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Environmental Protection  
Agency

Office of Mobile Source Air Pollution Control  
Emission Control Technology Division  
2565 Plymouth Road  
Ann Arbor, Michigan 48105

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Air

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# Near-Cylinder Dissociation of Methanol for Automotive Application

# **Near-Cylinder Dissociation of Methanol for Automotive Application**

by

Engine and Vehicle Research Division  
Southwest Research Institute  
6220 Culebra Road  
San Antonio, Texas 78284

Contract No. 68-03-1984

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Prepared for

ENVIRONMENTAL PROTECTION AGENCY  
Office of Mobile Source Air Pollution Control  
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## FOREWORD

This project was initiated by the Control Technology Assessment and Characterization Branch of the Environmental Protection Agency in September, 1984. The effort on which this report is based was performed by the Engine and Vehicle Research Division of Southwest Research Institute and was completed in July, 1988.

This project was identified within SwRI as 03-8352, and the Project Managers, in chronological order, were Mr. R. G. Phatak, Dr. Robert Thring (acting), Mr. Gerald Driscoll, and Mr. Gary Stecklein. This final report was compiled by Mr. Roy Hull and Mr. Charles Urban and was reviewed by Mr. Charles Urban and Mr. Gary Stecklein. Mr. Charles Urban also provided technical review of the heat exchanger subsequent to evaluation and recommended design improvements. The Project Officers at the Environmental Protection Agency over the course of this project were Mr. Robert Wagner, Dr. Karl Hellman (acting), and Mr. Robert Bruetsch.

## ABSTRACT

This report describes the design analyses and experimental evaluation toward developing a system of dissociating methanol for use in a spark-ignited passenger car engine. Maximum dissociation of methanol fuel attainable using exhaust gas heat was the basic goal of this project. The heating value of dissociated methanol is about 20 percent higher than that for liquid methanol. Therefore, significant energy savings appear to be attainable if a large percent of the engine fuel needs can be dissociated by use of the otherwise wasted heat of the exhaust gas. A heat exchanger consisting of a methanol evaporator, an injection system to provide fuel to the evaporator, and a dissociation catalytic reactor was designed, fabricated and tested. The dissociation efficiency of this initial reactor was not as good as expected. The relative poor performance of the dissociation reactor apparently was associated with fuel injector nozzle heating, blockage of passageways in the dissociation reactor, and an ineffective dissociation catalyst. The heat exchanger was redesigned to incorporate improvements, and four heat exchangers were fabricated using the final design.

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## SUMMARY

A program was conducted by SwRI to analyze, design, and test a methanol dissociation heat exchanger for automotive applications. The major objective for methanol dissociation is to provide improved engine operating efficiency compared to conventional operation with liquid methanol. In-cylinder dissociation of methanol was initially desired but was shown early in the program to be unachievable. An alternative approach was taken to locate the heat exchanger near the exhaust port and to inject the products of dissociation into the combustion chamber without prior mixing with combustion air. Maximum dissociation of methanol from available exhaust heat was a primary goal.

A gain in engine thermal efficiency is possible in theory, because the exhaust heat can be used to dissociate methanol into hydrogen and carbon monoxide according to the reaction  $\text{CH}_3\text{OH} \longrightarrow 2\text{H}_2 + \text{CO}$ . Through this dissociation process, the energy content (lower heating value) of liquid methanol is increased about 20 percent. Mathematical and design analyses were made of catalytic reactor and evaporator sections for use in a dissociation heat exchanger. These analyses were based on using a Nissan NAPS-Z two-liter engine. A counterflow design was chosen, whereby the exhaust gases flowed first over the catalytic reactor and then over the evaporator. This counterflow design was selected over crossflow or parallel-flow systems as being the most efficient for the dissociation process.

Based on the analyses, a heat exchanger approximately 52 cm (20.5 inches) long by 9.5 cm (3.75) inches outside diameter, including reactor and evaporator, was designed and fabricated. The Johnson Matthey Catalytic Systems Division was selected to provide the catalysts for the dissociation reactor. For the methanol dissociation catalyst, a proprietary base metal catalyst (Type H) was used. For the exhaust-side catalyst, precious metals (platinum and palladium) were used. The fuel system for injecting liquid methanol into the evaporator consisted of a modified Stanadyne DB2 distributor-type pump and an injector designed and fabricated by SwRI.

Performance evaluations of the prototype dissociation heat exchanger were conducted at selected engine speed and load conditions using the exhaust from one cylinder of the NAPS-Z engine. This engine was utilized as an exhaust generator, and the products of dissociation were not used as fuel for the engine in these evaluations. Dissociation rates in the reactor ranged from 1 to 96 percent of the total methanol injected into the evaporator; the higher dissociation rates being associated with low methanol injection rates. This represented from 0.6 to 9.8 percent of the engine cylinder fuel needs at the test points evaluated. The evaporator was adequately sized to vaporize 100 percent of the engine cylinder fuel needs at 3000 rpm, but only 50 percent at 1500 rpm. The vaporization rate was greater at 3000 rpm because of the higher exhaust temperature and flowrate at that engine speed.

Design improvements were made to the dissociation heat exchanger. These included a relocation of the methanol injector, a modification to the flow areas in the reactor, and the addition of fins to the evaporator. Four heat exchangers were fabricated to the final design specifications, and provided to the EPA.

## I. INTRODUCTION

This section discusses the objectives, background, and scope of work associated with development of a methanol dissociation heat exchanger.

### A. Project Objectives

The original goal was to provide reactors inside the cylinders of a methanol engine (in a pre-chamber) to vaporize and dissociate a significant portion of the total engine fuel needs. The dissociated methanol was to provide improved operating efficiency compared to conventional operation with liquid methanol. At the outset of the program, the in-cylinder dissociation was determined not possible given the limited volume (hence limited catalyst area), high temperature (potential catalyst damage), and presence of oxygen and combustion products (catalyst oxidation or poisoning) that are typically found in combustion chambers.

The project efforts were then directed toward the following objectives:

- ° Design, fabricate and test a heat exchanger for "near-cylinder" dissociation of methanol. This was to utilize a heat exchanger for each cylinder and discharge the dissociation products injected directly into the cylinder.
- ° Design and fabricate engine modifications to accommodate direct injection of the heat exchanger products into the cylinder.
- ° Procure or fabricate a fuel injection system to inject and meter fuel into the heat exchanger.
- ° Based on the analysis of test results, modify the heat exchanger design to optimize its performance.
- ° Fabricate four new heat exchangers to the optimized design.

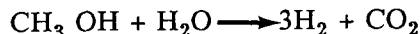
Design efforts in several areas were more extensive than originally planned, and major problems were experienced with the engine to be used in testing the methanol dissociation heat exchanger. In order to concentrate remaining efforts toward development of the dissociation heat exchanger, program requirements were subsequently redirected to omit the modifications to the engine (controls and intake valve) and the actual operation of the engine on the products of dissociation.

### B. Background Information

It is possible to enhance the energy content of liquid methanol by endothermically reacting it over a catalyst to form gaseous hydrogen and carbon monoxide. Dissociated methanol is methanol decomposed by one of two processes. The first approach separates neat methanol into hydrogen and carbon monoxide primarily in a reaction as follows:



The second approach uses an equimolar solution of methanol and water and is known as steam reformation. This method can be demonstrated by the following reaction:



Even though steam reformation provides more hydrogen, dissociation of neat methanol provides for greater improvement in thermal efficiency than that provided by steam reformation.

There are several reasons for the interest in using dissociated methanol versus neat methanol in internal combustion engines. The primary reason is to reduce specific fuel consumption. This can be accomplished because the lower heating value (LHV) of the dissociated products ( $\text{H}_2$  and  $\text{CO}$ ) is about 20 percent higher than that of liquid methanol and 13 percent higher than that of vaporized methanol. In addition, the engine can operate at very low equivalence ratios with the hydrogen-rich dissociated methanol as compared to liquid methanol. A second reason for using dissociated methanol is that harmful emissions are reduced. Hydrocarbon and aldehyde emissions are very low with dissociated methanol versus liquid methanol. Oxides of nitrogen are also lower with dissociated methanol when operating at low equivalence ratios in reciprocating engines.

The following comments on emissions are based on ideal mixtures of dissociated or reformed products of methanol. Actual emissions levels would probably be between those produced on liquid methanol and those produced on these ideal mixtures.

**Hydrocarbons** - Most of the literature suggests that hydrocarbon (HC) emissions should be very low with either reformed or dissociated methanol as compared to liquid methanol. This is because there are no hydrocarbon compounds in either reformed ( $3\text{H}_2 + \text{CO}_2$ ) or dissociated ( $2\text{H}_2 + \text{CO}$ ) methanol. Engines operating on mixtures of  $\text{H}_2$  and  $\text{CO}$  or  $\text{H}_2$  and  $\text{CO}_2$  generate hydrocarbons only from the lubricating oil that enters into the combustion chamber past the rings or valve stem seals. Thus, hydrocarbon emissions when using dissociated methanol are a function of engine condition, design and load. Hydrocarbon emissions from an engine fueled partially with dissociated methanol should at least be less than the HC emissions from the same engine fueled with liquid methanol.<sup>(1)\*</sup>

**Oxides of Nitrogen** -  $\text{NO}_x$  emissions are low at very lean equivalence ratios (low load) when operating on dissociated methanol.<sup>(1,2)</sup> No data were found in the literature for engine operation with dissociated (or reformed) methanol at high loads. Operation on dissociated methanol at high loads, with equivalence ratios of about 1.0, should produce somewhat higher  $\text{NO}_x$  emissions compared to liquid methanol because of the higher flame temperature of the  $\text{H}_2 + \text{CO}$  mixture.<sup>(2)</sup>

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\*Superscript numbers in parentheses designate references at the end of this report.

**Carbon Monoxide** - At very low equivalence ratios, CO emissions with dissociated methanol tend to be somewhat higher than with liquid methanol, because of passthrough of unburned CO. At higher equivalence ratios, CO emissions are typically less with dissociated methanol. (2)

**Aldehydes** - Aldehyde emissions are not readily formed from the primary methanol dissociation products: hydrogen and carbon monoxide. Because dissociation to  $H_2$  and CO is not complete and other products of dissociation have not been adequately defined, however, effect of dissociation on aldehydes is not currently known.

### **C. Scope of Work**

This program was directed toward dissociation of methanol in the combustion chamber or in a reactor located close to the combustion chamber, so the products of dissociation could be directly introduced into the combustion chamber. Three technical tasks were specified and included the development of design specifications, procurement and/or fabrication of hardware and engine components, and engine testing followed by system design improvements. A fourth task delineated the program reporting requirements.

### **D. Methanol Dissociation Heat Exchanger**

The term "heat exchanger", as applied in this report, refers to the assembly into which liquid methanol is injected and out of which dissociated products ( $2H_2 + CO$ ) are discharged. The heat exchanger is made up of two components. These are the "evaporator" into which the liquid methanol is injected and vaporized, and the "reactor" where the vaporized methanol is superheated and dissociated into hydrogen and carbon monoxide.

Heat exchanger design objectives were to:

- ° Make maximum use of exhaust heat down to about 400°F for dissociation in the reactor section and use heat below 400°F for vaporization in the evaporator section.
- ° Design for maximized dissociation of methanol under all engine operating conditions.
- ° Accommodate transient engine operating conditions through the use of an auxiliary fuel system. This auxiliary system would fuel the engine during start-up and would provide supplementary fuel when the amount of dissociated fuel was insufficient for the power requirements.

Heat exchanger design considerations included the following:

- ° The reactor design analysis was to be directed toward plate/fin and concentric tube designs with a counterflow configuration to provide maximum heat transfer area for a given mechanical volume. The design was to be based on analyses of steady-state conditions.

- ° The possibility of using fins on both sides (exhaust and methanol) was to be investigated.
- ° Depositing catalyst materials on both sides of the reactor was to be investigated. Catalyst material on the exhaust side could increase reactor temperature through oxidation of any HC and CO present in the exhaust.
- ° Vaporization of methanol in the evaporator was to occur under all operating conditions utilizing the residual exhaust heat energy after the exhaust gases have passed through the reactor.
- ° Pressure drop across the reactor and transient response of the heat exchanger under a range of engine operating conditions were to be calculated.

### E. Methanol Fuel

To meet future energy needs, a synthetic fuel derived from domestic coal, natural gas, and biomass would be especially attractive if the use of such fuel also led to increased engine efficiency and improved exhaust emissions. One favorable candidate that has emerged from extensive engine testing in the U.S.A. <sup>(3)</sup> and Germany <sup>(4)</sup> is methanol. Methanol can be made from synthesis gas using readily-available catalysts and reactor designs. Based on thermal cycles <sup>(5,6)</sup>, methanol appears to be the most cost-effective liquid fuel that can be made from coal. Projections <sup>(7)</sup> indicate that methanol could become economically competitive with gasoline.

The production of methanol from synthesis gas is an exothermic process (21.68 kCal/mole) by the reaction  $\text{CO} + 2\text{H}_2 \longrightarrow \text{CH}_3\text{OH}$ , which is carried out in a catalyst bed at relatively low temperatures and high pressures. Use of waste heat from a combustion engine to dissociate methanol back into carbon monoxide and hydrogen, an endothermic process, provides an opportunity to recover some of the energy lost during the coal to methanol conversion.

Although methanol has several good combustion qualities, namely, high octane number, high flame speed, and broad ignition limits, it also has some less desirable properties such as high heat of vaporization, a tendency to pre-ignite, and low heat of combustion. Problems with neat methanol include cold-start ignition, cylinder wear, and vehicle range. To alleviate difficulties with cold-start ignition, the volatility of methanol is increased by adding components such as gasoline or dimethyl ether. A system using exhaust heat to dissociate methanol would not enhance cold-start ignition in an engine, but it could improve thermal efficiency and reduce exhaust emissions. The main advantage of methanol dissociation is that it provides a method of utilizing waste heat and thus the potential for reducing the specific fuel consumption of the spark-ignition engine. <sup>(8-11)</sup>

## II. HEAT EXCHANGER - INITIAL DESIGN

The term "heat exchanger", as used in this project, includes the evaporator into which liquid methanol is injected, and the reactor where the methanol is dissociated into hydrogen and carbon monoxide.

### A. Fuel Injection System

The fuel injection system, consisting of a pump and a suitable injector for each evaporator chamber, must be capable of delivering the correct amount of fuel in a spray pattern that evenly covers the walls of the evaporator, to assure rapid vaporization. The pump can be a multi-cylinder, distributor-type pump capable of supplying fuel to each individual injector. Compatibility with methanol fuel is a requirement for both the pump and the injector as well as any connecting lines, fittings and gaskets. Pump and nozzle wear is a concern if the pump and nozzles are designed for diesel fuel but have to handle methanol. Materials changes are required to avoid wear and corrosion.

To provide the greatest possible vaporization, there is a need to spray the walls of the evaporator with a forceful impingement (to minimize boundary layer effects) of small droplets over the entire surface of the evaporator (to minimize evaporator volume).

**Development Effort** - An initial survey of SwRI engineers having experience with methanol-fueled engines and fuel injection systems in general failed to disclose any suitable pumps or injectors that would meet the requirements for the fuel system. Commercial suppliers of pumps and injectors were not surveyed at that time. SwRI experience had shown that use of neat methanol in standard diesel injectors and pumps results in early failures of these components due to lack of lubrication. Therefore, an in-house effort was made to design a pump and injector system based on the SwRI experience.

This fuel injection system design effort was directed towards providing a system that would:

- ° Deliver from 0.2 to 11 kg/hr (0.5 to 24.5 lbm/hr) of methanol per cylinder.
- ° Deliver fuel evenly from each injector.
- ° Atomize the fuel sufficiently to promote rapid vaporization.
- ° Provide injectors to operate at internal evaporator temperatures of up to 126°C (259°F) and external exhaust temperatures up to 177°C (350°F), and include a check valve feature to minimize vapor lock.
- ° Provide pump and injectors to generate and withstand fuel pressures up to 2100 kPa (300 psig). This value is the sum of the maximum reactor operating pressure of 700 kPa (100 psig) and the maximum expected pressure drop across the fuel nozzle required to achieve good atomization of 1400 kPa (200 psig).

- ° Assure that the injector produces a methanol spray pattern that maximizes coating the heated inside walls of the evaporator.
- ° Provide pump and injectors to perform reliably and with sufficient durability without the inherent lubricity provided by petroleum fuels.

Initial effort resulted in a workable system that produced good spray atomization and distribution at high flowrates, as observed within a clear plastic tube using Stoddard solvent. Testing of the SwRI designed pump and injectors is described in Appendix A. The pump had two separate pistons, each driven on the opposite side of the same eccentric. The outlet from each piston was sent to two of the four nozzles. Bench tests were performed using the pump (driven by an electric motor) connected to four nozzles. Each of the nozzles was installed in a clear plastic tube with an inside diameter of 7.9 cm (to simulate the 3.1 inches diameter of the evaporator). Each tube had provisions for collecting and draining the sprayed solvent, so that the quantity of solvent sprayed from each nozzle could be determined over a test period and compared to each other. This bench testing showed that the initial design had two major shortcomings: (1) lack of balanced fuel delivery between nozzles at all flowrates, and (2) poor atomization quality at low pump speeds (low flowrates). In order to overcome these shortcomings, a second generation pump was designed using the nozzles and pump eccentric housing from the first generation design. The second generation pump design (shown in Appendix A) uses a single piston that operates at constant speed to provide good atomization at all flowrates. Changes in flowrate were accomplished by adjusting the pressure regulator.

Subsequent to the in-house pump and injector design efforts, a search was conducted for commercially available injection systems that are compatible with methanol. Three manufacturers were contacted: Stanadyne, American Bosch, and Robert Bosch. Each was asked if one of their production fuel injection systems (pump and nozzle) or a modified production system would operate on neat methanol. Stanadyne responded with assistance applicable to the specific program needs, since they had experience in operating their distributor-type pumps with methanol. There is an inherent advantage in using a distributor pump over an in-line pump in that no other source of lubrication is required. An in-line pump typically uses engine oil for lubrication in the cam area, but a distributor pump uses only the fuel it is supplied with to lubricate the internal pump parts. Thus, if a distributor pump can be successfully used with methanol, contamination of the engine oil by methanol and contamination of the fuel with engine oil can be avoided. Engine oil in the methanol could have a deleterious effect on the dissociation catalyst. Internal changes to the distributor pump were necessary, however, to avoid wear and corrosion when using methanol instead of diesel fuel.

At this point in the program there were three possible directions to pursue to obtain a suitable fuel injection system. They were to:

- ° **Use internal design effort on the second generation pump.** This concept was designed to provide a balanced fuel delivery between each of the nozzles and to give good atomization. It was not a proven concept, so there was risk that it would not achieve these goals.

- ° **Use a completely commercial based (Stanadyne) system for the pump and nozzles.** This could be either an off-the-shelf unmodified system that has demonstrated reasonable life using neat methanol, or a modified commercial system that has demonstrated its durability. Some changes to the commercial nozzles would probably be required to obtain the desired spray pattern.
- ° **Use a combination of commercial pump and the existing nozzles.** This approach could be of value if the existing nozzles worked well with the commercial pump.

Each of these approaches would require some effort to adapt the pump to the engine and to the control system. The third approach (i.e., the combination of a commercial Stanadyne DB2 pump and existing SwRI designed injectors) was chosen at that time.

There was some difficulty in assessing the actual durability of standard or modified commercial pumps operating on methanol. Though there were some published data discussing hardware <sup>(12-14)</sup>, that typically was not the primary purpose for the publication. Published data did not involve extensive operating hours and discuss only limited experience. Discussions with manufacturers, likewise, indicate that their experience was limited.

The SwRI designed injector performed satisfactory in evaluations at room temperature but did not perform satisfactorily at elevated operating temperature. In addition, it was considered desirable to use injectors that were more readily available. The final system utilized a commercially modified fuel injection pump and modified commercially available injectors; these units are described as follows:

**Pump** - The Stanadyne DB2 distributor type pump is used commercially on small, high-speed diesel engines. To enable the pump to safely operate on methanol, the following pump modifications were made by Stanadyne:

- ° The housing was nickel plated to retard corrosion of the aluminum by methanol.
- ° Ceramic rollers were used in place of steel.
- ° Tool steel was used instead of sintered steel for transfer pump liners and rotor.
- ° The governor section and the valve cage were nickel plated.

**Injectors** - The Stanadyne Model 14 (or CVA Model 5760 403) poppet nozzle injector was modified to provide the wide spray pattern desired for the heat exchanger application. The spray pattern obtained is shown in Figure 1, and the modifications to the Stanadyne Model 14 injector necessary to achieve this pattern is shown in Figure 2.

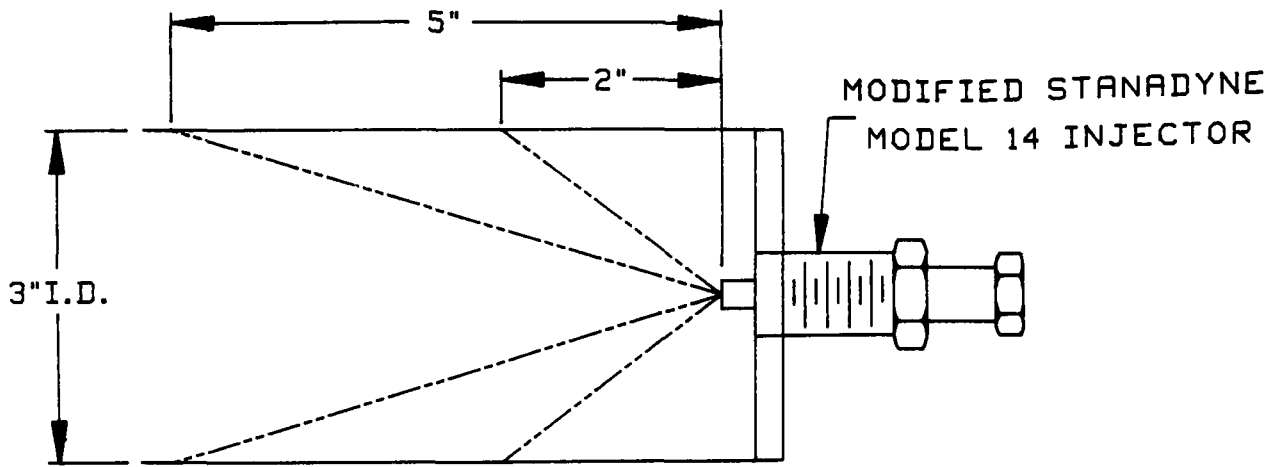


FIGURE 1. SPRAY PATTERN OF METHANOL INJECTOR.

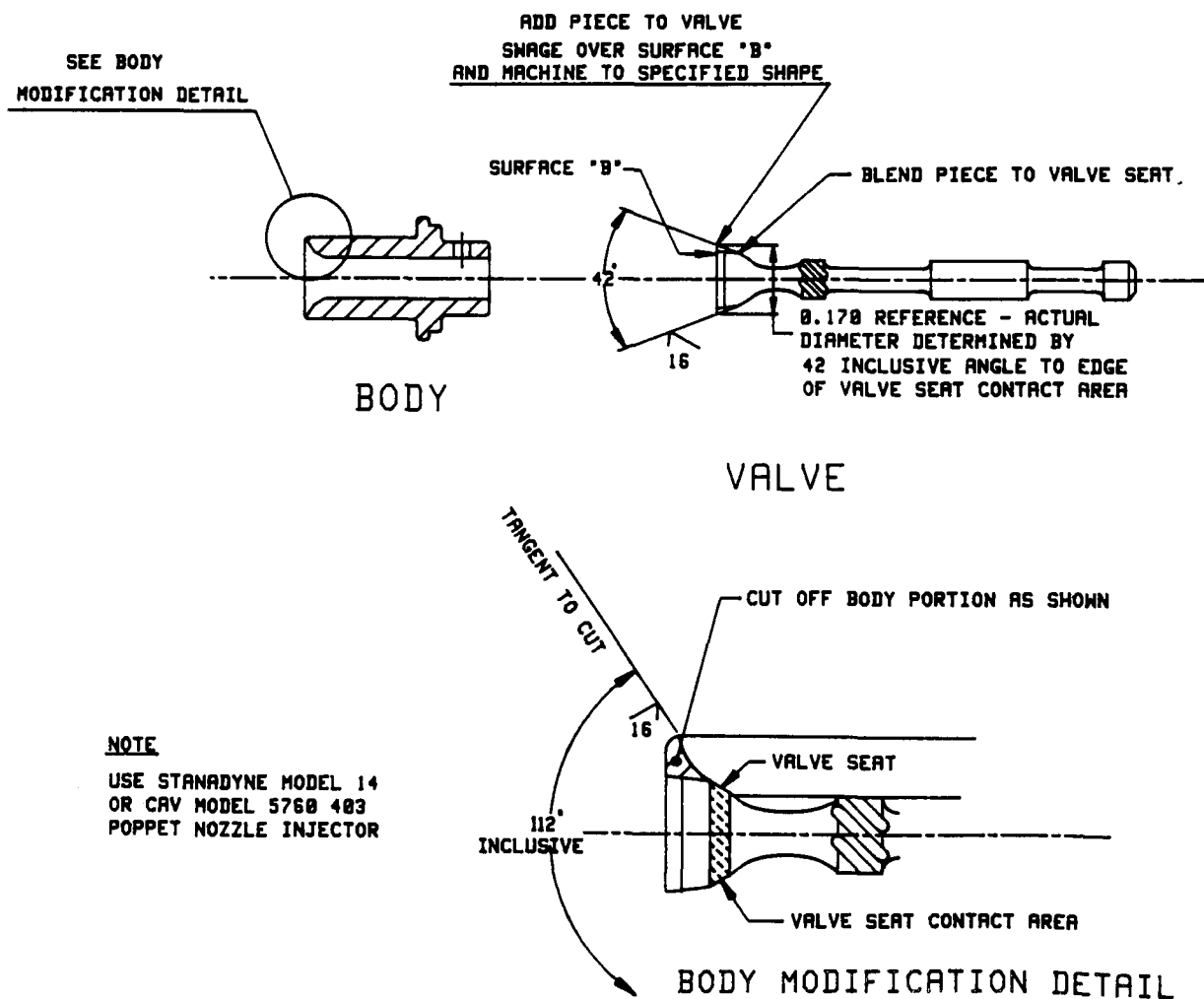


FIGURE 2. INJECTOR MODIFICATIONS TO OBTAIN SPRAY PATTERN.

## B. Evaporator and Reactor

The initial intent of this program was to have the dissociation of the liquid methanol occur in the combustion chamber. In the report Design Specifications for In-Cylinder Dissociation of Methanol (Appendix B), SwRI concluded that there would be several disadvantages to locating the catalyst within the combustion chamber. As stated in the design specifications, the major limitation was that the evaporator and reactor (catalyst) volumes required would be greatly in excess of space available in the combustion chamber. Additional stated disadvantages of in-cylinder dissociation were:

- ° Contamination of the catalyst with combustion products, rendering it useless in a short period of time.
- ° Heating of the catalyst would primarily occur during combustion, rather than from waste heat in the exhaust, and that results in lower cycle efficiency.
- ° The necessity of supplying methanol, and therefore dissociation, during the intake cycle, resulting in low volumetric efficiency of the engine.
- ° Premature combustion of dissociated methanol, resulting in loss of engine efficiency and damage to the engine's structure.

These limitations were eliminated by (1) separating the catalyst chamber from the engine's combustion space and (2) locating the catalyst chamber in the exhaust stream so that waste heat from the exhaust gases can readily be used. However, such design would still be a departure from previous work of others in that the dissociated gases would be inducted directly into the cylinder rather than through the intake manifold with combustion air. Products of dissociation were to be introduced into the cylinder through a separate induction valve. To conserve heat, the heat exchanger was to be located as close as possible to the exhaust port. Maximum dissociation of methanol was the goal, and the guidelines to be followed in designing the heat exchanger were:

- ° Use a counterflow heat exchanger, finned on both sides with either a plate-fin or concentric tube configuration.
- ° Provide sufficient area to handle maximum heat flux from the exhaust above 205°C (400°F.)
- ° Catalyze both sides of the heat exchanger.
- ° Investigate, by analysis, the transient behavior of the heat exchanger.
- ° Construct the exchanger so that low temperature exhaust is used for vaporization, with the higher temperature exhaust being used for dissociation of the vaporized methanol.

- ° Design the heat exchanger for steady state conditions, and provide separate fueling provisions for start-up and other transient conditions.

Design analyses of the heat exchanger were performed by SwRI and a consultant. Analysis of the evaporator by the consultant is contained in Appendix C. Initial heat exchanger analysis by SwRI (Appendix D) covered both the evaporator and the reactor. After reviewing the analyses and the related literature, an evaporator design was selected, and a decision was reached to perform a series of tests on a single unit on the engine to determine the actual performance of the evaporator and the reactor. Design specifications for the heat exchanger that was fabricated for testing are listed in Table 1. The heat exchanger was fabricated by SwRI using catalyst substrates provided by Johnson Matthey. Figures 3-7 are photographs of the heat exchanger showing the assembled heat exchanger and its component parts. These figures are described in the following paragraphs:

- Figure 3 -** The heat exchanger outer shell is shown attached to the exhaust manifold. Ports in the outer shell near the exhaust manifold were used to measure exhaust gas temperature and pressure as it enters the heat exchanger. Other ports in the outer shell were used to measure exhaust gas temperatures and pressures at locations between the reactor and evaporator and at the exit of the evaporator. The tube extending from the right side of the outer shell is for discharging exhaust gases.
- Figure 4 -** The heat exchanger is shown with the reactor (where dissociation takes place) at the left and the evaporator (where methanol vaporization takes place) to the right.
- Figure 5** A closeup of the junction of the evaporator and reactor is shown with the evaporator to the right. The single exhaust annulus around the evaporator is visible as are three of the four tubes that port the vaporized methanol from the evaporator to the reactor. The outer shells of both the evaporator and reactor were made from 0.127 mm (0.005-inch) thick stainless steel and served only to retain the metal substrate during fabrication.
- Figure 6 -** This view shows the top of the evaporator cover. The nozzle is in the center, with its fuel line extending upward and its spring tension adjustment on top.
- Figure 7** The reactor exhaust inlet and dissociated methanol outlet are shown. The manifold connects the two methanol annuli and has a flared connection that permits attachment to the outlet port welded to the outer shell. The metal catalyst substrate can be seen in the three exhaust annuli.

**TABLE 1. DESIGN SPECIFICATIONS FOR  
SwRI METHANOL DISSOCIATION HEAT EXCHANGER**

**Dimensions**

Heat Exchanger Housing:	58 cm (23 inches) long by 9.5 cm (3.75 inches) in diameter
Inside Housing: Reactor - Evaporator	20.4 cm (8.05 inches) long 10.2 cm (4.0 inches) long
Connection Between Evaporator and Reactor:	3.8 cm (1.5 inches)

Remainder of the length inside housing is for the fuel injection nozzle, exhaust discharge, and a manifold for the dissociated products.

**Design Flowrates**

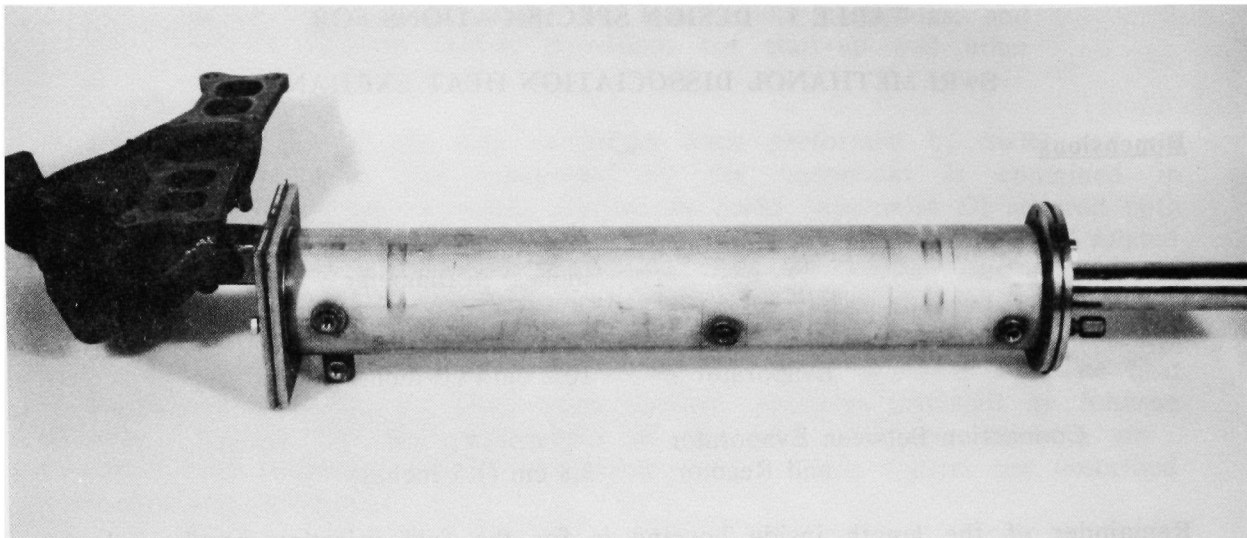
Exhaust Side:	64 kg/hr (141 lbm/hr) with less than 25 mm (1.0 in.) Hg. pressure drop
Methanol:	0.2 to 11 kg/hr (0.5 to 25 lbm/hr) injector rating

**Materials**

Housing and all structural parts are 304 L stainless steel.

**Reactor Catalyst Details**

Dissociation Catalyst Material:	Johnson Matthey Type H base metal (2 annuli)
Apparent Surface Yield:	3.9 kg/hr-m <sup>2</sup> (0.8 lbm/hr-ft <sup>2</sup> )
Actual Surface Yield:	1.8x10 <sup>-3</sup> kg/hr-m <sup>2</sup> (3.7x10 <sup>-4</sup> lbm/hr-ft <sup>2</sup> )
Specific Surface Area:	125 m <sup>2</sup> /g
Bulk Density:	0.5 g/cm <sup>3</sup>
Washcoat Thickness:	0.05 mm
Exhaust Catalyst Material:	Johnson Matthey precious metal; 9 Pt: 1 Rh (3 annuli)



**FIGURE 3.     HEAT EXCHANGER OUTER SHELL AND EXHAUST MANIFOLD.**



**FIGURE 4.     HEAT EXCHANGER SHOWN WITH REACTOR AT LEFT AND EVAPORATOR ON THE RIGHT.**

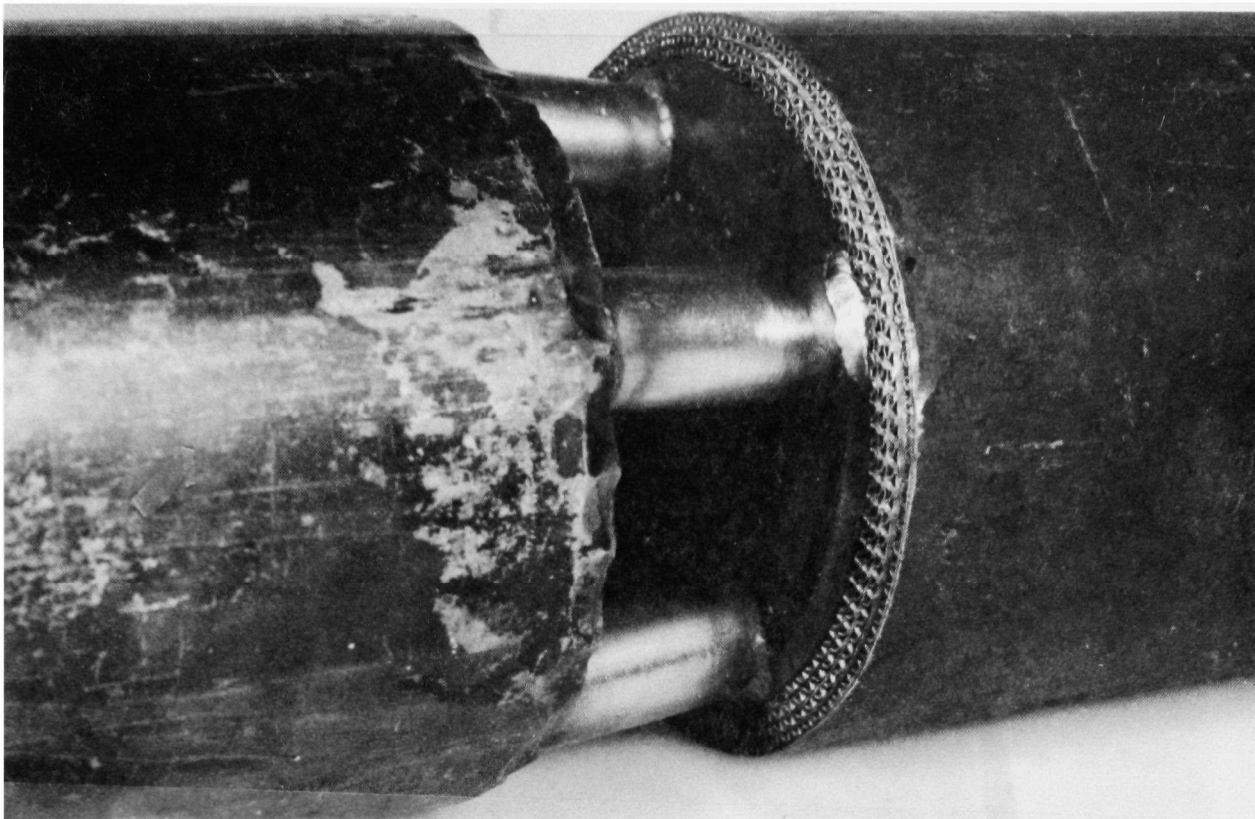


FIGURE 5. JUNCTIONS OF EVAPORATOR AND REACTOR WITH EVAPORATOR ON THE RIGHT.

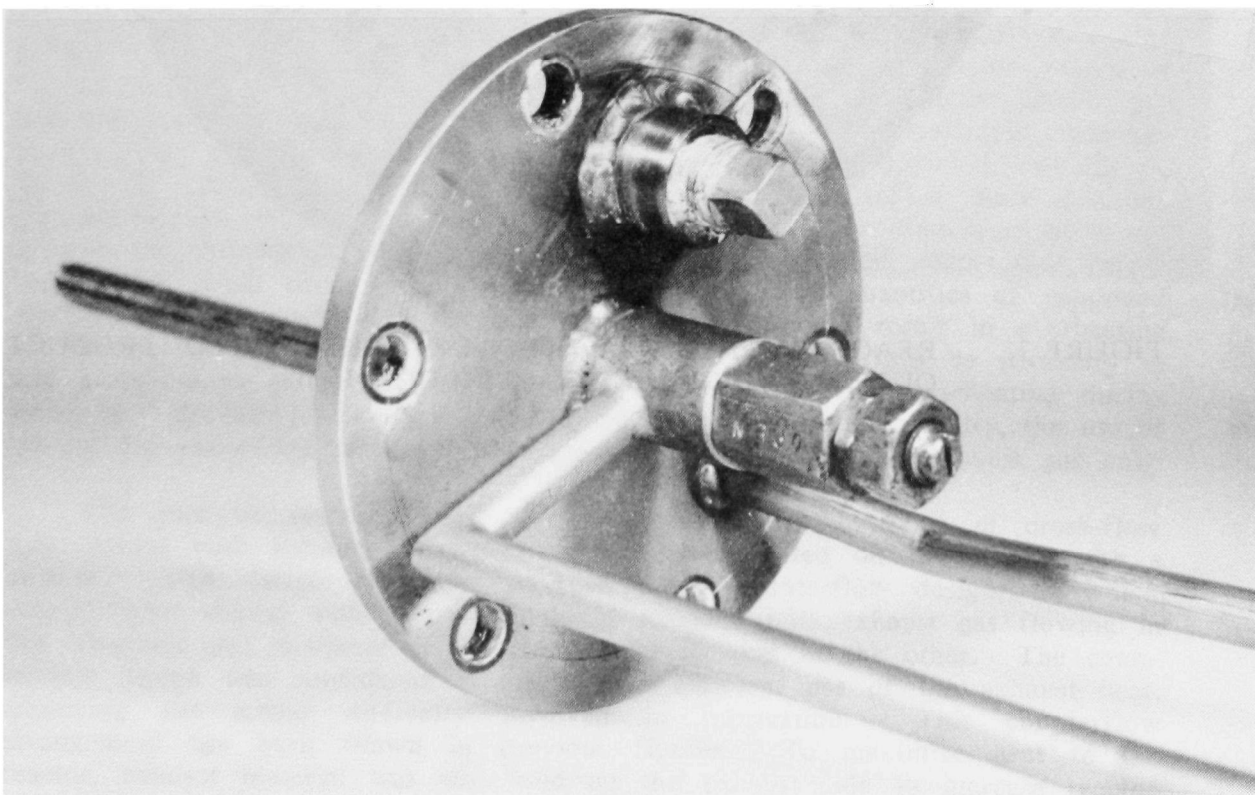


FIGURE 6. TOP VIEW OF EVAPORATOR COVER,

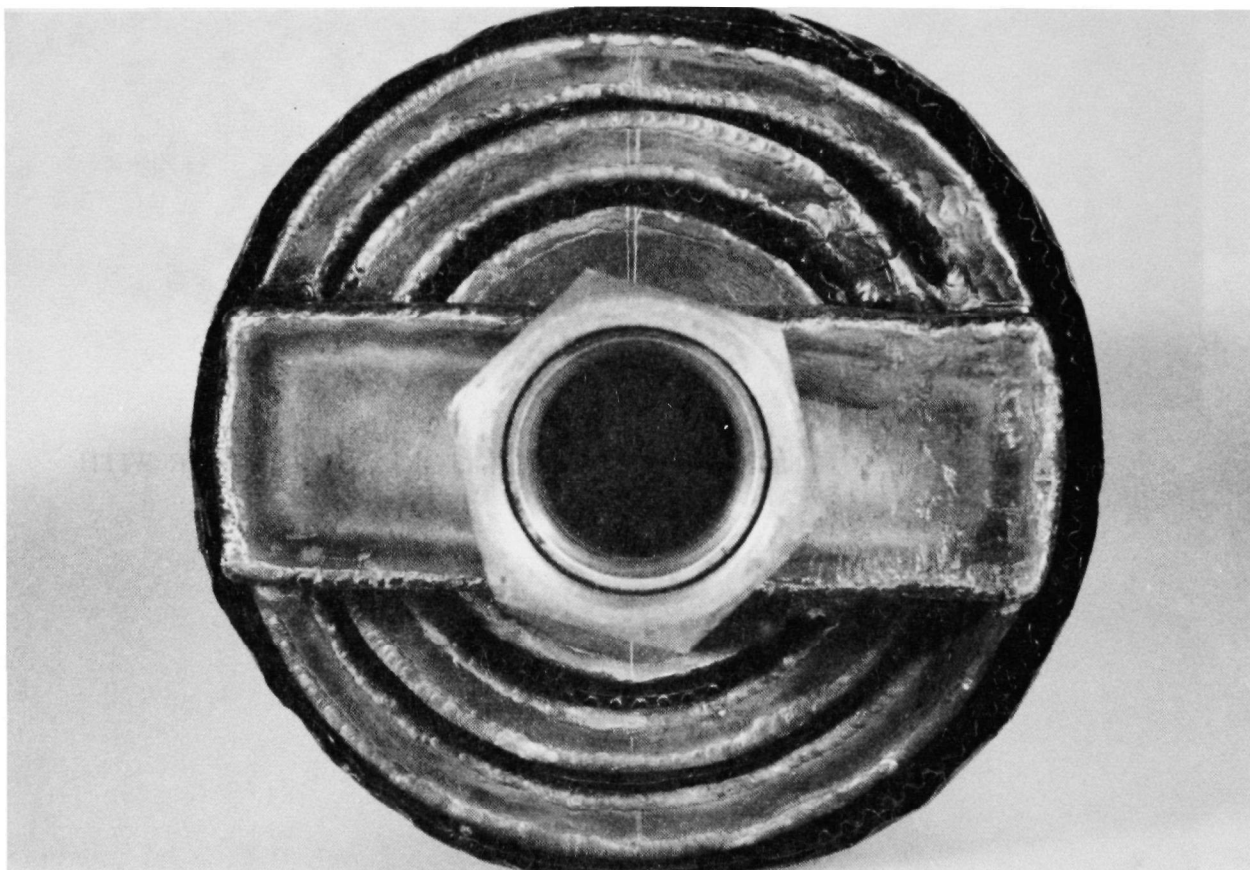


FIGURE 7. REACTOR END VIEW SHOWING DISSOCIATED PRODUCT  
OUTLET AND EXHAUST GAS INLET.

### C. Catalyst

The design criteria specified for the reactor catalysts were:

- ° Provide adequate heat at the required temperature to the catalyst active sites.
- ° Provide sufficient catalyst surface area.
- ° Have low pressure drop, allowing the product gases to charge the engine cylinder in the time available.
- ° Provide thermal control to maintain the catalyst in its optimum temperature range, or at a minimum, provide safeguards from overheating the catalyst material, which would result in permanent damage.
- ° Resist the potentially corrosive gases.
- ° Resist the vibration levels of an automotive engine operating at high speed.
- ° Provide low thermal inertia, thus enabling the reactor output to follow changing engine speed-load conditions.

Design concepts included (1) the use of the exhaust gas as the total source of heat and (2) the use of the exhaust gas and engine coolant. The first concept would be applied by locating the evaporator and the catalytic reactor directly in the exhaust stream. The second approach would use engine coolant to provide heat to the evaporator, and the catalytic reactor would be located in the exhaust stream. The advantages of using the engine coolant are that the vaporizer design could be compact due to the liquid-to-liquid heat exchange and that some of the coolant heat, otherwise rejected, would be recovered. Disadvantages of using the engine coolant are a more complex system, relative to using exhaust heat only, and a longer time for warm-up, because the coolant and engine block must achieve operating temperature before vaporization could occur. The time delay in producing quantities of vaporized methanol, which would then be fed to the reactor, could result in overheating of the reactor due to lack of methanol vapor. It would thus be necessary to add a device to divert exhaust from the reactor to prevent overheating during warm-up. Because of the long warm-up period and added complexity, the use of coolant for vaporizing methanol was rejected in favor of using exhaust gas only.

The catalytic reactor design was proposed by SwRI to be of cross-flow tube design with methanol flowing through tubes coated on the inside with a catalyst. This design was later replaced by a counterflow design, in which coaxial tubes coated with catalytic material would handle exhaust gas flowing in one direction and methanol or methanol vapor flowing in the other. The counterflow design was considered to make more efficient use of the exhaust heat, offsetting the added difficulty involved in fabrication. This counterflow arrangement has been shown in previous figures. To maximize heat to the reactor, catalyst material was also used on the exhaust side to increase reactor temperature through oxidation of any CO and HC remaining in the exhaust gases.

Three catalyst manufacturers were contacted for assistance in the analysis, design, and fabrication of the catalytic reactors. These manufacturers were Johnson Matthey (JM), Conoco, Inc., and W.R. Grace & Co.

Conoco supplied copies of patents and a report on their previous catalytic dissociation efforts. Catalyst yields were not given in the report provided. The patents described the catalyst composition, for each of the patent applications, the catalysts were applied to pellets in a fixed bed. Based on the geometric surface area of the pellets used in their supported bed simulation unit, a representative from Conoco calculated yields between 0.5 to 2.9 kg/hr-m<sup>2</sup> (0.1 to 0.6 lbm/hr-ft<sup>2</sup>) for idle to full load, respectively.<sup>(15)</sup> The product yield values were based on the throughput of methanol at 85% dissociation. The size for a single reactor for the engine would be approximately 8x18x38 cm (3x7x15 inches). Conoco's choice of catalyst was based on overall yield, yield at low temperatures, long-term stability, thermal stability, and physical integrity. It was mentioned that none of the better catalysts used at Conoco were substantially better (e.g., 2 times) than the others. Conoco was not selected to supply a catalyst, because their pellet-type catalyst applied to a crossflow reactor would result in an unuseably large heat exchanger.

W.R. Grace declined their involvement in supplying catalyst materials at that time.

Johnson Matthey proposed to design, build and catalyze a reactor. The proposed reactor was a single methanol annulus design similar to configuration number 6 in Figure 3B of Appendix D. Their preference for a single annulus design was to reduce cost and complexity. With connections, the length of the reactor unit would be less than 30 cm (12 inches). It would be capable of operating at 1035 kPa (150 psig) and would be catalyzed on both the methanol and exhaust sides. Subsequently, specifications for a double-annulus design were provided to JM for review. They replied that they could produce that design. Therefore, a decision was made to have JM fabricate the double annulus design. SwRI would design and build a separate evaporator to mate with the reactor. SwRI proposed to assemble and test one of these heat exchanger units on one cylinder of the NAPS-Z engine to obtain experimental data. The output of the reactor for this first test would not be injected into the engine, but would be analyzed to determine the product species, the mass flowrates of vaporized and dissociated products, and operating temperatures and pressures. Copies of correspondence with Johnson Matthey are contained in Appendix E.

Johnson Matthey provided the following specifications on their proposed catalysts:

<b>Dissociation Catalyst Material:</b>	<b>Johnson Matthey Type H Base Metal</b>
<b>Apparent Surface Yield:</b>	<b>3.9 kg/hr-m<sup>2</sup> (0.8 lb/hr-ft<sup>2</sup>)</b>
<b>Actual Surface Yield:</b>	<b>1.8 x 10<sup>-3</sup> kg/hr-m<sup>2</sup> (3.7x10<sup>-4</sup> lb/hr-ft<sup>2</sup>)</b>
<b>Specific Surface Area:</b>	<b>125 m<sup>2</sup>/g</b>
<b>Bulk Density:</b>	<b>0.5 g/cm<sup>3</sup></b>
<b>Washcoat Thickness:</b>	<b>0.05 mm</b>
<b>Exhaust Catalyst:</b>	<b>Precious Metal Proprietary (9Pt:1Rh)</b>
<b>Reactor Material:</b>	<b>Stainless Steel</b>
<b>Thermal Conductivity:</b>	<b>K = 24 W/m-k (14 Btu/hr-ft-°F)</b>

JM provided the catalyzed metal foil substrates and assembled the tubes and substrates into the reactor configuration. The tubes making up the concentric catalyst dividers were fabricated by SwRI and supplied to JM. The partially assembled reactor was delivered to SwRI, where it was visually inspected, prior to final assembly, to assure all passages in the methanol and exhaust catalysts were open.

After assembly of the evaporator to the reactor, thermocouples, pressure taps, and the injector nozzle were installed. The assembly did not leak when pressurized to 69.0 kPa (100 psi) while submerged in water. This prototype heat exchanger (evaporator/reactor) was then evaluated on a test engine, and the results of those tests and of a post-test analysis are covered in the following section.

### III. EVALUATION OF HEAT EXCHANGER

A test plan, contained in Appendix F, was prepared following an EPA/SwRI meeting in February, 1986. The purpose of the planned testing was to determine the performance of the heat exchanger, compare the experimental results with the desired and calculated values, provide data to optimize the heat exchanger design, and balance the individual reactor and evaporator designs. The test engine setup is shown in Figure 8. For these evaluations, the product output from the dissociation heat exchanger was sampled and evaluated but was not injected into the engine intake.

#### A. Test Engine

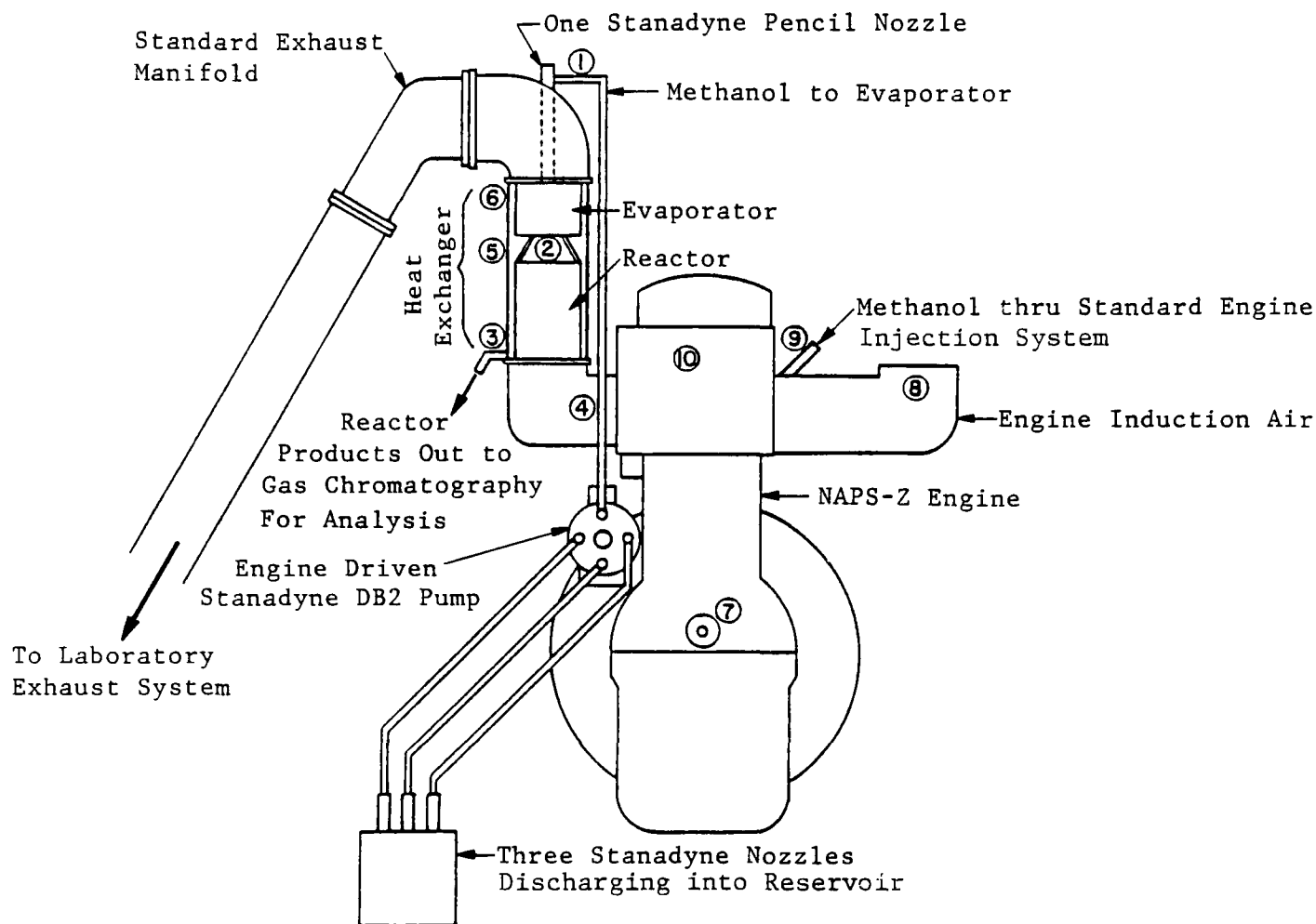
A Nissan NAPS-Z two liter engine was selected for the evaluation of the prototype methanol dissociation heat exchanger and this engine has two spark plugs per cylinder. Operating the engine on only one spark plug provides a convenient location in which to install a valve for induction of the products of dissociation. The combustion chamber, a crossflow design, is also well suited for these test purposes.

A cylinder head was sectioned to determine if a new cylinder head casting would be required or if existing heads could be altered for the test program. After layouts of heat exchangers were made, based on using a new head design and on using existing heads, a decision was made to use the existing head design. Appendix G contains design options for the heat exchanger gas admission valve and head modifications.

A NAPS-Z engine, received from EPA to use in the evaluation of the dissociation heat exchanger, was installed in a test cell and run on methanol at several points matching those in EPA test data provided to SwRI. Results of this initial testing are shown in Table 2. All fuel consumption data taken at SwRI exceeded that taken at the EPA. The specific fuel mass flowrate transducer used was a Micromotion unit calibrated for methanol. Its calibration, as well as that of the dynamometer, were checked and reconfirmed when this fuel consumption difference became apparent. A laminar-flow element was installed on the engine induction air system to permit measurement of air mass flowrate and calculation of equivalence ratios.

The engine was then operated at three test points, data from which are summarized in Table 3. The engine started and operated smoothly and steadily during this entire test sequence. The engine was then shut down to review the data. When preliminary testing was resumed, engine failure occurred. Repairs included honing the cylinder bores, installing new low-compression pistons and rings, and installing new connecting rods. The damaged pistons were inspected, photographed and sent to the EPA.

The cause of the engine failure was not conclusively determined. Damage such as this is usually caused by high temperatures that result from excessively lean operating and/or pre-ignition. However, test data shown in Table 3 indicate that the engine was running richer than stoichiometric. Subsequently, it was determined that the fuel-rich operation apparently resulted from misinstallation of an air-fuel ratio controller provided with the engine. Following repairs, to return the engine to standard overhaul condition, break-in



Data Acquisition		
No.	Location	Parameter
1	Methanol into the evaporator	Temperature, pressure Mass flowrate
2	Methanol between the evaporator and reactor	Temperature
3	Dissociated products out of reactor	Temperature, pressure Product analysis
4	Exhaust out of engine	Temperature, pressure
5	Exhaust between reactor and evaporator	Temperature, pressure
6	Exhaust after evaporator	Temperature, pressure
7	Engine crankshaft	Mass airflow
8	Engine intake	Mass flowrate
9	Methanol injected into manifold or ports	Temperature
10	Engine coolant	Temperature

FIGURE 8. TEST ENGINE SETUP TO EVALUATE HEAT EXCHANGER

**Table 2. Initial SwRI test Data on NAPS-Z Engine As Received**

<u>Engine Speed (rpm)</u>	<u>Spark Advance °BTDC</u>	<u>%Load</u>	<u>Torque (N-m)</u>		<u>Fuel Consumption (kg/hr)</u>		
			<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>	<u>% Difference</u>
1500	27.0	30	45	45	4.7	5.8	23
1500	18.0	70	96	96	7.6	8.2	8
1500	12.0	100	141	140	11.0	12.4	13
3000	39.0	30	44	45	9.2	11.4	25
3000	39.0	50	75	76	12.4	15.5	25
3000	32.0	70	105	104	15.9	19.1	20
3000	22.0	100	150	156	22.3	24.2	9
4500	45.0	30	42	42	14.2	19.7	39
4500	24.0	70	96	95	24.3	28.7	18
4500	24.0	100	140	141	32.2	37.8	18

**Table 3. Summary of Data from Engine Test on NAPS-Z Engine as Received**

<u>Engine Speed (rpm)</u>	<u>Spark Advanced °BTDC</u>	<u>Torque (N-m)</u>		<u>Fuel Consumption (kg/hr)</u>		<u>Air Consumption (kg/hr)</u>	
		<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>
4500	23.5	140	136	32.2	38.6	224	222
3000	32	105	104	15.9	16.8	142	105
1500	27	45	45	4.7	5.7	44	28
<u>Power Output (kW)</u>		<u>BSFC (kg/kW-hr)</u>		<u>A/F Ratio</u>		<u>Equivalence Ø Ratio</u>	
<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>	<u>EPA</u>	<u>SwRI</u>
64.9	63.9	0.496	0.604	6.9	5.8	0.93	1.25
33.0	32.8	0.482	0.512	8.9	6.2	0.72	1.03
7.1	7.0	0.662	0.814	9.4	4.9	0.70	1.32

running was performed. The engine continued to run fuel-rich, with equivalence ratios ranging from 1.5 at low loads and speeds to 1.15 at high loads and speeds. Following the break-in running, the engine was prepared for measuring heat exchanger parameters and dissociation product makeup.

## B. Heat Exchanger Test Results

The methanol dissociation heat exchanger was evaluated, using the exhaust from one cylinder, over a range of engine speeds and power outputs. Results for several test runs are summarized in Table 4 and 5. Appendix H contains a copy of the report submitted to EPA during September, 1987 covering the engine evaluation of the methanol dissociation heat exchanger.

**Table 4. Data from Evaluation of Methanol Dissociation Heat Exchanger<sup>a</sup>**

	<u>RUN 4</u>	<u>RUN 3</u>	<u>RUN 9</u>	<u>RUN 5</u>	<u>RUN 8</u>
<b><u>ENGINE OPERATION</u></b>					
Speed, rpm	1500	1500	1500	1500	3000
Torque, ft-lb	30	30	30	30	40
Methanol/Cylinder, lb/hr	11.7	12.7	10.8 <sup>b</sup>	12.7	28.2
Exhaust/Cylinder, lb/hr	813	791	840 <sup>c</sup>	773	1148 <sup>c</sup>
Exhaust Temperature, °F					
<b><u>DISSOCIATOR</u></b>					
Insulated <sup>d</sup>	NO	NO	YES	NO	YES
Methanol Flow, lb/hr	0.50	1.00	1.10	2.00	6.30
<b>Exhaust Temperature, °F:</b>					
Before Reactor	790	707	877 <sup>c</sup>	658	1167 <sup>c</sup>
After Reactor	652	419	721	171 <sup>b</sup>	863
After Evaporator	422	210	244	162	691
<b>Methanol Temperature, °F</b>					
In Evaporator	392	198	352	162	345
After Reactor	518 <sup>b</sup>	666	788	576	1140

<sup>a</sup>Data presented in order based on methanol flowrate into the dissociation.

<sup>b</sup>Data appears to be somewhat low.

<sup>c</sup>Apparent minor discrepancy in these data based on location in system.

<sup>d</sup>Around the outside of the heat exchanger unit.

Based on the temperature data given in Table 4, the evaporator was apparently unable to vaporize the total fuel needs of an engine cylinder at the 1500 rpm operating condition. This is concluded from the relatively low temperature (i.e., less than 200°F) in the evaporator in Runs 3 and 5. Insulating the heat exchanger assembly resulted in some improvement in vaporizing potential, as illustrated by the increased temperature in the evaporator in Run 9. At the 3000 rpm engine operating condition, the total methanol fuel needs of an engine cylinder could have been vaporized by the evaporator.

**Table 5. Methanol Mass Flowrate Versus Percent Dissociation**

<u>Run No.</u>	<u>Methanol Mass Flowrate (kg/hr)</u>	<u>% of Engine Cylinder Needs</u>	<u>Percent Dissociation</u>
6	0.01	1	96
4	0.2	19	22
7	0.4	29	7
3	0.4	31	5
9	0.5	35	5
5	0.9	63	1
8	2.9	89	11

---

<u>Run No.</u>	<u>Dissociated Products as of % Cylinder Needs</u>	<u>Engine Speed (rpm)</u>	<u>Torque (N-m)</u>	<u>Heat Exchanger Condition</u>
6	0.6	1500	41	Insulated
4	4.2	1500	41	<u>Uninsulated</u>
7	2.0	1500	41	<u>Uninsulated</u> /pressurized to 242 kPa
3	1.6	1500	41	<u>Uninsulated</u>
9	1.8	1500	41	Insulated
5	0.6	1500	41	<u>Uninsulated</u>
8	9.8	3000	54	Insulated

Conditions in the heat exchanger were stable at low to moderate engine speeds and loads, enabling determination of methanol dissociation rates. At high engine speeds and with high loads at lower engine speeds, the conditions in the heat exchanger were very unstable, and meaningful methanol dissociation rates could not be determined.

The mechanical design of the heat exchanger was generally satisfactory. An exception was the injector location in the exhaust stream; high injector temperatures at high speeds and loads were encountered. The lack of adequate injector cooling was a major factor in the inability to operate the heat exchanger at high engine speeds and loads because of the severe deterioration of injector spray characteristics.

For the evaluations shown in Table 5, the dissociation rates in the reactor ranged from 1 to 96 percent of the total methanol injected into the evaporator; the higher dissociation rates were associated with low methanol injection rates. These dissociation rates represented from 0.6 to 9.8 percent of the engine cylinder fuel needs at the test points evaluated. Heat exchanger performance versus methanol flowrate is shown in Figure 9 and the percent of cylinder fuel needs versus methanol flow rate is shown in Figure 10.

The evaporator was adequately sized to vaporize 100 percent of the engine cylinder fuel needs at 3000 rpm, but only about 50 percent at 1500 rpm. The vaporization rate was greater at 3000 rpm because of the higher exhaust temperature and flowrate at that engine speed.

### C. Analysis of the Catalyst

Following analysis of the heat exchanger test results and the conclusion that satisfactory heat exchanger performance was not achieved, the reactor was shipped to Johnson Matthey for a post-test analysis of the reactor catalyst. Specifically, JM was asked to determine the catalyst active surface area and the condition of the catalyst and to conduct other analyses, as appropriate, to determine why the dissociation yields were so low. Based on the catalyst design criteria, (e.g., optimum dissociation temperature of 370°C) dissociation yields should have been much higher.

The methanol dissociation and the engine exhaust catalysts were checked by the JM Analytical Lab for effective surface area (B.E.T.). These catalysts were also scanned by x-ray for the presence of catalyst poisons and the coke deposit at the reactor outlet was analyzed by x-ray fluorescence (XRF) for contaminants. Preliminary results of the analyses by JM are given in Appendix E.

The effective surface area measured for the dissociation catalyst was less than one meter squared per gram ( $\text{m}^2/\text{g}$ ). The corresponding result for the engine exhaust catalyst was just slightly over one  $\text{m}^2/\text{g}$ . Elements found on the dissociation catalyst were Al, Cr, Fe, and Zn, and elements found in the coke deposited on the dissociation catalyst were Ca, Cr, Fe, Pb, and Zn. Elements found on the exhaust catalyst were Al, Ca, Cr, Cu, Fe, Pt, and Zn. The high temperature resistant stainless steel metal support is an alloy containing Al, Cr, and Fe which could be picked up by the x-ray.

The expected effective surface area for a metal supported catalyst of the type used would be somewhere on the order of 8 to 13  $\text{m}^2/\text{g}$ , so the effective surface area of both catalysts was an order of magnitude lower than expected. Usual reasons for loss of surface area are poor washcoat adhesion, thermal sintering, and masking/poisoning. A scan with a 20-power lens did not reveal bare patches of metal which would indicate washcoat adhesion problems. The 600°C (1100°F) temperatures noted by SwRI are not as high as in automotive applications and would not seem to be a prime candidate for low surface area numbers. Welding the catalyst reactor could be a source of high temperatures (and metal poisons), and masking or poisoning effects are a definite possibility. The coke deposit scanned by XRF showed the presence of Ca and Pb as well as the expected Cr, Fe, and Zn, but the amount of each of these elements is unknown. Each could be a poison in large amounts on the catalyst surface.

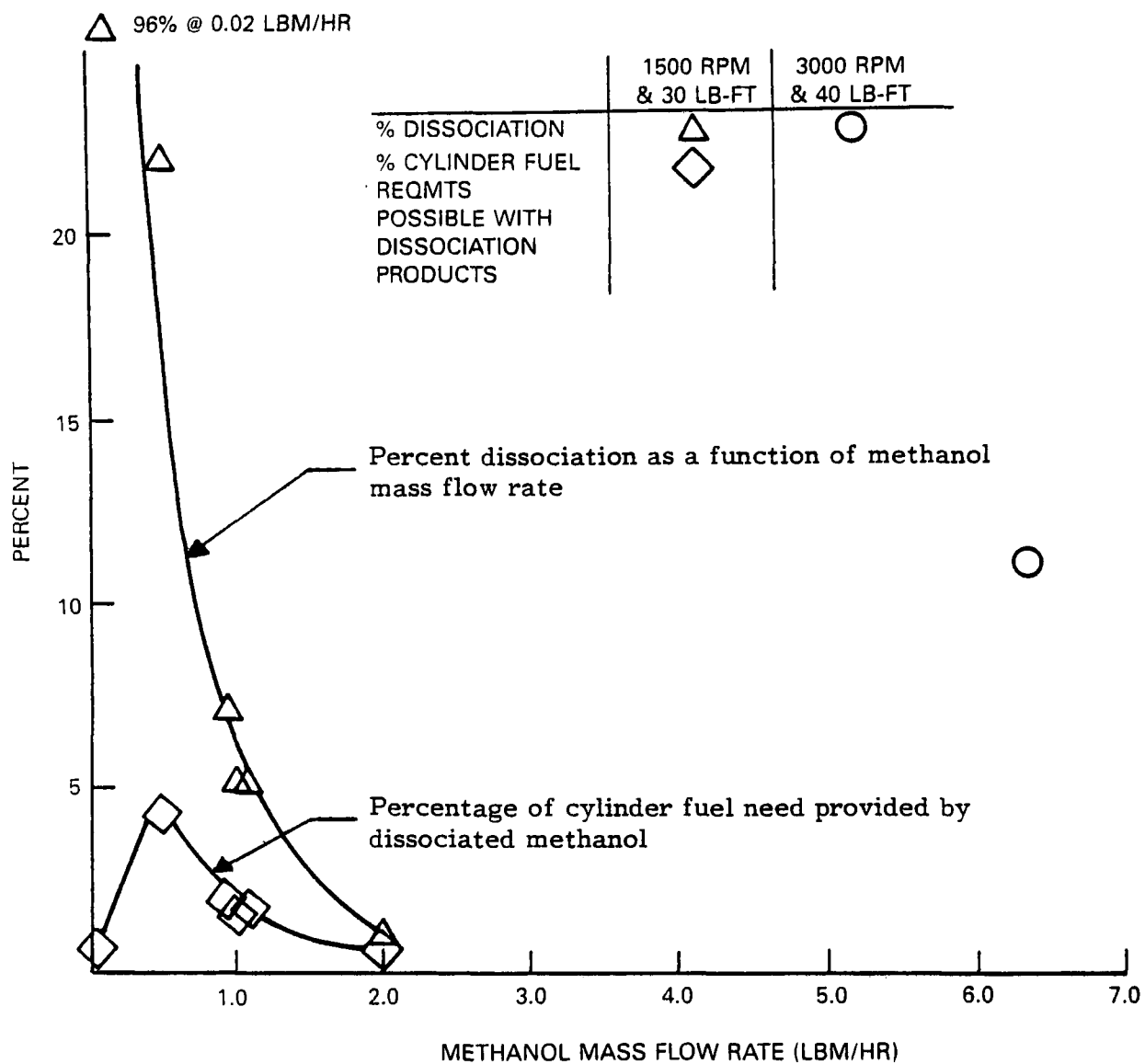


FIGURE 9. HEAT EXCHANGER PERFORMANCE VERSUS METHANOL MASS FLOWRATE.

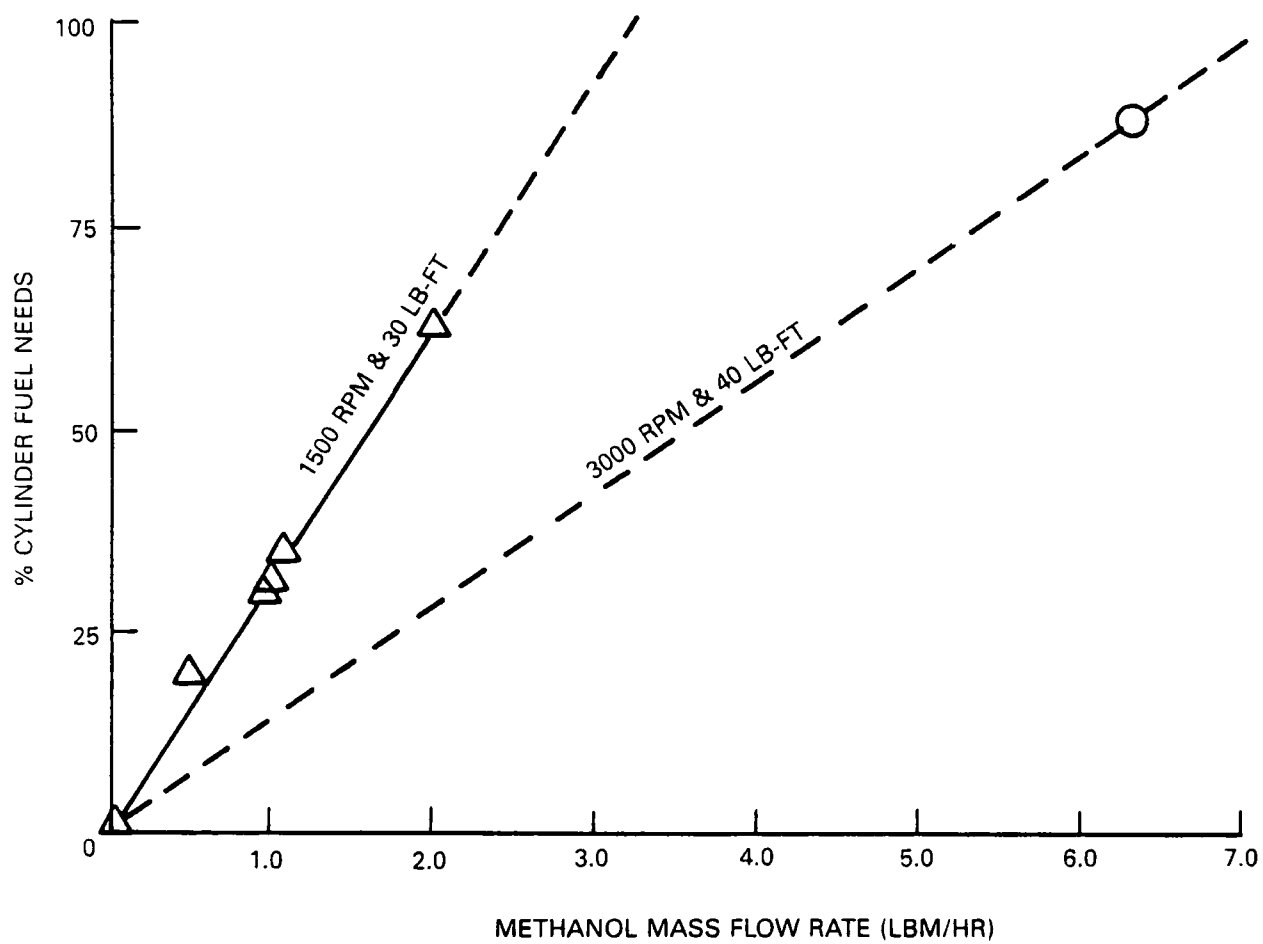


FIGURE 10. CYLINDER FUEL NEEDS VERSUS METHANOL MASS FLOWRATE.

The x-ray scan of the catalyst is not sensitive to the lighter elements, so a masking by carbon compounds would not be detected. The very fact that a coke deposit was produced within the reactor may indicate occurrence of some other undesired catalytic reactions.

A check of the heat exchanger design was made, and generally it appears that appropriate design criteria were used in all but a couple of areas. The primary design flaw observed was the location of the methanol injector in the exhaust stream without provisions for cooling.

In some areas, potential for design improvements were noted. One design improvement involved the exhaust flow through the reactor section of the methanol dissociation heat exchanger. With reference to the view of the reactor given in previous Figure 7, the center section of the exhaust catalyst was designed to carry the same exhaust heat per circumferential unit as the two outer sections of the exhaust catalyst. Since the center sections provides heat to methanol catalysts on both radial sides, it should be designed to carry more exhaust heat. Incorporating this design improvement involves only minor redesign. Another design improvement would be to insulate around the outer diameter of the reactor with a material such as 3M Interam heat expandable ceramic insulation. Due to the limitations on the outside diameter of the heat exchanger, however, incorporating such internal insulation would require extensive redesign of the reactor.

Based on the overall design criteria, the heat exchanger should have provided relatively good dissociation of methanol at several of the conditions over which it was operated. Some of the findings in the inspection of the heat exchanger assembly by SwRI and of the catalysts by Johnson Matthey probably explain the low dissociation efficiency. The primary finding was that the methanol catalyst had an effective area an order of magnitude less than anticipated. No specific cause was found for this major reduction in effective area. Other findings of potential significance were that the actual cross sectional flow area of the center section of the exhaust catalyst was less than half the designed area and that significant carbonaceous deposits were present on the methanol catalyst. A number of the outer flow tubes in the methanol catalysts were blocked by plugs of the carbonaceous material.

Fabrication of subsequent units should include additional inspection to assure meeting design specifications. With the catalyst, this should include determinations of the effective surface area and the dissociation efficiency of the actual batch of catalyst substrate to be used in the reactor assemblies. During assembly of the system, checks should be made to assure all important physical dimensions and criteria meet design specifications. Also, the type of catalyst used in the the prototype heat exchanger should be reconsidered as to whether it remains as the primary choice.

## IV. VALVE TRAIN AND CONTROL SYSTEM CONSIDERATIONS

Design considerations toward a valve train and control system for the methanol dissociation heat exchanger are discussed in this section.

### A. Valve Train Considerations

An initial objective of the program was to inject the products of dissociation directly into the combustion chamber without first mixing with the combustion air charge. To achieve that objective, a dissociated products inlet valve is required which operates independently of the engine intake and exhaust valves. The selected engine (Nissan NAPS-Z) has two spark plugs per cylinder. One of the spark plug holes can be used for the dissociated products inlet valve, and the engine can be run using the remaining spark plug per cylinder. The turbulence and mixing that will occur should assure that one spark plug per cylinder will be sufficient.

Several methods to actuate the valves for admitting dissociated products to the cylinders were considered. These included electronically-actuated assemblies that could be designed to perform both gas admission and flowrate control functions. While there appears to be some advantages to this method, it is the most expensive approach and also the most risky. The expense is due to the low volume production of suitable solenoids and the need for a separate control system to open and close the valves at the proper times. The risk is high, because the concept is not proven and it is not known whether development of working hardware could be achieved.

Mechanical valve actuation methods (overhead cam and overhead valve with rocker arm) were reviewed to determine which was the most suitable. The specific requirements of the dissociated product valve timing necessitate careful attention to valve dynamics. With the short duration ( $73^\circ$  of crank angle) and high maximum engine speed (6000 rpm), the valve will have to be accelerated quickly to achieve its full open position. The high accelerations will yield high forces, and such forces are best handled by a valve train of minimum mass and proven high speed potential. The short duration requires a cam profile without convex surfaces or a cam with an all-around convex surface of large diameter (approximately 15-cm base circle). An alternative to either of these would be to use a cam with a convex contour and a small lift, combined with a rocker arm, to increase the valve lift to the required amount. This approach, however, increases the total valve train mass and makes packaging impractical. After considering these various approaches, direct actuation using a small diameter cam was chosen. The layout for the heat exchanger was enlarged to include the valve gear and a computer program was written to calculate the cam profile and the valve accelerations. The dissociated products valve train design is contained in Appendices I through K.

### B. Control System Considerations

Because the dissociation of methanol will not occur at engine start-up (cold exhaust), and may not be adequate to fuel the engine at some operating conditions, a dual system for fueling the engine will be required. One of the systems is for port-injection fueling, and the other is for injection of methanol

into the catalytic reactor. Separate control systems could be required for the two systems. Parameters to be sensed for control purposes include:

- Evaporator temperature
- Catalytic reactor temperature
- Engine speed
- Engine load (throttle position or manifold vacuum)
- Exhaust oxygen content
- Exhaust temperature
- Hydrogen in reactor

At this time, no practical method is known for continuously measuring hydrogen concentration.

**Design Concept** - A conceptual design of a control system was developed following the testing of the heat exchanger. Operation of the heat exchanger made some of the desired characteristics of a control system apparent. Control of the engine is thought best done with two separate control loops. One loop would control the heat exchanger and maintain it at some condition, such as a predetermined evaporator temperature that was above the equilibrium point. The other control system would control the engine fuel system. Flow from the heat exchangers would be restricted or stopped for low fuel demand conditions. Otherwise all available reactor contents would be discharged into the combustion chamber each time the valve is opened and the manifold fuel injection system would make up for the balance of fuel needs.

**Reactor Variability** - It became apparent, when operating the heat exchanger that it is difficult to control the evaporator temperature. Also, exhaust temperature varied substantially from run to run and drifted even when the heat exchanger was operating under what should have been steady-state conditions. It appears unlikely that multiple heat exchangers (such as one for each cylinder) can be maintained at similar conditions. If each heat exchanger operates at different conditions, rates of dissociation will differ. With different rates of dissociation, the equivalence ratio in each cylinder will differ and it will be difficult to take full advantage of the extreme lean operation possible with hydrogen-rich mixtures. A single heat exchanger for the engine would eliminate such variation and be more space efficient than multiple units, but a single unit would likely present major challenges in the design of the evaporator and the dissociation reactor.

## V. HEAT EXCHANGER - FINAL DESIGN

A technical design review was conducted and the results were transmitted to the EPA for review. A copy of the design review and proposed improvements is given in Appendix L, and the findings are briefly summarized as follows:

**Dissociation Catalyst** - The base metal catalyst used in the initial heat exchanger did not provide satisfactory dissociation. From a brief review of the published literature and discussions with individuals at JM, EPA, and SwRI, it appears that a fully appropriate dissociation catalyst composition has not yet been identified. No catalyst composition has been found that will provide the essential characteristics of high dissociation efficiency at low temperature, durability at somewhat higher temperatures, and negligible coking characteristics. The primary requirement for developing a methanol dissociation heat exchanger is the identification of a suitable dissociation catalyst composition.

Until sufficient operating history has been developed on a specific catalyst composition, it is recommended that a sample from each batch be analyzed to assure it meets design specifications. At minimum, such analyses should include determination of effective surface area and bench determination of dissociation efficiency.

**Evaporator** - The present evaporator involves a closed cylinder wrapped with corrugated metal catalyst substrate. Because the engine exhaust gases first pass through the exhaust catalyst in the dissociation-reactor, which should oxidize essentially all available HC and CO, the catalyst wrapped around the evaporator appears to serve no useful function. Additionally, the corrugated catalyst substrate effectively isolates most of the exhaust flow away from the evaporator. By removing the catalyst substrate from around the evaporator and installing longitudinal fins onto the outer surface, heat transfer from the exhaust to the evaporator should increase significantly. Another potential improvement is to have the cone in the evaporator open to the exhaust, rather than closed as in the present design.

A commercially available injector, that can be utilized with only minor modification, is considered to be satisfactory and about as good as can be attained without major redesign effort. An essential design modification is relocation of the methanol injector out of the exhaust stream.

**Dissociation Reactor** - One design improvement involves the exhaust flow through the reactor section of the methanol dissociation heat exchanger. With reference to the original design of the reactor, the center section of the exhaust catalyst was designed to carry the same exhaust heat per circumferential unit as the two outer sections of the exhaust catalyst. Since the center sections provides heat to methanol catalysts on both radial sides, it should be designed to carry more exhaust heat. Another recommended improvement is to increase the methanol dissociation annuli from two to three. A third improvement would be to increase the void space at the entrance and exit of the dissociation annuli and to provide four exit ports from the annuli, rather than the two as in the initial design.

**Expected Result of Design Improvement** The mechanical design improvements described should improve the operation and dissociation efficiency of the heat exchanger. These improvements, however, are not expected to provide anywhere near the order of magnitude improvement desired. It appears that selection of the catalyst composition is the most important criteria toward meeting the desired dissociation efficiency.

## VI. CONCLUSIONS AND RECOMMENDATIONS

Tests of the heat exchanger showed the dissociation rates to be 1 to 96 percent of the total methanol injected into the evaporator. These rates, however, only represented 1 to 10 percent of the cylinder fuel needs at the engine test points evaluated. The catalytic reactor size or the effectiveness of the catalyst (or a combination of size and effectiveness) will have to be increased by roughly an order of magnitude to achieve the dissociation needed to meet 20-25 percent of the engine fuel needs at the lower range of power operating conditions.

The evaporator was adequate to vaporize 100 percent of the engine fuel requirement at 3000 rpm and 50 percent at 1500 rpm. Exhaust temperatures at the evaporator were higher than they would have been if the dissociation rate in the catalytic reactor had been higher. A more effective reactor would absorb more of the exhaust heat, and the evaporation rate would be reduced, possibly to the extent that the evaporator size or effectiveness would have to be increased.

Injector overheating occurred as a consequence of it being mounted in the exhaust stream. When injector temperatures exceeded 205°C (401°F), the injector nozzle spray pattern deteriorated. The lack of adequate injector cooling was a major factor in the inability to operate the heat exchanger at high engine speeds and loads. One flowrate of methanol was evaluated at a higher engine speed and load, 54 N-m (40 lb-ft) torque at 3000 rpm, and it resulted in the highest rate of dissociation (11 percent) and the highest percentage of cylinder fuel requirement (10 percent).

The catalyst used in this reactor to dissociate the methanol provided unsatisfactory dissociation yields at all engine power levels evaluated. The power levels evaluated are considered reasonably typical of engine operation for light-duty vehicles. Although exhaust flow through the reactor annuli was not optimum, it appears that a catalyst with higher dissociation effectiveness at lower temperatures is needed to enable a reasonable reactor size and mass.

Test results indicate that if a separate heat exchanger is used at each cylinder, variations in dissociation rates from cylinder-to-cylinder will occur and equivalence ratios will vary. Complex controls will likely be required to take advantage of the extreme lean operation possible with hydrogen fuel. A single catalytic reactor for the engine would eliminate cylinder-to-cylinder variations and be more space efficient. Evaporator and dissociation reactor design for a single unit, however, would likely become more complex.

Heat exchanger performance was shown to be inadequate because of the poor performance of the catalytic reactor and the injector. Cause for the poor performance of the injector has been determined. Specific cause for the poor performance of the catalytic reactor, however, can not be specifically determined from the available data. It is recommended that subsequent methanol dissociation heat exchanger development include bench testing in the catalyst selection process and baseline bench testing of the batch of catalyzed substrate actually used.

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## **APPENDICES**

- A - TESTING OF SwRI PUMPS AND INJECTORS**
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## **APPENDIX A**

### **TESTING OF S<sub>w</sub>RI DESIGNED AND FABRICATED PUMP AND INJECTORS**

## TESTING OF THE SWRI DESIGNED AND FABRICATED PUMP AND INJECTORS

### A. Fuel Injection System

Details of the fuel injection system are shown in Figures 1 and 2. The design is based on previous work at SwRI that includes a data base of results. Liquid methanol will be supplied by the engine-driven fuel pump to the electric motor-driven fuel pump shown in Figure 2. This pump consists of an electric motor driving two separate, but identical, positive displacement single piston pumps via an eccentric. The eccentric has a ball bearing mounted around it. The outer bearing shell contacts the plungers which eliminates sliding motion at their bases. Liquid methanol enters the ends of each pump through an inlet check valve as the plunger retracts under spring force. The inlet check valve is moved from its open to its closed position by friction between the plunger mounted O-ring and the internal check valve diameter. The trapped methanol is expelled through a second check valve to the pump outlet. The plunger rides on a teflon lip seal in the methanol end of the bore. An oil bath separates the plunger from the bore at the eccentric end. Methanol from each piston pump is directed to two evaporator nozzles. Each piston has been sized to provide methanol to two nozzles over the entire range of engine requirements (assuming all engine fuel demands are met through this pump).

A typical nozzle cross-section is shown in Figure 1. One of these is installed in each evaporator. Methanol enters the nozzle through the inlet port, goes through the fuel channels, and fills the void on both sides of the plunger piston. As each pressure pulse is provided by the pump, the valve unseats and ejects a quantity of liquid methanol into the evaporator. Because the pump is a positive displacement type, the metering of methanol into the evaporator is a direct function of the pump speed. The control system will provide a signal to the electric motor based on its measured speed. The adjusting screw on the nozzle is provided so that fuel flow rate from individual nozzles can be adjusted to the same value.

### B. Test Set-up

A series of bench tests was performed using the pump (driven by an electric motor) connected to the four nozzles. Each of the nozzles was installed in a clear plastic tube with a three-inch inside diameter (actual diameter to be 3.108 inches). Each tube had provisions for holding and draining the sprayed methanol so that the quantity of methanol sprayed from each nozzle could be determined over the test period and compared to each other. Stoddard solvent was used in place of methanol for testing.

The system was evaluated using the following test matrix showing nozzle number as a function of nozzle position and test number.

<u>Test Number</u>	<u>Nozzle Position</u>			
	A	B	C	D
1	1	2	3	4
2	2	1	4	3
3	3	1	4	2
4	2	4	1	3
5	1	2	3	4

Each test included operation at 600, 950, 1200 (except test No. 4), and 2400 pump rpm. Nozzle volume output and individual pump piston output were measured as a function of time at each of these speeds. Test number 5 is a repeat of test number 1, and was done to check repeatability of the system. The left pump piston output was always connected to nozzle positions A and C, while the right pump piston output was always connected to nozzle positions B and D. Pump and nozzle volume flowrates were plotted for each of the tests as shown in Figures 3 through 12.

The nozzles were adjusted to produce a balanced output at 2400 pump rpm as set up in test numbers 1 and 5. Test number 2 interchanged the two nozzles that were connected to each pump output so that each pump was delivering to the same two nozzles, but in different positions. Test numbers 4 and 5 exchanged nozzles so that each pump delivered fuel to one nozzle that previously received flow from the other pump.

Several observations are apparent from the plots:

1. For test numbers 1, 2 and 5 -
  - ° Volume flowrate while matched (cylinder to cylinder) at one pump speed is not matched at other pump speeds.
  - ° Nozzle flowrate versus pump speed is slightly non-linear (per nozzle flowrate plots).
  - ° Pump output (sum of both applicable nozzles) is not a linear function of pump speed (per pump flowrate plots).
2. For test numbers 3 and 4 -
  - ° Nozzle outputs are not balanced.
  - ° Pump output is not a linear function of pump speed.

From these observations we can conclude that:

- ° The system design (pump and nozzles) does not provide for equal output from each nozzle at all pump speeds after the nozzles are balanced at one pump speed.
- ° Pump output would not appear to be a linear function of pump speed. Part of this may be due to measurement methods, however, because nozzle output increases almost linearly with pump speed.

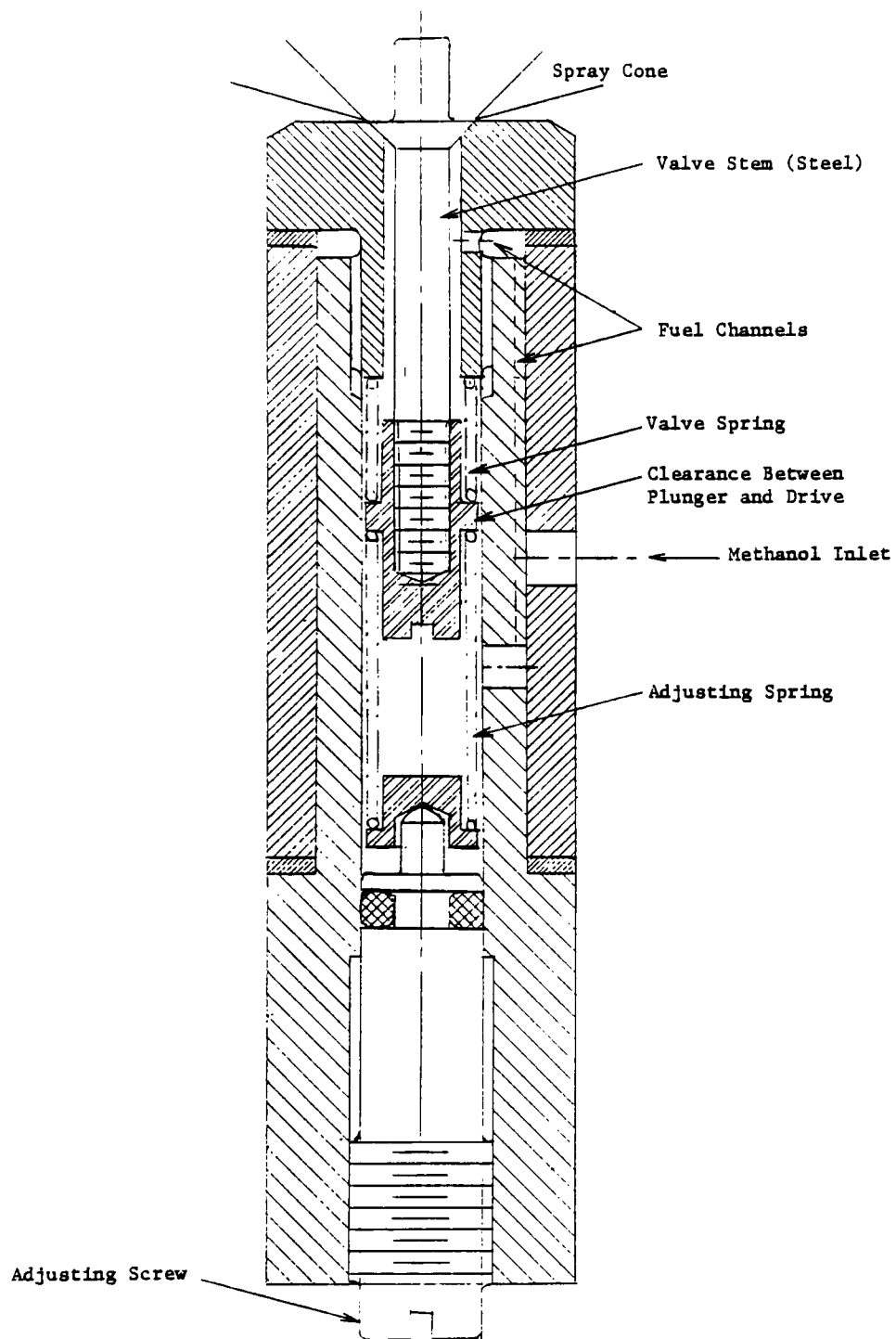
- ° Pump piston output characteristics differ even though they are dimensionally the same. This is based on results of tests 1 and 2 which show that interchanging nozzle positions so that they still receive fuel from the same pump piston does not appreciably change the nozzle flowrate characteristics versus pump speed. Changing nozzle position (tests 3 and 4) so that two of the four nozzles receive fuel from the other pump piston changes the relative flowrates between nozzle pairs.

In addition to these conclusions, it was apparent during the tests that atomization was poorer at low fuel flowrates than at high flowrates. Good atomization quality depends on both a high pressure drop across the nozzle and on a high frequency of fluid pressure pulses. Thus, the scheme to adjust fuel flowrate by changing pump speed will not provide for optimum atomization quality over the range of required flowrates.

### C. Second Generation Pump Design

The first generation design had two major shortcomings: (1) lack of balanced fuel delivery between nozzles at all flowrates, and (2) poor atomization quality at low pump speeds (flowrates). In order to overcome these a second generation pump was designed as shown in Figure 13. It uses the nozzles and pump eccentric housing from the first generation design.

The second generation design has a single piston that operates at constant speed to provide good atomization at all flowrates. Changes in flowrate are accomplished by adjusting the pressure regulator. Low flowrates are accomplished by reducing the spring tension in the regulator piston which allows it to displace as the pump cycles and accommodates the pump output. At higher flowrates, the spring tension on the regulator piston is increased so that part or all of the pump output is discharged through the nozzles. Discharge through the nozzles occurs when the pressure required to further displace the regulator piston exceeds that required to force fuel through the nozzle. Maximum flowrate occurs when the spring tension in the regulator piston is sufficiently high to preclude any piston displacement before the nozzles discharge fuel.



**FIGURE 1. SwRI-DESIGNED NOZZLE**

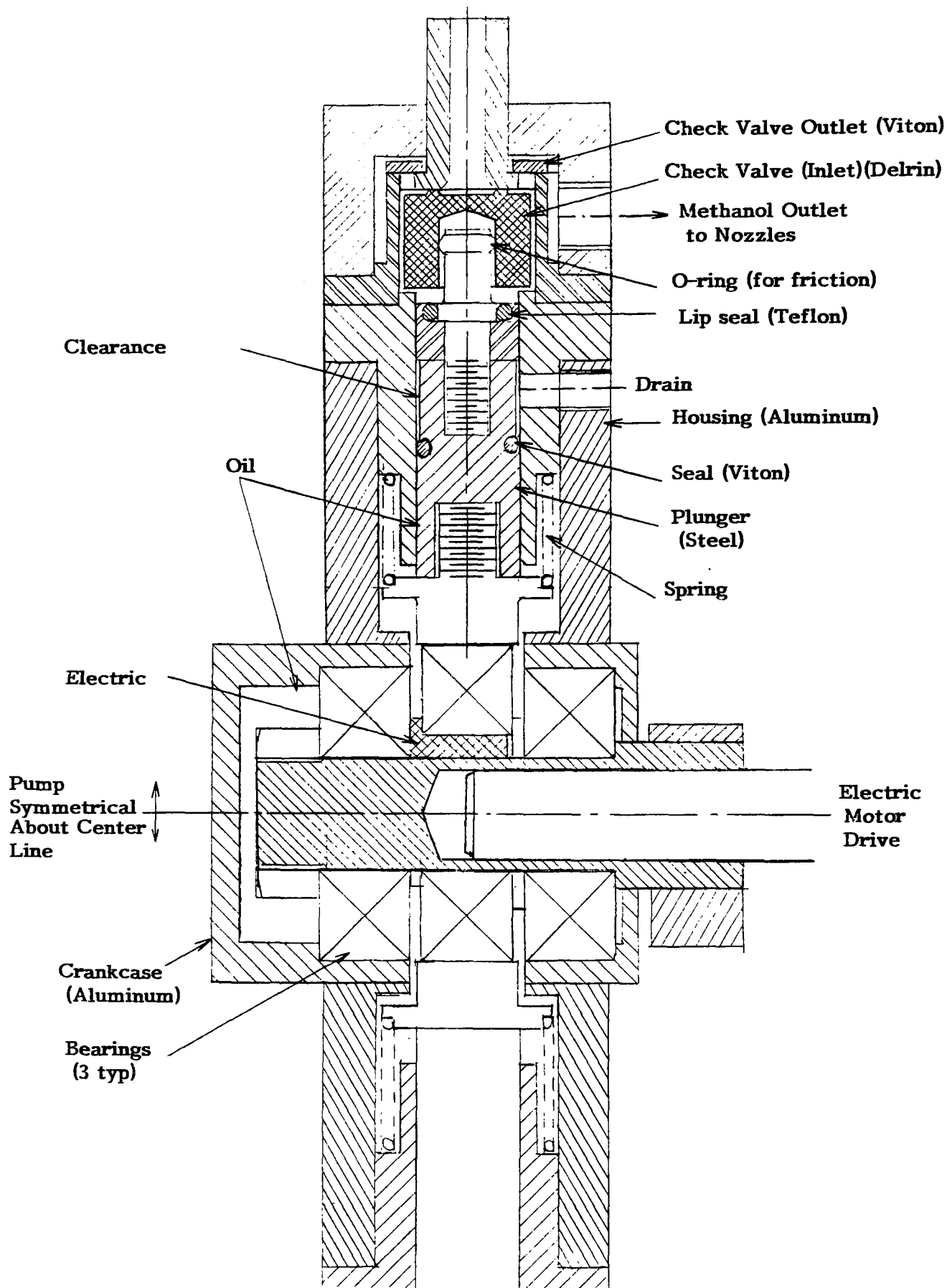
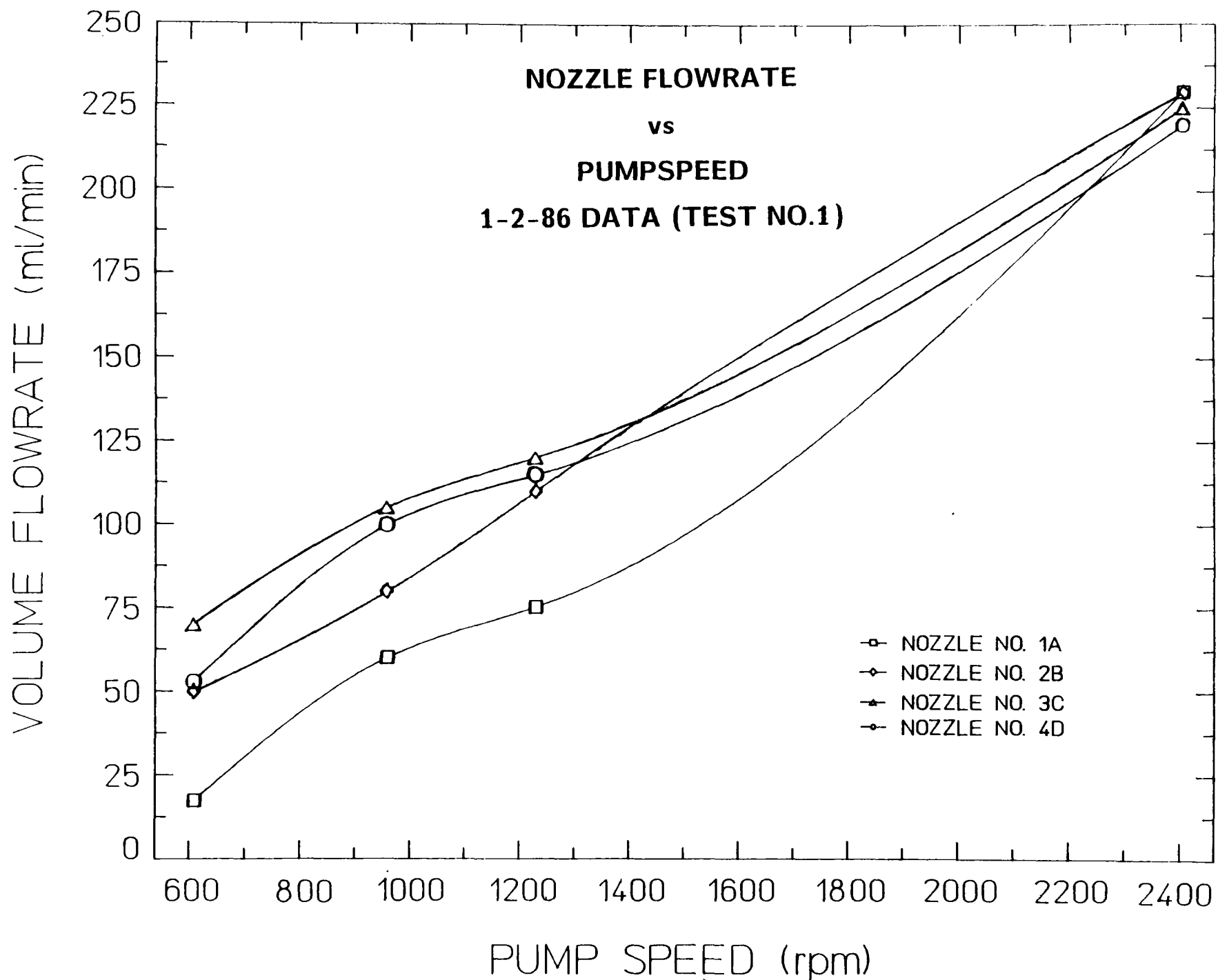


FIGURE 2. METHANOL FUEL PUMP



**FIGURE 3. NOZZLE FLOWRATE VS. PUMP SPEED**

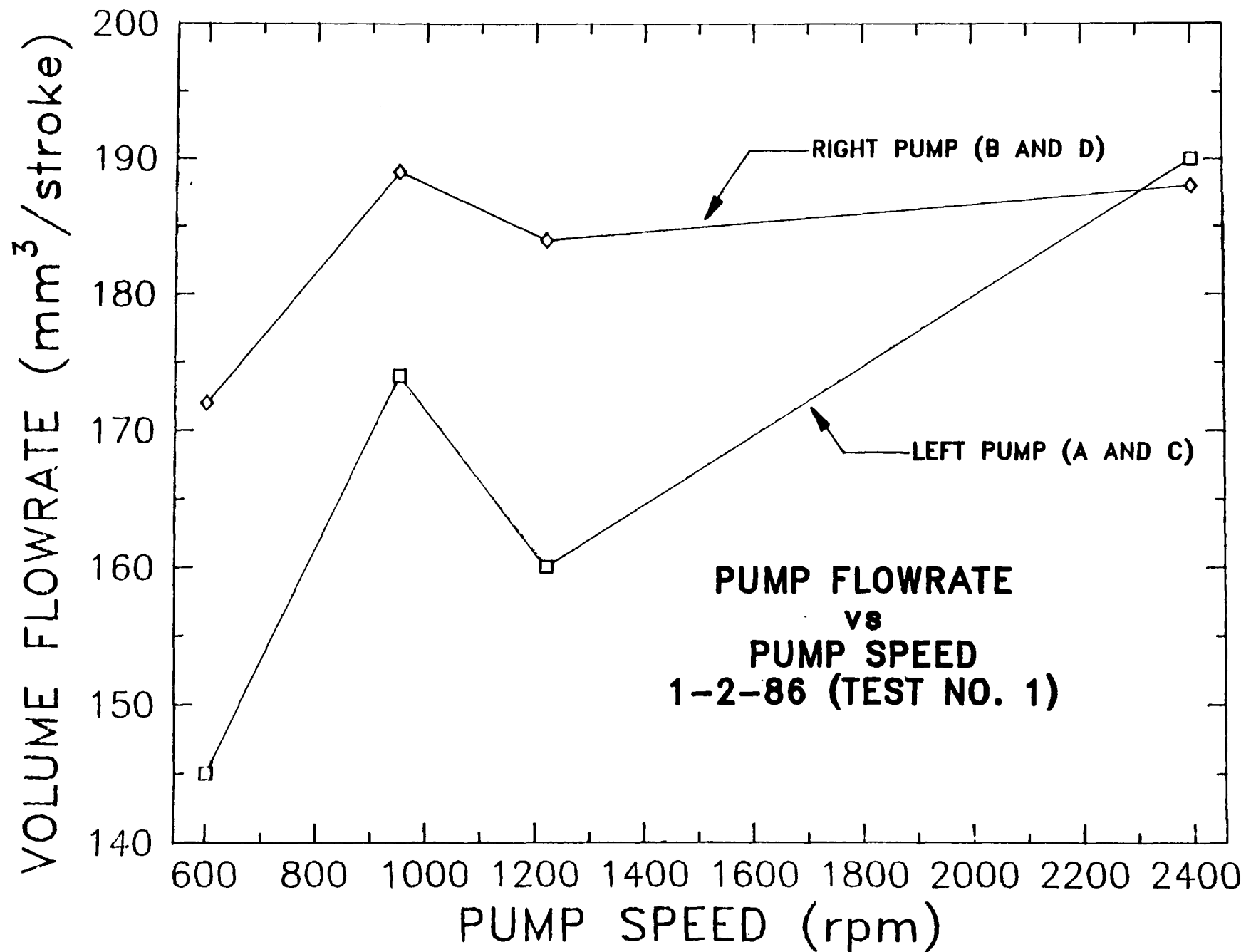


FIGURE 4. PUMP FLOWRATE VS. PUMP SPEED

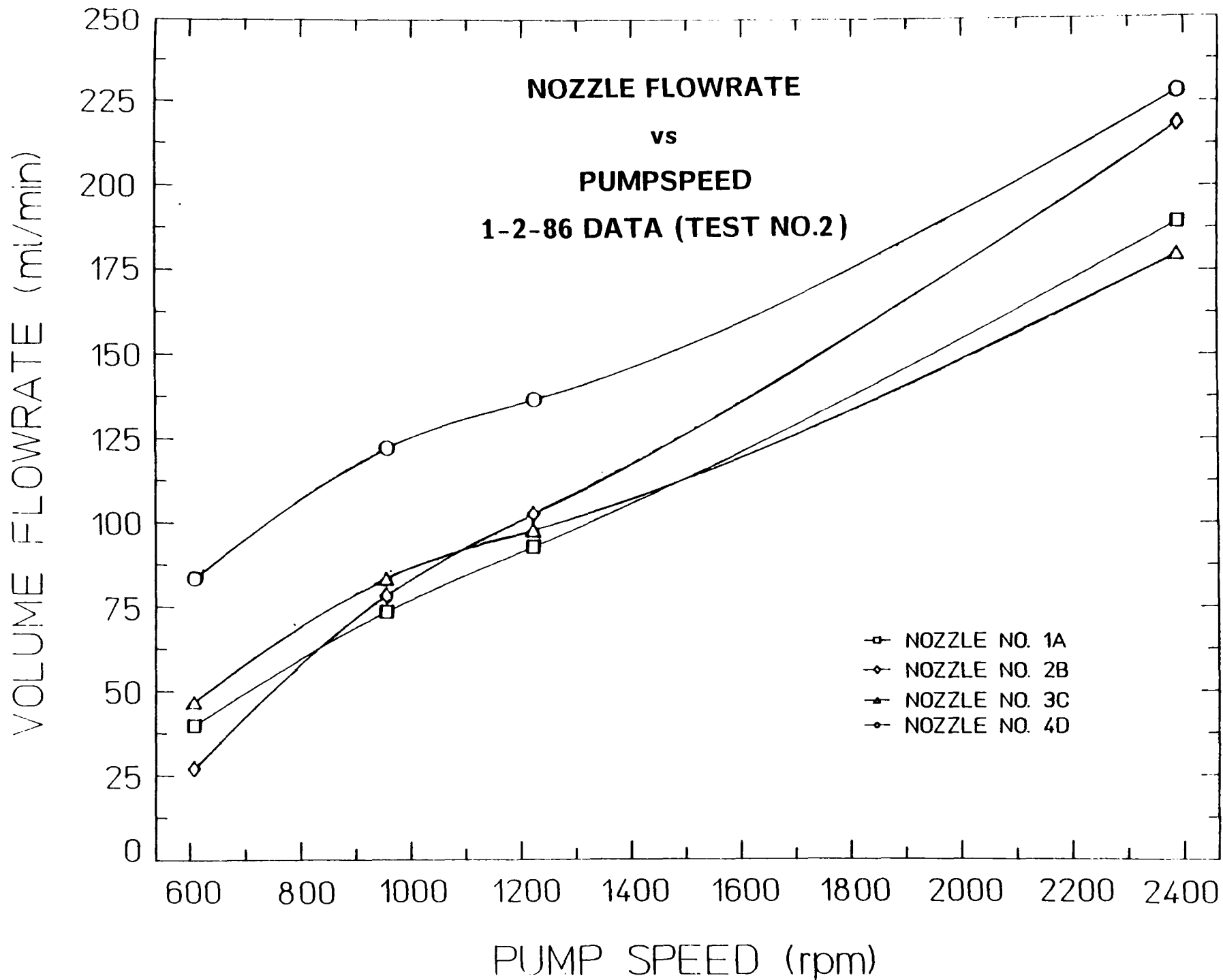


FIGURE 5. NOZZLE FLOWRATE VS. PUMP SPEED

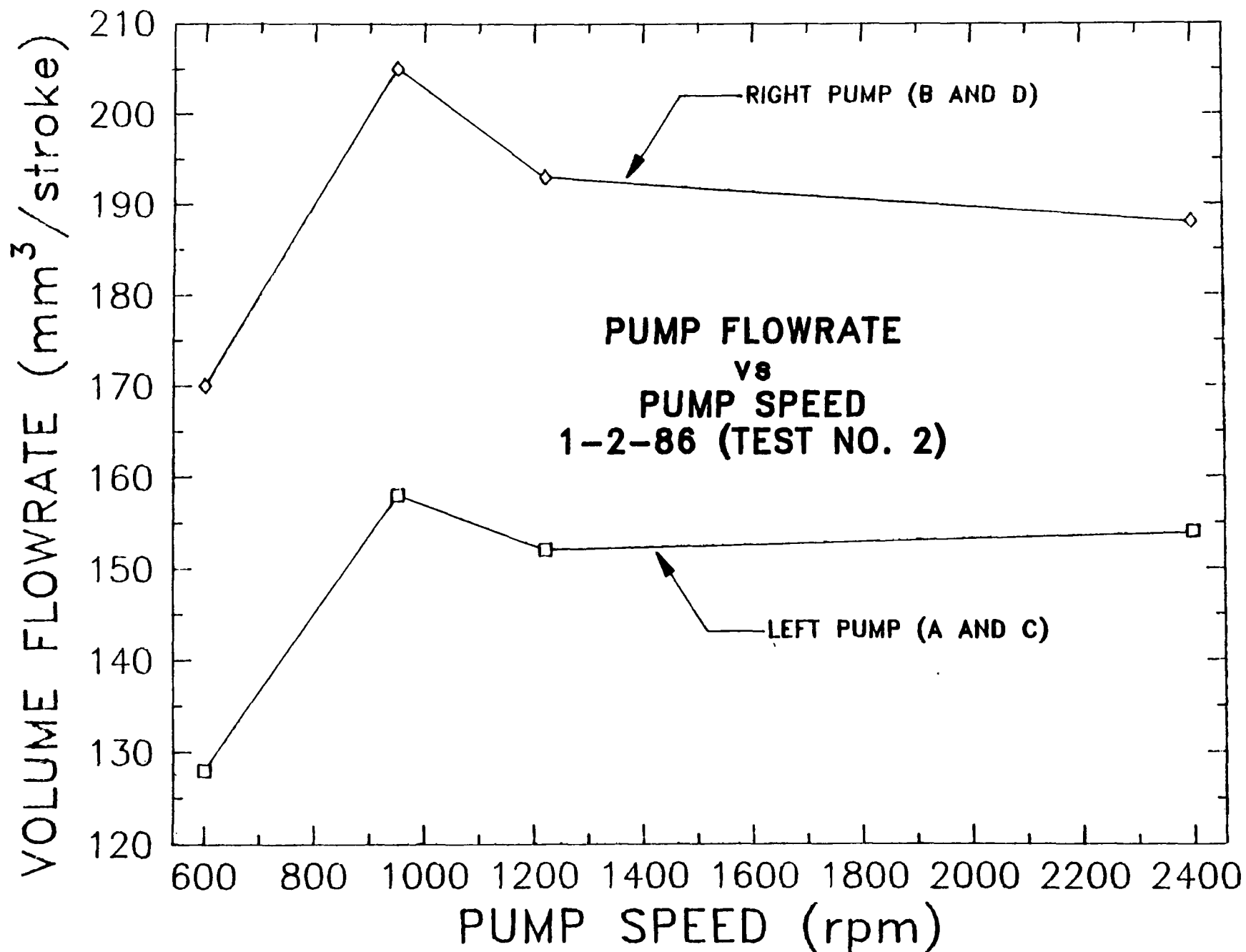
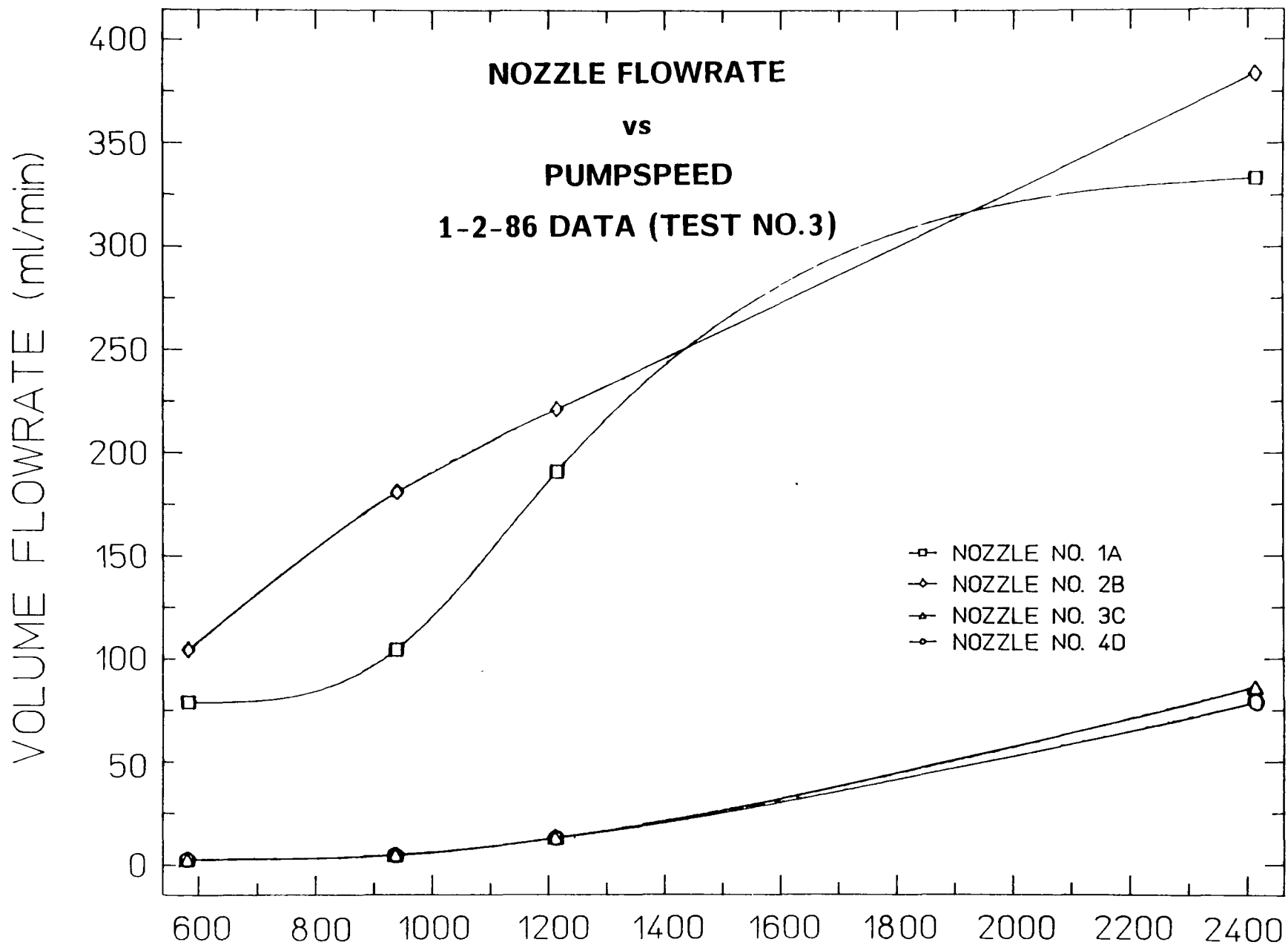


FIGURE 6. PUMP FLOWRATE VS. PUMP SPEED



**FIGURE 7. NOZZLE FLOWRATE VS. PUMP SPEED**

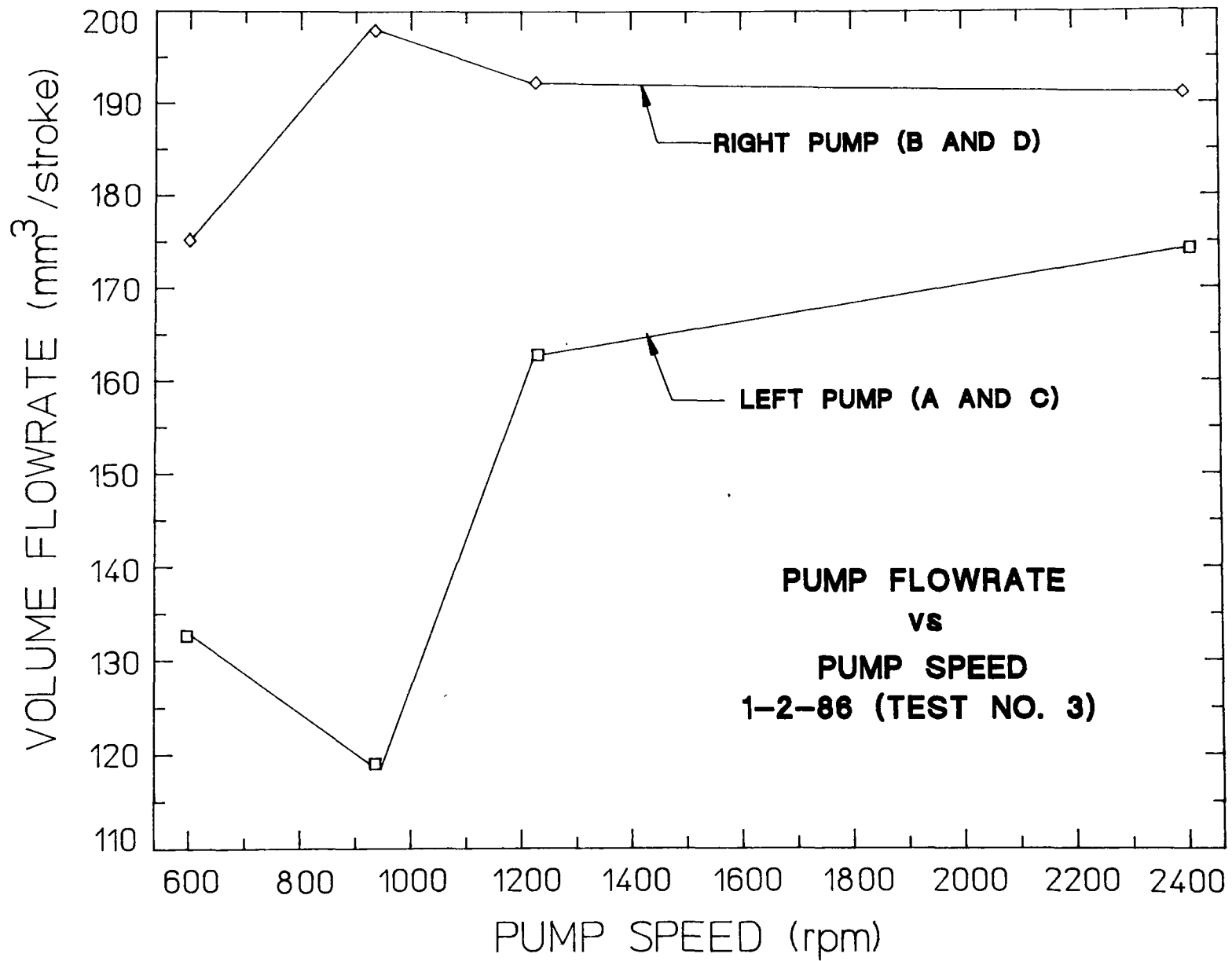


FIGURE 8. PUMP FLOWRATE VS. PUMP SPEED

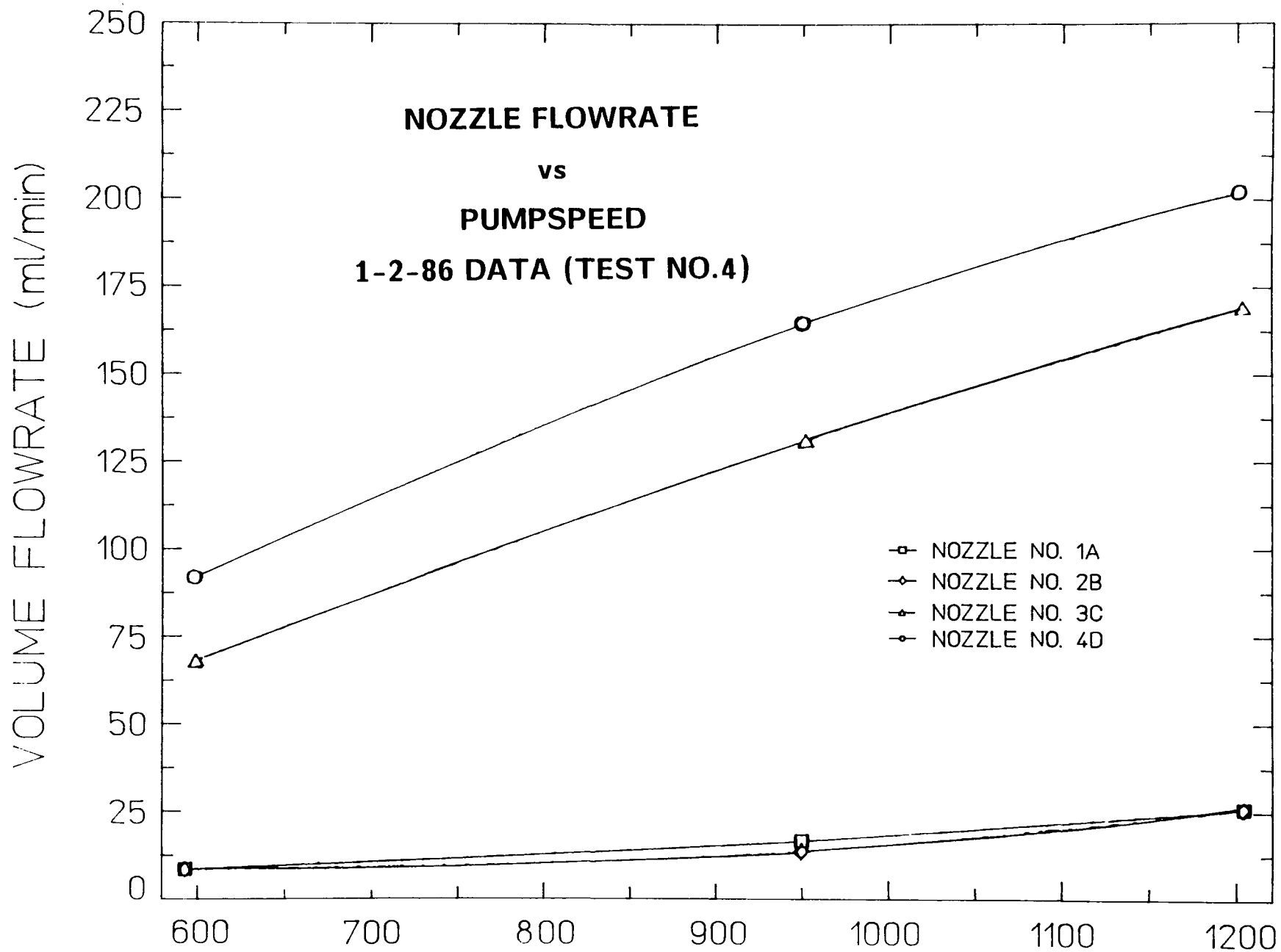


FIGURE 9. NOZZLE FLOWRATE VS. PUMP SPEED

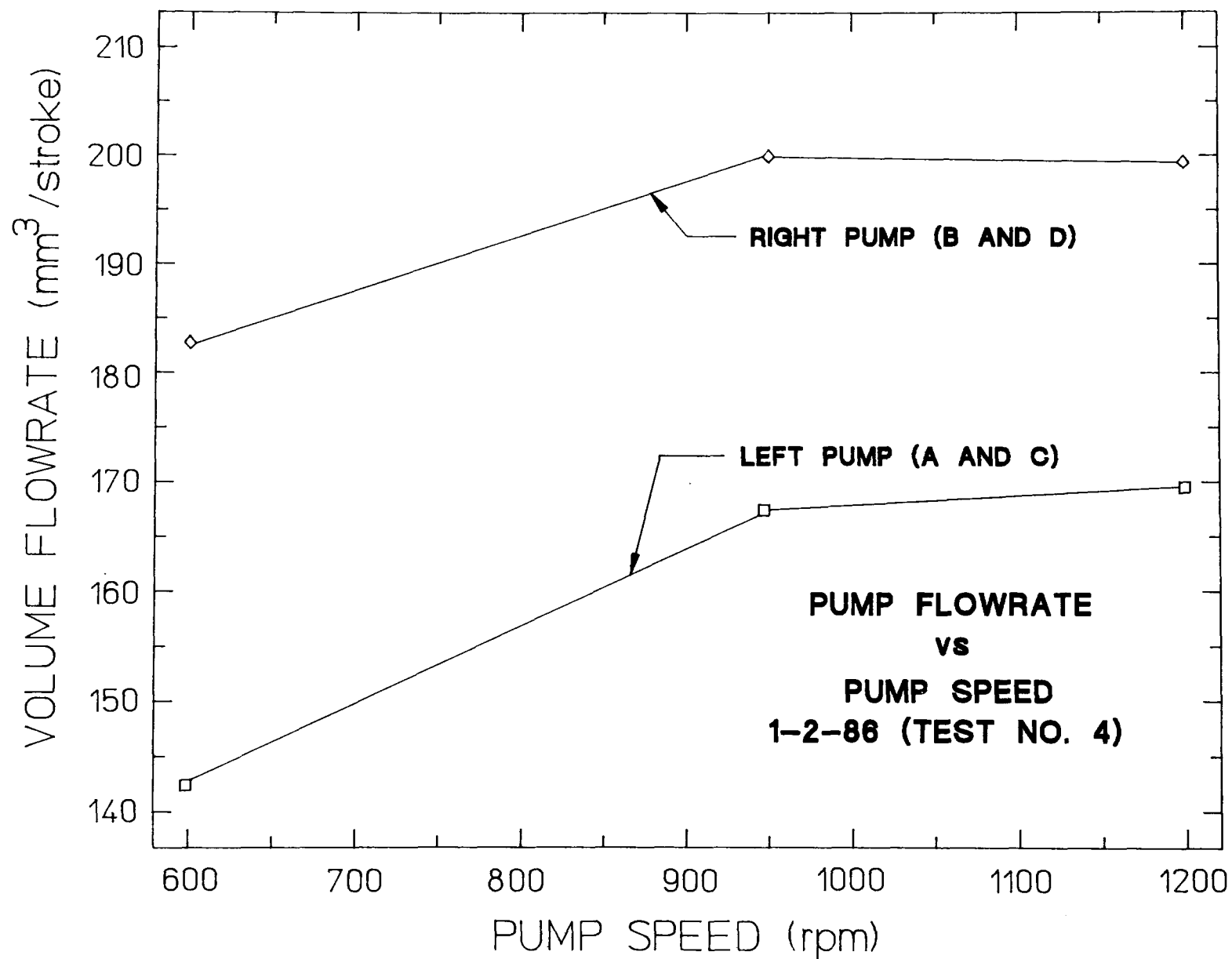


FIGURE 10. PUMP FLOWRATE VS. PUMP SPEED

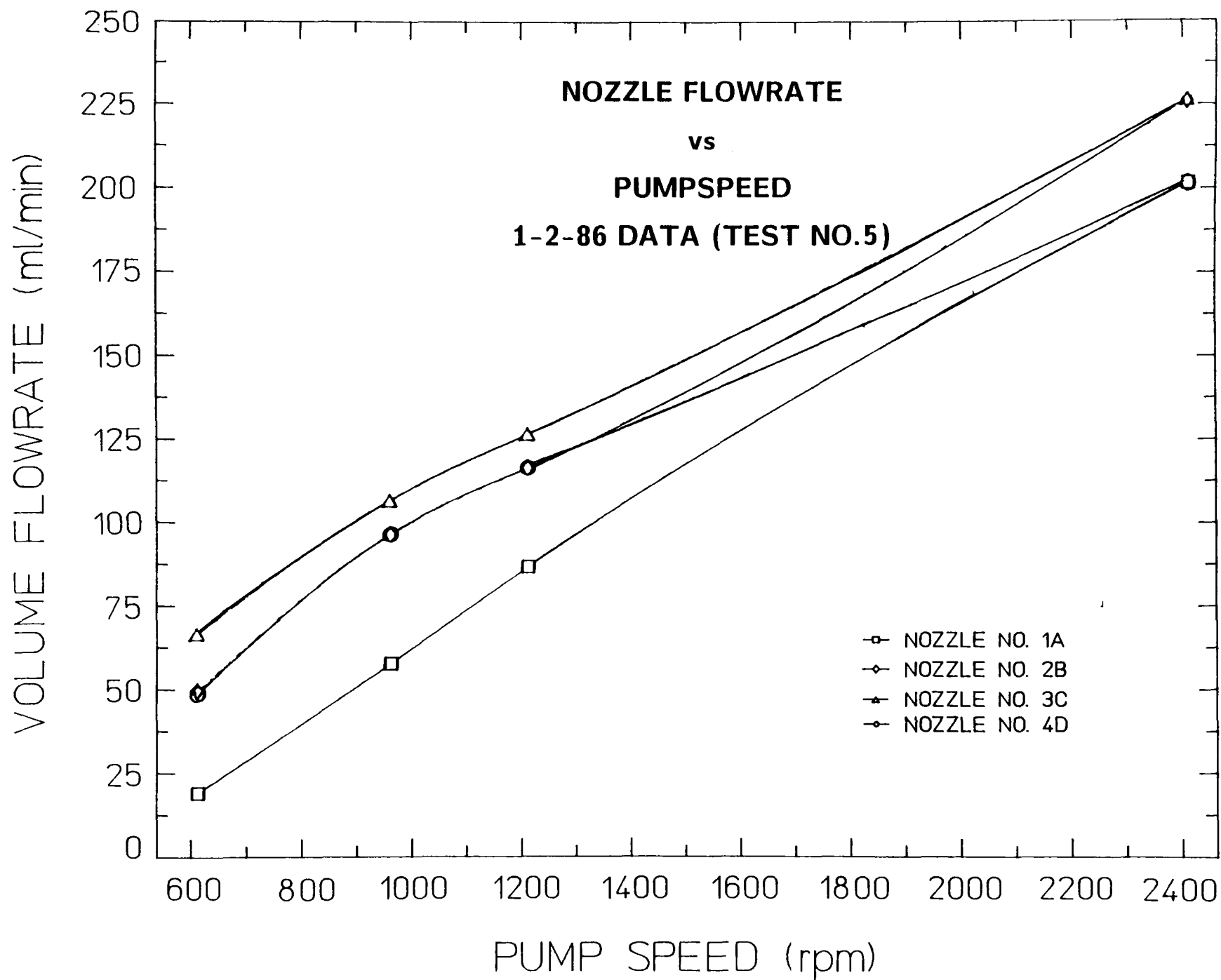


FIGURE 11. NOZZLE FLOWRATE VS. PUMP SPEED

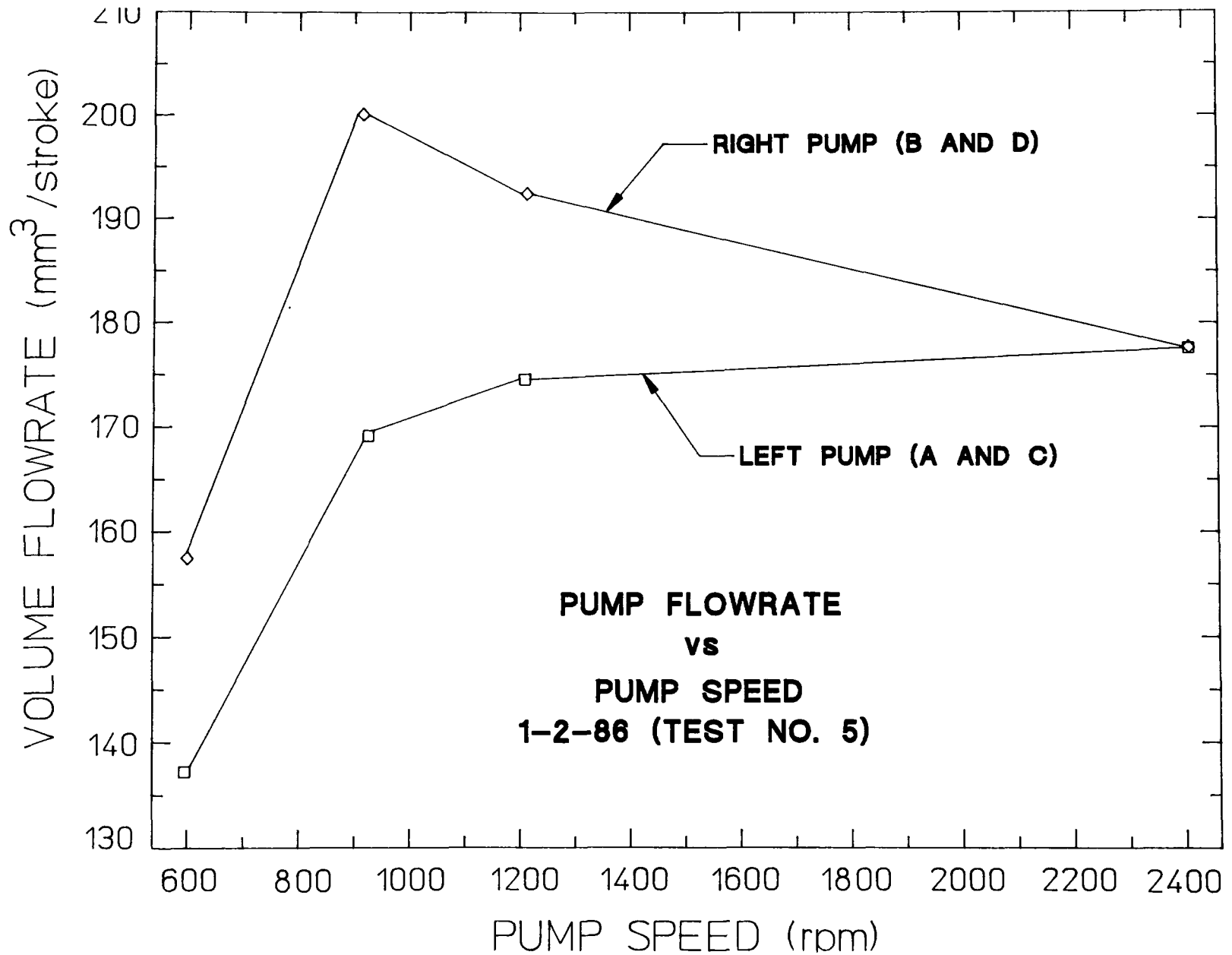


FIGURE 12. PUMP FLOWRATE VS. PUMP SPEED

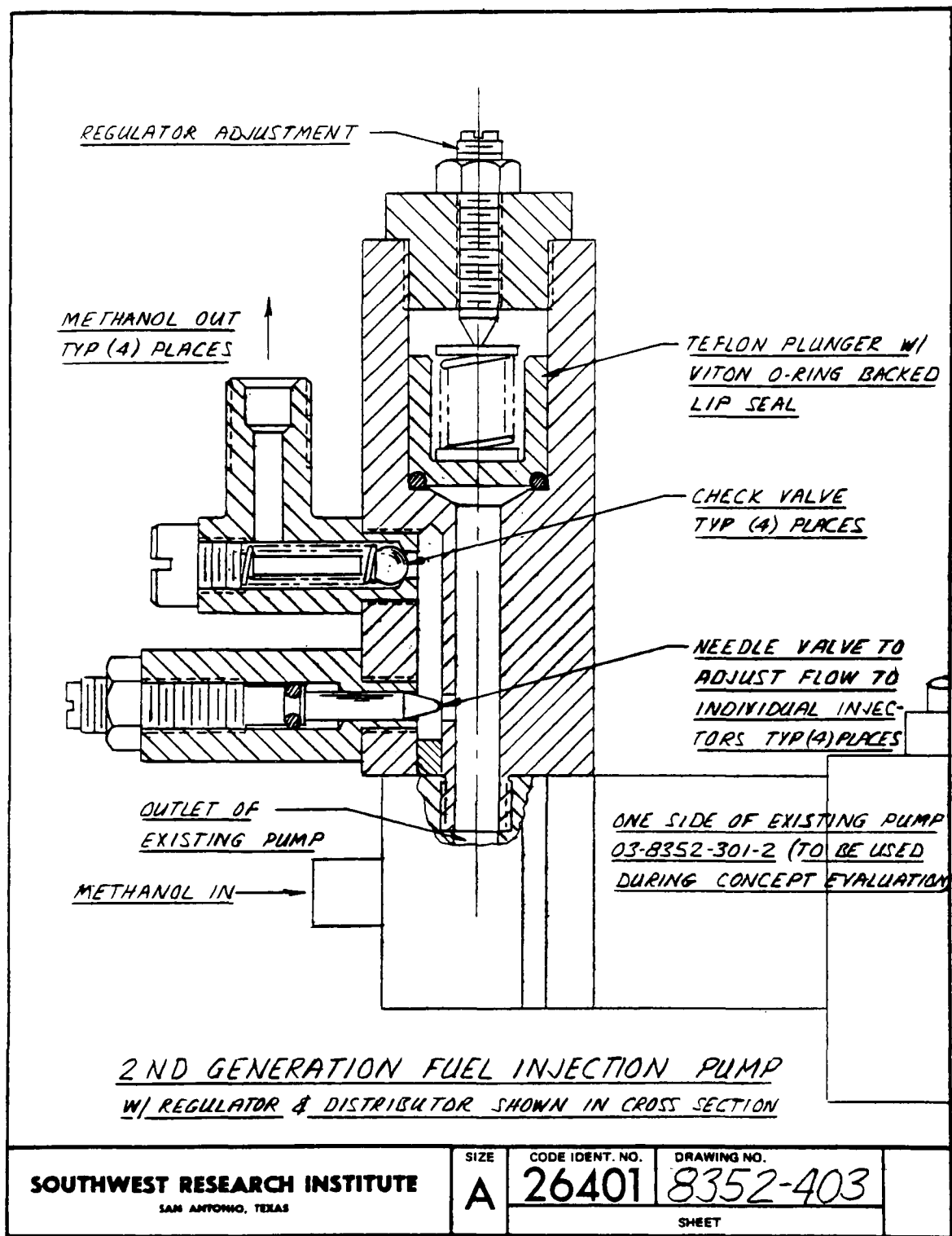


FIGURE 13. SECOND GENERATION SwRI-DESIGNED FUEL INJECTION PUMP

**APPENDIX B**  
**DESIGN SPECIFICATIONS**  
**IN-CYLINDER DISSOCIATION OF METHANOL**

**DESIGN SPECIFICATIONS**  
**"IN-CYLINDER DISSOCIATION OF METHANOL"**

SwRI Project No. 03-8352  
EPA Project No. 68-03-1984

Submitted by  
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Department of Engine and Vehicle Research  
Southwest Research Institute

November 30, 1984

## INTRODUCTION

The objective of engine design specifications is to provide a guideline for the project work. Consistent with the technical objective of the program "In-Cylinder Dissociation of Methanol," the various alternatives considered and the design specifications presented in this document are aimed at developing a methanol-operated engine with fuel economy, driveability and exhaust emissions at least equal to the automotive gasoline engine selected for the experiments. The method of achieving this goal are discussed in the appropriate section of this document.

## COMBUSTION CYCLES, LOCATION OF CATALYST AND FUEL CONSIDERATIONS

Automobile engines of the four-cycle type operate either on gasoline or diesel fuel. The combustion cycle of the gasoline engine is the Otto cycle, in which the charge induced during the suction stroke is a homogeneous mixture of fuel (gasoline) and air. The diesel engine operates on the diesel cycle, or constant pressure cycle, in which the charge induced into the engine's cylinder consists of air. Fuel is injected into the engine's cylinder at an appropriate time in the cycle. In Otto cycle engines, the combustion of the fuel/air mixture is initiated by high voltage electric sparks through the spark plugs. The combustion of diesel fuel in a diesel cycle engine is accomplished through self-ignition.

Because of the self-ignition properties of the fuel, diesel engines do not require any ignition assistance. However, to initiate this process, the fuel is required to be admitted to the engine when the combustion air temperature and pressure are sufficiently high to cause the fuel to self-ignite. In diesel engines, the required high pressures and temperatures are achieved through the use of a high compression ratio. Also, the self-ignition property of the fuel enables the engine to operate over a wide fuel/air ratio.

Change in load is achieved by altering the amount of fuel admitted into the combustion space of the engine. The air supplied to the engine is controlled only through the engine's design, and no provisions are required to alter the air flow to the engine. Use of higher compression ratios, and the engine's ability to operate on wide fuel/air ratios, makes the diesel cycle engine thermodynamically more efficient than

the Otto cycle gasoline engine. The compression ratio of Otto cycle gasoline engines is usually limited to 10:1 due to fear of preignition/detonation of the fuel/air mixture. Although combustion of fuel-air mixtures much leaner than chemically-correct (stoichiometric) is theoretically possible, burning in the internal combustion engine poses several problems. In conventional Otto cycle automobile engines, the fuel-air mixture is supplied at or very near stoichiometric, and load is controlled by regulating the amount of air and fuel induced into the engine's cylinder. The amount of air is varied by opening or closing a butterfly valve in the intake manifold/carburetor. Such an obstruction to the airflow reduces the volumetric efficiency of the engine. The low compression ratio, inability to burn a lean fuel-air mixture and loss of volumetric efficiency make the Otto cycle engine thermodynamically less efficient than the diesel cycle engine.

The concept of in-cylinder dissociation of methanol can be adapted to either diesel or Otto cycle engines; however, there are certain advantages and disadvantages associated with each approach. Before the applicability and suitability of the cycles are considered, it is essential to consider the possible locations of the catalyst in an engine. In the specific context of this particular project, it is possible to locate the catalyst chamber within the combustion space of the engine. Alternatively, a catalyst chamber can be designed as part of the cylinder head. The first approach has the following disadvantages:

- 1) contamination of the catalyst with combustion products, rendering it useless in a short period of time,
- 2) exposure of the catalyst to high combustion heat, causing a heat loss that results in lower cycle efficiency,
- 3) the necessity of supplying methanol, and therefore dissociation, during the intake cycle, resulting in low volumetric efficiency of the engine,
- 4) premature combustion of dissociated methanol, resulting in loss of engine efficiency and damage to the engine's structure,
- 5) inability to use exhaust heat (waste heat) for dissociation of methanol, thereby being unable to improve the thermodynamic efficiency of the engine.

These disadvantages can be eliminated if:

1. the catalyst chamber is isolated from the engine's combustion space,
2. the catalyst chamber location is designed to use the waste heat from the engines exhaust gases.

Since differences in the combustion cycle are due to the characteristics of the fuel, it is essential that the hydrogen (H) and carbon monoxide (CO) are characterized as fuel for an internal combustion engine. The primary products of dissociated methanol are 66 percent hydrogen, and 33 percent carbon monoxide. Both gases are suitable for internal combustion engines. Table 1 shows the typical properties of methanol, hydrogen, and carbon monoxide.

**Table 1. Properties of Fuels**

	<u>Methanol (MeOH)</u>	<u>Hydrogen (H)</u>	<u>Carbon Monoxide (CO)</u>
Heating Value BTU/lb	8471	51600	4321
Ignition Temperature °F	842	1040	1121
Theoretical air requirements lb/lb	6.4	34	2.5
Ignition Limit, air-fuel ratio			
Lower	5.5	4	12.5
Upper	26	77	75

For combustion cycles and operating efficiency, ignition temperature and lower ignition limits are important. Both gases have high ignition temperatures and a very wide ignition limit, which is highly desirable for fuel economy and power.

Another important consideration is the flame speed. Both gases have very high flame speeds. Use of hydrogen fuel in spark-ignition internal combustion engines is associated with several problems, such as flashback, preignition, severe cylinder

pressure oscillation, and rough running due to a high rate of pressure rise. However, the presence of CO in hydrogen suppresses all the above without affecting flame speed.

### **Combustion of Dissociated Methanol in a Diesel Cycle**

Combustion of dissociated methanol in a diesel cycle is possible. Because of high ignition temperatures, however, the compression ratio of such an engine must be in excess of 80:1. It would not be possible to convert an existing gasoline automotive engine to run at such a high compression ratio. Such an engine, if developed, would be very bulky and would result in a loss of overall fuel economy. Administering the gases to the cylinder would also be a problem. The pressure required to inject the gas into the combustion chamber would be more than 10,000 psi. Dissociation of methanol in a catalyst chamber results in pressure rise. The pressure depends on the catalyst used, the temperature, and the volume of the chamber. Preliminary calculations indicate that for a one liter engine under the best possible conditions, the pressure in the chamber will be approximately 150 psi. This being far less than the required injection pressure, additional power will have to be expended to increase the pressure of the gases. The additional work will obviously result in a loss in fuel economy.

The only advantage of using the diesel cycle would be an excellent control on the combustion by regulating the rate of fuel (gas) injection. However, the anticipated poor fuel economy and higher NO<sub>x</sub> emissions make this cycle unsuitable.

### **Combustion of Dissociated Methanol in Otto Cycle**

Conventional Otto cycle, in which a homogeneous fuel-air mixture is induced into the engine's cylinder, is certainly not suitable for this project. The fuel in the catalyst chamber at about 150 psi can be admitted to the engine during the induction stroke with the help of a third valve in the cylinder head. However, introduction of gas into the cylinder during the induction stroke will reduce the engine's power output considerably due to a loss in the volumetric efficiency. The fuel is required to be admitted only after the exhaust valve is closed; however, this would not be a problem. The combustion of fuel in such a cycle will be initiated through a spark at an appropriate timing. The high flame velocity means that the engine can run on a highly retarded

timing (an advantage to reduce the NO<sub>x</sub> emissions) and timing changes for various loads and speeds would be minimal. Engine load control will be accomplished through the metering of fuel and/or air induced into the engine. As stated earlier, the major disadvantage of the Otto cycle as described above is reduced power output.

### **Combustion of Dissociated Methanol in a Modified Otto Cycle**

Engine power can be considerably increased if the fuel is supplied after or just before the intake valve is closed during the compression stroke. The cylinder pressure at the time of intake valve closing is estimated to be equal to or slightly less than atmospheric pressure. Therefore, introducing the dissociated methanol fuel (already at approximately 150 psi) is not only easier but has other beneficial effects. It is expected that the effects of introducing the high pressure gas will be similar to a supercharged engine. Increased power and efficient combustion can be therefore expected from the engine. Furthermore, by shaping the port and suitably locating the fuel gas inlet valve in the cylinder head, air swirl can be generated. Air swirl in conjunction with the high flame speed is expected to improve the combustion efficiency.

It is well known that air standard efficiency of an engine increases with increases in the engine's compression ratio. Considering the high-octane rating of both the gases, it appears possible to increase the compression ratio of the engine. The actual increase will be decided upon the structural strength of the engine selected for the experiment.

Initiation of combustion will be through a spark plug. As discussed earlier, the engine can be operated with a highly retarded ignition timing. In addition, the required changes in the timing due to changes in speed and load will be minimum. Load control can be through regulation of both air and fuel; however, it is advantageous to operate the engine at open throttle to maximize power output.

Regardless of the combustion cycle selected, the engine will operate in different modes during starting/warm-up, and when the engine is warmed up. During the cold starting and warming up period, there would be insufficient heat available to cause dissociation of methanol. The fuel, therefore, will have to be admitted with the induction air. The fuel can be supplied either through a carburetor, a throttle-body fuel

injection system, or a port injection system. Once there is sufficient heat available for dissociation of methanol, the mode of fuel should be gradually changed from the liquid fuel in the induction manifold to dissociated methanol in the cylinder.

Based on the above descriptions, the following design specifications are suggested for the combustion cycle:

1. A modified Otto cycle engine operating in dual-mode; that is, a standard Otto cycle during starting and warming up and a modified Otto cycle during operation.
2. During starting, liquid methanol fuel will be supplied in the manifold or port injection.
3. During operation, dissociated methanol will be supplied to the engine cylinder through a third valve.
4. Dissociated methanol will be supplied to the engine cylinder after or just before the intake valve is closed.
5. Methanol will be injected into the dissociation chamber soon after the chamber is emptied into the engine cylinder.
6. The charge will be ignited with the help of a spark plug.
7. Open throttle (or no throttle) operation is desirable during the modified Otto cycle operation.

## DEVELOPMENT OF CATALYSTS AND CATALYST CHAMBER SPECIFICATIONS

The selection of catalyst materials, catalyst configuration, and the pre-chamber dimensions will be made following a bench type experiment to screen different materials and obtain other design data. Performance data on methanol dissociation catalysts for automotive use are reasonably well-known for steady-state atmospheric conditions. This data are not readily available for transients and high pressures in the range of 2 to 10 atmospheres. Such data are essential to the design of the pre-chamber-type dissociator proposed in this program.

Figure 1 shows the design of the reaction chamber for the test rig. The design is an approximation of the chamber to be used on the engine. The catalyst chamber is

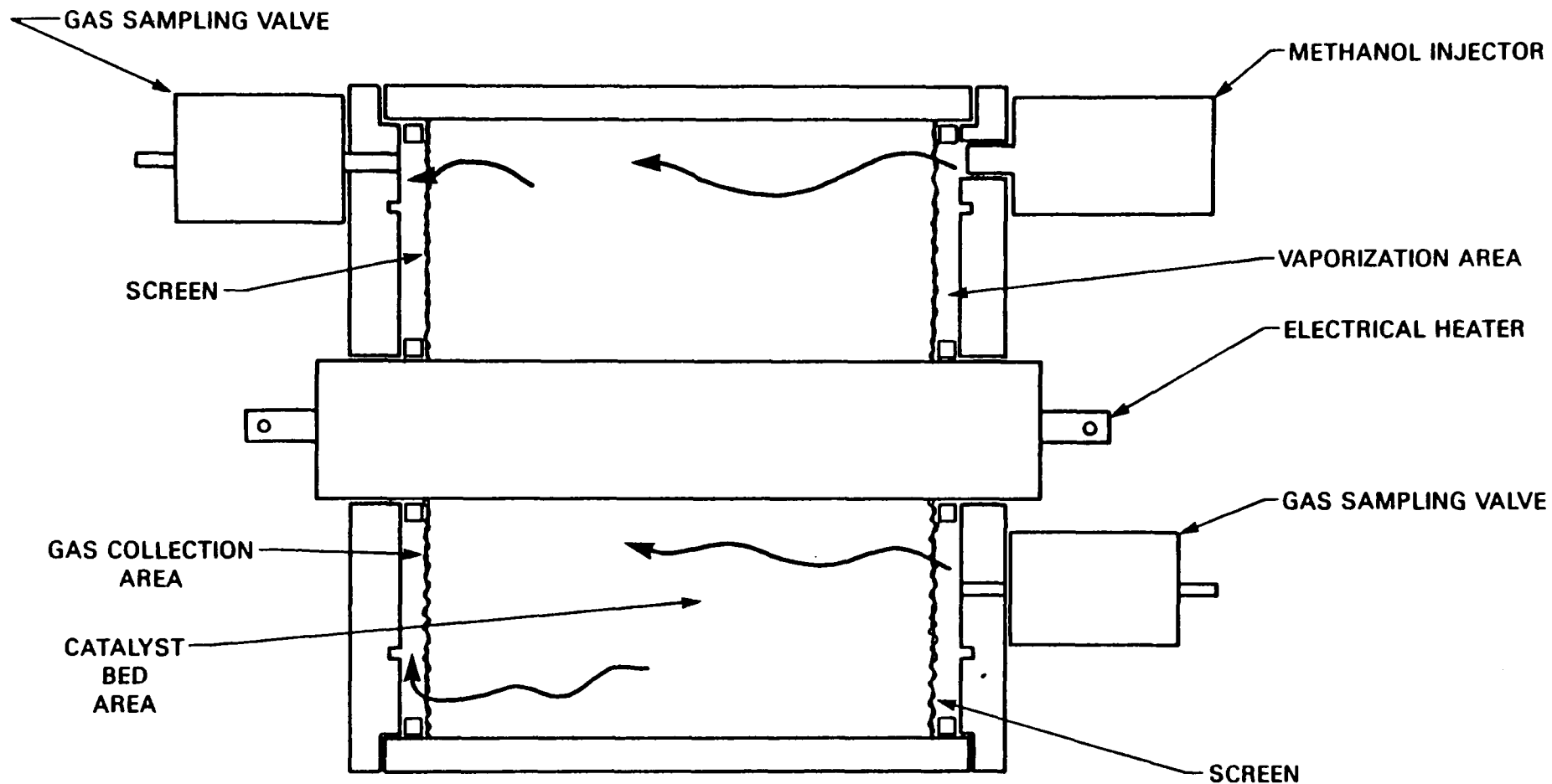


FIGURE 1. SINGLE PASS CATALYST TEST CHAMBER

annular in cross section with an electrical heater element through the center, representing the heat from the exhaust flow. The total volume of the chamber will be  $100\text{ cm}^3$ . A fuel injector will spray methanol onto a set of copper fins. This is to provide space and time for vaporization to take place. Methanol vapors will then travel through the catalyst bed. Following timing cycles as in the engine, a blowdown valve will open, simulating the release of dissociation products into the combustion chamber.

The experimental chamber will be instrumented for pressure rise, temperatures at several locations, and gas chromatography will be used to analyze the products of dissociation. The gas analysis will include the determination of  $\text{CO}$ ,  $\text{H}_2$ ,  $\text{CH}_4$ ,  $\text{H}_2\text{O}$ ,  $(\text{CH}_3)_2\text{O}$ , and unreacted methanol. Mass balances will be made in order to assess possible formation of solid carbon in the catalyst bed. By use of a high speed gas sampling valve, the gas analysis history can be attained at various segments of the pressure rise following the injection of methanol.

This experiment will provide information on the transport properties of the catalyst matrix, namely, the effects of conduction and heat capacity. These properties play a role during the thermal recharge cycle and the dissociation cycles. The overall reaction rate depends on both the chemical rate and the heat and mass transfer to the catalyst. At sufficiently high temperatures ( $300^\circ\text{C}$ ), the chemical reaction rate is quite fast and should not be rate-limiting. The transport steps are:

1. Mass transfer of reactants to the catalyst and the desorption of products.
2. Heat transfer to the catalyst bed.

In a closely packed bed, the gases are in intimate contact with the catalyst and diffusion lengths are short. However, if desorption of products is slow, the reaction rate will be limited by the number of available sites. If the rate is limited by desorption of products, the effect can be ascertained by varying the temperature and the catalyst particle size. Increasing the available surface area of the catalyst will increase the rate if mass transport and desorption of products is rate-limiting. Dissociation rates will be determined from pressure rise data.

The effects of bulk mass transfer could be examined by altering the geometry of the reaction chamber. Such a modification may take the form as shown in Figure 2. Here an internal cylinder has been added to the design, creating a longer flow path for the reactants, hence a higher flow velocity through the catalyst bed.

Heat transfer to the catalyst bed is an important aspect of the dissociation process. Both vaporization and dissociation of methanol are very endothermic processes, which require the maintenance of a high temperature (300°C). Several high-response thermocouples will be installed in the reaction chamber shown in Figure 2 to assess temperature gradients and rates of heat recharge.

Finally, the data from these tests, will be used to predict rates of dissociation in real engine tests. The simulated catalyst chamber test data will also be of value in measuring catalyst performance and longevity.

#### **DESIGN SPECIFICATIONS - ENGINE AND COMBUSTION CHAMBER CONSIDERATIONS**

Engine and the combustion chamber configurations must be selected to match the objective of the project and the above selected combustion cycles. Also important in the selection of the engine configuration is the development of hardware. In this particular project, due consideration must be given to the design and development of the cylinder head.

Since the objective of the project is to study the in-cylinder dissociation of methanol concept for an automobile engine, the selected engine must be suitable for automotive applications. A four-cycle engine is best suited for the experiments. From a dissociation point of view, an air-cooled engine may be preferred over a water-cooled engine; however, air-cooled gasoline engines are no longer used on automobiles. It is preferred that we select a late model automobile engine of the state-of-the-art design. On a four-cycle engine running at 6000 rpm, the injection event repeats every 20 milliseconds; therefore, regardless of how the fuel is admitted, the minimum time available for dissociation of methanol is at least 20 milliseconds. Since this available time is more than that required, engine speed is not likely to be a limiting factor. All

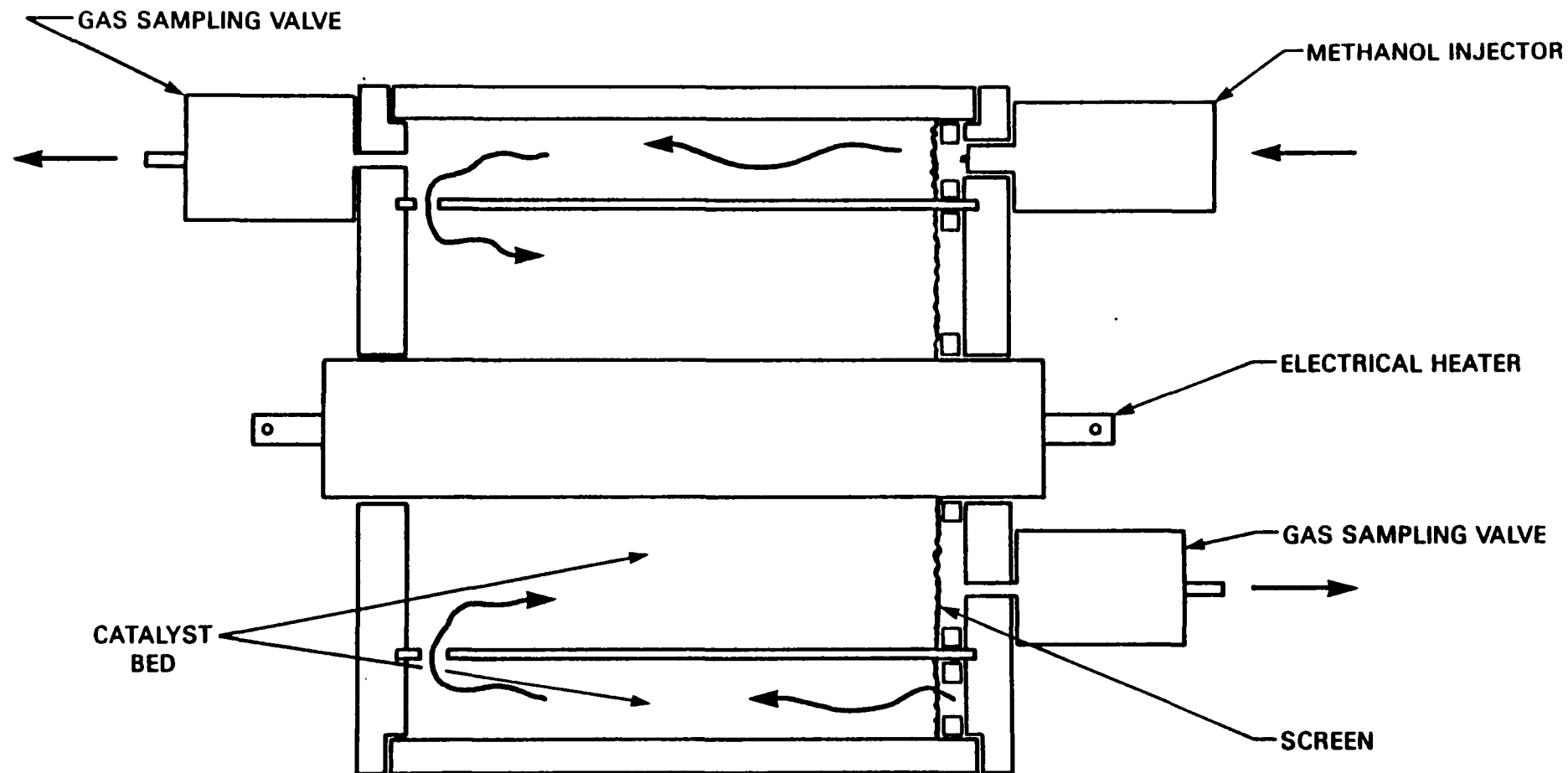
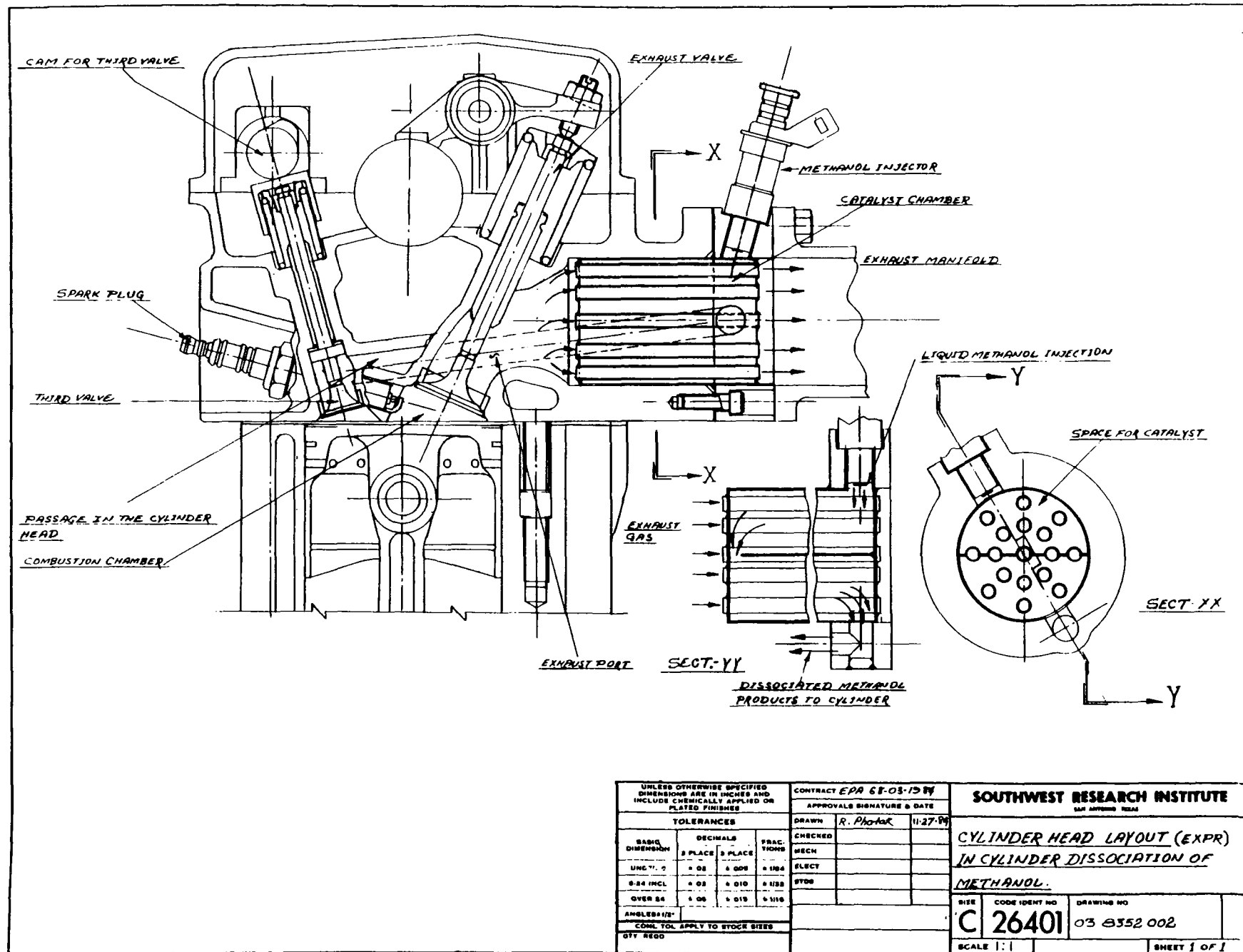


FIGURE 2. DOUBLE PASS CATALYST TEST CHAMBER

late model automotive engines are of the overhead valve type, a superior design as compared with the side valve engines. In this project, too, an overhead valve engine is highly desirable. A conservative engine design (structural) is more suitable. As discussed in the earlier sections, some thermal efficiency gains are likely if the engine's compression ratio is increased. Such an increase is possible only if the engine's structure can take the additional load due to higher working pressures. This particular point will be considered in the engine selection process.

The engine design configuration should be suitable for the proposed design modifications. As discussed earlier in this document, placing the catalyst chamber in the combustion space has many disadvantages and would require extensive modifications to the engine. The most promising alternative is the use of heat from the exhaust gases, and possibly from the cooling water jacket. In order to use heat from the exhaust gases, it is desirable that the catalyst chamber be located in the exhaust port of the cylinder head. For the combustion cycle selected, and for the highest volumetric efficiency, it is essential that the dissociated methanol be supplied to the cylinder just before or soon after the intake valve is closed. This requires that there is a fuel supply valve in addition to the intake and exhaust valves. Figures 3 and 4 show a conceptual layout for the cylinder head design. From this layout it is clear that we need ample space in the exhaust port to accommodate the catalytic chamber. It is therefore required that the engine's cylinder head design configuration has a cross-flow head, or that it be possible to convert the head to a cross-flow type. For efficient combustion and high BMEP, several automobile engines use hemispherical heads and four valves driven through double overhead cams. Although the hemispherical combustion chamber and four valves are advantageous, there are very difficult hardware problems. The hemispherical combustion chamber heads with four valves usually do not have the space to accommodate a third valve and the large space required for the catalytic chamber. Furthermore, machining the valve gear surface at complex angles (hemispherical heads) is much more difficult than valve gear surfaces parallel or at right angles to the cylinder axis. It is felt that the type of fuel, together with the intake swirl, will produce results comparable to a hemispherical combustion chamber with a much simpler "bathtub" shaped combustion chamber. From a hardware modifications point of view, an overhead cam is preferred. The engine will most likely need an additional camshaft to drive the third valve. In order to keep the hardware development costs to



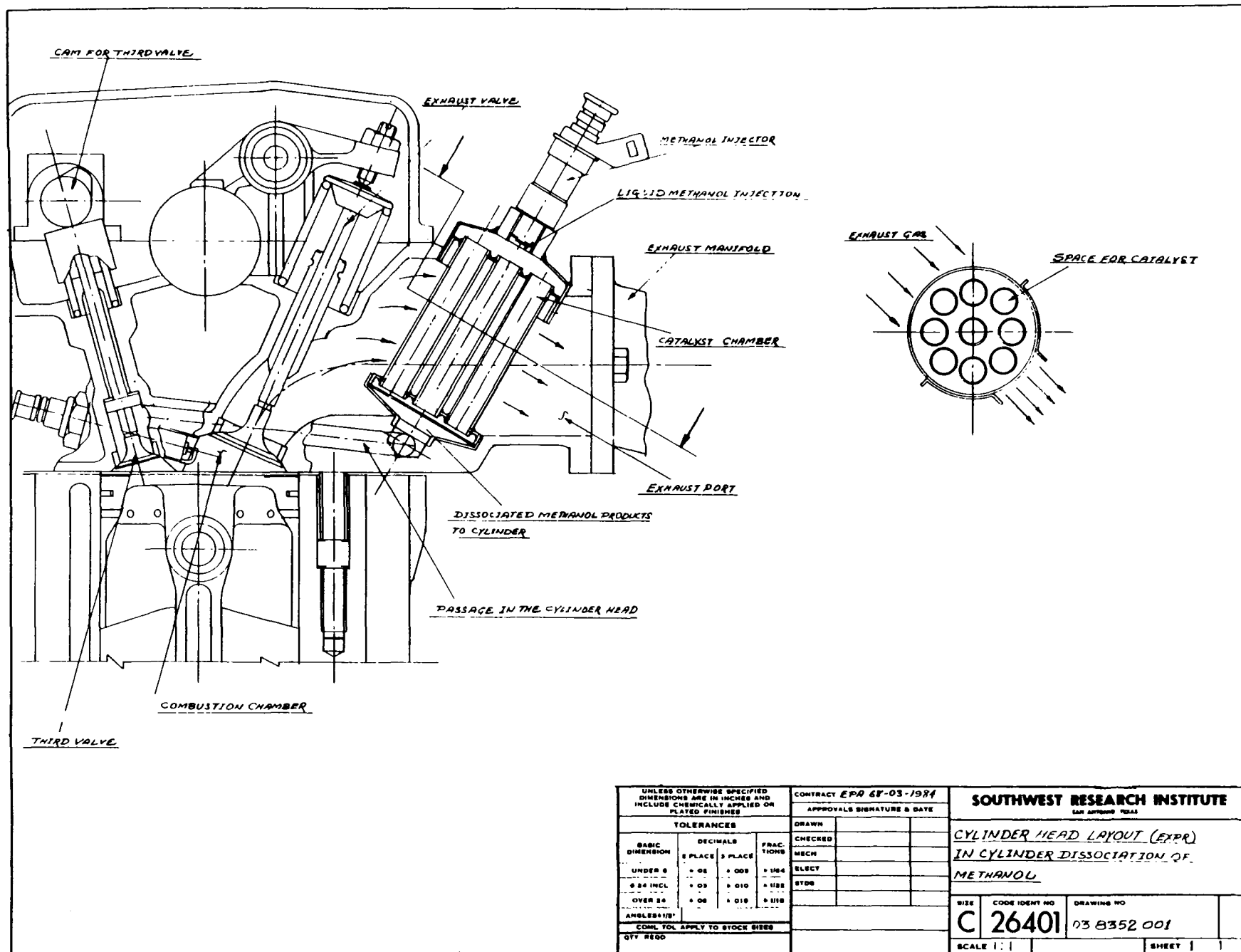


FIGURE 4. CYLINDER HEAD LAYOUT - SINGLE PASS CATALYST CHAMBER

a minimum, we are proposing a four-cylinder in-line engine. Also, it is desirable that we select an over-square engine.

Based on the above descriptions, the following set of design specifications are recommended:

1. A four-cylinder, spark-ignition automobile engine
2. Engine speed up to 6000 rpm
3. Larger bore engine; that is, stroke/bore ratio as small as possible
4. Two overhead valves, one cam engine
5. Cross-flow type cylinder head design
6. A conservatively designed engine

Based on the above requirements, two engines are considered suitable for the experiments. The engine specifications are shown in Table 2.

**Table 2. Engine Specifications**

	<u>1</u>	<u>2</u>
Make & Model	Datsun 200 SX, 1982	U.S. VW Rabbit
Bore x Stroke (mm)	84.5 x 88	79.5 x 86.4
Displacement (liters)	2.2	1.6
Cam	Single OH	Single OH
Maximum Power	102 Bhp @ 5200 rpm	74 Bhp @ 5000 rpm
Maximum Torque	129 lb ft @ 2800 rpm	90 lb ft @ 3000 rpm
Fuel System	Bosch L-Jetronics	Bosch K-Jetronics

The following modifications to the engine are recommended:

1. Fit a heat exchanger (catalytic chamber) into the exhaust port of each cylinder.
2. Provide the engine with a third valve to admit the fuel into the engine.
3. Provide valve gear for operating the third valve.
4. Design a new exhaust manifold.
5. Design/modify any other component as a result of the above modifications.

## **DESIGN SPECIFICATIONS FOR CATALYTIC CHAMBER**

The program objective is to use the waste heat (heat lost to cooling water and heat lost to exhaust gases). Although part of the cooling water's heat can be used for evaporation of methanol, the temperature of cooling water is far less when compared to the required temperature for dissociation of methanol. The primary heat source for methanol dissociation has to be the hot exhaust gases. Maximum heat transfer can be achieved if the heat exchanger is placed in the exhaust port and as close as possible to the exhaust valve opening. The size and surface area of the heat exchanger required cannot be finalized at this time. An experiment is being planned to determine the size of the heat exchanger. Two designs, shown in Figures 3 and 4, are possible. The material for the catalyst chamber will be either copper or stainless steel. The space provided in the catalyst chamber will be filled with the catalyst material. Liquid methanol will be supplied to the catalyst chamber through a fuel injector. In operation, the temperature and pressure in the catalyst chamber will be monitored. Detailed design specifications of the catalyst chamber can be determined at the completion of the experiments.

## **DESIGN SPECIFICATIONS - GOALS FOR DRIVEABILITY, FUEL ECONOMY, AND EXHAUST EMISSIONS**

The project's goal will be to achieve driveability, fuel economy, and exhaust emissions equal to or better than the engine selected for these experiments.

Driveability measurements/assessments are usually subjective in nature. For these discussions we are referring to the report on CRC Project No. CM-118-84. Appendix A shows the detailed procedure for evaluating driveability.

Individual raters are provided with a procedure to start and idle the engine and drive the car(s) at specified speeds and distances. The driveability assessment is based on the severity of the malfunctions, such as (1) hesitation, (2) stumble, (3) surge, (4) stall, and (5) backfire. The malfunctions are rated subjectively. For example, a trace of malfunction and heavy malfunction are rated as 1 and 4, respectively.

In the current project, testing of an automobile to CRC procedure for driveability rating is not planned. However, the malfunction factors suggested by CRC will be used to compare engine performance. In our experiments, the selected engines (baseline and after modifications to run on dissociated methanol) with all its controls will be suitably instrumented to measure hesitation, stumble, and surge. For example, the degree of time delay between opening the throttle and an increase in engine speed could be measured and compared to quantify hesitation. Likewise, surge characteristics of an engine can be assessed by monitoring the dynamometer output. For the engine running on dissociated methanol, acceptable driveability will be achieved by suitably modifying the fuel control system. As discussed elsewhere in this document, the engine will likely have the control systems, one for liquid injection of methanol in the ports, and the other for liquid injection of methanol in the catalyst chamber. It is anticipated that both systems will have to be tuned to achieve acceptable driveability.

The project's goal is to achieve fuel economy with dissociated methanol equal to or better than the selected engine. The fuel economy testing and evaluation will be based on dynamometer testing of the engine. The engine(s) will be dynamometer tested for predetermined speeds and loads and the fuel consumption will be measured. The first step in determining the speed and loads is to select a driving cycle. Using the in-house computer program and the selected engine/vehicle data, the operating speed and engine load will be calculated for the driving cycle. The fuel consumption of the engine operated on both gasoline and dissociated methanol will be compared to assess the fuel economy gained/lost. It is anticipated that improved fuel economy will be achieved through the use of dissociated methanol. Fuel economy goals will be achieved by

maximizing the use of waste heat and optimizing the engine to run on lean fuel-air mixture. Slight supercharging of the engine and air swirl will be attempted to improve the combustion efficiency of the engine.

Testing of the automobile with the dissociated methanol engine is not planned in this project. It is therefore not possible to relate the engine's emissions to 1975 Federal Test Procedure. Our emission goal, therefore, is to achieve identical steady-state exhaust emissions from the gasoline and dissociated methanol versions of the engine. In both cases the engine will be tested on a dynamometer for pre-determined speed-load conditions. It is possible to use the same speed-load point for both fuel economy and emissions testing. The emissions measurements will include total HC, CO,  $\text{No}_x$ , and aldehydes. The measurements will be made after the exhaust catalyst. The reduction in emissions will be achieved through combustion modifications. For example, our attempt will be to run the engine at or below an equivalence ratio of .5 with as retarded an ignition timing as possible.

## **DESIGN SPECIFICATIONS - AUTOMATIC CONTROLS**

The dissociated methanol operated engine will be equipped with two control systems: one for port injection of liquid methanol and the other for injection of methanol in the catalyst chamber. It is suggested that for liquid methanol injection in the ports, we replace the electronic control system on the engine with a new adjustable system. We are proposing two control systems, one each for liquid methanol and dissociated methanol. We are suggesting an intermittent fuel injection system(s) similar to Robert Bosch L-Jetronics or LH-Jetronics system. Intermittent fuel injection is considered to be advantageous for maximum dissociation of methanol. During start and warm-up the port injection of liquid methanol would be operational. The temperature in the catalyst chamber will be measured and an appropriate signal will be used to activate the methanol dissociation system. The in-port injection system will either be cut off or kept in operation; however, at a much reduced fuel injection rate. At low idling and very low loads, when the exhaust temperature is expected to be low, the fuel supplied to the engine will be suitably shared by the two systems. The engine will be fitted with both these systems at the beginning of engine testing. Initial engine tests will be run without the electronic controls. At each speed/load point, the

engine performance will be optimized by optimizing the spark-timing for the lowest possible equivalence ratio fuel-air mixture. Also, warm-up mixture and cold starting/warm-up spark timing requirements of the engine will be evaluated and optimized using the external controls. Also, engine tests will be performed to optimize the ratio of liquid injected methanol in the port and dissociated methanol system at several speed-load points. The above optimization tests will provide a guideline to program the microprocessor in the automatic control systems.

The control system will be used primarily for controlling spark timing, fuel-air ratio and, if required, exhaust gas recirculation. It is anticipated that  $\text{NO}_x$  emissions of the dissociated methanol engine will be lower than the gasoline engine due to the engine's ability to run on low equivalence ratio fuel-air mixture. Also, the retarded ignition timing will help reduce the production of  $\text{NO}_x$ . An EGR system will be introduced only if the lean mixture and retarded ignition timing fail to bring the  $\text{NO}_x$  equal to the gasoline engine. We are planning to use the fuel quantity supply signal to control the flow of exhaust gas to the engine.

Our preliminary calculations indicate that rate of heat transfer to the catalyst chamber will not require any control. Therefore, no attempt will be made to control the flow of exhaust gases over the catalyst chamber.

An alternative control system for this engine would consist of essentially a speed governor, controlling the RPM through the quantity of fuel injected. The system would be the electronic version of the diesel's engine-type governor. Depending on the load, the engine would operate unthrottled (middle to maximum load) or throttled (light load). The throttle plate will be required on this engine, unlike the diesel, because the charge is homogeneous. The leanest equivalence ratio obtainable is estimated to be 0.3 as demonstrated by the Solar Energy Research Institute (SERI). The diesel, on the other hand, can idle at an overall equivalence ratio of 0.01 due to charge stratification. Some charge stratification is anticipated in this design; however, to what degree is difficult to predict.

Figure 5 is a block diagram of the control system. A proportional-integral-derivative (PID) analog controller (or the digital equivalent), would be used. A PID controller uses both the integral and the derivative of the error (difference between the

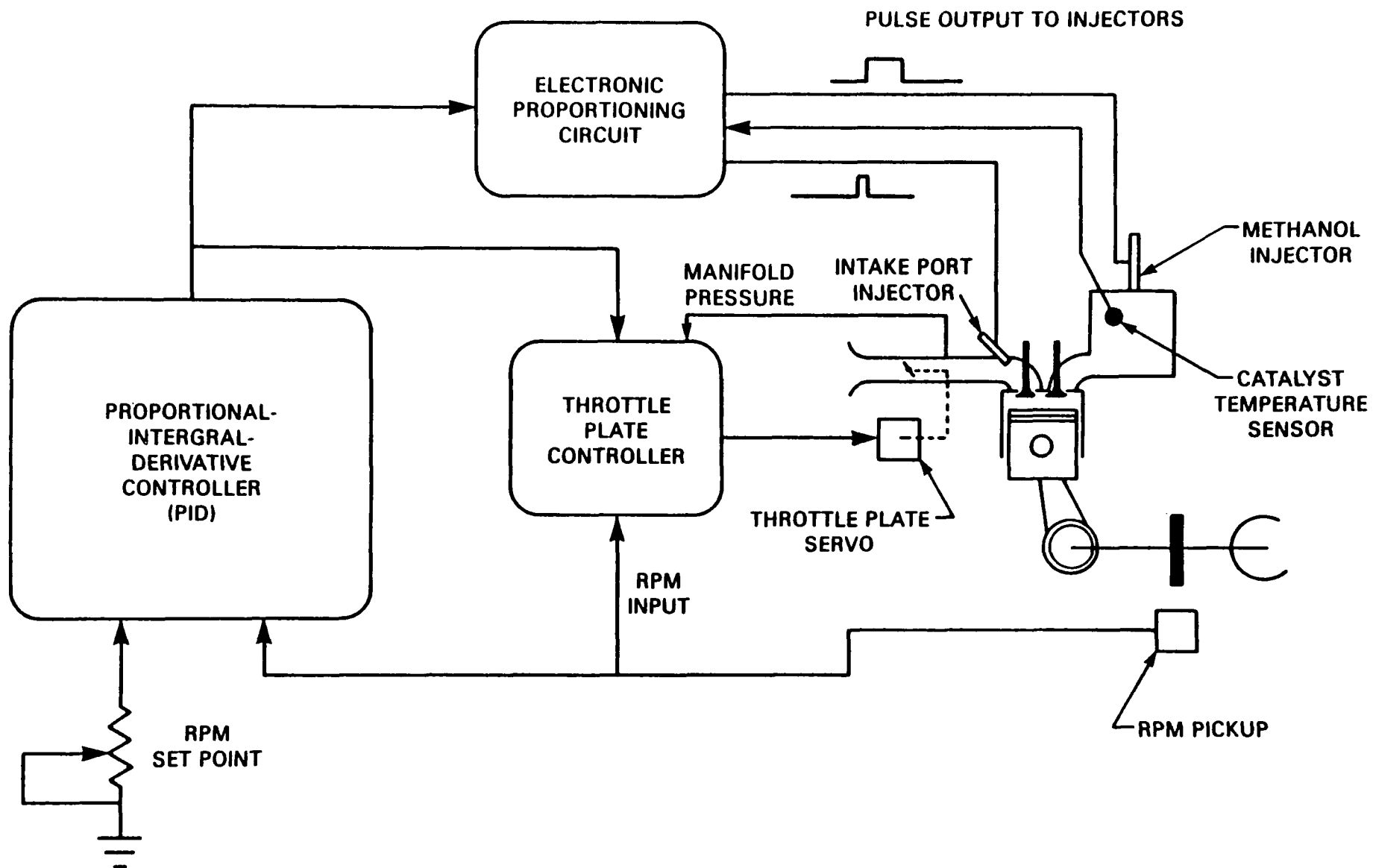


FIGURE 5. SIMPLIFIED BLOCK DIAGRAM OF ALTERNATIVE CONTROL SYSTEM

actual RPM and the setpoint) as well as the error itself to determine the control output. It would for example provide enrichment of the mixture during an acceleration due to the increase in the derivative of the error.

The output of the PID would then be divided between the intake port injector and the catalyst chamber depending on factors such as the catalyst temperature, the quantity of fuel required, and the rate of change of fuel delivery.

The temperature sensor in the catalyst bed would divert methanol to the port injectors if the temperature was too low. This condition would occur during cold start or high load conditions when there would not be sufficient heat to dissociate the fuel.

During conditions of acceleration and of increasing load but constant RPM, the heat supplied to the catalyst will lag the heat required for dissociation. By diverting methanol to the port injectors during these transient conditions, the thermal lag of the catalyst bed can be avoided.

While examining possible approaches in developing this control scenario, it is not yet clear whether analog is more appropriate than digital circuitry for this project.

## DESIGN SPECIFICATIONS - TEST PLAN

Engine testing will be done in three phases. During the first phase, called the baseline test, the engine will be tested on an engine dynamometer to establish fuel economy, exhaust emissions and driveability. For fuel economy and emissions measurements, the engine will be tested at the following speed-load conditions:

<u>Speed (rpm)</u>	<u>Load BMEP (psi)</u>
Idle	29.5
1750	10,18,35
1950	39
2150	11,43
2350	48
3000	Corresponding to max power
5000	Corresponding to max power

The speeds and loads in the first 6 rows are based on a vehicle fuel economy and performance simulation computer program. The input for the program was based on an average of 97 models of 1983 U.S. built cars (Table 3). Table 4 shows the output of the computer simulation program. Depending upon the engine and the car selected, the speed/load numbers in the first five rows will change slightly. The speeds selected in the last two rows will depend upon the speeds corresponding to the max torque and max power of the selected engine.

**Table 3. Input Data for Computer Program**

1983 U. S. Production Cars - 97 Models

**Average Statistics:**

Frontal Area: - 20.6 sq. ft.  
 Weight: - 2900 lbs (inclusive of driver and payload)  
 Displacement: - 183.7 in<sup>3</sup>  
 Bore: - 3.633 in  
 Stroke: - 3.306

Number of Cylinders: 5.361  
 Axle Ratio: 2.9965  
 Wheel Revolutions per Mile: 780 rpm (assume GR 78-14)  
 Wheel Base: 105 in.  
 Fuel/Air Ratio: 16 (14.93 stoichiometric, assumed)  
 Timing: MBT (assumed)  
 Compression Ratio: 8.575  
 Engine Speed, rpm: 2142 @ 55 mph

Four-speed Standard Transmission

**Computer Results**

	<u>AF = 26 ft<sup>2</sup></u>	<u>EFF. AF = 20.6 ft<sup>2</sup></u>
MPG	23.4 @ 55 mph	25.6
EPA City:	18.6	19.0
EPA Highway:	25.8 @ 50 mph	27.4
BMEP:	49.6 psi @ 55 mph	43.2
FMEP:	20.3 psi @ 55 mph	20.6
BHP:	24.6 @ 55 mph	21.5
BSFC:	.5458 lbs @ 55 mph	.5900

Engine rpm and load corresponding to about 20 mph will be used for evaluating

Table 4. SwRI Vehicle Fuel Economy and Performance Simulation

Vehicle: AVG,CAR  
 HP Req't Mode: RL  
 Engine Type: SI  
 Air/Fuel Ratio: 16.0  
 Pressures: 1)Exh (psia): 15.0 2)Baro (in-Hg): 29.92  
 Temperatures (F): 1)Air: 70 2)Coolant: 180  
 Stoich Air/Fuel Ratio: 14.93  
 Vehicle Eff Frontal Area (ft<sup>2</sup>): 20.60  
 Normal Loaded Weight (lb): 3200  
 Drivetrain Type: ST  
 N/V Ratio (Top Gear): 38.95  
 Piston Displacement (in<sup>3</sup>): 183.70 Cyls: 5  
 Bore x Stroke (in): 3.633 x 3.306 L/R Ratio: 1.70  
 Compression Ratio: 8.6 Rated rpm: 4000  
 Volumetric Efficiency: 85  
 Fuel LHV (BTU/lb): 19020  
 Fuel Density: 5.86  
 Electric Cooling Fan: NO Air Cond: NO  
 Ign Timing: (from MBT: +RTD, -ADV): 0  
 Gearbox Ratios: 3.000 2.200 1.500 1.000 MA

Specifications:  
 Max BHP @ rpm 120 @ 4000  
 Redline 4000 rpm  
 Adhesion Limit 1387.8 lbf  
 Track 57.7 in  
 Wheelbase 105.3 in  
 Height 30.0 in  
 Test Weight 3200 lbm  
 Weight Dist 50  
 Axle Ratio 2.997  
 mph/1000rpm 25.67  
 Gear Ratios:  
 Gear 1 3.000  
 Gear 2 2.200  
 Gear 3 1.500  
 Gear 4 1.000  
 Top Speeds in Gears:  
 Gear 1 34.2 mph  
 Gear 2 46.7 mph  
 Gear 3 68.5 mph  
 Gear 4 102.7 mph

Performance:  
 Max Speed 111.69 mph  
 Redline Limit 102.70 mph  
 Time to Speed  
 mph sec  
 0-90 29.58  
 0-80 21.37  
 0-70 14.78  
 0-60 10.83  
 0-50 7.98  
 0-40 5.43  
 0-30 3.46  
 0-20 2.28

#### Fuel Consumption

Idle @ 3.83 lbm/hr	Man Vac= 21.6 in-Hg		
MPG= 23.5 @ 20 mph	Man Vac= 19.4 in-Hg	RPM=1714 (2)	BMFP= 10.0 psi
MPG= 30.8 @ 25 mph	Man Vac= 18.8 in-Hg	RPM=2142 (2)	BMFP= 10.9 psi
MPG= 32.7 @ 30 mph	Man Vac= 18.1 in-Hg	RPM=1753 (3)	BMFP= 12.4 psi
MPG= 33.5 @ 35 mph	Man Vac= 15.5 in-Hg	RPM=1363 (4)	BMFP= 28.7 psi
MPG= 36.3 @ 45 mph	Man Vac= 14.0 in-Hg	RPM=1753 (4)	BMFP= 35.2 psi
MPG= 27.4 @ 50 mph	Man Vac= 14.0 in-Hg	RPM=1947 (4)	BMFP= 39.0 psi
MPG= 25.6 @ 55 mph	Man Vac= 13.1 in-Hg	RPM=2142 (4)	BMFP= 43.3 psi
MPG= 24.0 @ 60 mph	Man Vac= 12.2 in-Hg	RPM=2337 (4)	BMFP= 47.8 psi
BMFP (Acc# 1)= 42.8 psi	Man Vac= 13.0 in-Hg	A/F= 16.0	RPM= 1753 (1)
BMFP (Acc# 2)= 59.8 psi	Man Vac= 9.4 in-Hg	A/F= 16.0	RPM= 2142 (2)
EPA City Estimate: 19.0 MPG (LA4)			(Error Crit= .05000)
EPA Hwy Estimate: 25.0 MPG			
City/Hwy Composite: 22.8 MPG			

driveability. For better comparison between the gasoline engine and the dissociated methanol engine, we will try to quantify the malfunctions.

In the second phase of testing the engine will be dynamometer tested with the dissociated methanol as the fuel. These tests will be run with the fuel injection equipment hardware but without the electronic controls. For these tests the electronic controls will be replaced with the manual controls. The objective of these tests is to verify the suitability of the catalyst chamber design for engine operation. The engine will be tested for the following speed-load conditions.

<u>Speed (rpm)</u>	<u>Loads (F = Full Load)</u>
1000	F, 0.8F, 0.6F, 0.4F, 0F
2250	F, 0.8F, 0.6F, 0.4F, 0F
3000	F, 0.8F, 0.6F, 0.4F, 0F
4000*	F, 0.8F, 0.6F, 0.4F, 0F

(\*or rated speed of the engine)

Alternatively, the speed-load points used in the first set of tests can be used in place of the above speed-load points. At each speed-load point maximum fuel economy will be achieved by varying ignition timing and optimizing the use of dissociated methanol as engine fuel. The optimized ignition timing and the fuel delivery characteristics of both fuel injection systems for each speed-load point will provide input data for programming the electronic controller.

Prior to the third phase of testing the electronic controllers in the fuel injection systems will be programmed. In this phase the engine will be tested for fuel economy emissions and driveability with the electronic controllers. If the test results are found to be short of the goals, then further modifications will be considered for the catalyst chamber and control systems. For example, if the NO<sub>x</sub> emissions are higher than the goal, then an EGR system and a related control will be added to the engine.

## **APPENDIX C**

### **EVAPORATOR DESIGN ANALYSES PERFORMED BY A CONSULTANT**

## EVAPORATOR DESIGN FOR SOUTHWEST RESEARCH INSTITUTE

Use Configuration 4 in Table 3c. Design conditions are: Methanol saturation exhaust flow rates are 132 lbm/hr-cyl at 4500 rpm, gas pressure drop = 2.5 psi. Desire a set of hand calculations that outlines the design analysis and the

### DESIGN CONCEPT

A diesel spray nozzle will spray methanol droplets on the inner surface of the 3.358 in diameter evaporator tube. Heat transfer from the hot exhaust gases will vaporize the methanol. We will assume that the spray nozzle will fully wet the entire surface of the evaporator tube. The evaporator tube will be inclined at 45 degrees.

### POSSIBLE EVAPORATOR DESIGN CONCEPTS

There are two basic design concepts that may be considered:

1. A shell-and-tube boiler, having gas passing inside a bundle of small diameter horizontal tubes, with nucleate boiling of methanol on the outside of the tubes.
2. Evaporation of a thin methanol film that is gravity drained from the inside surface of a vertical (or inclined) tube. Exhaust gas flows parallel to the outer surface of the tube.

SwRI has specified the second type of evaporator. There are two possible methods of feeding the methanol to the evaporator:

1. Feed the liquid at the top of the evaporator tube.
2. Spray the liquid, as droplets, over the entire length of the

evaporator tube.

SWRI has specified that the second method is desired. The methanol will enter at ambient temperature, approximately 90 F. Hence, it must be heated to its vaporization temperature (259 F).

#### DESIGN CONSIDERATIONS

Because the methanol will form a film on the inner tube surface, it may rupture upon heating. Should film rupture occur, the dry heat transfer surface will be ineffective for evaporation. In order to assure surface wetting, use of capillary grooves or a porous surface coating would help to maintain surface wetting. When all of the methanol is evaporated, the tube wall will become dry.

It is unlikely that a "threaded" (axial or circumferential grooves) surface would provide an increase of surface area. It is probable that the tips of the v-threads would be unwetted, because of film rupture. The contact angle of the methanol should be small (15-20 deg). Hence, it is unlikely that such grooves would provide any significant film surface area increase. For an axial grooved surface, the forces acting on the film are gravity and surface tension forces (acting at the contact angle).

It is possible to solve the momentum and energy equations for a smooth inner tube surface and determine the liquid film thickness, assuming no film rupture. Since the film is laminar, the heat transfer coefficient is equal to the liquid conductivity ( $k$ ) divided by the film thickness ( $\delta$ ). The problem is complicated by two factors: 1. The wall temperature varies along its length, and 2. Uniform spray distribution along the tube length is more complicated than liquid supply at the top of the tube.

If an axial grooved inner tube surface were used, the solution would be

further complicated. However, I think the problem can be solved.

#### PRELIMINARY DESIGN

A hand calculation has been completed, which outlines the methodology of the evaporator design, assuming the methanol evaporation coefficient is known. This calculation is attached. It is noted that the thermal properties of methanol used are somewhat different than included in the SwRI report. My properties were taken from Perrys Chemical Engineer's Handbook, 6th ed., page 3-204.

The analysis assumes that axial threads are on the inner tube surface. Two thread heights are considered - 0.015 and 0.030 in. The analysis assumes that the thread grooves are filled to their tips with methanol. Thus, the film thickness (B) is the groove depth. It is assumed that the thread tips are not wetted. The evaporation coefficient is calculated as  $h = k/B$ . It is also assumed that the active inner surface area is the inner tube circumference. Methanol has a quite low thermal conductivity, approximately 0.095 Btu/hr-ft -F. The calculated evaporation coefficients are 38 and 74 Btu/hr-ft -F for  $B = 0.030$  and  $0.015$  in, respectively. Approximately 80% of the total thermal resistance is on the methanol side for  $B = 0.015$  in.

The analysis calculates the UA required to: 1. Raise the methanol to saturation temperature, and 2. To evaporate the methanol. I believe the analysis method is correct for liquid supplied at the top of the tube. However, I am not so sure about the situation for a spray of methanol over the entire tube length. For this case, liquid at 90 F is sprayed on the film surface. The mechanism by which the methanol is raised to saturation temperature and evaporated is unclear.

Using a methanol latent heat of 405 Btu/lb (rather than 500 Btu/lb as shown in the SwRI report), the calculated tube lengths are 2.92 and 1.63 ft

for  $B = 0.03$  and  $0.015$ , respectively. It is suggested that it may be difficult for a single spray nozzle to uniformly wet the entire length of a tube 2-3 ft long. Hence, the possibility of liquid supply at the top of the tube may be somewhat reasonable.

## CONCLUSIONS

The analysis has shown that the dominant thermal resistance is on the methanol side. For the chosen design concept, the required heat-exchanger length will decrease as the liquid film thickness is made smaller. A somewhat complex analysis would be required to estimate the film thickness for a tube having axial thread grooves; however, it is probable that such an analysis can be done. Consideration should be given to final selection of the method of liquid supply to the inner tube surface, e.g., whether spray distribution over the entire tube surface can be achieved.


## RECOMMENDATIONS

It is recommended that some further analysis be performed to estimate the probable methanol liquid film thickness, and the distribution of the heat transfer coefficient over the tube length.

The simplest concept for analysis would be a smooth inner tube surface. It is possible that this analysis can be extended to treat the axial thread groove geometry.

Should SWRI desire the Consultant to undertake the above analysis, I would estimate that 5-8 days would be required for the plain tube case. An additional 10 days may be required to extend the analysis to the axial thread geometry. The Consultant would hire the services of a Graduate Student to do detailed calculations. The cost of the Graduate Student would be in the \$800-1,000 range. Some computer time would be involved, perhaps \$300. Actually,

this problem would be a good one for an M.S. Thesis. This option may be of interest, if your time schedule permits. An alternate, or parallel approach would involve experimental investigation to determine the methanol film coefficient.

Submitted by 

Ralph L. Webb

July 17, 1985

DR. RALPH L. WEBB  
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STATE COLLEGE, PA 16801

August 9, 1985

Mr. William E. Likos  
Fuels and Lubricants Research Division  
Southwest Research Institute  
Post Office Drawer 28510  
San Antonio, TX 78284

Dear Bill:

This letter is in response to our telephone conversation on about July 31. You requested that I provide additional guidance on how one may predict the methanol film thickness in the evaporator, and thereby calculate the methanol heat transfer coefficient. I have spent approximately 12 hours on this question, and believe that I know how to perform the necessary calculations. However, it would be necessary to derive the applicable differential equations and perform a numerical solution. The problem of thin film evaporation of a uniform spray onto a grooved tube is not one, whose solution can be looked up in a book. Although I believe it should be possible to analytically solve this problem, some time would be necessary to do the job.

The purpose of this letter is to describe the fluid flow and heat transfer phenomena in the evaporator tube, and to describe how one may proceed to solve the problem.

If the methanol were added at the top end of a plain evaporator tube, the solution can be taken from Nusselts theory of film condensation. However, the evaporator design you envision introduces three additional complications. These are:

1. Introduction of the methanol via a uniform spray over the full length of the tube.
2. Introduction of a subcooled, rather than saturated fluid.
3. The use of axial grooves on the inner surface of the tube.

I will comment on the complications introduced by each of the above factors, and indicate how one may approach the problem analysis.

Consider, first, a vertical, plain evaporator tube. If saturated methanol were introduced at the top of the tube, Nusselt's theory of film condensation is directly applicable to the "reverse" problem of film evaporation. If the entering fluid

is subcooled, it is a fairly straight forward matter to calculate the tube length required to raise the subcooled fluid to its saturation temperature.

Introduction of the methanol by a uniform spray over the full length of the tube substantially changes the velocity and thickness of the liquid film. Attachment A outlines how one may proceed to derive and solve the differential equations for the film thickness. I think that the resulting film thickness will be smaller than that of a film introduced at the top of the tube. Contrary to the Nusselt theory, it appears that the differential equations must be numerically solved.

The use of an axially grooved evaporator tube introduces surface tension forces that act to slow the drainage of the film. Attachment B shows how one would calculate the static height of the liquid film inside a grooved evaporator tube. Note that there is no flow of the film for this analysis. However, the same surface tension forces would exist for the dynamic condition, when the film is gravity drained from the tube. Attachment C shows how one would approach this problem for the liquid introduced at the top of the tube. As shown by the analysis, it is necessary to write a force balance, which accounts for the pressure, gravity and surface tension forces on the liquid film.

Now, if one combines all of the above three special features (uniform spray over the tube length, grooved tube and entering subcooled liquid) the differential equations become more complex. However, I believe it is possible to formulate the necessary momentum and energy balances, which define the differential equations that must be solved. Another factor involved, that I have not discussed, is the inclination angle of the tube. However, one may easily account for this by including the component of the gravity force in the flow direction.

I think that the Nusselt solution for a plain tube, with all liquid introduced at the top would yield a conservative answer, relative to that for the uniform liquid spray. Furthur, I feel that the heat transfer coefficient for a plain tube would be higher than for a grooved tube. The main function of the grooved tube is to prevent surface dewetting, which is quite likely to occur for a plain tube. Attachment D contains calculations for the evaporation coefficient in a plain tube inclined at 45 degrees, having all liquid introduced at the top of the tube. Introduction of the liquid by a uniform spray over the full tube length will probably result in a higher evaporation coefficient, and the use of axial grooves will probably act to decrease the coefficient.

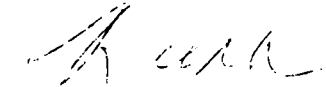
The above information is all I can accomplish in "eight hour analysis," which you specified. In regard to future evaluations for the evaporation coefficient, I will suggest two possibilities for your consideration:

1. Forget any further analysis, and experimentally determine the evaporator performance.
2. Attempt to solve the governing differential equations of the problem.

I would be pleased to attack either of the above approaches for you. Such work would probably best be performed under a research subcontract with Penn State. I believe it should be possible to set up an experimental apparatus to measure the evaporation coefficient. The analytical approach would require a matter of weeks to perform.

I hope this information is of value in identifying the probable value of the evaporation coefficient, and approaches to its more accurate determination.

With my best regards,



Ralph L. Webb

**APPENDIX D**

**HEAT EXCHANGER DESIGN ANALYSES**

**PERFORMED BY SWRI**

# **HEAT EXCHANGER DESIGN FOR DISSOCIATING METHANOL WITH EXHAUST HEAT**

## **1.0 INTRODUCTION**

This report covers the design specifications of the individual cylinder heat exchangers for vaporizing and dissociating methanol using exhaust heat. The following paragraphs discuss the specifics of the design analysis, the assumptions and methodologies used, and the results and recommendations. Included are a sketch of the design, and its details.

## **2.0 ASSUMPTIONS AND LIMITS (Used in the calculations)**

### **2.1 Catalyst**

#### **2.1.1 Recommendations by Johnson Matthey (J M)**

Catalyst formulation and required area were discussed with several people at J M. The required area to dissociate a pound of methanol per hour varied from 0.165 to 0.98 square feet. The catalyst material for these values is copper oxide and zinc oxide.

Catalysts containing copper were not recommended due to poor high temperature resistance. J M recommended catalysts using platinum, chromium, or palladium. Yields equal to or greater than the reported values were predicted by J M.

#### **2.1.2 Catalyst Material (Dissociation Side)**

No specific catalyst material was used in the calculations. Plots of reactor length versus catalyst area were made to finalize the reactor size once a value of yield was selected.

#### **2.1.3 Catalyst Material (Exhaust Side)**

None was assumed. However, addition of an oxidizing catalyst on the exhaust side would increase the total heat flux to the methanol side and improve the heat exchanger effectiveness.

#### **2.1.4 Heat Exchanger Surface Area Required for Catalyst**

This is considered as an independent variable in the reactor design and is discussed in the analysis section.

#### **2.1.5 Maximum Allowable Catalyst Temperature**

No means are provided to protect the catalyst from the maximum exhaust temperature.

#### **2.1.6 Minimum Catalyst Temperature to Achieve Significant Yields**

These are summarized in Table 3.

## 2.2 Reactor

### 2.2.1 Coefficients of Thermal Conductivity

17-7-PH Stainless steel = 22.0 BTU/(hr)(ft<sup>2</sup>)(°F/ft)

### 2.2.2 Specific Heats (BTU/lbm - °R)

Air = 0.24

Exhaust = 0.27

Methanol (vapor) = 0.41

### 2.2.3 Heat of Vaporization of Methanol

500 BTU/lbm

### 2.2.4 Heat of Dissociation of Methanol

1500 BTU/lbm

### 2.2.5 Structural Descriptions of 17-7-PH Stainless Steel

Ultimate Strength - 87 ksi

Yield Strength - 39 ksi

Endurance Limit - 31 ksi

### 2.2.6 Minimum Fin Spacing

The fins on both the exhaust and methanol sides can be no closer together than 0.05 inches (20 fins per inch) to assure that the wash coat follows the fin contours and does not bridge them.

### 2.2.7 Pressure Drop

The maximum allowable pressure drop on the exhaust side of the reactor and evaporator is 2.5 psig.

### 2.2.8 Methanol and Exhaust Flowrate Limits (lbm/hr - cylinder)

Extrapolated from EPA NAPS-Z Engine Data

<u>Engine Condition</u>	<u>Methanol</u>	<u>Exhaust</u>
Idle (500 rpm, $\Phi = 0.7$ )	0.7	8.0
Full Power (6000 rpm & 100% load, $\Phi = 0.93$ )	24.5	190.0

## 3.0 ANALYSIS

### 3.1 Required Reactor Pressures and Volume

- (1) Minimum Desirable Valve Size - The minimum preferable size for the gas inlet valve should be such that its mach index number does not

exceed 0.6. Using the following relationship (Reference 1) this valve size was determined:

$$z = \frac{A_p \times S}{A_i \times C_i \times a}$$

where:

z =	Valve mach index number = 0.6 maximum desirable
Ap =	Piston area = 8.8 in <sup>2</sup> (NAPS-Z engine)
Ai =	Inlet valve area, which calculates to 0.44 in <sup>2</sup>
S =	Mean piston speed = 1553 ft/min for NAPS-Z engine at 5500 rpm
a =	Sonic velocity of inlet gas = 1318 ft/sec under expected inlet conditions
Ci =	Mean valve flow coefficient = 0.65 typically for a well-designed poppet valve with its lift equivalent to 25% of its diameter

The Ai = 0.44 in<sup>2</sup> yields a minimum desirable valve diameter of 0.75 inches.

- (2) Maximum Allowable Valve Size - The NAPS-Z engine existing spark plug holes are approximately 0.5 inches in diameter. The sectioned engine head reveals that one of the spark plug holes in each cylinder could be enlarged to 0.625 inch in diameter without compromising the structural integrity of the head.
- (3) Critical Flow Through the Maximum Allowable Valve Size - The 0.625-inch diameter valve is smaller than the 0.75 inch minimum desirable size. It will yield a higher mach index at maximum inlet gas flowrates. The calculated mach indexes at 100% engine load are:

Engine Speed (rpm)	Mach Index
5500	0.85
4500	0.70

- (4) Valve Timing - The opening and closing locations of the methanol inlet valve are limited by the following engine parameter values as a function of crank angle:
  - Maximum spark advance
  - Induction air intake valve closing
  - Cylinder compression pressure

The maximum spark advanced shown in the Reference 3 test data was 45° BTDC. The point of induction air inlet valve closing was not documented but is assumed at a common value of 45° ABDC. The cylinder compression of induction air was assumed to be isentropic and raises the cylinder pressure to 72 psia with the crank at 45° BTDC. Given these constraints the valve opening was made at 45° ABDC and its closing at or before 45° BTDC. This allowed 90° of crank angle for the introduction of dissociated products into the cylinder. The corresponding time at this crank angle for several engine speeds is summarized below:

Engine Speed (rpm)	Maximum Valve Opening Time (ms)	Effective* Valve Opening Time (ms)
500	30.0	15.0
1500	10.0	5.0
4500	3.3	1.7
6000	2.5	1.3

\* 50% of maximum to account for reduced valve area during opening and closing.

#### (5) Required Reactor Pressures to Provide Adequate Product Flowrates

The reactor pressure must be maintained between 100 to 150 psig so that the required product mass can be delivered to the cylinder during the brief valve opening time. Flowrates were calculated using (Reference 1):

$$\dot{m} = A_2 \times a_{01} \times \rho_{01} \times \Phi_1$$

where:  $\dot{m}$  = Mass flowrate of product  
 $A_2$  = Valve port nominal area  
 $a_{01}$  = Sonic velocity at valve opening  
 $\rho_{01}$  = Density of dissociated products in reactor  
 $\Phi_1$  = Compressible flow function based on empirical data (Reference 1)

A summary of product flows per cylinder per cycle at 100 and 150 psig reactor pressures compared to the required amount of product to maintain 100% power is summarized as follows:

Engine Speed (rpm)	Amount of Products Entering per Cylinder (lbs x 10 <sup>-3</sup> )		Amount of Products Required per Cylinder (lbs x 10 <sup>-3</sup> )
	150 psig	100 psig	
500	4.3	2.6	---
1500	1.5	0.9	0.14
4500	0.5	0.3	0.14
6000	0.4	0.2	0.14

Mass flowrates in each case are below calculated critical values.

#### (6) Minimum Reactor Volume to Maintain Required Pressures

Assuming the isothermal expansion (worst case) of the reactor gases through the opened valve, a minimum of 6 inches<sup>3</sup> reactor plus evaporator volume is required to maintain 100 psig minimum pressure when the starting pressure is 150 psig and maximum product delivery is required.

### 3.2 Heat Balance

In the proposed reactor system liquid methanol is injected into an evaporator, where it vaporizes. The saturated methanol vapor is then superheated in the evaporator and enters the reactor where it dissociates into CO and H<sub>2</sub>. The exhaust gas from the engine provides the heat for all requirements: vaporization, superheat, and dissociation. The exhaust gas flows counter to the direction of

methanol flow, so heat is first transferred from the exhaust gas to the dissociation process and last to the vaporization process.

A primary question is what percentage of the total engine fuel flow can be processed in the manner described above, given the quantity and quality of the heat available in the exhaust. This discussion will concentrate on the engine operating conditions of 4500 rpm, 100% load and 500 rpm, 30% load.

Parameters of importance in the analysis were:

Heat of vaporization of methanol	500 BTU/lb
Heat of dissociation of methanol	1500 BTU/lb
Specific heat of liquid methanol	0.58 BTU/lb-°F
Specific heat of vaporized methanol	0.44 BTU/lb-°F
Exhaust flow rate at 4500 rpm; 100% load	132 lb/hr-cyl
Fuel flow rate at 4500 rpm; 100% load	20.5 lb/hr-cyl
Exhaust flow rate at 1500 rpm; 30% load	24 lb/hr-cyl
Fuel flow rate at 1500 rpm; 30% load	2.6 lb/hr-cyl
Minimum temperature for the dissociation reaction	400°F

The exhaust temperatures measured by EPA at 4500 rpm, full load, and 1500 rpm, 30% load were 1300°F and 851°F respectively. Our calculations show that, by insulating the exhaust port, these temperatures can be raised to 1400°F and 911°F, respectively. In our analysis, we considered the effect of the standard port (as used by the EPA) and an insulated port (giving the higher exhaust temperatures). Insulation would be accomplished, for instance, by a ceramic port insert.

In the proposed system, the pressure within the evaporator and reactor is uniform, and this pressure is defined solely by the temperature of the evaporator, since in the evaporator the methanol liquid and vapor exist in equilibrium. A few equilibrium states are:

<u>Pressure (psia)</u>	<u>Temperature (°F)</u>
150	289
100	259
29	180
14.7	149

Thus, if the evaporator temperature can be maintained at 289°F, the fuel pressure to the engine will be 150 psia. Since it is necessary to inject the fuel gases during the compression stroke, and since significant fuel pressure is required to do this in the time available, a high evaporator temperature (producing a high fuel pressure) is a necessity. A heat balance can determine the temperature of the evaporator, and hence the pressure, at least approximately. A first approximation can be readily obtained by assuming an infinite heat exchanger area, so that the complexities of varying heat transfer coefficients and fin efficiencies can be ignored. A more accurate approximation takes into account these factors. Both approximations will be made in this summary.

The quantity of heat required for processing the methanol was calculated and the effect upon the exhaust gas temperature was determined. For different temperature differences between methanol and exhaust gas, the maximum flow

rate of methanol was calculated. Figure 1 shows the percent of the total fuel flow needed to run the engine at 4500 rpm, fuel load that results in complete vaporization and dissociation by the available exhaust heat. Two cases are shown. The first is for an insulated exhaust port and an infinite heat exchanger where the exhaust gas temperature is equal to the liquid methanol temperature at the entrance to the vaporizer. The second is for a 100°F difference between the exhaust gas and the liquid methanol at the vaporizer entrance, which implies a small heat exchanger. A standard exhaust port is used. Thus, the upper curve shows the maximum amount of methanol that can be dissociated, and the lower curve provides a conservative estimate.

Figure 2 shows similar results for the engine condition of 1500 rpm, 30% load, and  $\eta = 0.7$ .

In either case, running the fuel pressure at 165 psia (as opposed to a lower pressure) has a relatively small penalty on the amount of fuel that can be processed through the reactor and evaporator. Note that increasing the fuel throughput decreases the fuel pressure, but even when the pressure is reduced to very low values, the fuel throughput has not reached 100%. This is because there is insufficient heat in the exhaust for dissociation and vaporization of 100% of the methanol even at reduced temperatures corresponding to low pressures.

Insulating the exhaust port will permit raising the fuel throughput by about 7% at 1500 rpm, 30% load, and by about 8% at 4500 rpm, fuel load, for the same evaporator design.

### **3.3 Heat Exchanger Design For Heat Transfer (Step 1)**

#### **3.3.1 Reactor**

- (1) Reactor Design - The reactor was designed to use all available exhaust heat from the engine down to 432°F (432°F exhaust gas temperature was calculated to yield a 400°F wall temperature). This temperature was chosen as the lowest point that significant yields of dissociated methanol could be produced from the best catalysts. The cross-sectional geometry was chosen based on a trade-off of outside diameter (limited by engine cylinder-to-cylinder spacing), number of annuli (a low number desired to reduce manifold complexity), available metal catalyst substitute material (from Behr) that can be coated (maximum of 20 fins per inch according to Johnson-Matthey).
- (2) Reactor Heat Transfer - The length of the reactor was determined from the chosen cross-sectional geometry and the calculated required heat transfer area necessary to cool the exhaust gases to 432°F. The maximum mass flow rate condition was determined to be the limiting case for heat transfer area. The NTU effectiveness method, as outlined in Reference 2, was used to perform the heat transfer calculations. The Reynolds number was calculated

from the cross-sectional geometry and exhaust mass flow rate. The heat transfer parameter and friction factor were selected from plots for each configuration as a function of Reynolds number. Fin effectiveness was calculated from the fin geometry. Heat exchanger exhaust side effectiveness was chosen and along with the fluid outlet temperature differences used to calculate the temperature change in the exhaust gas. This temperature difference and the capacity rate ratio were used to calculate the NTU. The NTU was then used to determine the required heat transfer area and, for a given cross-sectional geometry, the reactor length.

- (3) Pressure Drop - Pressure drop through the reactor exhaust side was calculated for each configuration using the formulas in Reference 2.
- (4) Summary of Reactor Designs - Figure 3 and Table 1 summarizes the various reactor geometries and their properties.

### **3.3.2 Evaporator**

- (1) Evaporator Design - The analysis of the evaporator was similar to that of the reactor in that it considered the temperature of the exhaust leaving the reactor and the minimum temperature (267°F exhaust temperature was calculated to yield 259°F wall temperature) at which methanol would vaporize under an elevated reactor pressure (150 psig).
- (2) Evaporator Heat Transfer - The same procedures discussed for the reactor were used to calculate the evaporator required heat transfer area.
- (3) Evaporator Pressure Drop - The pressure drop on the exhaust side was calculated using the same methods as that used for the reactor.
- (4) Summary of Evaporator Designs - Figure 3 and Table 2 summarize the various evaporator configurations and their properties.

## **3.4 Heat Exchanger Heat Transfer Optimization (Step 2)**

Design of the reactor/evaporator using the 432°F exhaust outlet temperature from the reactor resulted in a reactor that could dissociate more methanol than the evaporator could vaporize (on a heat transfer basis). To correct this a balanced design was sought by setting the yields of the evaporator and reactor equal. The parameters of one reactor configuration and one

evaporator configuration are summarized below:

<u>Component</u>		<u>Product Yield (lbm/hr)</u>	<u>Catalyst Area (ft<sup>2</sup>)</u>	<u>O.D. (in)</u>	<u>Length (in)</u>	<u>Δ P (psig)</u>	<u>Effectiveness</u>
Reactor	#6	17.9	2.57	4.0	1.8	0.15	0.85
Evaporator	#4	17.9		4.0	4.8	0.37	0.97

These values are based on a reactor inlet temperature of 1400°F, a reactor outlet and evaporator inlet temperature of 550°F and an evaporator outlet temperature of 267°F. The 1400°F exhaust temperature would be possible by insulating the exhaust port as discussed in paragraph 3.1.

### 3.5 Heat Exchanger Design for Catalyst Area (Step 3)

- (1) Catalyst Area - The available catalyst area for each reactor configuration was calculated based on the heat exchanger area and compared to the area requirements of Johnson Matthey. With all reactor designs, the required catalyst area (per Johnson Matthey) is greater than the required heat transfer area. The length of any design, therefore, must be increased to achieve the necessary catalyst area. This is shown on Figure 4 which plots % dissociation versus reactor length for both Johnson Matthey and Wei and Chen yield data. If a more appropriate catalyst surface yield value than that recommended by Johnson Matthey or that demonstrated by Wei and Chen is deemed appropriate, then the required reactor length can be determined.
- (2) Discussion of Catalysts and Surface Yields - A summary of catalyst properties is shown in Table 3. A review of the literature suggests that higher surface yields than those achieved by Johnson Matthey are possible (Wei and Chen data). If so, the length of the reactor could be reduced as discussed previously. In any case, however, the reactor would probably contain greater surface area than that required for heat transfer.
- (3) Effect of Catalyst Area Requirements on Pressure Drop - Increasing the reactor length to provide adequate catalyst area will result in an increase in pressure drop. This is shown in Figure 5, which plots catalyst surface area versus pressure drop for the various reactor configurations. The point representing the minimum heat transfer area is shown for each configuration.

### 3.6 Fabrication and Assembly Details

- (1) Separate reactor and evaporators are used for several reasons:
  - Design of the reactor and evaporator can be optimized independently. This is particularly important for the evaporator where the uniformity of spray impingement

necessitates a different configuration for the methanol side from that used on the reactor.

- Vaporization and dissociation function separation will minimize the possibility of reactor flooding.
  - Reactor and evaporator performance can be independently measured as can the state of the fluid in each during testing.
- (2) The reactor tubes and other structural parts are made of 0.030 inch or thicker material and the fins of 0.004 inch thick material. Type 17-7 PH stainless steel or an equivalent will be used for this application. This material and these tubing thicknesses will yield maximum tubing stresses of less than 15 ksi. This type of stainless steel permits welding, maintains high strength at high temperatures and contains aluminum which will provide better adherence of the alumina-based wash coat. Pieces will be furnace brazed with a high temperature brazing filler metal such as BNiCr and/or TIG welded.
- (3) Figure 3a shows the reactor and evaporator mounted in-line in one section of exhaust pipe. It may be necessary to mount the reactor above the evaporator and connect them with a "U" section of pipe to reduce the overall length of the assembly. Such an arrangement would not change the basic design or the operating characteristics of the system shown in the figure.

### 3.7 Transient Conditions

Changes in engine fuel requirements will necessitate a change in the flow rate of dissociated products into the engine. Under steady-state conditions dissociated product generation and mass flowrates will be a function of exhaust temperatures and mass flowrates. Because the reactor cannot supply 100% of the engine needs, direct methanol injection into the intake manifold will be used during steady-state conditions to supplement the reactor output. Mass flow rates of direct methanol injection will be a function of reactor output under these conditions. Under conditions where increased power is required, direct methanol injection will have to make up the difference in fuel demand during the period of the transient and until the reactor/evaporator reaches steady-state production. Lag in the output of the reactor is a function of the total internal volume and the mass and thermal conductivity of the heat transfer surfaces, and will need to be determined experimentally. Under transient conditions, the fuel control system using inputs from the engine, throttle position and reactor temperatures and pressure will be designed to meet engine fuel needs by correctly proportioning fuel delivery to both the intake manifold and the evaporator.

## 4.0 RECOMMENDATIONS

The final size of the reactor is determined by the catalyst yield predictions. SwRI has the most confidence in the yield data provided by J-M which was derived from a coated tube configuration. The combination of the reactor configuration number 6 and evaporator number 4, appears to be a reasonable design. This configuration, sized according to the catalyst activity of the J-M tube data,

results in a reactor length of 13.6 inches and an evaporator length of 4.8 inches. The total pressure drop would be 1.5 psid.

J M would provide an alumina washcoat to both sides of the reactor. The catalyst on each side would be dependent upon the final recommendation of J M or EPA.

This design provides a factor of safety of 7.6 for the heat transfer into the reactor. No safety factors exist for the catalyst yield predictions and the evaporator design. These safety factors could be provided at the expense of a higher pressure drop in the exhaust system.

## REFERENCES

1. Taylor, C.F., "Internal Combustion Engine in Theory and Practice," Volumes 1 and 2, 1980.
2. Kays, W.M., and A. L. London, "Compact Heat Exchangers," 2nd Edition.
3. EPA test data on 380 NAPS-ZMD engine - test numbers HD812481 and HD812489

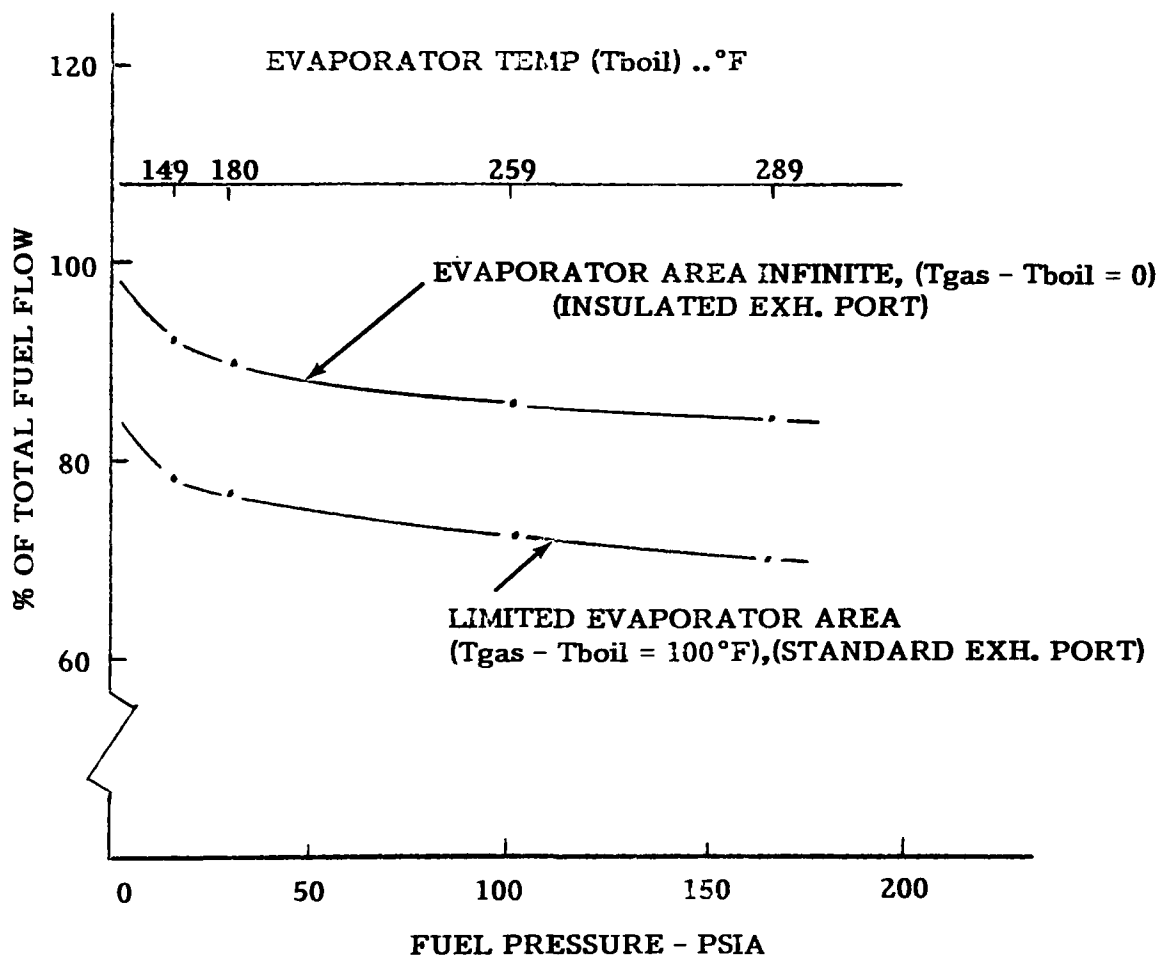


FIGURE 1 - FUEL THROUGHPUT AT 4500 RPM,  
FULL LOAD,  $\phi = 1.0$

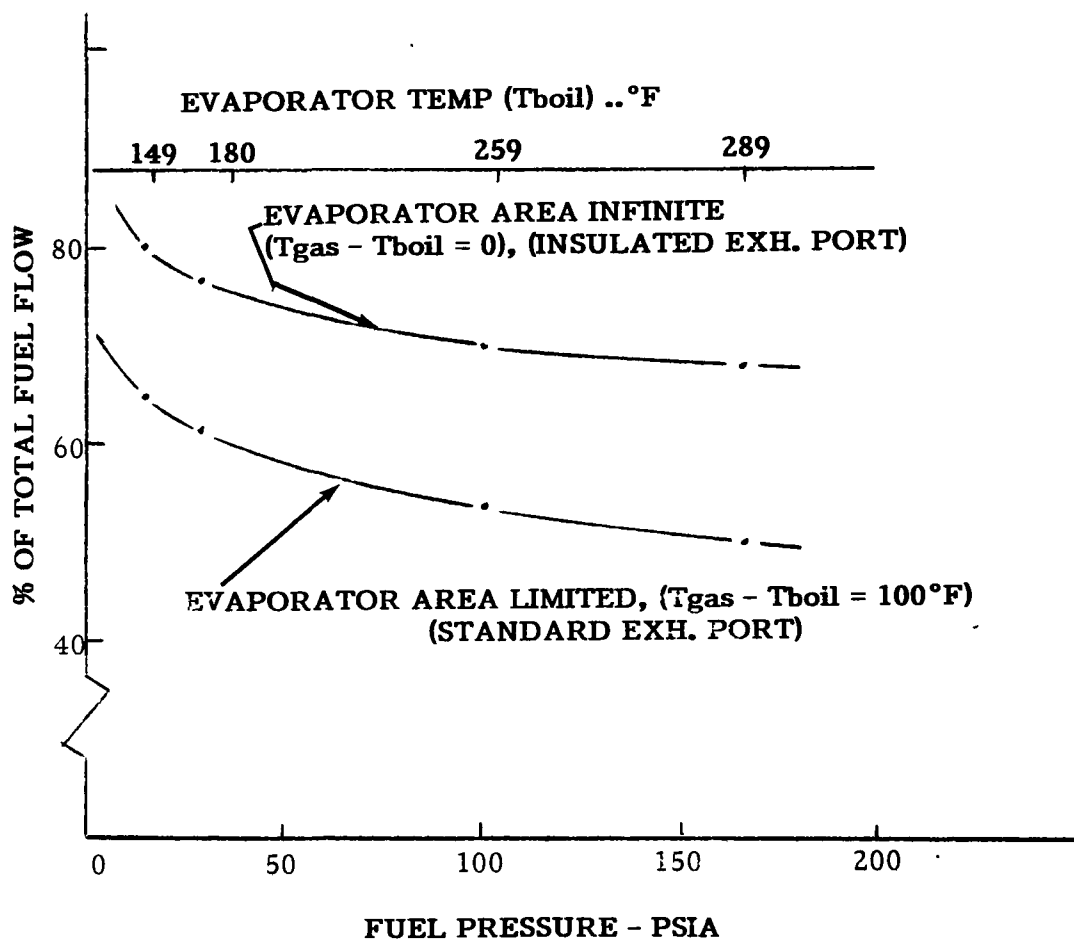
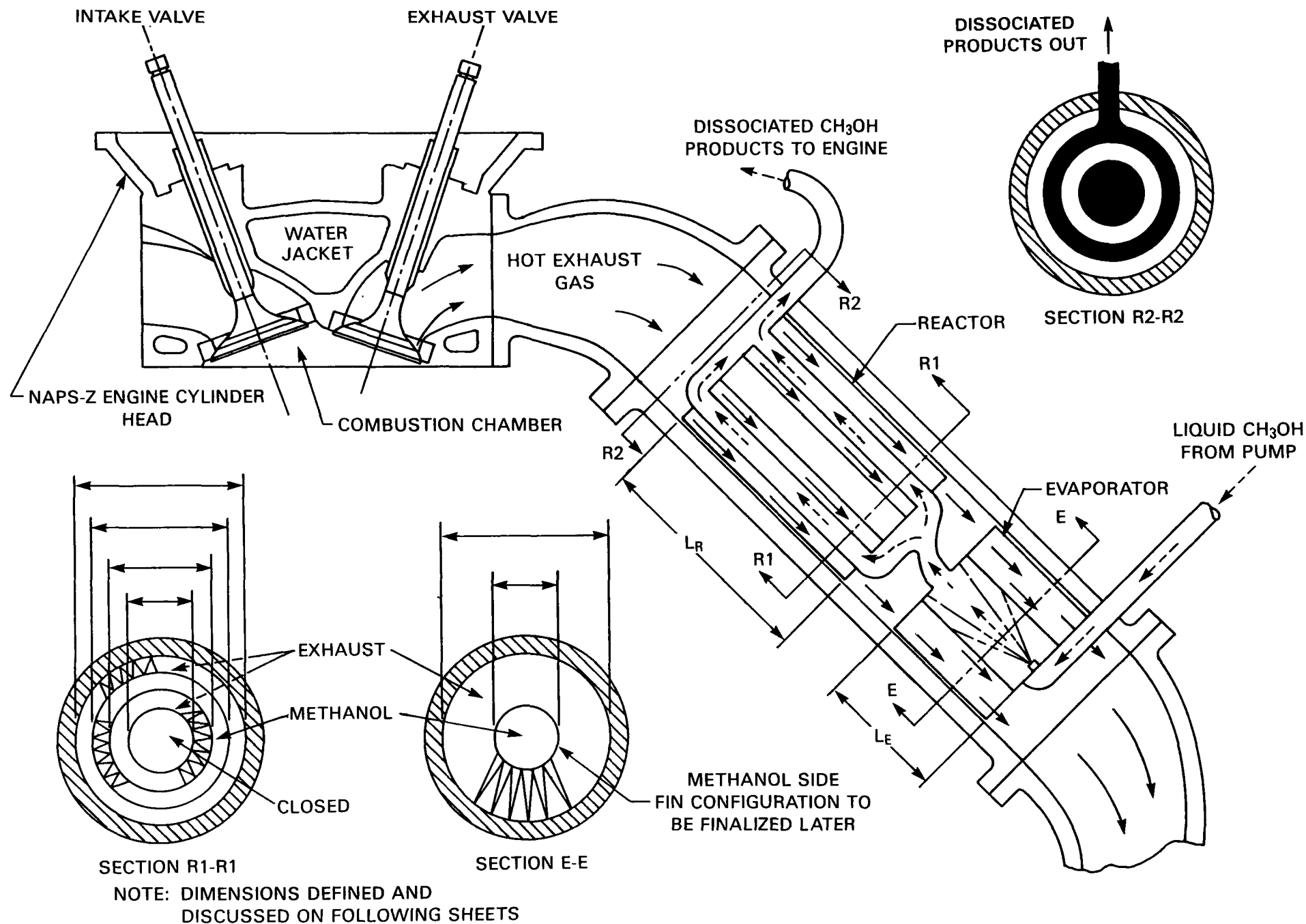


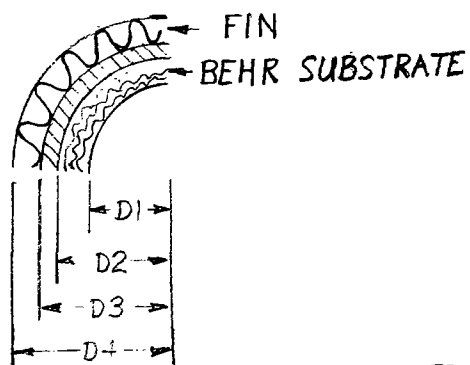
FIGURE 2 - FUEL THROUGHPUT AT 1500 RPM,  
30% LOAD,  $\phi = 0.7$



**FIGURE 3A - REACTOR ASSEMBLY FOR EVAPORIZATION AND DISSOCIATION OF METHANOL**

Configuration	Type	Diameters (inches)										Fin Description
		D <sub>1</sub>	D <sub>2</sub>	D <sub>3</sub>	D <sub>4</sub>	D <sub>5</sub>	D <sub>6</sub>	D <sub>7</sub>	D <sub>8</sub>	D <sub>9</sub>	D <sub>10</sub>	
1	A	1.000	1.100	1.140	1.336	--	--	--	--	--	--	Strip fin Figure 10-56 Kayes and London, 3rd Edition, .098" height, 20 per inch, 0.125 inch length in direction of flow
2	B	0.800	0.996	1.036	1.436	1.476	1.672	--	--	--	--	
3	B	0.800	0.996	1.036	1.436	1.476	1.672	1.712	2.112	2.152	2.348	
4	B	0.800	1.300	1.340	1.740	1.780	2.280	--	--	--	--	11 plain fin/inch: Figure 10-26 Kayes and London, 2nd Edition
5	A	3.544	3.744	3.804	4.000	--	--	--	--	--	--	Figure 10-56 Kayes and London, 3rd Edition
6	B	3.088	3.283	3.344	3.744	3.804	4.000	--	--	--	--	Figure 10-56, Kayes and London, 3rd Edition
7	B	2.372	2.568	2.628	3.028	3.088	3.284	3.344	3.744	3.804	4.000	Figure 10-56, Kayes and London, 3rd Edition

Type A	
Dimension	Description
D <sub>1</sub>	Inner closed cylinder
D <sub>2</sub>	Reaction side annulus
D <sub>3</sub>	Wall
D <sub>4</sub>	Fin - exhaust annulus



Type B	
Dimension	Description
D <sub>1</sub>	Inner closed cylinder
D <sub>2</sub>	Fin
D <sub>3</sub>	Wall
D <sub>4</sub>	Reaction side annulus
D <sub>5</sub>	Wall
D <sub>6</sub>	Fin
D <sub>7</sub>	Wall
D <sub>8</sub>	Reaction side annulus
D <sub>9</sub>	Wall
D <sub>10</sub>	Fin

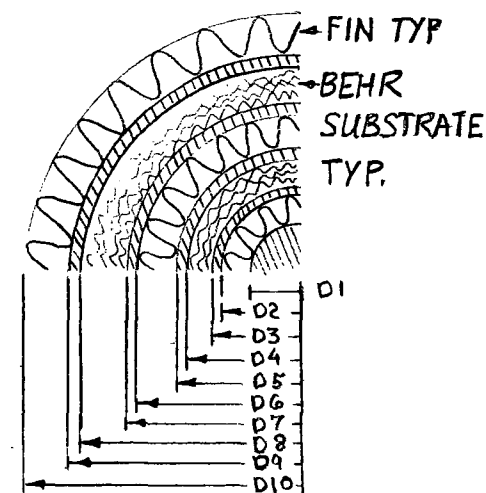


FIGURE 3B. CROSSECTIONAL GEOMETRIC DATA OF REACTOR CONFIGURATIONS

<u>Configuration</u>	<u>Type</u>	<u>D<sub>1</sub></u>	<u>D<sub>2</sub></u>	<u>D<sub>3</sub></u>	<u>Fin Description</u>
1	A	2.064	2.1040	2.300	Figure 10-56 Kayes and London, 3rd Edition
2	A	1.858	1.898	2.300	Figure 10-60 Kayes and London, 2nd Edition
3	A	3.744	3.804	4.000	Figure 10-56 Kayes and London, 3rd Edition
4	A	3.538	3.598	4.000	Figure 10-60 Kayes and London 2nd Edition

<u>Dimension</u>	<u>Description</u>
D <sub>1</sub>	Inside diameter of evaporation chamber
D <sub>2</sub>	Wall
D <sub>3</sub>	Fin

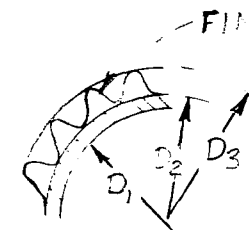


FIGURE 3C. CROSSECTIONAL GEOMETRIC DATA OF EVAPORATION CONFIGURATION

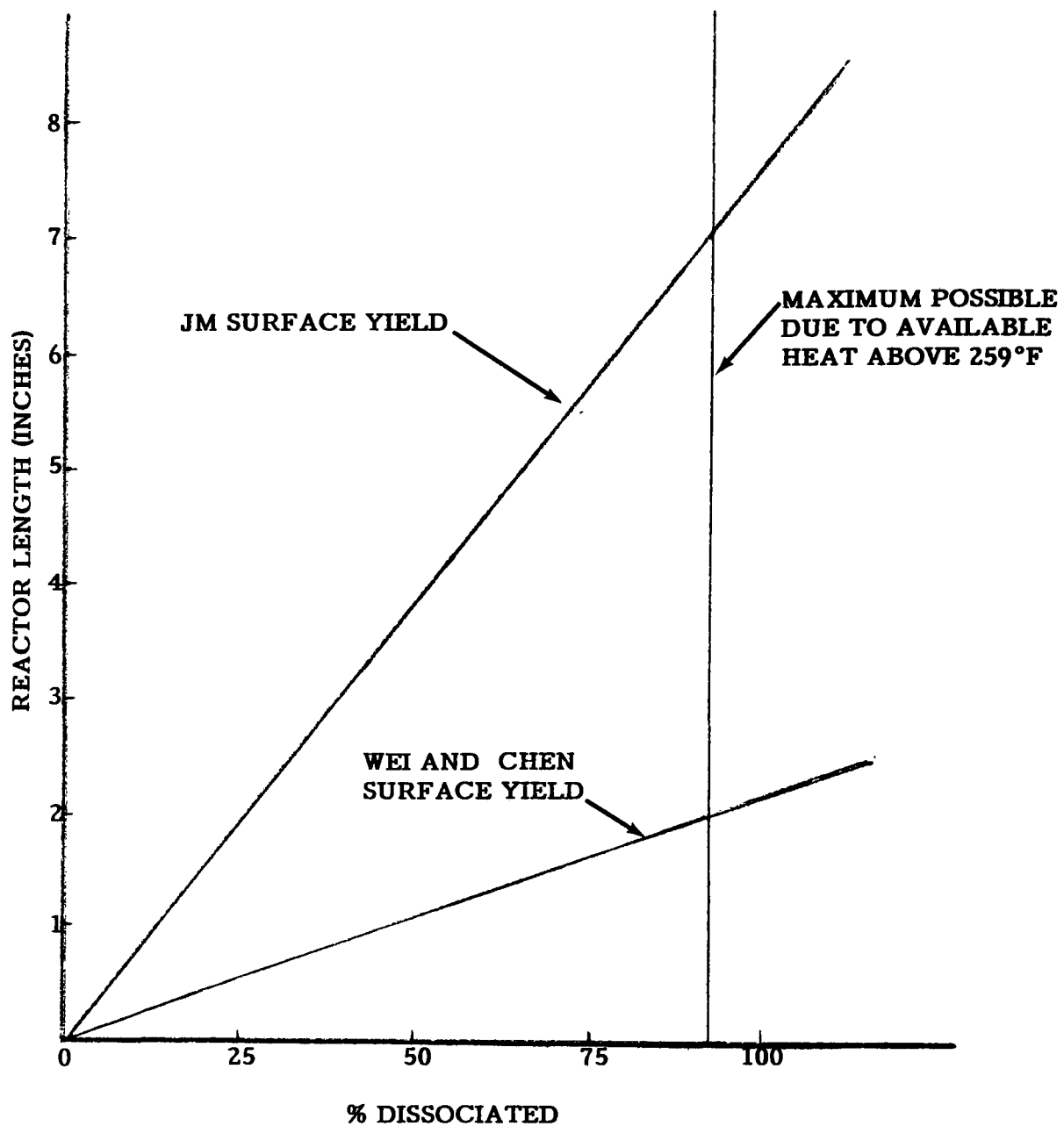


FIGURE 4 - REACTOR LENGTH (4 IN. DIA.) vs % DISSOCIATION

AT 4500 RPM,  $\Phi$  = % LOAD  
 $T_{exh}$  = 1400°F

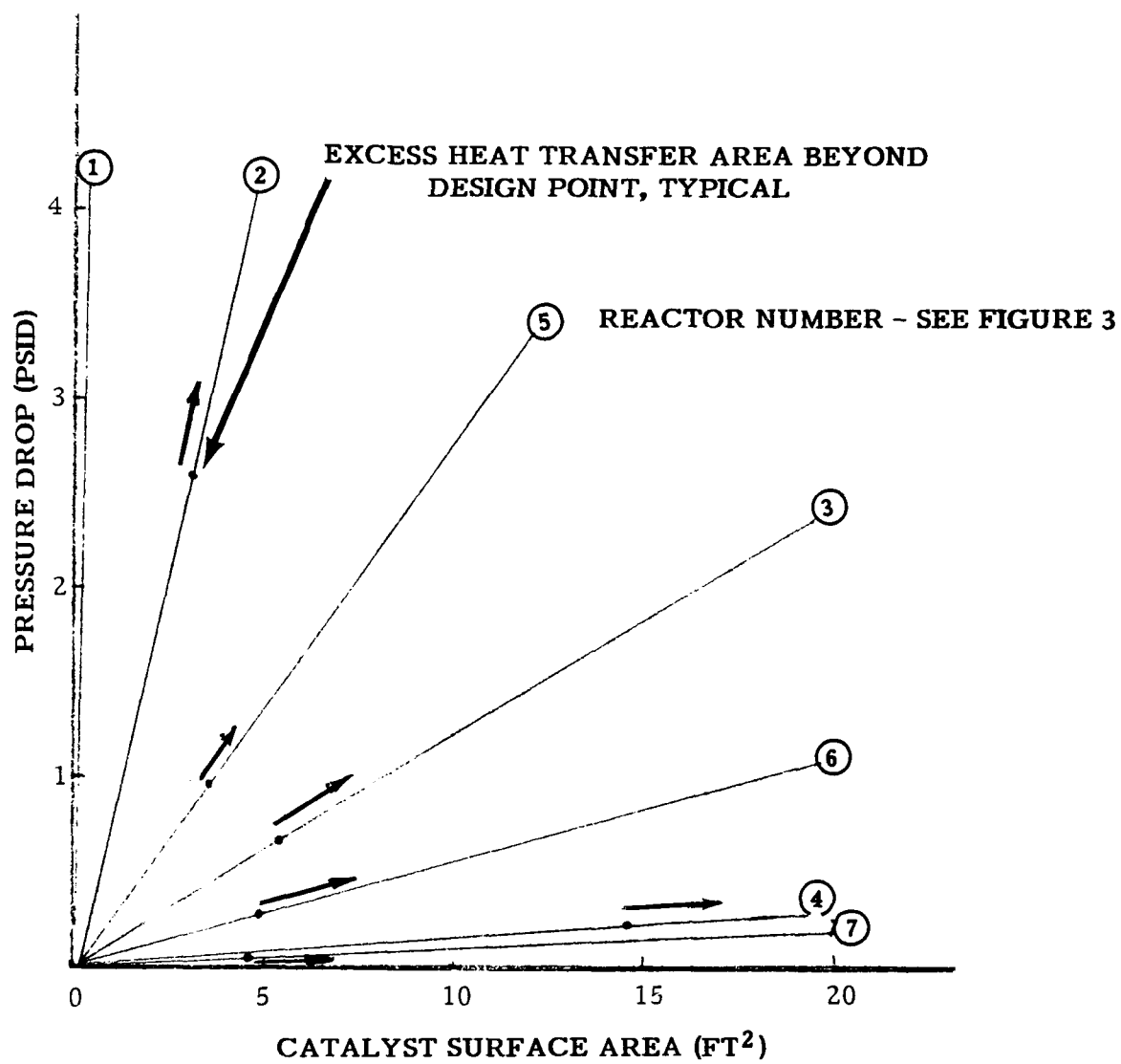


FIGURE 5. PRESSURE DROP VS. CATALYST SURFACT AREA

Table 1. Reactor Configurations

<u>Configuration</u>	<u>Exhaust Annuli</u>	<u>Reaction Annuli</u>	<u>Length (in)</u>	<u>Outer Diameter (in)</u>	<u>Pressure Loss (psid)</u>	<u>Volume Catalyst (in<sup>3</sup>)</u>	<u>Catalyst Area (ft<sup>2</sup>)</u>
1	1	1	8.90	1.336	14.9	0.716	0.45
2	2	1	6.09	1.672	2.6	4.70	3.0
3	3	2	4.262	2.348	0.632	8.43	5.35
4	2	1	23.70	2.28	0.220	22.9	14.5
5	1	1	5.442	4.000	0.950	5.44	3.45
6	2	1	3.36	4.000	0.277	7.48	4.79
7	3	2	1.68	4.000	0.040	6.75	4.28

Table 2. Evaporator Configurations

<u>Configuration</u>	<u>Exhaust Annuli</u>	<u>Evaporation Annuli</u>	<u>Length (in)</u>	<u>Outer Diameter (in)</u>	<u>Pressure Loss (psid)</u>
1	1	1	3.810	2.300	2.93
2	1	1	6.200	2.300	1.15
3	1	1	4.078	4.000	0.816
4	1	1	4.085	4.000	0.316

Table 3 - Summary of Catalyst Properties

Catalyst	T (°F)	Surface Yield lb/hr-ft <sup>2</sup>	Surface Area Required to Produce 19.1 lb/hr CO + 2H	Comments
JM CuO ZnO pellets	698	0.165	116	<ul style="list-style-type: none"> <li>o Laboratory pellet data is similar in yield rates</li> <li>o Space velocities ( 1/hr) are lower than what has been used in automotive reactors</li> </ul>
JM 1/4" tube coated with CuO ZnO	698	0.98	19.5	Based on an <b>actual coated tube, which we can duplicate</b> . JM suggest that it may have been heat limited, implying that higher yields may be possible by improving the heat flux. Higher temp. resistance of Cu is poor, other catalyst materials (Pt, Cr <sub>2</sub> O <sub>3</sub> , Pd) can be used with similar or improved yields.
Co Sch of Mines Pd/La pellets	572	0.15	119	Higher temp. resistance of Cu is poor, other catalyst materials (Pt, Cr <sub>2</sub> O <sub>3</sub> , Pd) can be used with similar or improved yields.
Conoco	560			Awaiting report from EPA
Wei and Chen Methane formation from CO + H <sub>2</sub> Raney Nickel	*	4.2	4.5	An example of possible rates for the decomposition reaction if the heat and mass transfer limits are higher than those obtained by pellet-filled tubes
Mass diffusion of CO into methanol limit on rate		.16	119	Similarity between mass diffusion rate and pellet data rates in which the velocities were low suggest that diffusion may be limiting

**Addendum to Appendix D**

**Letter to EPA Containing Follow-up  
Discussions and Clarifications/Revisions  
to Heat Exchanger Design Analysis**

# SOUTHWEST RESEARCH INSTITUTE

POST OFFICE DRAWER 28510 • 6220 CULEBRA ROAD • SAN ANTONIO, TEXAS, USA 78284

ENGINES, EMISSIONS AND VEHICLE RESEARCH DIVISION

June 25, 1985

Mr. Carl Hellman  
United States Environmental Protection Agency  
Motor Vehicle Testing Laboratory  
2565 Plymouth Road - ECTD  
Ann Arbor, MI 48103

**Subject: Follow-up Information on Monthly Progress Report No. 8, Dated May 31, 1985**

Dear Mr. Hellman:

The following paragraphs contain our responses to the questions you raised during our June 17 telephone call. Where applicable, page numbers refer to the sequential order of pages in the technical discussion attached to our Monthly Progress Report No. 8 (MPR #8).

## Parameter Values on Page 5

The values for fuel and exhaust mass flowrates used in paragraph 3.2 were those assigned originally to this analysis. The values used in the final calculations (as summarized in MPR #8) are shown below along with the appropriate values from the EPA test results (Test No. HD-812489) on the NAPS-Z engine.

<u>Engine Condition</u>	<u>Mass Flow Rate Parameter</u>	<u>SwRI Value Used (lbm/hr-cyl)</u>	<u>EPA Test Data (lbm/hr-cyl)</u>	<u>% Difference</u>
4500 rpm, 100% load	Fuel	17.8	17.7	0.6
4500 rpm, 100% load	Exhaust	142.8	141.3	1.1
1500 rpm, 30% load	Fuel	2.6	2.6	0.0
1500 rpm, 30% load	Exhaust	25.8	26.7	3.4

Most of the differences in values used versus the values from the EPA data are small enough not to appreciably affect the results of the heat balance analysis.

## Values of Dissociated Products Mass Flow Versus Choking Flow on Page 4

Table 1 summarizes the values of maximum possible product flow into the cylinder and required product flow for 100% cylinder requirements. The table includes values of maximum possible product flow per cylinder for reactor pressures at 100 and 150 psig and product temperatures at 400°F and 1200°F. These temperature values represent the boundaries for the product as it is discharged into the cylinder. The number after the virgule in each case represents the choking flow at that condition. The maximum possible amount of product injection is the lower of the two values. This is because further decreases in downstream pressure (cylinder pressure) such as that which occurs at product

valve start to open (14.2 psia) and full valve open positions (23.9 psia), will not cause an increase (or decrease) in the choking flow rate.

The phenomenon of choking flow and the values of mass flow rates at a mach number of 1 is discussed in some thermodynamic texts. The particular one used was written by G. J. Van Wylen, entitled "Thermodynamics" and was published in 1963 by John Wiley and Sons.

Also, the equation for calculating mass flow rate, given the proposed valve size, is not sensitive to the value of absolute pressure.

It can be concluded, by looking at Table 1, that the maximum possible product flow in most cases is at or near choking flow. (It is this at both reactor pressures because of the large pressure differential.) This poses no problem, however, because the required amount of products for 100% fuel needs is well below these maximum possible values as shown in the far right column. In addition, the section on heat balance (MPR #8), calculates that there is not sufficient exhaust heat to vaporize and dissociate 100% of the engine fuel needs, so somewhat less that the required amount of fuel will be injected each cycle (not considering the increased heat of combustion of the dissociated products relative to liquid methanol). Even if the dissociated product valve duration is reduced to 73° from 90° Crank angle (19% reduction in duration), the maximum possible amount of product flow will still exceed the amount required.

### **Sensitivity of the Heat of Dissociation to Pressure**

The heat of dissociation is independent of pressure for an ideal gas and nearly so for other reactions. Pages 70 and 77 in "Thermodynamics for Chemists," by Samuel Glasstone, D. Van Nostrand Company, discusses this. The actual value of the heat of dissociation and, for that matter, the heat of vaporization vary depending on the reference, but tend to cluster about certain values as shown in Table 2.

## Connector Between Reactor Housing and Cylinder Head

This can be reduced to virtually zero length which will shorten the overall size of the heat exchanger and reduce heat losses. We will look at exhaust gas distribution as it exits the port to assure that the transition to the reactor provides uniform flow through the annulus. Insulation can also be applied to the outside of the connector (if a connector is required) and the heat exchanger housing to minimize heat loss.

## Value for Thermal Conductivity

The value for thermal conductivity used in the calculations in MPR #8 was 22 Btu/(hr)(ft<sup>2</sup>)(°F/ft). Discussions with Professor Webb indicate that this was in error and a value of 8 to 10 Btu/(hr)(ft<sup>2</sup>)(°F/ft) would be more appropriate. This change has no effect on the final reactor design because the catalyst area requirements exceed those for heat transfer. The evaporator lengths shown on Table 2 of MPR #8 will be increased by about 31% to the values below:

Configuration	New Length (in.)
1	5.0
2	8.1
3	5.3
4	5.4

We will, however, investigate other materials for the evaporator that may have higher coefficients of thermal conductivity. There is no need for material compatibility between the evaporator and reactor. In addition, the evaporator is exposed to lower exhaust temperatures and does not need to have a surface compatible with the catalyst washcoat. An evaporator material with a higher thermal conductivity will reduce the overall size of the heat exchanger.

## Evaporator Flooding

During our June 10 telephone conversation you mentioned your concern over reactor flooding with the inclination of the reactor and evaporator as shown on Figure 3A in MPR #8. We had considered this possibility in configuring the reactor/evaporator as shown. We theorized that the lower evaporator would prevent liquid fuel from entering the reactor and, if insufficient vaporization did occur then vapors would not be passed into the reactor which would mean that the exhaust gas temperatures would not decrease appreciably as it passed through the reactor. These higher temperatures would then be available to vaporize the liquid methanol in the evaporator. This does not mean that liquid methanol could not build up in the evaporator. This is a possibility, particularly as the evaporator heat transfer effectiveness is lowered with the presence of the bulk liquid rather than having it spread out on the evaporator surfaces.

The disadvantage of having the reactor/evaporator inclined downward toward the engine is that liquid methanol could enter the reactor. Its presence

will force the reactor to operate at the saturation temperature of the vaporized methanol (289°F at 150 psig reactor pressure) which is below the minimum temperature for significant dissociation. While vaporization may occur, the engine will receive either liquid or vaporized methanol. This may be a less objectionable consequence of overfueling than puddling of fuel in the evaporator. In any case it may be necessary to include a safety valve in the line between the evaporator and reactor or at the reactor outlet.

Sincerely,



Gerald Driscoll  
Senior Research Engineer  
Vehicle Systems  
Department of Engine and Vehicle Research

/tme  
Attachments

**Table 1. Maximum Possible and Required Product Flows Per Cylinder  
Per Cycle at Various Engine and Reactor Conditions**

Engine speed (rpm)	Maximum Possible Amount of Products Entering/Cylinder/Cycle (lbm x 10 <sup>-3</sup> )				Required Product Flow (lbm x 10 <sup>-3</sup> )
	Reactor Pressure at 150 psig		Reactor Pressure at 100 psig		
	400°F*	1200°F	400°F	1200°F	
500	4.7/4.4**	3.6/3.4	2.9/3.1	2.1/2.3	---
1500	1.5/1.5	1.2/1.1	1.0/1.1	0.7/0.8	0.14
4500	0.5/0.5	0.4/0.4	0.3/0.3	0.5/0.3	0.14
6000	0.4/0.4	0.3/0.3	0.3/0.3	0.2/0.2	0.14

\* Temperature of dissociated products.

\*\* First value in each cell indicates product quantity based on pressure difference between reactor and cylinder at 45° BTDC. Second value indicates choked or maximum amount of products.

NOTE: Slight differences between values shown here and in our MPR #8 are due to the use of different values for the ratio of specific heats (k). This table uses k = 1.4. The data in MPR #8 uses k = 1.3.

**Table 2. Values of the Heats of Vaporization and  
Dissociation of Methanol**

**CH<sub>3</sub>OH HEAT OF VAPORIZATION**

<u>Value (Btu/lbm)</u>	<u>Reference</u>
545	Lalk, T.R., "Evaluation of Dissociated and Steam Reformed Methanol as an Automotive Engine Fuel," May 1984, NASA CR 168242, DOE/NBB-0064, May 1984, p. 48.
474	Taylor, C.F., "The Internal Combustion Engine in Theory and Practice," Vol. I, p. 46.
482	Baumeister and Marks, "Standard Handbook for Mechanical Engineers," pp. 4-14.
481	Bechtold and Timbario, "The Theoretical Limits and Practical Considerations of Decomposed Methanol as a Light-Duty Vehicle Fuel," 1984 Alcohol Fuels Symposium, pp. 1-24.

**CH<sub>3</sub>OH HEAT OF DISSOCIATION  
(Not including heat of vaporization)**

<u>Value (Btu/lbm)</u>	<u>Reference</u>
1500*	Lalk, T.R., p. 48.
1202	Finegold, J.G., "Dissociated Methanol Vehicle Results," April 1984, SERI/TP-234-2245, p. 2.
1188	Bechtold, pp. 1-24.

\* This may include some specific heat used to raise the temperature of the vapors to the point where dissociation may occur.

## **APPENDIX E**

### **CORRESPONDENCE WITH CATALYST MANUFACTURER**

# SOUTHWEST RESEARCH INSTITUTE

POST OFFICE DRAWER 28510 • 6220 CULEBRA ROAD • SAN ANTONIO, TEXAS, USA 78284

ENGINES, EMISSIONS AND VEHICLE RESEARCH DIVISION

August 16, 1985

Dr. Alan D'Alessandro  
Johnson-Matthey Inc.  
436 Devon Park Drive  
Wayne, PA 19087

**Subject: EPA Reactor Specifications for Dissociating Methanol**

Dear Dr. D'Allesandro:

I have attached specification sheets that EPA recently sent to us listing reactor parameters and values that they would like used. These are the ones I mentioned in our recent telephone conversation. Would you please review these and tell me if you can comply with them, if you would recommend other valves or materials, and if you would like me to set up a conference call with EPA to discuss concerns that you have?

As defined in the attachments I sent you previously, the EPA would like to use reactor configuration number 7 rather than number 6. To permit the reactor to fit inside a tube with an 3.584 inch inside diameter, the exact dimensions of the tubes and the mesh and fin material need to be changed from the values previously listed. You may want to adjust these dimensions to fit available fin and mesh thicknesses and tubing sizes. The length will need to be calculated to achieve the desired catalyst EPA recommends or what you feel is necessary.

## NEW DIAMETER DIMENSIONS FOR CONFIGURATION NO. 7

<u>DIAMETER DESIGNATION</u>	<u>DIMENSIONS (IN)</u>	
	<u>DIAMETER</u>	<u>DIAMETRAL DIFFERENCE</u>
D <sub>1</sub>	1.942	0.196
D <sub>2</sub>	2.138	0.060
D <sub>3</sub>	2.198	0.400
D <sub>4</sub>	2.598	0.060
D <sub>5</sub>	2.658	0.196
D <sub>6</sub>	2.854	0.060
D <sub>7</sub>	2.914	0.400
D <sub>8</sub>	3.314	0.060
D <sub>9</sub>	3.374	0.196
D <sub>10</sub>	3.570	

I will be on vacation from August 20 through September 3. I will call you when I return to ask you for your decision on building the reactor to configuration 7 and to discuss any questions you may have. If it appears that we can go ahead with fabrication, I would like to pursue this with a minimum of delay.

If you have any questions while I am on vacation, please feel free to contact Bill Likos at (512) 684-5111, x-3135.

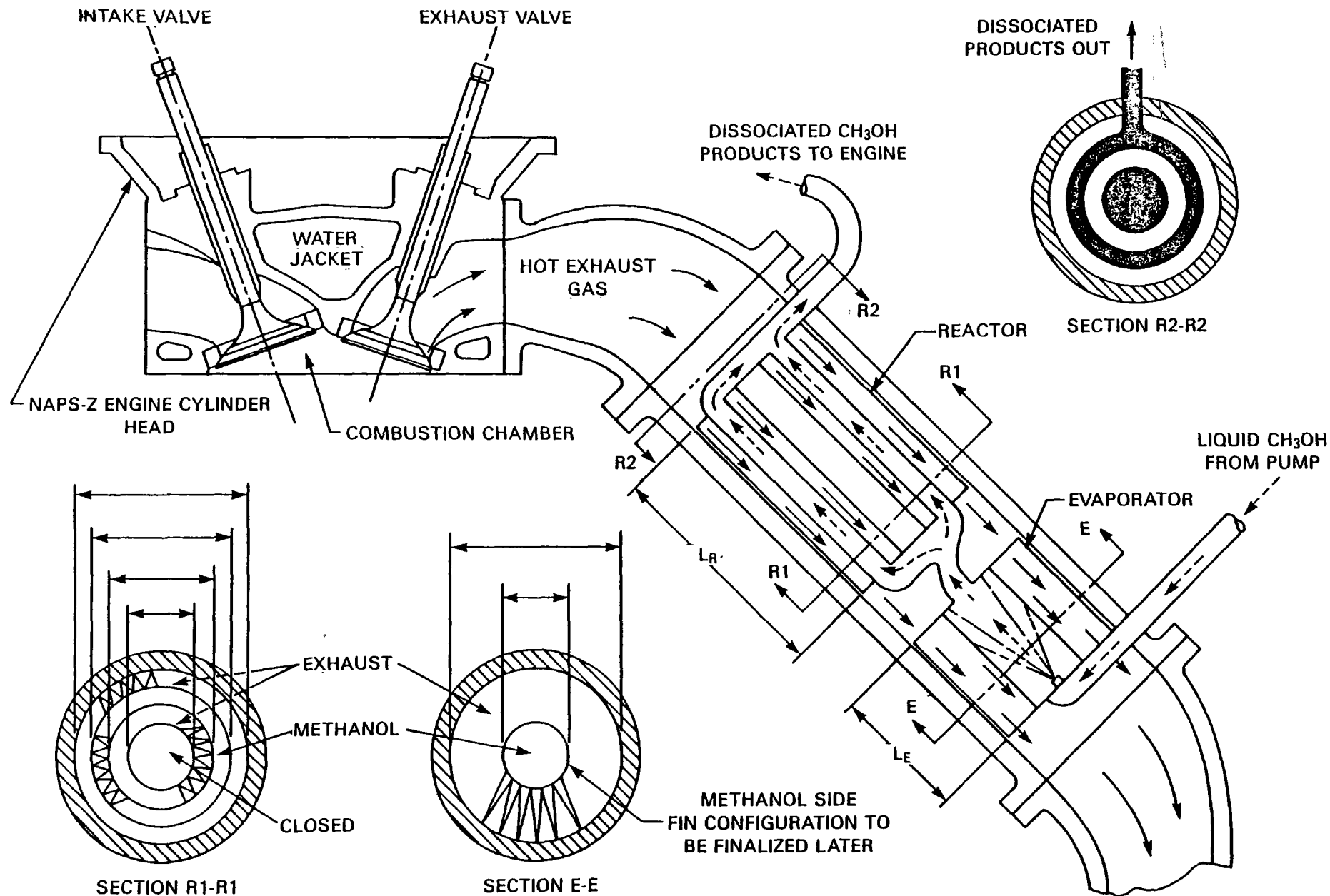
Sincerely,

A handwritten signature in cursive script that reads "Gerald D. Driscoll".

Gerald D. Driscoll  
Senior Research Engineer  
Vehicle Systems  
Department of Engine and Vehicle Research

/ds

cc: R. H. Thring  
B. Likos (02)



NOTE: DIMENSIONS DEFINED AND  
DISCUSSED ON FOLLOWING SHEETS

REACTOR-EVAPORATOR ASSEMBLY  
FOR EVAPORIZATION AND DISSOCIATION  
OF METHANOL

FIGURE 3A

Configuration	Type	Diameters (Inches)										Fin Description
		D <sub>1</sub>	D <sub>2</sub>	D <sub>3</sub>	D <sub>4</sub>	D <sub>5</sub>	D <sub>6</sub>	D <sub>7</sub>	D <sub>8</sub>	D <sub>9</sub>	D <sub>10</sub>	
1	A	1.000	1.100	1.140	1.336	--	--	--	--	--	--	Strip fin Figure 10-56 Kayes and London, 3rd Edition, .098" height, 20 per inch, 0.125 inch length in direction of flow
2	B	0.800	0.996	1.036	1.436	1.476	1.672	--	--	--	--	
3	B	0.800	0.996	1.036	1.436	1.476	1.672	1.712	2.112	2.152	2.348	
4	B	0.800	1.300	1.340	1.740	1.780	2.280	--	--	--	--	
5	A	3.544	3.744	3.804	4.000	--	--	--	--	--	--	Figure 10-56 Kayes and London, 3rd Edition
6	B	3.088	3.283	3.344	3.744	3.804	4.000	--	--	--	--	Figure 10-56, Kayes and London, 3rd Edition
7	B	2.372	2.568	2.628	3.028	3.088	3.284	3.344	3.744	3.804	4.000	Figure 10-56, Kayes and London, 3rd Edition

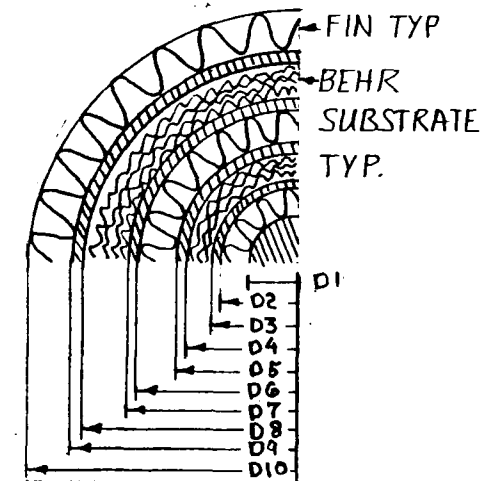
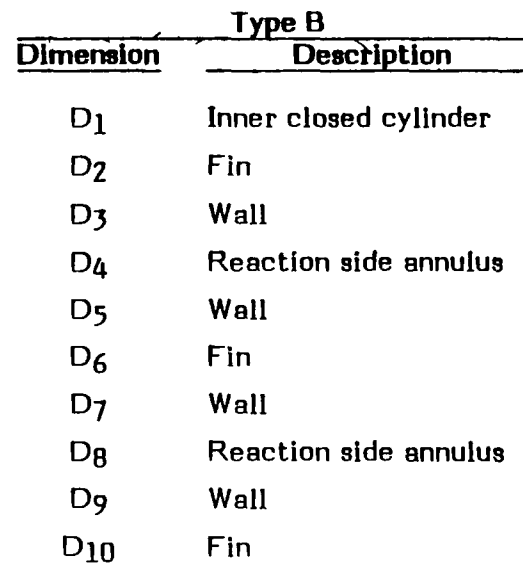
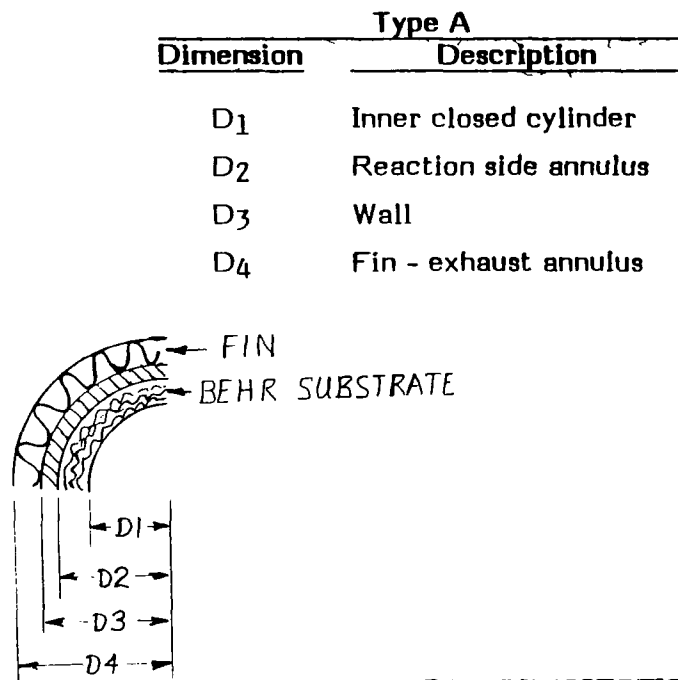


FIGURE 3B. CROSSECTIONAL GEOMETRIC DATA OF REACTOR CONFIGURATIONS

<u>Configuration</u>	<u>Type</u>	<u>D<sub>1</sub></u>	<u>D<sub>2</sub></u>	<u>D<sub>3</sub></u>	<u>Fin Description</u>
1	A	2.064	2.1040	2.300	Figure 10-56 Kayes and London, 3rd Edition
2	A	1.858	1.898	2.300	Figure 10-60 Kayes and London, 2nd Edition
3	A	3.744	3.804	4.000	Figure 10-56 Kayes and London, 3rd Edition
4	A	3.538	3.598	4.000	Figure 10-60 Kayes and London 2nd Edition

<u>Dimension</u>	<u>Description</u>
D <sub>1</sub>	Inside diameter of evaporation chamber
D <sub>2</sub>	Wall
D <sub>3</sub>	Fin

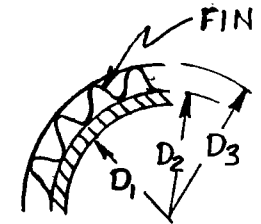


FIGURE 3C. CROSSECTIONAL GEOMETRIC DATA OF EVAPORATION CONFIGURATION

# SOUTHWEST RESEARCH INSTITUTE

POST OFFICE DRAWER 28510 • 6220 CULEBRA ROAD • SAN ANTONIO, TEXAS, USA 78284

ENGINES, EMISSIONS AND VEHICLE RESEARCH DIVISION

June 18, 1985

Dr. Alan D'Alessandro  
Johnson-Matthey Inc.  
436 Devon Park Drive  
Wayne, PA 19087

**Subject: Catalyst Selection and Application to a Reactor for Dissociating Methanol**

Dear Dr. D'Alessandro:

I am writing with regard to our recent telephone conversation to provide you with some information concerning the reactor that we are designing, and to ask for some information that we need to finalize this design.

We are conducting a program for the EPA to evaluate direct injection of dissociated methanol (CO and H<sub>2</sub>) into the combustion chamber of an engine. We need a catalyst manufacturer to provide an appropriate catalyst and to apply it to a reactor that we would supply.

With regard to this we would like to ask, first of all, if Johnson-Matthey would be willing to assist us by recommending a catalyst and applying it to the fin tube surface of our reactor. The reactor will operate at 100 to 150 psig and we would like the catalyst to survive maximum exhaust temperatures of about 1300°F. A catalyst that would produce significant product yields at temperatures as low as 400°F is also desired. The primary products of dissociation should be CO and H<sub>2</sub> under these conditions. The attachments show the basic reactor configurations we are considering.

If you can assist us, we need certain information about your selected catalyst to permit us to finalize the reactor design:

1. Catalyst yield at the elevated pressures and at several temperatures.
2. Approximate degradation of catalyst yields as a function of time and temperature.
3. Maximum allowable temperature the catalyst can be exposed to and retain its function.
4. Minimum temperature at which significant (e.g. 50%) yields may be realized.

5. Description of product species at the elevated pressure.
6. Materials that the reactor should be made of to provide good adherence for the wash coat.
7. Minimum substrate fin spacing that will permit the wash coat to conform to the substrate and not bridge the fins.
8. Suggested prefabricated high density fin or substrate material to provide maximum catalyst surface area in a minimum volume.
9. Approximate cost and time required to perform the application.

Your early response to our inquiry would be appreciated. Please call me at 512/684-5111, extension 2047.

Sincerely,



Gerald D. Driscoll  
Senior Research Engineer  
Department of Engine and Vehicle Research

/tme  
Attachments  
cc: R. Thring  
W. Likos

## **APPENDIX F**

### **TEST PLAN FOR EVALUATING HEAT EXCHANGER WITHOUT OPERATING ENGINE ON PRODUCTS OF DISSOCIATION**

# **SUMMARY OF PREPARATIONS FOR HEAT EXCHANGER LABORATORY TESTING**

## **Purpose of Testing**

To measure heat exchanger performance under actual engine operating conditions so that a comparison of analytical and experimental results can be made, the actual capabilities to dissociate methanol can be assessed and the final heat exchanger design details can be determined.

## **Preparations**

### **1.0 Heat Exchanger**

- 1.1 Complete fabrication of heat exchanger shells and ship to Johnson Matthey (J M).
- 1.2 Have J M apply substrate, catalyze and assemble tubes.
- 1.3 Finish heat exchanger plugs, ports, ducts, and mounts
- 1.4 Design provisions for mounting nozzle to heat exchanger after decision on nozzle is made.

### **2.0 Fuel Injection**

- 2.1 Need information from Stanadyne on the suitability of their nozzles for this application and a design for the nozzle tip to spray methanol over the inside evaporator surface.
- 2.2 If Stanadyne nozzles appear suitable they need to be evaluated for their spray pattern on the test stand at SwRI.
- 2.3 If the Stanadyne nozzles cannot be made suitable then the existing SwRI design can be used.

### **3.0 Engine Modifications**

- 3.1 Prepare package of existing calculations and send to EPA.
- 3.2 Design modifications to adapt Stanadyne DB2 pump to NAPS-Z engine (need engine).
- 3.3 Complete engine design modifications with regard to valve train and cam drive and submit drawing package to EPA (need engine).

### **4.0 New Parts Required to Mate Engine and Heat Exchanger**

Design and fabricate parts to connect the engine and heat exchanger; the heat exchanger and exhaust manifold; and the heat exchanger to various sensors.

## 5.0 Control System

No control system design efforts need to be accomplished other than to provide for adjustment and locking of the Stanadyne pump rack.

## 6.0 Test Setup

- 6.1 The NAPS-Z engine would be installed in a standard test cell and connected to a dynamometer, coolant pipes, and the cell exhaust system.
- 6.2 The engine would operate on its existing unmodified fuel injection system. It would require no modifications other than the addition of the Stanadyne pump.
- 6.3 The heat exchanger would be mounted in one housing that connected one cylinder exhaust port to the exhaust manifold. The other exhaust ports would be connected by housings that did not contain heat exchangers. Exhaust from one cylinder would flow through the reactor, then through the evaporator, counterflow to the methanol.
- 6.4 Methanol would be pumped at high pressure by the Stanadyne pump to the nozzles. One nozzle would be mounted in the evaporator and spray methanol on its inside surface. The other nozzle discharges would be routed back to the methanol fuel supply. Methanol would be vaporized in the evaporator and these vapors would flow into the reactor. Reactor discharge would be collected for analysis via gas chromatography. The dissociated products would not be injected into the engine.

## 7.0 Test Instrumentation

The engine and heat exchanger would be instrumented to monitor the following parameters. The values of these parameters would be used to measure the performance of the heat exchanger (MPR #10).

<u>Parameter</u>	<u>Location</u>
Temperature Pressure Mass flowrate	Methanol into the evaporator
Temperature	Methanol between the evaporator and reactor
Temperature Pressure Product analysis	Dissociated products out of reactor

<u>Parameter</u>	<u>Location</u>
Temperature Pressure	Exhaust out of engine
Temperature Pressure	Exhaust between reactor and evaporator
Temperature Pressure	Exhaust after evaporator
Engine speed	Engine crankshaft
Mass airflow	Engine intake
Mass flowrate	Methanol injected into manifold or ports
Temperature	Engine coolant

## 8.0 Test Procedure

The engine would be operated over a matrix of loads and speeds. These would represent steady-state conditions. The heat exchanger would be subjected to a matrix of pressures and flowrates at each engine test point. Measurements from the instrumentation listed in paragraph 7.0 would be obtained at each test point.

## 9.0 Use of Results

The test results will be used to define the following:

- 9.1 Heat exchanger, evaporator, and reactor exhaust side effectiveness in terms of methanol and exhaust temperatures at each test point.
- 9.2 Efficiency of the dissociation process in terms of methanol dissociated versus total methanol flow at each test point.
- 9.3 Heat exchanger total, evaporator and reactor pressure drops at each test point.
- 9.4 Comparison of above experimental results with calculated design specifications.
- 9.5 Qualitative and quantitative analysis of all product constituents to determine if compounds or elements other than hydrogen, carbon monoxide, and vaporized methanol are present at each test point.
- 9.6 Optimum Heat exchanger total size and relative sizes for the reactor and evaporator.

## **APPENDIX G**

### **CYLINDER HEAD AND CATALYTIC REACTOR DESIGN OPTIONS**

## CYLINDER HEAD AND CATALYTIC REACTOR DESIGN OPTIONS

Four layout drawings were made which show two possible arrangements, one which would make use of the existing cylinder head and one which would use a new, modified cylinder head casting.

Layout drawing number 03-8352-003 shows the overall assembly of the cylinder head with the catalytic converters. An independent catalytic converter is planned for each cylinder. In this layout only the exhaust port configuration along with the converter housing and the converter are shown. A casting is being prepared for the converter housing. This casting will have provision for accommodating either two or four converters. The converters will be bolted onto the housing. Depending upon the design selected (two or four converters per housing), one or two converter housings will be built. The advantages or disadvantages of each of the arrangements are discussed later in this report. The housing(s) will be bolted to the cylinder head in the existing holes for the exhaust manifold. Also, the hole patterns on the converter housing's outlet flange are such that the exhaust manifold can be used without any modifications.

The layout drawing also shows the initially proposed construction of a crossflow catalytic converter. The converter consists of header tanks at both ends. Stainless steel tubes of approximately 0.125 and OD x 0.015 inch wall thickness would form the body to support the catalyst. The tubes would provide large surface areas for catalytic reaction and heat transfer from the hot exhaust gases to the catalyst. A methanol fuel injector would be accommodated in one of the header tanks. The header tank on the other side will be used to collect the dissociated products. This crossflow design was discarded in favor of a counterflow design which is more efficient for a dissociation reactor application.

In the above design configurations, no cylinder head modifications were contemplated. However, adoption of this design means some heat loss will occur from the exhaust gas to the water jacket. In the present cylinder head design, a portion of the exhaust port is surrounded by the water jacket. The heat loss to the cooling water can be eliminated if the cylinder head casting is modified as shown in drawing 03-8352-005. In this design modification, a cored air space is added between the port wall and the water jacket. Alternatively, ceramic lining of the port surfaces or a port liner made up of an insulating material will be considered to reduce the heat loss.

Layout drawings 03-8352-004 and -006 show the gas (dissociated products of methanol) admission valve. In drawing 03-8352-004, the valve is designed to fit into the spark plug hole adjacent to the exhaust valve/port. Although some enlargement of the existing 14 mm spark plug hole seems possible, this design will restrict the gas flow area to slightly more than 0.1 square inch. It is estimated that, at 5200 rpm engine speed, the dissociated products will have to be admitted to the cylinder in 1.6 milliseconds. This result was based on the assumption that the gas admission valve will be opened for a period of 50 crank degrees during the compression stroke of the engine. The volume of the dissociated methanol produced in the catalytic converter at full load-rated speed of the NAPS-Z engine is estimated to be 1.6 cubic inches. In reality, however,

the construction features of the converter and the joining passages are the limiting factors. Based on current design of the converter, it is estimated that the volume of dissociation products to be transferred to the cylinder is about 3.5 cubic inches. The calculations indicate that the velocity of the gas through the valve would be in excess of 1000 ft/sec. Such a high velocity is considered to be undesirable; therefore, it is essential that, among other things, the gas inlet valve be designed as large as possible. Depending upon the decision made, this issue will be suitably addressed in the detailed design of the components.

Layout drawing 03-8352-006 shows the gas inlet valve in a modified (new casting and machining) cylinder head. By providing an independent boss in the casting the valve size is considerably enlarged.

It can be seen that, due to the large size of the converter, which is necessary for heat transfer and catalyst area considerations, it has not been possible to incorporate the converter within the confines of the cylinder head. however, the essence of in-cylinder dissociation has been retained, since the dissociated products are still admitted directly to the cylinder, without being first mixed with incoming air.

Valve operating mechanism is another important factor in the design of the in-cylinder methanol dissociation scheme. Both modified and unmodified cylinder head layouts show the valve operating mechanism. A separate camshaft driven by the engine is being considered. The cam is designed to directly operate on the follower attached to the valve stem. No difficulties are anticipated in the design of the cam/follower assembly and the camshaft drive arrangement. However, for the existing unmodified cylinder head, lubrication of the valve stem and the drive mechanism is likely to be far more complex than the one for the modified cylinder head. In the modified cylinder head design the camshaft supports, the cam, the follower and valve stem are all accommodated on the cylinder head. The new design has larger modified rocker covers to house the gas inlet valve and the valve train. A modified rocker cover will be used to house the entire valve gear (intake, exhaust and gas inlet valve).

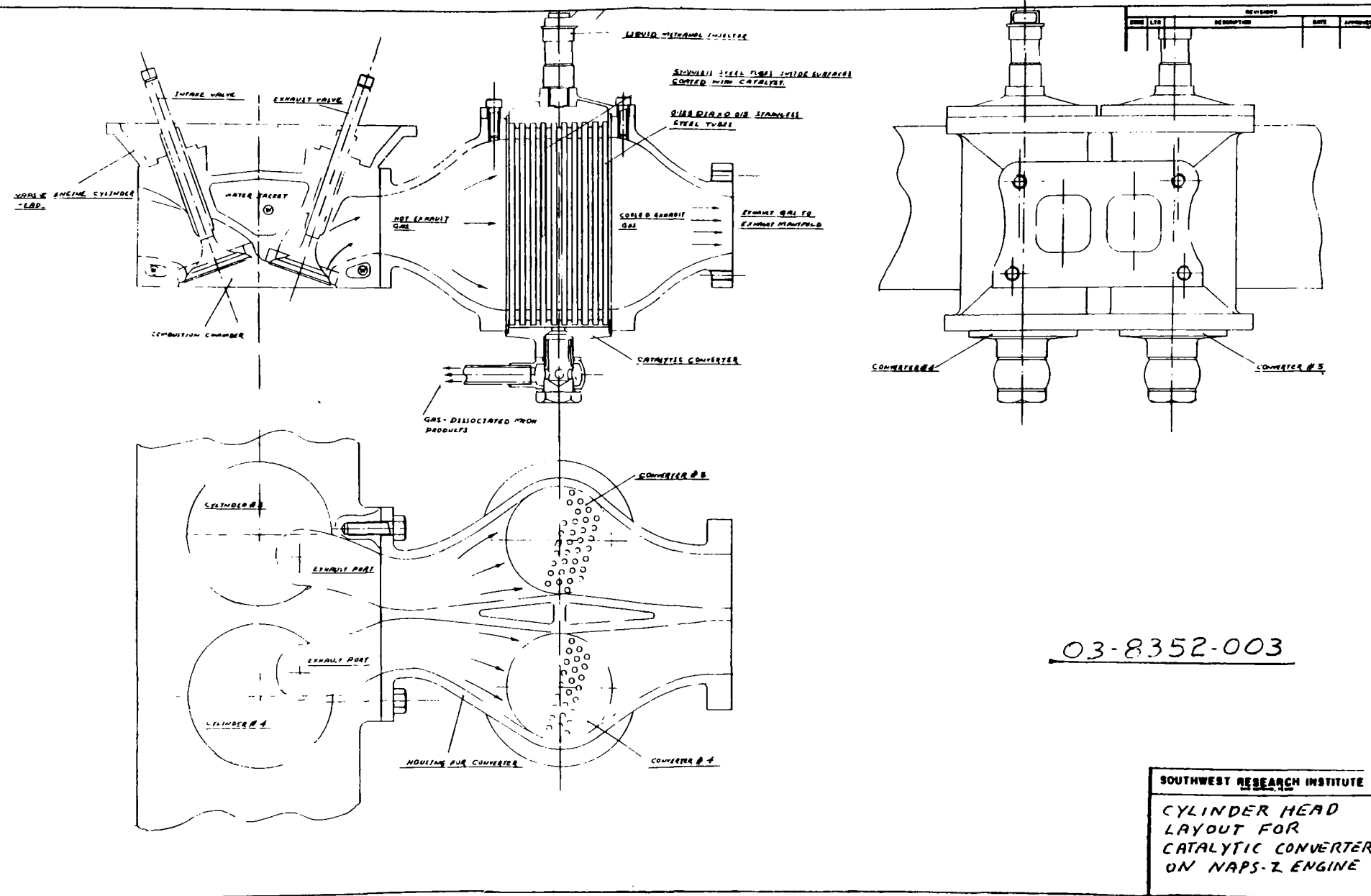
As an alternative to the mechanically operated valve, consideration is being given to an electrical solenoid-operated valve design. The possibility of electrical valve operation depends upon the existence of an electrical solenoid with large force and displacement and capable of operating at a frequency of at least 2600 cycles/minute.

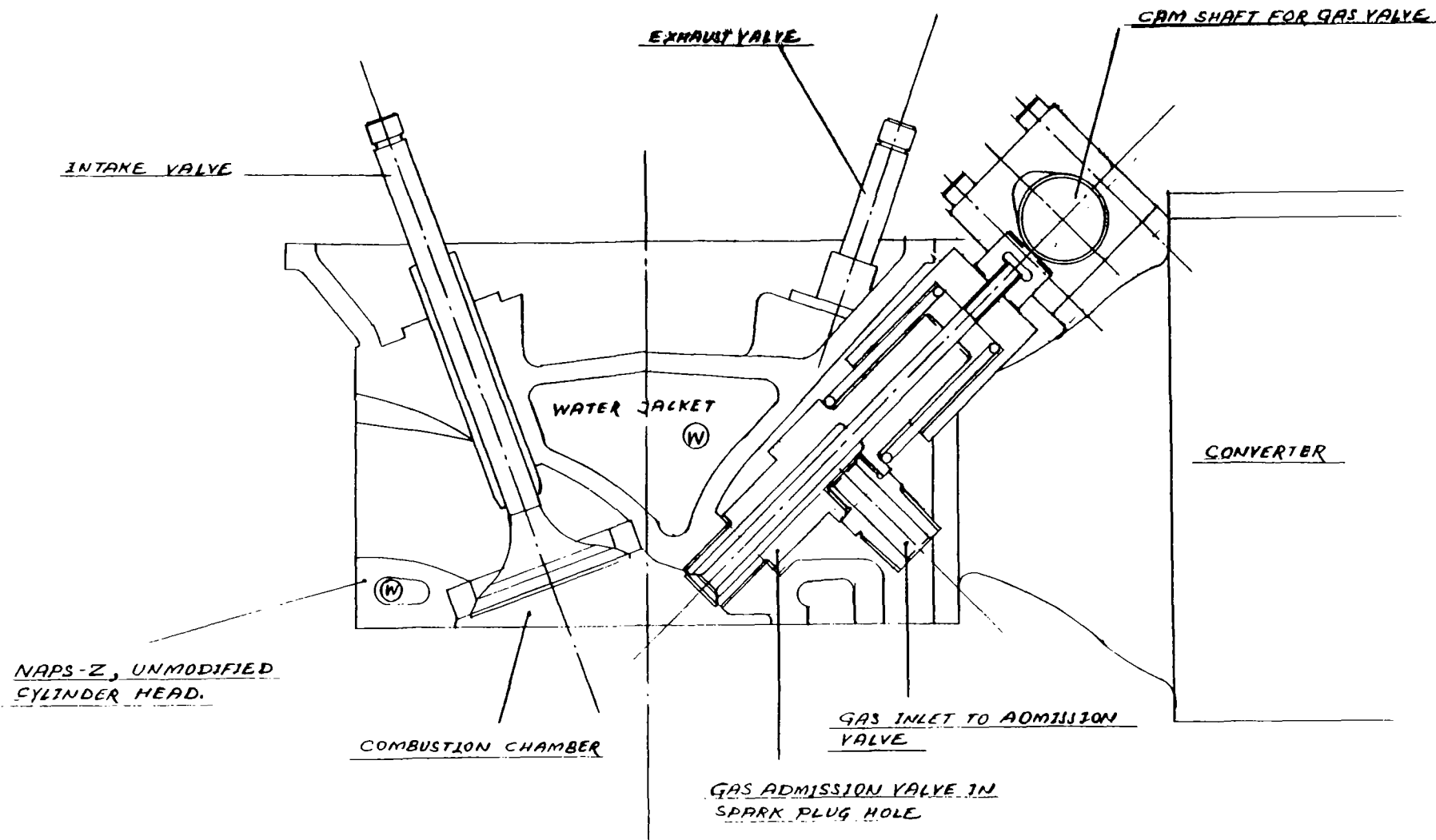
Either of the two approaches discussed above is possible. The modified cylinder head approach, though advantageous, is considerably more complicated since an entirely new head must be developed. The use of the existing cylinder head design has some functional disadvantages; however, from an execution point of view it is a much simpler and less time-consuming approach. As already mentioned, after considerable thought, the unmodified cylinder head was chosen for future work.

Reasons for this recommendation are as follows. There are four main factors involved: (1) the location of the converter; (2) the gas velocity in the transfer valve; (3) the insulation of the exhaust port; and (4) the valve train. As far as the location of the converter is concerned, due to the heat transfer and catalyst area considerations, the size of the converter is such that it cannot be fitted within the confines of the cylinder head (neither the existing

head nor redesigned head). There is not benefit, therefore, in designing a new head from this point of view. The gas velocity in the transfer valve would be too high with the standard cylinder head, using the 14 mm spark plug hole, but enlarging that hole will reduce the gas velocity to a reasonable level. The production of a new cylinder head would enable the exhaust port to be more effectively insulated, but adequate insulation with the standard head can be achieved by fitting an exhaust liner. The valve train will be somewhat more difficult to lubricate with the unmodified cylinder head, but this problem can be overcome.

The time required to design and develop the new cylinder head is estimated to be about 24 weeks. If the existing cylinder head is used, the time required to design and build the converter housing, converters, valve and valve gear is estimated to be 10 weeks. Most of the above parts are common to the existing cylinder head or a new cylinder head design.

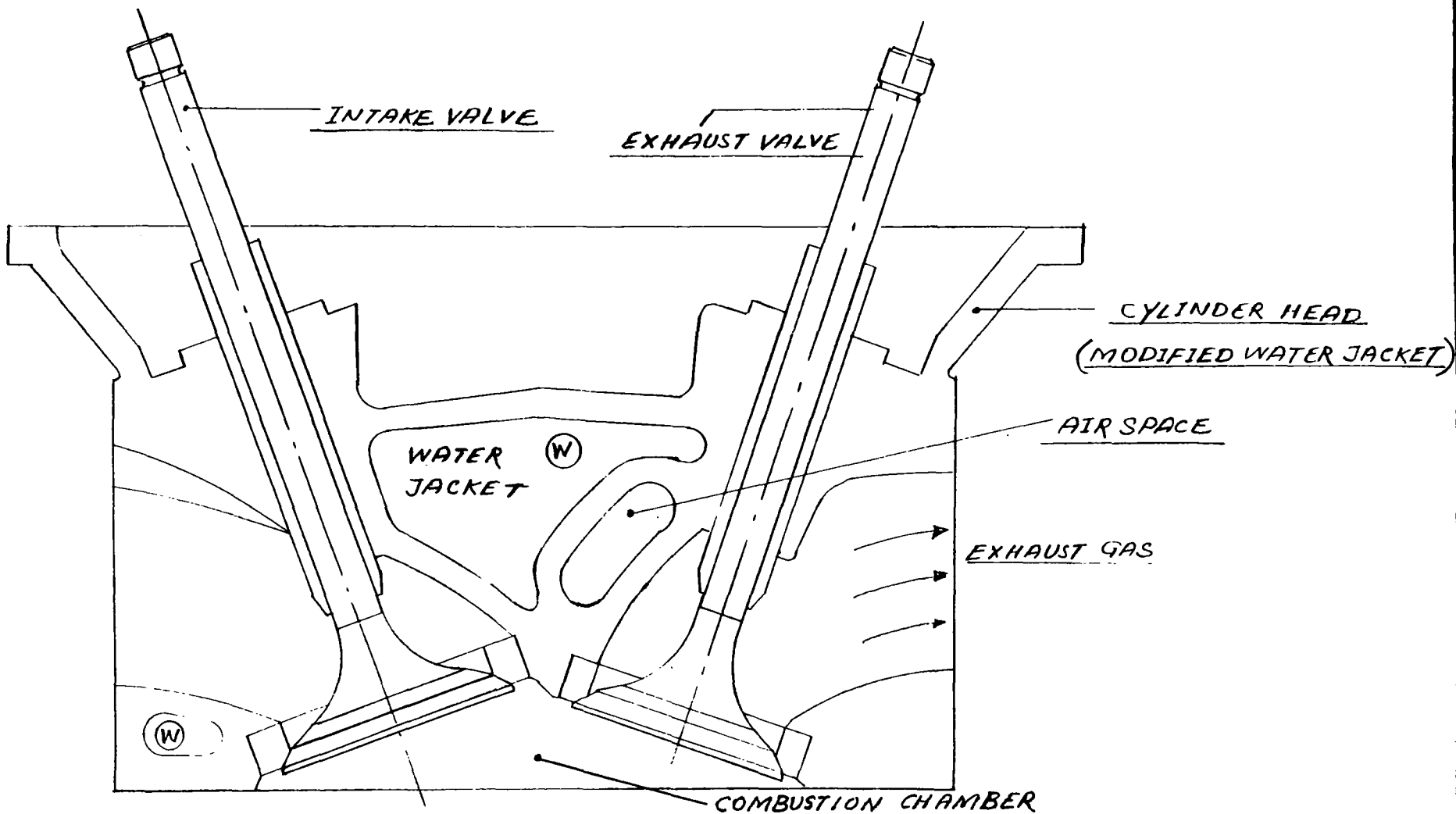




# **SOUTHWEST RESEARCH INSTITUTE** SAW ANTONIO, TEXAS

EXPR. CYLINDER HEAD LAYOUT  
 GAS ADMISSION VALVE IN  
 SPARK-PLUG HOLE. UNMODIFIED  
 CYLINDER HEAD CASTING.

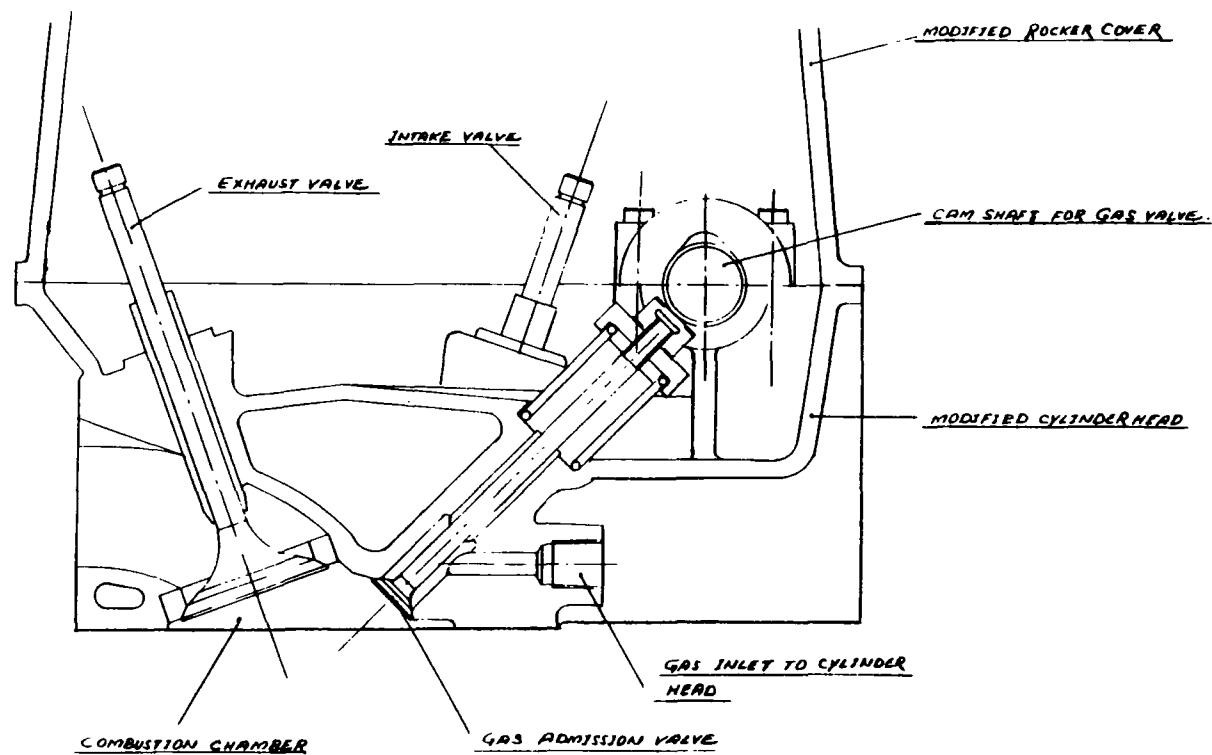
SIZE	CODE IDENT NO.	DRAWING NO.
<b>D26401</b>		03 8352 004



**SOUTHWEST RESEARCH INSTITUTE**  
SAN ANTONIO, TEXAS

CYLINDER HEAD LAYOUT  
CASTING MODIFICATION

SIZE	CODE IDENT. NO.	DRAWING NO.
A	26401	03-8352-005



# **SOUTHWEST RESEARCH INSTITUTE**

SAN ANTONIO, TEXAS

EXPR: CYLINDER HEAD LAYOUT  
GAS ADMISSION VALVE IN CASTING  
NEW- MODIFIED CYLINDER HEAD  
CASTING

SIZE	CODE IDENT NO.	DRAWING NO.
C	26401	03-8352-006

SCALE 1:1	SHEET
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## **APPENDIX H**

### **EVALUATION OF THE METHANOL DISSOCIATION HEAT EXCHANGER**

**(Includes a Table of Additional Data)**

**SPECIAL TECHNICAL PROGRESS REPORT**

**EVALUATION OF THE METHANOL DISSOCIATION HEAT EXCHANGER**

**SwRI Project 03-8352**

**EPA Contract 68-03-1984**

**Prepared by**

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**Submitted to**

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United States Environmental Protection Agency  
Motor Vehicle Testing Laboratory  
2565 Plymouth Road - ECTD  
Ann Arbor, Michigan 48103**

**September 1987**

## INTRODUCTION

A heat exchanger system has been evaluated to determine its effectiveness in dissociating methanol into hydrogen and carbon monoxide. This system consists of evaporator and reactor sections that are heated by engine exhaust gases. Methanol is injected into the evaporator and, after being vaporized, passes over a dissociation catalyst in the reactor. This heat exchanger system, designed for application to only one engine cylinder, is 10 cm (four inches) in diameter by 50 cm (20 inches) long. Background information on the design of the evaporator and the reactor is given in the section "Heat Exchanger Design Considerations."

## SUMMARY

The methanol dissociation heat exchanger was evaluated over a range of engine speeds and power outputs. Conditions in the heat exchanger were stable at low to moderate engine speeds and loads, enabling determination of methanol dissociation rates. At high engine speeds and with high loads at lower engine speeds, the conditions in the heat exchanger were very unstable, and meaningful methanol dissociation rates could not be determined. The lower engine power operating conditions are considered to be representative of typical steady-state engine operating conditions for light-duty vehicles.

The mechanical design of the heat exchanger was generally satisfactory, but some additional improvements in injector mounting and injector cooling are needed. The lack of adequate injector cooling was a major factor in the inability to operate the heat exchanger at high engine speeds and loads.

In these evaluations, the dissociation rates in the reactor ranged from 1 to 96 percent of the total methanol injected into the evaporator; the higher dissociation rates being associated with low methanol injection rates. This represented from 0.6 to 9.8 percent of the engine cylinder fuel needs at the test points evaluated. The reactor size, or the effectiveness of the catalyst, will have to be increased by a factor of 2 to 4 to achieve sufficient dissociation to meet 20 to 25 percent of the total fuel needs of the engine at the lower power operating conditions.

The evaporator was adequately sized to vaporize 100 percent of the engine cylinder fuel needs at 3000 rpm, but only 50 percent at 1500 rpm. The vaporization rate was greater at 3000 rpm because of the higher exhaust temperature and flowrate at that engine speed.

## TEST MATRIX

The engine, with the heat exchanger mounted, was operated at engine speeds that ranged from 1500 rpm to 4500 rpm and loads that ranged from 30 lbs-ft to 110 lbs-ft. During initial testing, however, it became apparent that the evaporator reached excessive temperatures when operating at high exhaust temperatures and flowrates. A major factor was overheating of the methanol injector, resulting in injector malfunction. This limited testing to low load conditions at 1500 and 3000 rpm.

Evaluations conducted involved the determination of dissociation, with several methanol flowrates through the heat exchanger at two engine operating

conditions. Also, evaluations were conducted to determine the effect of reactor pressure and temperature on the rate of dissociation.

## METHANOL DISSOCIATION IN HEAT EXCHANGER

A summary of the test results is given in Table 1. Table 1 includes the dissociation rate in percent on a mass basis versus methanol mass flowrate into the heat exchanger. The amount of dissociated products as a function of total engine cylinder fuel needs at these test points varied from 0.6 to 9.8 percent. The reactor performed more efficiently at the higher engine speed and load conditions, because of the high exhaust temperatures and flow rate.

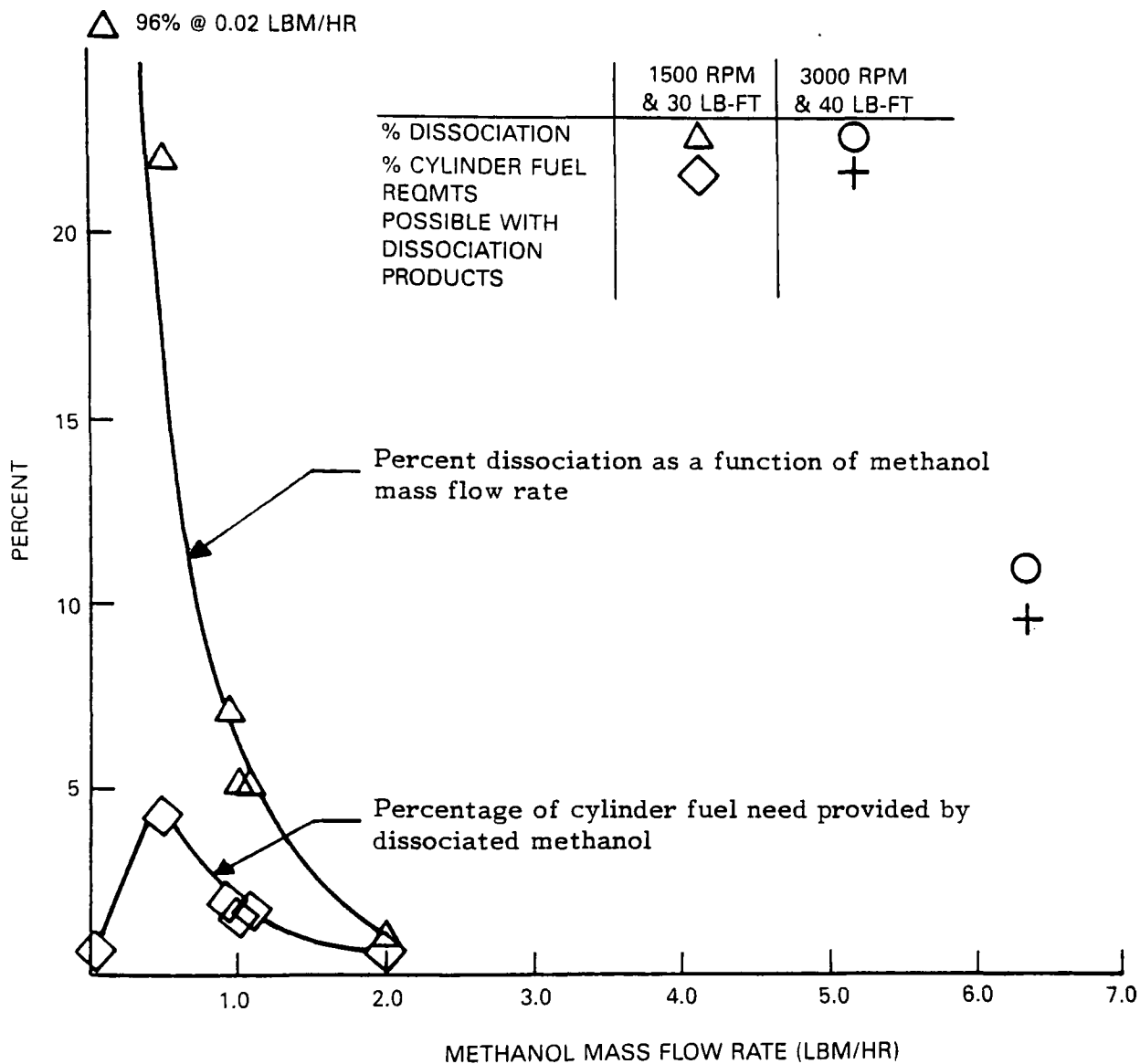
### Effects of Fuel Rate

A comparison of dissociation rate, as a function of methanol mass flowrate into the heat exchanger, is included in Table 1 and shown in Figure 1. There is the expected inverse relationship between the percent of dissociation and fuel rate.

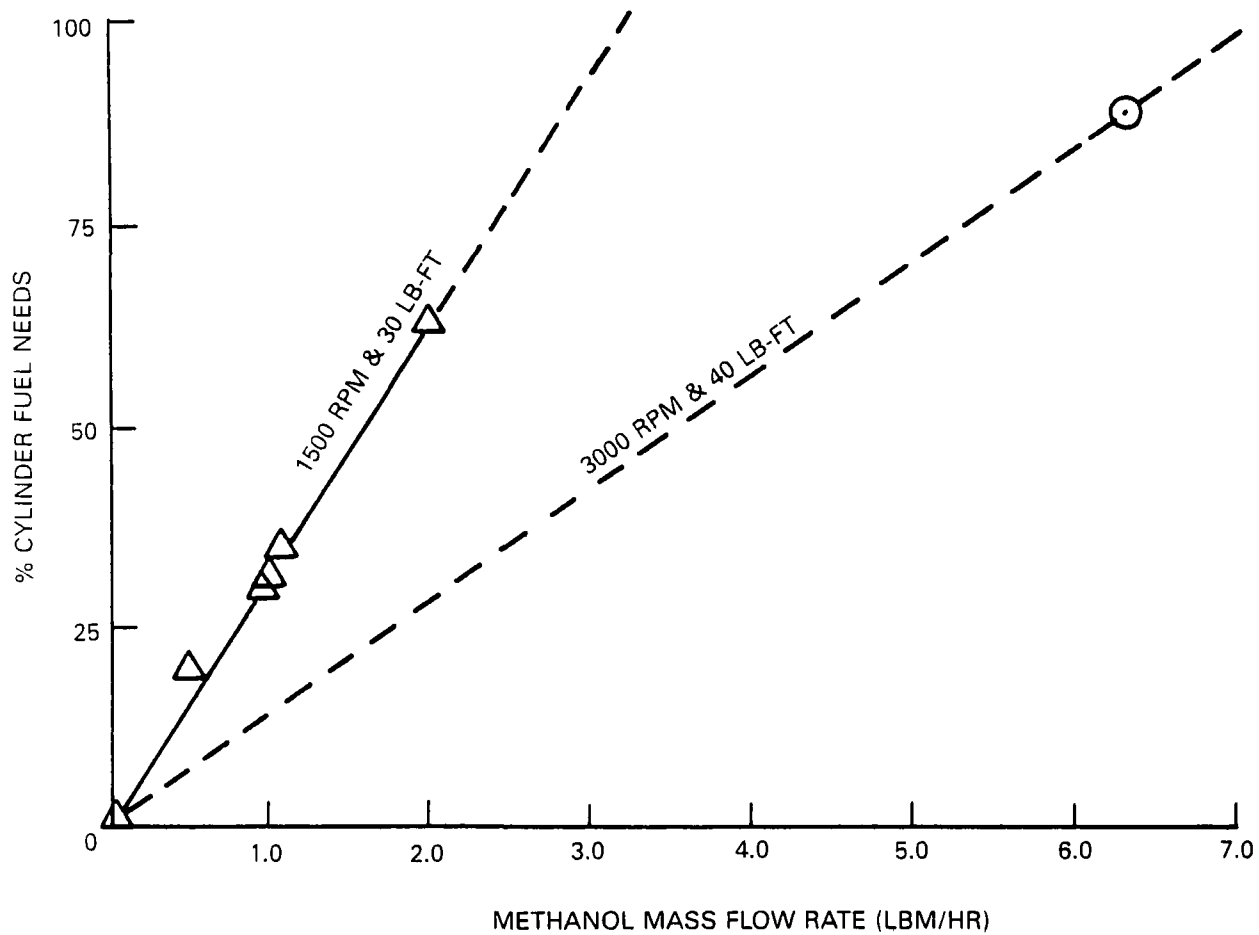
Figure 1 also shows the product of the dissociation rate and the percent of engine cylinder fuel need. This product represents the amount of dissociated products that could be supplied as a percent of the total cylinder fuel needs at a specific engine operating condition. The dissociation rate as a function of cylinder requirements at the 1500 rpm test point appears to reach a maximum of 4.2 percent of requirements at about 0.5 lbs/hr methanol flow through the heat exchanger. Only one flowrate was used at the higher engine speed and load, and it resulted in a relatively high rate of dissociation (11.0 percent) and the highest percentage of cylinder fuel need (9.8 percent). Excessive temperatures in the heat exchanger at higher engine speeds and loads eliminated the possibility of testing at those conditions. The percent of cylinder fuel needs, as a function of heat exchanger methanol mass flowrate, is shown in Figure 2.

### Effects of Internal Pressure

Two comparative evaluations (Test runs 3 and 7) were performed at the same test conditions, except for an elevated evaporator and reactor pressure in Run 7. Results of these two tests are given in Table 2. There was little difference in the rates of dissociation, between these two tests. This result was to be expected because Johnson-Matthey reported that the dissociation at 8 atmospheres of pressure would be about 93 percent of the dissociation at 1 atmosphere. Although the literature discusses the tendency of the reaction to slow down and reverse at higher pressures, change in pressure should have negligible effect over the range of pressures expected in this application.



**FIGURE 1. HEAT EXCHANGER PERFORMANCE VERSUS METHANOL MASS FLOWRATE**



**FIGURE 2. CYLINDER FUEL NEEDS VERSUS METHANOL MASS FLOWRATE**

Table 1. Methanol Mass Flowrate Versus Percent Dissociation

Run* No.	Methanol Mass Flowrate (lbm/hr)	% of Engine Cylinder Needs	Percent Dissociation	% Dissociation x % Cylinder Needs	Engine		Heat Exchanger Condition
					Speed (rpm)	Torque (lb-ft)	
6	0.02	0.6	96	0.6	1500	30	Insulated
4	0.5	19	22	4.2	1500	30	<u>Un</u> insulated
7	0.95	29	7	2.0	1500	30	<u>Un</u> insulated/pressurized to 35 psig
3	1.0	31	5	1.6	1500	30	<u>Un</u> insulated
9	1.1	35	5	1.8	1500	30	Insulated
5	2.0	63	1	0.6	1500	30	<u>Un</u> insulated
8	6.3	89.4	11	9.8	3000	40	Insulated

\* Analysis of heat exchanger products for run numbers 1 and 2 could not be made because test equipment was not set up to handle the significant quantities of methanol in the sample.

**Table 2. Effects of Evaporator Internal Pressure on Rates of Dissociation**

Run Number	3	4
MeOH Mass Flowrate (lbm/hr)	1.0	0.95
Average Reactor Pressure (psig)	0	33
Percent Dissociation	5	7
Average Reactor Temperature (°F)*	432	236
Insulation	Uninsulated	Uninsulated

**Effects on Temperature**

Two comparative evaluations (Runs 3 and 9) were made at the same test conditions, except that the heat exchanger was wrapped in an insulated blanket for Run 9. Results of these two tests are summarized in Table 3. The dissociation rates were the same for both tests, although the average evaporator/reactor temperature for Run 9 was 138°F higher than that for Run 3. Johnson-Matthey indicated that maximum dissociation occurred with this catalyst at 370°C (698°F) and that there were significant yields at 300°C (572°F). For Run 9, the average temperature between inlet and outlet of the reactor was 300°C (570°F). This temperature is lower than that for maximum dissociation, but it is at the point of significant yields. Operation at an average reactor temperature of 222°C (432°F) in Run 3 should have resulted in a lower dissociation rate.

**Table 3. Effects of Temperature on Rates of Dissociation**

Run Number	3	9
MeOH Mass Flowrate (lbm/hr)	1.0	1.1
Average Reactor Pressure (psig)	0	0
Percent Dissociation	5	5
Average Reactor Temperature (°F)*	432	570
Insulation	Uninsulated	Insulated
Evaporator Temperature (MeOH)(°F)	198	352
Reactor Temperature (MeOH)(°F)	666	788
Exhaust Temperature Before Reactor (°F)	707	877
Exhaust Temperature Between Evaporator and Reactor (°F)	419	721
Exhaust Temperature After Evaporator (°F)	210	244

\*Average reactor temperature is average of internal evaporator and reactor outlet (MeOH) temperatures.

## Effects of Changes in Engine Load and Speed

Run 8 was at higher engine load and speed than the other tests and had a higher methanol flowrate through the heat exchanger. The results are summarized in Table 1 and Figure 1. It was not possible to lower the methanol flowrates in this test because the evaporator temperature would have become excessive. The dissociation rate in Run 8 was 11 percent. It should be noted that the average reactor temperature for this test was 395°C (742°F), which is higher than for any other run and was close to the optimum temperature of 370°C (698°F). The combination of higher reactor temperature and higher heat flowrate was apparently responsible for the dissociation rate being higher than in any of the tests at the engine speed of 1500 rpm. In addition, the test at 3000 engine rpm had the highest portion of dissociated products as a function of total cylinder fuel needs.

## RESULTS OF EVAPORATOR MAPPING

### Approach

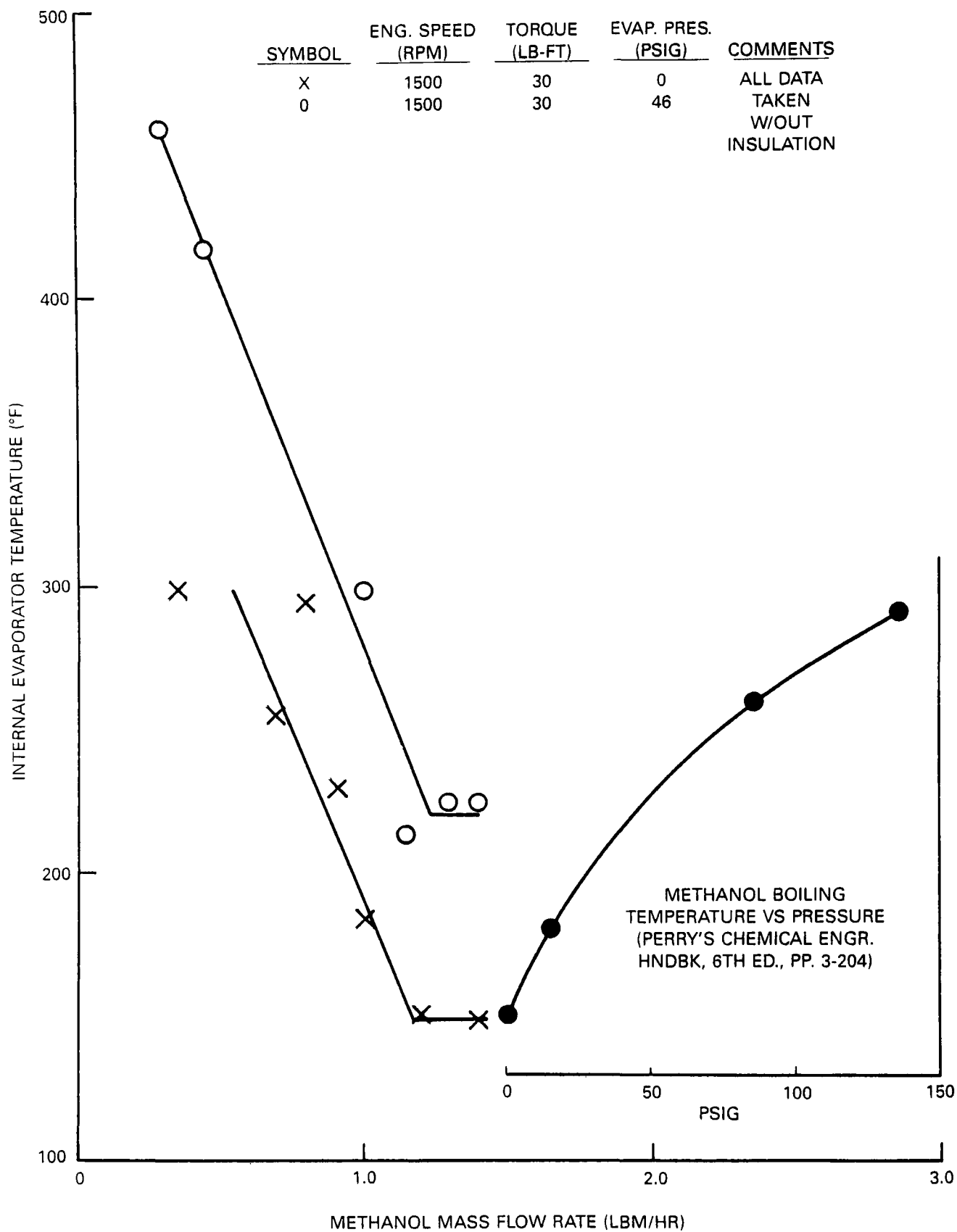
The capacity of the evaporator to vaporize methanol as a function of flowrate was also determined. All testing of the heat exchanger was accomplished with the evaporator at a temperature higher than the boiling point (equilibrium temperature) of methanol. To determine the maximum capacity of the evaporator to completely vaporize the methanol, a series of tests were conducted. Evaporator internal temperature as a function of flowrate was determined at 1500 engine rpm and 30 lbs-ft torque at ambient and high pressures, with and without insulation. Testing was also done at 2000 engine rpm and 35 lbs-ft. Testing at higher speeds and loads, however, was difficult for two reasons. First, once the temperature was above the equilibrium point it was difficult to achieve stability; the internal evaporator temperature changed at a rate of up to 2°C per second. Second, attempts to find the minimum fuel flowrate that still maintained the evaporator at the equilibrium temperature were unsuccessful, because after any excess fuel vaporized in the evaporator, the temperature would rise rapidly. Control problems were even more severe when the heat exchanger was wrapped in an insulating blanket.

Testing the evaporator, by measuring its internal temperature and plotting it as a function of fuel mass flowrate through the evaporator, assumes that the evaporator vaporizes all of the fuel once the internal temperature exceeds the equilibrium temperature. This seems correct in theory, but has not been verified. An attempt toward verification through a heat balance between the exhaust and methanol sides of the evaporator was unsuccessful.

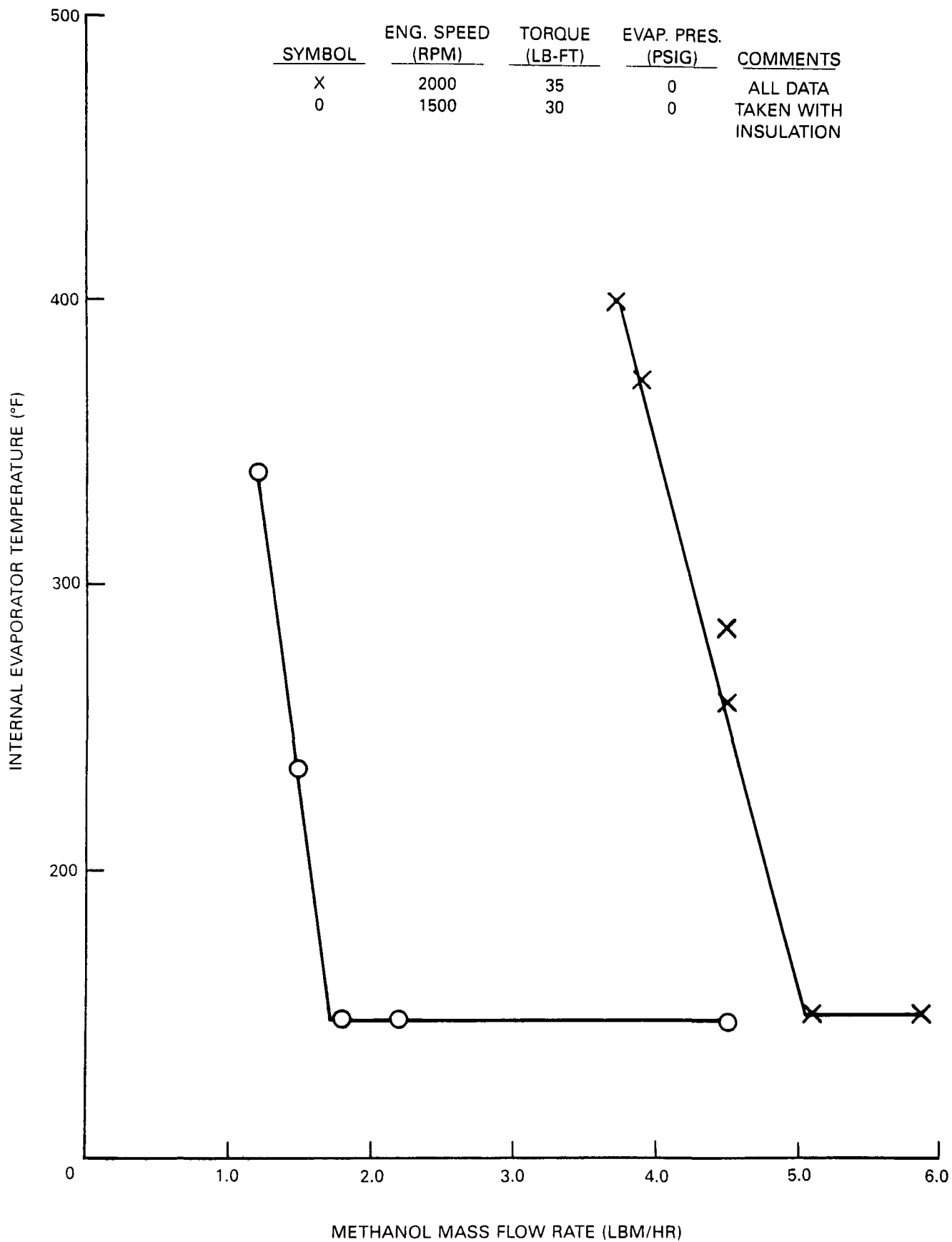
### Results

Results of evaluations without insulation at low and high pressure in the heat exchanger with the engine operating at 1500 rpm and 30 lbs-ft of torque are shown in Figure 3. Pressure versus boiling point for methanol is also included. The equilibrium temperature for each test closely matched the theoretical value. Results of evaluations with insulation are shown in Figure 4.

The maximum fuel rate at which complete vaporization can be expected is 1.17 lbs/hour without insulation and 1.7 lbs/hour with insulation with the engine operating at 1500 rpm and 30 lbs-ft of torque. Insulation increases the capacity of the evaporator about 45 percent at this engine operating condition. The



**FIGURE 3. EVAPORATOR TEMPERATURE VERSUS METHANOL MASS FLOWRATE WITHOUT INSULATION**



**FIGURE 4. EVAPORATOR TEMPERATURE VERSUS METHANOL MASS FLOWRATE WITH INSULATION**

evaporator capacity at the higher engine speed test point was three times what it was at the lower speed, while the engine only consumed about 35 percent more fuel. These data are summarized in Table 4. The evaporator maximum capacity, as defined by the maximum flowrate that yields an evaporator temperature slightly over equilibrium temperature, is less than the engine cylinder needs at 1500 rpm and 30 lbs- ft, but it exceeds the cylinder needs at 2000 rpm and 35 lbs-ft.

**Table 4. Maximum Evaporator Flowrates**

<u>Engine</u>		<u>Insulation</u>	<u>Evaporator Pressure (psig)</u>	<u>Evaporator Maximum Mass Flowrate (lbm/hr)</u>	<u>Maximum Flowrate as a Portion of Cylinder Needs (%)</u>
<u>Speed (rpm)</u>	<u>Torque (lb-ft)</u>				
1500	30	Uninsulated	0	1.17	37
1500	30	Uninsulated	46	1.22	38
1500	30	Insulated	0	1.70	54
2000	35	Insulated	0	5.05	112

## EVAPORATOR SIZE

The maximum allowable evaporator flowrates can be determined at any engine test point as discussed in the previous paragraph. The evaporator size is adequate at 2000 engine rpm and 35 lbs-ft and at higher loads and speeds. In Run 8, at 3000 rpm and 40 lbs-ft, the evaporator temperature was well above the equilibrium temperature, and the methanol flowrate through the heat exchanger was about 90 percent of the cylinder fuel needs. If the slope of the evaporator temperature versus fuel flowrate is similar to that at 2000 rpm and 35 lbs-ft, then the maximum fuel rate at the equilibrium temperature would be about 110 percent of the cylinder requirements. Again, it is assumed that maximum flowrate can be defined as a function of evaporator temperature.

It should be noted that all evaporator testing was done with the current-sized reactor. The current reactor does not produce high dissociation, so it does not use large amounts of exhaust heat. Therefore, more exhaust heat is available for vaporization of the methanol. A more effective reactor could require a larger evaporator.

While evaporator mapping indicated that the evaporator could not handle 100 percent of the cylinder fuel needs at the lower power level, the evaporator could easily vaporize the fuel rates required to achieve the optimum dissociation rates in terms of the maximum percent of the cylinder fuel needs.

## REACTOR SIZE

### General

From the data summarized in Table 1, it is apparent that this reactor will not provide high dissociation rates at low engine loads and speeds. Also, the

percent of cylinder fuel needs that can be met by dissociation products will be fairly low. Based on the test data, a reactor two to four times the capacity of the present one (8.05 inches long) would be required to provide dissociated products accounting for 20 to 25 percent of the cylinder fuel needs at low to moderate engine power levels.

### **Adding Heat to the Exhaust Side of the Reactor**

Improvements in overall reactor dissociation effectiveness at low engine power output, without increasing the size or effectiveness of its catalyst, requires an increase in exhaust temperature. There is little temperature loss between the engine exhaust port and the inlet to the reactor based on test data. Insulation could decrease the heat loss, but the benefit would be minimal. Exhaust temperature could be increased by burning additional fuel in the exhaust side of the reactor. The exhaust side of the reactor is coated with an oxidizing catalyst, and adding fuel would increase the exhaust temperature. However, the gain in dissociation and engine efficiency would not offset the reduction in thermal efficiency from adding fuel into the exhaust.

### **ANALYSIS OF SAMPLES**

Samples for analysis were taken from the base of the heat exchanger and routed through a heated line to a series of impingers. The first impinger was chilled to approximately 4°C with an ice-water bath. The second and third impingers were cooled to about -50°C with an isopropyl alcohol-dry ice bath. The temperature of the effluent leaving the condensers was sufficiently low to assure that almost all of the water, methanol, and dimethyl ether were condensed out, and the essentially dry gas was collected in a Tedlar bag. This sample bag and the liquid samples were then transported to the Gas Chromatograph Laboratory for analysis.

The gas chromatograph (GC) utilized a 15' x 0.125" S.S. column packed with Parapak Q 80 - 100 mesh, and was equipped with a Valco six-port gas sampling valve and a thermoconductivity detector. Calibration standards, containing measured volumes of hydrogen, nitrogen, carbon monoxide, carbon dioxide, methane and methanol, were prepared using a Tracor-Atlas 10 liter gas-blending cylinder. These standard blends were injected into the GC; then the identified peaks were integrated, and the response factors for each compound were calculated. The gas samples were injected and analyzed in the same manner as the standards.

The liquid samples were analyzed for water, DME and methanol. The volume of the water was determined by coulometry using a Photovolt Titrator. The volume of DME was determined by gas chromatography using a fused-silica, open-tubular column. The amount of methanol was determined by the difference between these two compounds and the total for all three compounds.

The results of these analyses for the tests conducted are summarized in Table 5. This table also includes the calculated value for the rate of dissociation for each test.

**Table 5. Gas Chromatograph Analysis of Heat Exchanger Samples**

Date	8/12/87	8/13/87	8/17/87	8/25/87	8/27/87	9/4/87	9/4/87
Time	14:30	15:45	11:30	16:18	11:25	12:15	14:05
Test Code (Run Number)	3	4	5	6	7	8	9
Hx Fuel Flow (lbm/hr)	1.0	.5	2.0	0.02	.95	6.3	1.1
Cylinder #1 Exhaust Mass Flow (lbm/hr)	16.3	17.11	17.36	17.26	17.90	46.3	17.20
<b><u>Air</u></b>							
Amount Liquid Condensed (g)	200	93.4	215.5	0	71.3	42.2	200.0
Volume Gas Collected (l)	107.5	142	13	9	4.3	14.0	25.0
Sampling Time (minutes)	25	30	13.7	30	30	15	30
H <sub>2</sub> /CO Mol Volume Ratio	6.3	3.2	3.5	1.7	3.7	2.3	2.1
<b><u>Gas Sample</u></b>							
Air (N <sub>2</sub> /O <sub>2</sub> ) Mol Volume Ratio	61.8/16.4	44.7/11.6	57.4/14.6	0.007/0.002	3.6/0.2	3.9/0.2	5.1/1.1
Volume % MeOH	—	1.9	4.3	1.6	17.5	8.1	1.7
Volume % H <sub>2</sub>	17	30	16.6	57.2	54.8	60.0	61.0
Volume % CO	2.7	9.5	4.7	33.8	14.9	25.7	28.7
Volume %CH <sub>4</sub>	0.2	0.3	0.4	1.8	2.2	1.1	0.7
Volume % CO <sub>2</sub>	1.9	2.0	2.0	4.7	6.8	1.1	1.3
<b><u>Condensate</u></b>							
Weight % H <sub>2</sub> O	3.2	3.9	.3	None	2.8	0.98	0.83
Weight % DME	1.0	3.1	.4	None	3.5	0.4	N/A
Dissociation (%)	5	22	1	96	7	11	5

## HEAT EXCHANGER

### History

The basic concept of a counter-flow heat exchanger made up of concentric tubes for the reactor was proposed by the EPA. The heat exchanger includes an evaporator to vaporize the methanol and a reactor to dissociate the methanol vapor. SwRI undertook the detailed design of the reactor and enlisted the assistance of Dr. R. Webb of Pennsylvania State University, as recommended by the EPA, to help design the evaporator. Fuel is injected into the evaporator from an engine-driven, specially modified, distributor-type pump built by Stanadyne. Modifications to the pump included nickel plating the interior and using ceramic rollers in the precharge section. The methanol injection nozzle, custom designed and built by SwRI, differed from existing production nozzles in that it provided full spray impingement on the evaporator walls for maximum evaporation. The reactor substrate and the methanol and exhaust side catalyst coatings were recommended and provided by Johnson-Matthey. Assembly specifications and instrumentation to monitor the heat exchanger performance were defined by SwRI. The selection of the catalysts and the basic design and dimensions were approved by the EPA in a July 31, 1985 letter to SwRI concerning design specifications.

### Current Design Consideration

Several design considerations became apparent during testing of the prototype heat exchanger. Selected considerations are discussed as follows.

**Methanol Injector** - The methanol fuel injector is currently located within the exhaust stream in the heat exchanger. With lower than maximum fuel flowrates through the evaporator, the evaporator temperature could exceed 205°C (340°F). When the internal evaporator temperature exceeded 205°C, the quality of the spray deteriorated. The primary cause of deterioration of the spray characteristics was a reduction in the injector cracking pressure (cracking pressure was monitored continuously). Reduction in cracking pressure was apparently caused by a loss in spring tension at the elevated temperatures. Vapor lock can occur with loss in cracking pressure. The seal in the top of the injector lost its elastic properties and allowed methanol to leak directly into the exhaust stream. The methanol injector should be relocated outside the exhaust stream and incorporate provisions for additional cooling.

**Evaporator** - Significant temperature instabilities were noticed during testing, particularly with the heat exchanger insulated. The cause appeared to have been the thermal lag in increasing and decreasing the temperature of the metal in the heat exchanger as conditions changed. Consideration needs to be given toward evaporator performance under transient engine operation.

Evaporator capacity, defined as the maximum fuel rate that can be injected and still maintain the internal temperature above the boiling point of methanol, is very sensitive to injector spray quality. A slight drip from the injector can reduce the maximum vaporization rate by 50 percent, based on observations during testing. The degree of atomization from the injector is a function of the cracking pressure; the droplet size decreases as the cracking pressure is increased. Atomization is advantageous when injecting fuel into a combustion chamber for immediate burning. However, in this case where it is desirable to propel the methanol against the entire surface of the wall of the evaporator, the optimum droplet size is that which allows the evaporator to

operate at maximum capacity under a given exhaust gas flowrate and temperature. Moving the injector outside the exhaust stream, where it would be exposed, would enable adjustment of the cracking pressure while observing the evaporator temperature. This would permit adjustment of the cracking pressure to achieve optimum droplet size.

The catalyst used in this reactor to dissociate the methanol provided unsatisfactory yields at low to moderate engine power levels; these power levels are considered representative of typical light-duty engine use. A catalyst with higher dissociation effectiveness at lower temperatures is needed to enable a reasonable reactor size and mass. The catalyst furnished by Johnson-Matthey is their proprietary Type H. This catalyst has a maximum dissociation rate at 370°C (698°F), with significant yields at 300°C (572°F). In the evaluations conducted, the average methanol-side reactor temperatures with insulation were generally at or above 300°C. At lower loads and speeds, such as idle, lower temperatures with reduced dissociation can be expected. Higher loads and speeds will generate temperatures considerably higher than the 370°C optimum temperature.

**Exhaust Back-Pressure** - The increase in exhaust back-pressure was significant, being about 1.6 inches of Hg with the engine operating at 3000 rpm and 40 lbs-ft. This increase in back-pressure was sufficient to increase the exhaust temperature at the cylinder by about 80°C at this engine operating condition.

## CONCLUSIONS AND RECOMMENDATIONS

Given the current catalyst effectiveness, it appears that satisfactory heat exchanger performance cannot be achieved with a design that will fit reasonably under the hood of a vehicle. Redesign of the existing reactor would require that it be increased in size by a factor of two to four to provide minimum satisfactory dissociation rates at low engine power levels. Such an increase in size would result in increased thermal lag and could require an increase in evaporator size to offset lower exhaust temperatures exiting from the larger reactor.

Given the low dissociation effectiveness at low to moderate engine speeds and loads, it is doubtful the current heat exchanger design would prove satisfactory under transient operation in a vehicle. Most advantageous would be a dissociation catalyst that is more effective over a wider temperature range. There is, however, no known source for such a catalyst.

**ADDITIONAL DATA FROM EVALUATION OF METHANOL DISSOCIATION HEAT EXCHANGER DISSOCIATOR<sup>a</sup>**

<u>PARAMETER</u>	<u>RUN 6</u>	<u>RUN 4</u>	<u>RUN 7</u>	<u>RUN 3</u>	<u>RUN 9</u>	<u>RUN 5</u>	<u>RUN 8</u>
Date	08/25/87	08/13/87	08/27/87	08/12/87	09/04/87	08/17/87	09/04/87
Time	1618	1545	1125	1430	1405	1130	1215
<b><u>ENGINE OPERATION</u></b>							
Speed, rpm	1500	1500	1500	1500	1500	1500	3000
Torque, ft-lb	30	30	32	30	30	30	40
Methanol Consumption, lb/hr	12.8	11.7	13.2	12.7	10.8 <sup>b</sup>	12.7	28.2
Intake Air, lb/hr	56.3	56.7	58.4	52.6 <sup>b</sup>	58.0	56.7	157.0
Spark Advance, °BTC	20	20	20	20	22	20	28
Exhaust/Cylinder, lb/hr	17.3	17.1	17.9	16.3 <sup>b</sup>	17.2	17.4	46.3
Exhaust Temperature, °F	881 <sup>c</sup>	813	822	791	840 <sup>c</sup>	773	1148 <sup>c</sup>
<b><u>AMBIENT</u></b>							
Temperature, °F	96	92	89	97	87	90	88
Barometric Pressure, in.Hg	29.1	29.0	29.3	29.0	29.2	29.2	29.2
<b><u>DISSOCIATOR</u></b>							
Insulated <sup>d</sup>	YES	NO	NO	NO	YES	NO	YES
Methanol Flow, lb/hr	0.02	0.50	0.95	1.00	1.10	2.00	6.30
Nozzle Pressure, psig	225	135	110	90	45	150	175
<b>Exhaust Pressures, in. Hg:</b>							
Before Reactor	0.3	0.1	0.3	0.0	0.2	0.1	1.1
After Reactor	0.2	0.0	0.2	0.0	0.1	0.0	0.5
After Evaporator	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>Exhaust Temperature, °F:</b>							
Before Reactor	905 <sup>c</sup>	790	763	707	877 <sup>c</sup>	658	1167 <sup>c</sup>
After Reactor	908 <sup>c</sup>	652	--	419	721	171 <sup>b</sup>	863
After Evaporator	732	422	165	210	244	162	691
Backpressure on Evaporator, psig	0.0	0.0	33	0.0	0.0	0.0	0.0
<b>Methanol Temperature, °F:</b>							
In Evaporator	--	392	176	198	352	162	345
After Reactor	--	518 <sup>b</sup>	--	666	788	576	1140

<sup>a</sup>Data presented in order based on methanol flowrate into the dissociation.

<sup>b</sup>Data appears to be somewhat low.

<sup>c</sup>Apparent minor discrepancy in these data based on location in system.

<sup>d</sup>Around the outside of the heat exchanger unit.

## **APPENDIX I**

### **ENGINE MODIFICATIONS FOR A DISSOCIATED PRODUCT VALVE**

## SUMMARY OF ENGINE MODIFICATIONS FOR OPERATION AND CONTROL OF DISSOCIATED PRODUCT VALVE

### 1. General

The dissociated product valve for each cylinder will be actuated by a separate additional camshaft that will be driven via a short chain from an additional sprocket attached to the existing camshaft sprocket. The drive will be purely mechanical. This simplicity has the advantages of providing reliable and repeatable valve operation. It has the disadvantage of not allowing variation in valve opening duration which could be used to control the flow of dissociated products to the cylinder. Approaches using solenoid operated valves were considered, but they were expensive, were still in the development stage and their full-time control would have added substantially to the demands of the control system.

### 2. Dissociated Product Inlet Valve Assembly

In order to save project time and money and to reduce development risks, we chose an existing valve assembly for this purpose. The valve is designed as an exhaust valve for a Honda motorcycle engine. Given its design and proven street performance we feel that it will perform adequately as a dissociated products inlet valve. The motorcycle exhaust valve is exposed to high accelerations given the engine redline of approximately 10,000 rpm, and high temperature gas flows over 1500°F. The valve face will be exposed to somewhat lower combustion chamber temperatures in the NAPS-Z engine operating on methanol than those of the gasoline fueled Honda engine. Also, the dissociated product maximum temperature of about 600°F means that the dissociated product inlet valve will be exposed to lower gas flow temperatures than it would on the engine it is designed for.

The stock NAPS-Z engine head is aluminum and it has steel valve seats pressed into it to provide adequate durability. Our design provides for a "caged" valve assembly similar in design concept to that used on large bore low speed diesel engines and to the third valve in Mitsubishi MCA jet engines. Diesel engines contain this feature to minimize the time required to perform valve overhaul or replacement. This design feature was included in our design to provide a material suitable for hardening at the valve seat, to provide a guide and mount for the valve and valve spring, and to port dissociated products from the reactor outlet to the cylinder. Providing a valve seat that adequately resists wear is important particularly with hydrogen and carbon monoxide as the primary products being transmitted through this valve. Dry gases like natural gas or propane, and we suspect, hydrogen and carbon monoxide, cause an increase in valve wear over that experienced with unleaded gasoline.

### 3. Pushrod

A short pushrod is provided between the overhead cam and the valve stem. Its primary purpose is to provide a mechanical link between the cam surface and the valve stem. If the valve chosen had a longer stem it would not be necessary to have the pushrod. In fact, an extension could be friction welded to the valve stem to provide the additional length needed. However, the pushrod performs two other functions which make this concept desirable. Most importantly, it accommodates side loads induced from the cam. This arrangement minimizes bending loads on the valve stem and friction between the stem and the valve guide. It also permits the cam follower to be integrated with the pushrod so that the valve will accurately follow the cam profile (which includes concave surfaces) and so that an adequately wide surface can be

provided to reduce wear to acceptable levels. Calculations covering contact loads are discussed in paragraph 10.

#### 4. Overhead Cam

The cam profile was defined using a computer program written especially for that purpose. A number of general purpose cam profile and valve train analysis programs are available in the department, but they are not suitable for the unique cam shape required for this application. The concave surfaces of the cam are necessary given the short duration of valve lift, the small diameter cam defined by the engine configuration, and the desire to keep the valve train mass to a minimum. Calculations summarizing the cam profile design and the computer listing and output are attached in Appendix IVB.

#### 5. Dissociated Product Valve Cam Chain Drive

The NAPS-Z engine manual that we purchased and the documentation you sent us are adequate to define the cam drive concept. We do have a head that provides some dimensions, but practical determination of details requires an engine complete with all valve train components. A general concept using a chain drive between the existing and new camshafts has been devised. The specifics will be worked out after the engine is received.

#### 6. Dissociated Product Valve Temperature and Pressure Characteristics

The temperature environment for the valve is less stringent than that which it is designed for (exhaust). The back of the valve will be exposed to the reactor pressure of up to 100 psig, but it will be prevented from opening by sufficient preload on the valve spring. We had considered some pressure balanced valve designs to remove variation in reactor pressure as a consideration in determining valve spring rate, but the added complexity, particularly with regard to sealing and lubrication of the balancing piston, made this concept impractical.

#### 7. Valve Assembly Details

Appendix J summarizes the calculations for these. Some specific values are summarized below.

Parameter	Value
Required valve lift	0.156 in.
Design Cam Speed (@ 4500 engine rpm)	2250 rpm
Minimum spring force required to seat valve against maximum (150 psig) reactor force	46 lbf
Combined spring rate (as measured)	330 lbf/in.
Combined maximum allowable spring compression	0.50 in. (0.557 in. for outer) (0.510 in. for inner)
Spring force available at zero lift	113.5 lbf ( 46 lbf required)

<u>Parameter</u>	<u>Value</u>
Available spring force at maximum valve lift	165 lbf
Valve assembly dynamic weight	0.194 lbf
Maximum allowable cam generated deceleration (spring controlled)	328,639 in/sec <sup>2</sup>

## 8. Cam Profile

The equations and the computer program used for developing the cam profile are listed in Appendix K along with the cam radius versus degrees. A summary of critical values are as follows:

Ramp height = 0.034 in.

Maximum acceleration between stations 2-3 = 217,809 in/sec<sup>2</sup>

Maximum acceleration between stations 3-4 = 138,569 in/sec<sup>2</sup>

Maximum valve displacement = 0.177 in.

Maximum valve displacement needs to be between 0.156 inches minimum lift and 0.190 inches maximum lift (sum of ramp and required lift).

## 9. Follower Radius

The cam profile listed in Appendix K was drawn approximately 20 times larger over the approximately 45° one-half lift duration to provide a visual check that the calculated cam profile was acceptable. This large scale drawing of the cam profile also provided a useful tool for determining the maximum allowable follower radius of 0.06 inches.

## 10. Contact (Hertz) Stresses

The contact stresses between the cam surface and the curved follower on the pushrod were checked to see if these were excessive. Maximum Hertz stresses which are a result of both static (spring) and dynamic forces were calculated as follows (Reference 2, pg. 87):

<u>Cam Width (in.)</u>	<u>Maximum Stress (psi)</u>
0.5	231
0.625	207
0.75	189

Hertz stresses are not a problem so cam and follower design will primarily consider wear as the limiting constant.

## 11. Follower Jumping Speed

The speed at which the follower will no longer maintain contact with the cam surface is a function of the cam profile, camshaft speed and natural frequency of the valve gear. Using the methods outlined in Reference 1, Volume II, page 541, the natural frequency of the valve train was found to be excited at 3868 crankshaft rpm. This is well within the operating speed range of the engine. A change to correct this will be made (one man-day effort).

## 12. Valve Guide Material Considerations

The preferred material for the valve guide is cast iron. It is usually chosen for production applications because of its low cost and resistance to wear. In this case a high carbon low-alloy tool steel will be chosen because of ease in machining, medium strength and wear resistance.

## 13. Valve Guide and Cam Follower Lubrication

A thin film of oil must be established between the cam follower and the cam surface and some oil must be available at the valve guides and pushrod guides. Given the conceptual design shown on our layout drawings it will not be a problem in providing oil to the pushrod guide. Oil supplied to the cam and follower will drain down over the pushrod guide and then to the valve guide. In conventional engine design some care is taken to assure that the valve guide is not covered with oil but does receive lubrication from oil splashed in the rocker cover volume. The reason for avoiding an accumulation of oil at the top of intake valve guides is that the differential pressure between the rocker box and the intake port tends to drive oil into the port and then to the cylinder thus causing excessive oil consumption and exhaust emissions. This particular application has a pressure differential between the dissociated product port and the rocker, but the pressure on the valve side will most often be greater than that in the valve cover. Nonetheless, oil needs to be directed at the dissociated product valve guide and not allowed to submerge it. An oil drain back to the engine sump will be provided at the base of the dissociated product valve assembly.

## 14. Valve Seat Material

The dissociated product valve seat will be incorporated in the sleeve that is part of the valve assembly. This assembly will be made up outside the engine then inserted in the head and fastened in place. It is a "caged" valve concept, much like those used on larger engines. The sleeve material will be a medium carbon, medium alloy, heat treatable steel such as SAE 3140 or 4140. It will be hardened after initial machining and before final grinding to 40-46 R<sub>C</sub>.

The basic attributes are that the seat must resist pound-in, hot hardness, abrasion, corrosion, and creep at high temperature. Because of assembly considerations, the head material (aluminum alloy) was never considered for a valve seat. It would be poorly suited for this purpose. This particular application may be more severe given the essentially dry gas composition (CO and H<sub>2</sub>) from the reactor. However, the less than 100% reactor efficiency will mean that some vaporized methanol will be passing and this will be to the benefit of the valve seat by reducing the tendency to wear.

Thermal expansion and thermal conductivity of the valve seat are of some concern also. The application of similar alloy steels in valve seats in aluminum-based heads is fairly common. A nominal press fit of 0.003 in./in. diameter is suggested in SAE Recommended Practice J610b for cast iron or aluminum heads. Because the dissociated product valve seat will be exposed to lower gas temperatures than the exhaust valve seat and because coolant passages are about the same distance from each, this basic approach is considered satisfactory.

## 15. References

- 15.1 Taylor, C. F., "The Internal Combustion Engine in Theory and Practice," Volumes I and II, The MIT Press, Revised Edition, 1985.
- 15.2 Shigley, J. E. and Mitchell, L. D., "Mechanical Engineering Design," Fourth Edition, 1983.

**APPENDIX J**  
**VALVE ASSEMBLY CALCULATIONS**

## SUMMARY OF CONDITIONS FOR CAM DESIGN

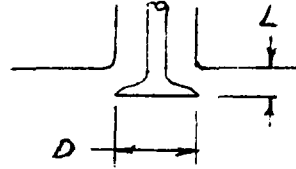
### 1. Valve Lift

$$A_{\text{port}} = A_{\text{valve opening}}$$

$$\frac{\pi D^2}{4} = \pi D L$$

$$L = D/4$$

$\frac{D}{0.75}$	$\frac{L}{0.1875}$
0.625	0.156*



### 2. Cam Speed

(= ½ engine speed)

		<u>rpm</u>	
Eng Speed	6000	5000	4500
Cam Speed	3000	2500	2250
		<u>rad/sec</u>	
Cam Speed	~314	~262	~236
			$37.5 * 2 * \pi$

### 3. Minimum Spring Force Required (to seat valve with reactor pressure)

	<u>Valve Diameter (in.)</u>	
	<u>0.75</u>	<u>0.625</u>
100 psig	44 lbf	31 lbf
150 psig	66	46

### 4. Spring Rate

$$(150 + 180 \text{ lbf/in}) = 330 \text{ lbf/in}$$

### 5. Allowable Compression

Large: 0.557 inch

Small: 0.510 inch

Allow.: 0.5 inch

### 6. Required Lift

$$L = 0.156 \text{ in. (see paragraph 1)}$$

### 7. Force Available with Zero Lift

$$0.5 - 0.156 = 0.344 \text{ inch}$$

$$.344m(180 \text{ lbf/in} + 150 \text{ lbf/in}) = 113.5 \text{ lbf}$$

$$113.5 \text{ lbf} > 66 \text{ lbf required minimum}$$

**8. Maximum Force at Maximum Lift**

$$0.5 \text{ in. } (180 \text{ lbf/in.} + 150 \text{ lbf/in.}) = 165 \text{ lbf}$$

**9. Valve Assembly Weight**

	<u>grs</u>	<u>With ½ Spring</u>
Valve	26.0	26.0
Two springs	54.5	27.3
Keeper and washer	9.9	9.9
Pushrod (assume)	25	25.0
		<hr/> 88.2 grs

$$88.2 \text{ grs} \times \frac{2.205 \text{ lbm}}{1000 \text{ grs}} = 0.194 \text{ lbm}$$

**10. Maximum Allowable Cam Deceleration**

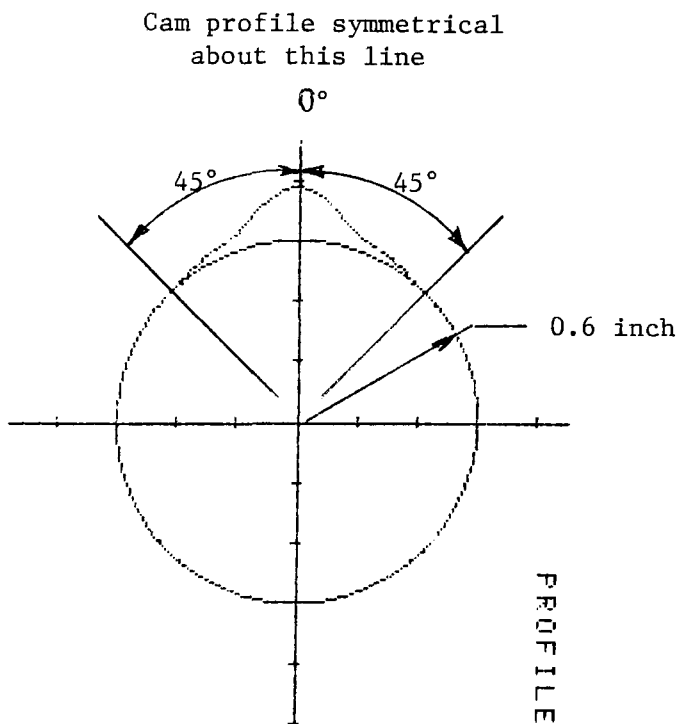
$$F = ma, a = \frac{F}{m} = \frac{386.4 \text{ in.} \times 165 \text{ lbf}}{0.194 \text{ lb-sec}^2}$$

$$= 328,639 \text{ in/sec}^2$$

## **APPENDIX K**

### **CAM PROFILE PROGRAM AND OUTPUT**

# CAM PROFILE FOR DISSOCIATED PRODUCT INLET VALVE



DEGREES	(INCHES) RADIUS
0	77697
1	77406
2	7704
3	76599
4	76083
5	75495
6	74835
7	74106
8	73309
9	72448
10	71526
11	70546
12	6953
13	68526
14	67578
15	66711
16	65946
17	65295
18	6476
19	64338
20	64012
21	63762
22	6356
23	63378
24	632
25	63022
26	62844
27	62667
28	62489
29	62311
30	62133
31	61956
32	61778
33	616
34	61422
35	61244
36	61067
37	60889
38	60711
39	60533
40	60356
41	60178
42	6
43	6
44	6
45	6

```

10 ! EPACAM
20 ! CALCULATE CAM PROFILE
30 ! G. DRISCOLL, JULY 1985
40 K=.0983 ! DISP UNDER ACCEL
50 L=.156 ! IN
60 W=75*PI ! RAD/SEC (3000 RPM)
62 A6=0
63 A7=0
64 V5=0
65 V6=0
66 V7=100
67 S6=0
68 S5=0
70 T1=0
80 D=1/13500 ! TIME INCREMENT
90 B=.6 ! BASE CIRCLE RADIUS
100 INTEGER I,J
110 SHORT A(1000),V(1000),S(1000)
    ,H(1000)
120 PRINT "K=";K
130 PRINT "L=";L;"IN"
140 PRINT "W=";W;"RAD/SEC"
150 PRINT "B=";B;"IN RADIUS"
155 PRINT "D=";D;"SEC INCREMENT"
160 RAD
170 V9=24 ! IN/SEC RAMP SPEED
180 FOR J=1 TO
185 ! J=5
190 GCLEAR
200 IF J=2 THEN 290
210 IF J=3 THEN 350
220 IF J=4 THEN 410
230 SCALE 0, .02, -500000, 500000
    J=1
240 XAXIS 0, .002, 0, .02
250 YAXIS .01, 100000, -500000, 500
    000
260 MOVE 014, 400000
270 LABEL "ACCEL"
280 GOTO 460
290 SCALE 0, .02, -250, 250 ! J=2
300 XAXIS 0, .002, 0, .02
310 YAXIS .01, 50, -250, 250
320 MOVE 014, 200
330 LABEL "VELOCITY"
340 GOTO 460
350 SCALE 0, .02, 0, .2 ! J=3
360 XAXIS 0, .002, 0, .02
370 YAXIS .01, .02, 0, .2
380 MOVE 014, .18
390 LABEL "DISPL"
400 GOTO 460
410 SCALE -1.2, 1.2, -.9, .9 ! J=4
420 XAXIS 0, 2, -1, 1
430 YAXIS 0, 2, -1, 1
440 MOVE .5, .8
450 LABEL "PROFILE"
460 MOVE 0, 0
470 FOR T=0 TO 0134 STEP D
480 I=T/D
490 T1=.77166706*PI/W
500 T2=7*PI/8/W
510 T3=15*PI/16/W
515 T4=PI/W
520 T5=17*PI/16/W
530 T6=9*PI/8/W
540 T7=0
550 T8=0
560 IF T<T1 THEN 660 ! DWELL
570 IF T<T2 THEN 790 ! RAMP
580 IF T<T3 THEN 950 ! ACCEL
590 IF T=T3 THEN 1130
600 IF T<T5 THEN 1140 ! DECEL
610 IF T=T5 THEN 1350
620 IF T<T6 THEN 1360 ! ACCEL
630 IF T=T6 THEN 1530
640 IF T<T7 THEN 1540 ! RAMP
650 IF T<=T8 THEN 1700 ! DWELL
660 A=0
670 A(I)=A
680 V=0
690 V(I)=V
700 S=0
710 S(I)=S
720 H=S+B
730 H(I)=H
740 IF J=1 THEN DRAW T,A
750 IF J=2 THEN DRAW T,V
760 IF J=3 THEN DRAW T,S
770 IF J=4 THEN DRAW H*COS(T*W),
    H*SIN(T*W)
780 GOTO 1820
790 A=0
800 A(I)=A
810 V1=V
820 V=V9
830 V(I)=V
840 S1=S
850 S=V9*D+S1
860 S(I)=S
870 H=S+B
880 H(I)=H
890 ! PRINT A;V;S
895 IF J=1 THEN DRAW T,A
900 IF J=2 THEN DRAW T,V
910 IF J=3 THEN DRAW T,S
920 IF J=4 THEN DRAW H*COS(T*W),
    H*SIN(T*W)
930 S3=MAX(S1,S)
940 GOTO 1820
950 A1=A ! A1=PREVIOUS A
960 A=(T4/(T3-T2))^2*W^2*K*L*SIN
    (T4/(T3-T2)*W*(T-T2))
970 A(I)=A
980 A6=MAX(A6,A)
990 V1=V
1000 V=0*(A+A1)/2+V1
1005 ! V=-((16.6751*K*L*W*COS(16.
    6751*W*(T-T2)))+V9+16.6751*
    K*L*W

```

```

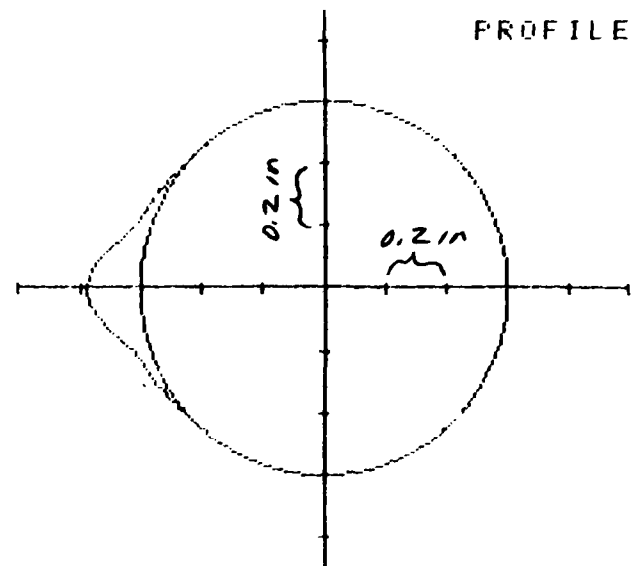
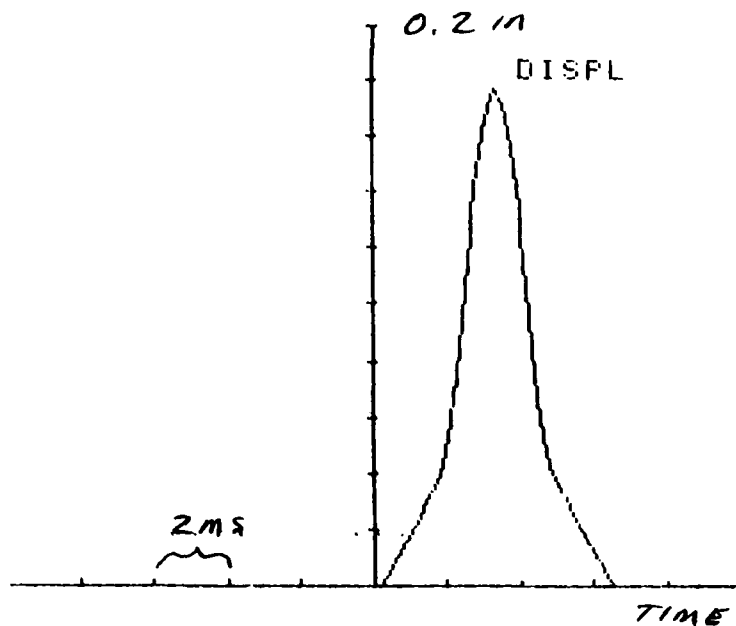
1007 V5=MAX(V5,V)
1010 V(I)=V
1020 S1=S
1025 ! S=K*L*SIN(16.6751*W*(T-T2)))+S3
1030 S=D*(V+V1)/2+S1
1035 S5=MAX(S5,S)
1040 S(I)=S
1050 ! PRINT T;S
1060 H=S+B
1070 H(I)=H
1080 IF J=1 THEN DRAW T,A
1090 IF J=2 THEN DRAW T,V
1100 IF J=3 THEN DRAW T,S
1110 IF J=4 THEN DRAW H*COS(T*W),H*SIN(T*W)
1120 GOTO 1820
1130 A=0
1135 S2=S
1136 V2=V
1140 A1=A
1150 ! A=-((69.5149*(1-K)*L*W^2*SIN(8.3376*W*(T-T3)))
1155 A=-((T4/(T6-T2))^2*W^2*L*SI
N(T4/(T6-T2)*W*(T-T2)))
1157 ! PRINT T;A
1160 A(I)=A
1170 A7=MIN(A7,A)
1180 V1=V
1190 V=D*(A+A1)/2+V1
1195 ! V=4.1688*W*L*(1-K)*COS(4
1688*W*(T-T2))
1200 V(I)=V
1210 V6=MAX(V6,V)
1220 V7=MIN(V7,V)
1230 S1=S
1240 S=D*(V+V1)/2+S1
1245 ! S=(1-K)*L*SIN(4.1688*W*(T
-T2))+S2
1250 S6=MAX(S6,S)
1260 S(I)=S
1270 ! PRINT T;S
1280 H=S+B
1290 H(I)=H
1300 IF J=1 THEN DRAW T,A
1310 IF J=2 THEN DRAW T,V
1320 IF J=3 THEN DRAW T,S
1330 IF J=4 THEN DRAW H*COS(T*W),H*SIN(T*W)
1340 GOTO 1820
1350 A=0
1360 A1=A
1370 A=278.0596*K*L*W^2*SIN(16.6
751*W*(T-T5))
1380 A(I)=A
1390 V1=V
1400 V=D*(A+A1)/2+V1
1410 V(I)=V
1420 S1=S
1430 S=D*(V+V1)/2+S1
1440 S(I)=S
1450 ! PRINT A;V;S
1460 H=S+B
1470 H(I)=H
1480 IF J=1 THEN DRAW T,A

```

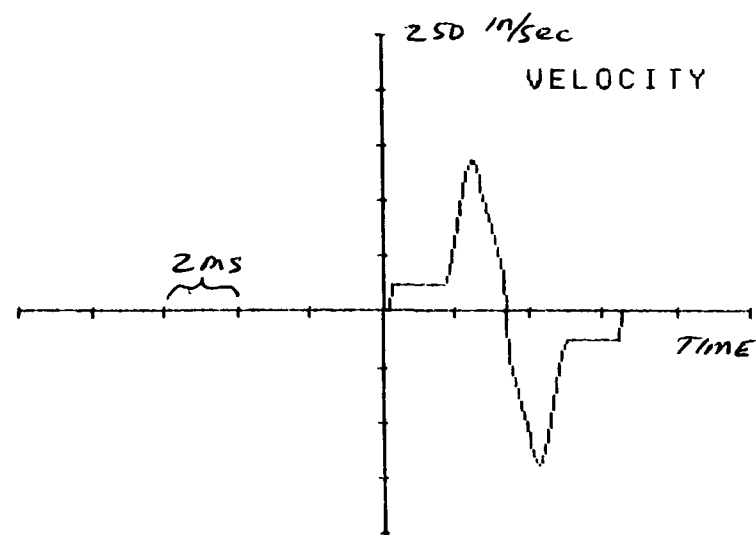
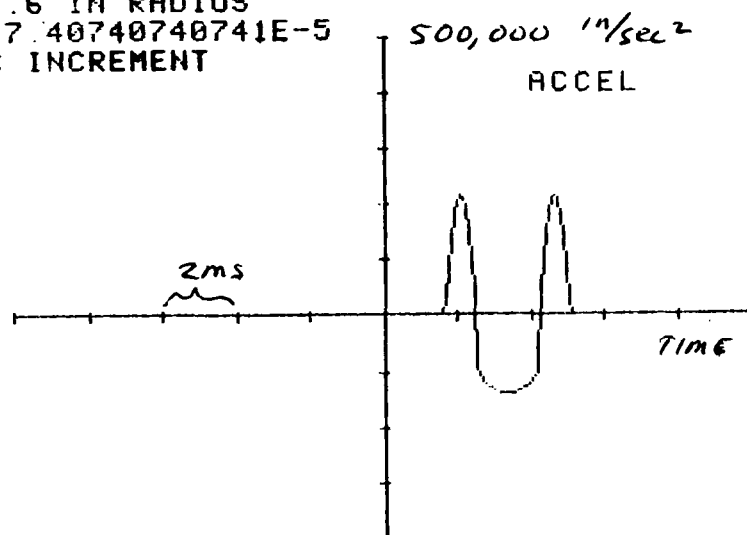
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1490 IF J=2 THEN DRAW T,V
1500 IF J=3 THEN DRAW T,S
1510 IF J=4 THEN DRAW H*COS(T*W),H*SIN(T*W)
1520 GOTO 1820
1530 A=0
1540 A1=A
1550 A=0
1560 A(I)=A
1570 V1=V
1580 V=-V9
1590 V(I)=V
1600 S1=S
1610 S=V*D+S1
1620 S(I)=S
1630 H=S+B
1640 H(I)=H
1650 ! PRINT A;V;S
1660 IF J=2 THEN DRAW T,V
1670 IF J=3 THEN DRAW T,S
1680 IF J=4 THEN DRAW H*COS(T*W),H*SIN(T*W)
1690 GOTO 1820
1700 A=0
1710 A(I)=A
1720 V=0
1730 V(I)=V
1740 S=0
1750 S(I)=S
1760 H=S+B
1770 H(I)=H
1780 IF J=1 THEN DRAW T,A
1790 IF J=2 THEN DRAW T,V
1800 IF J=3 THEN DRAW T,S
1810 IF J=4 THEN DRAW H*COS(T*W),H*SIN(T*W)
1820 NEXT T
1830 FOR I=1/75/D-1 TO 0 STEP -1
1840 T=2/75-I*D+D
1850 IF J=1 THEN DRAW T,A(I)
1860 IF J=2 THEN DRAW T,-V(I)
1870 IF J=3 THEN DRAW T,S(I)
1880 IF J=4 THEN DRAW H(I)*COS(T*W),H(I)*SIN(T*W)
1882 ! PRINT
1883 ! PRINT "DEGREES","RADIUS"
1884 ! FOR I=180 TO 120 STEP -1
1885 ! PRINT 180-I,H(I)
1886 ! NEXT I
1890 NEXT I
1900 IF J<4 THEN 1940
1910 FOR Z=0 TO 2/75 STEP D
1920 DRAW B*COS(Z*W),B*SIN(Z*W)
1930 NEXT Z
1940 COPY
1950 PRINT
1960 PRINT
1970 NEXT J
1980 PRINT "SRAMP=";S3
1990 PRINT "MAXA(ACCEL)=";A6
2000 PRINT "MINA(DECCEL)=";A7
2010 PRINT "MAXV(DECCEL)=";V6
2020 PRINT "MINV(DECCEL)=";V7
2030 PRINT "MAXS(TOTAL)=";S6
2035 PRINT "MAXS(ACCEL)=";S5
2040 END

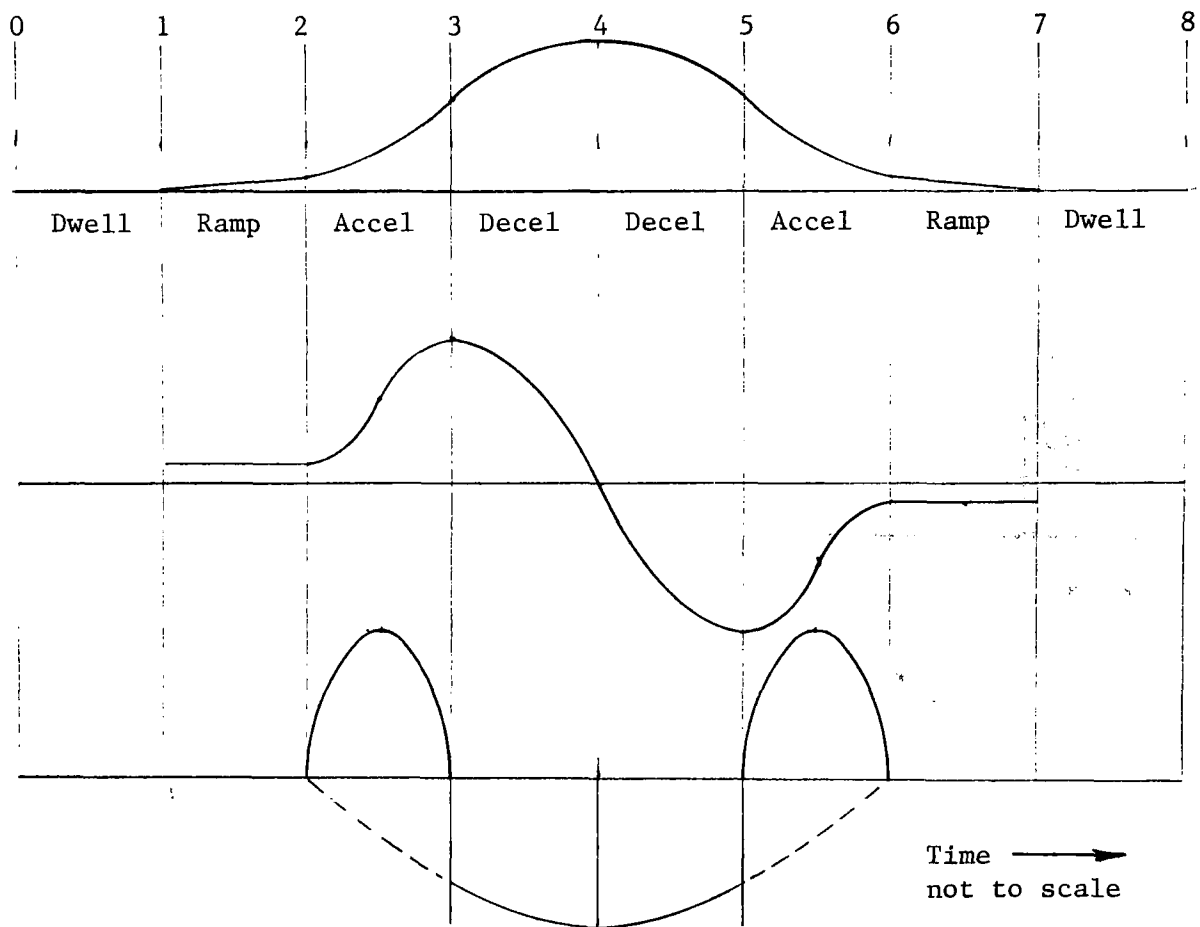
```



K = .0983  
L = .156 IN  
W = 235.619449019 RAD/SEC  
B = .6 IN RADIUS  
D = 7.40740740741E-5  
SEC INCREMENT



# C1. Cam Profile



For Stations 2-3 and 5-6 ( $\beta = 16$ )

$$y = -KL \sin \beta W (t - t_2) + V_{\text{ramp}} (t - t_2) + KL \beta W (t - t_2)$$

$$\dot{y} = -KL \beta W \cos \beta W (t - t_2) + V_{\text{ramp}} + KL \beta W$$

$$\ddot{y} = KL (\beta W)^2 \sin \beta W (t - t_2)$$

For Stations 3-4 and 4-5 ( $\alpha = 4$ )

$$y = L \sin \alpha W (t - t_2)$$

$$\dot{y} = \alpha W L \cos \alpha W (t - t_2)$$

$$\ddot{y} = -(\alpha W)^2 L \sin \alpha W (t - t_2)$$

## C2. Equations for Cam Development

<u>Station</u>	<u>Portion</u>	<u>Function</u>
0-1	Dwell	$H = B$
1-2	Ramp	$H = S + B$ $S = V_{\text{ramp}}(\Delta T)$ $A = 0$
2-3	Acceleration	$A = KL\beta^2W^2 \sin\beta W(t - t_2)$ $V = \int A dt + V_{\text{ramp}}$ $S = \int \int A dt + \int V_{\text{ramp}} dt$
3-4	Deceleration	$A = \alpha^2W^2 L \sin\alpha W(t - t_2)$ $V = \int A dt + V_3$ $S = \int \int A dt + \int V_3 dt$
4-8	Remainder	Symmetrical with first 180° generated

### C3. Variable Definitions for Equations in Paragraph C2

<u>Label</u>	<u>Definition</u>
H	Cam radius ( = S + B)
S	Valve displacement (0 is equivalent to valve closure)
B	Cam base circle radius = 0.600 inch
K	Coefficient applied to acceleration function for station 2-3 to make the cam profile equal at the junction of stations 2-3 and 3-4.
L	Desired valve lift above ramp (0.156 inch)
W	Rated cam speed = 22500 rpm (4500 engine rpm)
A	Acceleration of valve assembly
V	Velocity of valve assembly
V <sub>ramp</sub>	Ramp velocity = 24 in/sec as per Taylor, Vol. II, pg. 539.
t <sub>n</sub>	Time at station assuming zero elapsed time at station 0 and cam at rated speed (W).
t	Current time
$\beta$	Ratio of camshaft displacement to displacement of angle generating sinusoid between stations 2-3 ( = 16).
$\alpha$	Ratio of camshaft displacement to displacement of angle generating sinusoid between stations 3-4 ( = 4).

#### C4. List of Variables in Program "EPACAM"

B	=	base circle radius	T	=	time
D	=	time increment	T1	=	end of dwell
A	=	acceleration	T2	=	end of ramp
A1	=	previous acceleration value	T3	=	end of acceleration
A7	=	minimum acceleration	T5	=	end of deceleration
A(I)	=	acceleration array	T6	=	end of acceleration
A6	=	maximum acceleration	T7	=	end of ramp
			T8	=	"0" point
			V	=	velocity
H	=	cam final radius	V1	=	previous value of velocity
I	=	array subscript	V2	=	maximum velocity at end of acceleration
J	=	defines acceleration, velocity, displacement, or profile	V6	=	maximum velocity during acceleration
K	=	ratio of displacement under acceleration to displacement under deceleration	V5	=	maximum velocity during acceleration
			V7	=	minimum velocity during acceleration
L	=	maximum lift	V(I)	=	velocity array
S	=	displacement	W	=	camshaft speed
			Z	=	factor used to generate base circle
S1	=	previous value of displacement			
S(I)	=	displacement array			
S3	=	displacement at end of ramp			
S6	=	maximum displacement (total) during deceleration			
S2	=	maximum displacement end of acceleration			

## **APPENDIX L**

### **METHANOL DISSOCIATION HEAT EXCHANGER DESIGN REVIEW**

# SOUTHWEST RESEARCH INSTITUTE

POST OFFICE DRAWER 28510 • 6220 CULEBRA ROAD • SAN ANTONIO, TEXAS, USA 78284

February 12, 1988

ENGINE AND VEHICLE RESEARCH DIVISION

Mr. Robert Bruetsch  
United States Environmental Protection Agency  
Motor Vehicle Testing Laboratory  
2565 Plymouth Road - ECTD  
Ann Arbor, MI 48103

**Subject: Methanol Dissociation Heat Exchanger - Design Review and Proposed Improvements, EPA Contract No. 68-03-1984, SwRI Project No. 03-8352.**

The technical design review findings and proposed improvements presented are primarily based on observations of the preparer since he became involved with this project in December of last year. In keeping within project constraints, the design review has been limited. The proposed improvements are considered to be incremental and should not be misconstrued as changes that will assure satisfactory methanol dissociation performance. Areas of technical concern or improvement are discussed as follows:

**DISSOCIATION CATALYST** - The base metal catalyst used in the initial heat exchanger did not provide satisfactory dissociation. A copy of the preliminary results of the catalyst analyses by JM is included as Attachment A. From a brief review of the published literature and discussions with individuals at JM, EPA, and SwRI, it appears that a fully appropriate dissociation catalyst composition has not yet been identified. The writer has been unable to find a catalyst composition that will provide the essential characteristics of high dissociation efficiency at low temperature, durability at somewhat higher temperatures, and negligible coking characteristics. The primary requirement for developing a methanol dissociation heat exchanger is the identification of a suitable dissociation catalyst composition.

**VERIFICATION OF CATALYST EFFICIENCY** - Until sufficient operating history has been developed on a specific catalyst composition, it is recommended that a sample from each batch provided be analyzed to assure it meets design specifications. At minimum, such analyses should include determination of effective surface area and bench determination of dissociation efficiency.

**CATALYST RECOMMENDATION** - The representative from Johnson Matthey, like the writer, feels that reconsideration of catalyst composition and bench evaluation of samples of the actual batch to be used are essential. From the first contact in December of last year, the JM representative has emphasized their current overload with high priority programs. Johnson Matthey will be unable to schedule review, formulation, fabrication, and bench evaluations of methanol dissociation catalysts for several months. Total time to obtain catalyst substrates is estimated to be six months. If a currently applied catalyst composition, such as platinum, is used and no bench evaluations are required, it was indicated that such substrates could likely be provided within a couple of months. As previously discussed, however, the writer has been unable to find any reasonable basis on which to recommend any specific catalyst composition.

**EVAPORATOR** - The present evaporator involves a closed cylinder wrapped with corrugated metal catalyst substrate. Because the engine exhaust gases first pass through the exhaust catalyst in the dissociation reactor, which should oxidize essentially all available HC and CO, the catalyst wrapped around the evaporator appears to serve no useful function. Additionally, the corrugated catalyst substrate effectively isolates most of the exhaust flow away from the evaporator. By removing the catalyst substrate from around the evaporator and installing longitudinal fins onto the outer surface, heat transfer from the exhaust to the evaporator should increase significantly. Another potential improvement is to have the cone in the evaporator open to the exhaust, rather than closed as in the present design.

**DISSOCIATION REACTOR** - One design improvement involves the exhaust flow through the reactor section of the methanol dissociation heat exchanger. With reference to the original design of the reactor shown in Attachment B, the center section of the exhaust catalyst was designed to carry the same exhaust heat per circumferential unit as the two outer sections of the exhaust catalyst. Since the center sections provides heat to methanol catalysts on both radial sides, it should be designed to carry more exhaust heat. Incorporating this design improvement involves only minor redesign. Another recommended improvement is to increase the methanol dissociation annuli from two to three as illustrated in the revised design shown in Attachment B. A third improvement would be to increase the void space at the entrance and exit of the dissociation annuli and to provide four exit ports from the annuli, rather than the two as in the initial design.

**INJECTOR DESIGN AND LOCATION** - The commercially available injector that can be utilized with only minor modification is illustrated in Attachments C and D. This configuration is considered to be satisfactory and about as good as can be attained without major redesign effort. An essential design modification is relocation of the methanol injector out of the exhaust stream. Relocation is shown conceptually in Attachment E.

**INTERNAL INSULATION** - Inclusion of internal insulation, such as 3M Interam, around the outer diameter of the dissociation reactor would provide for good conservation of heat, and it would also provide for a much more professional appearance than does insulation installed around the overall heat exchanger assembly. The disadvantage of internal insulation is the resultant 17 percent loss of potentially useable cylindrical area. That loss in area can be made up by addition of the smaller annulus in the center of the dissociation reactor as illustrated by the revised design shown in Attachment B. Adding internal insulation in the area around the evaporator will result in the necessity to also reduce the diameter of the evaporator, as illustrated in Attachment D.

A possible solution to the current size limitation of 3.75 inches overall outside diameter on the heat exchanger would be to make the heat exchangers elliptical. Without extensive design and fabrication efforts, however, an elliptical shape would be impractical. Fabrication and assembly of the current

cylindrical design are extremely difficult, and an elliptical design would increase the fabrication difficulty severalfold.

**HEAT EXCHANGER ASSEMBLY** - It is proposed to fabricate two separate two-unit assemblies. Attachment of each two-unit assembly to the Nissan NAPS-Z engine will make use of existing exhaust manifold attachment bolt holes. Attachment of four separated individual units to the engine appears to be impractical, and fabrication of a single four-unit assembly is considered significantly more difficult.

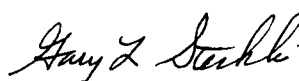
**EXPECTED RESULT OF DESIGN IMPROVEMENT** - The mechanical design improvements described should improve the operation and dissociation efficiency of the heat exchanger. These improvements, however, are not expected to provide anywhere near the order of magnitude improvement desired. It appears that selection of the catalyst composition is the most important criteria toward meeting the desired dissociation efficiency.

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Staff Engineer  
Engine Systems Research & Development

Submitted by:



Gary L. Stecklein  
Director  
Vehicle Systems Research Department

/ew

Attachments

## ANALYSIS OF CATALYST BY JOHNSON MATTHEY

FAX TO: SOUTHWEST RESEARCH INSTITUTE  
FROM: R.MCDOWELL  
DATE: 4 JAN 88  
SUBJECT: PRELIMINARY RESULTS - METHANOL REACTOR

ATTN: MR. C. URBAN FAX # (512) 684-7523

Both the MeOH dissociation and the engine exhaust catalyst have been checked by our Analytical Lab for B.E.T. surface area. These catalysts were also scanned by xray for the presence of catalyst poisons. A coke deposit discovered at the product outlet (Figure 9 in the SWRI report) was analyzed by XRF for contaminants.

The surface area (S.A.) measured for the dissociation catalyst was less than one meter squared per gram ( $m^2/g$ ). The corresponding result for the engine exhaust catalyst was  $1.2 m^2/g$ . Elements found on the dissociation catalyst were Al, Cr, Fe, and Zn. Elements found on the exhaust catalyst were Al, Ca, Cr, Cu, Fe, Pt, and Zn. Elements found in the coke deposit were Ca, Cr, Fe, Pb, and Zn. The high temperature resistant stainless steel metal support is an alloy containing Al, Cr, and Fe which could be picked up by the xray.

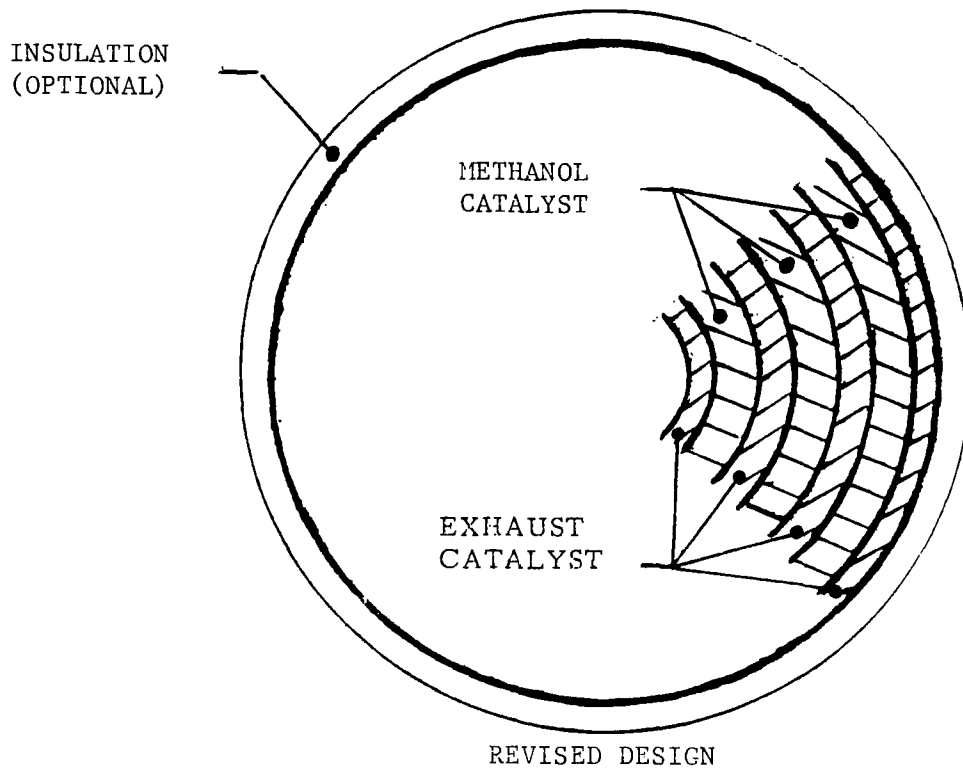
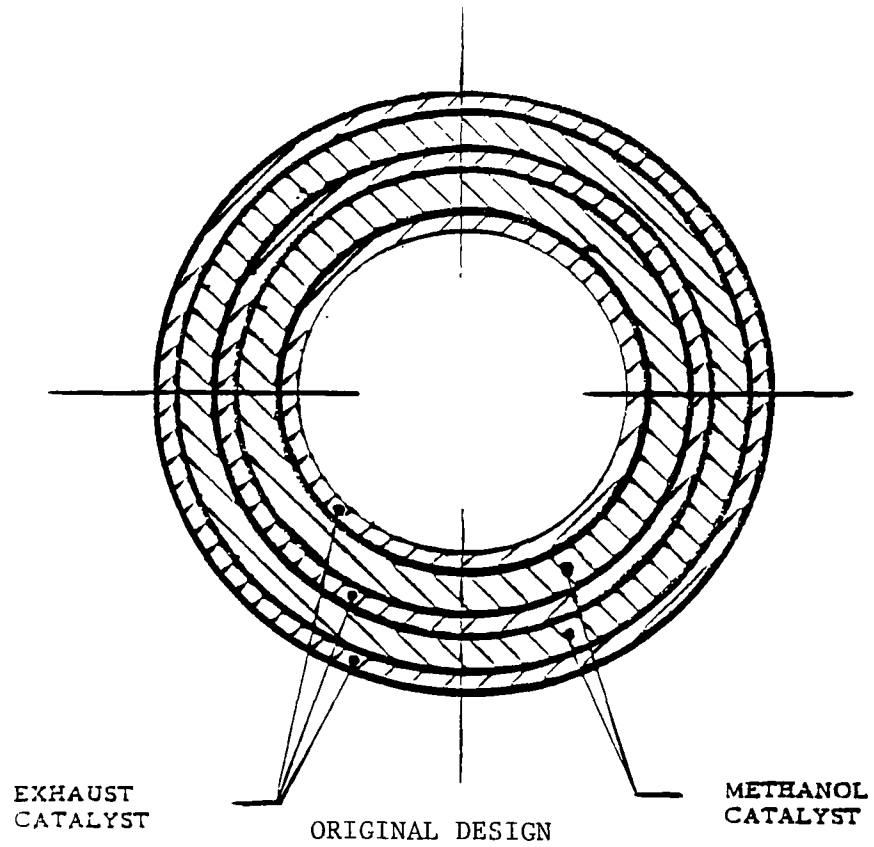
The expected B.E.T. surface area for a metal supported catalyst would be somewhere on the order of 8 to  $13 m^2/g$ , so the low result on both catalysts is surprising. Usual reasons for loss of S.A. are poor washcoat adhesion, thermal sintering, or masking/poisoning. A scan with a 20x lens did not reveal bare patches of metal which would indicate washcoat adhesion problems. The 600 degree C. temperatures noted in the SWRI report are not as high as we see in automotive applications and would not seem to be a prime candidate for low S.A. numbers. Welding the catalyst reactor may be a source of high temperatures ( and metal poisons ). Masking or poisoning effects are a definite possibility. The coke deposit scanned by XRF shows the presence of Ca and Pb as well as the expected Cr, Fe, and Zn. However, the amount of each of these elements is unknown. Each could be a poison in large amounts on the catalyst surface. The xray scan of the catalyst is not sensitive to the lighter elements, so a masking agent of carbon compounds would not be detected. The very fact that a coke deposit was produced at the exit port of the reactor may indicate some other undesired catalytic reactions going on, perhaps caused by these other materials.

A meeting to discuss the problem and your potential need for four additional prototypes will be held early this week. Dr. Paul Ellgen or Jay Hoffman will phone you to let you know where we stand.

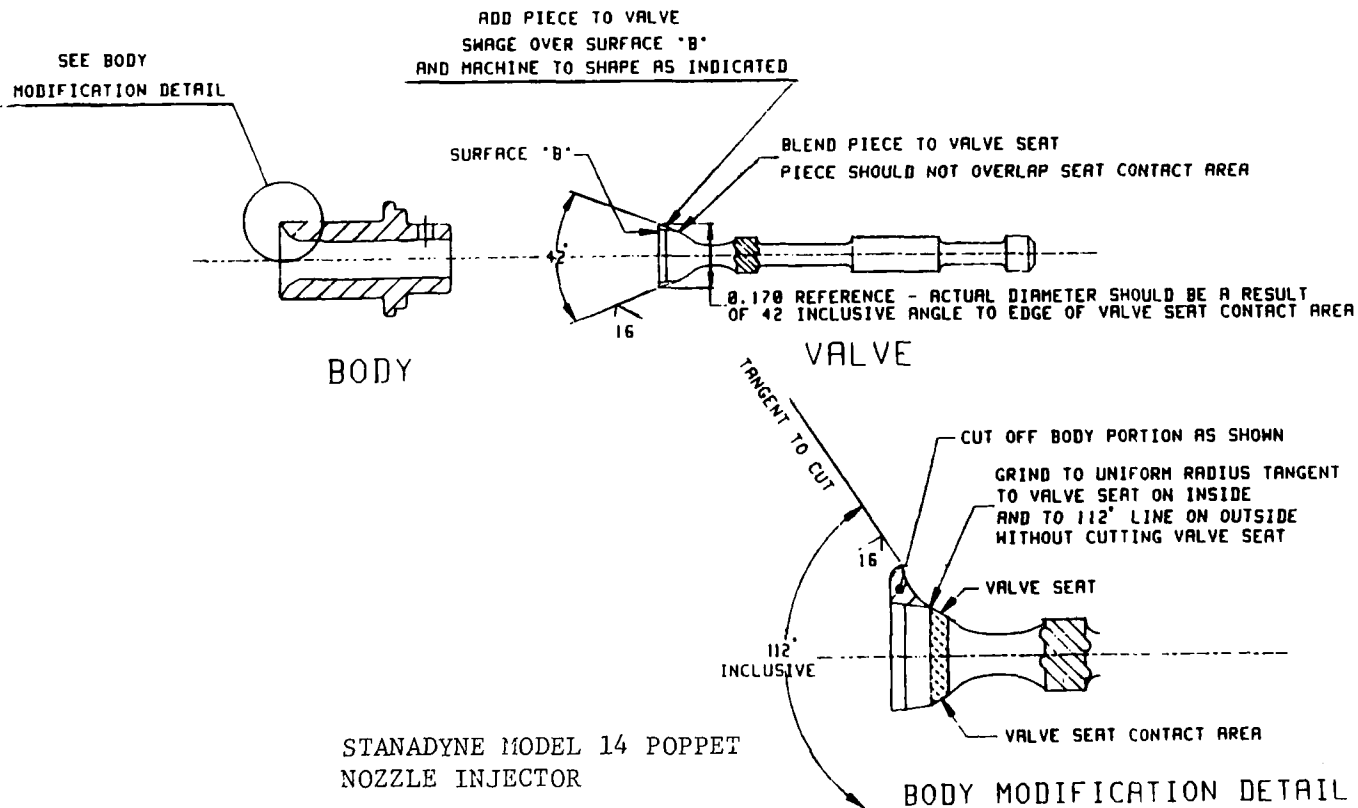
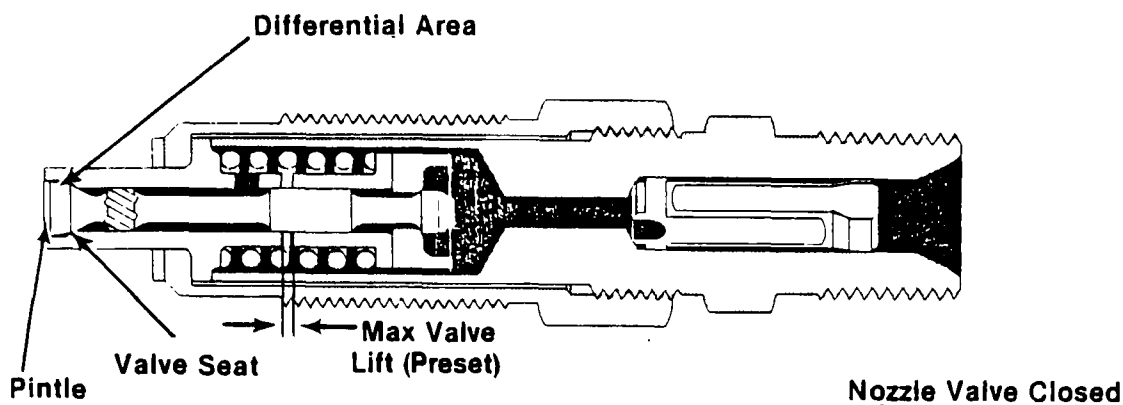
## Johnson Matthey

CATALYTIC SYSTEMS DIVISION  
436 DEVON PARK DRIVE, WAYNE, PA 19087

METHANOL DISSOCIATION REACTOR

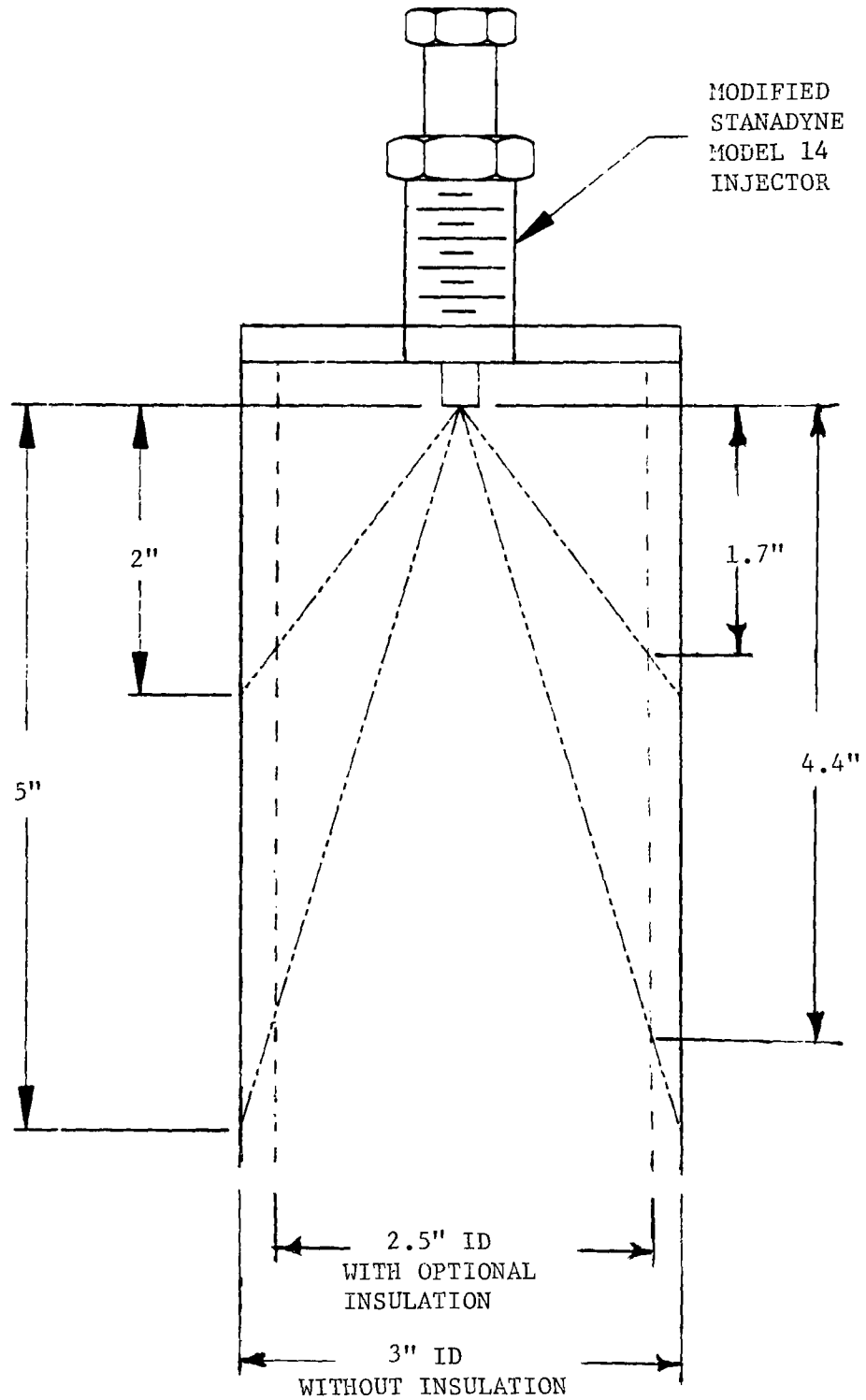


# METHANOL FUEL INJECTOR

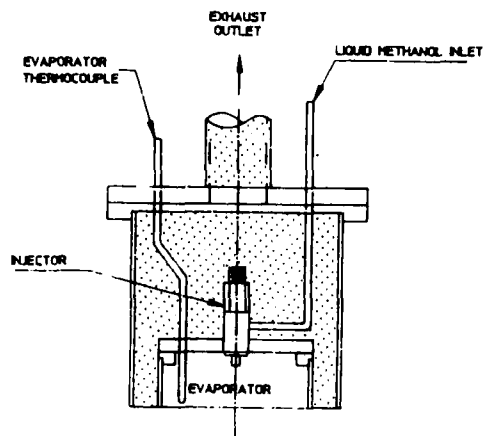


ATTACHMENT D

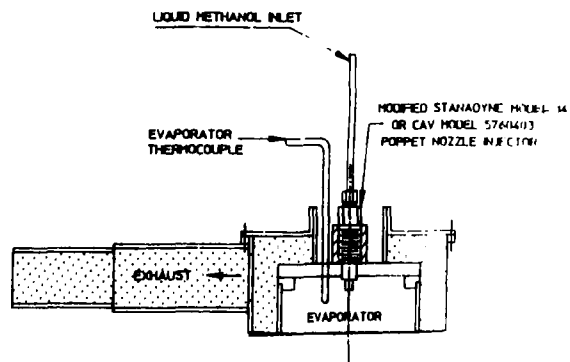
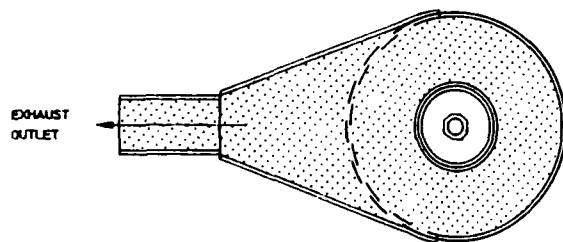
METHANOL INJECTOR SPRAY PATTERN



# RELOCATION OF METHANOL INJECTOR



ORIGINAL DESIGN



REVISED DESIGN

# **TECHNICAL REPORT DATA**

*(Please read Instructions on the reverse before completing)*

1. REPORT NO. <b>EPA-460/3-88-002</b>		2.	3. RECIPIENT'S ACCESSION NO.	
4. TITLE AND SUBTITLE <b>NEAR-CYLINDER DISSOCIATION OF METHANOL FOR AUTOMOTIVE APPLICATION</b>			5. REPORT DATE <b>July 1988</b>	
			6. PERFORMING ORGANIZATION CODE	
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12. SPONSORING AGENCY NAME AND ADDRESS			13. TYPE OF REPORT AND PERIOD COVERED	
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15. SUPPLEMENTARY NOTES				
16. ABSTRACT  <p>This report describes the design analyses and experimental evaluation toward developing a system of dissociating methanol for use in a spark-ignited passenger car engine. Maximum dissociation of methanol fuel attainable using exhaust gas heat was the basic goal of this project. The heating value of dissociated methanol is about 20 percent higher than that for liquid methanol. Therefore, significant energy savings appear to be attainable if a large percent of the engine fuel needs can be dissociated by use of the otherwise wasted heat of the exhaust gas. A heat exchanger consisting of a methanol evaporator, an injection system to provide fuel to the evaporator, and a dissociation catalytic reactor was designed, fabricated and tested. The dissociation efficiency of this initial reactor was not as good as expected. The relative poor performance of the dissociation reactor apparently was associated with fuel injector nozzle heating, blockage of passageways in the dissociation reactor, and an ineffective dissociation catalyst. The heat exchanger was redesigned to incorporate improvements, and four heat exchangers were fabricated using the final design.</p>				
17. KEY WORDS AND DOCUMENT ANALYSIS				
a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS		c. COSATI Field/Group
<b>Methanol</b> <b>Methanol Exhaust Emissions</b> <b>Motor Vehicles</b>		<b>Methanol Fueled Vehicles</b> <b>Light-Duty Vehicles</b>		
18. DISTRIBUTION STATEMENT  <b>Release Unlimited</b>		19. SECURITY CLASS (This Report) <b>Unclassified</b>		21. NO. OF PAGES <b>182</b>
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