diesel fuel quality and its relationship with emissions from diesel engines

Prepared for the CONCAWE Automotive Emissions Management Group based on the work carried out by the Special Task Forces on Diesel Fuel Quality/Engine Emissions (AE/STF-2, AE/STF-4 and AE/STF-5).

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SUMMARY

CONCAWE predicts future (year 2000) diesel fuel properties to be essentially in the range of 43 to 54 cetane number (median value: 48.5) and 0.825 to 0.870 density (median value: 0.846). Compared with present average commercial European diesel fuels this means a drop in cetane number by 2 and an increase in density by 0.006, however the spread in quality remains similar.

Operating costs for the EEC oil industry to compensate for these changes would amount to some $US 38 to 45 million per year if ignition improvers were employed and $US 1.3 to 1.7 billion/year if hydrogenation processes were installed. The latter figure is based on capital costs of some $US 3.5 to 4.5 billion. The ignition improver approach is clearly less expensive than the processing route but it will not change other parameters such as density/aromaticity. The costs and energy requirements to compensate for the anticipated changes in diesel fuel quality are very high when compared to any marginal improvement in emissions performance of today's engines.

Updating the diesel engine homologation fuel specification to reflect changes in commercial fuel properties would reliably ensure that certified emissions standards will be met in the field, despite variations in fuel quality. In addition, advances in engine technology, which are already emerging in the USA, represent viable measures for improving the emissions performance of diesel engines.

1. INTRODUCTION

At the request of the European Commission, a Steering Committee comprising CCMC, representatives from the other European vehicle manufacturers and CONCAWE was established. The purpose of this committee was to conduct a joint study programme to assess the implications of future diesel fuel characteristics on diesel emissions performance. The principal objective was to provide the European Commission with a basis, agreed by both the oil and motor industries, for establishing realistic regulations for the control of diesel vehicle exhaust emissions.

An essential element of the regulatory process involves the certification or homologation of the vehicle, or its engine, against the permitted emissions levels. Emissions have to be measured according to set procedures using a standard reference fuel. Because fuel properties can influence the emissions performance of diesel engines it is important that the reference fuel reflects the properties of fuels marketed within the European Community. In its contribution to the study, CONCAWE therefore presented findings on the relationship between automotive diesel fuel characteristics and engine performance (1) as well as a study of likely future diesel fuel quality (2).

Following discussion of these reports within the Steering Committee and with the EEC Ad Hoc Group "Motor Vehicle Emissions" (MVEG) CONCAWE was asked to extend the study on future diesel fuel quality to address:

- the effects of two additional cloud point specifications on the other properties of the diesel fuel (representing typical production in winter for Northern Europe and typical production in summer for Southern Europe);
- the effect of hydrocracking;
- the feasibility and costs of refinery processes for upgrading diesel fuel quality;
- the technical background and costs of increasing cetane quality by additives.

The following report summarises the CONCAWE findings with respect to future diesel fuel quality and compares these data with current European diesel fuels. The findings take into account the original study (2) and the additional work outlined above. The influence of the predicted changes in fuel characteristics on emissions are discussed and compared with the cost of raising cetane number. In addition, the results have provided CONCAWE with a basis for proposing appropriate properties for a future diesel engine homologation fuel.

2. DIESEL FUEL QUALITY

Throughout the earlier CONCAWE work (2) the cloud point of the diesel fuel was fixed at 0°C. In order to more fully assess the range of future diesel fuel properties, the work was extended to include additional cloud points of -8°C and +4°C, representing typical North European winter and South European summer qualities. (It should be noted that cloud points in Scandinavian winter diesel fuels are as low as -20 to -30°C).

Some additional data for a refinery configuration including crude, vacuum, hydrocracking and visbreaking units was also incorporated. Comparison of the new data with that generated in the original programme indicates that the new information is consistent with that reported in (2). The inclusion of the hydrocracking case has had a negligible impact and other predicted properties (volatility, viscosity) remain essentially unchanged.

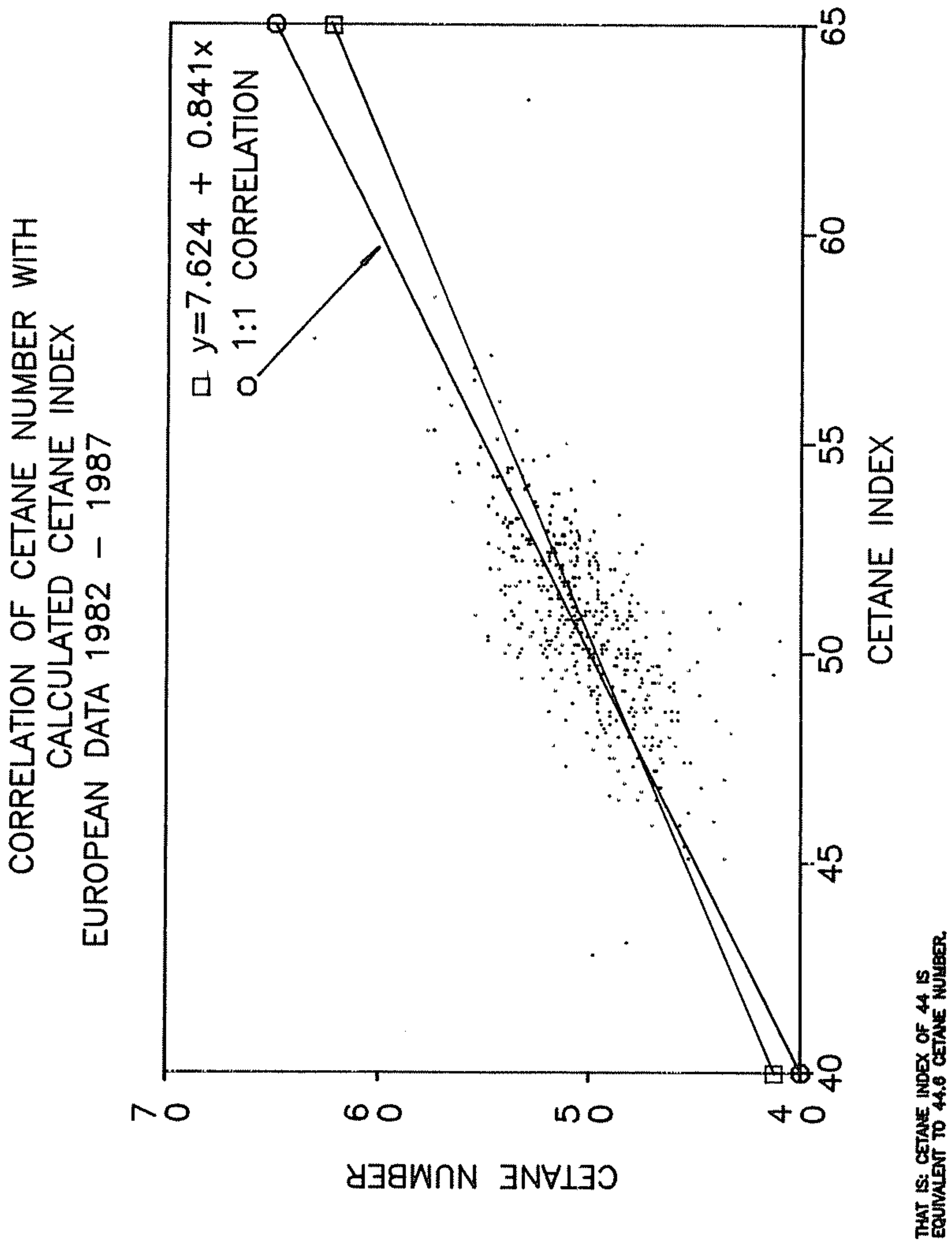
Predicted future cetane quality derived from computer linear programming models is based on cetane indices. For the purposes of this study a 1:1 correlation between cetane number and cetane index has been assumed. Fig. 2/1, which plots the relationship between cetane number and cetane index calculated by ASTM D 976-80 for over 400 European diesel fuels, reveals no bias between cetane number and cetane index in spite of the scatter in data points which are due to the inaccuracy of the cetane number measuring procedure. It should be noted that in spite of these findings, specifications for the homologation fuel as well as for commercial fuels are (and will be) on the basis of cetane number (and not cetane index).

Fig. 2/2 shows that the span of predicted cetane numbers lies between 43 and 54 with a median value of 48.5. If it is assumed that the cloud point differential between typical European summer and winter quality is 8°C, then the average difference between seasonal median diesel fuels is approximately one cetane number (i.e. winter median value of 48 cetane number, summer 49). Fig. 2/3 presents the predicted range for density, which lies between 0.825 and 0.870 with a median value of 0.846. Again, differences between typical summer and winter qualities are observed. The median value of winter density will lie around 0.842, rising to 0.848 during the summer.

To demonstrate the realism of these findings, published market surveys of European diesel fuel quality from 1982 to 1986 have been sales-weighted and plotted in the same way. These plots have been superimposed on the prediced fuel quality curves and are shown in Figs. 2/4 and 2/5. For simplicity the extremes of quality found over several years have been presented. These "envelopes" therefore encompass variations in processing and, more particularly, crude sourcing patterns. Seasonal variations in density and cetane number will generally fall within the envelopes. These market data indicate that the range of cetane values is similar, 43 to 57, with an average of 50.5, whilst density lies between 0.820 and 0.855, with an average of 0.840. It should also be noted that the shape of the distribution curves is basically the same in both the actual and predicted cases which confirms that the predicted distribution curves are established on a realistic basis.

The slight overall lowering of cetane number combined with the small rise in density is totally consistent with the anticipated increased use of cracked components. These materials have higher densities and lower cetane numbers because of the lower hydrogen content of their constituent hydrocarbons. It should be emphasised, however, that the difference between the situation today and that foreseen for the year 2000 is relatively small.

Fig. 2/1 Correlation of cetane number with calculated cetane index
European data 1982 - 1987



Cetane Number = 7.624 + 0.841 Cetane Index

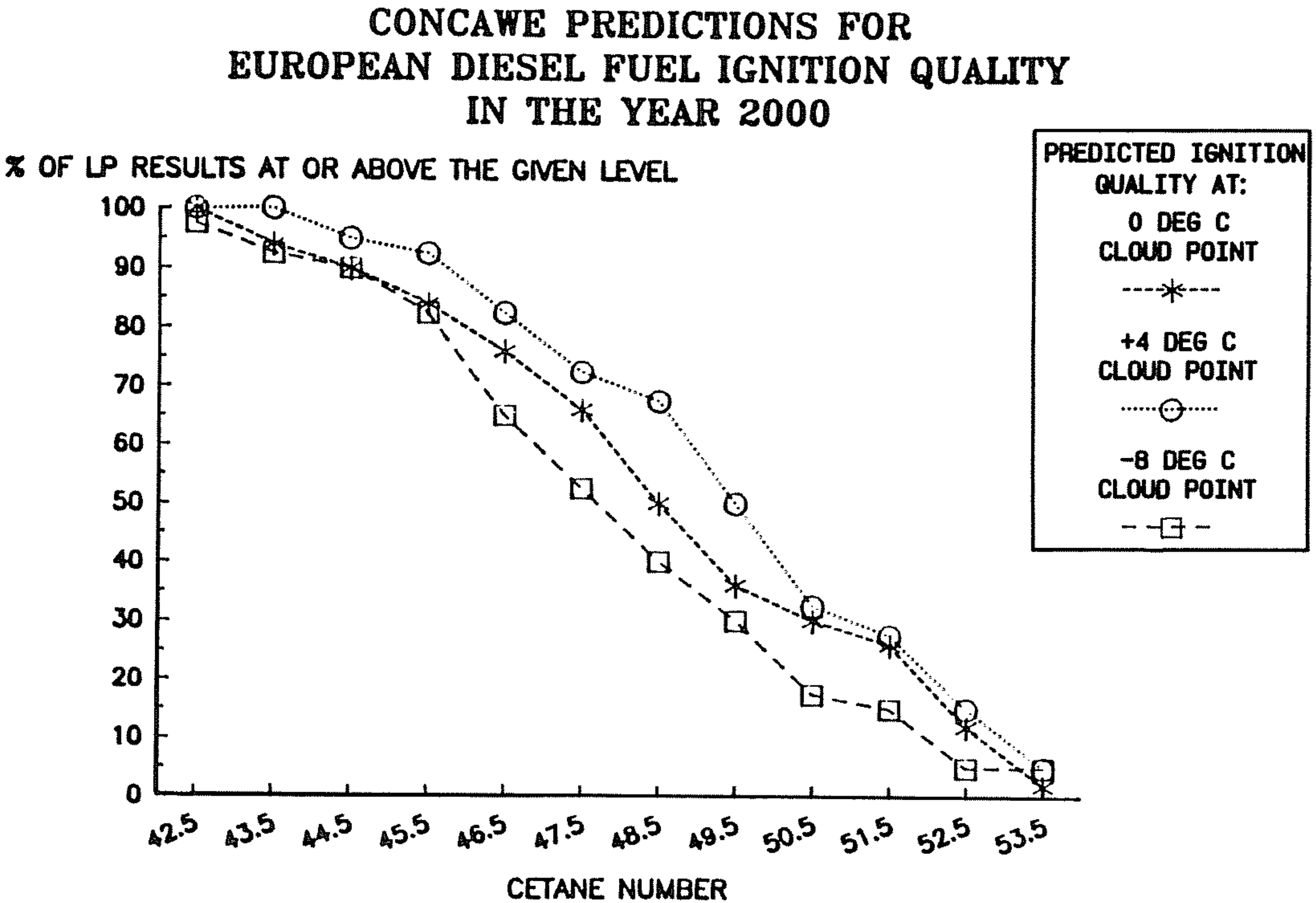


Fig. 2/2 CONCAWE predictions for European diesel fuel ignition quality in the year 2000

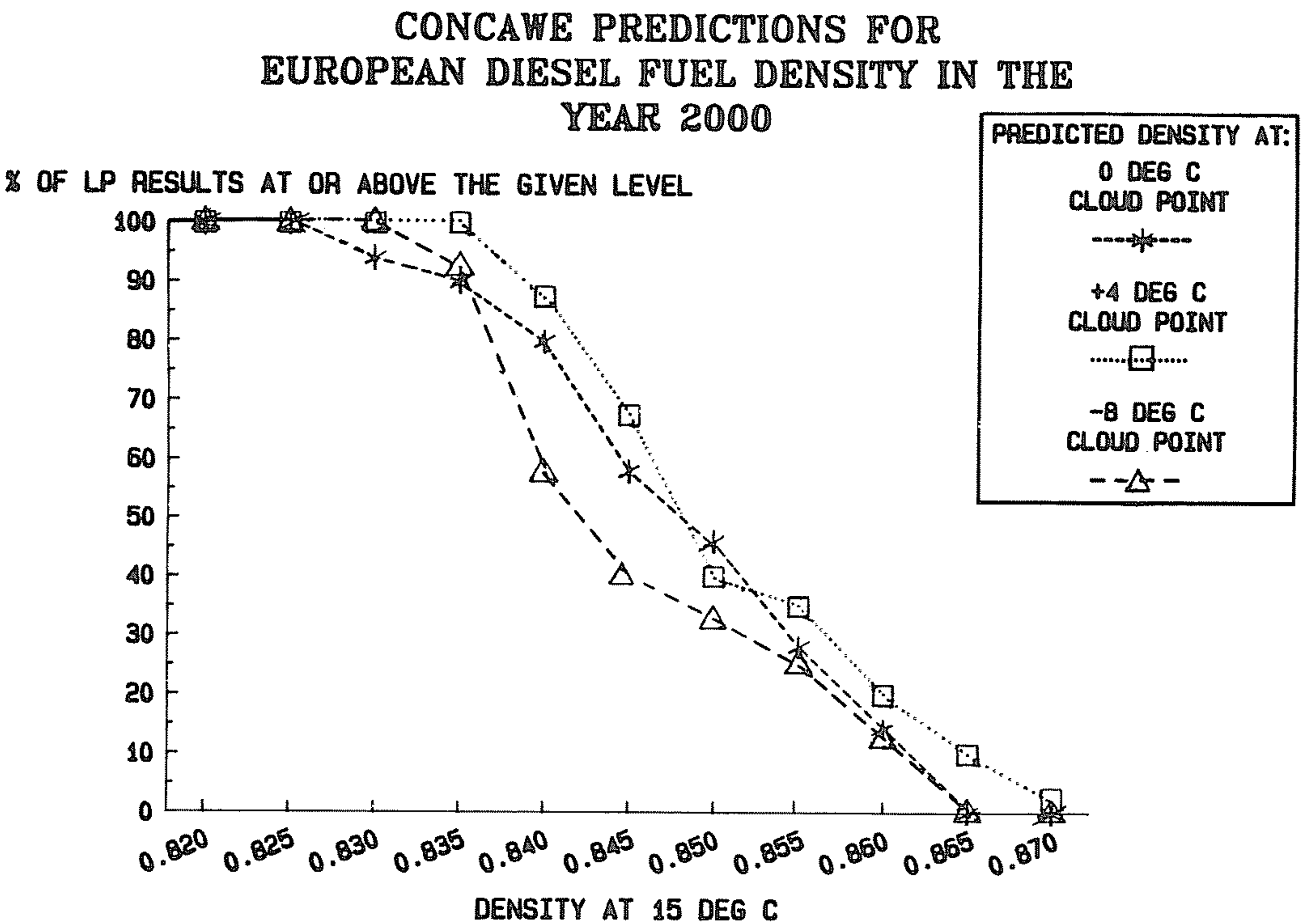


Fig. 2/3 CONCAWE predictions for European diesel fuel density in the year 2000

COMPARISON OF CURRENT AND PREDICTED RANGES OF IGNITION QUALITY

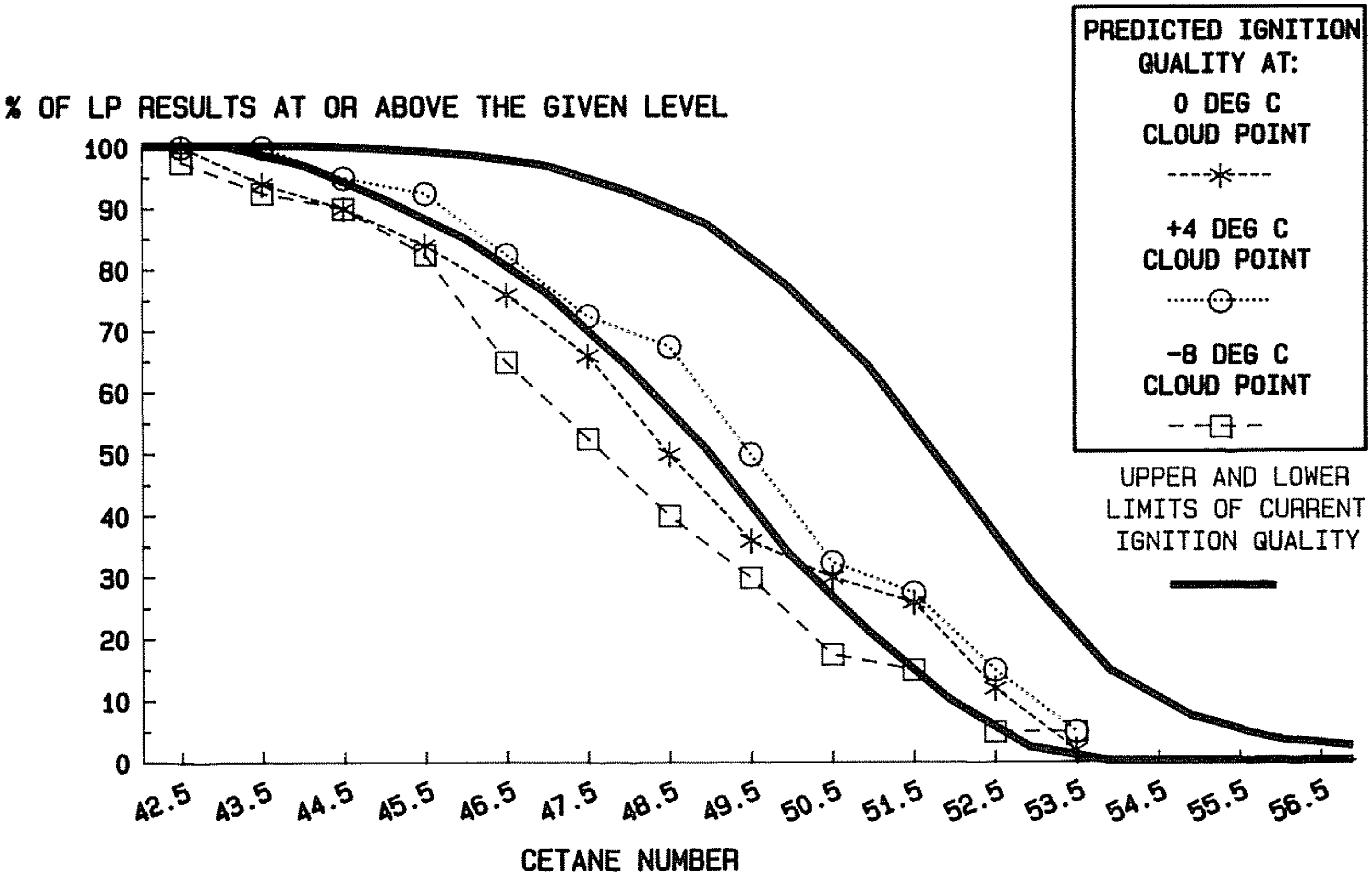
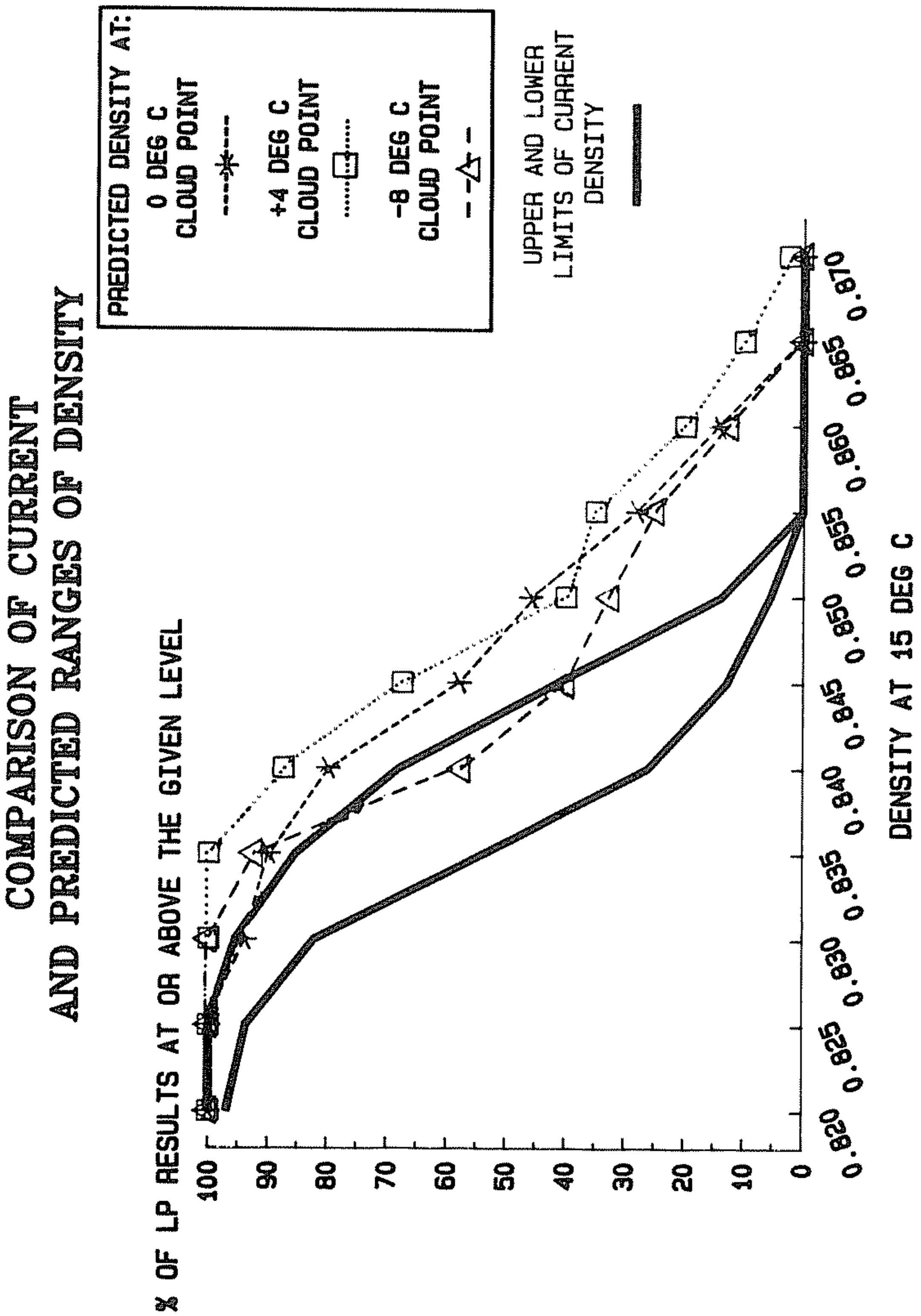


Fig. 2/4 Comparison of current and predicted ranges of ignition quality

Fig. 2/5 Comparison of current and predicted range of density



3. DIESEL FUEL QUALITY AND ITS INFLUENCE ON EMISSIONS

A previous CONCAWE report (1) assessed the influence of a wide range of diesel fuel characteristics on the emissions performance of current production engines certified on the present homologation fuel. At the time that report was published, the levels and ranges of predicted future diesel properties were not defined so that the report could not provide quantitative estimates of changes in emissions.

CONCAWE has now reassessed the position on the basis of the "95% worst case" fuel (cetane number 44, density 0.865) predicted in Section 2. The performance of current production engines, certified on the existing homologation fuel, is compared over the fuel quality range 50 to 44 cetane number and 0.840 to 0.865 density. The estimates are based on investigations reported in (4), (5), (6) and (7). Correlations between United States and European test procedures have been taken from published sources (8), (9) and private communications (10).

The results are summarised below and compared with the Ricardo estimate, published in their report DP 86/1946 (11). The results show reasonable agreement, remembering that the Ricardo figures are based on a fall in cetane number from 50 to 45 and their report does not quote any density change.

Table 1 Estimated % increase in emissions over given cetane number range

Emissions Species	% increase	
	CONCAWE 50 - 44	Ricardo 50 - 45
NO_x	0 - 4	3 - 7
HC	0 - 21	15 - 25
CO	8 - 35	0 - 10
Particulates	0 - 12	0 - 20

Note that particulates data for all engines have been taken from unpublished sources available to CONCAWE.

It is important to place these percentages increases in perspective as they represent the extreme case of engines homologated on the current certification fuel running on the "95% worst fuel" predicted for the year 2000. The median shift in quality of about two numbers is so small that CONCAWE estimates that existing engines, homologated on the current certification fuel, will on average show the following performance deterioration when future fuels are employed.

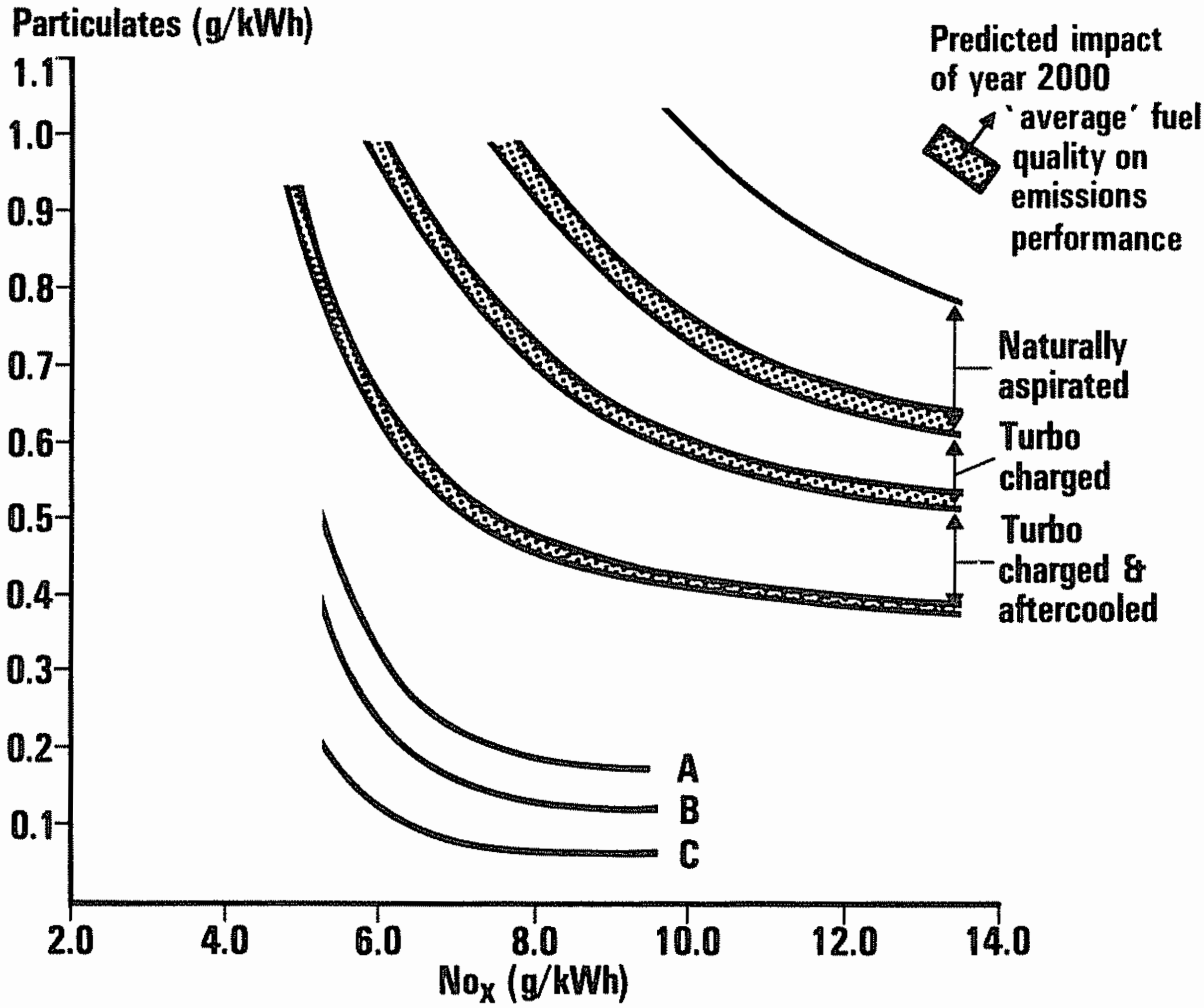
Table 2 Estimated % increase in emissions as result of predicted *average* fuel quality change

Emissions Species	% increase
NO_x	0 - 2
HC	0 - 7
CO	3 - 12
Particulates	0 - 6

These increases are far lower than the variability between different engine types and are negligible in comparison with the influence of engine design, as illustrated in Fig. 3/1. The performance bands for each generic engine type are quite wide, with emissions performance improving as one moves from naturally aspirated, through turbo-charged, to turbo-charged and after-cooled engines. The estimated effect of the predicted *average* fuel quality change has been superimposed on the best performance curve for each engine type and clearly demonstrates the overriding influence of engine design. Moreover, the curves A, B and C in Fig. 3/1 show the potential of further improvements in engine technology to reduce emissions.

CONCAWE recognises that many of these engines are designed for a non-legislated emissions regime and accepts that in the future this engine model variability may be reduced. However, current evidence suggests that engines developed and adjusted to meet more stringent emissions legislation are less susceptible to fuel quality effects. The influence of fuel characteristics on future engines will therefore be further reduced or virtually eliminated. Data supporting this view are presented in (9), (10) and (12).

Fig. 3/1 Particulates - NO_x trade-off for heavy duty DI diesels tested over the US transient cycle (from SAE 860456)



Ricardo predictions for improved performance

A = Turbocharged and aftercooled with pump injectors and electronic control

B = A with reduced oil consumption

C = B with particulate trap (50% efficiency)

4. COSTS TO UPGRADE DIESEL FUEL QUALITY

The scope for upgrading diesel fuel quality is limited in comparison with the process options available for gasoline. It should be stressed that diesel fuel quality is essentially a resultant of crude oil quality and its distillation, coupled with the need to absorb components from conversion processes.

In principle there are three routes available for upgrading diesel fuel quality:

- selective blending;
- processing;
- the use of cetane number improving additives.

4.1 SELECTIVE BLENDING

Selective blending involves segregating high cetane number components for automotive diesel fuel which, in turn, reduces the cetane quality and increases the aromaticity of the remaining non-automotive gas oil pool. There is a limit to how much aromaticity can be absorbed in heating/bunker gas oil and this is normally considered to be equivalent to 40 cetane number.

The CONCAWE study described in section 2 assumed this cetane level for the non-automotive gas oil pool, so there is little or no scope for additional cetane number improvement by selective blending.

4.2 PROCESSING

Three processing options are available:

- aromatics extraction;
- hydrocracking;
- hydrogenation.

The first two routes result in significant changes in product yield whereas the last option has only a marginal impact on product balances.

Solvent extraction of aromatics from highly aromatic gas oil components would represent both a significant loss of gas oil yield and a disposal problem for the aromatics. This route is therefore not considered to be a viable solution except in highly localised circumstances.

Hydrocracking produces good quality gàs oils and acceptable feedstocks for further upgrading to motor gasoline. However, CONCAWE Report No. 5/86 (3) has shown that currently planned and on-site conversion capacity can meet foreseen fuel oil and distillate demand up to the year 2000. Building additional hydrocrackers to produce good quality gas oils would therefore compete with catalytic crackers to use the available vacuum distillate feedstock, resulting in the shut down of existing conversion capacity. Such a move would also require the construction of new gasoline upgrading plants, e.g. catalytic reformers. This is not a generally acceptable economic solution. However, there may be specific local circumstances where some additional hydrocracking capacity is required to meet distillate demand.

Hydrogenation

Gas oil hydrodesulphurisation typically operates at relatively low pressure and has only a small effect on aromaticity. Conventional desulphurisation only increases the cetane number of the feedstock by one or two numbers. The CONCAWE computer model runs have assumed that all the cracked components are treated to meet storage stability and sulphur content requirements so that any small cetane number improvement has already been accounted for in the year 2000 predictions.

However, high pressure hydrogenation of cycle oils would provide significant cetane number improvements. Such technology does exist but it must be emphasised that no commercial units have yet been built for this application. The process has the added advantage that increasing the hydrogen content of the product reduces its density.

If it is assumed that a two cetane number improvement would be required across the EEC-12 diesel fuel pool (estimated at 75 million t/yr in year 2000) this would represent 150 million cetane tonnes upgrading. Some 15 million tonnes of light cycle oil will be available from cat. crackers which means an average cetane number improvement of 10 per tonne of light cycle oil would be required. The capital costs for EEC-12 countries based on hydrogenation unit capacities of 1,000 to 1,500 t/d is estimated to be $US 3.5 to 4.5 billion for some 30 to 45 units. Annual costs, including a 25% capital charge and direct/indirect fuel costs are estimated at $US 1.3 to 1.7 billion/year. In addition some 3 million t/yr extra hydrocarbons would be required for energy and hydrogen manufacture.

4.3 THE USE OF CETANE NUMBER IMPROVING ADDITIVES

A wide range of compounds have been studied as diesel fuel ignition improvers, the most common being nitrate esters. Peroxides and other reactive compounds have generally been discarded in view of their hazardous nature and/or ability to promote harmful side effects in the fuel. As a consequence virtually all currently available improvers are based on 2 - Ethyl Hexyl Nitrate or mixed Octyl Nitrates. Based on third quarter 1987 information, bulk deliveries of cetane improvers in Western Europe are in the price range of $US 1,250 to 1,500 per tonne.

If cetane number of diesel fuels is boosted to successively higher levels, the response to cetane improvers decreases and hence additive concentration per unit of cetane improvement increases exponentially.

A typical additive response for a 45 cetane number diesel fuel is 0.017% volume per unit of cetane improvement. The EEC-12 diesel fuel consumption is expected to increase to some 75 million tonnes/year by the year 2000. A cetane improvement of 2 numbers would therefore require 30,000 tonnes of additive giving a cost of $US 38 to 45 million per year.

Costs would also be incurred for storage and handling of the additive, for the provision of a cetane number test engine according to ASTM D-613 and for the manpower to operate and maintain the engine. It is estimated that this would increase the cost for a two cetane number improvement by additive treatment to $US 42 to 50 million per annum.

Clearly the additive route is less expensive than hydro-processing, but other quality parameters such as density and aromaticity are not changed. On the other hand, additive dosage can be easily adjusted for fluctuating cetane levels which may occur in refineries because of crude oil changes, seasonal demand variations, etc. Capital intensive processing is, by contrast, a continuing cost situation largely independent of requirement.

5. DIESEL ENGINE HOMOLOGATION FUEL

The currently proposed homologation fuel RF-03-A-84 (established by CEC in 1984 to replace the 1980 - or earlier - versions in the legislation) specifies its key properties as follows:

- cetane number - minimum 49, maximum 53;
- density - minimum 0.835, maximum 0.845.

If the median specifications of the homologation fuel for cetane number (51) and density (0.840) are compared with the properties of current marketed fuels, then the homologation fuel is fairly representative of the 50 percentile commercial quality.

Previous experience with the actual properties of diesel homologation fuels indicates, however, that quality levels are generally close to the maximum cetane number and minimum density specifications. For example, measured cetane numbers of various batches of RF-03-A-84 varied between 52 and 53, while densities were close to the minimum level of 0.835. Similarly, in the United States of America the actual cetane number of the 2 D homologation fuel has been about 48, while the allowed specification range is 42 to 48.

About 70% of currently marketed fuels therefore have densities above, and cetane numbers below, the respective measured values of the homologation fuel. This demonstrates that, even today, the actual properties of RF-03-A-84 no longer represent typical market quality.

Before addressing the question of cetane number and density levels for any future homologation fuel, it would be appropriate to discuss those presently agreed for RF-03-A-84. On the basis of the experience noted above, CONCAWE considers that the current approach is not precise enough for specifying a legislative homologation fuel in the future. Thus the 1984 specification, for example, would more accurately reflect the current 50 percentile market fuel if the cetane number and density were controlled to 51 and 0.840 respectively, with no margin around these values. This ideal is impracticable and debate on the technically feasible minimum tolerance is beyond the scope of this report. CONCAWE believes, however, that multiple testing of each batch of homologation fuel is entirely feasible, follows US practice, and would allow much closer definition of a fuel which is, after all, an essential part of the certification process.

For the purposes of this report, CONCAWE has therefore only quoted the absolute values it believes should be introduced in any future homologation fuel. It is suggested that the question of allowable tolerances should be taken up by the Reference Fuels Group of the Co-ordinating European Council (CEC CF5).

Engines and vehicles need to be homologated to meet exhaust emissions throughout the year. It would therefore be prudent to ensure that the homologation fuel reflects the variation in key properties which results from seasonal changes to marketed fuel, i.e. lower ignition quality in winter and higher density during the summer. If the rationale for defining properties of the homologation fuel is to be based on average seasonal market quality, then the CONCAWE study suggests the following absolute values (note that the following figures have been rounded to the nearest cetane number and 0.005 density):

- cetane number 48;
- density 0.850.

Instead, however, CONCAWE suggests a 70% market coverage rather than an average quality. In this case the absolute values for the future homologation fuel should be:

- cetane number 46;
- density 0.855.

The reasons for proposing a 70% market approach are summarised below:

- CONCAWE's predictions on the future diesel fuel quality are based on pan-European frequency distributions. In view of regional differences in crude supply, domestic heating oil / diesel fuel ratios, climatic conditions etc., predicted extreme fuel qualities might have significant market shares in certain parts of Europe. Hence, the adjustment of vehicles/engines on a homologation fuel covering 70% of the European market would ensure that most vehicles meet legislated exhaust emission limits in spite of varying commercial fuel properties. Furthermore, reference fuels for engine development purposes are often specified in terms of the "90% worst case fuel". Such an approach could be adopted for a homologation fuel but is probably too stringent as it would erode any margin of performance required to ensure engine conformity during series production and service;

- engine builders have expressed a strong interest in maintaining the longest possible lifetime for a homologation fuel. They stress that this lifetime should not be less than that of a major engine development programme (5 to 7 years).

  In addition, engine builders requested a period of two years between the publication of any newly defined homologation fuel and the date of adoption of that fuel.

  Under these circumstances, any new homologation fuel established in 1988 would still be in use in the years 1995/1997. Diesel vehicles certified at this time will still be on the market for another 10 to 15 years, i.e. until the beginning of the next century. It would therefore be prudent from an environmental viewpoint to specify the homologation fuel properties closer to the expected minimum cetane/maximum density levels. This would cater for further changes of commercial fuel properties beyond the year 2000;

- it should also be noted that manufacturers tend to adjust diesel engines for maximum possible power within the constraints of power output and emission standards. Under these circumstances, even small differences between homologation and market fuels might cause relatively large changes in the emissions performance of critical engines. Hence, a homologation fuel designed to cover 70% of the expected market would offer a "built-in" safety margin and therefore minimise the risk of deteriorating emissions performance in the field;

- the proposed specification for the homologation fuel at 70% market coverage is representative of the minimum cetane number and maximum density limits currently stipulated in many of the national standards in Europe.

CONCLUSIONS

- Within a cloud point spread of minus 8°C and plus 4°C (representative of typical winter and summer qualities in North and South Europe respectively) cetane number and density levels of future diesel fuels are predicted to range between 43 to 54 and 0.825 to 0.870. Other diesel fuel properties such as viscosity and distillation characteristics are not expected to vary significantly from current market levels.

- Inclusion of some additional data for a refinery configuration with a hydrocracker had little effect on the overall results for ignition quality and density. As there are very few hydrocrackers in the EEC their influence on future diesel fuel quality will be marginal.

- A comparison between the frequency distribution curves of present and predicted cetane number and density levels indicates the following typical changes between now and the year 2000.

    - cetane number - reduced by two numbers.
    - density - increased by .006.

- The typical changes in fuel quality, quoted above, will have a very small impact on the regulated emissions performance of current production engines certified on the current homologation fuel. Even the "95% worst case" year 2000 fuel increases emissions by less than the variability between one engine type and another.

- Advances in engine technology and/or adjustment of current DI and IDI engines on future type diesel fuels represent viable measures for effectively improving the emissions performance of diesel vehicles. Such technology is already making an impact in the United States (13) where more stringent emission standards than those proposed for Europe are in place and where fuel quality can be lower today than that predicted for the EEC in the year 2000.

- High pressure hydrogenation is not in commercial operation and is highly capital intensive. A two cetane number increase in the EEC-12 countries would require a capital investment of $US 3.5 to 4.5 billion, a yearly total cost of $US 1.3 to 1.7 billion and an additional hydrocarbon consumption of some 3 million tonnes/year for energy and hydrogen manufacture.

- The use of additives to improve cetane numbers, including dosing facilities and testing, would cost $US 38 to 45 million/year for a similar pool cetane improvement. This option is clearly less expensive than the processing route and is more flexible. However, other important quality parameters such as density and aromaticity are not changed.

- Costs and energy requirements to compensate for the expected changes in diesel fuel properties are therefore very high when compared to any marginal improvement in emission performance of today's diesel engines. The reformulation of the present homologation fuel RF-03-A-84 would effectively ensure that certified emissions standards could be met in the field despite varying fuel quality.

- Setting homologation fuel properties at a 70% market coverage (only 30% of future commercial European diesel fuels would have cetane numbers below or densities above the homologation fuel properties) would result in a cetane number absolute value of 46 and absolute value for density of 0.855 respectively. Such a fuel would minimise the risk of emissions performance deterioration in the field and would ensure harmonisation with commercial fuels produced to meet existing European national diesel fuel standards.

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