57 + 0.219[1.8(65%) - 459.72] - 0.375[1.8(85%)
- 459.72] + 0.759[1.8(97%) - 459.72] + 0.165[1.8(98%) - 459.72] | 0.960                 | 5.1(9.17)            |
### Table V. - Equations for Estimating Bulk Properties of Kerosene Fuels (Ref. 3)

<table>
<thead>
<tr>
<th>Equations</th>
<th>Std. Correl. error coeff. of est.</th>
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| °API = 100.42 - 0.147[1.8(10%) - 459.72] + 0.306
   [1.8(20%) - 459.72] - 0.195 [1.8(35%) -
   459.72] - 0.098[1.8(65%) - 459.72] | 0.950 0.97(°API) |
| Flash Point (K) = -29.63 + 0.210[1.8(IBP - 459.72]
   + 0.191[1.8(5%) - 459.72] + 0.257
   [1.8(25%) - 459.72] - 0.049
   [1.8(FBP) - 459.72] - 0.458(API) | 0.989 1.1K(2.1°F) |
| Viscosity = 22.58 + 0.042[1.8(10%) - 459.72] + 0.027
   [1.8(50%) - 459.72] + 0.027[1.8(97%) -
   459.72] - 0.184(API) | 0.991 0.3(CS) |
| Distillation Points (IBP, 5%, 10%, etc.) are from D2887 Test, K |
| API = Gravity in °API |
### TABLE VI. - \( \text{n-ALKANE CONTENT OF JP-5 TYPE JET FUELS} \)

294 - 561 K (250-550°F)

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<th>( C_{14} )</th>
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### TABLE VII. - D86 DATA POINTS CALCULATED FROM EQUATIONS OF TABLE IV

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**IBP-561K (IBP-550°F)**

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**Coal**  
**IBP-561K (IBP-550°F)**

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**Shale**  
**394-561K (250-550°F)**

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**Coal**  
**394-561K (250-550°F)**

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TABLE VII. - Concluded.

Shale
394-616K(250-650°F)

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<td>K °F</td>
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Coal
394-616K(250-650°F)

| IBP         | 428(311)    | 427(310) | 425(306)    |     |             |     |
| 10          | 434(322)    | 442(337) | 438(329)    |     |             |     |
| 20          | 446(343)    | 461(371) | 456(361)    |     |             |     |
| 50          | 478(402)    | 507(454) | 498(437)    |     |             |     |
| 90          | 555(539)    | 571(569) | 569(565)    |     |             |     |
| FBP         | 589(601)    | 584(592) | 586(596)    |     |             |     |

Shale
IBP-616K(IBP-650°F)

| IBP         | 382(229)    | 379(223) | 349(169)    | 353(177) |     |     |
| 10          | 417(292)    | 409(277) | 395(252)    | 397(255) |     |     |
| 20          | 438(330)    | 430(314) | 419(295)    | 420(297) |     |     |
| 50          | 497(436)    | 488(419) | 481(407)    | 480(404) |     |     |
| 90          | 578(582)    | 572(570) | 575(575)    | 570(567) |     |     |
| FBP         | 590(602)    | 585(593) | 585(593)    | 583(590) |     |     |

Coal
IBP-616K(IBP-650°F)

<p>| IBP         | 387(238)    | 384(232) | 366(199)    | 360(189) |     |     |
| 10          | 407(274)    | 422(301) | 401(262)    | 399(259) |     |     |
| 20          | 427(310)    | 425(306) | 427(310)    | 425(306) |     |     |
| 50          | 475(395)    | 469(385) | 492(426)    | 500(440) |     |     |
| 90          | 550(531)    | 544(520) | 569(565)    | 567(561) |     |     |
| FBP         | 592(607)    | 580(585) | 586(595)    | 585(593) |     |     |</p>
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<th>Flash Point °F</th>
<th>Viscosity, CS at 239K(-30°F)</th>
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<td>314(106)</td>
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<td>45.6</td>
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<td>315(108)</td>
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<td>323(123)</td>
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<td>24</td>
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TABLE IX. - D2887 AND D86 - AVERAGE DISTILLATION TEMPERATURES,

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<th>Fuel No.</th>
<th>IBP-561K (IBP-550)</th>
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<th>D86 (10% + 50% + 90%)</th>
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<td>462(372.2)</td>
<td>466(379)</td>
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<td>5</td>
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<td>460(368.6)</td>
<td>466(379)</td>
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<td>6</td>
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<td>461(371.1)</td>
<td>467(382)</td>
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<td>464(378.9)</td>
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<th>D86 (10% + 50% + 90%)</th>
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<tbody>
<tr>
<td>9</td>
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<td>478(401.7)</td>
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<td>479(402.4)</td>
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<th>D86 (10% + 50% + 90%)</th>
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<th>D86 (10% + 50% + 90%)</th>
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<td>485(414.3)</td>
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<td>478(401)</td>
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<td>478(402)</td>
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Figure 1. Typical D2887 boiling range distribution curve for a jet fuel.

Figure 2. Typical distillation curves by D86 and D2887 methods.
Figure 3. Comparison of measured and calculated D86 data points for shale fuels, IBP-561 K (550°F).
Figure 4. - Comparison of measured and calculated D86 data points. Coal fuels, IBP=561 K (500° F).
Figure 5. - Comparison of measured and calculated D86 data points. Shale fuels, 394-561 K (738°F-1042°F).
Figure 6. - Comparison of measured and calculated D86 data points. Coal fuels, 394-561 K (728°F-1042°F).
Figure 7. - Comparison of measured and calculated D86 data points. Shale fuels, 394-616 K (230°-650°F).
Figure 8. - Comparison of measured and calculated D86 data points. Coal fuels, 394-616 K (790°-1150° F).
Figure 9. Comparison of measured and calculated D86 data points. Shale fuels, IBP-616 K (1050°F).
Figure 10. - Comparison of measured and calculated D86 data points. Coal fuels, IBP-616 K (1150°F).
Figure 11. - Difference between measured D86 data points and data points calculated from D2887.
Figure 12. Comparison of calculated and measured °API for JP-5 and diesel no. 2 type fuels.
Figure 13 - Comparison of calculated and measured flash points.
Figure 14. Comparison of calculated and measured viscosity at 239 K (330°F) for JP-5 type fuels.
Figure 15. - Comparison of D2887 and D86 average distillation temperatures.
Figure 16. - Plot of freezing point against n-alkane concentration (Σ of C_{14} to C_{17}) of JP-5 type fuels.

Figure 17. - Freezing point of jet fuels as function of n-C_{16} concentration, wt %.