Waste Heat Recovery in SI Engines by the Dissociation of Methanol Fuel

N. R. van der Walt,* C. J. Rallis†
University of the Witwatersrand, Johannesburg

Abstract

Methanol is the most likely replacement for petroleum as a liquid fuel for automotive engines. By using the thermal energy of the engine coolant and exhaust gases to dissociate methanol into hydrogen and carbon monoxide, regeneration can be achieved. A single cylinder SI engine was instrumented to investigate this technique. Dissociation was simulated by fuelling the engine simultaneously with dissociated methanol from a gas cylinder and liquid methanol. Improvements in efficiency of up to 27% over normal throttled operation on methanol were achieved. The proportion of dissociated methanol in the fuel which gave maximum efficiency varied from 100% at no load to 40% at maximum power. Analysis of combustion chamber pressure data showed that the addition of dissociated methanol significantly increases the rate of combustion and limits of flammability of methanol. The use of a small dissociator which always operates at maximum capacity is recommended as the best compromise between engine efficiency and cost.

Introduction

Keller [1] has estimated that the world supply of petroleum will be exhausted by the end of the century. Alternative fossil fuels are oil shale, tar sands and coal, but these are all solids and the world's transportation today demands liquid fuels. The most likely replacement for petroleum as a liquid fuel in Southern Africa is methanol which can be extracted from our abundant supplies of coal.

Regenerative Fuelling

In an internal combustion engine approximately two thirds of the chemical energy of the fuel that is supplied is rejected to the surroundings as heat via the exhaust and cooling systems. If this energy could be recovered and reused in the engine there would be an increase in its overall thermodynamic efficiency. One way in which this can be achieved is through the catalytic dissociation of methanol.

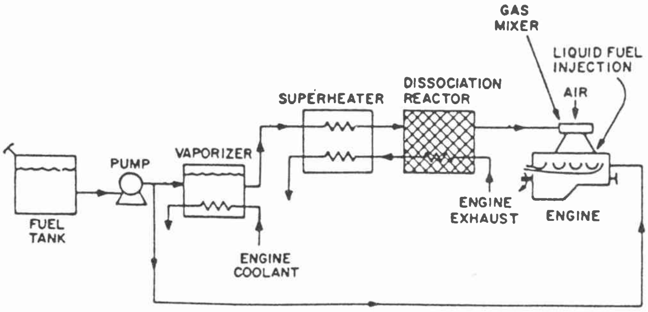

Figure 1 – Waste heat recovery through vaporisation and dissociation [1]

$$CH_3OH_{(l)} + \triangle q \Rightarrow CO_{(g)} + 2H_{2(g)}$$

Since this is an endothermic reaction the heat of combustion of the products is higher than that of liquid methanol. By using the thermal energy of the engine coolant and exhaust gases to drive this reaction and then fuelling the engine with the dissociated methanol (DM) regeneration can be achieved. Figure 1 shows the schematic layout of an engine modified in this way.

Previous Engine Tests

The tests performed can be divided into two groups: those in which an engine was fitted with a dissociator [2,3,4,5] and those in which dissociation was simulated by fuelling the engine with DM gas from cylinders [6,7]. In the latter case the engine was fuelled either with methanol alone or DM alone, not combinations of the two. In the first method the results obtained are dependent on the heat exchanger and catalyst used, thus restricting their generality. Also, since only the methanol flowrate into the dissociator was measured, the proportion of methanol which was dissociated was unknown making it difficult to draw conclusions on the effect of the degree of dissociation on engine performance. For the purpose of optimising the engine/dissociator configuration this information is vital.

Increases in efficiency of between 7 percent and 35 percent compared to methanol were reported in the literature, these improvements being primarily due to the increase in the heat of combustion of the fuel. All the researchers except Yamaguchi *et al* [4] found that for high concentrations of DM in the fuel, engine performance was limited by backfiring through the inlet system. Dramatic reductions in aldehyde emissions were also reported in references, 2, 3 and 7. This is significant since this is the only type of emission for which methanol does not better the standard set by petrol.

Only Sato *et al* [2] had instrumentation to measure combustion chamber pressure. They reported that the

---

*MSc Student (1989)
†Professor, School of Mechanical Engineering, Wits 2050. Honorary Fellow.

combustion duration and cycle-to-cycle variations in pressure decreased as the proportion of fuel supplied to the dissociator was increased. Data of this type can give a valuable insight into the effect of dissociation on the combustion characteristics of methanol and its effects on the engine cycle.

Specific Objectives

In view of the foregoing the specific aims of this study were:

- To determine experimentally the improvement in engine performance that can be achieved through regeneration by the dissociation of methanol
- To investigate the effect of the degree of dissociation of methanol on engine performance and combustion phenomena

This paper is based on the dissertation of N.R. van der Walt [8].

Experimental equipment and procedure

The Engine

A single cylinder CFR spark ignition engine usually used for the octane rating of fuels was used for the tests. Specifications are given in [9]. A Mikuni slide/needle type carburettor was used to fuel the engine on liquid methanol. This item was modified so that the flowrates of methanol and air into the engine could be controlled independently. Premixed DM fuel from a gas cylinder was supplied directly to the inlet manifold downstream of the carburettor. The engine was loaded by a hydraulic dynamometer which was coupled to the flywheel.

Instrumentation

The flowrate of air into the engine was measured with an orifice plate manufactured and installed according to British Standards [10] and those of the methanol and DM fuels were measured with variable area flowmeters. The temperatures of the inlet air, fuel/air mixture and exhaust gases were measured with thermocouples. The combustion chamber pressure was measured by a quartz piezoelectric transducer and was recorded for eighteen cycles of the engine at 0,2 degree increments of crankshaft rotation. A mercury U-tube manometer was used to measure the pressure drop across the inlet system. Ignition timing was measured by the use of a timing light. The engine torque was measured by a load cell which restrained the rotation of the trunion mounted dynamometer.

Procedure

Tests were conducted at a compression ration of 8:1, an engine speed of 1360 revs/min and with wide open throttle operation. Spark timing was optimised to give maximum efficiency. This was achieved by conducting preliminary tests so that the optimum spark advance could be expressed as a function of the methanol and DM equivalence ratios. The actual test procedure was as follows:

- The flowrate of DM into the engine was set to a given value
- The methanol flowrate was set so that a fuel rich mixture was obtained
- The methanol flowrate was decreased in steps
- At each of these steps the spark timing was set to the optimum and measurements were recorded.

This procedure was repeated for various DM flowrates.

Energy Release Model

The combustion chamber pressure data were used to calculate the approximate rate at which energy was released by combustion of fuel. This was achieved by using the following equation derived by Obert [11]:

$$\frac{dq}{d\Theta} = \frac{\gamma - n}{\gamma - 1} p \frac{dV}{d\Theta}$$

where:

dq = Differential energy transfer to the system
dV = Differential change in volume
$d\Theta$ = Differential crank rotation
p = Combustion chamber pressure
γ = Isentropic index
n = Polytropic index for process

The polytropic index was calculated from the change in pressure and volume over each increment. The value of γ used was that for air expressed as a function of temperature only. The heat term was split into the chemical energy liberated by the combustion of fuel and the energy transferred to the walls of the combustion chamber. This latter term was approximated by using the relationships recommended by Annand [12].

Results and Discussion

As expected the onset of backfiring limited the operating range of the engine for mixtures with a large proportion of DM in the fuel. The output of the engine could be

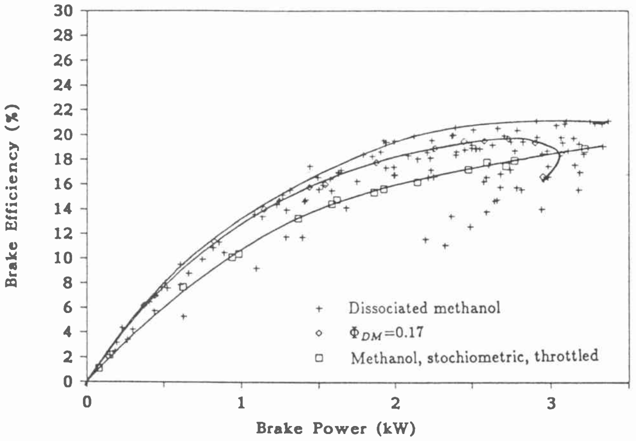

Figure 2 – Engine efficiency with differend fuel compositions.

increased by increasing the equivalence ratio (ϕ) until a point was reached where flashback in the inlet system occured. Once backfiring began it persisted until the supply of DM to the engine was completely shut off. This condition began earlier for higher proportions of DM in the fuel. The backfiring is a result of the low activation energy required for the combustion of hydrogen. Hot spots in the combustion chamber possessed enough energy to ignite the incoming charge.

There was also a reduction in the maximum power of the engine as the proportion of DM in the fuel increased due to the displacement of air from the combustion chamber by the gaseous fuel.

Efficiency Improvements

Figure 2 shows the results of all the tests. The top curve is the envelope of the data points obtained for operation on combinations of methanol and DM. It represents the best possible operation of the engine. For comparison the data for operation on methanol alone where power was controlled by throttling is shown. This represents normal operation on liquid methanol fuel. The efficiency was calculated by dividing the brake power by the product of the mass flowrate of fuel into the engine and the heat of combustion of *methanol*. This is the efficiency if the DM had been produced by a dissociator driven by the engine.

The third curve is the data for the test in which the equivalence ratio of DM (ϕ_{DM}) was fixed at 0.17 while the equivalence ratio of methanol was varied. Thus at the left end of the curve the mixture had a high proportion of DM and was fuel lean whereas at the right hand end of the curve it had a high proportion of methanol and was fuel rich. The hook shape at the end of the curve is due to a reduction in efficiency and thus power as the mixture becomes very fuel rich. This curve is representative of the results one would expect if a small dissociator which operates at maximum capacity all the time were used.
Thus the supply of DM to the engine would be fixed and power could be increased by increasing the supply of methanol to the engine. The improvement in efficiency for this configuration over methanol is close to the maximum which can be achieved for most powers.

Figure 3 shows the improvement in efficiency over throttled methanol operation as a percentage of this efficiency. The curves both pass through the origin since at zero brake power the efficiency is zero regardless of the fuel flowrate. The improvements in efficiency which were achieved are substantial.

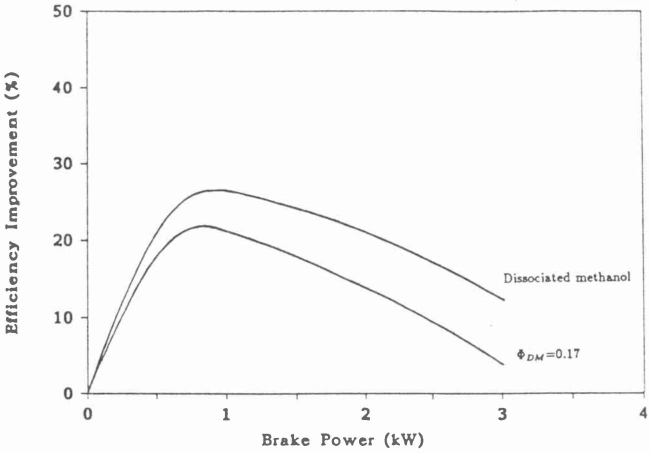

Figure 3 – Efficiency improvement

Figure 4 shows data obtained by interpolation of the results in Figure 2. The curve shows how the efficiency varied for a given power as the proportion of DM in the fuel changed. The locus of the maxima is plotted. This represents the proportion of DM in the fuel which gave maximum efficiency. If the curve is extrapolated it passes through 100% at zero power. At 3 kW power, maximum efficiency occurred when there was only 40% DM in the fuel mixture. The proportion of DM in the fuel which gave maximum efficiency decreased as the power output increased. This curve for optimum operation could be approximated in practice by having a small dissociator operating at maximum capacity as mentioned earlier.

Effect of DM on Combustion

Figure 5 shows how the pressure/volume (*pV*) diagram for the engine changes as the fraction of DM in the fuel is increased. For all these curves the fuel/air mixture was stoichiometric and the spark timing was kept constant at 10° before top dead centre (BTDC). There is virtually no difference between the curves up to the point where ignition occurs after which they diverge noticeably. As the fraction of DM in the fuel increases the rate of pressure rise during combustion becomes much higher as does the peak pressure of the cycle. The curve with 37% DM in the fuel is much closer to the ideal constant volume combustion cycle than that for operation on methanol alone.

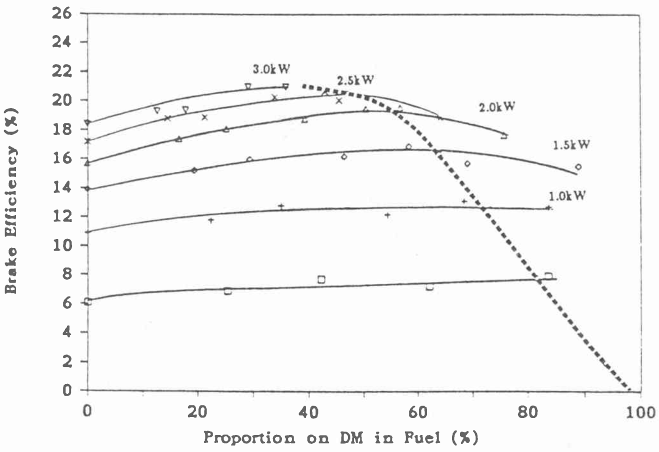

Figure 4 – Efficiency curves for different powers

During expansion the curves cross over. The reason for this is that, although the equivalence ratio is the same, the mass of fuel in the combustion chamber decreases as the fraction of DM in the fuel is increased. This is so because the gaseous DM fuel is displacing air so that less fuel is required to give the same equivalence ratio. Thus the pressure must eventually be higher for pure methanol fuel since there is more fuel to burn in the combustion chamber.

Figure 6 shows the output of the energy release model corresponding to the *pV* diagrams in Figure 5. As the

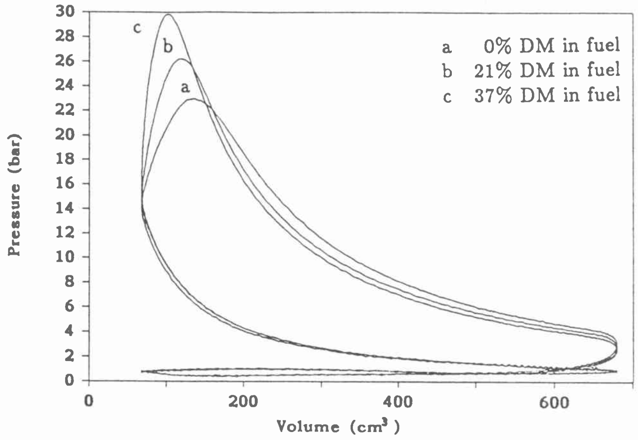

Figure 5 – Effect of DM on *pV* diagram

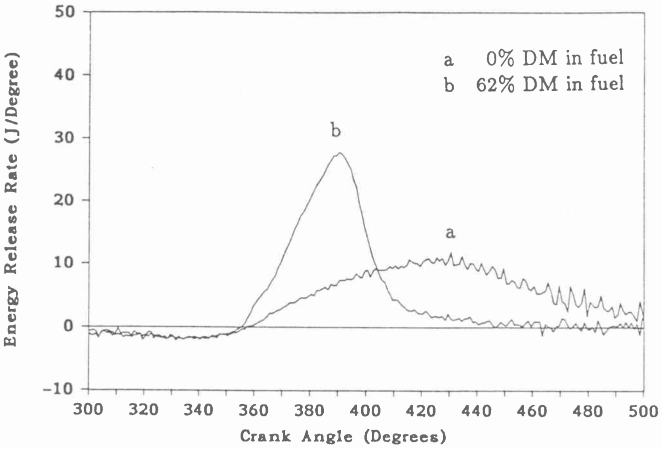

Figure 7 – Effect of DM on combustion rate for lean mixtures

amount of DM in the fuel increases the rate of combustion increases and the duration of combustion decreases. This can be attributed to the hydrogen rich DM fuel having a higher burning velocity than methanol. Surprisingly, the maximum rate of energy release is virtually constant. This is probably due to the decrease in the mass of fuel in the combustion chamber as the fraction of DM in the fuel increases. The negative rate of combustion before ignition is a result of the energy release model not accounting adequately for heat transfer to the combustion chamber walls.

Figure 7 shows the effect of DM on combustion for an overall equivalence ratio of 0.7. Again the ignition timing was fixed at 10° BTDC. The difference in the curves is much more pronounced than for the case when the fuel/air ratio was stochiometric. For the curve with methanol alone, the fuel is still burning when the exhaust valve opens at 500°, a full 150° after ignition occurred. When there was 62 percent DM in the fuel, combustion was almost complete 70° after ignition.

The difference between the curves is far more pronounced than that between the curves in Figure 6. This can be attributed to two reasons. Firstly, the range of proportions of DM is greater for Figure 7 than Figure 6. Secondly, in Figure 7 the overall equivalence ratio of 0.7 is close to the lean misfire limit of methanol, where the burning velocity becomes very low. DM, on the other hand, is far from its lean misfire limit at this equivalence ratio, and consequently its addition will have a significant effect on the combustion velocity of the mixture.

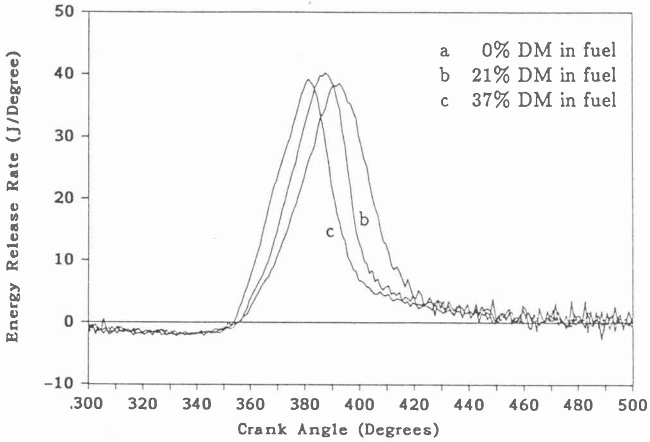

Figure 6 – Effect of DM on combustion rate for stochiometric mixtures

These results highlight an important advantage of dissociated methanol: its ability to extend the limits of combustion of methanol. During tests performed with methanol fuel at wide open throttle, the engine misfired when the equivalence ratio was less than 0.7 and the spark timing had to be advanced to as much as 60° BTDC for maximum efficiency. If a small quantity of DM was added to the fuel the engine would run smoothly for an equivalence ratio of less than 0.2.

The importance of these results is that the engine can be operated at wide open throttle all the time. The output of the engine can then be controlled by adjusting the quantity of fuel supplied to the engine rather than by throttling the engine. The latter method results in high pumping losses which decrease the part load efficiency of an engine. Carburettion would also be simplified since the flowrates of air and fuel into the engine do not need to be metered accurately to keep the equivalence ratio between certain limits to avoid misfiring.

Small Dissociator

There are several factors which favour the use of a small dissociator:

- The problem of backfiring will be eliminated
- The reduction in maximum power would be reduced
- A large proportion of the maximum improvement in efficiency possible could be achieved
- There would be cost, space and weight savings compared to a large dissociator

Conclusions

- Improvements in efficiency of up to 27 percent over throttled operation on liquid methanol can be achieved
- The proportion of dissociated methanol in the fuel which gives maximum efficiency varies from 100 percent at no load to 40 percent at maximum load
- The addition of dissociated methanol increases the rate of combustion and the limits of combustion of methanol fuel.

Acknowledgements

The Fuels and Power Plant Programme has been in operation in the School of Mechanical Engineering at the University of the Witwatersrand for some years has been supported financially by AECI, the Anglo American Corporation of South Africa Limited, the Foundation for Research Development of the Council for Scientific and Industrial Research and by the University. The support of all these institutions is gratefully acknowledged.

References

1. Keller J. L. Alcohols as a motor fuel? *API refining meeting*, May 1979.
2. Sato T., Tanaka M. and Agawa K. A study of the reformed methanol engine. *SAE Technical Paper Series*, No. 861237, Sept. 1986.
3. König, A. Ellinger K. W. and Korbel K. Engine operation on partially dissociated methanol. *SAE Technical Paper Series*, No. 850573, Feb. 1985.
4. Yamaguchi I., Toshio T., Takayuki S., Tadashi A. and Yong K. K. Development research on dissociated methanol fuelled spark ignition engine. *SAE Technical Paper Series*, No. 852201, 1985.
5. Finegold J. G. Dissociated methanol vehicle test results. *Proceedings of VI International Symposium on Alcohol Fuels Technology*, Ottawa, May 1984.
6. Adams T. G. A comparison of engine performance using methanol or dissociated methanol as the fuel. *SAE Technical Paper Series*, No. 845128, 1984.
7. McCall D. M., Lalk T. R., Davison R. R. and Harris W. B. Performance and emissions characteristics of a spark ignition engine fuelled with dissociated and steam reformed methanol. *SAE Technical Paper Series*, No. 852106, Oct. 1985.
8. Van der Walt, N. R. Waste heat recovery in spark ignition engines by the dissociation of methanol fuel. MSc Dissertation, University of the Witwatersrand, Johannesburg, 1989.
9. ASTM manuel for rating motor fuels by motor and research methods, Fourth Edition. *American Society for Testing Materials*, Pasedena, 1960.
10. British Standard BS 1042. Measurement of fluid flow in closed conduits. Part 1: Pressure differential devices. *British Standards Institution*, London, 1984.
11. Obert E. F. Internal combustion engines. *Harper and Row*, New York, 1973.
12. Annand W. J. D. Heat transfer in the cylinders of reciprocating internal combustion engines. *Institution of Mechanical Engineers*, Vol. 177, No. 36, pp 973-996, 1963.