

# Chemistry and Mixing Effects in Reburning

Study Report 1999

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## Research Summary

**TITLE:** Chemistry and Mixing Effects in Reburning

**CONTRACTOR:** Technical University of Denmark (DTU),  
Danish Gas Technology Centre (DGC)

**PRINCIPAL INVESTIGATOR:** Peter Glarborg and Anker Jensen (DTU)  
Lone Schmidt and Niels B.K. Rasmussen (DGC)

**REPORT PERIOD:** January 1999 – March 2000

**OBJECTIVES:** The objective of the work was to develop an engineering model for gas injection systems with detailed chemistry that in a simple manner can be used to simulate processes like Natural Gas Reburning. The work involves improvement and validation of detailed kinetics models for hydrocarbon oxidation and hydrocarbon/nitrogen interactions, based on flow reactor data covering a wide range of hydrocarbon fuels, temperature and stoichiometry. Furthermore, a systematic analysis and evaluation of different approaches for modeling of jet mixing systems with simplified fluid dynamics and detailed chemistry was planned. The preferred mixing model was to be validated through comparison with literature results on reburning.

**TECHNICAL PERSPECTIVE:** Presently, design of gas injection systems may rely on CFD modeling, physical (cold flow) modeling, scaling of pilot scale work, and/or experiences from previous full scale tests. Proper design of gas injection systems would be facilitated considerably, if simple and reliable modelling tools for the chemistry of jet mixing systems were available. In the present work an engineering model of jet mixing systems with simplified fluid dynamics and full chemistry was to be developed and validated, emphasizing Natural Gas Reburning.

**RESULTS:**

The project, planned to last three years, was terminated shortly into the second year, following the discontinuance of the GRI Basic Research Program. The emphasis during the first part of the project has been on the chemistry of the reburn process. The major uncertainties are associated with 1) the hydrocarbon oxidation chemistry, in particular prediction of the concentration of the HCCO radical largely responsible for NO removal in Natural Gas Reburning, and 2) rate constant and product channels for the HCCO+NO reaction. A comprehensive experimental database on hydrocarbon oxidation in a flow reactor under a wide range of fuels (C1 and C2 hydrocarbons) and reaction conditions (temperature, stoichiometry, pressure) has been established and compared with modeling predictions with our current reburn mechanism as well as GRI Mech 3.1. In general, both mechanisms perform satisfactorily, but important deviations have been identified, which need to be addressed in future work.

In order to characterize HCCO reactions, in particular HCCO+NO and HCCO+O<sub>2</sub>, flow reactor experiments with a convenient precursor for HCCO, carbon suboxide (C<sub>3</sub>O<sub>2</sub>), have been conducted. The oxidation of C<sub>3</sub>O<sub>2</sub> with and without presence of NO was investigated at different temperatures and stoichiometries. Data are interpreted in terms of a detailed chemical kinetic model.

A preliminary mixing model, based on the approach by Zwietering, in combination with the detailed reaction mechanism has provided a satisfactory description of bench and pilot scale data on reburning from literature.

**PROJECT  
IMPLICATIONS:**

GRI contract 5035 has provided fundamental research that has helped in the evaluation and design of gas injection processes for NO<sub>x</sub> reduction (related to reburn processes and their various modifications). It has continued to provide new results on, and advance the understanding of, the chemistry of hydrocarbon oxidation and its interactions with nitrogen species, and has validated and compared detailed kinetics models for these interactions. The results have been important in developing a working knowledge of the advantages and limitations of natural-gas-based reburn technologies, and

NOx emission control strategies.

The research work had progressed to a new phase, aiming to develop a usable engineering model for simulating gas injection reburn systems that incorporates both detailed chemistry and jet mixing effects. The work of the initial year of this phase established a comprehensive data base on hydrocarbon oxidation in a flow reactor for a wide range of fuels and reactor conditions. This was used to compare and test against modeling predictions and kinetic mechanisms, helping to identify model deviations in need of further resolution.

However, in order to optimize benefits to its supporters and its customers under new financial circumstances, GRI's program of Research, Development, and Commercialization has been restructured and its program priorities have been re-ordered. As a result, GRI will not support further research under this contract. However, the results and deliverables obtained to date from the research are expected to provide value to GRI and its investors in connection with gas-based reburn processes.

**PROJECT  
MANAGERS:**

Robert V. Serauskas, Gas Research Institute  
Bent Karll, Danish Gas Technology Centre

## INTRODUCTION

Natural gas injection is an efficient way of reducing emissions of NO [1] as well as N<sub>2</sub>O [2] from a significant range of combustion systems. During the 1980's Natural Gas Reburning has matured through a number of pilot scale studies, and full scale tests primarily on coal-fired units have generally been successful [1]. An emerging application of Natural Gas Reburning is use in connection with combustion of biomass and coal/biomass blends. Selective catalytic reduction (SCR) is not presently applicable for NO<sub>x</sub> control in biomass combustion facilities due to catalyst poisoning, and a number of conventional NO<sub>x</sub> control technologies such as low-NO<sub>x</sub> burners are generally incompatible with furnace design in these systems.

Presently, design of gas injection systems may rely on CFD modeling, physical (cold flow) modeling, scaling of pilot scale work, and/or experiences from previous full scale tests. A combination of these methods, possibly supplemented with ideal-reactor detailed kinetics modeling, have proven to be efficient in the design process. Direct implementation of detailed kinetics in CFD models is not at this point an option, even though significant efforts are undertaken to develop efficient ways of handling the chemistry in these codes and to improve the understanding of turbulence/chemistry interactions.

Proper design of gas injection systems would be facilitated considerably, if simple and reliable modelling tools for the chemistry of jet mixing systems were available. Different approaches for modeling of jet mixing systems with simplified fluid dynamics and (potential of) full chemistry have been suggested in literature (e.g. [3, 4, 5, 6, 7, 8]), but strengths and limitations of these schemes have not been investigated systematically over a wider range of conditions.

Gas injection systems, such as Natural Gas Reburning, are very challenging to simulate numerically, due to the combination of a very complex chemistry and the occurrence of mixing/chemistry interactions. Our present understanding of the reburn chemistry is still incomplete [9, 10] and detailed kinetics modeling can only be used cautiously to assess the process potential, even under ideal reactor conditions. Furthermore, ideal reactors cannot be expected to provide a sufficient description of flow and mixing conditions in a practical application. Here a secondary fuel, representing typically only a few percent of the mass of the bulk flow, is injected through one or several injection nozzles, creating a complex mixing zone, where the degree of mixing will be affected both by the



momentum of the secondary jet(s) and by the bulk flow characteristics. In this region, macro and micro mixing are expected to play a significant role for the reburn chemistry, but little is known about the effect of mixing. Contrary to a fuel oxidation process, processes such as reburning and SNCR involve a reaction selectivity, which will depend on mixing conditions.

The present project aimed at developing a model for gas injection systems with detailed chemistry that in a simple manner can be used to simulate processes like Natural Gas Reburning. The work planned had three major components:

1. Improvement and validation of detailed kinetics models for  $C_1/C_2$  hydrocarbon oxidation and hydrocarbon/nitrogen interactions.
2. Experimental study of the effect of mixing on reburning with  $C_1/C_2$  hydrocarbons in a laminar flow diffusive mixing reactor.
3. Systematic analysis of different approaches for modeling of jet mixing systems with simplified fluid dynamics and detailed chemistry (the chemical engineering model approach as opposed to the CFD modeling approach).

1)

In this part of the work the detailed reaction mechanism developed in previous GRI/DGC funded work was to be refined in order to provide a better description of reburning with  $C_1$  and  $C_2$  hydrocarbons. The experimental database established in our group as well as reported experimental data mainly from University of Zaragoza would form the basis for the analysis, supplemented by new flow reactor experiments emphasizing specific reactions or subsets in the reburn mechanism.

2)

A systematic investigation of the effect of mixing on reburning with  $C_1$  and  $C_2$  hydrocarbons was to be undertaken in a laboratory Burke–Schumann type set-up under isothermal conditions. The mixing takes place by diffusion in a laminar co-flow reactor, where temperature, stoichiometry and mixing conditions could be varied.

3)

The following approaches for modeling of jet mixing systems with simplified fluid dynamics and full chemistry were to be evaluated: a) the Zwietering non-ideal

plug reactor approach [3] where one stream is uniformly and continuously distributed along the other stream; b) the droplet diffusion model, where micromixing is modeled empirically in terms of a molecular diffusion process in a number of hypothetical droplets surrounded by bulk fluid [5]; and c) the Two-Stage Lagrangian model [6] developed in GRI funded work to describe detailed chemical kinetics in turbulent flames, using experimental correlations for entrainment and mixing. The chemical engineering models would be evaluated by comparison with CFD predictions as well as pilot scale results from literature. Based on this analysis, the applicability of the mixing models would be assessed and the model that provides the best description of the investigated jet-mixing systems selected. The preferred mixing model with the updated detailed kinetics were then to be further validated against pilot scale results on natural gas/methane reburn from literature.

## **PROJECT OBJECTIVES**

The objective of the present project was to develop a model for gas injection systems with detailed chemistry that in a simple manner can be used to simulate processes like Natural Gas Reburning. The work involved improvement and validation of detailed kinetics models for hydrocarbon oxidation and hydrocarbon/nitrogen interactions, based on flow reactor data covering a wide range of hydrocarbon fuels, temperature and stoichiometry. The effect of mixing on reburning would be evaluated through experiments with a laminar diffusion mixing reactor. Furthermore, a systematic analysis and evaluation of different approaches for modeling of jet mixing systems with simplified fluid dynamics and detailed chemistry were to be undertaken. The preferred mixing model would be validated through comparison with bench and pilot scale results on reburning.

## **OBJECTIVES FOR THE FIRST YEAR**

The principal objectives of the first year included:

1. evaluation of the predictive capabilities of the current hydrocarbon oxidation mechanism by comparison with flow reactor results obtained for  $C_1$  and  $C_2$  hydrocarbons over a range of stoichiometries and temperatures, with and without NO addition.

2. flow reactor experiments on carbon suboxide oxidation in the presence and absence of nitric oxide, in order to derive rate constants for critical reactions of the HCCO radical.

## WORK PERFORMED

### Evaluation of the hydrocarbon oxidation mechanism

In order to evaluate the predictive capabilities of the present hydrocarbon oxidation mechanism [10, 11], modeling predictions were compared with flow reactor results obtained for C<sub>1</sub> and C<sub>2</sub> hydrocarbons over a range of stoichiometries and temperatures, with and without NO addition. The experiments were conducted in previous work, much of which presently unpublished. Selected experiments from the database were early on made available for the GRI mechanism development group for validation of version 1.2.

#### *Experimental*

The experiments were conducted in specially designed isothermal laminar flow quartz reactors that provide well defined reaction conditions in the temperature range of interest. The experimental setup has been used previously in a number of studies on gas phase processes [13, 14, 15] and its suitability for studies of detailed gas phase kinetics has been evaluated previously [16, 17].

The flow system is designed to mix a reactant gas consisting of up to 8 different components and water. The reactant gas is led through the flowsystem to the reactor. The reaction takes place in a quartz reactor which is placed in a three-zone oven. After reaction the product gas is led to the analysis equipment where species concentrations are measured. The system is connected to an automated control and data acquisition system.

The different gases that make up the reactant mixture are supplied from gas cylinders, led through reduction valves and dosed by eight mass flow controllers. The three first inlets are used for the main gas flow, which normally contains nitrogen and oxygen. The main flow can be dried by passing through a bed of water absorption material, or a part of the main stream can be led through an evaporator for addition of water.

The remaining five inlets are used to inject gases containing reactant components such as hydrocarbons, CO, NO, and NH<sub>3</sub> into the reactor. The five inlets to the injection system is mixed to obtain three separate flows to the reactor, ensuring that no reaction takes place in the injection tubes.

After reaction but prior to gas analysis water is removed in a cooling tube. The flow system is build of 1/4 and 1/8 inch PTFE tubes, while the valves are made of either PTFE, PVC or brass, and the mass flow controllers of stainless steel. It is possibly to deliver total flows in the regime from 200 ml/min to 2000 ml/min (1 atm, 293 K).

A number of quartz flow reactors of varying volume, all designed to achieve a good plug-flow approximation in the laminar flow regime, are available for the experiments. To achieve a well defined reactor volume the main stream and the three injector streams are heated separately and mixed in cross flow at the reactor inlet. Figure 1 shows the reactor design. CFD calculations [17] show that the mixing time is of the order of 5 ms in the large reactor.

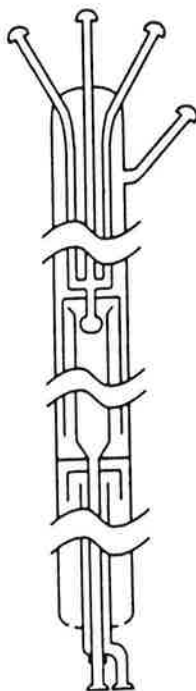


Figure 1: Schematic of the reactor design.

The flow-reactor system is placed in a three zone oven with individual control

of the three heating sections to provide good temperature control. The oven operates in the temperature range 800–1500K. The varying size of the reactors (from  $0.40 \times 5.6$ cm to  $0.89 \times 18.5$ cm) allows for a considerable variation in residence time (30 to 600 ms) in the present flow and temperature range. It also allow us to investigate the impact of surface reactions on the quartz reactor walls.

After reaction the flue gas is conditioned for the analysis equipment by removing water in a cooling tube and adjusting the gas flow. The concentration of hydrocarbons are measured by FTIR, while CO, CO<sub>2</sub>, O<sub>2</sub>, NO and N<sub>2</sub>O are measured by spectrophotometric analyzers. HCN and NH<sub>3</sub> are measured with wet chemical methods or by FTIR. Reactor temperature is measured with a NiCrNi thermocouple protected from the gas by a quartz tube. The pressure is measured in the main stream just before the reactor.

#### *Chemical kinetic modeling*

The chemical kinetic model used was developed for nitrogen conversion in reburning and hybrid reburning/SNCR [10, 18, 19]. A few modifications were made to the methane oxidation subset in a recent work related to methane emissions from lean-burn gas engines [11]. In the current evaluation of the mechanism, predictions are compared with flow reactor data using application codes from the CHEMKIN library [20], primarily Senkin [21].

The kinetic model consists of oxidation mechanisms for C<sub>1</sub>–C<sub>2</sub>-hydrocarbons, HCN and NH<sub>3</sub> together with a subset describing reactions between hydrocarbon and nitrogen species. The most reliable parts of the mechanism are the subsets for moist CO oxidation, CH<sub>4</sub> oxidation and HCN oxidation. We consider the C<sub>2</sub> oxidation chemistry to be considerably more uncertain, in particular that of acetylene. Until recently, the most controversial part of the kinetic model was the subset describing selective non-catalytic reduction of NO by NH<sub>3</sub>. Significant advances in the understanding of this subset [22, 23] have led to the development of a model that provides a satisfactory description of this process over a wide range of conditions. This enhances the possibilities of establishing a reliable model for the advanced reburn (*i.e.* hybrid reburn/SNCR) chemistry.

### Comparison of model predictions with experiment

A systematic experimental investigation of the hydrocarbon oxidation chemistry in the 800–1500 K range has been conducted for methane and ethane, as well as for selected intermediate hydrocarbons (ethylene, acetylene, acetaldehyde) under flow reactor conditions at a range of stoichiometries. Typical results obtained for CO in the outlet under slightly fuel-rich conditions are shown in Fig. 2.

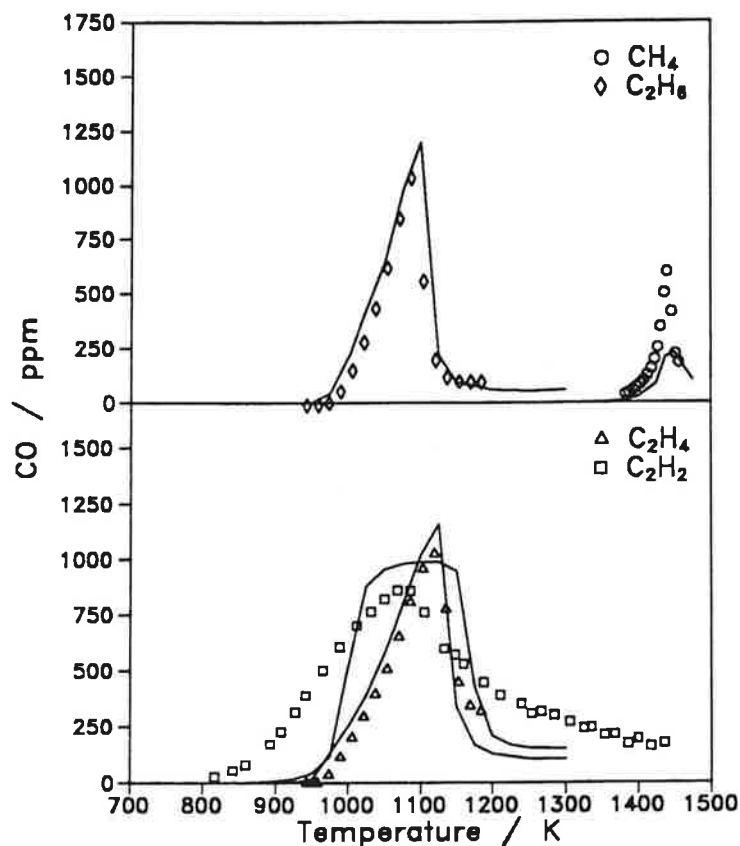


Figure 2: Comparison between experimental data and modeling predictions for methane, ethane, ethylene and acetylene oxidation in a flow reactor under slightly fuel-rich conditions. The excess air ratio  $\lambda$  is about 0.9 and the residence time is of the order of 100 ms.

As expected, the characteristic temperature regime for oxidation of the hydrocarbon to CO at the present reaction times differ widely between fuels (Fig. 2). Compared to methane, the C<sub>2</sub> hydrocarbons are consumed at much lower temperatures at a given reaction time. This is consistent with shock tube ignition

delay experiments reported in literature [24].

Both our current mechanism [10, 11] and GRI-Mech 3.1 were compared with the available experimental database. The comparison of Fig. 2 (for our mechanism) indicate the level of agreement obtained. While both mechanisms in general provide a satisfactory description of the hydrocarbon oxidation chemistry, neither scheme is able to describe correctly acetylene oxidation. The major uncertainties in this subset of the mechanism relates to the  $C_2H_3/C_2H_2/HCCO$  link and to reactions of HCCO. Since HCCO is also the major radical responsible for removing NO in reburning with natural gas [10], this subset is important to improve.

### Experiments to characterize HCCO reactions at high temperature

In the reburning process it is important to obtain a good reduction of NO formed in the primary combustion zone. In Natural Gas Reburning, this reduction occurs primarily by reaction of NO with the HCCO radical. Unfortunately neither the HCCO+NO reaction or the formation and consumption of HCCO in  $C_1$  and  $C_2$  hydrocarbon oxidation are presently well characterized. For the HCCO+NO reaction, the overall rate constant is known, but the branching ratio between the two product channels, one leading to HCNO (which is largely recycled to NO) and one forming HCN is controversial [10]. Furthermore, there is considerable uncertainty about the rate of the HCCO+ $O_2$  reaction at high temperatures; this reaction is presumably the most important consumption step for HCCO and competes with the HCCO+NO reaction.

For these reasons we wish to characterize the reactions of HCCO with NO and  $O_2$ . In order to investigate these steps experimentally at high temperatures without interference from side reactions of  $CH_i$  radicals, it is necessary to use a fuel which do not produce  $CH_i$  radicals. For this purpose, carbon suboxide ( $C_3O_2$ ) has been chosen.

Carbon suboxide is a linear molecule ( $O=C=C=O$ ), which forms HCCO radicals by reaction with H and OH radicals [25, 26, 27, 28]. By using  $C_3O_2$  as precursor for HCCO, some of the complexities of using for instance  $C_2H_2$  can be avoided. However, other complications arise, since some uncertainty in the  $C_3O_2$  oxidation chemistry remains.

## *Experimental*

The experiments are performed in the flow reactor set-up described above. The carbon suboxide used for experiments was synthesised by thermal decomposition of malonic acid using the procedure of Glemser [29]. The purified product was dosed by leading nitrogen through a tube containing liquid  $C_3O_2$  cooled in an acetone dry ice cooling bath (195 K). The stream was analysed using FTIR; the  $C_3O_2$  product gas contained some CO as well as small amounts of  $CO_2$ . These impurities are taken into consideration in the data interpretation. FTIR calibration spectra was made as well, measuring the carbon suboxide concentration by subsequent oxidation to  $CO_2$  at 1300 K. The  $CO_2$  concentration was measured both using FTIR and an IR analyzer. During the experiments the concentration of  $O_2$  was measured with a paramagnetic analyzer, CO and  $CO_2$  were detected by IR analyzers, and NO was measured using a UV analyzer. At the same time the FTIR was used to determined concentrations of  $C_3O_2$  and  $CO_2$  because the  $CO_2$  analyzer is cross sensitive to  $C_3O_2$ .

## *Preliminary results*

In order to characterize the  $C_3O_2$  oxidation chemistry and, based on that, derive rate constants/branching ratios for the reactions of HCCO with  $O_2$  and NO, a number of experiments have been conducted. These include pyrolysis of  $C_3O_2$ , lean and rich oxidation of  $C_3O_2$ , and reaction of  $C_3O_2$  with NO. All experiments were conducted with about 2% of water vapor in order to introduce hydrogen to the reaction system. Formation of H and OH radicals is required to ensure that  $C_3O_2$  is converted primarily to HCCO radicals.

Figure 3 shows typical results on the reaction of carbon suboxide with nitric oxide in the presence of small amounts of oxygen. Above 800 K a significant reduction of NO is observed, which can be attributed to the HCCO+NO reaction. Data interpretation is currently undertaken.

## **Preliminary evaluation of the Zwietering mixing approach for modeling reburning**

A preliminary mixing model, based on the approach by Zwietering [3], in combination with the detailed reaction mechanism has been tested against bench and pilot scale data on reburning from literature [18, 30, 31]. Figure 4 compares pilot



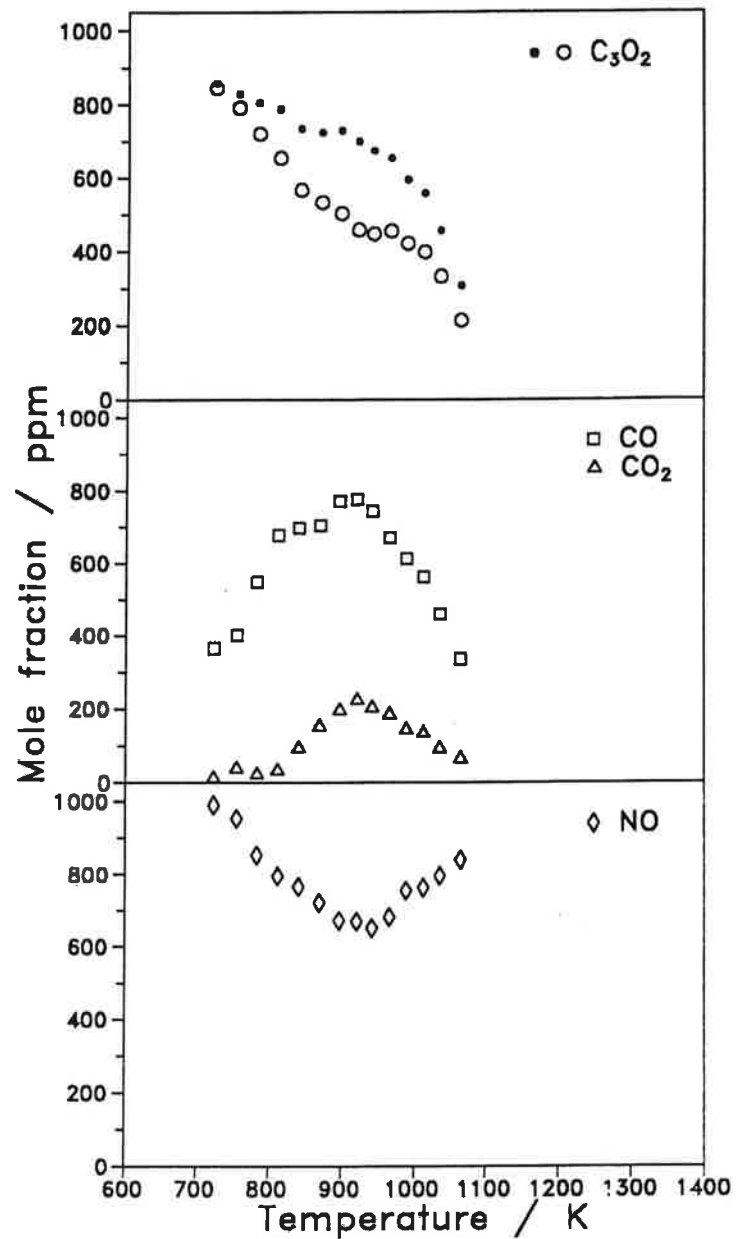


Figure 3: Experimental results on carbon suboxide oxidation with NO present. Due to problems of maintaining a steady feed of  $C_3O_2$ , the inlet concentration (shown as filled circles) varies. The  $O_2$  level was 1000 ppm,  $H_2O$  was 2%, and the reaction time about 100 ms.

scale data on reburning with natural gas or gasification gas with modeling predictions. Results are generally encouraging, but for a more thorough validation of the model, pilot scale experiments with better defined mixing conditions are required.

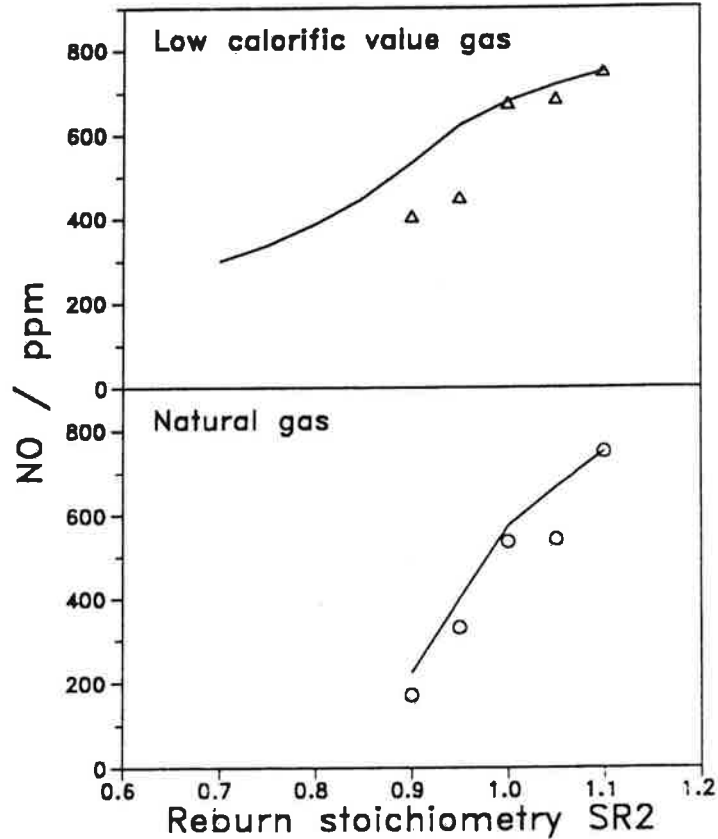


Figure 4: Comparison between pilot scale data and modeling predictions on reburning with low calorific value gas and natural gas. The pilot scale data are from Bortz and Offen [32].

## WORK PLANNED

The work to be performed in year 2000 was as follows:

1. Characterize the reactions of HCCO with  $O_2$  and NO from the  $C_3O_2$  experiments

2. Refine and validate hydrocarbon/reburning mechanism based on HCCO reaction data as well as flow reactor results.
3. Perform mixing experiments to assess the effect of mixing on reburning
4. Perform initial evaluation of chemical engineering model for reburning

Due to the termination of the contract by February 2000, none of these tasks were completed.

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