#### PROGRESS REPORT NO. 12

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

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PERIOD: February 1, 1970 to February 28, 1970

February 1970

This project is under the technical supervision of the:

Coordinating Research Council ARPAC-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

February 23 marked the completion of the first year of this three-year program. As yet a contract has not been executed for the second year. We will be working on a month-to-month basis until a contract is negotiated.

#### PHASE I PROGRESS

Baseline evaluation of the 350 CID engine is virtually complete. Installation of the duPont reactors may begin in March. The two-tank reactor

system fabrication has still not been completed. We expect delivery during March from Walker Manufacturing.

The hydrogen meter fabrication has been completed and this unit has been checked out with calibration gases for response to hydrogen and interference from other combustion products. No major problems are anticipated in the measurement of hydrogen as part of the exhaust gas mix.

The exhaust system of a single cylinder engine has been modified to permit installation of a laser-schlieren system. Temperature and flow data obtained will be used as inputs for the computer model.

#### PHASE II PROGRESS

A simulation on a single arm of an exhaust manifold (7.5 cu in. volume) receiving exhaust from a single cylinder has been completed. Inlet exhaust conditions entering the manifold were the same as those previously used for exhaust gas entering the 300 cu in. exhaust reactor; i.e., temperature cycling between 1200 and 2000°F, hydrocarbon (as methane) cycling between 250 and 2500 ppm, and carbon monoxide constant at 0.8%. Air was introduced at 100°F to achieve an overall dilution ratio of 1.4 as before; however, flow rate of air was staged to give 10% of the average rate over the 75°-interval of crank angle of maximum exhaust flow and a higher rate which resulted in the correct average over the remaining 645° of a 720°-cycle.

Resulting temperatures, pressures, and concentrations as a function of crank angle were observed to exhibit periodic oscillations of wide amplitude, as would be expected from the pulsing input and small manifold volume. Changes

in hydrocarbon and carbon monoxide during the period after exhaust flow ceased for a cycle were represented by an exponential-type decline as combustion and dilution by the continuing flow of air dropped concentrations to near zero at the end of each 720°-cycle. Perhaps the most significant finding was that conversion of CH<sub>4</sub> was 70% and the conversion of CO 20% within the small volume of the exhaust manifold. It should be remembered that these conversions are based on selected literature values of kinetic constants (Yuster for carbon monoxide and Koslov for methane) and are subject to an unknown error for the conditions of this problem. However, the tenative conclusion is that the manifold may be highly important in predicting overall conversions between the exhaust port and the tailpipe of an exhaust system. Its importance may however be less than that shown due to imperfect mixing of air and exhaust within the small volume of the manifold.

Modeling of the 300 cu in. CSTR reactor is continuing at higher levels of CO and with  $\rm H_2$  added as an additional combustible species. For exhaust containing several percent CO, the amount of  $\rm H_2$  entering is assumed to be predicted by equilibrium for the water gas shift reaction at a K of 3.5 corresponding to a reaction temperature of 2640°F. A similar assumption has been used by Eltinge in computing fuel/air ratios from exhaust analyses and by Schwing in studies of exhaust oxidation. No applicable values of kinetic constants have been found in the literature for oxidation of hydrogen; and an assumption will be made that its oxidation in the CSTR reactor is essentially complete.

Calculations were performed on the mass balance for CO, based on the kinetics used previously, to predict conversion versus reaction temperature. The

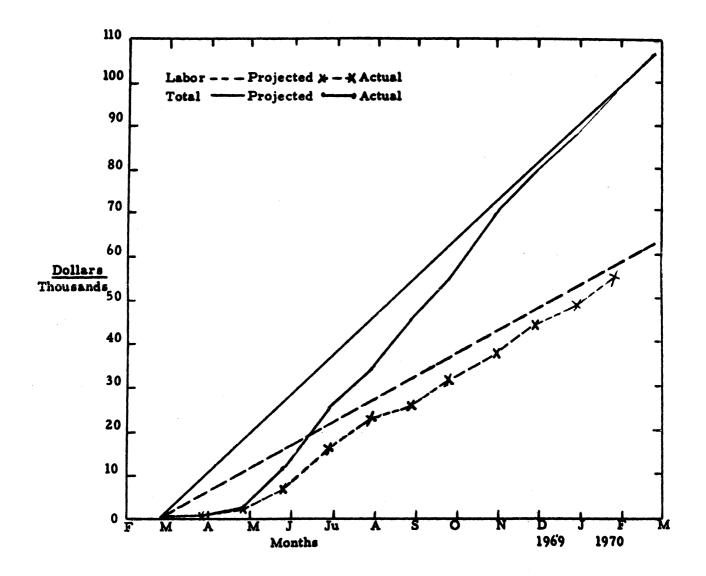
conversions calculated were in close agreement with those obtained in previous simulations of the CSTR reactor, which predicted a conversion of 56% for CO at 1200°F reactor temperature. This method of determining conversions for CO from intercepts between the mass balance and the energy balance (the method used by Schwing) is being used here to identify the inlet temperature below which conversions of CO drop precipitously (blowout). A range of temperature close to the calculated value will then be investigated using the CSTR simulation at the higher percentages of CO and H<sub>2</sub> mentioned earlier to confirm that the simulation correctly predicts the blowout phenomenon.

#### PHASE III PROGRESS

No progress this month.

## OVERALL FINANCIAL SUMMARY

Program Total: February 24, 1969 - February 23, 1970	\$106,455
Cumulative Expenditures through January 23, 1970	98,103
Balance	\$ 8,352



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