# PROCEEDINGS OF THE FIFTH ASIA-PACIFIC INTERNATIONAL SYMPOSIUM ON COMBUSTION AND ENERGY UTILIZATION

Shanghai, October 24-29, 1999

Edited by
HUANG ZHAO XIANG
and
Liu Xin



**International Academic Publishers** 

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Edited by

Huang Zhaoxiang and Liu Xin

Proceedings of the Fifth Asia-Pacific International Symposium on Combustion and Energy Utilization

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### PREFACE

After 10 years' cooperation with all the scientists of the field in thermal science we have organized 4 International meeting of Asia Pacific International Symposium on Combustion and Energy Utilization (APISCEU) successfully in Beijing, Hong Kong and Bangkok respectively. More than 500 participants from approximately 40 countries and/or territories gathered together to present papers and discuss mutual interesting problems with great enthusiasm. Scientists from Asia, America, Europe, Africa and Oceania discussed and exchanged their academic ideas and made acquaintance with each other, new friends and old colleagues communicate with each other even after our meetings. This is really my great pleasure through the successful serve in each meeting.

Energy science is intimately connected with thermal science, especially with combustion science, hence a great number of paper on combustion field come to our symposium and deeply interest us for a rather long time. The environmental protection technology is now the most important problem especially in recent 10 years, the air pollution is now more serious than before, the combustion scientists all over the world now prefer to concentrate their attention to air pollution, hence we try to organize a special session "The Environmental Protection Technology and Air Pollution Problem in China", many combustion scientists devote themselves to the air pollution field by using their knowledge on combustion field.

Welcome all the participants from different continents, congratulate the success of our meeting, wish you to increase your new scientific ideas through a serious of discussion, and please enjoy yourselves in Shanghai and other cities in China.

Have a good time with us!

Prof. HUANG, Zhao Xiang Executive Chairman, APISCEU IET/CAS, Shanghai, China July 1, 1999

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### 5th Asia-Pacific International Symposium on Combustion and Energy Utilization

### **Alternative Diesel Fuels**

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It is now almost thirty years since the global oil crises of the 1970s precipitated the search for alternative nonpetroleum fuels. In recent years this on-going search to find cheaper and more readily available alternative fuel supplies has been heightened by the need to address the intensified international concerns about the adverse impacts on global climatic change and public health of petroleum fuel usage. Moreover, even the most optimistic forecasts suggest that the world's crude oil supplies will be exhausted before the middle of the next century. There are, therefore, a number of factors driving the modern efforts to develop alternatives and replacements for petroleum fuels. The two main fuels derived from petroleum oil are gasoline and diesel, the former being the dominant product. Diesel fuels are associated with the compression-ignition (diesel) engine. Such engines are more efficient than gasoline (spark-ignition) engines and emit lower rates of criteria pollutants such as carbon monoxide, nitrogen oxides and unburnt hydrocarbons. Diesel engines are used extensively in commercial transportation and stationary power generation applications and because of their fuel economy are becoming increasing popular in private and light-duty vehicle applications. However, the exhaust gas pollutants produced from the use of current commercial diesel fuels are, deservedly or not, becoming viewed as environmentally unacceptable and as posing a serious health risk. If the diesel engine is going to survive then cleaner, safer fuels must be used. In this paper an overview is presented of some of the wider issues currently being addressed regarding alternative fuel usage and in particular alternative diesel fuels.

Keywords: alternative fuels, diesel engines, biodiesel, DME, CNG

### SETTING THE SCENE

The production of mechanical power from the burning of combustible fuels was a well established technology long before the dawn of the "petroleum age" at the start of this century. Biomass (mainly wood), coal and, to a lesser extent, non-petroleum oils and gases were the primary fuel sources at this time combustion steam engines when the external dominated both stationary power generation and transportation. In fact in terms of global energy production biomass fuel sources dominated until the late 19th century and even today play a significant role in meeting the energy needs of many nations. The industrial revolutions in 18th and 19th century Britain and early 20th century North America were fuelled by coal and muscle-power although petroleum products were available in the late 1800s. However, the invention of the spark-ignition and compression

ignition reciprocating internal combustion (IC) engines in the late 1800s and their rapid development in the first quarter of the 20<sup>th</sup> century especially in the transportation sector not only benefited from the growing availability of cheap petroleum based fuels such as gasoline and diesel oils but in turn the IC engine developments provided the impetus for the exploration of the raw feedstock for the production of such fuels

However, the compression-ignition engine, commonly if not wholly-accurately known as the Diesel engine, can be operated using a number of different fuels which combust in the presence of air or oxygen. Before the arrival of petroleum-based (PB) fuels, diesel engines were designed and developed to operate on fuels derived from coal or vegetable oils and even solid fuels such as pulverised coal. Indeed, in times of crises such as the 1939-45 War, when petroleum fuels were scare or not available, nations

have had to use engine fuels produced from nonpetroleum sources such as coconut oil. Nevertheless, apart from these occasional temporal exigencies, petroleum-based fuels have held a dominant position in the global transportation sector for almost 7 decades and in terms of worldwide energy production has been equally dominant for at least the latter half of this century. By 1996, crude oil and NGPL (Natural Gas Plant Liquids), were responsible for 146 Quad (quadrillion -10<sup>15</sup>) Btu of global energy production compared to 96 Quad Btu from Coal the next most used fuel<sup>[1]</sup>.

As shown in figure 1 as global energy production has increased over the last quarter-century by some 52% so has the use of crude oil increased although as a proportion of the total production, crude has diminished to just over 36% from almost 48%[1]. Moreover, the primacy of fossil fuels is generally confined to the industrialized world and nowhere more so than the United States and Canada. The peoples of latter two countries represent less than 5% of the world's total population but by 1996, over 20 million barrels per day of petroleum were being consumed in North America, almost twice as much as in 1973 and 28% of the present total global production. Consequently, when considering the subject of alternative petroleum fuels, the situation in North America will inevitably be the major focus of the discussions. In terms of the use of diesel fuels in the land transportation sectors, commercial and personal, Europe also plays a very significant role. In particular, the dieselcar is becoming increasingly popular in the countries of the European Union and in Austria, for example, diesel road vehicles have a similar market share to the gasoline fuelled vehicles. In the USA diesel fuel serves primarily the commercial heavy-duty vehicle market.

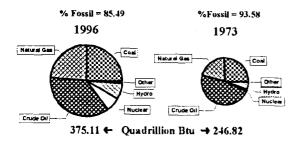


Fig.1 Global energy production

After the 1939-45 War many Western industrialised nations gradually moved to an oil-based economy turning away from indigenous fuel resources

such as coal. Crude oil was cheap, plentiful and readily available not only in North America but also in the Middle East. By the start of the 1970s, global reliance on Middle East supplies had increased as dramatically as the demand for petroleum products had increased in the industrialized nations. However, political changes and instability in the Middle East lead to many foreignowned oil companies being wholly or partially nationalized, and oil producing cartels being formed resulting not only in enormous increases in crude oil prices but also in a series of supply embargoes. Between, 1971 and 1981 (the all-time high) the price of oil rose by almost a factor of five, figure 2. This situation lead to heavily-funded national and international efforts to develop alternative fuels and energy conversion systems with cost and availability being the prime drivers of the efforts. Moreover by the start of the 1980s increasing international concerns were being expressed about airborne pollutants and their possible links with health risks, climate change and global warming.

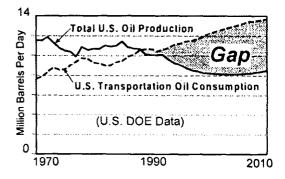


Fig.2 Historical trend - oil prices

However, as can be seen from figure 2, oil prices dropped in the 1980s almost as sharply as they had risen in the preceding decade and research and development funding on alternative fuels and energy systems noticeably diminished. Although a number of technology breakthroughs were achieved the omnipresent barrier to the widespread use of alternative fuels especially in the transportation sector was the "at-pump" retail price. Subsequently, a series of events changed the alternative fuels panorama to what it is today. These were:

- The burgeoning public and political acceptance of the need for pollution control, especially in the personal transportation sector and urban areas.
- The Gulf War, which once again raised the questions of crude oil availability and the political use of oil resources.

The growing "petroleum-gap" in the USA, i.e., the increasing reliance of the USA on imported petroleum products, figure 3.

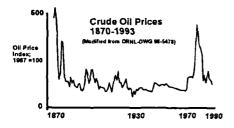


Fig.3 The USA petroleum "Gap"

This combination of factors lead to the formulation of national alternative fuel policies in the USA, the passing of national and international environmental legislation and protocols, such as the Kyoto Agreement, the US Clean Air Acts, the European Union Standards and so on.

Energy demand and consumption are closely linked with the economic activity and the well-being of a nation. The more industrialized countries use more energy both in total and per capita than less well developed countries. Thus, regardless of any nation\*s altruistic or security credos, national economics will play a dominant role driving the development of alternative petroleum fuels. For example, it has been estimated by one source that if the cost of prosecuting the Gulf War and maintaining a military presence since its end is added to the price of crude oil imports to the USA from the Middle East then the "real" cost to the nation of each barrel of crude oil is likely to be closer to \$120 than the \$12-\$18 paid by the oil importing companies<sup>[2]</sup>. It could be argued that such cost estimates are somewhat simplistic but the point to be made is that there is more to fuel costs than the at-pump prices. Public cognisance of such hidden costs are rarely apparent although it is usually taxpayers who will have to pay the bill in one form or another.

Subsequently, market forces of cost and supply invariably play crucial roles in any change from existing practices to alternatives. Interest-group lobbying, public acceptance and Government intervention are also constituent elements in such transformations. Since the mid-1980s comprehensive studies on alternative transportation fuels such as ethanol, methanol, and natural gas have emphasized the significant impact thatchanging crude oil prices have on the market and that, historically, interest in alternative fuels tends to follow

these prices<sup>[3-5]</sup>. However, these relationships are neither simplistic nor straightforward. Over the past thirty years when the profit margins of crude-oil production has been low Governments have intervened in the form of incentives designed to bolster the cash flow of producers of non-renewables to prevent the consequent societal problems such as, unemployment, lower tax revenues and so on. Similarly, when fuel prices at the pump have become too high, regardless of profit margins, Governments have encouraged the search for and development of cheaper alternatives in an attempt to secure significant independence from the vagaries of the oil market and the national security implications of nonguaranteed supplies. However, in many instances the alternatives are only cheaper because of the indigenous tax structure and other Governmental financial incentives. This situation is unlikely to change dramatically for the next decade or two especially in North America and Europe.

In the personal transportation sector, performance level and range of gasoline powered vehicles passenger engines and their life cycle cost provide the benchmarks against which alternative fuels and energy convertors have to compete<sup>[5]</sup>. To-date other than in freight-carrying applications the gasoline powered SI engine has proven to be a formidable, dominating and technologically advanced competitor. This situation has proven to be the main hurdle to the acceptance of alternatives. This barrier is now becoming less surmountable because of the superior environmental characteristics of some of the alternatives and the growing realization and acknowledgment by industry and governments of the crucial importance of such characteristics. Hence, the main factors affecting the acceptance of alternative fuels and energy convertors in the passenger vehicles sector are, in comparison to the ubiquitous gasoline fueled SI engine:

- Relative performance, life cycle cost and technical maturity
- Environmental emission generation especially, Particulate Matter (PM), CO<sub>2</sub> and NOx
- The level of Governmental financial incentives regarding technical developments and usage of alternatives.

In other words, in the personal transportation sector, the diesel engine regardless of the fuel used has an omnipotent competitor - the SI engine. Thus, in this application, the compression ignition engine is still establishing itself an alternative prime mover. A suitable alternative diesel fuel in this sector will not only have to demonstrate advantages over existing PB diesel fuel but also ensure that the compression ignition engine itself can meet the SI benchmarks.

However, even if a technical mature,

environmentally friendly and market acceptable alternative fuel vehicle were available and significant government assistance was provided, the infrastructure costs associated with the production and supply to the consumer may be prohibitive. For example, although the use of natural gas vehicles has increased significantly in the USA there are only just over 1,000 filling stations supplying the fuel nationwide<sup>[6]</sup>. Another factor, often overlooked, is that most of the vehicles on the road are not new and therefore would need to be retrofitted to use the alternative fuel, not only could this be expensive up to \$9,300 for a Ford E-250HD van<sup>[7]</sup> but it could invalidate the warranty of the vehicle and the insurance coverage.

Clearly, as long as there are cheap and plentiful supplies of petroleum based fuels available then the case for the total replacement of such fuels by more expensive alternative fuels and alternative energy conversion systems will require arguments that are economically and politically irrefutable and which have sufficient societal acceptance. Simplistic environmental polemics alone will not suffice. More efficient fossil fuel burning engines and more effective emission regulations devices have ameliorated to some extent both environmental concerns and problems. There is, however, a growing awareness that the regulation and monitoring of tailpipe or stack emissions levels by themselves are only part of the overall environmental canvas. Life-cycle (cradle-to-grave) emissions are a crucial measure of the environmental characteristics of the use of a particular fuel and energy system. For example, as will be discussed later in this paper, while diesel fuel produced from biomass (biodiesel) may reduce some tailpipe emissions, in comparison with the use of PB diesel fuel, the processes which are used to manufacture this alternative fuel may lead to more not less of some of the criteria pollutants being emitted into the atmosphere. Nevertheless from the public's point-of-view they will be as interested, if not more so, in the tailpipe/stack emissions which effect local environmental quality as in life-cycle emissions which are more important regionally, nationally and globally.

In cost terms, apart from the upheavals of the short-lived oil crises of the 1970s, the much shorter Gulf War of 1990, and the market forces caused by the occasional mismatching of supply and demand by OPEC and other oil producing concerns, oil prices has been very stable for the last thirty years. In general, if the price of crude had kept up with inflation in the G7 countries from the 1960s then it would cost in the region of \$70 US per barrel today. In the transportation sector, the rise in the at-pump prices, especially in Europe and particularly of gasoline, is due to national tax policies and not increases in the cost of the raw feedstock or fuel production. However, there is no denying that oil is a

finite stock and although new sources are located every day, existing sources are also being continuing depleted and often exhausted. Although estimates vary widely and wildly, it would appear that the Governments of the large industrialized nations consider that if crude oil is consumed at its present rate then global resources will become exhausted by the middle of the 21st century or maybe a decade earlier. Thus, regardless of economic and environmental precursors there is a need to search for alternative fuels since in the not too distant future omnipresent crude oil products will not be available and will never be available again.

The strategic question for nations with an oil-based economy is when to start looking for alternatives, clearly that question has already been answered in the USA - the time is now- and they are not alone in that assessment. Brazil, for example, has developed a massive biomassethanol production capacity to alleviate its PB gasoline problems. The USA have adopted a pragmatic approach to the gradual replacement of PB diesel and gasoline fuels rather enforce a discrete and rapid change. Consequently a number of different alternatives are being considered. It has also become clear that a single universal PB replacement may not evolve and that the type of replacement could be geographically driven, e.g., in agriculturally fertile areas the replacement fuels could emanate from biomass sources whereas in other areas, natural gas or coal resources could provide the basic feedstock. For the internal combustion engine this means that multi-fuel capabilities could become paramount. Similarly, the use and development of renewable energy conversion systems, such as tidal, solar, hydro and wind power are very regionalised in all countries. At the moment the only obvious universal source of energy is electrical power but discussions on that issue are out of the scope of this paper other than to say that electrical road vehicles are unlikely to replace many, if any, diesel powered vehicles in the foreseeable future.

There are some 200 million diesel engines in use worldwide[8] and in recent years their popularity in the small-to-medium stationary power generation and heavyduty transportation sectors has spilled over to light-duty and personal transportation applications. Initially this trend was driven by fuel economy and then, additionally, by environmental concerns. However, it is now these latter type of anxieties that are causing a reaction against the use of the diesel engine or more accurately the use of conventional PB diesel fuel. Concern over the carcinogens in diesel engine exhausts has been voiced over the last few years especially in the Unites States. PB Diesel fuels also contain more sulfur than gasoline and hence proportionately diesel exhaust makes a greater contribution to the acid rain problem. Thus, apart from the greenhouse gases and the NO<sub>x</sub> issues there are a number of other environmental matters that need to be addressed. In 1998, the US Government levied, after negotiation, a fine of \$1 Billion on US diesel engine manufacturers for emission violations and US Federal laws now require that diesel emissions be reduced by 50% by 2004. It could be then that if alternatives to the currently used PB diesel fuels are not found the demise of the diesel engine itself will be inevitable.

Thus, in summary when assessing the attractiveness and viability of candidate alternative diesel fuels the following factors have to be considered:

- National Strategic Security Policies
- Life-cycle and Local Emissions National and International Compliance
- Personal and National Economic Factors
- Geography and Logistics of Raw Feedstock supplies
- Applicability of Existing Infrastructure and Commercial Off-The-Shelf Technologies
- Competing Technologies

Nevertheless, it is a sobering statistic, as Gerpen and Reitz<sup>[9]</sup> have pointed out, that it is still more cost effective to invest in changes in engine technology rather than all but the most inexpensive fuel changes since the cost of fuel burned by a typical diesel engine significantly exceeds the cost of the engine.

# ENVIRONMENTAL CHARACTERISTICS AND LEGISLATION

In the past alternative fuels have struggled to achieve any significant market share because they were invariably more expensive to produce and could not make use of the existing engines or delivery and distribution infrastructures. Although such economic factors still dominate fuel choice whether for power generation or transportation applications, growing environmental concerns and legislation necessitate that factors other than production costs alone must be considered in future choices. In particular, solutions will have to be found to the problems of achieving the required reductions in so-called greenhouse emissions. improvements in urban air quality and the elimination of health risks associated with fossil fuel usage. As shown on figure 4, despite the successful efforts to improve engine efficiency and design and exhaust after-treatment, the emissions of carbon dioxide - one of the main greenhouse gases - over the last ten years has increased albeit marginally. This trend has been manifest globally and in most of the industrialised countries including the USA and Canada.

In fact North America has consistently accounted for over 25% of such emissions with Canada producing more than countries such as Italy which has almost three times Canada\_s population and almost three-quarters of that produced by the whole of Central and South America. In the USA although some headway has been made in reducing emissions of non-methane VOCs and carbon monoxide, little impression has been made on NOx emissions and carbon dioxide emissions (in terms of metric tons of gas) are 17% higher—overall than they were in 1985. Against this background the Kyoto target of a 7% reduction below the 1990 levels of carbon dioxide emissions by 2012 does not appear to be quite as modest as some perceive.

The environmental attraction of the diesel engine is that is produces lower rates of CO, hydrocarbons and NOx but particulate matter emissions are higher and an increasing cause for concern. The sulphur and heavier hydrocarbons (especially aromatics) content of diesel fuel is much higher than gasoline and the result is a greater tendency to produce particulates especially since the combustion temperatures are lower. In the USA, diesel-powered vehicles produced almost 63% of the particulate matter emissions from highway vehicles, some 172,000 tons(short) in 1996 alone. Of this total 59.1% was from heavy-duty trucks<sup>[10]</sup>. The US Federal Emission Control Requirement from 1998-on for PM for such trucks is 0.1 grams/bhp-hr, six times less than the benchmark of a decade ago and since 1995 the PM requirement for automobiles and light-duty trucks has been 0.08 grams/bhp-hr.

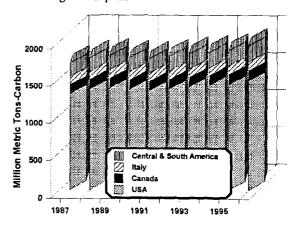


Fig.4 CO<sub>2</sub> emissions 1987-97

In terms of sulphur emissions - once again in the USA - the transportation sector contributes only 3.5% of the total but PB diesel contains more than 90 times the sulphur of PB gasoline. Almost 90% of all SO<sub>2</sub> comes from stationary source combustion (heavy oils and coal). Thus, there are efforts to produce even lower sulphur PB diesel fuels for both transportation and stationary power generation purposes. In a recent press release, 2 July 1999, BP-Amoco announced they are to make available

an Ultra Low Sulphur Diesel (ULSD) in Paris, France from September 1999. This PB diesel fuel will be provided at no extra cost and it is claimed will reduce sulphur emissions by 90%, meet the anticipated 2005 EU emission standards and enable new PM technologies to be fully effective. The chemical composition of many alternative diesel fuels is such that the sulphur emission problem would become a non-issue but the PM problem will still persist in many cases.

Many nations and international groups are legislating for increasing stringent environment standards both for light duty and automotive vehicle emissions and stationary power generation. Imposed emission standards have been to slower to appear for the heavy duty land vehicles and marine engines but are now rapidly catching up. Thus, there are a multitude of regulations available specifying allowable current and future emission standards some of which are fuel specific. The challenge for engine and alternative fuel systems designers is demonstrated very clearly by the California regulations, Table 1. This US state has been setting the benchmarks for environmental air quality for a number of years and is a region that has exhibited a growing political and social intolerance to the internal combustion engine.

Table 1 California	Air Resources Board
Standards	for LEVs

Vehicle Type Passenger Cars and	Emission Reduction From Basic Standards				
Light-Duty Trucks	(www.arb.ca.gov)				
	HC	CO	NO <sub>x</sub>		
Transitional Low-	50%	<b>©</b>	<b>6</b>		
Emission		to	to		
		Basic	Basic		
Low-Emission	70%	<b>B</b>	50%		
	1	to			
		Basic			
Ultra-Low-Emission	85%	50%	50%		
Zero-Emission	100%	100%	100%		

### CANDIDATE FUELS AND SYSTEMS

The initial searches for alternatives to petroleum-based (PB) Diesel and gasoline fuels concentrated mainly on finding fuels that could wholly replace the petroleum products but in recent years more emphasis has been placed on the use of blends, i.e., mixtures of alternative liquid and PB I fuels and on developing IC engines that can operate with two or more different fuels. In the vehicular sector this new trend has lead to the development of three new categories of vehicle<sup>[11]</sup>:

- (1) The Bi-fuelled Vehicle. This type of vehicle can operate on either an alternative fuel or a conventional fuel. There are separate tanks for each fuel and the operator can switch being the two kinds of fuel thus eliminating refuelling problems in situations where the alternative fuel is not available. Currently, most bi-fuelled in-service vehicles use gasoline with either CNG or LPG.
- (2) The Flexible (or Variable) Fuelled Vehicle. With this class of vehicles only one type of fuel storage tank or tanks is used. The tank contains mixtures of the alternative fuel and the conventional PB fuel. A sophisticated electronic sensor/management system is required to automatically adjust the engine\_s operating characteristics in harmony with the amount of alternative fuel in the mixture. The favoured fuels option for flexible-fuelled vehicles in the USA is alcohol derivates and gasoline. Methanol and Ethanol will become more popular as a distribution network for such fuels is developed.
- (3) The Dual-Fuelled Vehicle. The Dual-fuelled vehicle uses two separate fuel systems but unlike the bifuelled vehicle the engine can burn both fuels at the simultaneously in the same cylinder. This is the preferred approach for diesel engine powered vehicles and the technology for gas-diesel dual-fuelled engines is now sufficiently mature for large scale production to be viable. In the stationary power generation sector dual-fuel diesel-generators are now relatively common-place commercial off-the-shelf (COTS) items.

The main alternative fuels that have been investigated to replace, wholly or partially PB Diesel are:

- Dimethyl Ether (DME)
- Biodiesel
- Compressed Natural Gas (CNG)
- Liquid Petroleum Gas (LPG)
- Methanol
- ✓ Coal
- Fischer-Tropsch Liquids

Fuel oils produced from coal and fuel blend using dimethyl oxygenates other than DME such as dimethyl carbonate (DMC) have also been investigated.

Although PB based diesel fuels will dominate the market for the foreseeable future, even a modest level of success for alternative fuels whether used neat, blended or in dual-fuel situations would provide a significant market. For example, if alternative diesel fuels were to achieve a 10% penetration in the existing US diesel market that would represent a requirement for—some 10

billion gallons per annum. Moreover, if alternative engine lubricants obtained a 5% US market penetration then this share would require an annual production of some 50 million gallons<sup>[12]</sup>.

As previously discussed the choice of alternative fuel - whether for usage or development - is dependent upon many inter-related factors and will not be made or should not be made on the technical characteristics of the fuel in isolation. Nevertheless the fuel characteristics are important and particular fuel properties are crucial, e.g., octane number for gasoline engine fuels and cetane number for diesel engine fuels. For hydrocarbon based fuels the constituent chemical and physical properties, especially those associated with aromatics and linear paraffins, that produce high octane numbers also produce low cetane numbers[11]. This usually means that alternative fuels than are well suited for use in gasoline engines are not well suited to diesel engine use and vice versa. That is not to say that fuels such as Methanol (cetane number less than 15) cannot be used in both types of engines but if methanol is to be used in a diesel engine then some form of ignition assistance such as a spark or a glow plug will be have to be fitted to the modified engine.

All the fuels listed above can be used in a diesel engine and depending upon the scenario a strong case could be made for each one being the "best" choice. However, from the literature it would appear that DME, Biodiesel and CNG are the most promising alternative diesel fuels at the moment. Hydrogen may well be the fuel of the fuel and coal-derived fuels may well attract increasing attention<sup>[3,14]</sup>. However, perhaps the most exciting new development is the synthetic diesel fuels that can be produced by using the Fischer-Tropsch technology. Thus, in the remainder of this paper these latter fuels will be considered in more detail and the Fischer-Tropsch developments mentioned.

### **FAVORABLE OPTIONS**

### (A) Dimethyl Ethers

Dimethyl Ether (DME), CH<sub>3</sub>-O-CH<sub>3</sub>, is the simplest ether compound and it is both nontoxic and chemically benign. It has a boiling point of -25°C and at standard temperature and pressure it is a colourless and odourless gas which becomes a liquid under modest pressure of about 0.5 MPa. It is fortunate that DME is not particularly reactive since as it is heavier than air it could collect in cavities. If used as a publically available fuel it would need to be "odourized" to prevent undiscovered leaks. As a chemical product DME has two main uses currently:-

As a aerosol propellant for cosmetic sprays - in

Japan alone some 8,000 tonnes are used for this purpose annually. Unlike chlorofluorocarbons, DME is not harmful to the ozone layer and easily degrades in the troposphere<sup>[15]</sup>.

As an ignition enhancer for the cold weather starting of IC engines because it has an inherently higher cetane number, i.e.,55-60, than the commercial grade diesel fuels<sup>[16]</sup>.

The main physical properties of DME are given in Table 2 along with those of other fuels for comparison purposes. The key properties that make DME so attractive for compression ignition engines are the combination of the high cetane number, a high inherent molar oxygen content of 35% and the boiling point of -25°C for these provide:

- Fast combustible mixture formation
- Reduced ignition delay
- Excellent cold starting
- Smokeless combustion
- Lower particulate matter and high EGR tolerance<sup>[17]</sup>. {Indeed under most operating conditions the emission levels associated with DME usage would be lower than those required by the very stringent Californian ULEV regulations}.

Moreover since diesel engines have a lower greenhouse gas impact (on a CO<sub>2</sub> equivalent basis) than comparable gasoline engines and the transportation sector is a major contributor to CO<sub>2</sub> emissions (in Canada it is the largest generating sector) then a DME fuelled diesel engine has the potential to be an attractive prime mover especially for transportation applications. However, in comparison with PB diesel fuel, the volumetric energy content of DME is much lower and to obtain a power output from a DME fueled engine equal to that of a PB fueled diesel engine, assuming constant engine efficiency, the volumetric fuel flow must be increased by a factor of up to 1.8<sup>[17]</sup>.

Unlike methanol, DME is non-corrosive to metals and does not require special materials for fuel system structural components. Some elastomers, however, are not chemically compatible with DME and will deteriorate after prolonged exposure to it. Therefore, careful selection of seal material is necessary. The lubrication characteristics of DME, which has a lower viscosity than PB oil, have not yet been fully investigated. As DME is a liquid under moderate pressure the handling characteristics of DME are very similar to liquefied petroleum gas (LPG). In comparison to other alternative fuels such as methanol or ethanol the energy density of DME (kJ/kg) is higher.

Table 2 Properties of DME compared to other fuels (Fleisch et al, 1995; Verbeek and Van der Wiede, 1997)

Property	DME	Diesel	Propane	Butane	CNG	Methanol	Ethanol	Gasoline
Lower Heating value MJ/kg	28.8	42.7	46.35	45.72	49	19.8	26.4	43.2
Density kg/m³	667	831	500.5	578.8		795	789	750
Auto ignition temperature C	235	250	470	365	650	450	420	
Cetane number	>55	40-55				~5	40/50	1
Vapour Pressure kPa @ 20 ℃C	530		830	210		37	21	45/90
Stoichiometric A/F Ratio	8.99	14.7			_	6.5	t ——	
Boiling Pt./Range C@ 1 bar	-25	71 to 193	1			65	i	
Liquid Density g/ml @ 20 C	0.66	0.8-0.84	1			0.79	1	

DME can be produced from a number of carbonaceous sources including biomass, coal and natural gas as well as from waste. Currently, DME is produced in commercial quantities in a two step process involving the dehydration of methanol, the annual world wide production being between 100,000 and 150,000 tonnes. However, the Danish Company, Haldor Topsoe has developed and successfully demonstrated, in pilot scale, a catalytic process with which DME can be efficiently produced directly from syngas, a mixture of H2, CO and CO<sub>2</sub> that is often used by industry as an intermediate step in the production of chemicals and also for power generation<sup>[16,18]</sup>. Syngas can be made from a wide variety of fossil feedstocks and wastes. About a year before its merger with British Petroleum, the US oil and gas company Amoco was planning to build a large DME production plant in Venezuela using the Haldor Topsoe process with a capacity of 42,000 barrels per day, equivalent to 4,900 tonnes of diesel fuel, generated from eight million m<sup>3</sup> of gas feedstock. Coal-derived syngas can be converted to methanol and researchers at the University of Akron, Ohio, have developed a process for one-step synthesis of DME from syngas[19].

The production of DME from natural gas is particularly attractive both economically<sup>[20]</sup> and strategically for countries with large reserves or ready access to the basic feedstock, e.g., Canada andVenezuela<sup>[21,22]</sup>. Moreover, since the known global reserves of natural gas are estimated to be far greater than those of crude oil then DME, especially as a PB diesel replacement, would appear to be a secure option at least for the next century and until the forecast demise of the dynamic heat convertor.

In determining the end-user/at-pump price of DME, the manufacturing, infrastructure and transportation costs must be taken into account. If the Venezuelan DME

plant used natural gas feedstock priced at \$0.8 MM Btu then the manufacturing cost of DME would be 84% of that of diesel oil and 45% of that of gasoline produced from an existing, paid-off refinery using crude oil costing \$18 per barrel<sup>[17]</sup>. As DME is transported, stored and dispensed as a liquid fuel in the same manner as LPG or propane then the same technology, with the exception of some plastic seals, could be used. Thus, the retrofitting and infrastructure costs will depend on the extent of the existing facilities.

Obviously, transportation costs will be depend on the distance from the refinery to the market. Fleisch and Meurer<sup>[17]</sup> considered a scenario where the DME from the proposed Venezuelan plant would be used on the US Gulf Coast and compared the end-user costs of DME, diesel oil and gasoline, Figure 5. With this set of circumstances the end-user cost of DME were 29% lower than gasoline but 35% higher than diesel oil. In countries such as Canada, with have abundant natural gas

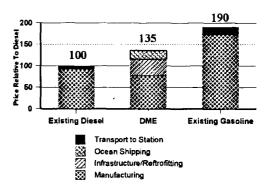


Fig.5 DME end-user costs[17]