Evaluation of Pure Hydrocarbons as Jet Fuels

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AIRCRAFT traveling at supersonic speeds require fuels with a greater heat sink capacity than that offered by petroleum fuels in current use because of the aerodynamic heating attendant with such speeds. The heat generated at subsonic flight speeds is readily dissipated by air cooling. At supersonic speeds, however, the rate of heat dissipation is inadequate. Fuels that can absorb this extra heat without undergoing adverse chemical change offer an answer to this cooling problem. The requirements for such fuels are thermal stability, good combustion characteristics, closely defined properties, and the best low temperature properties possible, commensurate with the first three requisites.

A thermally stable fuel would not decompose at the high temperatures caused by supersonic speed and thus would not form deposits that would hamper fuel pumping and vaporizing systems.

High heat of combustion means high energy release which increases flight range or payload.

Close definition of properties refers to the reproducibility of properties by whatever method the fuel is produced and to careful minimization of contaminants. Impurities such as nitrogen and sulfur compounds will adversely affect the thermal stability of the fuel by causing deposit formation.

Good low temperature properties, that is, low freezing point and low viscosity, are required for cold-climate, trouble-free performance in the fuel pumping system, effective atomization in fuel nozzles, and also for effective heat transfer in the cooling process.

This investigation has as its over-all objective, the synthesis and evaluation of various classes of saturated hydrocarbons for potential jet fuel use. The evaluation program is concerned with the determination of properties required for such fuels. The actual selection of fuels, however, is the responsibility of the U. S. Air Force. Also, the results of this study should be of value to the petroleum refiner in refining and blending operations toward the selection of the most promising hydrocarbon types for jet fuel application. Finally, an important adjunct of this program has been the determination of basic properties of saturated hydrocarbons.

The evaluation of 38 saturated hydrocarbons is presented as part of a continuing study.

RESULTS AND DISCUSSION

Synthesis Program. The saturated hydrocarbons involved in this program were selected as representative of the following classes: acyclics, monocyclics, bicyclics—both condensed and isolated ring systems, and polycyclics—both condensed and isolated ring systems.

Of the 38 compounds studied, 24 were synthesized in this laboratory. In general, commercial feasibility from the standpoint of availability of raw materials and synthetic methods has governed the synthesis program. Reactions used to prepare the aromatic or unsaturated precursors included Friedel-Crafts alkylations and acylations, acid-catalyzed condensations, Diels-Alder additions, Grignard additions, and bimolecular reductions. The aromatic and unsaturated precursors were reduced over a nickel catalyst at high pressure and carefully fractionated before evaluation.

In most cases stereomeric mixtures were not separated because of the inherent difficulties involved. In some cases position isomers were not separated since such mixtures would result from commercial processes and remain liquids at lower temperatures than the pure isomers.

Purity estimation of the compounds studied was effected by vapor phase chromatography and infrared and ultraviolet spectrophotometry. The estimated purities, reported in vapor phase chromatography as area per cent, are given in Table I. Over 80% of the compounds studied possessed purities greater than 98 area % with a minimum of 93.5 area % observed.

For the 24 compounds synthesized in this laboratory, knowledge of the synthetic routes was an important purity criterion. Because of the nature of their preparation, these compounds were virtually free of sulfur, nitrogen, and halides. High pressure reduction over a nickel catalyst removed traces of sulfur compounds; the synthetic methods did not employ nitrogen-containing compounds; and negative Beilstein tests indicated halogen content of less than 5 p.p.m. (*3*).

The synthesis program included some compounds of unusual structure, the preparation of which until recently would have prohibited their consideration as potential fuels. Cyclododecane (I) is conveniently prepared in two steps; butadiene is trimerized with a Ziegler catalyst, and the resulting cyclododecatriene is catalytically reduced (*8*).

I

Evaluation Program. The evaluation program has been concerned with the determination of properties defining the following performance characteristics of jet fuels:

- Cooling capacity
  - Heat sink capacity
    - Thermal stability
    - Heat capacity
  - Heat transfer properties
    - Viscosity
    - Thermal conductivity
    - Heat capacity
- Combustion characteristics
  - Heat of combustion
    - Weight basis, B.t.u. per pound
    - Volume basis, B.t.u. per gallon
  - Burning characteristics
    - Luminosity (Luminometer)
    - Deposit formation (Phillips microburner)
  - Low temperature properties
    - Viscosity
    - Freezing point

The results of this program are summarized in Table I which lists the properties of some of the hydrocarbons examined to date. This investigation is currently in progress, and at its completion a rather full study of most saturated hydrocarbon types will have been made.

Thermal Stability. The most important property to be evaluated is thermal stability. Unfortunately, it is also the property which is most difficult to define and measure. Basically, the thermal stability of interest is related to the amount of deposit which, because of heating, forms in the fuel handling system of the aircraft before the fuel is burned. The thermal stability, as defined above, is influenced by the chemical structure of the fuel, the presence of contaminants, and the fuel system design. By using pure materials of known structure an attempt has been made to limit this investigation to thermal stability as influenced by the chemical structure of the fuel.

At present there is no accepted laboratory test using a pint of fuel or less that will reliably determine the thermal stability of fuels. The development of such a suitable thermal stability test is currently in progress under U. S. Air Force sponsorship.

Until a suitable test has been developed, a very simple determination of the thermal decomposition temperature

Table I. Physical Constants of Hydrocarbons

	Compound	Thermal Decomp. Temp., °F.	Heat Capacity, Cp.[B.t.u./Lb. °F.]			Thermal Conductivity, k, $\left[\frac{\text{B.t.u.}}{\text{Hr. Ft.}^2(^\circ\text{F./Ft.})}\right]$			Net Heat of Combustion, $-\Delta H$		Purity VPC Area %
			100° F.	200° F.	300° F.	145° F.	219° F.	316° F.	B.t.u./Lb.	B.t.u./Gal.	
1	Cetane	705	0.512	0.560	0.608	0.0760	0.0748	...	18,940	122,300	96.9
2	*n*-Undecane	700	...	...	...	...	...	...	...	...	...
3	*n*-Dodecane[a]	700	...	...	...	0.0738	0.0668	...	18,944	120,000	99.5
4	Diethylcyclohexane (mixed isomers)[b]	716	0.447	0.495	0.579	0.0606	0.0594	...	18,590	124,670	99.8
5	Cyclododecane[b]	740	...	...	...	...	...	...	18,667	136,632	100.0
6	1,2,3,4,5,6-Hexaethylcyclohexane[b]	650	...	...	...	...	...	...	18,735	124,212	99.0
7	Decalin (mixed isomers)[c]	780	0.379	0.437	0.495	0.0614	0.0630	...	18,361	137,798	94.9
8	β-Methyldecalin[b]	770	0.397	0.464	0.529	0.0559	0.0583	...	18,278	132,574	99.5
9	α-Methyldecalin[b]	750	0.422	0.482	0.542	0.0564	0.0614	...	18,340	135,470	98.5
10	β-Ethyldecalin[b]	750	0.417	0.474	0.532	0.0571	0.0588	...	18,374	135,108	99.8
11	α-Ethyldecalin[b]	740	0.436	0.489	0.543	0.0583	0.0625	...	18,370	135,998	99.2
12	α-Isopropyldecalin[b]	730	0.419	0.481	0.543	0.0593	0.0591	...	18,420	137,400	98.9
13	α-*n*-Propyldecalin[b]	720	0.445	0.499	0.554	0.0571	0.0617	...	18,379	135,800	98.2
14	α-*n*-Butyldecalin[b]	710	0.439	0.478	0.525	...	...	...	18,317	136,000	99.5
15	α-sec-Butyldecalin[b]	700	0.431	0.487	0.552	0.0571	0.0586	...	18,442	137,700	98.3
16	Hydrindan[d]	770	0.423	0.472	0.569	0.0668	0.0637	...	18,341	135,400	99.8
17	Methylhydrindan[d]	740	...	...	...	0.0608	0.0589	0.0588	18,145	132,600	95.9
18	Ethylhydrindan[d]	730	0.442	0.499	0.553	0.0611	0.0598	0.0598	18,437	135,000	99.4
19	Isopropylhydrindan[b]	690	0.474	0.515	0.542	0.0612	0.0589	0.0584	18,123	133,150	93.5
20	Pinane[b]	700	0.400	0.449	0.527	0.0588	0.0569	...	18,695	134,272	98.0
21	Dimethyldecalin (mixed isomers)[b]	760	...	...	...	...	...	...	18,423	134,800	99.9
22	Isopropylbicyclohexyl[b]	715	0.479	0.524	0.569	0.0617	0.0618	0.0604	18,430	136,442	99.6
23	Bicyclopentyl[d]	750	0.397	0.428	0.497	0.0653	0.0623	...	18,297	132,864	98.9
24	Bicyclohexyl[b]	745	0.432	0.465	0.536	0.0615	0.0612	...	18,403	137,580	99.2
25	Cyclohexyl(2-ethylcyclohexyl)methane[e]	...	0.472	0.512	0.565	...	...	...	18,682	138,457	99.8
26	1,1-Dicyclohexylheptane[d]	670	0.480	0.536	0.577	0.0691	0.0657	0.0628	18,556	138,000	95.7
27	1,2-Dicyclohexylpropane[b]	680	...	...	0.571	0.0648	0.0628	0.0602	18,486	137,200	100.0
28	Cyclohexyl(ethylcyclohexyl)methane[b]	705	...	...	0.564	0.0630	0.0603	0.0589	18,485	133,000	100.0
29	Dicyclohexylmethane[b]	...	0.471	0.517	0.571	0.0649	0.0622	0.0616	18,476	135,388	99.9
30	Tricyclo[7.1.1.0^{4,6}]decane[b]	...	...	...	...	0.0666	0.0640	...	18,474	142,697	95.1
31	1-Cyclohexyl-1,3,3-trimethylhydrindan[b]	665	0.440	0.508	0.569	0.0567	0.0581	0.0571	18,368	145,200	99.3
32	9-Methylperhydrofluorene[f]	730	...	...	...	0.0614	0.0583	0.0584	18,265	142,600	99.9
33	Tetracyclo[6.2.1.1^{3,6}]dodecane[a,g]	740	0.407	0.458	0.509	...	...	...	18,121	152,132	98.5
34	3-Ethylperhydropyrene[h]	...	0.446	0.476	0.518	0.0574	0.0569	...	18,064	148,490	99.9
35	4′-*n*-Heptyl-*m*-tercyclohexyl[i]	...	0.461	0.514	0.563	0.0647	0.0682	...	18,414	140,683	99.0
36	Cyclopentylbicyclohexyl[b]	675	0.439	0.502	0.536	...	...	...	18,369	142,729	99.7
37	*o*-Tercyclohexyl[b]	...	0.408	0.472	0.537	0.0627	0.0615	...	18,287	142,000	97.8
38	*m*-Tercyclohexyl[b]	730	0.440	0.479	0.524	...	...	...	18,241	...	99.0

	Compound	Luminometer No.	Viscosity, Cs.				Freezing Pt., ° F.	Molecular Weight	H/C Wt. Ratio
			−30° F.	100° F.	210° F.	300° F.			
1	Cetane	140.1	Solid	3.05	1.31	0.845	+65	226.4	0.178
2	*n*-Undecane	157.9	. . .	. . .	. . .	. . .	+14	156.3	0.183
3	*n*-Dodecane[a]	157.8	. . .	. . .	. . .	. . .	+16.8	170.3	0.182
4	Diethylcyclohexane (mixed isomers)[b]	80.7	4.41	1.07	0.57	. . .	<−70	140.2	0.168
5	Cyclododecane[b]	106.1	Solid	Solid	2.28	1.18	~110	168.3	0.168
6	1,2,3,4,5,6-Hexaethylcyclohexane[b]	69.6	Solid	11.2	2.01	1.07	−16	252.5	0.168
7	Decalin (mixed isomers)[c]	46.5	16.5	2.35	1.04	0.655	−92	138.2	0.151
8	*β*-Methyldecalin[b]	. . .	11.1	1.82	0.86	0.558	. . .	152.3	0.153
9	*α*-Methyldecalin[b]	. . .	15.0	2.20	0.98	0.623	. . .	152.3	0.153
10	*β*-Ethyldecalin[b]	. . .	22.0	2.38	1.04	0.655	. . .	166.3	0.154
11	*α*-Ethyldecalin[b]	. . .	22.0	2.38	1.04	0.655	. . .	166.3	0.154
12	*α*-Isopropyldecalin[b]	. . .	. . .	3.22	1.25	0.780	<−75	180.3	0.155
13	*α*-*n*-Propyldecalin[b]	. . .	. . .	2.90	1.13	0.710	. . .	180.3	0.155
14	*α*-*n*-Butyldecalin[b]	. . .	103.1	3.80	1.32	0.850	<−70	194.3	0.156
15	*α*-sec-Butyldecalin[b]	. . .	126.0	3.90	1.32	0.820	<−70	194.3	0.156
16	Hydrindan[d]	49.5	7.74	1.95	0.86	0.550	−48	124.2	0.149
17	Methylhydrindan[d]	45.9	9.47	1.67	0.81	0.542	<−75	138.2	0.151
18	Ethylhydrindan[d]	51.3	11.2	1.76	0.85	0.570	<−75	152.3	0.153
19	Isopropylhydrindan[b]	50.9	12.7	2.10	0.97	0.630	<−75	166.3	0.154
20	Pinane[b]	50.8	11.5	1.85	0.85	0.535	<−75	138.2	0.151
21	Dimethyldecalin (mixed isomers)[b]	47.5	22.6	2.35	1.04	0.600	<−75	166.3	0.154
22	Isopropylbicyclohexyl[b]	58.2	Solid	6.2	1.82	1.03	−29	208.4	0.157
23	Bicyclopentyl[d]	52.2	4.22	1.35	0.72	0.502	−35	138.2	0.151
24	Bicyclohexyl[b]	. . .	Solid	3.15	1.18	0.737	. . .	166.3	0.154
25	Cyclohexyl(2-ethylcyclohexyl)methane[e]	. . .	. . .	5.2	1.62	0.95	−20 to −22	208.4	0.157
26	1,1-Dicyclohexylheptane[d]	81.8	16,700	19.0	3.1	1.46	−42	264.5	0.159
27	1,2-Dicyclohexylpropane[b]	69.6	827.3	6.5	1.87	1.22	<−75	208.4	0.157
28	Cyclohexyl(ethylcyclohexyl)methane[b]	72.3	416.6	7.0	1.75	1.0	<−75	208.4	0.157
29	Dicyclohexylmethane[b]	74.8	Solid	4.1	1.44	0.86	+2	180.3	0.155
30	Tricyclo[7.1.1.0^{4,6}]decane[b]	23.1	Solid	2.75	1.09	0.69	+50	120.1	0.134
31	1-Cyclohexyl-1,3,3-trimethylhydrindan[b]	46.4	Solid	31.0	4.10	1.84	−10	248.4	0.149
32	9-Methylperhydrofluorene[f]	33.2	86.9	4.3	1.52	0.92	<−75	192.3	0.144
33	Tetracyclo[6.2.1.1^{3,6}]dodecane[g]	17.7	. . .	. . .	. . .	. . .	+62	162.3	0.126
34	3-Ethylperhydropyrene[h]	35.1	Solid	17.5	3.3	1.61	+25	264.4	0.140
35	4′-*n*-Heptyl-*m*-tercyclohexyl[i]	72.7	Solid	240	12.0	3.79	+68	346.6	0.155
36	Cyclopentylbicyclohexyl[b]	57.2	Solid	14.5	3.2	1.52	+38 to 42	234.4	0.148
37	*o*-Tercyclohexyl[b]	. . .	Solid	. . .	. . .	. . .	+20 to 25	248.4	0.149
38	*m*-Tercyclohexyl[b]	70.3	. . .	. . .	. . .	. . .	. . .	248.4	0.149

[a] Humphrey-Wilkinson. [b] Monsanto. [c] Du Pont. [d] Applied Science. [e] NASA-NBS. [f] Union Carbide. [g] Shell. [h] Denver Research. [i] Olin-Mathieson.

of fuels is being made in a high pressure, high temperature isoteniscope (Figure 1). This instrument measures the temperature at which the fuel begins to decompose and evolve gas, but does not measure deposit formation.

Thermal decomposition temperature for a compound is defined as that temperature at which the fuel decomposes at the rate of 1 mole % per hour. Two assumptions are made in calculating this quantity: the decomposition is unimolecular, and 1 mole of gas is formed by the decomposition of 1 mole of pure compound.

Thus, for pure saturated hydrocarbons, the thermal stability given by this method would probably be the minimum temperature at which the fuel becomes unsuitable for use, since it is unlikely that deposit formation would occur before decomposition to gaseous products. The fuel may decompose to gas without forming deposits; if this is the case, the fuel could be used at temperatures higher than those indicated by the isoteniscope.

This method is not applicable to ordinary jet fuels which may contain unsaturates or trace impurities such as nitrogen and sulfur. Unsaturates can polymerize to give deposits with a decrease in vapor pressure.

The following tabulation summarizes, in general, the high pressure, high temperature isoteniscope decomposition temperatures for a number of representative hydrocarbon classes examined so far. The three most thermally stable groups were the unsubstituted condensed bicyclics, the lower monoalkylated condensed bicyclics, and the monocyclics. The condensed polycyclics examined, dimethanodecalin and 9-methylperhydrofluorene, exhibited thermal stabilities approximately equivalent to the lower monoalkylated condensed bicyclics.

Thermal Decomposition Temperatures

	T_d, ° F.
Bicyclics, condensed	
Decalin	780
Hydrindan	770
α- or β-Methyldecalin	750–770
α- or β-Ethyldecalin	740–750
Methylhydrindan	740
Monocyclics	
Diethylcyclohexane	716
Cyclododecane	740
1,2,3,4,5,6-Hexaethylcyclohexane	650
Polycyclics	
Tetracyclo[6.2.1.1^{3,6}]dodecane[a]	740
9-Methylperhydrofluorene	730
m-Tercyclohexyl	730
Cyclopentylbicyclohexyl	675
1-Cyclohexyl-1,3,3-trimethylhydrindan	665
Acyclics and dicyclic alkanes	
Cetane	705
n-Dodecane	700
Cyclohexyl(ethylcyclohexyl)methane	705
1,1-Dicyclohexylheptane	670

[a] Dimethanodecalin.

Of particular interest is the decrease in thermal decomposition temperature of the decalins with increasing chain length of substituted alkyl groups: decalin (780° F.), α-methyldecalin (750° F.), α-ethyldecalin (740° F.), α-*n*-propyldecalin (720° F.), α-*n*-butyldecalin (710° F.), and α-*sec*-butyldecalin (695° F.).

The thermal decomposition temperature range of the butyldecalins is approximately that observed for the *n*-alkanes such as cetane (705° F.) and *n*-dodecane (700° F.). The same trend is noted in alkylated hydrindans: hydrindan (770° F.), methylhydrindan (740° F.), ethylhydrindan (730° F.), and isopropylhydrindan (690° F.).

Thus, as the chain length of alkyl substituents of such condensed bicyclics increases, the thermal decomposition temperatures approach those for the *n*-alkanes.

This same general trend is observed for other saturated hydrocarbons with a high degree of nuclear alkylation. The net effect is a relatively low thermal stability as measured by this method. 1-Cyclohexyl-1,3,3-trimethylhydrindan has a thermal decomposition temperature of 665° F. and 1,2,3,4,5,6-hexaethylcyclohexane a value of 650° F.

Heat Capacity. Heat capacities have been determined over the temperature range 100° to 300° F. using a differential heating method and apparatus previously described in the literature (*5–7*).

Of the compounds studied so far, the normal alkanes were observed to have the highest heat capacities.

Heat Capacity

	Cp. (B.t.u./Lb. ° F.)		
Compound	100° F.	200° F.	300° F.
Cetane	0.512	0.560	0.608
1,1-Dicyclohexylheptane	0.480	0.536	0.577
Isopropylbicyclohexyl	0.479	0.524	0.569
Dicyclohexylmethane	0.471	0.517	0.571
α-*n*-Propyldecalin	0.445	0.499	0.554
Diethylcyclohexane	0.447	0.495	0.579
Bicyclohexyl	0.432	0.465	0.536
α-Methyldecalin	0.422	0.482	0.542
Decalin	0.379	0.437	0.495

Next in order are the alkylated noncondensed bicyclics, followed in turn by the alkylated condensed bicyclics, alkylated monocyclics, and unsubstituted bicyclics. Alkylation of the nucleus increases heat capacity, and the heat capacity increases linearly with increasing temperature over the range studied.

Thermal Conductivity. A highly refined modification of the hot wire method has been adopted to measure the thermal conductivity of organic liquids. The cell developed by Cecil and Munch (*1*) is designed to place the results on an absolute basis and to enable accurate thermal conductivity measurements to be made on small samples of liquid (~20 ml.). For measurements at elevated temperatures, the thermal conductivity cell is immersed in an insulated silicone fluid bath, the temperature of which is maintained by a condensing vapor bath (*2*).

The following tabulation extracted from Table I shows that the normal paraffins have the highest thermal conductivity of the compounds tested. Next in order were long-chain, alkyl-substituted di- and tricyclics, followed by a number of compounds containing the 5-membered ring system.

Of lower conductivity than this latter category is a large group of compounds of varied structure for which no obvious correlation is apparent. The poorest group of compounds with respect to this property contained many of the alkylated decalins. There is no apparent uniform change in thermal conductivity with temperature in the ranges studied.

Thermal Conductivity

	K[B.t.u./Hr. Sq. Ft. (° F./Ft.)]		
Compound	145° F.	219° F.	316° F.
Cetane	0.0760	0.0748	. . .
4-*n*-Heptylbicyclohexyl	0.0708	0.0711	0.0609
Bicyclopentyl	0.0664	0.0642	. . .
Dicyclohexylmethane	0.0649	0.0622	0.0616
o-Tercyclohexyl	0.0627	0.0615	. . .
Decalin	0.0614	0.0630	. . .
9-Methylperhydrofluorene	0.0614	0.0583	0.0584
Pinane	0.0588	0.0569	. . .
α-Methyldecalin	0.0564	0.0615	. . .

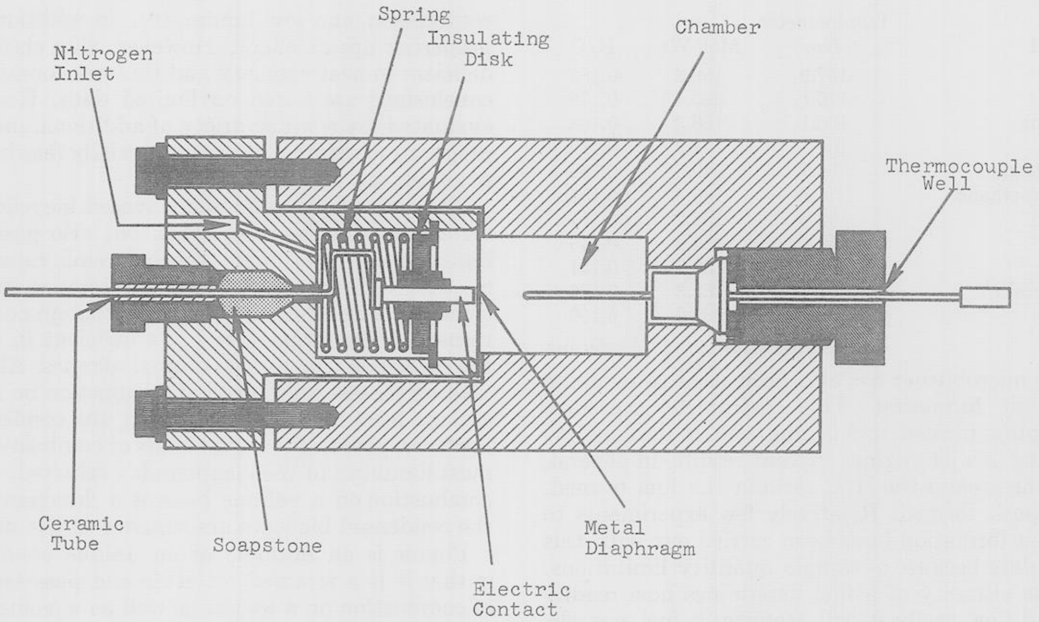

Figure 1. High temperature, high pressure isoteniscope

Heat of Combustion. Net heats of combustion were obtained with a Parr Oxygen Bomb Calorimeter according to A.S.T.M. D240-57T and are listed in Table I.

It is desirable to have as high a heat of combustion as possible on a weight and a volume basis. In unstrained compounds, a compromise must be made because as the former decreases the latter increases. In short range, high load missions, a high heat of combustion per unit weight is more important than a high volume-based heat of combustion. In long range, low load missions, a high heat of combustion per unit volume becomes important. Thus, it is impossible to define the best fuel without specifying its end use. In fuels such as cyclohexyl(2-ethylcyclohexyl)-methane and pinane, both high weight- and volume-based heats of combustion are obtained. These would be good compromise fuels. Normal paraffins such as cetane are outstanding on a weight basis and dimethanodecalin has the highest volume-based heat of combustion of the compounds evaluated so far.

Data in Table I clearly show that as the hydrogen-to-carbon (H/C) ratio increases, the heat of combustion (British thermal unit per pound) increases. This correlation is more clearly seen in Figure 2. Exceptions to this generalization exist for those cases where strain occurs in the molecule; examples of such compounds are pinane and tricyclo$[7.1.0.0^{4,6}]$decane.

The heat of combustion on a volume basis, in general, increases as the H/C ratio decreases because of the overriding effect on heat of combustion of the density increase as compared to the H/C ratio decrease. *n*-Dodecane, with and H/C ratio 0.182, has a value of 120,000 B.t.u. per gallon, whereas dimethanodecalin, with an H/C of 0.126, has a value of 152,100 B.t.u. per gallon.

Burning Characteristics. It is important that fuels burn cleanly in a jet engine. Deposits caused by poorly burning fuels decrease the efficiency of the power plant. Another problem is that of increased engine temperatures caused by radiant heating as described by Droegemueller (*4*). Fuels burning with a luminous flame should be avoided, since the additional heat produced by the emitted radiation may seriously damage the engine burner walls and other engine parts, making frequent overhaul necessary.

Evaluation of the radiation emitted during burning was carried out with the Luminometer (*4*). The method is described in (*9*).

As outlined in the following tabulation extracted from Table I, normal alkanes have the highest Luminometer numbers (that is, are the least luminous) of the compounds tested. Next in order are monocyclics and isolated ring bicyclics, followed by condensed ring compounds. In general, the lower the molecular weight, the higher the H/C ratio, and the less the branching, the higher the Luminometer number (the lower the luminosity). Also, 6-membered ring compounds appear to burn less luminously than their 5-membered counterparts.

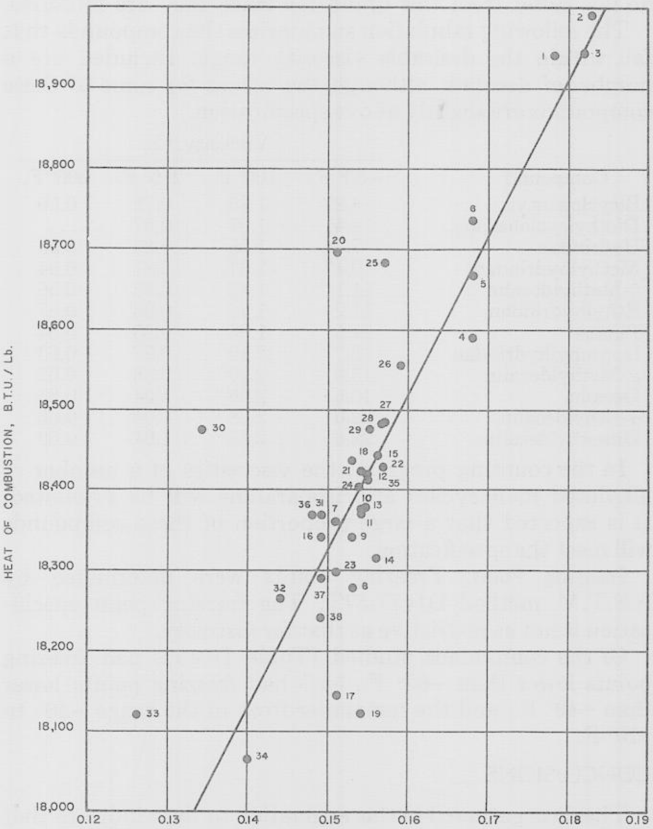

Figure 2. Variation in heat of combustion with hydrogen-to-carbon ratio

Compounds referred to by number are listed in the table

Compound	Luminometer No.	Mol. Wt.	H/C
n-Undecane	157.9	156.3	0.183
Cetane	140.1	226.4	0.178
Cyclododecane	106.1	168.3	0.168
Iso-octane	100[a]	114.2	0.188
Diethylcyclohexane	80.7	140.3	0.168
Dicyclohexylmethane	74.8	180.3	0.155
Bicyclopentyl	52.2	138.2	0.151
Hydrindan	49.4	124.2	0.149
Decalin	46.5	138.2	0.151
Dimethanodecalin[b]	17.7	162.3	0.126
Tetralin	0[a]	132.2	0.150

[a] By definition.

[b] Tetracyclo[6.2.1.1^{3,6}]dodecane.

The Phillips microburner has also been used to evaluate fuels for deposit formation. This instrument measures deposits and gums formed in burning and is designed to simulate burning in a jet engine. Present results, in general, indicate that the greater the H/C ratio in the fuel burned, the less the deposit formed. Relatively few experiments to evaluate deposit formation have been carried out with this instrument to date because of sample quantity limitations.

Viscosity. The viscosity of a fuel determines how readily it will flow and how easily it will atomize in fuel nozzels. Low viscosity makes for efficient fuel pumping and atomization. In addition, low viscosity is a desirable characteristic for good heat transfer properties.

The specification for this property is a maximum of 15 cs. at −30° F. For the pure compounds evaluated to date this viscosity limit would appear to be the most restrictive requirement. It is possible that this requirement can be met by mixtures of pure compounds. Also, given a fuel outstanding in all properties, except for its low temperature viscosity, it may be possible to design around this deficiency. Some of the pure compounds studied in this program have been found to be solids or highly viscous liquids at −30° F.; petroleum fractions, on the other hand, do not suffer from this limitation since they are mixtures.

The following tabulation summarizes the compounds that fall within the desirable viscosity range. Included are a number of decalins, although the values for some of these compounds are slightly above specification.

	Viscosity, Cs.			
Compound	−30° F.	100° F.	210° F.	300° F.
Bicyclopentyl	4.22	1.35	0.72	0.50
Diethylcyclohexane	4.41	1.07	0.57	...
Hydrindan	7.74	1.95	0.86	0.55
Methylhydrindan	9.47	1.67	0.81	0.54
β-Methyldecalin	11.1	1.82	0.86	0.56
Ethylhydrindan	11.2	1.76	0.85	0.57
Pinane	11.5	1.85	0.85	0.54
Isopropylhydrindan	12.7	2.10	0.97	0.63
α-Methyldecalin	15.0	2.20	0.98	0.62
Decalin	16.5	2.35	1.04	0.66
α-Ethyldecalin	22.0	2.38	1.04	0.66
Dimethyldecalin	22.6	2.35	1.04	0.60

In the counting program, the viscosities of a number of alkylated monocyclics and isoparaffins will be evaluated. It is expected that a large proportion of these compounds will meet the specification.

Freezing Point. Freezing points were determined by A.S.T.M. method D1477-57T. The freezing point specification is not as restrictive as that for viscosity.

Of the compounds studied (Table I) 43% had freezing points lower than −60° F., 55% had freezing points lower than −40° F., and the remainder froze in the range −40° to 110° F.

CONCLUSIONS

The data gathered in this evaluation to date indicate that saturated monocyclics may be the most promising compromise fuel based on an over-all consideration of all the properties determined. This class, as typified by diethylcyclohexane, has high thermal stability, high heat of combustion, and low luminosity. In addition, its viscosity properties are excellent. However, this class is somewhat deficient in heat capacity and thermal conductivity. These conclusions are based on limited data. Remaining to be evaluated are a wide variety of additional monocyclics, the preparations of which are commercially feasible from readily available raw materials.

The normal alkanes and condensed bicyclics each possess certain outstanding properties, but also possess important limitations. For example, the heat sink capacity is related to the thermal decomposition temperature and heat capacity. The condensed bicyclics, though outstanding with respect to the former, are quite deficient in heat capacity; the reverse is true for the normal alkanes. Also, the normal alkanes possess high heats of combustion on a weight basis and are least luminous in burning; the condensed bicyclics, however, possess the lowest heats of combustion and are the most luminous of the compounds evaluated. If the heat of combustion on a volume basis is a dominant requirement, the condensed bicyclics are superior to the normal alkanes.

Pinane is an example of an unique condensed bicyclic in that it is a strained molecule and possesses a high heat of combustion on a weight as well as a volume basis. This compound also has good low temperature properties and is commercialy available.

Within comparable molecular weight ranges, the condensed bicyclics possess better low temperature properties. Although the evaluation of the condensed bicyclics is essentially complete, examination of the alkanes (normal and isoalkanes) is as yet incomplete.

The noncondensed bicyclics—e.g., isopropylbicyclohexyl, are not outstanding in any one property. The most serious deficiency of this class is the low temperature viscosity; in any fuel application where a high viscosity is not limiting, the noncondensed bicyclics would be good compromise fuels.

From over-all considerations the condensed polycyclics examined to date appeared to be the least promising of the classes considered. Although they possess good thermal stability, they are deficient in heat of combustion on a weight basis. They do, however, possess good heats of combustion on a volume basis. Their burning characteristics and low temperature properties also are poor.

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