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INTRODUCTION

The United States Department of Energy, Office of Advanced Automotive Technologies and Office of Heavy Vehicle Technologies, requested that J.E. Sinor Consultants Inc. carry out a state-of-the-art survey on the use of dimethyl ether (DME) as a transportation fuel. This was done by starting with a conventional computerized search of the literature through several commercial databases. For items which appeared to be of preliminary interest, abstracts were printed out. For abstracts which appeared promising, the referenced publications or reports were obtained and examined. A bibliographic database was prepared on Microsoft Access, and a printout is attached as an appendix to this report.

All of the items in the database were examined and a list of key organizations and key individuals in those organizations was compiled. These individuals were then contacted by telephone, facsimile or e-mail. Questions were asked about their involvement in DME research and development and about their views concerning the need for further research and development efforts.

Using both the literature references and the results of the personal interviews, a summary of the state-of-the-art in DME development and of known ongoing activities was prepared.

FUNDAMENTAL ASPECTS OF DIMETHYL ETHER

GENERAL

An ether is a chemical compound with a C-O-C linkage. Dimethyl ether CH_3OCH_3 is the simplest of all ethers. It is a synthetic fuel, not occurring naturally in petroleum. Dimethyl Ether (DME) has been detected in interstellar space, and for many years it was the largest organic compound that had been detected in space. The overall formula for DME is the same as that for ethanol C_2H_6O; thus DME could be considered to be an isomer of ethanol.

DME can be made from almost any carbonaceous feedstock by first making synthesis gas (a mixture of carbon monoxide and hydrogen) and then allowing synthesis gas to react over a catalyst.

The largest current use for DME is as a propellant in aerosol spray cans. Total world production is estimated to be about 100,000 to 150,000 tons per year.

DME has been investigated as a chemical reagent for the desulfurization of lignite (2).

DME has been investigated for use as the working fluid in Rankine cycles for power and refrigeration. Kustrim and Tuma (19,67) concluded that, compared to other organic fluids which are frequently used in Rankine cycles, DME:

- Would be quite efficient
- Is thermally stable to 220°C
- Costs less than other proposed CFC replacements

PHYSICAL PROPERTIES

Dimethyl ether (or methoxymethane) is a colorless, almost odorless gas at room temperature and atmospheric pressure. Basic physical properties from several sources are given in Table 1.

Liquid density as a function of temperature and pressure is given in Figure 1.

DME is reported to have a lower viscosity than either butane or isobutane.

Thermal conductivity as a function of temperature is compared to butane and isobutane in Table 2.

Vapor pressure data for DME are given in Table 3 (52).

The modulus of elasticity for liquid DME as a function of temperature and pressure is given in Figure 2.

TABLE 1

PHYSICAL PROPERTIES OF DME REPORTED BY VARIOUS SOURCES

Property	Unit	Ref. 78	Ref. 17	Ref. 67	Ref. 68	Ref. 58	Ref. 74	Ref. 24	Ref. 69	Ref. 112
Molecular Weight		46.07		46.07		46.07				
Boiling Point	K	248.3		248.4	248.3	249.5	248.1	248.2		248.2
Freezing Point	K	131.7		141.0		134.7				
Vapor Density (air)		1.59		1.59	1.59	1.59	1.59			
Critical Pressure	atm	52.5		53.7						
Critical Temperature	K	402.0		400.0						
Heat of Melting	cal/g	25.6								
Heat of Vaporization	cal/g	111.6		98.0			111.7			109.9
Specific Heat @ 246 K	cal/g	0.535								
Liquid Specific Gravity			0.66	0.67	0.668		0.67	0.668	0.665	0.66
Viscosity, Kinematic	cSt		<1							
Viscosity	kg/m-s							0.15		
Viscosity	cP				0.15					
Velocity of Sound	m/s		960							
Modulus of Elasticity	N/m^2		$637x10^6$							
Discharge Coefficient			0.53							

CHEMICAL PROPERTIES

DME is actually a quite stable compound which reacts or decomposes only at rather severe conditions. The estimated decomposition rate at 493K is on the order of 1 percent per year. It is basically inert chemically. However, it is a powerful solvent, and much attention will have to be devoted to the compatibility of elastomeric gasket and sealing materials if DME is adopted for automotive use. It has a high solubility for both polar and non-polar substances.

Up to 7 weight percent of water can be added to DME or 34 weight percent of DME to water before a second phase is formed at the ambient temperature of 20°C. An addition of 7 weight percent of methanol to the DME/water formulation makes it miscible at all concentrations. These properties may be important because DME synthesis can result in a mixture of DME, alcohol and water. It would be most economical if the reaction product mixture could be used directly as fuel rather than having to separate and purify a single-component product.

The solubility of DME in unleaded gasoline is shown in Table 4.

THERMODYNAMIC AND COMBUSTION PROPERTIES

Chlorofluorocarbons (CFCs) have been widely used as working fluids for organic Rankine cycles. However, because of their destructive effect on stratospheric ozone, they are being phased out. Replacements such as DME are under consideration (67). DME looks useful for this application because its atmospheric lifetime is about 5 to 7 days (67, 75), the same as ethanol, compared to years or even decades for the CFCs.

The thermodynamic properties of DME are similar to those of refrigerant R12. An enthalpy-entropy chart for DME was calculated and published in reference 67. A

FIGURE 1

LIQUID DENSITY AS A FUNCTION OF TEMPERATURE AND PRESSURE

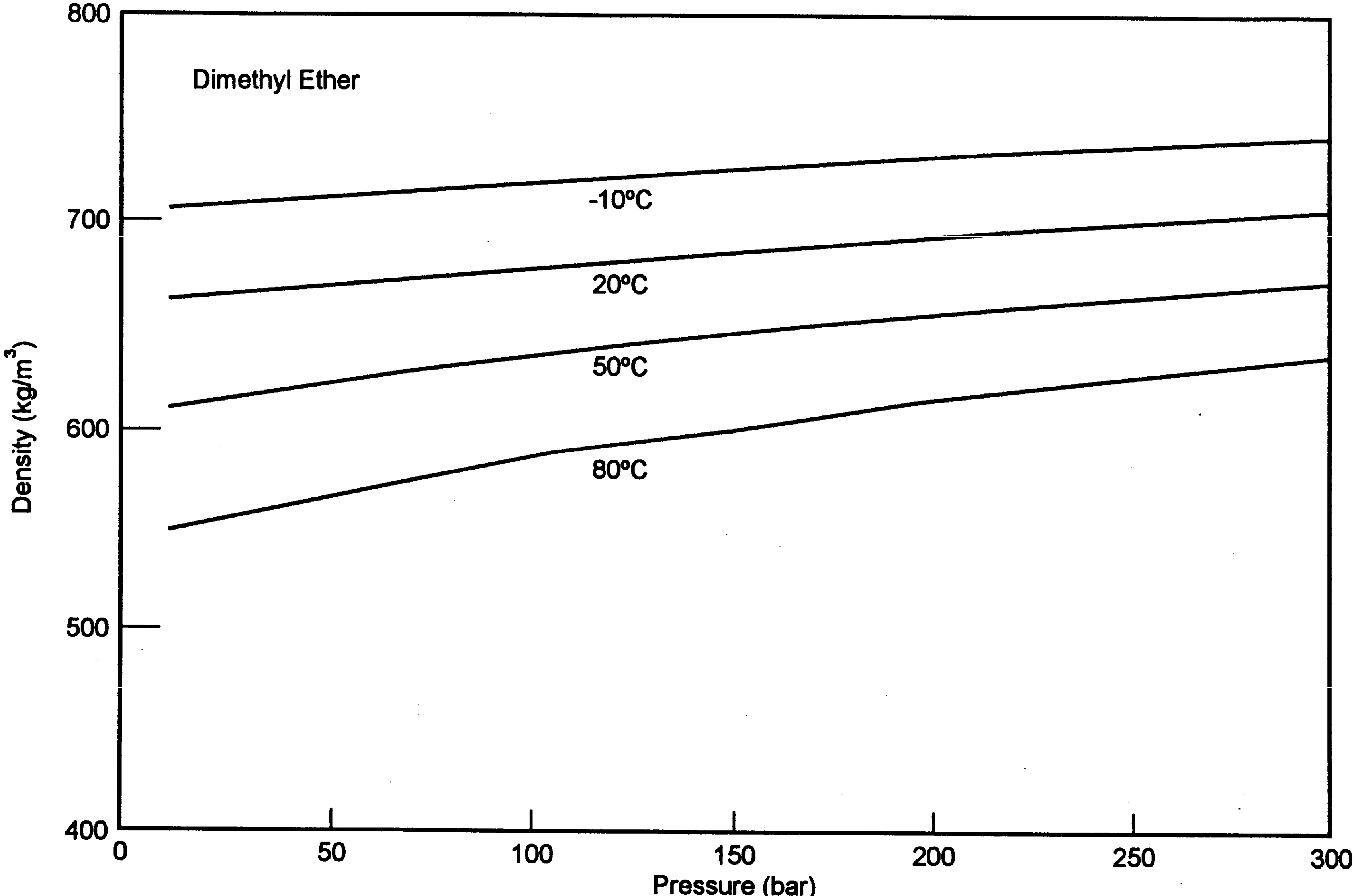

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TABLE 2

SATURATED LIQUID THERMAL CONDUCTIVITIES OF BUTANE, ISOBUTANE AND DME

Temp. (°C)	Butane (W/mK)	Isobutane (W/mK)	DME (W/mK)
0	0.1448	0.1389	0.1486
20	0.1348	0.1282	0.1365
40	0.1242	0.1168	0.1235
60	0.113	0.1046	0.1096
80	0.101	0.0912	0.0941
100	0.0878	0.0576	0.0523

temperature-entropy chart is available in reference 25. Calculated perfect-gas thermodynamic properties for DME are given in reference 57.

Vapor-liquid equilibrium data are available for a number of mixtures of DME with other compounds:

- DME/Water (108, 109)
- DME/Methane (53)
- DME/Methanol (52)
- DME/n-Butane (48)
- DME/1-Butene (106)

Basic combustion characteristics from various sources are listed in Table 5.

The variation of certain physical and thermodynamic properties as a function of temperature may be found in Table 6 (78).

CETANE NUMBER

Because of its importance for diesel engine operation, much attention is focused on the cetane number. The cetane number is a measure of the auto-ignition properties of a fuel. In Europe, diesel fuel has a cetane number between 46 and 55 (most commercially available diesel fuels are between 48 and 50). The cetane number of DME is higher; values from 55 to 60 are generally mentioned. This property makes DME very suitable for use in compression ignition engines.

Surprisingly, not everything is known yet about the cetane number of DME and some researchers expect the true value to be higher than 60, perhaps as high as 70. Cetane

TABLE 3

VAPOR PRESSURE DATA FOR DIMETHYL ETHER

Temp. (K)	Pressure (kPa)
253.85	128.07
258.63	155.49
258.64	155.59
261.08	171.07
261.08	171.17
265.41	201.98
268.25	224.34
273.22	267.41
278.00	315.19
287.94	434.55
292.93	506.08
297.60	580.96
302.93	675.74
303.01	677.34
307.57	767.74
312.95	885.28
317.62	997.92
320.40	1,069.90
320.51	1,072.80

numbers are particularly useful when blending fuels. Usually, a linear blending relationship may be assumed.

MISCELLANEOUS PROPERTIES

Reference 120 contains several pages of miscellaneous physical property data and references to safety and handling procedures that were obtained by an Internet search on the words dimethyl ether.

FIGURE 2

LIQUID MODULUS OF ELASTICITY AS A FUNCTION OF TEMPERATURE AND PRESSURE

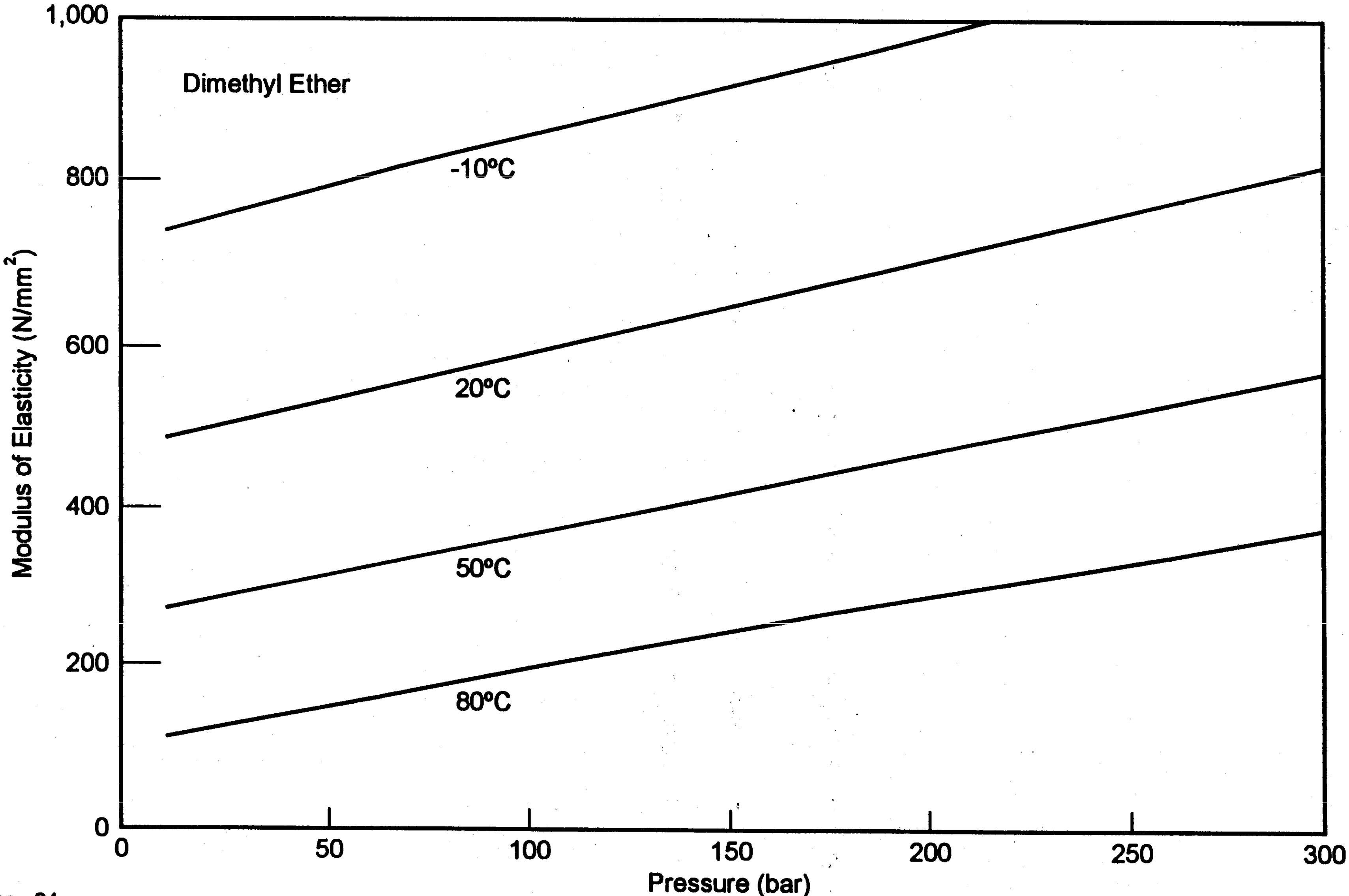

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TABLE 4

SOLUBILITY OF DME IN UNLEADED GASOLINE

Temperature	Wt.% DME
-40°C	64
0°C	19
25°C	7

TABLE 5

DME COMBUSTION CHARACTERISTICS

Property	Unit	Ref. 74	Ref. 67	Ref. 24	Ref. 69	Ref. 112	Ref. 113
Burning Velocity	cm/sec	50					
Ignition Energy	10^{-6} J	45					
Ignition Temperature	K	623	508			508	
Cetane Number		55-60		»55	55-60	»55	55
Net Calorific Value	kcal/m^3	14,200					
Net Calorific Value	kcal/kg	6,903					
Heat of Combustion	MJ/kg		31.75	28.8	28.2	27.6	27.6
Volumetric Heating Value	MJ/liter						18.2

TABLE 6

SOME PHYCIAL AND THERMODYNAMIC PROPERTIES OF DIMETHYL ETHER AT VARIOUS TEMPERATURES

Temp. °C	Vapor Pressure atm	Density Liquid g/ml	Density Vapor g/ml	Dielec-tric Cons-tant	Heat of Vapori-zation kcal/kg	Enthalpy Liquid kcal/kg	Enthalpy Vapor kcal/kg	Entropy Liquid cal/(g) (°K)	Entropy Vapor cal/(g) (°K)
-40	0.392	–	–	–	116.13	77.58	193.71	0.9109	1.4090
-30	0.741	–	–	–	113.17	83.08	196.28	0.9342	1.3996
-20	1.35	0.7174	0.0027	–	110.12	88.64	198.76	0.9568	1.3918
-10	1.97	0.7040	0.0039	–	106.95	94.23	201.23	0.9787	1.3851
0	2.80	0.6905	0.0055	–	103.64	100.00	203.64	1.0000	1.3794
10	3.86	0.6759	0.0076	–	100.17	105.79	205.96	1.0206	1.3744
20	5.24	0.6610	0.0104	5.15	96.44	111.75	208.19	1.0410	1.3700
30	7.00	0.6455	0.0142	4.90	92.64	117.60	210.24	1.0604	1.3660
40	9.06	0.6292	0.0188	4.67	88.43	123.63	212.11	1.0795	1.3620
50	11.6	0.6116	0.0241	4.41	–	–	–	–	–
60	14.7	0.5932	0.0306	4.18	–	–	–	–	–
70	18.4	0.5735	0.0385	3.93	–	–	–	–	–
80	22.7	0.5517	0.0484	3.70	–	–	–	–	–
90	27.4	0.5257	0.0623	3.48	–	–	–	–	–
100	33.0	0.4950	0.0810	3.25	–	–	–	–	–
110	39.5	0.4575	0.1060	3.00	–	–	–	–	–
120	46.6	0.4040	0.1465	–	–	–	–	–	–

HISTORY OF EFFORTS TO INTRODUCE DME AS A TRANSPORTATION FUEL

EARLY REFERENCES TO DME AS A MOTOR FUEL

A search through commercial databases back to 1906 did not reveal any mention of using DME as a motor fuel before the modern era (1980+). A 1984 German patent (86) describes a methanol base fuel consisting of non-distilled technical methanol, water, dimethyl ether and further additives.

A 1986 U.S. patent (105) describes a method of operating a diesel engine with a fuel consisting of 95 to 99.9 percent DME.

DME AS AN IGNITION IMPROVER FOR METHANOL

The first extensive literature references to using DME as a motor fuel involve the use of DME as an additive to methanol in order to improve its ignition characteristics. This can be helpful in two ways. First it can improve the cold-start performance of high-methanol fuels in spark-ignited engines. The low vapor pressure of methanol makes cold starts difficult. Second, DME can improve the cetane number of methanol for use in diesel engines. Methanol has a high octane number and correspondingly low cetane number, making it difficult to burn in compression ignition, or diesel, engines.

Considerable work was carried out at the Petroleum Energy Center, Japan, on the use of methanol with added DME in spark-ignited, or Otto-type, engines (70). Exxon Research and Engineering (84) and the University of Toronto (93) also did some work in this area.

Another concept involved splitting a portion of the methanol/air stream going to the engine and running it over a catalyst to decompose the methanol to DME + water, then mixing this stream with the remainder of the alcohol/air charge. This concept was tested in Germany (83), Japan (38) and Colorado (92).

Probably the most research was completed while looking for a way to improve the performance of methanol in heavy-duty applications such as city buses. Several publications on this subject came from:

- University of Witwatersrand (54)
- Sypher-Mueller (31, 50)
- TDA Research (33)
- Hokkaido University and Riken Corporation, Japan (35, 36)

Simple aspiration of DME into the engine air intake was found to work but this method suffers from poor emissions performance and requires large amounts of DME. The use of the plasma torch concept (35) appears more promising. The amount of DME required was only 5 percent of the total fuel supplied or one-tenth that required by the aspiration method.

DME AS A TOTAL FUEL FOR DIESEL ENGINES

The use of DME as a total replacement for diesel fuel began to attract worldwide attention after a key set of five papers (17, 20, 21, 23, 68) was published in 1995 by personnel from Amoco, AVL List, Haldor Topsoe, Navistar and the Technical University of Denmark. These papers covered emissions from both light-duty and heavy-duty engines burning DME, the development of fuel injection equipment for such engines, and the costs of large-scale manufacture of DME.

ENGINE PERFORMANCE WITH DME

Thus far, only a few engines have been tested on DME and conclusions must still be considered somewhat preliminary. Nevertheless, excellent results have been obtained. These include:

- Smooth compression ignition achieved in unmodified diesel engines
- Effective cetane number (55-60) much higher than conventional diesel fuel
- Successful cold-start down to -24°C without ignition aids (68)
- Especially under part load, DME engines produce less noise (15 dBA) than diesel engines--comparable to gasoline engines (112)
- Low emissions achieved with much lower fuel injection pressures
- Lower rates of pressure buildup and lower maximum cylinder pressures
- Overall thermal efficiency similar to that for diesel fuel
- Almost zero particulate (smoke) and low NO_x emissions

TESTS WITH 0.273-LITER DIRECT INJECTION ENGINE

Tests were carried out at Technical University of Denmark (68) in a small, single-cylinder, non-turbocharged, direct-injection diesel engine. Engine efficiency was the same for DME and diesel fuel, within experimental variations. The DME engine was quieter as a result of lower rates of pressure rise and lower maximum pressure.

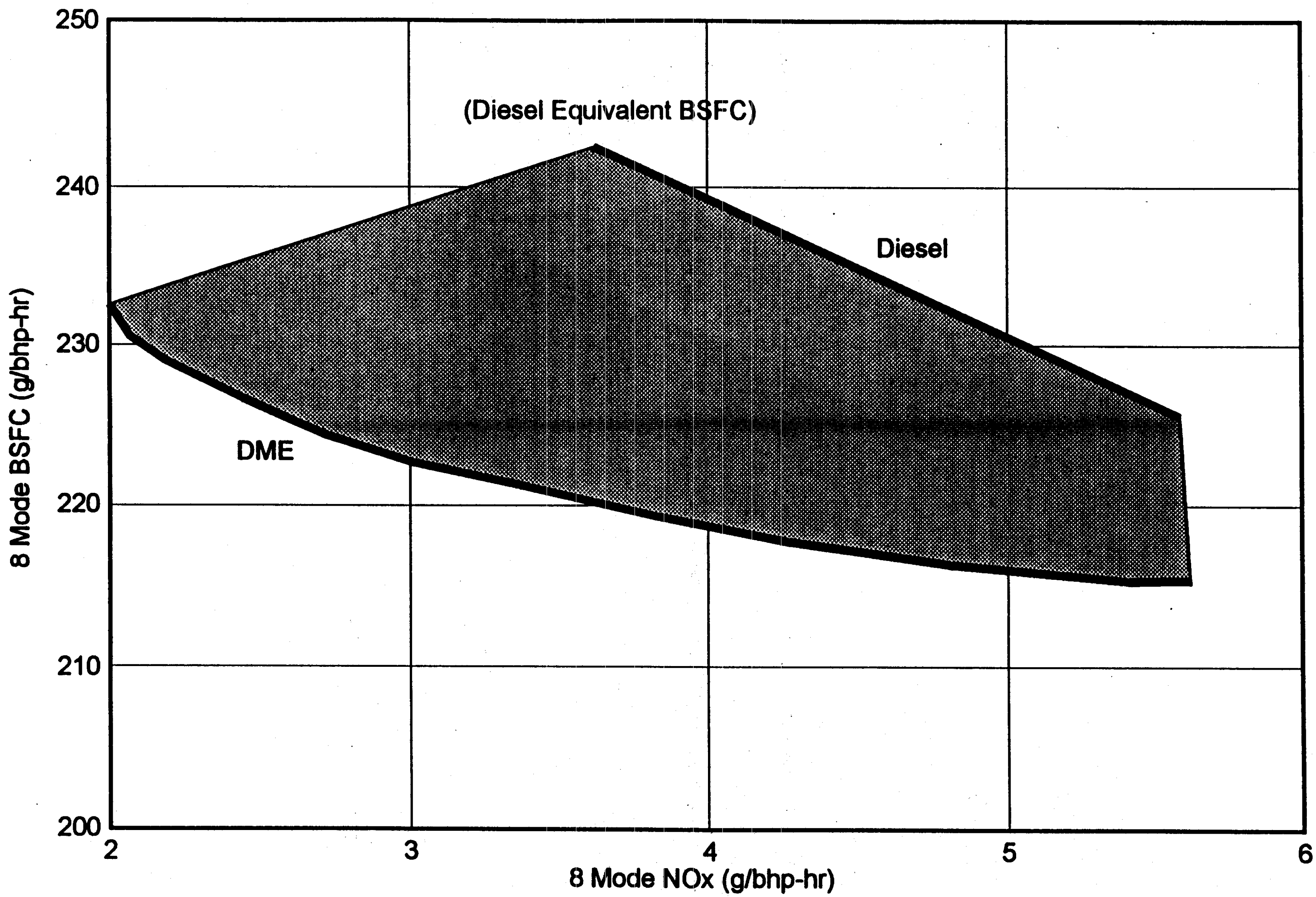
TESTS WITH NAVISTAR ENGINE

DME was tested in a Navistar 7.3-liter, V-8, direct-injected, turbocharged diesel at the AVL facility in Graz, Austria (20). This Navistar T444E engine is widely used in Class 2-7 trucks and buses. Results showed that brake-specific fuel consumption (on an energy-content basis) was lower for DME than for diesel fuel at any given level of NO_x emissions (Figure 3). To obtain acceptable NO_x emissions with diesel fuel, engine adjustments are required that reduce thermal efficiency on the order of 10 percent.

TESTS WITH 2.0-LITER AVL ENGINE

AVL List GmbH carried out tests with DME in a 2-liter, 4-cylinder, direct-injected, turbocharged and intercooled passenger car diesel engine (17). Because passenger car emission regulations are primarily based on gasoline-engine technology (stoichiometric engine operation with three-way catalytic converters), meeting the NO_x standards with a diesel-type engine is more difficult than meeting the heavy-duty vehicle NO_x standards with DME. Test results showed that for a comparable specific

FIGURE 3
NO_x/BSFC TRADEOFFS



Source: 20

fuel consumption, the DME engine exhibits NO_x emissions about one-third of the diesel fuel engine in combination with a combustion noise about 10 dB(A) lower.

It was concluded that the rate of heat release exhibited by an optimized DME combustion system comes relatively close to a constant pressure combustion. Consequently the peak firing pressure hardly exceeds the peak motoring pressure. This fact allows consideration of engines with a lighter structure than current diesel engines for DME operation. Such an engine type would then exhibit the energy consumption of a diesel engine but in combination with a less costly engine structure.

COMPARISONS OF FUEL CONSUMPTION FOR DIFFERENT FUELS

Considerable caution is advised when reviewing the literature for fuel consumption comparisons between DME and other fuels. Slight differences in various basic assumptions can significantly change the comparison. Diesel fuel does not have a fixed composition, and DME properties depend on the purity assumed. Starting with a typical comparison of key properties (Table 7) it is easy to calculate that the volumetric energy content of DME is half that of diesel fuel. Therefore, if energy efficiencies are the same in both cases, it will take 2 gallons of DME to propel a vehicle as far as it can go with 1 gallon of diesel fuel. Yet several papers in the literature suggest that only 1.8 or even 1.7 gallons of DME would be equivalent to a gallon of diesel. Generally such comparisons are derived by considering that a DME engine will have a higher efficiency than a diesel engine <u>at the same NO_x emission level</u>. However, this is unlikely to reflect actual choices that will be available in the real world. When both are optimized for energy efficiency, there is probably not a large difference in thermal efficiency between using diesel fuel and DME, although there are reasons to expect DME to be somewhat better.

One must also note the imprecise use of the term "fuel tank volume required." When one considers that a DME tank must have 15 or 20 percent ullage to allow for possible thermal expansion of the liquid, the actual volume required for a DME tank is certain to be more than twice that of an equivalent diesel tank.

TABLE 7

COMPARISON OF KEY PROPERTIES OF DIFFERENT FUELS

Property	Diesel	CNG	LNG	DME	Fischer-Tropsch	Gasoline
Lower Heating Value (MJ/kg)	43	50	50	27.6	43	43
Volumetric Heating Value (MJ/l)	36.5	8	21.1	18.2	33.1	32.2
Density (gm/ml)	0.85	0.16 @3,000 psi	0.422	0.66	0.77	0.75
Cetane Number	45	--	--	55+	80	--

Source: 113

EMISSIONS FROM DME ENGINES AND VEHICLES

The most exciting results from DME engine testing have been the almost total lack of particulate emissions and extremely low levels of NO_x emissions. The small amount of particulates that is formed probably comes from the lubricating oil. The lack of particulate emissions is attributed to three or four major factors:

- The lack of carbon-carbon bonds in DME. All smoke particles are based on carbon-carbon bonds.

- The extremely good atomization created when DME is injected at temperatures above its boiling point results in efficient combustion.

- The high cetane number of DME results in low ignition delays and efficient combustion.

- The oxygen content of the DME molecule improves combustion.

Low NO_x emissions are aided also by the fact that the combustion characteristics of DME result in less premixed burning, a lower rate of pressure rise, lower maximum pressure and lower maximum temperature.

TESTS WITH 0.273-LITER DIRECT-INJECTED ENGINE

Tests at the Technical University of Denmark with a 0.273-liter, single-cylinder, non-turbocharged, direct-injected diesel engine showed that the emission trends for HC and CO from DME and diesel fuel were essentially the same (68). However, it should be pointed out that the HC emissions from DME operation are basically methane and DME, both of which have low photochemical reactivity.

With respect to particulate and NO_x emissions, large differences were observed between DME and diesel fuel. Throughout the entire power range, the NO_x emissions from DME were only about 25 percent of those from diesel fuel.

Smoke from DME was basically too low to measure. Typically the smoke number for the engine operated on DME was around 0.1 to 0.2, which is at or below the detection limit. These numbers were achieved regardless of load. The corresponding mass particulate emissions were estimated to be below 0.1 gram per kilowatt-hour.

Further tests were carried out on the effect of adding Exhaust Gas Recirculation (EGR). Further reductions in NO_x (total of 80 to 90 percent reduction from diesel fuel) were demonstrated with no loss in thermal efficiency up to 30 percent EGR. However, the HC and CO emissions are increased with EGR. Particulate emissions were still negligible.

Tests On New Yanmar Diesel

After the above-discussed tests, additional studies were carried out on a new 0.273-liter, single-cylinder, direct-injected Yanmar diesel engine (24). These tests showed that the major components in DME engine exhaust were DME and methane. Essentially no hydrocarbons above C_2 were found. Formaldehyde emissions were on the order of 3 to 5 parts per million. Other than methane, the total amounts of light hydrocarbons in DME exhaust are about an order of magnitude lower than for diesel fuel.

TESTS WITH NAVISTAR ENGINE

Emissions tests carried out with the Navistar T444E 7.3-liter turbocharged diesel engine demonstrated results below the 1998 California Ultra-Low Emission Vehicle (ULEV) regulation for medium-duty vehicles without the use of exhaust aftertreatment (20). See Figure 4. This regulation limits NO_x plus hydrocarbons to 2.5 g/bhp-hr and caps particulates at 0.05 g/bhp-hr. In addition, emissions of formaldehyde (HCHO) are restricted to 0.025 g/bhp-hr and CO emissions are limited to 7.2 g/bhp-hr. The proposed EURO III heavy-duty truck standards also appear to be satisfied (Table 8).

Soot-free combustion was achieved at all speeds and loads, even at air/fuel equivalence ratios below 1. This "sootless combustion" permitted the use of high EGR flows, which produced low specific NO_x emissions.

In addition, emissions were estimated for the U. S. Federal Test Procedure (FTP) cycle corrected to a 2.0-liter (passenger car) engine displacement. A 1,650 kilogram vehicle weight was used. These calculations suggest that 1996-2000 U.S. passenger car standards can be achieved with some additional development. These standards limit NO_x to 0.4 grams per mile.

RESULTS WITH 2.0-LITER AVL ENGINE

AVL tests with a 2.0-liter passenger car direct-injected diesel engine showed promising results with respect to meeting ULEV NO_x emissions without any soot emissions and without the need for a $DeNO_x$ catalyst (17). An oxidation catalyst will be necessary to meet the stringent CO and HC emission limits in the ULEV standard.

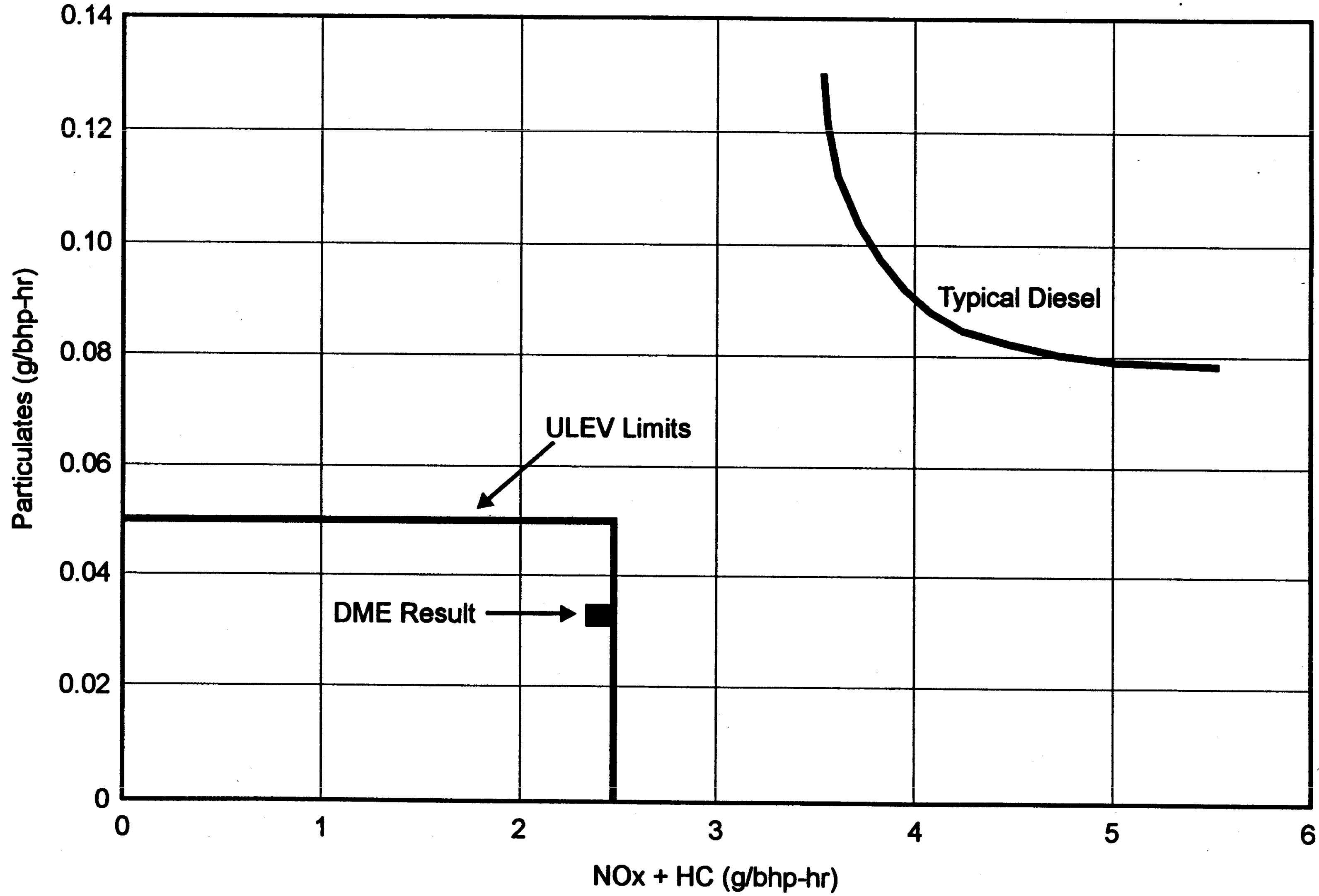
Heavy-duty (HD) vehicle emission legislation is primarily based on direct-injected diesel engine technology. Because of lean operation, an effective catalyst for NO_x reduction is not available. Additionally, the load/speed profile of the driving cycle is completely different for HD vehicles and for passenger cars. The passenger cars test cycle is operated in the low load/low speed region whereas HD vehicles have to pass a high load/high speed test cycle.

Thus DME results derived from HD development programs cannot easily be transferred to the requirements of passenger car engines. So the target for the AVL tests was to clarify whether the emission potential of a DI passenger car engine operated on DME is good enough to meet the low emission levels of a gasoline engine equipped with a three-way catalyst.

During testing it was found that, due to the high cetane numbers, fuel injection during the ignition delay period can be kept to a low value thus leading to a low amount of fuel injected for the premixed burn period. Then the pressure rise caused by the premixed

FIGURE 4

PARTICULATE VERSUS NO_x EMISSIONS FOR DME



Source: 20

TABLE 8

ESTIMATED ECE R49 EMISSIONS
(g/kWh)

	Euro III Proposal	DME Results
THC	0.60	0.20
CO	2.0	2.17
NO_x	5.0	3.85
PM	0.10	~0.05 est.

Source: 20

---

burn exhibits the same low values as on gasoline engines. Consequently the combustion noise can be kept near 80 dB(A), which is comparable to part-load noise levels on gasoline engines. Additionally, the low degree of premixed burning favors low NO_x formation during early combustion.

Based on steady-state test results of a refined DME system, engine exhaust emissions of the DME engine were projected in the FTP 75 cycle for an Audi 100 vehicle (3,000 pounds weight). With the DME engine it seems possible to just meet the ULEV emission limits with an oxidation catalyst (Table 9). The catalyst is needed to oxidize HC and CO engine-out emissions, which increase due to the high EGR rates required.

TESTS WITH AVL HEAVY-DUTY ENGINE

Considerable research work with DME fuel was performed by AVL on a 2.0-liter, single-cylinder, turbocharged, intercooled research engine. A summary of data projected from these tests is shown in Table 10 in comparison to typical state-of-the-art data from diesel engines developed to meet the U.S. 1998 federal regulations.

The data show the dramatic reductions in NO_x and particulate emissions that can be achieved with DME at equal power/torque and equal fuel economy on an energy basis.

The DME-fueled truck/bus engine meets the California ULEV standards without EGR and without any exhaust gas aftertreatment.

The fact that there is no acceleration smoke with DME can be used to improve the load response.

TABLE 9

COMPARISON OF DME TO ULEV LIMITS IN AN FTP 75 CYCLE SIMULATION

	DME	ULEV Limits
NO_x, g/mi	0.2	0.2
PM, g/mi	0	0.04
HC, g/mi	0.4 w/o cat. 0.04 with cat.	0.04
CO, g/mi	6.0 w/o cat. 0.6 with cat.	1.7

Source: 17

TABLE 10

DME EMISSIONS IN HEAVY-DUTY ENGINE TEST
(DME Data Projected From Steady-State Tests)

	Diesel	DME
Rated Power/Torque	equal	equal
Fuel Economy (energy basis)	equal	equal
Transient Cycle Emissions		
NO_x, g/bhp-hr	3.8	1.6
THC, g/bhp-hr	0.3	0.3
Total Particulates, g/bhp-hr	0.08	0.02 (from lube oil)
Peak Accel. Smoke, % opacity	5%	0%
Max. Combustion Noise, dB(A)	88	78

Source: 21

OZONE-FORMING POTENTIAL OF DME EMISSIONS

Laboratory research has been carried out to compare the reactivity, or ozone-forming potential, of DME along with other oxygenated compounds (37, 71, 75).

At a typical urban atmosphere NMOC/NO_x ratio, the reactivity of DME has been found to be "less than or equal to that of the typical urban NMOC mix." Thus the use of DME, even if emitted at the same rate as conventional fuels, could have a beneficial impact on urban ozone levels (71). The tropospheric lifetime of DME itself was calculated to be about 5 to 6 days (75).

SAFETY AND HEALTH

FLAMMABILITY

DME has a relatively high flammability rating. The lower explosive limit is reported to be 3.4 percent by volume in air.

Table 11 contains a compilation of fire and hazard characteristics of DME listed by various sources. More data on explosion limits may be available in reference 107 which was not obtained for this study.

DME burns with a visible flame similar to natural gas; therefore there is no safety hazard due to possible invisible flames such as with methanol and hydrogen.

Because DME vapors are heavier than air--approximately the same as propane--released vapors can settle in low spots and create an explosion hazard, the same as for propane. Therefore, good ventilation practices must be observed in maintenance areas.

DME/AIR DETONATIONS

Loss analysis studies in the hydrocarbon process industry have concluded that explosion, not fire, is the principal risk to be avoided when low molecular weight molecules (less than five carbon atoms) are involved (49). These substances have sufficiently high vapor pressure to support a gaseous hydrocarbon/air detonation. Work carried out at Lawrence Livermore National Laboratory and Sandia National Laboratory compared the "detonation cell width" of DME and a number of hydrocarbon and substituted-hydrocarbon compounds. They concluded that sensitivity to detonation increased in the following order:

- Branched chain alkanes (least sensitive)
- Straight chain alkanes

TABLE 11

FIRE AND HAZARD CHARACTERISTICS OF DME

Property	Units	Ref. 58	Ref. 74	Ref. 67	Ref. 78	Ref. 24	Ref. 112
Flash Point	K	232			232		
Autoignition Temp.	K	623	623	508	623	508	508
Lower Explosion Limit	vol.%	3.5	3.4	3.4	3.4	3.4	3.4
Upper Explosion Limit	vol.%	18.0	17.0	17.0	26.7	18.0	18.0
Ignition Energy	10^{-6} J		45				
Burning Velocity	cm/s		50				

- Cyclic alkanes
- Alkenes and alkynes
- Molecules with functional groups such as nitro, nitrate, epoxy and ether

Thus DME may represent more of a detonation hazard than the typical petroleum-derived hydrocarbon fuel and could be measurably more of a detonation hazard than propane.

STORAGE STABILITY

Heavier ethers (heavier than DME and methylal) are known to form peroxides upon standing and exposure to air. If these materials become concentrated they can then explode upon heating. This is not believed to be a problem with DME. First of all, the problem arises from CH_3-CH_2-O- groups which are not present in either DME or methylal. Second, DME is always stored under its own vapor pressure so there is no possibility of exposure to air.

TOXICITY

Based on existing toxicological data, DME is considered to have a low order of acute, subacute and subchronic inhalation toxicity. Other toxicological data on pharmacokinetics, blood resorption, and mutagenicity provide evidence that DME has no toxic effects during normal use. No adverse effects have been observed from (vaporized) DME contact with the skin.

Toxic hazard rating factors include (58):

- Acute local: Irritant 1
- Acute systemic: Inhalation 2; skin absorption 2; ingestion 2

The "ether" commonly used in the past as an anesthetic is diethyl ether.

CRASH HAZARDS

Crash tests and fire tests with LPG vehicles at TNO Road-Vehicles Research Institute have shown that LPG systems are safer than gasoline systems. Because of the similarities in physical properties of DME and LPG, the safety of DME in crashes is expected to be similar (69). DME vehicles might even be slightly safer than LPG vehicles because:

- It takes more heat to vaporize DME than LPG. In case of fire this results in lower tank pressures and lower discharge rates.

- The minimum amount of DME in air needed to form an explosive mixture (lower explosion limit) is higher than for LPG.

LEAKS AND SPILLS

With few exceptions, leaks and spills of DME will present little environmental hazard because the DME will evaporate rather than percolating into the groundwater system.

DISTRIBUTION AND DISPENSING REQUIREMENTS

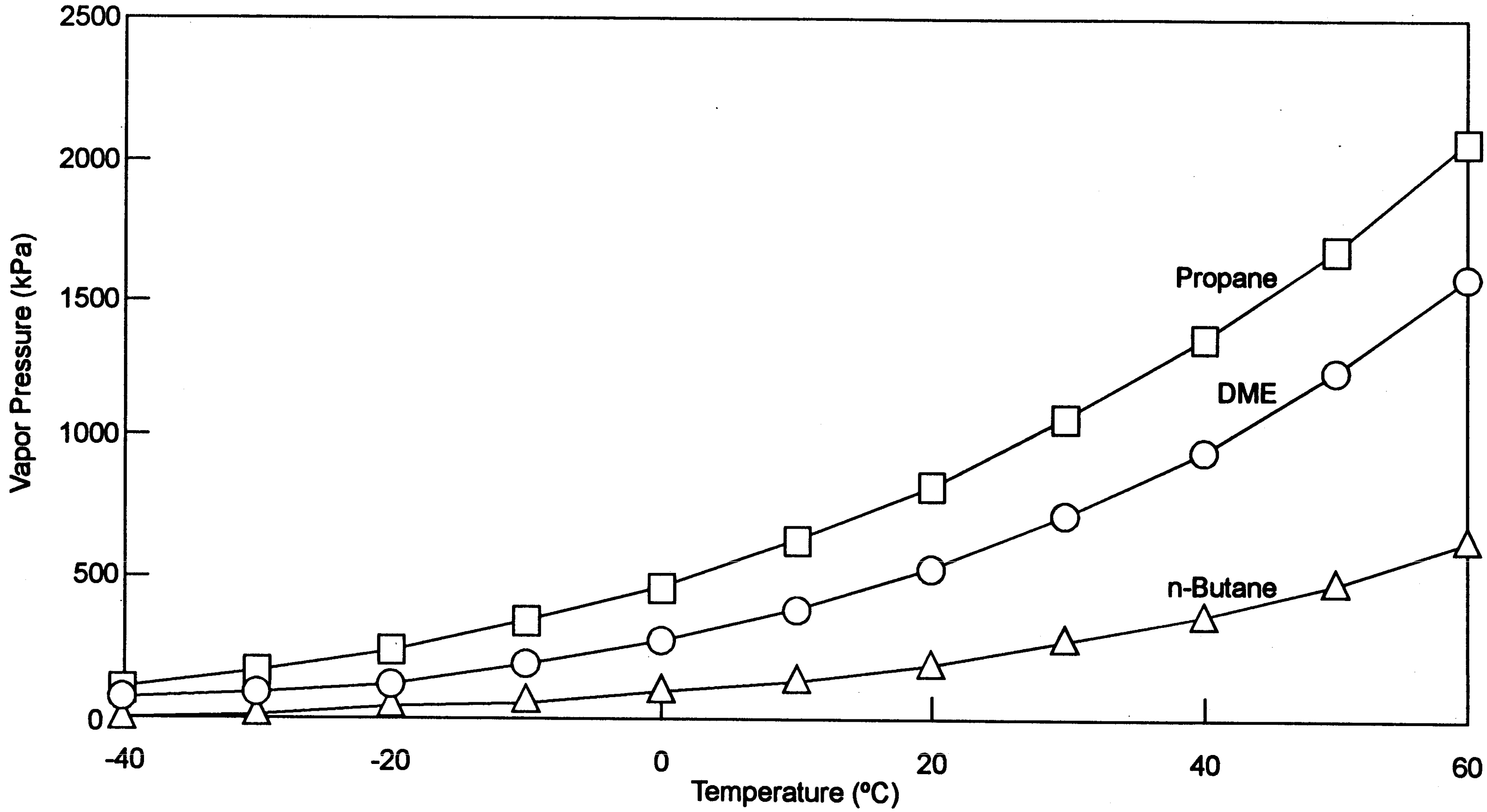
For the most part, discussion in the literature of the distribution and dispensing requirements for DME has been glossed over with the simple statement that the requirements "will be similar to those for LPG," or "will be exactly like those for LPG."

A comparison of the vapor pressure curves for DME, propane and butane (Figure 5) obviously suggests that tank pressure design criteria will be similar. The vapor pressure curve for DME falls between those for propane and butane--the two major constituents of LPG.

Other factors must be carefully considered, including the rate of decrease of liquid density with temperature (see Figure 1). This fixes the amount of ullage space required to be left in a tank after refueling so as to allow for liquid phase expansion. Another important subject is the compatibility of DME with materials used in seals and gaskets, pumps, valves, pressure relief devices, metering devices, level detection devices, etc. Reference 69 notes that the typical rubber refueling hose used with LPG vehicles would be unsuitable for DME.

FIGURE 5

VAPOR PRESSURE OF DME COMPARED TO LPG



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ONBOARD FUEL STORAGE AND SUPPLY SYSTEM

PURGE SYSTEM

Similar to systems for LPG, DME is held in the saturated state in the vehicle fuel tank. This means that the lowest pressure existing in the DME system is the saturation pressure which, at 20°C ambient temperature, is about 5 atmospheres. If this pressure would remain in a conventional diesel injection nozzle during engine shutdown, DME would certainly leak into the combustion chamber because the injector needle valve seal is a metal to metal contact. Compared to LPG this leakage is more of a problem with DME because it would then self-ignite uncontrollably during the next engine start (25).

It may therefore be necessary to depressurize the injector during normal engine shutdown. One way of doing this (25) is to provide a low pressure reservoir or purge tank. In both the purge system and the decompressed parts of the injection system, the DME is in a gaseous state. A compressor is required to recompress the gas into the storage tank and to control the purge tank pressure below a certain level (approximately atmospheric pressure). The compressor is not driven by the engine but by an external drive which is also able to operate when the engine is shut down.

Purge systems are being provided for prototype systems used in vehicles. It is not possible to say whether such systems eventually can be avoided while maintaining adequate safety standards.

LOW PRESSURE FUEL PUMP

In other respects, it appears that an onboard fuel system based upon LPG technology which has been modified to be compatible with DME should be suitable. Fuel must be provided as a subcooled liquid to the injection system. Any flashing at the intake to the injection pump must be avoided. Otherwise fueling problems occur and cavitation can damage the pumps.

Within the storage tank the fuel is usually kept in the saturated state, and tank pressure is determined by the vapor pressure of the fuel. A subcooled liquid state at the inlet of the injection pump is achieved by increasing the pressure of the saturated liquid fuel using a pump which preferably is located inside the tank (to eliminate leakage).

TANK DIMENSIONS

As with LPG, refueling systems must be designed so that a maximum of about 80 percent of the storage tank volume may be filled with liquid. The remaining gas volume is necessary to stay within reasonable pressures if the ambient temperature increases and the liquid volume expands.

This necessary extra tank volume, or ullage space, is sometimes overlooked when comparisons are made between various alternative fuels. It results in extra weight and volume allocations for the fuel system from the total available vehicle design space. Liquid fuels or compressed gaseous fuels do not have the same problems.

DESIGN OF INJECTION SYSTEMS FOR DME

The major technical problem to be solved for commercial use of DME in diesel engines is the design of a direct injection system (21, 25, 26, 64). The technical issues include:

- Because of the lower volumetric energy content of DME, approximately twice as much fuel has to be injected.
- DME has a much lower viscosity (0.25 centistoke) than diesel fuel (2.5 centistoke) and has poor lubricity, resulting in low durability.
- The high vapor pressure and low viscosity causes leakage through injection needle valves, pump seals, etc.
- The high compressibility of DME and its high variability with temperature along with the low viscosity cause pressure oscillations and variable injection pressures.

Solutions to these problems are under development at AVL Powertrain Engineering (26), AVL List GmbH (21), Advanced Engine Technology and Volvo .

INJECTION PRESSURES

DME does not produce soot emissions, and because it immediately vaporizes upon injection into the cylinder, high injection pressures are unnecessary. The pressure requirements are dictated primarily by the needed differential pressure across the nozzle to produce the required fuel delivery rate, and by nozzle opening and closing pressure considerations.

Required injection pressures (250 bar) are only about one-fifth those required to achieve low particulate emissions in diesel engines.

Lower injection pressures mean that lighter and less expensive injection systems can be developed.

ENVIRONMENTAL LIFE-CYCLE ANALYSIS

Environmental life-cycle analyses, comparing DME to other fuels, have been carried out (66, 102, 114). Global Assessment of Dimethyl Ether as an Automotive Fuel was published by TNO Road-Vehicles Research Institute in 1996 (114). A synopsis of that report follows.

POSITION OF DME IN WORLD ENERGY SUPPLY

DME can be made from a variety of carbonaceous energy sources. Among these are natural gas, coal, crude oil, oil sands and renewable sources such as wood, straw and crop residues. From a CO_2 emissions point of view, DME can best be made from biomass or natural gas.

For future energy supply, it will be necessary to start exploiting "remote" natural gas sources. DME is especially interesting when the energy is needed as a transportation fuel and when it has to be transported over increasingly long distances.

EXHAUST EMISSIONS WITH DME

DME appears to be an excellent fuel for diesel-cycle engines (compression ignition).

For light-duty engines a comparison was made with 1993 production engines fueled with diesel, gasoline, LPG and CNG. It was found that the DME engine can have the same NO_x emissions level as Otto engines with three-way catalysts. With medium- and heavy-duty engines the NO_x emission of the DME engine over the European R49 test cycle is in the same range as the lean-bum gasoline engines.

The CO and HC emissions levels are low when an oxidation catalyst is used. However, without catalyst they are somewhat higher than the engine operating on diesel fuel.

With respect to non-regulated exhaust emissions:

- Because of the simple molecular structure of DME no significant emissions of polycyclic aromatic hydrocarbons or BTX should occur.

- Because of the oxygen atom in the DME molecule, there is some risk of emissions of lower aldehydes (as with methanol and ethanol).

- SO_2 emissions will be low because of the absence of sulfur in DME.

WELL-TO-WHEEL COMPARISON

With respect to energy efficiency and CO_2 emissions, a "well-to-wheel" comparison was made using different fuels.

Overall energy efficiency with DME is lower than with diesel fuel because of the relatively high losses (almost 30 percent) occurring during production of DME from natural gas. Compared to other fuels in Otto-cycle engines, however, there is compensation because of the high diesel-cycle efficiency.

For light-duty vehicles the overall well-to-wheel energy efficiency of DME is about the same as with gasoline and CNG, but much better than methanol (16.4 percent versus 12.5 percent). With heavy-duty vehicles the overall energy efficiency using gas engines, especially the lean-burn engines, is better than with DME. For urban bus application the numbers are: DME 19 percent, CNG lean-burn 22 percent, LPG lean-burn 24 percent and diesel fuel 26.5 percent.

Carbon dioxide emissions are primarily dependent on the energy efficiency and the hydrogen to carbon ratio of the feedstock. In the well-to-wheel comparison with light-duty vehicles DME together with diesel fuel and CNG are the lowest CO_2 emitters (Figure 6). With heavy-duty engines DME is still about equal to diesel fuel, but CNG and LNG are 5 to 12 percent lower (Figure 7).

The lowest CO_2 emissions are naturally achieved when the fuel is made from renewable feedstock. This is possible for DME, methanol and ethanol. In that case the net CO_2 emission drops to 20 to 40 percent of the diesel fuel value (Figures 6 and 7).

FIGURE 6

WELL-TO-WHEEL NET CO_2 EMISSIONS FOR LIGHT DUTY VEHICLES (Mix of Urban, Suburban and Motorway)

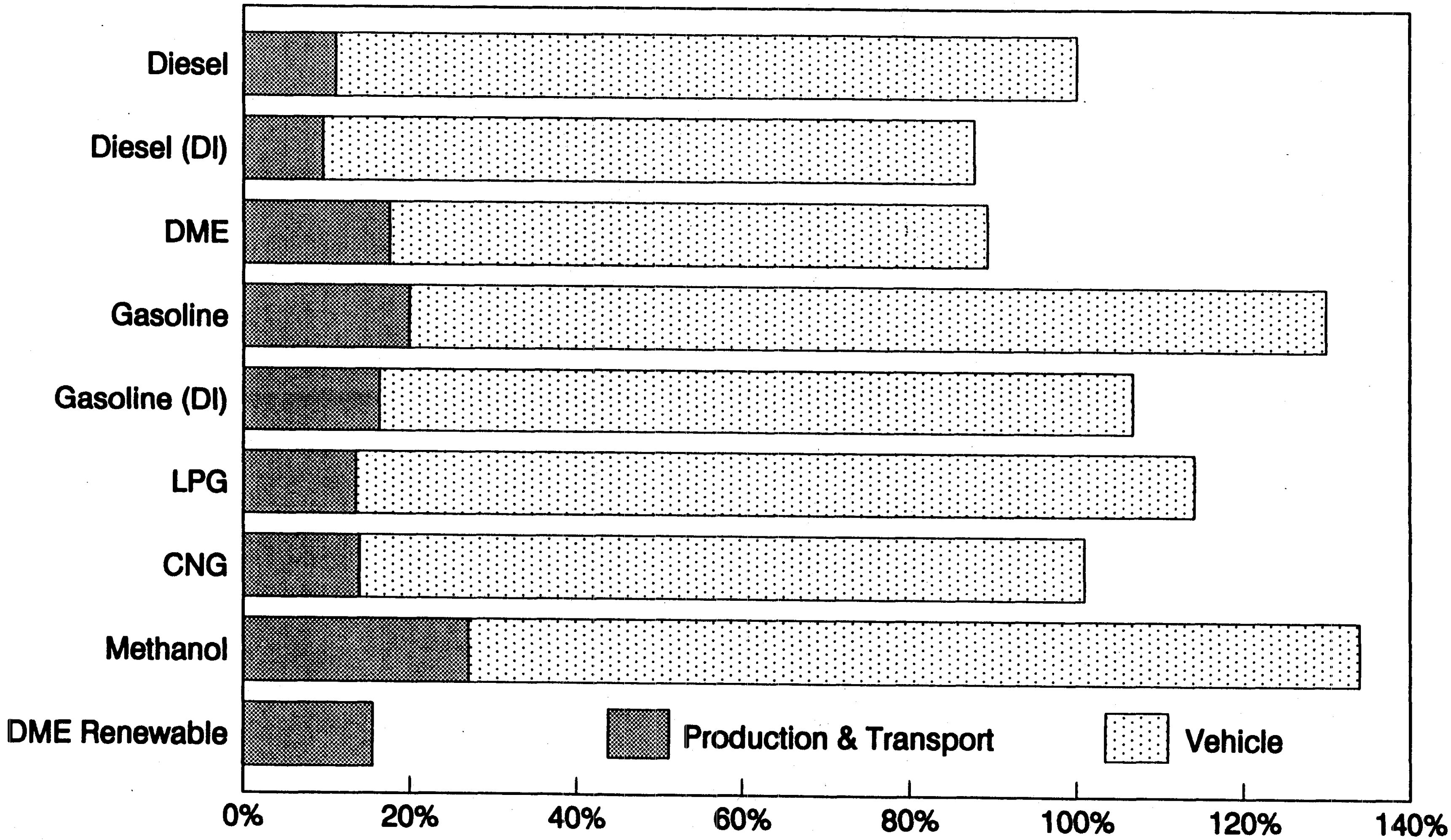

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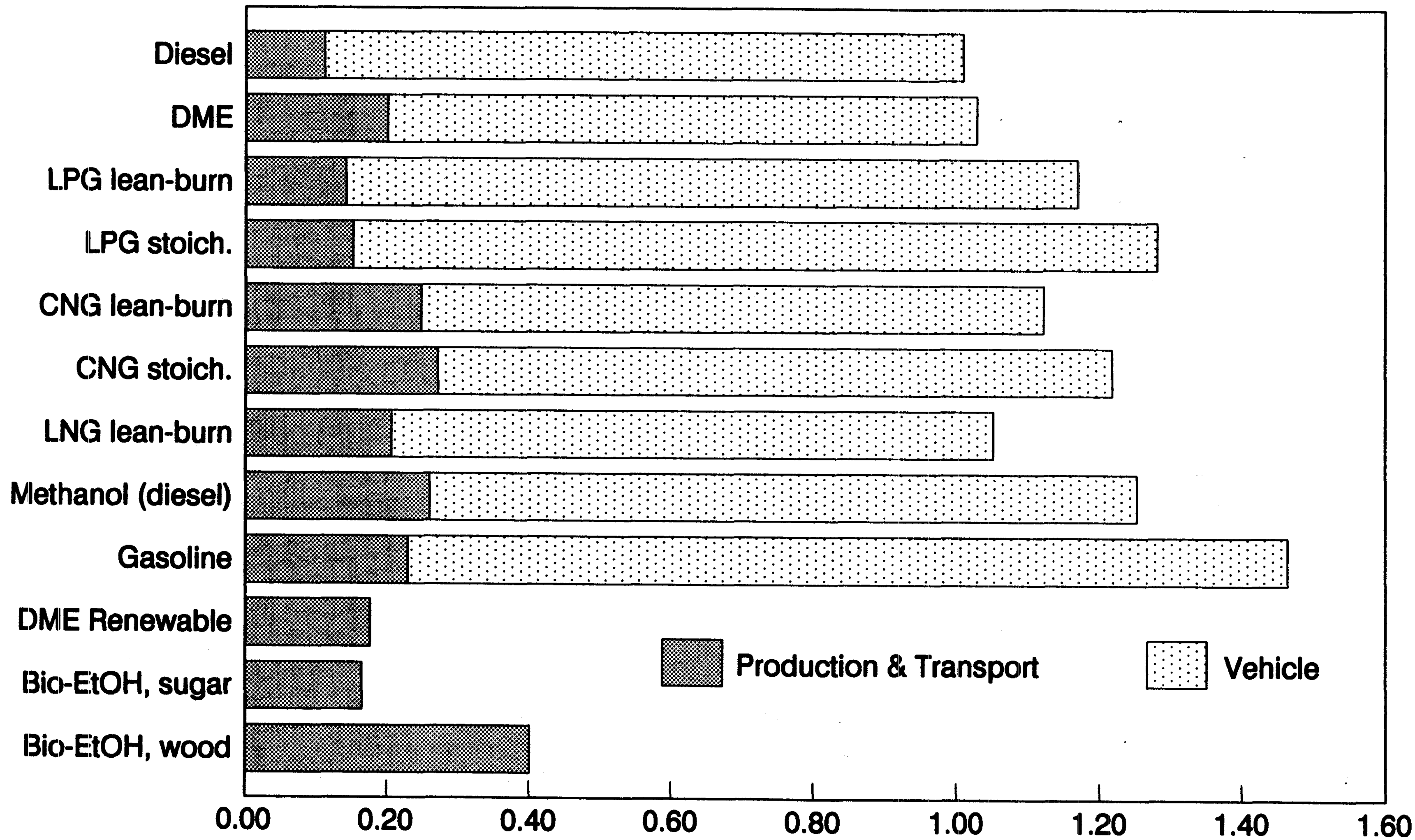
FIGURE 7

WELL-TO-WHEEL NET CO_2 EMISSIONS FOR HEAVY-DUTY VEHICLES (Urban Bus Application)



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DME PRODUCTION PROCESSES AND COSTS

There is a long history of commercial production of DME. However, in the current process, it is made by dehydration of methanol. This means it would always be more expensive than methanol. Current market prices for DME are about US$0.90 per kilogram, or roughly US$2.27 per gallon. In order for DME to find a place in the transportation energy system, a lower cost process will be necessary. Haldor Topsoe has developed one such process (23).

Current world production capacity for DME is around 150,000 metric tons per year (mtpy). The methanol dehydration process provides DME of the high purity required by the aerosol industry.

Despite the present limited production of DME as an end-product, it is an important intermediate in the manufacture of synthetic gasoline, in the synthesis of light olefins and more recently, in a novel process for the production of acetic acid and acetic anhydride.

Large-scale standalone production of DME would be based directly on synthesis gas (a mixture of hydrogen and carbon monoxide). Such synthesis gas can be generated from almost any carbon-containing material ranging from hard coal and heavy refinery residues to biomass. At present, DME production from natural gas represents the lowest energy and investment alternative and can take advantage of the abundance of cheap natural gas.

Haldor Topsoe's approach is to combine methanol and DME synthesis into one single process for the conversion of synthesis gas directly into DME. This is done by permitting the methanol, water gas shift and dimethyl ether reactions to take place simultaneously.

In the conventional methanol synthesis, methanol yield is restricted by an unfavorable equilibrium which requires high synthesis pressure (80 to 120 bar) in order to reach an acceptable conversion. The introduction of the dimethyl ether reaction serves to relieve the thermodynamic constraints inherent to the methanol synthesis by transforming the methanol immediately into DME. In this reaction the formation of DME is favored by equilibrium. The combination of these reactions results in a strong synergistic effect which dramatically increases the synthesis gas conversion level.

Haldor Topsoe developed a new dual catalyst system and built a 50 kilogram per day DME pilot plant at the Haldor Topsoe facilities in Copenhagen, Denmark.

EARLY MANUFACTURE OF DME

The early introduction of DME as a diesel fuel substitute is most likely to take place by increasing the capacity of small methanol dehydration plants, perhaps also by revamp of existing methanol plants for DME coproduction or manufacture of DME as primary product. Basically, the revamp of an existing methanol plant into coproducing DME can be done quite simply by replacing the methanol catalyst in the existing reactor with the dual function DME catalyst.

In the longer term, however, large, new, standalone DME plants based on natural gas are the most economical route.

STANDALONE DME PLANTS

According to Haldor Topsoe (23), an economical scale of production of DME for use as an alternative diesel fuel would call for standalone DME plants ranging from about 2,500 to 10,000 mtpd capacity.

In this context it is relevant to consider the technology for large methanol plants because the process layout for methanol and standalone DME plants is quite similar. A typical investment breakdown by major units would be (23):

- Synthesis gas preparation, 53 percent
- Synthesis loop, 8 percent
- Distillation section, 14 percent
- Utilities, 25 percent

It is clear that the selection of the synthesis gas preparation technology is of the utmost importance because it accounts for more than 50 percent of the total investment.

A conceptual DME process would consist of the following main steps:

- Desulfurization of the feed gas
- Autothermal reforming
- CO_2 removal
- Combined methanol and DME synthesis
- Final purification unit

COMBINED METHANOL AND DME SYNTHESIS

The synthesis takes place over the multiple function methanol/DME catalyst in a loop comprising three adiabatic reactors with interstage cooling to attain a high conversion of CO and CO_2. The selection of three adiabatic reactors with interstage cooling rather than a cooled reactor layout is made for economical reasons. For capacities greater than 1,000 to 1,500 mtpd, adiabatic reactors are the cheapest. Furthermore, by using spherical reactors, a single loop can be constructed with a capacity of up to 10,000 mtpd.

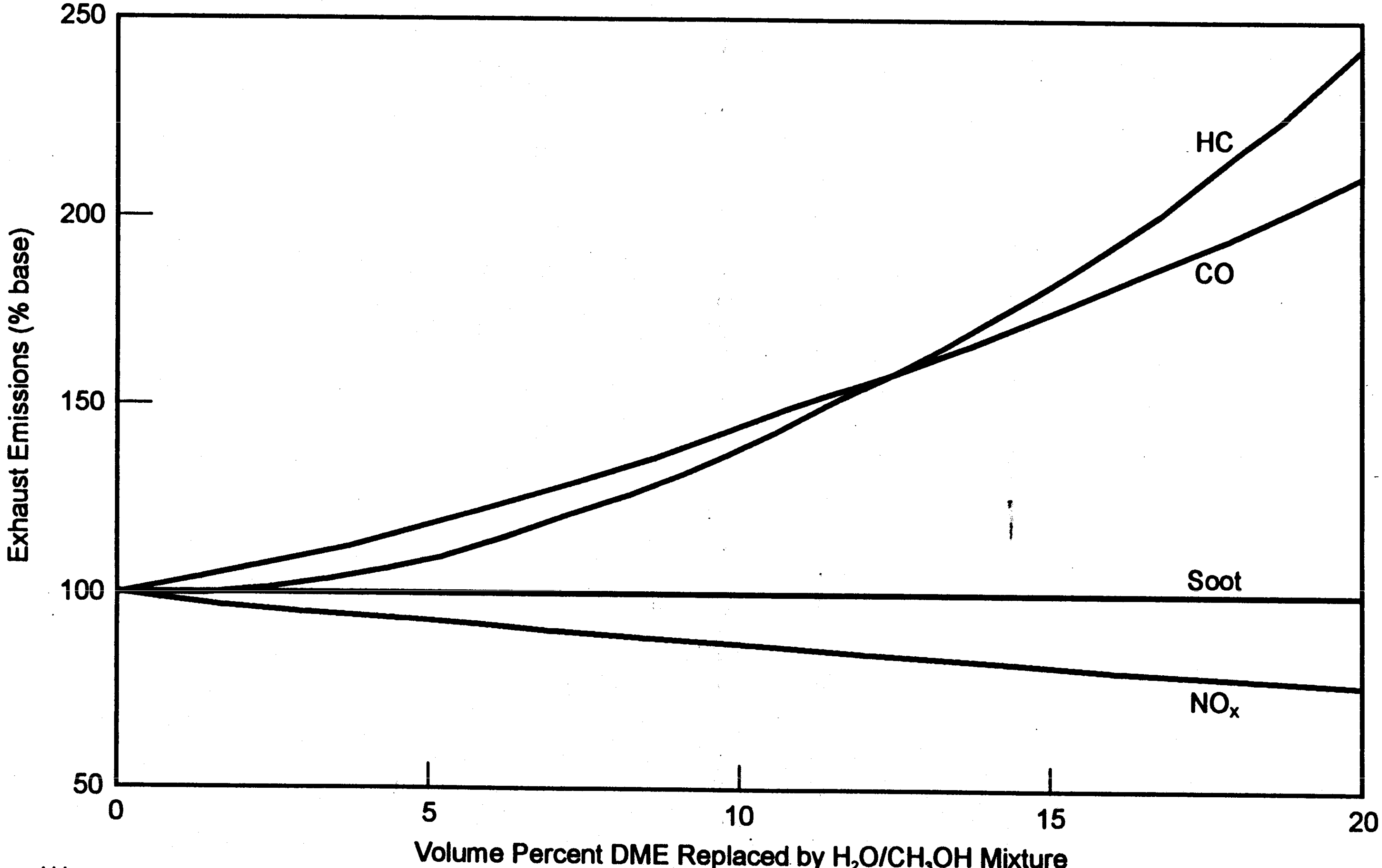
PRODUCTION OF FUEL-GRADE DME

Considerable cost savings are possible if high-purity DME is not required. The synthesis process naturally produces a mixture of DME, methanol and water.

The effects of water and methanol dilution were determined by repeating the 8-mode emissions test using fuel diluted with 3 percent water and 3 percent methanol (6 percent total dilution), and then with 10 percent water and 10 percent methanol (20 percent total dilution). Figure 8 shows the effects of this fuel dilution on emissions.

FIGURE 8

EFFECT OF DME DILUTION BY EQUAL PARTS OF H_2O & CH_3OH



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Overall, these data show that relatively large amounts of dilution can be tolerated without exceeding the ULEV emissions regulations.

Additional studies were performed to determine the ignition qualities of DME. Various mixtures of DME, methanol and water were tested to see if they would give satisfactory ignition and engine operation. The results are shown in Figure 9.

For mixtures without water, suitable ignition is obtained with methanol concentrations up to 19 mass percent. The addition of water reduces the area of good ignition. In the case of water addition to DME alone, two liquid phases are formed above 6 mass percent. Results suggest that it should be possible to satisfactorily use typical technical grades of DME.

Optimization results for different DME plant designs producing both pure DME and a fuel-grade DME are summarized in Table 12.

COST OF DME VERSUS DIESEL FUEL

Assessing the difference in production cost of DME and ordinary diesel fuel depends on assumptions about several parameters, including:

- The relationship between crude oil and natural gas prices
- The actual natural gas price for the DME plant
- The capacity and location of the DME plant
- The return required on the investment capital
- The cost of ocean freight
- Added transport to station and station costs
- Added vehicle costs

The comparison is complicated further because it is debatable whether one should use the cost of diesel fuel from an already depreciated refinery complex or the cost of a low-sulfur diesel fuel from a new refinery complex.

Using reasonable assumptions for all of the above parameters, Haldor Topsoe A/S and Amoco have calculated that it should be possible to make DME at a cost "equivalent to the cost of diesel fuel when the environmental benefits of DME are considered" (23).

Based on Haldor Topsoe's extensive experience in syngas production, methanol synthesis and their pilot plant work on DME synthesis, it is claimed that they can build large greenfield DME plants consisting mostly of single-train process units with capacities ranging from about 1,800 to 7,200 mtpd (approximately 10,000 to 40,000 barrels per day of diesel fuel equivalent) without any further plant scaleup studies. The current world-scale methanol plants have capacities of about 2,500 mtpd methanol (equivalent to about 1,800 mtpd DME). The capital cost of such a 42,000 barrels per day plant is probably close to $1 billion.

Figure 10 shows a simplified comparison of end-user costs of diesel, DME and gasoline before tax on the U.S. Gulf Coast. All costs are relative to the cost of diesel fuel manufactured from $18 per barrel crude oil in an existing, paid-off refinery. The diesel

FIGURE 9

IGNITION LIMITS FOR MIXTURES OF DME, METHANOL AND WATER

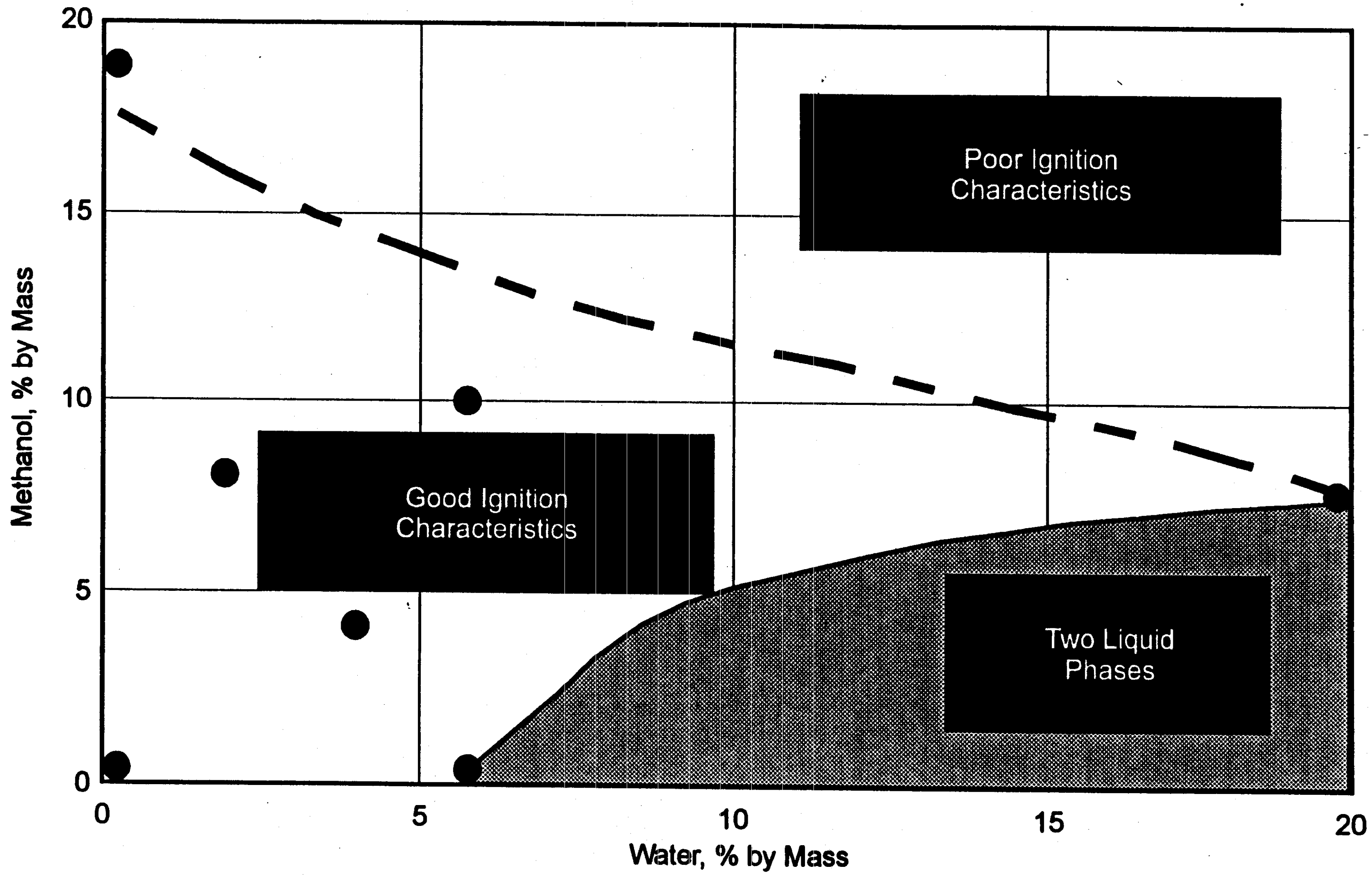

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TABLE 12

COMPARISON OF DIFFERENT PLANT DESIGNS
(Metric Tons Methanol Equivalent)

Capacity MTPD	Product	Relative Investment per MT	Nat. Gas Consumption GJ/MT	Power Export kWh/MT
2500	MeOH	100	30.6	9
2500	Pure DME	96	29.1	76
2500	Fuel DME	92	29.1	76
6000	Pure DME	84	29.1	76
6000	Fuel DME	80	29.1	76

fuel cost was set at 100 with 93 being the plant-gate cost and 7 the cost for transport of the diesel fuel to the service station.

Relative to the diesel fuel cost of 100, the manufacturing cost of DME in a large, new plant in Venezuela, with a capacity of 42,000 barrels per day and natural gas feedstock cost of $0.80 per million BTU, is 78. After ocean shipping of DME to the Gulf Coast, the cost is about the same as diesel fuel. However, this is not the final cost. DME requires a new infrastructure such as pipelines, trucks and pumps, and a retrofit of existing vehicles. All these costs add another 38, and make the DME end-user cost before taxes about 35 percent higher than diesel.

Another comparison shown in Figure 10 is the cost of reformulated gasoline expressed on a diesel gallon equivalent basis. After adjusting for the lower energy content of gasoline versus diesel, and especially for the lower energy efficiency of spark-ignited engines, the end-user cost of gasoline per mile of travel is nearly twice that of diesel fuel in a mixed city/highway driving pattern.

A more attractive picture is shown in Figure 11 for the European market, including all fuel taxes. The pump price of diesel fuel manufactured from $18 per barrel crude oil in an existing refinery was set at 100. DME is produced in a large plant in the Middle East with the feedstock cost of $0.80 per million BTU. Because of the high tax load, the pump price of DME, including the cost of infrastructure and retrofits, is only about 6 percent higher than diesel fuel. Gasoline is, again, overall more expensive than either diesel fuel or DME.

According to economic studies by Amoco, DME will cost more to make than diesel fuel on an energy equivalent basis, but less than methanol or ethanol. Costs could be

FIGURE 10

DME ECONOMICS: END-USER COSTS BEFORE TAX (Year 2000, U.S. Gulf Coast)

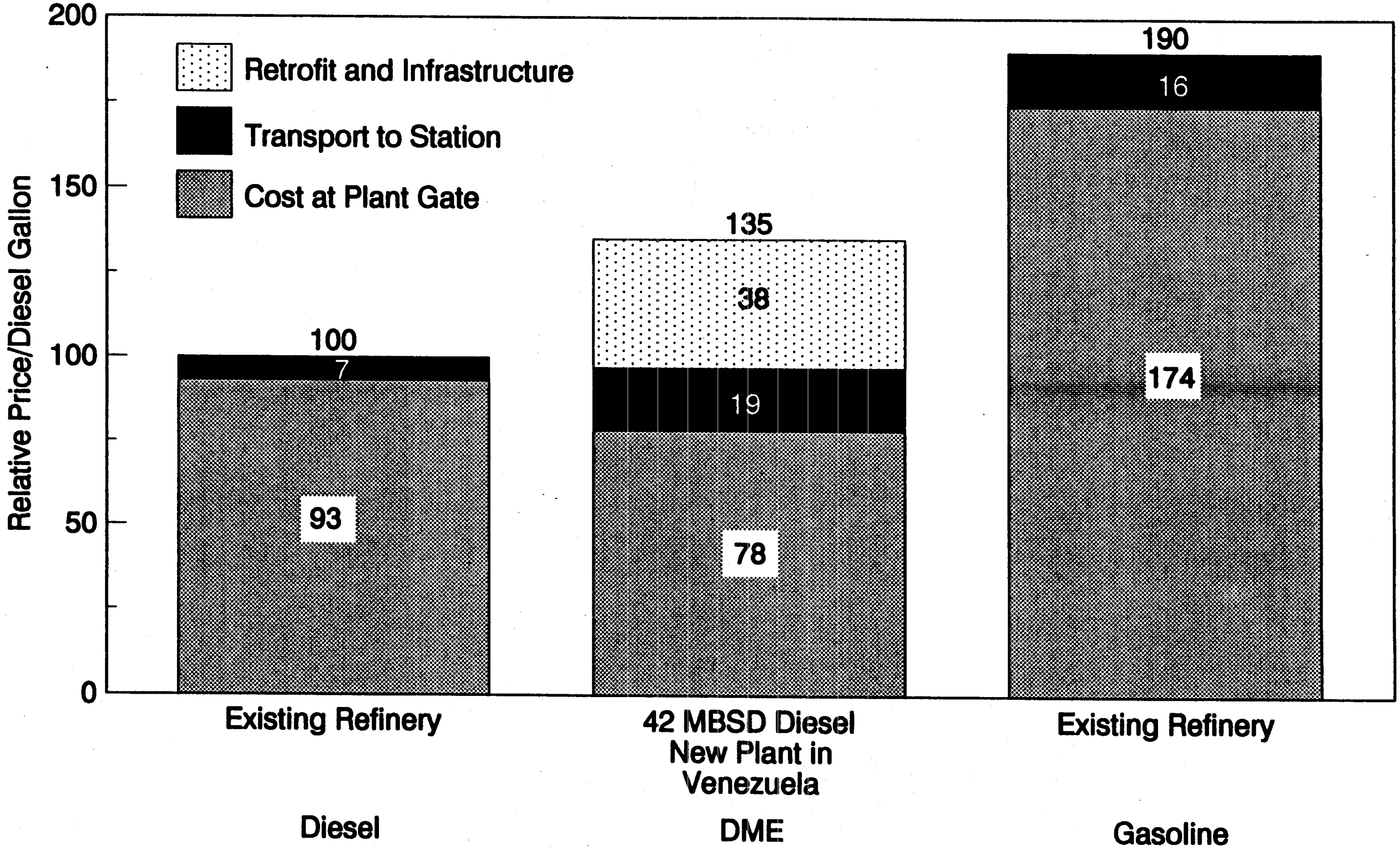

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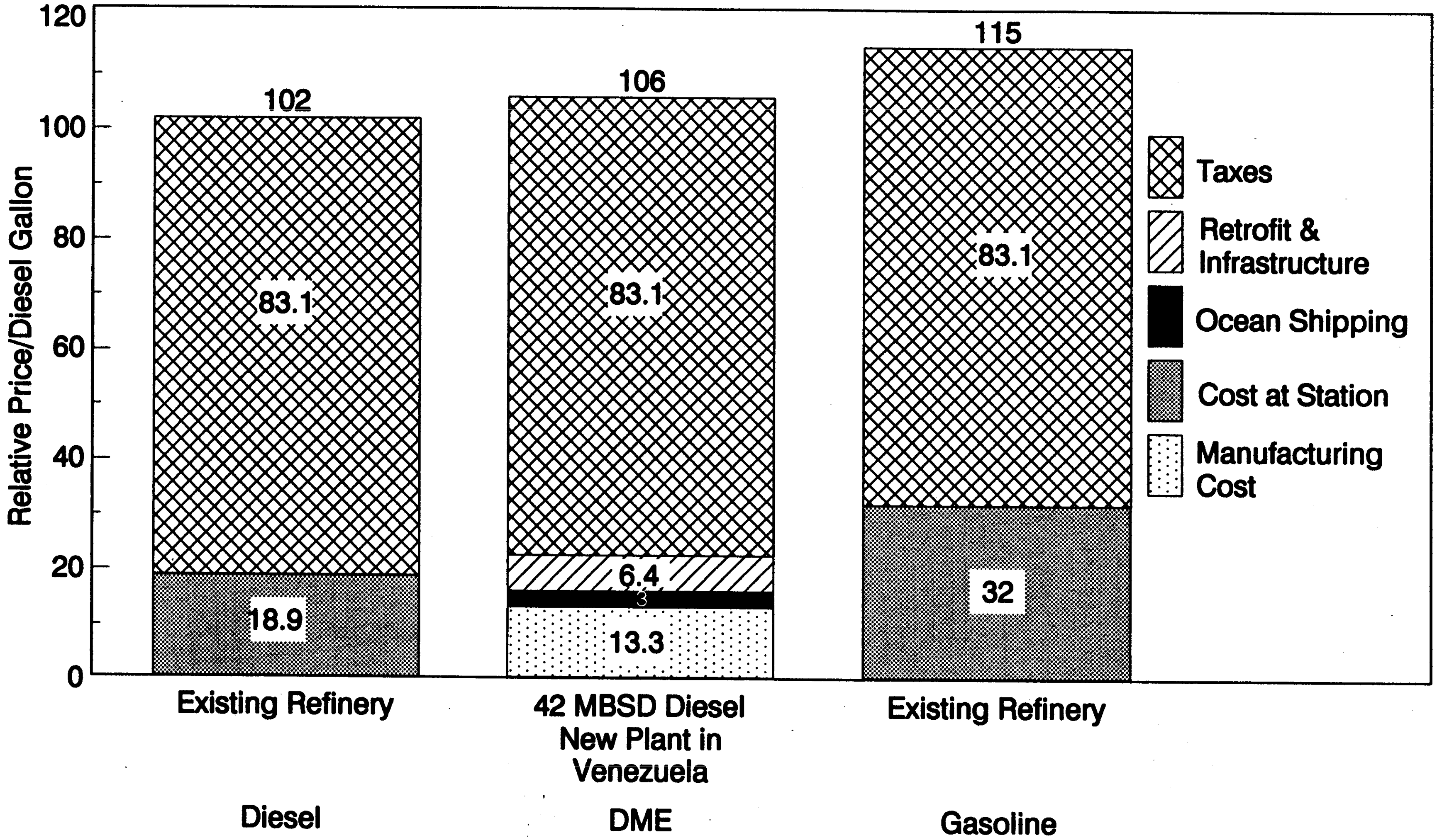
FIGURE 11

DME ECONOMICS: END-USER COSTS AFTER TAX
(Year 2000, European Market)



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similar to compressed natural gas or liquefied natural gas when DME is produced in world-scale production units (46).

OTHER DME PROCESS RESEARCH

Basic research on the reaction chemistry of DME has been under way in laboratories around the world for some time (103, 91, 90, 89, 88, 87, 85, 81, 80, 74, 72, 63, 62, 61, 60, 59, 56, 3, 4, 18, 39, 40 42). In the U.S. in particular, extensive process development work has been carried out by Air Products and Chemicals. Under U.S. Department of Energy sponsorship, Air Products has been developing a slurry phase reactor for methanol synthesis (73, 41, 95, 96, 99, 100, 101). The feasibility of making DME in the liquid phase slurry reactor was first demonstrated in 1991.

The most prolific center of DME synthesis research is the Chemical Engineering Department at the University of Akron (16, 13, 15, 11, 12, 10, 8, 9, 7, 6, 5, 1, 65, 94, 97). Lee and coworkers have investigated a number of processes involving DME, such as:

- DME to hydrocarbons
- DME from CO_2-rich syngas
- DME to oxygenates
- DME to olefins
- Single-stage DME synthesis
- Dual catalyst, DME/methanol
- Liquid phase DME
- DME from CO-rich syngas
- DME to petrochemicals
- Coproduction of DME and methanol
- DME to gasoline

At this point it seems that the chemistry of DME production and use as an intermediate is fairly well known. Process refinement and optimization studies will be continuing. However, most of the cost of production is accounted for by feedstock cost and the cost of converting that feedstock to synthesis gas. These elements are independent of the synthesis of DME.

Another source of information on DME production costs should be a study carried out for Air Products by Bechtel. The study was based on using the Air Products slurry phase reactor. To date, no details have been released, although it is believed that the study will show DME to be less expensive than diesel fuel from Fischer-Tropsch processes.

Also, Fluor Daniel is beginning a study, funded by Natural Resources Canada, to compare the cost of producing DME via the Haldor Topsoe process to the cost of producing DME via the Air Products slurry phase reactor process.

ONGOING DEVELOPMENT EFFORTS

Interest in DME as a fuel for diesel engines has grown rapidly since the publication of the key papers in 1995. Some of the major threads of DME activities are listed in the following.

INTERNATIONAL ENERGY AGENCY TASK FORCE

Under the leadership of TNO Road-Vehicles Research Institute, a task force has been formed by the International Energy Agency (IEA) under its Implementing Agreement "Alternative Motor Fuels" to put together a comprehensive program of Research and Development for DME. The task force last met in March 1997 in Charleston, South Carolina. It hopes to reach agreement on a statement of work and funding commitments from several national governments sometime this year. Joint research is proposed to be carried out in the following areas (27):

- Fuel quality evaluation and definition of fuel standards
- Fuel costs during market introduction
- Fuel properties and characteristics
- Materials compatibility
- Life-cycle analysis
- General safety evaluation
- Design guidelines

According to the IEA, the most important reasons to stimulate the development of DME are:

- Energy security: DME can be produced from a variety of feedstocks such as natural gas, coal, heavy crude oil, heavy residual oil, coal, waste and biomass.

- Clean and efficient transportation fuel: DME combines high (diesel cycle) engine efficiency with exceptionally clean exhaust gases.

AVL LIST PROJECTS INVOLVING DME

At AVL List GmbH several projects involving DME are ongoing. These involve both in-house work supported by AVL and other client-supported projects. AVL is pursuing a comprehensive strategy to provide all the technology needed to get DME vehicles on the road for fleet tests. Several DME-fueled engines are being built for a client-supported project that intends to have both trucks and buses on the road for a demonstration before the end of 1997. Operation of a 1.9-liter auto engine on DME has been studied for Ford Motor Company.

DENMARK DEMONSTRATION OF DME IN BUSES

A project is under way to carry out a fleet trial of DME in public transit buses in Denmark. Volvo is developing the six-cylinder engine technology. Three different transit agencies will test the buses. The first phase, involving one bus at each of the three agencies, is planned to begin around March 1998. Total project budget (exclusive of the engine development funded entirely by Volvo) is about US$2.7 million. The Danish Ministries of Transport and Environment are providing substantial funding.

AMOCO AND HALDOR TOPSOE

These companies are putting together another phase of development efforts concerning production of DME but no details had been made available at the time of writing this report.

NATURAL RESOURCES CANADA

Advanced Engine Technology (AET) is developing a DME injection system. Project funding is supplied by Natural Resources Canada and others. Project participants include Cummins Engines, Chrysler Canada, Robert Bosch, Dupont, Southwest Research Institute and Warner Pumps.

The approach being used by AET is different from that at AVL List and elsewhere, where sophisticated and expensive electronically controlled fuel injection systems are being developed. AET, along with Robert Bosch, is developing a simpler, less-expensive, mechanical injection system. A Chrysler pickup truck with a Cummins 5.9-liter diesel engine that is sold with a propane fuel option will be converted to DME. It is expected that the propane tanks will be suitable for DME. Road tests should begin by the end of 1997.

Natural Resources Canada is also funding four other DME projects:

- Fluor Daniel will compare the estimated cost of producing DME via the Haldor Topsoe process versus the Air Products and Chemicals process.

- A collaborative effort with Amoco will study certain safety issues.

- Blends of DME and propane will be studied.

- In cooperation with Sasol, the effects of methanol and water contaminants in DME will be studied. A question to be addressed is whether there is a critical purity level that affects process economics.

AVL POWERTRAIN ENGINEERING

Using funding from the United States Department of Energy Office of Heavy Vehicle Technologies and the California South Coast Air Quality Management District, AVL Powertrain Engineering is developing a common-rail injection system for DME. A three-phase program is envisioned (64):

- Phase I: Design, simulate, build and bench test a common-rail fuel injection system

- Phase II: Test engine, demonstrate emissions capability
- Phase III: Demonstrate technology in medium-heavy trucks, probably in California

FORD MOTOR COMPANY

In connection with its work on hybrid electric vehicles, Ford is investigating the use of DME as the fuel for a small (1.9-liter) diesel engine. Some of this work has been funded under the umbrella of the Partnership for a New Generation of Vehicles (PNGV). Some engine design work was contracted to AVL List and other work is being done in-house at Ford. At this time, Ford does not consider DME to be the prime candidate for use in meeting PNGV goals, but it will be used as a backup alternative.

GENERAL MOTORS

General Motors' assessment is that the time required to adapt a vehicle to use DME would be less than the time required to develop an infrastructure for fuel supply. Therefore, the auto manufacturers can wait for signs of a developing DME infrastructure before committing to engine development. GM will continue some low-level activity such as comparing the merits of DME versus Fischer-Tropsch fuels.

CHRYSLER

Chrysler has looked at DME as a potential fuel under the umbrella of the PNGV program. The company believes that DME is not a strong candidate at present because of infrastructure and injection unknowns. Because the physical properties of DME are similar to LPG (propane), Chrysler Canada's experience in making factory-built, dedicated LPG vehicles could be useful.

TANK AUTOMOTIVE COMMAND--U.S. ARMY

The U.S. Army's Tank Automotive Research Center participated in the work at Ford Motor Company and AVL List involving a 1.9-liter engine converted to DME. The Army is not considering the use of DME on its own, but simply wants to be prepared to adapt if the civilian sector should convert to DME in a big way.

BUS DEMONSTRATION IN THE NETHERLANDS

Gastec of The Netherlands is trying to raise funds for a 100-vehicle (probably buses) fleet demonstration in The Netherlands. DME would be produced on-site in a cogeneration application, which should reduce production costs.

TECHNICAL UNIVERSITY OF DENMARK

DME combustion chamber work is being carried out with funds from the Ministries of Environment and Transport.

UNIVERSITY OF CALIFORNIA-BERKELEY

Research at University of California-Berkeley involves engine testing with a variety of ethers and blended fuels. Funding is being provided by the National Renewable Energy Laboratory.

BECHTEL

Bechtel, under subcontract from Air Products, with funding from the U.S. Department of Energy, is preparing a cost estimate for large-scale production of DME using the Air Products slurry phase reactor process. Two cases are being studied:

- Coproduction of DME in an integrated gasification combined-cycle powerplant built next to an oil refinery

- Standalone DME production plant using "remote gas" feedstock

The report is expected to be released by June 1997.

U.S. ENVIRONMENTAL PROTECTION AGENCY (EPA)

The EPA is currently (under PNGV funding) running emissions tests on a variety of diesel fuels, including California reformulated diesel and Swedish "city diesel." EPA plans to add DME to the test schedule sometime this year, but funding has not been approved as yet.

SOUTHWEST RESEARCH INSTITUTE (SwRI)

Southwest Research Institute is studying the concept of "homogenous charge, compression ignition" of dimethyl ether. This would solve some of the problems of trying to maintain DME in a liquid state at all times right up to the injection nozzle.

SwRI has also been working on the basic chemical kinetics and ignition properties of several ethers.

U.S. DEPARTMENT OF COMMERCE

Under the Partnership for a New Generation of Vehicles, considerable effort is being devoted to Compression Ignition Direct Injection (CIDI). Within the CIDI effort there is an alternative fuels advisory group. Research area III for this group concerns dimethyl ether.

SURVEY CONSENSUS ON UNRESOLVED TECHNICAL ISSUES

SUMMARY OF DME BENEFITS

The conversion of specific types of diesel engines to DME fuel has demonstrated extremely low emissions and low noise levels without a loss in efficiency.

Emissions tests have demonstrated the potential to achieve California ULEV standards for medium- and heavy-duty engines. Also importantly, these emissions levels can be reached with a naturally aspirated (non-turbocharged) diesel engine. This suggests that these existing diesel engines can be retrofitted for low-emissions operation on DME.

With conventional diesel engines, there is a loss of efficiency when engines have to be adjusted to achieve low smoke and low NO_x emissions. With DME there is no smoke and little NO_x, so that a DME-fueled naturally aspirated engine could operate at about a 10 percent higher fuel efficiency than a similar diesel-fueled engine (22). The fact that there is no acceleration smoke with DME can be used to improve the load response.

The DME-fueled diesel engine meets California ULEV standards without EGR and without any exhaust aftertreatment. If cooled EGR is used with DME, it is believed that NO_x emissions can be reduced to 1.0 gram per brake horsepower-hour with practically no increase in particulates but with some loss in fuel economy.

With conventional direct-injected diesel engines, improved fuel atomization leads to a reduction of soot and therefore to reduced particulate emissions. This improvement in atomization is obtained by increasing the injection pressure and reducing the diameter of the spray holes. Diesel engines designed before the era of emissions legislation operated with fuel injection pressures some 800 bar lower than today's engines. Heavy-duty engines meeting future emissions requirements will need injection systems with even higher pressures (28). The peak injection pressures required for passenger car and truck engines are approaching 1,500 to 2,000 bar, while the pressures for construction machinery engines in the lower power ranges will be 800 to 1,200 bar.

With such injection systems, special attention must be paid to the fuel filtration systems to ensure reliability, efficiency and long service life. For example, fuel contaminated with rust particles of 10 to 12 microns or with water can damage injection nozzles and pistons/cylinder liners beyond repair. With DME, much lower injection pressures (250 to 300 bar) can be used, leading to more reliable operation.

DME engines exhibit a lower rate of pressure rise and lower maximum pressure. Thus fully optimized DME engines may have a lighter structure than conventional diesel engines and consequently can be cheaper. The reduced weight will also improve fuel economy.

MODIFICATIONS NEEDED TO ACCEPT DME

DME should be compatible with most direct-injected diesel engines. The key changes that will be needed include:

- Modification of fuel injection system to inject larger quantities of low-lubricity fuel

- Rematching of turbochargers to engine with addition of an EGR system

- New pressurized fuel storage and supply system

SURVEY OF DME EXPERTS ON UNRESOLVED TECHNICAL ISSUES

To ascertain the current status of DME development efforts and to determine a consensus of expert opinion on remaining unresolved technical issues, a telephone survey was carried out in April 1997. The following organizations were contacted: Advanced Engine Technology, Akzo Nobel, Amoco, AVL List GmbH, AVL Powertrain Engineering, Bechtel, ECN--Netherlands Energy Research Foundation, Caterpillar, Ford Motor Company, Gastec, Haldor Topsoe, Innas BV, IEA AFIS, Navistar, Natural Resources Canada, Novem BV, Oak Ridge National Laboratory, South Coast Air Quality Management District, Statoil, Technical University of Denmark, TNO Road-Vehicles Research Institute, U.S. Army Tank Automotive Command, U.S. Department of Commerce, U.S. Department of Energy, U.S. Environmental Protection Agency, Volvo.

Because several persons contacted did not wish to have their remarks published, individual company comments are not listed. However, there seemed to be general agreement on most issues, and there were no widely divergent opinions. Thus the following summary presents most, although not all, viewpoints concerning unresolved technical issues.

Physical, Chemical and Thermodynamic Properties of DME

The properties of DME are well enough known for all engineering needs at the moment with the possible exception of two areas. The first area concerns certain critical data needed for design of sophisticated injection systems. These include:

- Viscosity as a function of temperature and pressure over the whole range of values encountered in the injection system

- Compressibility as a function of temperature and pressure over the whole range and particularly near the critical point

- Orifice discharge coefficients

- Velocity of sound

- Cavitation factors

Although injection systems are being designed with the aid of calculated values for these parameters (obtained from computerized correlations), actual data would be desirable in some cases.

The second area concerns the effect of methanol and water on basic physical, chemical and thermodynamic properties of DME. It is hoped that "fuel grade" DME containing small amounts of methanol and water will be cheaper to produce without sacrificing the favorable engine performance that has been obtained with pure DME.

DME Production Processes and Costs

Most respondents believe that low-cost supplies of DME are of utmost importance if DME is to become a commercial motor fuel. They believe that the work already accomplished at Haldor Topsoe, Air Products, etc. is sufficient to provide the engineering basis for building the next scaleup of a DME production process. True long-term production costs will not be known until sufficiently large plants have been built and operated.

Design of Distribution and Dispensing Systems

No survey participants listed this as an area with major unresolved technical issues. Most, if not all, believe that LPG design experience will be adequate.

Design of Onboard Fuel Systems

No survey participants listed this as an area with major unresolved technical issues. Again, most, if not all, believe that LPG design experience can handle the problems. One unsolved technical issue, but not believed to be major, is whether a purge system will be necessary to remove DME from the injector and injector fuel system during engine shutdown and to capture this material in a purge tank.

Design of Fuel Injection Systems

Almost all respondents agree that this is the key area with unresolved technical issues or barriers. Ways must be found to:

- Avoid leaks through the injector due to DME's low viscosity and high vapor pressure.

- Obtain satisfactory life from injector, valve and pump parts when operating with low-lubricity DME. In one of the early tests (68) the fuel pump was worn out after 500 hours of operation on DME. It is always possible to add a lubricity enhancer to the fuel, but this should be avoided if possible.

Materials Compatibility

All survey participants agree that materials compatibility is a problem for seals and gaskets. DME is a powerful solvent for most elastomeric materials.

Although pure DME is not expected to exhibit corrosion problems such as have been seen with alcohol fuels, fuel-grade DME containing water and methanol is mostly an unknown. Materials compatibility requires more research.

Safety and Health

Survey respondents generally believe that there are no unresolved safety and health issues concerning DME. They feel that experience with LPG will be sufficient for handling safety concerns and that the data accumulated in getting DME approved for aerosol use will allay all concerns about health effects.

Environmental Life-Cycle Effects

Although survey respondents thought the analyses carried out to date were a good starting point, they acknowledged that a more detailed analysis could be useful. Energy consumption and emissions arising from DME production and distribution systems could be analyzed more thoroughly.

Engine Tests

Most survey respondents are associated with, or closely following, some kind of engine test program with DME. They felt that it was important to more closely define the power and fuel economy tradeoffs that are possible with DME-fueled engines. Most believe that DME engines can be optimized to give both lower emissions and better fuel economy than the best diesel fuel engine tuned to meet future emission standards for NO_x and particulates.

Fleet Tests

All survey participants agreed that it is crucial to start getting some on-road operating data with DME as soon as possible. No commitment to commercial production of DME engines or to production of DME itself will be possible until some fleet operating data have been obtained.

As an example, the bus fleet test planned for Denmark is designed to answer the following questions (77):

- Is it possible to retrofit from diesel to DME operation on existing city buses?
- What are the total environmental benefits (air quality and noise) achievable by using DME as fuel for buses?
- What is the overall energy consumption and reliability of DME-fueled buses?
- What is the overall fleet operating cost compared to diesel fuel?
- How is it possible to store, distribute and refuel DME most effectively and safely?

SURVEY OF DME EXPERTS ON THE FUTURE FOR DME

In addition to the questions concerning unresolved technical issues, the telephone survey posed the following questions:

- Where do you think DME is most likely to be used (public transit, heavy trucks, light-duty vehicles, etc.)?
- What do you see as the relative advantages for DME versus clean-burning diesel from Fischer-Tropsch plants?
- Are you considering or do you see a place for DME blends with any other materials?

The responses to the first question were varied. Some replied that they could not yet see a specific market niche for DME. Because DME costs more than diesel fuel, a market niche will develop only if created by legislation. Most survey participants agreed, however, that the market niche for DME will consist of centrally fueled fleet vehicles in urban areas with major pollution problems. Only such areas will be willing to pay the price and develop the necessary legislation. The fleets could consist of public transit buses, of medium- and heavy-duty commercial and industrial vehicles operating solely within the urban area, or of light-duty fleets like taxi cabs.

With respect to Fischer-Tropsch (F-T) diesel, respondents noted that F-T diesel fuel provides incremental improvements in emissions but DME provides a step change. Particulate emissions are not just lower, they are essentially zero. NO_x emissions are not just lower, they are dramatically lower. If new environmental legislation should specify "the cleanest diesel fuel possible," that would be DME. DME is expected to be equal or lower in cost because it is a simpler production process. F-T liquids have the advantage that no engine changes are required and that the liquids can simply be blended into conventional refinery streams.

Several respondents acknowledged that they have studied or considered blends of DME with other fuels, and that patents have been filed, but none seemed convinced that anything other than DME will find a market niche.

IMPACT ON DOE DIESELIZATION STRATEGY

The Office of Heavy Vehicle Technologies of the U.S. Department of Energy (DOE) is working on an integrated national strategy for transportation fuels in which a key element calls for "The Dieselization of America" (115). DOE notes that if the U.S. had dieselized its light-duty vehicle fleet at the same rate as France since the 1970s, in 1992 there would have been a saving of over 0.5 quadrillion BTU (80 million barrels of oil). In addition, carbon dioxide emissions would have been reduced by over 45 million tonnes.

In order to achieve the potential increase in energy efficiency while at the same time increasing energy security and not increasing pollutant emissions, DOE plans to focus on the use of diverse feedstocks to manufacture Fischer-Tropsch diesel fuel. The same efficiency and energy security benefits along with much greater emissions benefits could be obtained by using DME instead of F-T liquids. The disadvantages of DME are that engine and vehicle modifications are required and instead of being able to use the existing diesel fuel infrastructure for distribution it will be necessary to use the existing LPG infrastructure. However, the key point is that infrastructure exists in both cases. Thus it appears that the use of DME could be entirely complementary to the use of F-T liquids. In one scenario, F-T liquids would be promoted for use in existing, heavy-duty and over-the-road types of diesels where a widespread infrastructure is critical. In the light-duty field, where fleet turnover is more rapid, engine and vehicle modifications could be introduced more quickly for use in centralized fleets where infrastructure is less of a problem.

RECOMMENDATIONS

A SEARCH FOR OTHER ETHERS

Dimethyl ether seems to have almost ideal combustion characteristics for a diesel fuel. However, its high vapor pressure creates problems with bulk transport and distribution and with onboard fuel storage and feed systems. Therefore it seems logical to inquire whether there might be another fuel candidate with the same combustion benefits but a lower vapor pressure. Diethyl ether, for instance, has been used as a fuel for race cars.

An elementary consideration of the chemistry of DME suggests that a major reason for the absence of soot and smoke when DME is burned, is due to the fact that there are no carbon-carbon bonds in the DME molecule. Soot and smoke largely consist of carbon-carbon bonds that are difficult to break. If the fuel has no carbon-carbon bonds to begin with, they are much less likely to form during combustion. The only other major alternative fuels without carbon-carbon bonds are methane, methanol and hydrogen. Methane and hydrogen in particular are extremely clean burning, due at least in part to their gaseous state; but none of the 3 make a good diesel fuel.

Other than DME the only way to make an ether fuel without carbon-carbon bonds is to make a linear polymethoxy compound. The first compound in this series would be dimethoxymethane or methylene dimethyl ether (CH_3-O-CH_2-O-CH_3). The common name for this compound is methylal, and it finds use as a solvent. Its boiling point of about 108°F would make it much more convenient to handle as a fuel than DME. However, higher molecular weight generally brings higher possibility of unfavorable toxicology. Moreover, the high vapor pressure of DME is one of the factors that improves atomization and makes it possible to achieve good combustion and low emissions without relying on high injection pressures. The high vapor pressure also means that liquid fuel is less likely to accumulate in the cracks and crevices within the combustion chamber and lead to emissions of unburned or partially burned fuel late in the cycle.

Technologists working with DME are somewhat divided as to whether its favorable combustion behavior is due to the vapor pressure effects on atomization and mixing or due to the chemical combustion effects arising from DME's high cetane number. Undoubtedly, both are important, and while going to a higher molecular weight, lower vapor pressure ether such as methylal could preserve the cetane advantage, the atomization advantage would be lost. Also, the fuel could be more toxic, and it would undoubtedly be more expensive.

DME's high vapor pressure could actually be considered a blessing in disguise because it will require totally enclosed fuel storage and handling systems. DME vehicles will therefore qualify as Inherently Low Emitting Vehicles (ILEVs) because there will be no evaporative fuel losses.

If there are advantages to be gained by considering ethers other than DME, they are likely to be proposed by industry. There is believed to be a great deal of activity at the moment with respect to patent applications in this area. From an overall viewpoint, there appears to be no need at this time to focus a large effort on an ether other than DME. The United States Department of Energy, through the National Renewable Energy Laboratory, is already funding some research in this area at the University of California. Some investigation of methylal is certainly warranted; less with respect to other ethers. Any candidates other than DME would not be so fortunate with respect to having already available the great mass of toxicology data that was there for DME.

DESIGN OF INJECTION SYSTEMS

The primary technical barrier to the use of DME as a replacement diesel fuel, is the availability of a proven, durable, reliable, fuel injection system. The fact that DME is a liquefied gas rather than a normal liquid, introduces a number of technical challenges.

Because the major vehicle manufacturers are not yet convinced that there will be a market niche for DME, they are reluctant to invest the funds and time required to solve the technical problems associated with direct injection of DME. The outstanding environmental benefits possible with DME suggest that government support for injection system development is well justified. Strong support in this area is recommended.

Some work is already supported directly by the United States Department of Energy, and other work is supported somewhat indirectly by the Partnership for a New Generation of Vehicles (PNGV) program, which is coordinated through the United States Department of Commerce.. Participation in the IEA effort is likely in the future. All of these efforts should be coordinated so as to avoid duplication and obtain the maximum value per dollar of research funds.

As a supporting task to the injector design effort, a laboratory investigation of certain basic physical properties of DME and its mixtures with methanol and water is needed.

MATERIALS COMPATIBILITY

Materials compatibility (elastomeric materials in particular) is an important factor in designing distribution and dispensing systems, onboard fuel systems, fuel injection systems, and any component that could possibly come in contact with the fuel. This type of applied research sometimes requires appreciable effort that cannot be conveniently fitted into the task schedule and budget for, say, an injection system design project.

SAFETY AND HEALTH

The one possible red flag uncovered by this effort that is not currently being addressed anywhere is the potential detonation sensitivity of DME vapor clouds. If it turns out that special handling procedures are warranted during bulk storage and transfer operations, it would be desirable to have this knowledge as early as possible. Therefore, it seems that a careful review of the operating history of DME production plants to date, and discussions with producers about any past incidents of fire and explosions should be carried out soon.

New testing--perhaps using different techniques--of the detonation sensitivity of DME vapor clouds may be justified.

VEHICLE FIELD TESTS

All survey respondents agreed that field tests are an area in which government support is highly desirable. Fleet tests are expensive and time consuming. For best results they may require participation of various government agencies concerned with such things as emissions, safety and health, etc. Although some field tests are in the early stages of planning, much more needs to be done. It is believed that government participation and government aid in this area could accelerate the achievement of commercial status.

PRODUCTION OF DME

DME process research has been funded in various ways as outlined in this report. Much progress has been made. Although the technical knowledge appears to be available to design large-scale production plants, there is likely to be a period of intermediate need. More DME will be needed at lower cost than can easily be obtained from the present sources of supply. It may be desirable to build a "demonstration plant," larger than a pilot plant, to provide the DME needed for a number of fleet demonstrations and early commercialization efforts. Such a plant is unlikely to be profitable on its own, and could require government support of some type.

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