PROGRESS REPORT NO. 20

KINETICS OF OXIDATION AND QUENCHING OF COMBUSTIBLES IN EXHAUST SYSTEMS OF GASOLINE ENGINES

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PERIOD: October 1, 1970 to October 31, 1970

October, 1970

This project is under the technical supervision of the:

Coordinating Research Council
APRAC-CAPE 8-68 Steering Committee

and is work performed by the:

Department of Mechanical Engineering
The University of Michigan
Ann Arbor, Michigan

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LONG-RANGE OBJECTIVES

It is well-known that a significant amount of CO and unburned fuel may be consumed in the exhaust system of gasoline engines. Such combustion phenomena in exhaust reactors may be used to advantage to reduce the emission of these undesirable constituents. This process is the basis of exhaust air injection systems currently installed on some automobiles.

The overall objectives of this three-year research program are:

- To determine the chemical and physical processes which affect the emission characteristics of exhaust reactors installed on selected typical engines operating at various conditions on a dynamometer test stand.

- To identify the chemical species and significant chemical reactions present before, within, and after the reactor.

- To obtain information which will be helpful in predicting the design of the next generation of gasoline engine exhaust reactors.

GENERAL

This month a preliminary work statement for the third year was submitted to the Coordinating Research Council.

FIRST ANNUAL REPORT

Several corrections and modifications were made to the first annual report. The text has been submitted for final publication.

PHASE I PROGRESS

MULTICYLINDER REACTOR

Hysteresis curves of duPont reactor performance were developed this month. Tests were run to show the effect of air injection fraction and previous state of warm up on corrected CO, HC, and reactor core temperature. Temperature was measured by a shielded chromel-alumel thermocouple installed at the geometric center of the reactor core. The 350-CID Chevrolet engine was operated at 1200 rpm, 50% load (30 hp) with MBT spark. Both reactors were installed.

Emission concentration was measured at the tailpipe and a correction factor applied for dilution air. This correction factor is the ratio of the mole carbon atom concentration in undiluted exhaust to that in diluted exhaust. The fraction (by volume) of dilution air is calculated from the carbon atom concentration in a similar manner.

Figures 1 and 2 show the emission and temperature results for air fuel ratios of 12.5:1 and 13.8:1. Air injection fraction was varied from zero to about 1.8 or 80% dilution air by volume. The tests were run in the sequence suggested by the arrows. The first point was run with no added air. Subsequent points were run with increasing air injection fraction until an arbitrary maximum flow was reached. Then the air flow was reduced in steps to zero. At each step, adequate time was allowed for temperature and concentration stabilization.

At 12.5:1 air fuel ratio, good HC reduction occurred at relatively low air flows and remained low at higher air flows as Figure 1 shows. Especially

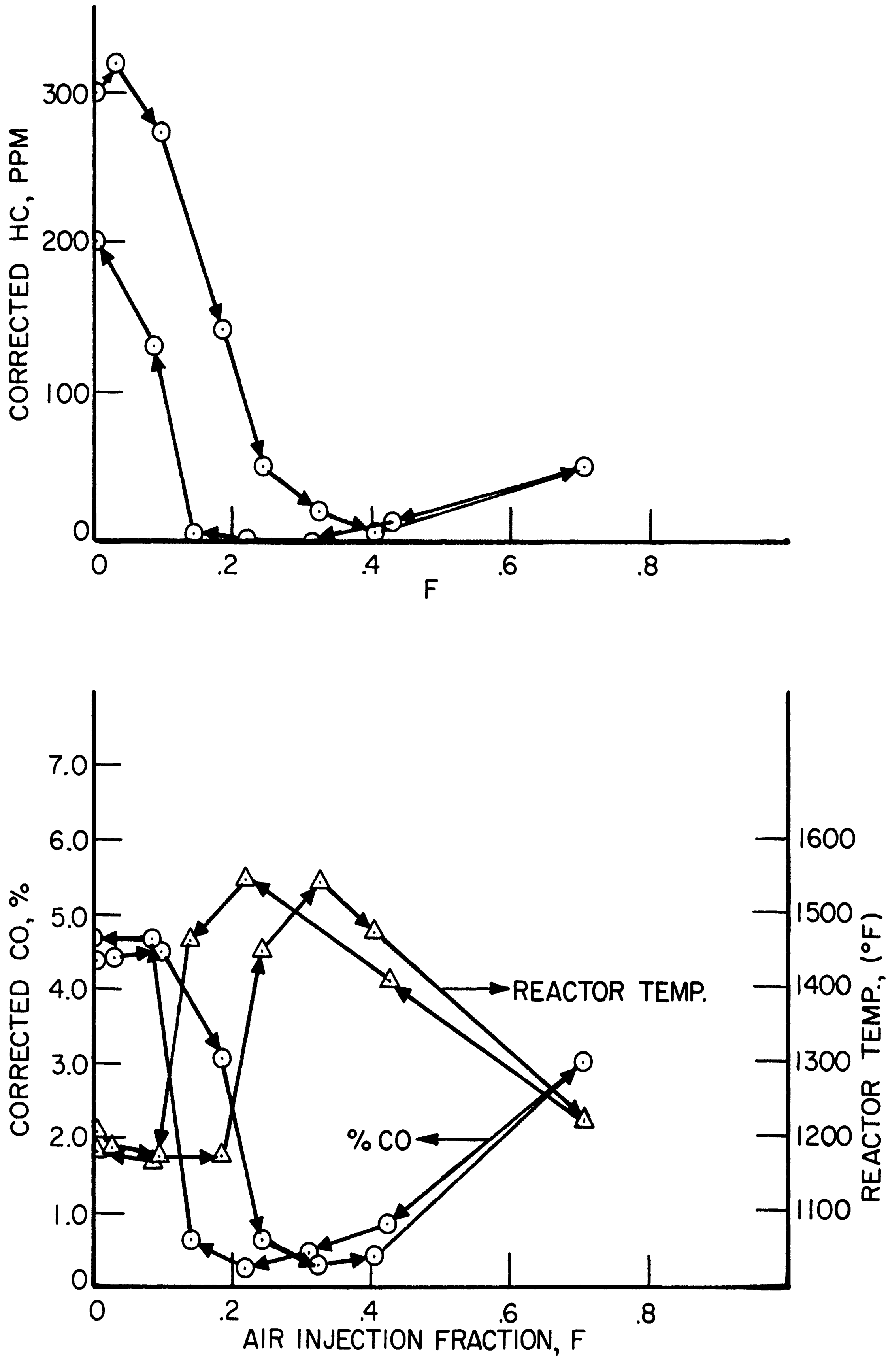


Figure 1. Exhaust emissions with duPont reactors as a function of air injection fraction. 1200 rpm, 50% load, 12.5:1 air-fuel ratio, MBT spark of 33°.

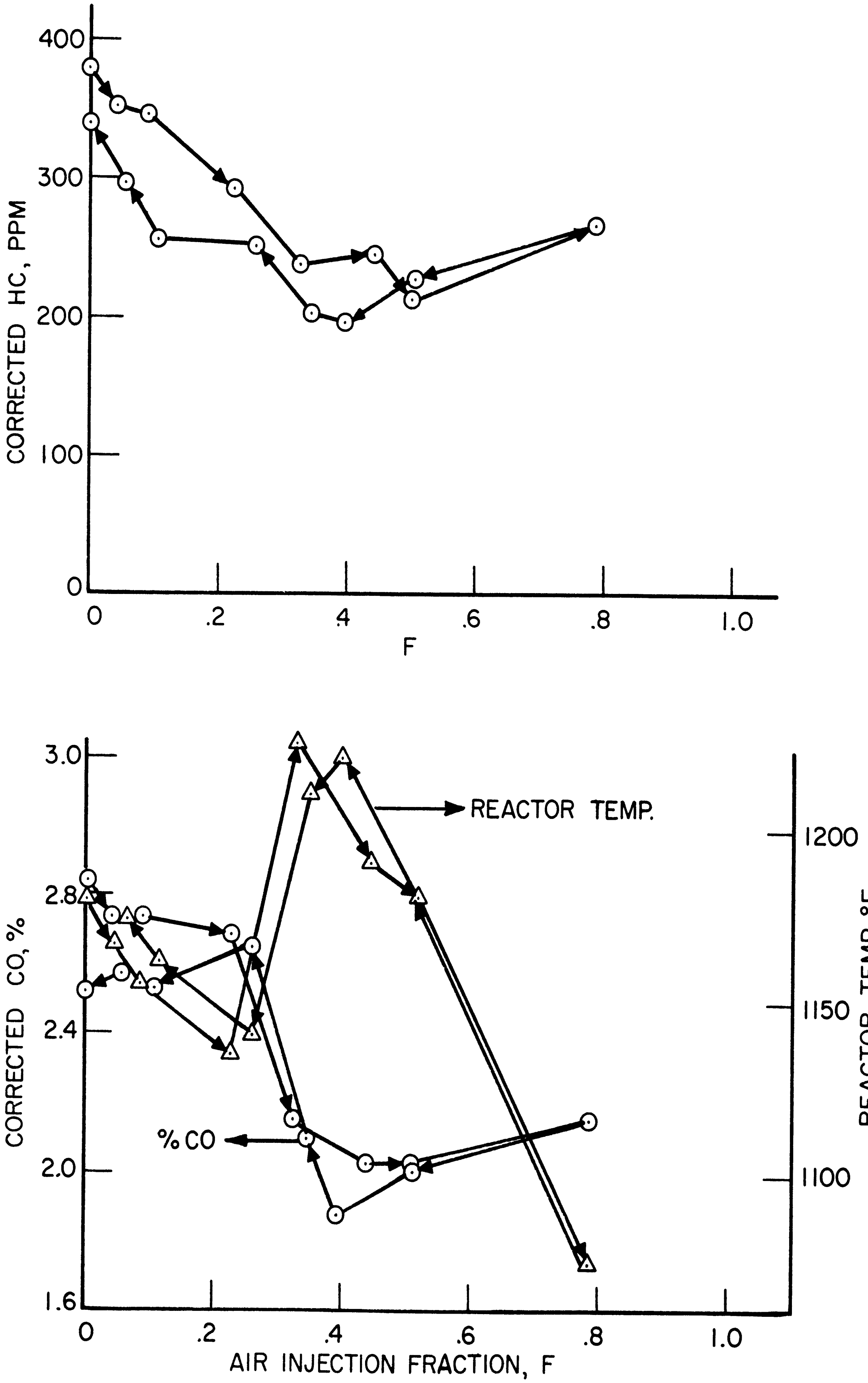


Figure 2. Exhaust emissions with duPont reactors. Air/fuel ratio 13.8:1.

good HC cleanup was observed at low dilution air flows when the reactor was previously hot (decreasing air fraction). Good carbon monoxide reduction was more dependent on air injection fraction. Like HC reduction, better performance at low air injection rates occurred when the reactor had been hot previously.

At 13.8:1 air fuel ratio, the exhaust contained fewer combustibles (2.8% CO vs. 4.5% at the richer mixture). Consequently the peak reactor temperature was only 1225°F compared to 1550°F with the richer mixture as Figure 2 shows. The hysteresis loop persisted and was similar but less pronounced than that of Figure 1. Note that he absolute HC emission levels are about the same or slightly greater for the leaner mixture. Normally leaner mixtures emit fewer hydrocarbons. The discrepances in this data result from day-to-day engine emission variations. The data in Figures 1 and 2 were taken on different days.

One obvious conclusion is that the prior state of warm-up can have an important effect on HC and CO clean-up depending on air injection fraction. CO has less tolerance to air injection fraction variation than hydrocarbons. Rich operation provides lower tailpipe emissions, but at the expense of fuel economy. Maximum emission reduction can only be achieved by reasonably close regulation of air injection fraction. Present automotive systems vary air injection volume flow with engine speed. Consideration should be given for controling air flow at a given speed as a function of load (for example, by manifold vacuum) and also as a function of temperature or rates of temperature change.

SINGLE CYLINDER REACTOR

Work on the two-tank reactor system this month was directed toward measuring the residence time distribution in the reactor and modifying the reactor geometry in order to more closely approach a well-stirred distribution. The use of a hot-wire anemometer to detect a change in the thermal conductivity of a room temperature helium-air mixture when the trace of helium is suddenly interrupted has proved successful. The three different geometrical configurations described below have been studied.

1. Initial Geometry—A set of residence time distribution traces obtained with the initial geometry indicated the presence of an unacceptably large plug flow component.
2. Baffle Removed—Upon examining the internal geometry in light of the above, it appeared that the end baffle might tend to promote plug flow behavior in the volume between it and the end wall, so it was removed. However, this left four holes in the end of the sparger tube pointed directly at the reactor exit, so in order to prevent short circuiting of the flow these holes were plugged. These modifications resulted in little if any improvement in the residence time distribution.
3. Conical Flow Director—On the assumption that plugging the end holes in the reactor had resulted in inadequate mixing in the end portion of the reactor, they were reopened. In order to prevent short circuiting of the flow from these end holes, a conical flow director was attached to the end of the sparger to deflect the jets away from the exit. In addition, the 1-1/2 inch diameter exit hole was covered by a plate containing about one hundred fifty 3/32 diameter holes to eliminate the possibility of large eddies being swept out of the

reactor. Measurements with this system indicated a substantial improvement in mixing. Typical traces indicated at most a few percent of the volume devoted to plug flow. Figure 3 is a typical photograph of three traces obtained at one condition.

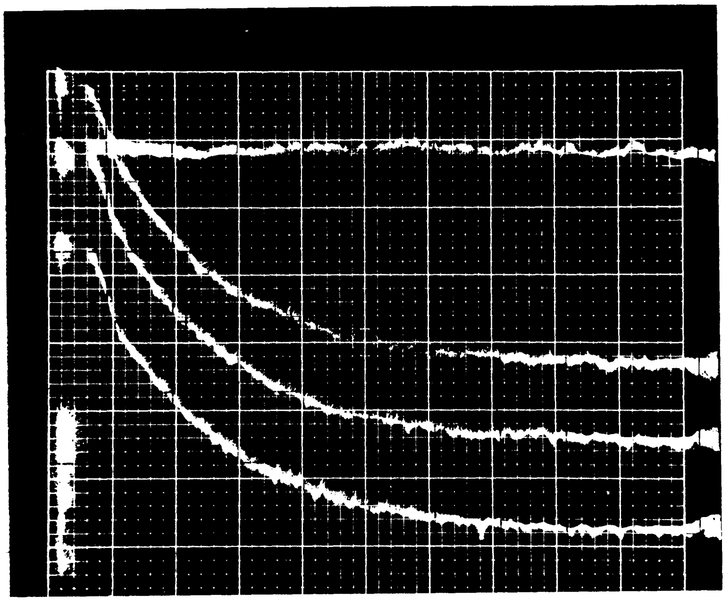


Figure 3. Typical residence time distribution traces showing change in hot-wire anemometer signal at exit of reactor vs. time.

It was next decided that the volume of the sparger tube should be reduced from its present volume of about 5% of the reactor volume, since even a small plug flow section upstream of a stirred tank can have a substantial effect upon total conversion under some conditions. This will be done by inserting a stainless steel plug in the sparger tube so that the flow will occur in an annulus of about 1/10 of the present volume, or about 0.5% of the total reactor volume. Figure 4 is a sketch of the reactor geometry at this stage, including the plug. A set of residence time distribution measurements will be made with this geometry next month.

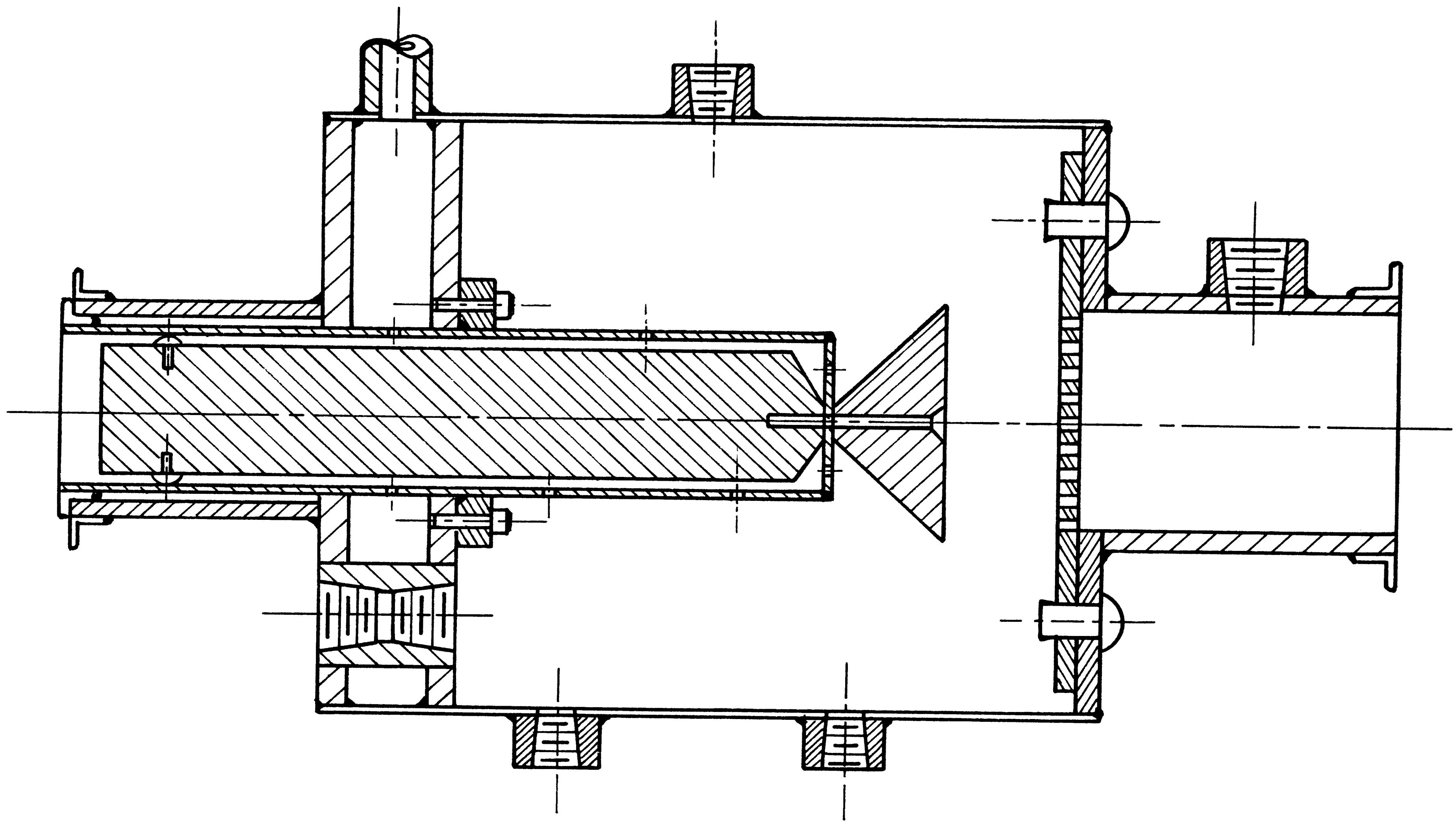


Figure 4. Experimental reactor in modified form.

PHASE II PROGRESS

During the last month, debugging was completed on the computer simulation "EXHAUST," which computes reactor performance for periodically varying inputs based on complete and instantaneous mixing within the reactor. The last efforts centered on generalizing previous work for obtaining a smooth approach from some arbitrary initial condition to a final condition characterized by nearly complete depletion of one or more of the combustible species. The final result is completely general in the sense that any reaction with known kinetics can be entered, and the program satisfactorily converges for both low and high temperature (ignition) modes of operation.

It should be stressed that the program EXHAUST is fully capable of simulating reactor warm-up, provided only that reactor wall temperatures are specified as a function of time for a series of simulations of short duration. These metal temperatures can be estimated from basic heat transfer considerations, as was done in one of the previous reporting periods; or perhaps still better, they can be specified from available experimental data. The series of required short-duration runs that are required to simulate warm-up can be accomplished with an acceptible economy of computational effort despite the necessity for small step size.

A general program was written previously for reducing the experimental data from Phase I on oxidation of various combustible exhaust species to a form which can be linearly regressed to obtain kinetic constants in a simplified rate correlation equation ($R = K e^{-E/RT} P_s^A P_{O_2}^B$). This program operates on flow rates for air and exhaust and concentrations entering and leaving the reactor to compute oxidative conversions. In turn, the conversions are related to the rate of reaction using the reactor design equations for an ideal back-mix reactor. Finally, logarithms are obtained for the rate R and for partial pressures P_s and P_{O_2} so that a linear regression can be performed on the log form of the rate equation.

The regression program that is being used performs an in-place inversion on the matrix of correlation coefficients using maximum pivot points. The program gives us the best values for the regression coefficients and a complete analysis of variance for the estimated value of the rate and for the contribution of each individual term within the regression equation.

Since the residence time distribution studies in Phase I have indicated a behavior which is very close to an ideal stirred tank for the reactor in the two-tank system, the existing data reduction program should yield good order of magnitude results. These results can be corrected on an iterative basis for small series and/or parallel plug flow components which may be inferred from the tracer curves. That is, by taking the rate constants from an initial calculation based on an ideal stirred tank, a correction can be computed for the amound of reaction occurring in the plug flow components. Application of these corrections will lead to an improved set of constants. The procedure can be repeated as many times as is warranted (therefore iteratively).

The development of a reactor simulation which treats non-ideal mixing of air and exhaust is being studied. Current thinking calls for a development based on an analysis of the relationship between mixing and the amount of turbulence which can be generated within a reactor subject to constraints on size and pressure drop. The specific effects of turbulence on mixing is a subject area which is not well treated in reactor design theory, and hence considerable effort may be required before the details of the next generation simulation are worked out. This more general approach is being pursued as an alternative to previous plans for a simulation based specifically on what could be learned about mixing in a particular device (the duPont reactor).

PHASE III PROGRESS

MEASUREMENT OF EXHAUST GAS VELOCITY

Effort for obtaining an instantaneous schlieren photograph for the flow pattern has been continued during the month of October. It was found during the process of optical alignment that the single flash spark source showed a poor performance by producing a large focal image of the spark at the knife edge and erroneous changes in position of the spark itself.

Since rebuilding of the spark source unit is impractical for this project and the theoretical analysis predicted approximately the same results as measured, we redirect our effort into a system change for measuring the instantaneous temperature of the exhaust gas. This will be attempted by measuring the sonic velocity of a shock wave in the gas. Two main jobs will be construction of a device for generating a shock waves inside of the exhaust pipe and an investigation of the proper speed of the rotating mirror in the camera system. Necessary changes in set-up will be followed accordingly

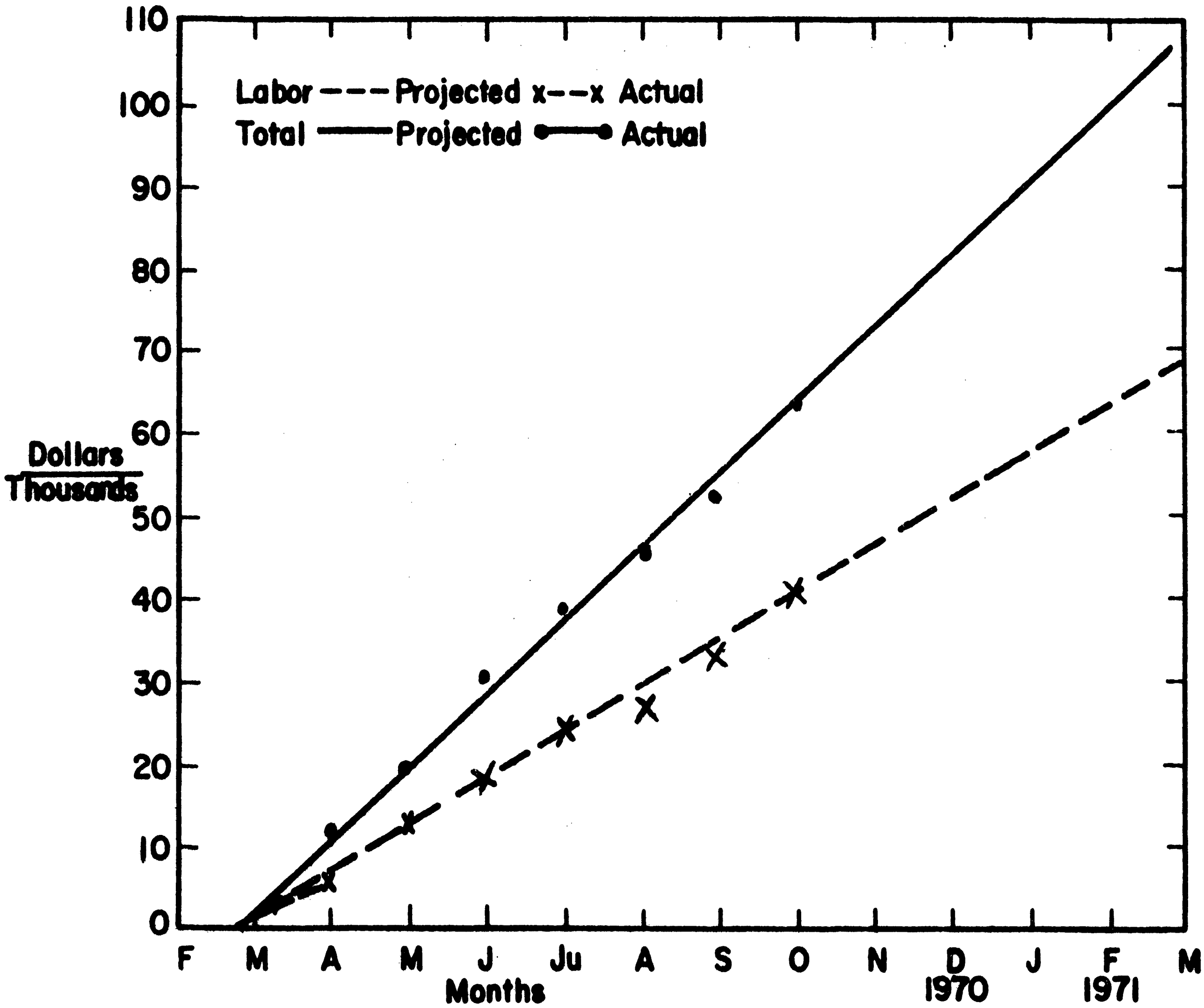
GAS CHROMATOGRAPH

Good progress has been made on the gas chromatograph. All stability problems have been eliminated. A digital integrator has been located to process the output. Karen Balaska, a Ford engineer, has agreed to set our unit up based on the Ford analysis system. She will work evenings and weekends. We plan to use the Ford data reduction program. In addition we have hired Mr. Albert Martin, a University of Michigan doctorial student in Chemical Engineering and an experienced GC operator, to assist with set up and analyses during the day.

It is the hope of The University of Michigan group that the GC log jam has been broken.

CRC CAPE 8-68 PROGRAM
OVERALL FINANCIAL SUMMARY

Program Total: February 24, 1970 - February 23, 1971		$106,500
Cumulative Expenditures through September 1970		62,000
	Balance	$ 44,500



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