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ABSTRACT

Due to the accumulation of deposits in the combustion chamber, the "appetite" of an engine for octane increases with mileage. Depending on the type of engine, driving conditions, and gasoline, this octane requirement increase (ORI) ranges from 3 to 10 octane numbers.

Because of ORI, national specifications for octane number of gasoline must be based on engines' octane requirement at equilibrium. Applying the incremental analysis technique to refining economics, F. Bernasconi calculated that the incremental cost of producing each extra octane number by refining ranges from \$2 to \$6 per ton. It is generally well accepted that an increase of one octane number will lead to a loss in refinery yield of 4 to 6%.

Octane requirement increase can be controlled with a new type of ashless, non-metallic additive. An ORI reduction of 50 to 80% has been observed, opening the route to decreasing national gasoline octane specifications. Savings of millions of dollars and up to 20% of crude are possible. Emissions are reduced.

DISCUSSION

In terms of combustion, a fuel for spark ignited engines is commonly characterized by its resistance to knock.

Toward the end of the 1920's, an experimental engine was designed in the USA to determine resistance to knock. It was called the CFR engine. The first method for classifying knock resistance

was developed in 1931; it was very similar to the current method for research octane number (RON). A little later in the 1930's, a second procedure was developed which gave rise to the motor octane number (MON). Both methods are still used worldwide; all specifications of gasolines in every country include one or both of these numbers.

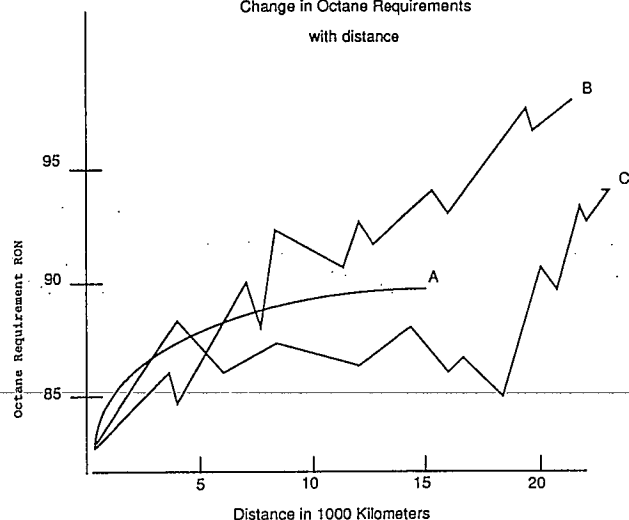
A spark ignited engine is well characterized by its octane requirement, which is the lowest octane of a fuel necessary for the engine to avoid any knock. At the minimum, the octane of a gasoline must satisfy the octane requirement of the engine, over the range of the running conditions of the vehicle.

The octane requirement increase of an engine over time was investigated as early as the mid 1920's (1)* and has been studied extensively over the years (2) (3). In an excellent recent literature review on deposits in gasoline engines (4), Kalghatgi reported variation of octane requirement with distance or engine operating time.

Basically, this increase can be very sharp right from the beginning (Figure 1, curve A), more continuous (curve B), or in a Z shape (curve C). An equilibrium is generally reached even if a plateau is not obvious. Depending upon the type of engine (compression ratio, shape of the combustion chamber, etc. . .), the driving conditions, weather, and the type of gasoline used (leaded, unleaded), the equilibrium octane requirement increase can range from 3 to 15 numbers. (5) (6) (7) (8).

*Numbers in parentheses designate references at end of paper.

Figure 1
Change in Octane Requirements
with distance



The main contributors to ORI are the combustion chamber deposits, even if, in the same engines, intake system deposits also contribute to ORI (4). In the combustion chamber, the deposits involved in ORI are those on the piston top, on the intake and exhaust valve surface, and in the end gas region. These deposits are related to both fuel and lubricating oil.

The nature of the fuel has a direct effect on the physical properties of the deposits: high boiling point components, for instance, are detrimental (9). Another large contribution to ORI is related to the type of gasoline detergents and carrier oils associated with the detergent to improve inlet valve cleanliness (11). These either add to the ORI problem or, in the best case, have no effect at all on ORI.

Lubricating oil also contributes to combustion chamber deposit levels. Large percentages of high molecular weight ingredients (bright stock, for instance) or high levels of sulphated ash increase deposit accumulation (4).

Three possible mechanisms through which combustion chamber deposits could effect octane requirement have been considered (2):

- Volume effect - the space occupied by the deposits increases compression ratio. This effect would be small (about 10%)
- Chemical/catalytic effect - deposits may change the combustion chemistry during flame propagation. There is some evidence against this mechanism (2).

- Thermal effect - deposits store heat in one cycle and give it up to the fresh charge in the next cycle. This is the most likely mechanism.

The control of octane requirement increase while maintaining induction system cleanliness is the real challenge of the 90's.

RECENT DEMANDS ON ENGINE PERFORMANCE AND FUELS

Environmental concerns and public pressure have forced automobile manufacturers to produce spark-ignition (SI) engines that operate reliably with reduced evaporative and exhaust emissions and improved fuel economy while using low lead or unleaded gasoline. These needs have been met by using increasingly sophisticated intake, piston/combustion chamber, exhaust, and control systems.

Performance of these systems has placed demands on gasoline quality which are being met by bulk treatment with special purpose detergent and dispersant additives and by using higher octane gasoline.

Detergent and dispersant additives quite effectively deal with intake system deposits, but have not been effective in preventing octane requirement increase. In fact, the reverse is frequently true - these additives often are contributors to ORI through increased combustion chamber deposits.

Refiners are experiencing growing difficulty in meeting octane demand. The rapid elimination of tetraethyl lead, changes in crude supply and availability, and environmental demands for reduction in aromatic components are forcing substantial reformulations of gasoline. To meet the demand for increasing octane levels, refiners have resorted to (a) increasingly severe catalytic cracking and (b) expanded use of octane enhancing oxygenates. Both approaches are expensive, and the use of oxygenates reduces the energy potential of the fuel, thus increasing overall fuel consumption.

The additive described in this paper is a multifunctional concentrate for use in gasoline. It has been shown to reduce ORI from 50% to 80%, which allows use of lower octane gasoline (8). Extensive testing shows improved fuel mileage (4.5% average increase) and substantially re-

duced exhaust emissions (10% average hydrocarbon emission reduction). This testing includes both laboratory and fleet use, with over 70,000,000 gallons (262,500,000 litres) of fuel treated since introduction of the additive. No deleterious effects have been noted with recommended use levels.

ADDITIVE HISTORY The additive discussed herein was initially developed to improve fuel economy of internal combustion engines without degradation of exhaust emission control systems. It was subsequently observed that the additive had a knock-reduction effect in SI engines. Hydrocarbon emissions were reduced. This behavior suggested the additive might have an important effect in modifying the combustion process and in controlling combustion chamber deposits.

ADDITIVE DESCRIPTION The additive is a patented multi-component mixture of materials containing only carbon, hydrogen, and oxygen. It is a blend of oxygenated aliphatic hydrocarbon liquids, glycol ethers, and hydrocarbon fuel stabilizers, with specific gravity and fuel value similar to gasoline. The active materials include a polar material, compatibilizers for the polar material and hydrocarbon fuels, and a compound for enhancing the water tolerance of the additive. The additive has been designated "substantially similar" by the US Environmental Protection Agency, and may therefore be used for bulk treatment of unleaded gasoline.

Table 1
Typical Properties of the Additive

Appearance	Clear Liquid
Color	Amber
Specific Gravity	0.875 15/15° C (60/60° F)
Vapor Pressure	0.86 kPa (6.5torr) @ 22° C (72°F)
Flashpoint (TCC)	43.3° C (110°F)
Boiling Range	104-316° C (220-600° F)
Water Content	< 0.5% by Wt.
Viscosity	4.1 cSt @ 15.6° C (60° F)
Heat of Combustion	45.00 MJ/kg (19,350 BTU/lb)

The additive has been tested in the laboratory and through fleet use in commercial fuels with most currently commercially available detergents

and carrier oils. Representative classes of such detergents include polybutene succinimides, polybutene amines, polyether amines, and polyisobutylene amines. There is no degradation in the effectiveness of these detergents in controlling intake system cleanliness.

SPARK-IGNITION ENGINE LABORATORY AND ROAD TESTS

OCTANE REQUIREMENT INCREASE - Octane requirement increase is observed with extended operation of gasoline engines. In order to maintain normal engine performance under these conditions, a higher octane fuel is often required. Although a number of factors may be involved in ORI, combustion chamber deposits are recognized as a major contributor to the problem. The effect of the additive on ORI was determined by Laboratories L-3, L-4, and L-6 using three different test procedures and five engine/base fuel combinations.

10 Car Road Test - Laboratory L-3 tested six (6) 1985 cars manufactured by Company A and four (4) 1984 cars manufactured by Company B. The Group A cars were equipped with 3.0 litre V-6 port injected engines and automatic transmissions. The Group B cars were equipped with 2.3 litre 4-cylinder carbureted engines and automatic transmissions. Cars within Group A consisted of three each of two body styles of the same size. All cars in Group B had the same body style.

In preparation for testing, the cylinder heads of each of the cars were removed and the combustion chambers cleaned. The valve train assemblies (especially the valve guide clearances) were inspected to insure that undue amounts of lubricating oil would not enter the combustion area and thus effect the test results. Crankcase oil was changed and oil, air, and fuel filters were replaced, together with spark plugs, EGR and PCV valves. Each of the engines was then tuned to the manufacturer's specifications.

The gas tanks were drained and filled with a commercially available unleaded regular fuel obtained from a single batch. The cars were driven for approximately 100 miles, under identical conditions, in an attempt to equalize combustion chamber deposits. At this point, octane require-

ment evaluations were made with a chassis dynamometer, using the CRC designated E-15-87 test procedure. The initial octane requirements for each of the ten cars was thus established.

Fuel for half of each of the Group A and B cars was treated with the additive at a concentration level of 667 ppm. A closed route representing both city and country driving conditions was followed with all of the vehicles traveling in line. The 100 mile route was traversed at an average speed of about 64 kph (40 mph), with maximum speed limited to 97 kph (60 mph). Vehicle order in the line and vehicle-driver combinations were rotated.

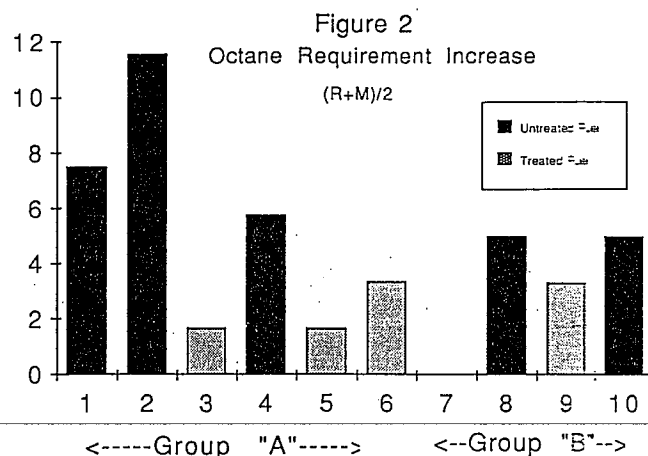
Octane requirement levels were determined for each of the cars after 2,500 and 5,000 miles. Based on the trends for the results, the Group A cars were subsequently run to 8,000 miles. The Group A tests were then terminated, since the laboratory judged that the octane requirements had essentially stabilized.

The octane requirement increases among the Group B vehicles were smaller than the Group A vehicles. Therefore, Group B test duration was extended to 10,000 miles to assure that equilibrium had been reached.

The octane requirement results are shown in Table 2 and the ORI's are summarized in Figure 2. Mean ORI with the additive treated fuel was 6.0 octane numbers lower than with untreated fuel for Group A cars and 3.3 octane numbers lower with Group B cars. The photographs are from Group B.

TABLE 2
OCTANE REQUIREMENT
(R+M)/2

		Miles Accumulated					
Car No.	Concn.						Final
Group A	ppm	0	2,500	5,000	8,000	10,000	ORI
1	0	81	87	87	88	—	7
2	0	81	84	91	92	—	11
3	667	83	84	84	84	—	1
4	0	83	88	88	88	—	5
5	667	83	84	—	84	—	1
6	667	81	84	—	84	—	3
Group B							
7	667	78	78	78	—	78	0
8	0	78	83	83	—	83	5
9	667	78	81	81	—	81	3
10	0	78	81	83	—	83	5



1.6 Litre Engine Test — An additional ORI evaluation was made by Laboratory L-4, using a European 1.6 litre, 4-cylinder, crossflow 4-stroke engine with a compression ratio of 9:1. The twin choke carburetor was modified to permit air/fuel ratio adjustment by control of float chamber pressure.

The engine was initially run in for 20 hours over a range of speeds and loads. The test schedule in this case took the form of a 200 hour mixed-cycle run, with octane requirement, part-load exhaust emissions, and fuel consumption determined at 50 hour intervals. Octane requirement was determined from the spark advance producing borderline knock. The cycle used in this test program is listed in Table 3. It is representative of a typical European duty cycle.

TABLE 3
TEST SCHEDULE
1.6 L 4-Cylinder Engine

Condition	Engine Speed rev/min	Engine Load BMEP	Time Minutes
1	2400	2.5 bar	20
2	3600	4.0 bar	20
3	3000	Full Load	5
4	2400	5.5 bar	20
5	1200	5.5 bar	20
6	1200	1.5 bar	20
7	850	Idle	15

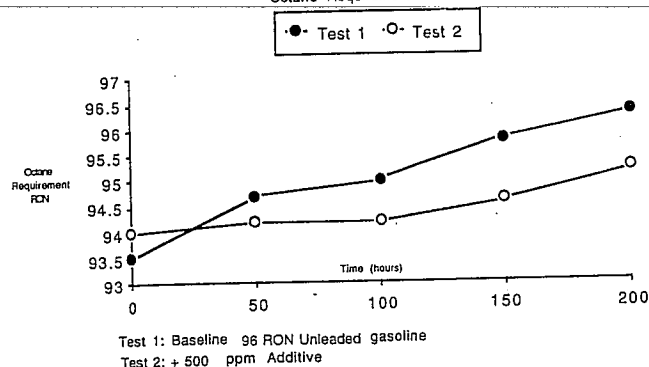
The 200 hour test was completed twice, first with the baseline fuel and then with 424 ppm of the additive. Prior to each test the engine was stripped, cleaned, and measured.

The initial octane requirement of the engine

at the start of the baseline fuel test was 93.5 RON. After the 200 hour run, this increased by 2.8 to 96.3, as shown in Figure 3.

After rebuilding the engine, the initial octane requirement was 94 instead of 93.5. After the 200 hour run with the additive, the octane requirement had increased by 1.2 to 95.2. Thus, ORI with the additive was reduced 1.6 RON from that for the baseline gasoline, or a 57% reduction in ORI.

Figure 3
Additive Tests
Octane Requirement Increase



10,000 km Road Tests — Laboratory L-6, a major European petroleum company, also ran some extended road tests on a car equipped with a 4-cylinder gasoline engine. These were four 10,000 km tests run in series with a different fuel in each test. The combustion chamber was cleaned between tests. Octane requirement for each cylinder was determined from the spark advance producing borderline knock. The knock and octane requirement characteristics of this engine were very well known to this laboratory. Based on this experience, the ORI reductions due to the additive as shown in Table 4 were "considered very significant."

TABLE 4

OCTANE REQUIREMENT INCREASE +
1.6L 4-CYLINDER ENGINE

	Untreated	Treated	ORI Reduction	Percent Reduction
Leaded gas	4.6	0.8	3.8	82%
Unleaded gas	1.5	0.3	1.2	80%

+ Average values of the 4 cylinders

ECONOMY AND SAVINGS

With the lead phase down in the United States and Japan, production of gasoline has become more and more sophisticated. It will do so in Western Europe and other areas in the very near future.

To produce gasoline, a refiner can mix different types of major blending stocks, representing more and more complete types of refining:

- Light naphthas — these have a rather low octane. This octane can be increased significantly by isomerization.
- Reformates — while reformat octanes can be high, they are very dependent on the severity of refinery operation. The highest practical clear RON level (no additive) is around 100.
- Alkylates - good blending stocks, with a reasonably high clear RON level and very low sensitivity. Alkylates show a very small difference between RON and MON.
- Fluid Catalytic Cracked (FCC) gasoline — again, a relatively low octane product. FCC gasolines exhibit high sensitivity, with a big difference between RON and MON.
- Oxygenates — provide flexibility through their high RON, but are available only in limited quantities. MTBE and ETBE can contribute to front end octane number (FEON) while benefiting volatile organic compound emissions control.

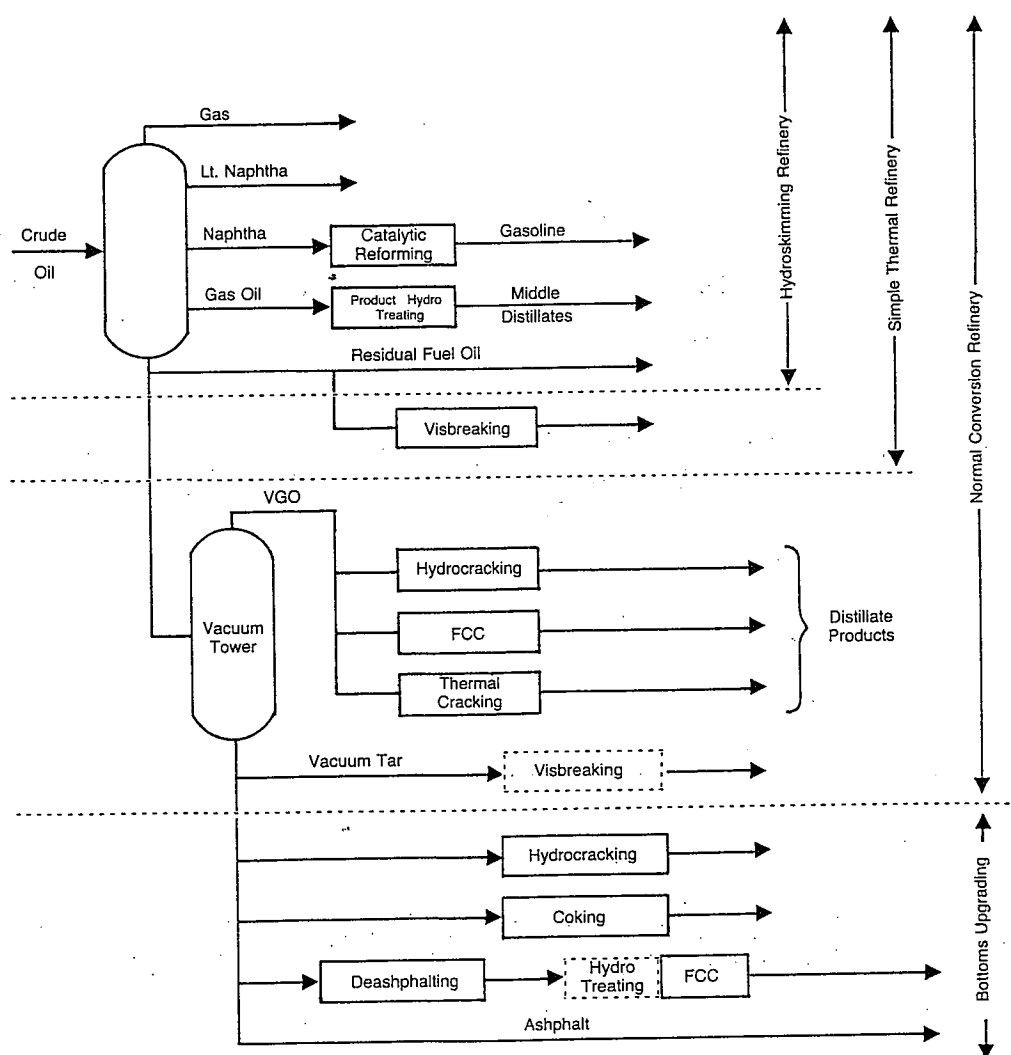
COST OF PRODUCING EXTRA OCTANE —

The challenge is to produce extra octane numbers at the lowest cost. By applying the incremental analysis technique to refining economics, F. Bernasconi has been able to calculate the incremental cost of producing gasoline with one extra octane number. (12). The gasoline production cost is assessed by incremental analysis as a function of the refinery feedstock (crude oil) and the main byproduct associated with gasoline production (residual fuel oil) for different refinery configurations. He identifies two general classifications for this analysis:

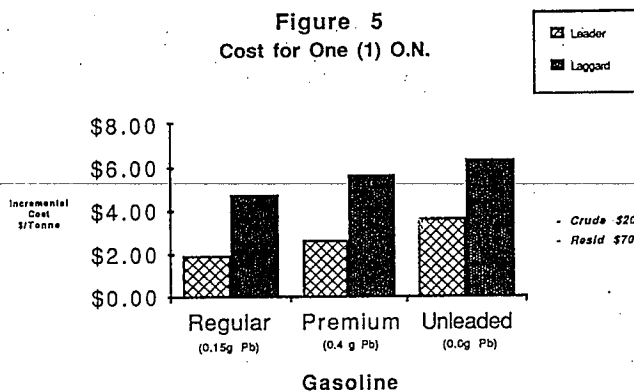
- "Leader" — a refinery equipped with residue upgrading facilities, such as hydrocracking, fluid catalytic cracking and thermal cracking or visbreaking.
- "Laggard" — a simple hydroskimming refinery

A typical schematic for these types of refineries is shown in Figure 4 (13).

Figure 4: Upgrading Stages



Depending on the type of refinery and the type of gasoline produced (leaded or unleaded), and using a crude oil price of \$20 per barrel and a residual fuel oil price of \$11 per barrel, the cost of a single extra octane number can range anywhere from \$2 to \$6 per metric ton (Figure 5).



This is very consistent with the numbers published by Turner, Mason, and Company in their report US Gasoline Outlook 1989-96 summarized in reference (14), where numbers of \$.30 to \$.60 per incremental octane number per barrel (ION.B) are reported. This equates to \$2.5 to \$5 per incremental octane number per metric ton (\$2.5 to \$5 per ION.T).

Generating this single extra octane number will also reduce yield. This results in increased consumption of crude for a given amount of gasoline production.

It is generally well accepted that in a semi-complex type refinery, if everything remains constant (type of crude feedstock, general process settings, etc. . .) an increase of one octane number over normally attainable octane will lead to a reduction in yield of gasoline per barrel of crude oil of about 5%. For example, if the basic yield is 30%, increasing refining severity to get one more octane number will reduce the yield to 25%. In order to provide the same total quantity of gasoline, you will consume 20% more crude oil.

On the other hand, if someone can satisfy the octane requirement of engines while decreasing the octane level of the gasoline by one octane number, he can potentially save:

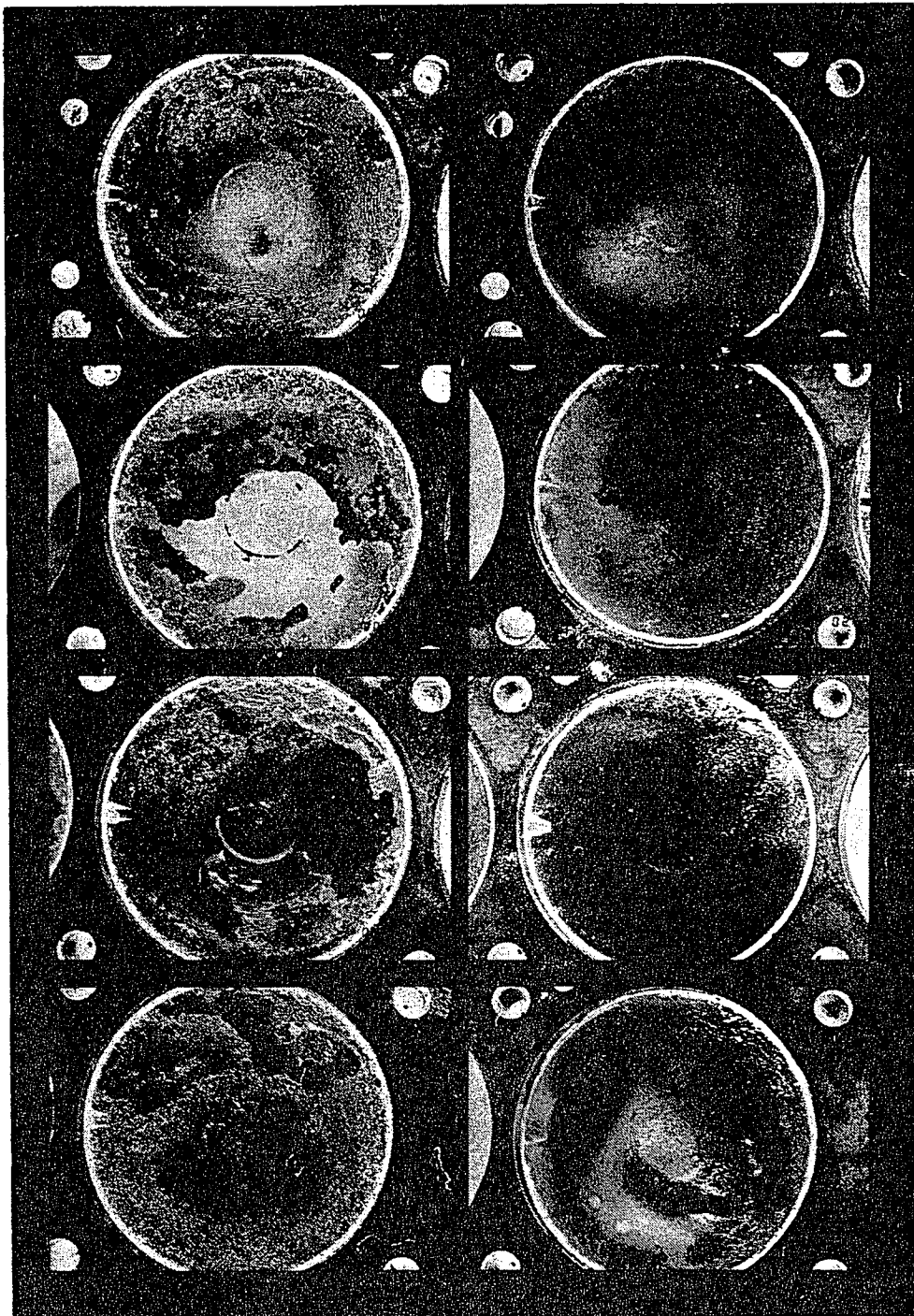
- \$2 to \$6 per metric ton of gasoline produced, and
- 20% of his crude oil consumption.

SAVINGS THROUGH ORI CONTROL — As we have seen previously, it is now possible to control the octane requirement increase of engines with ashless non-metallic additives comprised solely of carbon, hydrogen, and oxygen. A dramatic reduction of 50% to 80% of ORI has been observed (8), in current mass-produced engines. This opens the route to a decrease in national gasoline octane specifications, with no degradation in engine performance. Additional benefits also accrue, as reported in the referenced paper (Table 5).

TABLE 5
ADDITIONAL BENEFITS

- * Intake system cleanliness - neutral (CEC procedures)
- * Corrosion protection
fuel systems - improved
- * Spark plug cleanliness - improved
- * Gasoline consumption - reduced 4.5% (average)
- * Emissions reduced

hydrocarbons	10% (average)
carbon monoxide	neutral
nitrogen oxides	neutral
- * Valve recession reduced 40% to 60%



Untreated

Treated

Piston Tops

Group B

If one applies a national octane decrease specifications policy, huge savings can be achieved. For example, reducing the national gasoline octane specification by one octane numbers in various countries could produce the following savings (Table 6):

TABLE 6
POTENTIAL SAVINGS
Reduction of ONE Octane Number

	Annual Production Metric Tons/Year (000,000)	Annual Saving Potential @ \$(000,000)
Argentina	3	12
Brazil	7	28
Mexico	15	60
Venezuela	7	28

@ Based on \$4 per metric ton average saving

CONCLUSION

The octane requirement of an engine is known to increase with mileage by 3 to 15 octane numbers, averaging 6 to 7. For that reason the national specifications in octane number of gasolines have to be based not on the original octane requirement of the engine, but on its octane requirement when, after mileage is accumulated, an equilibrium octane requirement is established.

By using a new generation of ashless additive, it is possible to reduce that octane requirement increase by 50% to 80%, opening a new route to control waste of octane with no performance penalty. The savings in both money and crude oil are substantial:

- Decreasing the octane number by ONE units saves \$2 to \$6 per metric ton of gasoline produced.
- Decreasing the octane number by ONE units saves up to 20% of the crude oil feedstock requirement.

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APPENDIX A LABORATORY KEY

National Institute for Petroleum and Energy
Research (USA) L-3

RICARDO Consulting Engineers (UK) L-4

A Major European Petroleum Company ... L-5