CORRELATION OF CHEMICAL CHARACTERISTICS WITH FUEL PROPERTIES BY GAS CHROM. (U) SOUTHWEST RESEARCH INST SAN ANTONIO TX ARMY FUELS AND LUBRICA.

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CORRELATION OF CHEMICAL CHARACTERISTICS WITH FUEL PROPERTIES BY GAS CHROMATOGRAPHY

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and Development Command
Energy and Water Resources Laboratory
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December 1981
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**Title:** Correlation of Chemical Characteristics with Fuel Properties by Gas Chromatography  
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**Author(s):** D.L. Present, L.L. Stavinoha, F.M. Newman  
**Abstract:** Standard tests such as those published by ASTM are used to determine a fuel's properties. As new fuels are introduced, it becomes necessary to characterize them by applying available standard test methods and chemical/physical characterization techniques in a process which is costly, time consuming and developmental by its very nature. Because of the technical advances in digital computers and gas chromatography, it has become feasible.
20. ABSTRACT (Cont'd)

to attempt to develop correlations between gas chromatographic data and some chemical/physical properties. These, in turn, may be related to a fuel's performance. Eight test fuels were selected for this preliminary work because of their known stability and chemical/physical properties. A modified ASTM D 2887 boiling point distribution (BPD) method was developed to yield component specific identification in addition to BPD consistent with the conventional D 2887 method. The data from this modified method may be used in correlation equations to automatically calculate Reid Vapor Pressure, ASTM D 86, ASTM D 1160, API gravity, flash point, viscosity, and freeze point. In addition, the capability to "profile" several chromatograms for direct visual comparison has been developed and added to the system. Other analytical techniques, such as NMR, were evaluated for their possible contribution to this correlation development.
The work reported herein was conducted at the U.S. Army Fuels and Lubricants Research Laboratory (AFLRL), Southwest Research Institute, San Antonio, TX, under Contracts DAAK70-80-C-0001 and DAAK70-82-C-0001 during the period August 1980 through December 1981. The work was funded by the U.S. Army Mobility Equipment Research and Development Command (MERADCOM), Ft. Belvoir, VA. Contracting Officer's representative was Mr. F.W. Schaekel, Fuels and Lubricants Division, Energy and Water Resources Laboratory (DRDME-GL). Project technical monitor was Mr. M.E. LePera, MERADCOM, DRDME-GL.
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I. INTRODUCTION

As part of the major thrust within the Alternative and Synthetic Fuels Program, the Department of Defense (DOD) specified in late 1979 a task to "develop more efficient military fuel qualification procedures to effect capacity to react quickly to changes encountered in the petroleum refining industry." The normal time required for qualification of a new fuel for the engine and powerplant accessory systems is approximately 5 to 8 years. As an example, the transition to unleaded gasoline within the Department of the Army took 4 to 5 years.(1)* As shown in Figure 1, the first step in evaluating and qualifying new/modified fuels involves both laboratory characterization and specification testing.

![Diagram of process for evaluating new/synthetic fuels]

* Underscored number in parentheses refer to the list of references at the end of this report.
Fuel characterization is an important consideration for effective spark ignition, compression ignition, and turbine engine fuel utilization. Military mobility equipment depends upon fuels which provide reliable vehicle operation and performance. Military and federal specifications are designed to help control fuel quality for government use by providing the refiner with a guide which aids in producing an acceptable product. Specifications serve this purpose by listing physical and chemical fuel properties provided with maximum and/or minimum data value requirements which a fuel must meet. Table 1 provides a summary of properties and Specification (VV-F-800C) (2) limits for diesel fuels which are used to fuel the majority of Army ground tactical/combat vehicles.

As new fuels are introduced, it becomes necessary to characterize them by applying the available standard test methods and chemical/physical characterization techniques. The standard test methods are both costly and time consuming. When the candidate fuel has been defined by the standard tests, it can then be used in actual engine test stand operation to determine its engine performance characteristics. Engine test stand operation is very costly. At times, the use of a new fuel not previously screened for deleterious properties, can lead to serious engine malfunctions requiring extensive and expensive engine overhaul.

The objectives of this program are (1) to define those fuel properties and characteristics which are the most significant with regard to engine performance, and (2) to attempt to determine those fuel properties and characteristics from a minimum amount of laboratory analytical data through the use of correlation techniques. This report presents the initial results of this program.
TABLE 1. SUMMARY OF PROPERTIES AND SPECIFICATION LIMITS IN FEDERAL SPECIFICATION VV-F-800C FOR DIESEL FUELS

<table>
<thead>
<tr>
<th>Properties</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, kg/L @15°C</td>
<td>Report</td>
</tr>
<tr>
<td>Flash point, °C min</td>
<td>38</td>
</tr>
<tr>
<td>Cloud point, °C max</td>
<td>-51</td>
</tr>
<tr>
<td>Pour point, °C max</td>
<td>Report</td>
</tr>
<tr>
<td>Kinematic viscosity @40°C</td>
<td>1.1 to 2.4</td>
</tr>
<tr>
<td>Distillation, °C:</td>
<td>Report</td>
</tr>
<tr>
<td>50% evaporated</td>
<td>288</td>
</tr>
<tr>
<td>90% evaporated, max</td>
<td>300</td>
</tr>
<tr>
<td>End point, max</td>
<td>3</td>
</tr>
<tr>
<td>Residue, vol%, max</td>
<td>3</td>
</tr>
<tr>
<td>Carbon residue on 10% bottoms, mass %, max</td>
<td>0.10</td>
</tr>
<tr>
<td>Sulfur, mass %, max</td>
<td>0.25</td>
</tr>
<tr>
<td>Copper strip corrosion, 3 hrs. @ 50°C</td>
<td>3</td>
</tr>
<tr>
<td>Ash, mass %, max</td>
<td>0.01</td>
</tr>
<tr>
<td>Accelerated stability, total insolubles</td>
<td>1.5</td>
</tr>
<tr>
<td>mg/100 mL, max</td>
<td>1.5</td>
</tr>
<tr>
<td>Neutralization number, TAN, max</td>
<td>0.05</td>
</tr>
<tr>
<td>Particulate contamination, mg/liter, max</td>
<td>10</td>
</tr>
<tr>
<td>Cetane number, min</td>
<td>40</td>
</tr>
</tbody>
</table>

1/ DF-2 intended for entry into the Central European Pipeline System shall have a minimum value of 58°C.

2/ As specified by the procuring activity based on guidance in Appendix A of the Specification. DF-2 for Europe and S. Korea have a maximum limit of minus 13°C.

3/ As specified by the procuring activity. DF-2 for Europe and S. Korea shall have a maximum limit of minus 18°C.

4/ See Appendix B of the Specification. If the fuel contains cetane improvers, the test must be performed on the base fuel blend only.

5/ This requirement is applicable only for military bulk deliveries intended for tactical, OCONUS, or long-term storage (greater than 6 months) applications (i.e., Army depots, etc.).
II. BACKGROUND

Considerable effort has been expended by many researchers to fully identify all the compounds present in petroleum products. Early work by API Project 44 attempted separation and identification by careful distillation and purification. Beginning in the early 1940's, the use of ultraviolet/visible and infrared spectroscopy gave additional insight into the complex structure of fuels.

The advent of gas chromatography (GC)* presented new opportunities and opened new approaches,(3) but the many primary compounds with their isomers were not well resolved, and identification of all components continued to be elusive. High-resolution GC with both Support Coated Open Tubular (SCOT) and Wall Coated Open Tubular (WCOT) capillary columns showed that resolution of most compounds in the gasoline range could indeed be accomplished, but identification proved to be an insurmountable task because standard compounds of required purity did not exist for a sufficient number of components to produce detailed results. In addition, the large volume of data involved became a monumental task for reduction and presentation. The refinement and maturation of GC coupled to rapid mass spectrometers (GC/MS) made identification of the hundreds of components appear to be attainable. Employment of other specific detectors such as those which each respond to sulfur, nitrogen, and aromatics further enhanced the possibility of confirming compound identification. The recent use of nuclear magnetic resonance spectrometers as an analytical tool in fuel chemistry has enabled an even closer look into the structure of the many compounds present in a fuel.

Two technical advances have now made this highly desirable goal of complete identification approach a reasonable and attainable level. The widespread use of digital computers as controllers and data processors for analytical instrumentation has increased the capability of the analytical laboratory to handle the mass of data generated by sophisticated instrumental analyses.

Also, the improved system stability and performance of the hardware make more reliable data possible.

In 1979, a study was initiated at the U.S. Army Fuels and Lubricants Research Laboratory (AFLRL) to determine the feasibility of combining traditional analytical/chemical instrumentation, engine, and laboratory bench tests into a concise analytical methodology, and from a minimal quantity of compositional and physical data, characterize a substance in terms of its performance as a fuel.

In support of this effort, literature pertaining to physical and chemical methods of characterizing fuels has been reviewed. During this review, it was noted that most physical/chemical fuel properties must be determined directly. However, data for some properties could be calculated using correlative methods. (4,5) A correlative method is an analytical method by which a property can be mathematically determined by using data directly obtained for another property. For example, data from ASTM D 2887 (Boiling Range Distribution of Petroleum Fractions by Gas Chromatography) and ASTM D 3710 (Boiling Range Distribution of Gasoline and Gasoline Fractions by Gas Chromatography) can be used to calculate data for Reid Vapor Pressure and ASTM D 86 (Distillation of Petroleum Products) through mathematical correlation.

As a result of this effort, a report (6) was published providing a reference tabulation of over 100 physical and chemical fuel properties, chemical compounds, and compound classes identified during the literature review along with brief outlines of literature-derived methods for their determination. Methods not treated extensively in this review are developmental methods used primarily in areas of research and development such as fuel lubricity, elastomer compatibility, fuel stability, fleet testing, etc. Many methods of this type are not yet standardized, and various approaches using these methods have been and are being used in fuels and fuels-related research. A great deal of literature exists which discusses these developmental procedures' applications and results in detail. (7-14) Other reports in this general methodology development area at AFLRL have been prepared. (15-17)
III. APPROACH

Another result of the literature survey leading to development of the review discussed in the Introduction (Reference 6), was a directive to evaluate traditional analytical chemical instrument, engine, wet chemical, and bench tests as to their effectiveness in accurately determining physical and chemical fuel properties. Then, by selecting critical fuel-definitive properties, analytical techniques can be developed which will correlate these critical properties with fuel composition and other predetermined physical properties at a high level of confidence by the application of mathematical models.

The literature review afforded various test methods for the determination of over 100 fuel properties calling for utilization of analytical chemical instruments (chromatographs, spectrophotometers, etc.), engines, and bench apparatus. From the review, it appeared that a sophisticated gas chromatographic technique should be explored in a correlative approach to defining fuel physical/chemical properties. The use of external calibration, multicolumns and multidetectors could potentially provide mapping of petroleum and synthetic fuels correlatable to known or definable properties. While this task will not be easily accomplished because of its complexity, the extent of identification will improve with time as the details of the methodology are developed.

IV. DISCUSSION

Several vendors marketing gas chromatographic equipment with the high level of sophistication needed were contacted. After a thorough review and evaluation with consideration toward interfacing with data-handling systems already in-house, it was decided that Hewlett-Packard's 5880A Gas Chromatographic System was the best fit (Figure 2). The 5880A gas chromatograph can contain level 4 BASIC programming, allowing preprogrammed calculation procedures, with access to the GC report information to permit further automatic processing of the GC information. In addition, it has the ability to totally control all GC variables through the use of microprocessors. It can utilize dual capillary columns with the latest innovations in sampling
techniques, and is capable of housing up to four detectors. This multi-detector capability permits the use of selective detectors to minimize downtime for switching between them. The 5880A GC can have Hewlett-Packard's proven cartridge tape unit as a built-in feature. This would provide mass storage for analytical programs, calibration tables, reports, keystroke, and BASIC programs.

The instrumentation purchased incorporates several detectors capable of yielding component and/or element specific information. The capability of detailed composition fingerprinting of the neat fuel as well as the nitrogen and sulfur-containing components and aromatic components will aid in developing correlation of performance properties of experimental and test fuels with the performance properties of known fuels.

Other analytical techniques which would add to the ability to characterize a fuel were developed prior to the installation and operation of the H-P 5880A GC equipment. An infrared technique for the determination of oxygenate concentration of gasoline/oxygenate blends was developed and evaluated. (22) This method proved to be both qualitative and quantitative with a high potential for speed, low cost, and specificity. Additionally, a rapid and inexpensive ultraviolet spectroscopic method for determining the aromaticity of turbine and diesel fuels has been developed. (23) The method yields weight percent ring carbon in substituted benzenes, naphthalenes, and phenanthrenes/anthracenes. The precision and accuracy of the method are good for both standards and fuel blends. The method is currently in use for correlation work for both turbine combustors and diesel engines.

Initially, eight fuels that had previously undergone extensive analyses, and about which much information was available, were selected as a base from which correlative methods might be developed (Table 2). These fuels were derived from a variety of sources, i.e., petroleum, shale, tar sand, and covered turbine and diesel operation. They appeared to be stable over relatively long-term storage conditions, and so could be used over a period of time as an analytical base with a very low probability of changing or degrading.
FIGURE 2. GAS CHROMATOGRAPH SYSTEM FOR DEVELOPMENT OF METHODOLOGY FOR FUEL CHARACTERIZATION
### TABLE 2. STANDARD BASE TEST FUELS

<table>
<thead>
<tr>
<th>Code Number</th>
<th>Type</th>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL-8436-F</td>
<td>JP-5</td>
<td>MIL-T-5624L</td>
<td>Shale-Paraho-II</td>
</tr>
<tr>
<td>AL-6354-T</td>
<td>JP-5</td>
<td>MIL-T-5624L</td>
<td>Tarsand</td>
</tr>
<tr>
<td>AL-6526-T</td>
<td>JP-5</td>
<td>MIL-T-5624L</td>
<td>Shale</td>
</tr>
<tr>
<td>AL-7247-T</td>
<td>JP-5</td>
<td>MIL-T-5624L</td>
<td>Petroleum</td>
</tr>
<tr>
<td>AL-9089-SP</td>
<td>JP-8</td>
<td>MIL-T-83133</td>
<td>Shale-Paraho-II</td>
</tr>
<tr>
<td>AL-8907-F</td>
<td>JP-8</td>
<td>MIL-T-83133</td>
<td>Petroleum</td>
</tr>
<tr>
<td>AL-8437-F</td>
<td>DFM</td>
<td>MIL-F-16884G</td>
<td>Shale-Paraho-II</td>
</tr>
<tr>
<td>AL-9847-SP-T</td>
<td>JP-4</td>
<td>MIL-T-5624L</td>
<td>Shale-Geokinetics</td>
</tr>
</tbody>
</table>

High Performance Liquid Chromatography (HPLC) was used to effectively separate the saturates from the olefinic, heteroatomic, and aromatic components of each of the eight test fuels (Figure 3). The separations were clean with only a minimum amount of solvent carryover in some cases. (19)

Each of the eight test fuels and their saturate and aromatic/polar fractions obtained by HPLC fractionation, were analyzed by conventional, packed column GC utilizing flame ionization detectors for ASTM D 2887, "Boiling Range Distribution of Petroleum Fractions by Gas Chromatography" (BPD) (24) (Figures 4, 5, and 6). Table 3 gives the operating parameters for this method using Hewlett-Packard 5711 gas chromatograph. These data were stored on disc in the Hewlett-Packard 3354B/C Laboratory Data System computer used for calculating the boiling point distribution.
FIGURE 3. HPLC SEPARATION OF SATURATES AND AROMATIC/POLAR FRACTIONS OF PETROLEUM JP-5
FIGURE 4. ASTM D 2887 BOILING POINT DISTRIBUTION OF PETROLEUM JP-5
FIGURE 5. ASTM D 2887 BOILING POINT DISTRIBUTION OF AROMATIC/POLAR FRACTION PETROLEUM JP-5
TABLE 3. OPERATING PARAMETERS
HEWLETT-PACKARD 5711 GAS CHROMATOGRAPH

Sample Size: 1 microliter
Flow Rate: 25 cc/min Helium

DETECTOR

Flame Ionization:
Temperature: 400°C
Hydrogen: 35 cc/min
Air: 360 cc/min
Helium (makeup): 25 cc/min

OVEN TEMPERATURE

Programmed: 0° to 390°C
Rate: 16°C/min
Initial Hold: 0 minutes
Final Hold: 4 minutes

DATA PROCESSING

Hewlett-Packard 3354 Laboratory Data System

COLUMN

6 ft x 1/3 inch SS, 5% SE-30 on Chromosorb G,
AW-DMCS, 80/100 mesh

In addition to the neat fuels, aliphatic and aromatic/polar fractions of each of the fuel samples were analyzed by high-resolution-capillary column GC, and their "fingerprint" patterns were obtained; examples of which are given in Figures 7, 8, and 9. The analyses were performed utilizing flame ionization (in Figures 7-9) and nitrogen-specific detectors. Table 4 gives the operating parameters for this process. The chromatographic data obtained were stored on data cartridges for future use in component identification and correlations.

Boiling point distribution is the predominant analytical method used in the characterization of a fuel. The ASTM D 2887 Boiling Point Distribution (BPD) method utilizes conventional, packed column, low-resolution GC. This method does not yield detailed component or element specific information.
| OPERATING PARAMETERS--  |
|________________________|
| HEWLETT-PACKARD 5880A GAS CHROMATOGRAPH DUAL CAPILLARY COLUMNS--  |
| HIGH RESOLUTION  |

Sample Size: 1 microliter  
Split Ratio: 200:1  
Flow Rate (Linear Velocity) 17.4 cm/sec Helium  
Injector Temperature: 350°C

**DETECTORS**

<table>
<thead>
<tr>
<th>Flame Ionization:</th>
<th>Nitrogen/Phosphorus:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature: 400°C</td>
<td>Temperature: 400°C</td>
</tr>
<tr>
<td>Hydrogen: 30 cc/min</td>
<td>Hydrogen: 3 cc/min</td>
</tr>
<tr>
<td>Air: 350 cc/min</td>
<td>Air: 100 cc/min</td>
</tr>
<tr>
<td>Helium (makeup): 25 cc/min</td>
<td>Element Power: 100 (Zero=16)</td>
</tr>
<tr>
<td></td>
<td>Helium (makeup): 25 cc/min</td>
</tr>
</tbody>
</table>

**OVEN TEMPERATURE**

<table>
<thead>
<tr>
<th>Programmed: 0° to 200°C</th>
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</thead>
<tbody>
<tr>
<td>Rate 1: 4°/min</td>
</tr>
<tr>
<td>Initial Hold: 1 min</td>
</tr>
<tr>
<td>Final Hold: 0.1 min</td>
</tr>
<tr>
<td>Rate 2: 25°/min</td>
</tr>
<tr>
<td>Final Temperature: 320°</td>
</tr>
<tr>
<td>Final Hold: 15 min</td>
</tr>
</tbody>
</table>

**DATA PROCESSING**

H-P 5880 Lab Basic  
Norm % Compensated Analysis

**COLUMNS**

1 and 2: SE-54, 50 meter x 0.3 mm ID Fused Silica Capillary Column

---

It would be advantageous if a D 2887 BPD could be obtained from a chromatographic analysis that was capable of yielding some component and/or element specific information at the same time. Earlier attempts to develop such a technique were unsuccessful because of chromatographic data storage limitations. This technique yields data for several hundred individual components in a fuel, and this data, together with the programming necessary for D 2887, exceeds the memory capacity of the Level 4 HP 5880 Gas Chromatograph.
FIGURE 7. HIGH-RESOLUTION CAPILLARY COLUMN GC "FINGERPRINT" OF PETROLEUM JP-5
<table>
<thead>
<tr>
<th>OT</th>
<th>AREA</th>
<th>TYPE CAL</th>
<th>AMOUNT</th>
<th>NAME</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.15</td>
<td>7.79</td>
<td>BV</td>
<td>4 1.7614E-05 H-C4</td>
<td></td>
</tr>
<tr>
<td>5.79</td>
<td>6.65</td>
<td>BV</td>
<td>1.8444E-02 H-C6</td>
<td></td>
</tr>
<tr>
<td>5.94</td>
<td>5.25</td>
<td>BV</td>
<td>4 1.0645E-04 C6</td>
<td></td>
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<tr>
<td>9.90</td>
<td>23.32</td>
<td>BV</td>
<td>1.5934E-02 C6</td>
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</tr>
<tr>
<td>11.47</td>
<td>3.83</td>
<td>BV</td>
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FIGURE 8. HIGH-RESOLUTION CAPILLARY COLUMN GC "FINGERPRINT" OF AROMATICS/POLAR FRACTION OF PETROLEUM JP-5
### FIGURE 8. HIGH-RESOLUTION CAPILLARY COLUMN GC "FINGERPRINT" OF AROMATICS/POLAR FRACTION OF PETROLEUM JP-5 (CONT'D)

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**Figure 9.** High-Resolution Capillary Column GC "FingerPrint" of Saturate Fraction From Petroleum JP-5 (Cont'd)
A medium resolution chromatographic analysis was successfully developed. The operating parameters are shown in Table 5. The BPD reported by this technique is in close agreement with the BPD reported by the conventional D 2887 technique (Figures 10 and 10a, respectively). Figure 11 graphically illustrates the close agreement between the conventional and medium resolution D 2887 techniques. In addition, it can yield component and/or element specific information, however, not quite to the extent of a high-resolution analysis (as in Table 4). Note that the GC Distillation Report in Figure 10 is based on Boiling-Point Distribution by Gas Chromatography (BPDGC) software upgrade as presented in an earlier report.(25)

### TABLE 5. OPERATING PARAMETERS--
HEWLETT-PACKARD 5880A GAS CHROMATOGRAPH DUAL CAPILLARY COLUMN--
MEDIUM RESOLUTION

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<td>Simulated Distillation-D 2887 Software</td>
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<td>Figure 10--H-P-3354 Laboratory Data System</td>
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GC DISTILLATION REPORT

CHANNEL # 3
REPORT # 13
SAMPLE: AL-7247-T-II
INJECTED AT: 13:14:56 ON APR 10, 1981
FID DETECTOR EXTERNAL CALIBRATION
METHOD : SD/FUL SEQ : *SEQ03
PROC DATA FILE: *PRC03 RAW DATA FILE: *RAW03

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INT. STD. = 0 %

STANDARD RESPONSE FACTOR = 1
SAMPLE RESPONSE FACTOR = 1

FIGURE 10. D 2887 GC DISTILLATION REPORT BY CONVENTIONAL SIMULATED DISTILLATION

27
**FIGURE 10a. D 2887 GC DISTILLATION REPORT BY MODIFIED SIMULATED DISTILLATION**
For ease in comparing the standard ASTM D 2887 and two modified D 2887 capillary column techniques (Tables 4 and 5), Figure 12 provides a plot of Kovats Indices ($I_R$) versus retention time for the n-saturates. The conditions in Table 5 appear to provide peak resolution comparable to, but somewhat improved over those currently in use at the Aero Propulsion Laboratory where similar fuels are being investigated.
In addition to calculating the ASTM D 2887 BPD, the program is capable of reporting the correlation to ASTM D 86, "Distillation of Petroleum Products" (wide range) or ASTM D 1160, "Distillation of Petroleum Products at Reduced Pressure" (Table 6).

Equations for calculating the correlation of the modified D 2887 BPD to Reid Vapor Pressure (RVP) have been developed (28), but require some refining to bring the results into agreement with experimental results (Table 6). Other correlations have been developed equating the D 2887 BPD data to "API gravity, flash point, and viscosity."(4) However, the application of these correlation equations requires some additional refinement of the constants and selected data points to allow their use.
Analysis by proton ($^1$H) and carbon-13 ($^{13}$C) nuclear magnetic resonance (NMR) was explored to determine if NMR can be a useful technique in the characterization of fuels. Samples of the eight test fuels were sent to a commercial laboratory for this analysis. Interpretation of the spectral data along with UV aromaticity, BPD for carbon number range and molecular weight were expected to yield percent CH$_3$, CH$_2$, CH, aromatic carbon, amount of substitution on aromatic rings, number of fused rings, length of side chains, and degree of branching. Since no standard data requirements existed, considerable effort was expended in establishing the most dependable and significant values to report as shown in Table 7.(29) However, examination of the NMR analytical data of the eight test fuels showed significant differences compared to the results of the standard analytical procedures for aromatic and aliphatic compounds in Table 8, and no immediate benefit could be derived from the use of this technique.
### TABLE 7. MOLE PERCENT CARBON AND HYDROCARBON DISTRIBUTIONS USING NMR

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<tr>
<th>Sample</th>
<th>Aromatic</th>
<th>Aliphatic</th>
<th>Protonated Aromatic</th>
<th>Substituted Aromatic</th>
<th>n-Paraffin</th>
<th>Cyclo Paraffins</th>
<th>Aromatic</th>
<th>Aliphatic</th>
<th>CH&lt;sub&gt;x&lt;/sub&gt; O</th>
<th>CH&lt;sub&gt;2&lt;/sub&gt;</th>
<th>CH&lt;sub&gt;3&lt;/sub&gt;</th>
<th>( \phi )</th>
<th>Average n-Paraffin Chain Length (N C)</th>
<th>CH&lt;sub&gt;3&lt;/sub&gt;/CH&lt;sub&gt;2&lt;/sub&gt;</th>
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<td>54.7</td>
<td>32.7</td>
<td>0.43</td>
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<td>84.5</td>
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<td>7.6</td>
<td>33.9</td>
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<td>3.9</td>
<td>96.1</td>
<td>8.0</td>
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<td>0.49</td>
<td>12.5</td>
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<td>8907-F</td>
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<td>93.4</td>
<td>3.6</td>
<td>3.0</td>
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<td>56.9</td>
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<td>8.8</td>
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1. \( \phi \) - That fraction of aromatic edge atoms which are substituted.
2. This sample contains some olefins (0.4% olefinic hydrogen distribution).
<table>
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<tr>
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<th>8437-F</th>
<th>8907-F</th>
<th>9089-SP</th>
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(1) Wt% Aromatic Ring Carbon; net volume of aromatic hydrocarbon, see Reference 23.
* Fluorescent Indicator Absorption (ASTM D 1319).
** Includes Olefins.

Table 9 lists the chemical/physical properties initially explored for compatibility with correlative methods. These properties rank high in importance in determining a fuel's properties and have been the subject of considerable exploratory correlative work. (4)

The problem of analyses comparison is frequently encountered in gas and liquid chromatography, e.g., when a comparison of the analytical results of
TABLE 9. CHEMICAL/PHYSICAL PROPERTIES:
INITIAL CANDIDATES FOR CORRELATION TECHNIQUES
UTILIZING D 2887 DATA

- D 86 Correlation
- Reid Vapor Pressure Correlation
- Degrees API Correlation
- Flash Point Correlation
- Viscosity Correlation
- Freezing Point Correlation

the fractions of a chromatographic run is required, or a survey of the
concentration distribution of a chemical substance over several samples
would be advantageous. In these and other fields of application, a visual
display of the results can be a useful aid when drawing conclusions con-
cerning the chemical differences between similar samples with differing
physical parameters.

In order to obtain this type of data, the Hewlett-Packard 3354B/C Laboratory
Data System was updated to allow the use of graphics terminals for obtaining
"profiled" plots of multiple chromatographic analyses. The necessary pro-
gramming was entered and stored in the computer memory. A graphics CRT
terminal and printer were utilized to test the profiling capability. The
results were conditionally successful. Because of the large size of the
program, it must be divided into several programs, all linked together.
Figure 13 is an example of the results which can be achieved when four
chromatograms (in this case for four different JP-5 samples) are profiled
for comparison.
V. CURRENT STATUS

As stated previously, boiling point distribution by gas chromatography in a sophisticated mode appears to be the method of choice in establishing a number of correlations to individually determined experimental values.

The modified ASTM D 2887 method employing capillary columns yields BPD data consistent with the conventional packed column method. In addition, it is capable of giving component identification data and data to perform mathematical correlations. The equations for calculating the correlation to RVP, D 86, D 1160, "API gravity, flash point, and viscosity have been determined. However, in some cases, the constants and/or the data points used need adjustment to bring the results into closer agreement with the experimentally derived results.

Initial attempts to generate a "profiled" gas chromatogram of several similar fuels from different sources using graphics computer terminals has been successful. However, the programming requires some additional refining.

A gas chromatographic method for performing detailed component analysis, or "fingerprinting", of fuels utilizing fused silica capillary columns, temperature programming with subambient temperature capability, and selective detectors has been developed. Initial work has been performed with a flame ionization detector (FID) for a complete hydrocarbon presentation and some limited work with a nitrogen-phosphorus sensitive detector (NPD) to look at only those components containing nitrogen.

More than 40 compound identifications have been made with the FID system. To date, no work has been initiated toward identifying the nitrogen-containing compounds. Additionally, while a UV specific detector has been installed, no work has been done to demonstrate the specificity of this detector for aromatics. The need for a sulfur detector has been identified, but has yet to be purchased, installed, or demonstrated.

VI. CONCLUSIONS AND RECOMMENDATIONS

Development of a modified D 2887 boiling point distribution method to yield
component specific identification in addition to BPD consistent with the conventional D 2887 method has been successful. The modified D 2887 uses fused-silica capillary columns and will be capable of supplying the data necessary to calculate automatically correlations to RVP, ASTM D 86, D 1160, °API gravity, flash point, and viscosity already under investigation. These correlations, together with the method for "fingerprint" or more detailed chromatographic analysis of fuels, other correlations such as freezing point, and the capability to "profile" several chromatograms for direct visual comparison, can prove to be a very powerful tool in the characterization of candidate fuels with a minimal amount of laboratory analytical testing, thus effectively complementing the testing of candidate fuels both in the laboratory and by actual engine testing.

With the exception of the modified ASTM D 2887 boiling point distribution method discussed earlier, most of the work reported is in the initial stages of development. The sophisticated gas chromatographic instrumentation necessary for the approach taken was delivered in mid-March 1981 and required installation and check-out. The graphics computer terminals and computer programs necessary for profiling were not available until late September 1981, and are not dedicated to the GC system.

Because the key to the development of correlations and profiling was a form of ASTM D 2887, which would yield acceptable BPD data and the capability of component identification, emphasis was placed on the development of a modified ASTM D 2887 method and the development of a gas chromatographic method for obtaining detailed "fingerprints" of fuels. Work on the development of correlations and profiling did not start until September 1981.

The indications are that the development of correlations from BPD data is a viable and practical approach. Therefore, it is recommended that:

(1) Efforts to refine the correlation equations already developed for RVP, °API, flash point, and viscosity to bring them into closer agreement with experimental results should be continued, but with an expanded set of sample fuels covering a broader boiling point range. This expanded set of sample fuels should be sufficiently large to establish a fuel
identification approach similar to that in Reference 30.

(2) The development of correlations for other characteristic parameters such as freezing point should be investigated.

(3) A quantitative sample introduction approach should be investigated which may allow external calibration for calculation of heat of combustion, noncombustible components, etc.

(4) The development of the use of computer-assisted chromatogram profiling should be continued to include dedicated use of graphics terminals, both CRT type and plotting type. This would allow the generation of this type of reporting data to be effectively utilized.

(5) The modified ASTM D 2887 method should be expanded and demonstrated using property specific detectors to include nitrogen, sulfur, and the aromatic sensitive UV detector. Thermal conductivity detectors should be evaluated as to their ability to provide volumetric rather than gravimetric data as does the FID for lower boiling materials.

(6) The use of other instrumentation such as GC/MS, HPLC, IR, and UV/VIS, and NMR should be explored further to determine what additional contributions each might be able to make toward the expanded/rapid characterization of fuels.

(7) Expand collaborative effort with other Federal/Military Laboratories developing glass capillary gas chromatographic methods for characterizing military fuels.

(8) Expand analytical approach, where necessary, to assure program is in concert with and applicable to the emerging AIRLAND 2000 Battle Concept (31), which places emphasis on use of other than just conventional fossil fuels.
VII. LIST OF REFERENCES


CDR US ARMY MATERIEL ARMAMENT READINESS CMD ATTN DRSAR-LEM ROCK ISLAND ARSENAL IL 61299

CDR US ARMY COLD REGION TEST CENTER ATTN STECR-TA APO SEATTLE 98733
HQ, DEPT. OF ARMY ATTN: DAEW-RDZ-B WASHINGTON, DC 20310

CDR US ARMY RES & STDZN GROUP (EUROPE) ATTN DRXSN-UK-RA BOX 65 FPO NEW YORK 09510
HQ, US ARMY AVIATION R&D CMD ATTN DRDAV-GT (MR R LEWIS) DRDAV-D (MR CRAWFORD) DRDAV-N (MR BORGMAN) DRDAV-E 4300 GOODEFELLOW BLVD ST LOUIS MO 63120

CDR US ARMY FORCES COMMAND ATTN AFLG-REG AFLG-POP FORT MCPHERSON GA 30330

CDR US ARMY ABERDEEN PROVING GROUND ATTN: STEAP-MT-U (MR DEAVER) ABERDEEN PROVING GROUND MD 21005

CDR US ARMY YUMA PROVING GROUND ATTN STEYP-MT (MR DOEBBLER) YUMA AZ 85364

MICHIGAN ARMY MISSILE PLANT OFC OF PROJ MGR, ABRAMS TANK SYS ATTN DRCPM-GCM-S WARREN MI 48090

MICHIGAN ARMY MISSILE PLANT PROJ MGR, FIGHTING VEHICLE SYS ATTN DRCPM-FVS-SE WARREN MI 48090

PROJ MGR, M60 TANK DEVELOPMENT USMC-LNO, MAJ. VARELLA US ARMY TANK-AUTOMOTIVE CMD (TACOM) WARREN MI 48090

PROJ MGR, M113/M113A1 FAMILY OF VEHICLES ATTN DRCPM-M113 WARREN MI 48090

PROJ MGR, MOBILE ELECTRIC POWER ATTN DRCPM-MEP-T 7500 BACKLICK ROAD SPRINGFIELD VA 22150

OFC OF PROJ MGR, IMPROVED TOW VEHICLE US ARMY TANK-AUTOMOTIVE R&D CMD ATTN DRCPM-ITV-T WARREN MI 48090

CDR US ARMY EUROPE & SEVENTH ARMY ATTN AEAGC-FMD APO NY 09403

PROJ MGR, PATRIOT PROJ OFC ATTN DRCPM-MD-T-G US ARMY DARCOM REDSTONE ARSENAL AL 35809

CDR THEATER ARMY MATERIAL MGMT CENTER (200TH) DIRECTORATE FOR PETROL MGMT ATTN AEAGD-MM-PI-Q (MR PINZOLA) ZWIEBRUCKEN APO NY 09052

CDR US ARMY RESEARCH OFC ATTN DRXRO-2C DRXRO-EG (DR SINGLETON) DRXRO-CB (DR CHIRARDELLI) P O BOX 12211 RSCH TRIANGLE PARK NC 27709

12/81 AFLRL No. 153 Page 2 of 5
DIR
US ARMY AVIATION R&T LAB (AVRADCOM)
ATTN DAVDL-AS (MR D WILSTEAD) 1
NASA/AMES RSCH CTR
MAIL STP 207-5
MOFFIT FIELD CA 94035

CDR
TOBYHANNA ARMY DEPOT
ATTN SDSTO-TP-S 1
TOBYHANNA PA 18466

DIR
US ARMY MATERIALS & MECHANICS
RSCH CTR
ATTN DRXMR-EM 1
DRXMR-R 1
DRXMR-T 1
WATERTOWN MA 02172

CDR
US ARMY DEPOT SYSTEMS CMD
ATTN DRSDS 1
CHAMBERSBURG PA 17201

CDR
US ARMY WATERVLIET ARSENAL
ATTN SARWY-RDD 1
WATERVLIET NY 12189

CDR
US ARMY LEA
ATTN DALO-LEP 1
NEW CUMBERLAND ARMY DEPOT
NEW CUMBERLAND PA 17070

CDR
US ARMY GENERAL MATERIAL &
PETROLEUM ACTIVITY
ATTN STSGP-PW (MR PRICE) 1
SHARPE ARMY DEPOT
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CDR
US ARMY FOREIGN SCIENCE & TECH
CENTER
ATTN DRXST-MT1 1
FEDERAL BLDG
CHARLOTTESVILLE VA 22901

CDR
DARCOM MATERIEL READINESS
SUPPORT ACTIVITY (MRSA)
ATTN DRXMD-MD 1
LEXINGTON KY 40511

HQ, US ARMY T&E COMMAND
ATTN DRSTE-TO-O 1
ABERDEEN PROVING GROUND, MD 21005

HQ, US ARMY ARMAMENT R&D CMD
ATTN DRDAR-LC 1
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HQ, US ARMY TROOP SUPPORT &
AVIATION MATERIAL READINESS
COMMAND
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4300 GOODFELLOW BLVD
ST LOUIS MO 63120

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P O BOX 4005
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BALLISTIC RESEARCH LAB
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PROPULSION LABORATORY
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21000 BROOKPARK ROAD
CLEVELAND OH 44135

CDR
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ATTN DRDNA-YEP (DR KAPLAN) 1
NATICK MA 01760

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ATTN ATSP-CD-MS 1
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ATSM-CDM 1
ATSM-TNG-PT 1
FORT LEE VA 23801

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CDR
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CODE 2830 (MR G BOSMAJIAN) 1
CODE 2831 1
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JOINT OIL ANALYSIS PROGRAM -
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PENSACOLA FL 32508

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CDR, NAVAL MATERIEL COMMAND
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MAT-08E (MR ZIEM) 1
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