

# MASTER

ARI-RP-52

SIXTH QUARTERLY TECHNICAL SUMMARY REPORT  
ON THE  
HOMOGENEOUS PRODUCTION AND REMOVAL OF NO<sub>x</sub>  
FROM COMBUSTION EXHAUST GASES

By

J.A. Silver, C.M. Gozewski, and C.E. Kolb

Aerodyne Research, Inc.  
Bedford Research Park  
Crosby Drive  
Bedford, MA 01730

Prepared Under DOE Contract No. T-78-C-01-3183  
Period Covered: December 1, 1979 to February 29, 1980

Submitted to  
The Division of Fossil Energy Utilization  
U.S. Department of Energy

March 1980

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

## ABSTRACT

The final reaction rate constants for  $\text{NH}_2 + \text{NO}$  have been determined. A measurement of the fraction of product channels which form OH provides an approximate value of 0.2, but the uncertainties in the method used make this value a lower limit.

Preliminary rate measurements for the reaction of  $\text{OH} + \text{NH}_3 \rightarrow \text{NH}_2 + \text{H}_2\text{O}$  agree well with previous room temperature experiments and appear to show a simple Arrhenius dependence with temperatures to 1200 K.

A chemical model of the  $\text{NO}_x$  chemistry has been developed and includes approximately 50 reactions at this time. Preliminary runs using this set have reproduced the gross temperature dependence of the thermal  $\text{deNO}_x$  process.

## TABLE OF CONTENTS

| <u>Section</u> |   | <u>Page</u> |
|----------------|---|-------------|
|                | ABSTRACT.....   | ii          |
| 1              | INTRODUCTION .....  | 1           |
| 2              | TECHNICAL SUMMARY PROGRESS REPORT.....                                | 3           |
| 3              | NH <sub>x</sub> /NO RATE MEASUREMENTS .....                           | 6           |
|                | 3.1 Task Goals and Milestones .....                                   | 6           |
|                | 3.2 Technical Discussion .....  | 6           |
|                | 3.2.1 Rate Measurements for the NH <sub>2</sub> + NO<br>Reaction..... | 6           |
|                | 3.2.2 Branching Ratio of NH <sub>2</sub> + NO to OH<br>Products ..... | 8           |
|                | 3.2.3 NH Radical Source .....   | 11          |
|                | 3.3 Work Forecast.....  | 11          |
| 4              | NH <sub>x</sub> OXIDATION MEASUREMENTS .....                          | 12          |
|                | 4.1 Task Goal and Milestones.....                                     | 12          |
|                | 4.2 Technical Discussion.....   | 12          |
|                | 4.3 Work Forecast .....   | 13          |
| 5              | CHEMICAL MODEL FOR NO CHEMISTRY.....                                  | 16          |
|                | 5.1 Task Goals and Milestones .....                                   | 16          |
|                | 5.2 Technical Discussion.....   | 16          |
|                | 5.3 Work Forecast.....  | 18          |
| 6              | REFERENCES.....   | 19          |

# 1. INTRODUCTION

The production and removal of  $\text{NO}_x$  and other combustion products during fossil fuel combustion is a serious environmental problem for both stationary and mobile combustion driven energy systems. Since stationary systems are faced with increased utilization of coal, synthetic fuel oils derived from coal, or oil shale, and since all of these fuels have significant levels of fuel-bound nitrogen,  $\text{NO}_x$  formation may become acute.

Recent studies of the production of  $\text{NO}_x$  due to oxidation of fuel nitrogen strongly indicate that a critical role is played by the interaction of  $\text{NH}_x$  ( $x = 1,2,3$ ) species with  $\text{NO}$ ,  $\text{O}$ ,  $\text{OH}$  and  $\text{H}$ . Studies have also shown that these reactions play a vital role in the efficient homogeneous removal of  $\text{NO}_x$  from combustion exhaust streams upon the addition of  $\text{NH}_3$ .

The work in progress has three basic objectives. The first objective is to determine rate constants for several of the basic chemical reactions which govern the formation of  $\text{NO}_x$  in the combustion of fuel-bound nitrogen and which also play a key role in the thermal  $\text{deNO}_x$  process. The specific reactions to be studied include the reactions of  $\text{NH}_3$ ,  $\text{NH}_2$ , and  $\text{NH}$  with  $\text{NO}$  (Task 1), and the reactions of  $\text{NH}_3$ ,  $\text{NH}_2$ , and  $\text{NH}$  with the combustion radicals  $\text{O}$ ,  $\text{OH}$ , and  $\text{H}$  (Task 2). This report focuses on the measurement of reaction rates for  $\text{OH} + \text{NH}_3$  over the temperature range of 294 - 1200 K.

The second objective is to utilize the kinetic data obtained in Task 1 and Task 2 to identify the key  $\text{NO}_x$  radical scavenging species. Once the key  $\text{NH}_x$  radical(s) has been identified, gas additives other than  $\text{NH}_3$  which can efficiently produce this  $\text{NO}_x$  scavenger will be evaluated under combustor exhaust flow conditions. This work may allow a major improvement in the efficiency of the homogeneous  $\text{NO}_x$  scavenger concept (Task 3).

The third objective is to evaluate the impact of the kinetic and mechanistic data gathered in Tasks, 1,2, and 3 on the design of coal and synfuel combustors and on the implementation of homogeneous  $\text{NO}_x$  exhaust scavenging schemes. This will be accomplished by modeling the processes in the combustion stream (Task 4). This modeling will utilize existing computer codes, including Aerodyne's PACKAGE code. This modeling will allow assessment of the impact of the measured chemical parameters on exhaust  $\text{NO}_x$  content. The results of this computer modeling will be translated into conceptual designs for pilot scale experiments which demonstrate achievable impacts on exhaust  $\text{NO}_x$  content (Task 5). A set of rate equations has been selected and preliminary runs have been made which reproduce the gross features of the thermal de $\text{NO}_x$  process.

## 2. TECHNICAL SUMMARY PROGRESS REPORT

A summary of progress achieved during the last quarter is presented below. A time-phasing schedule for each key subtask is shown in Fig. 2.1.

### Task 1: Measurement of $\text{NH}_x + \text{NO}$ Rate Constants

The rate measurements for the reactions of  $\text{NH}_2 + \text{NO} \rightarrow \text{products}$  and  $\text{NH}_3 + \text{NO} \rightarrow \text{NH}_2 + \text{HNO}$  have been completed over the temperature range of 294 - 1200 K. The  $\text{NH}_2$  reaction rate decreases substantially as the temperature is raised. Reaction of NO with  $\text{NH}_3$  is extremely slow and probably plays no role in the  $\text{NO}_x$  system kinetics. The hydroxyl radical has been identified as a reaction product in at least 20% of the product channels. Attempts at producing a nonchemiluminescing NH source have been unsuccessful but a few methods still hold promise and are discussed in Section 3.

### Task 2: Rate Data for $\text{NH}_x$ Oxidation

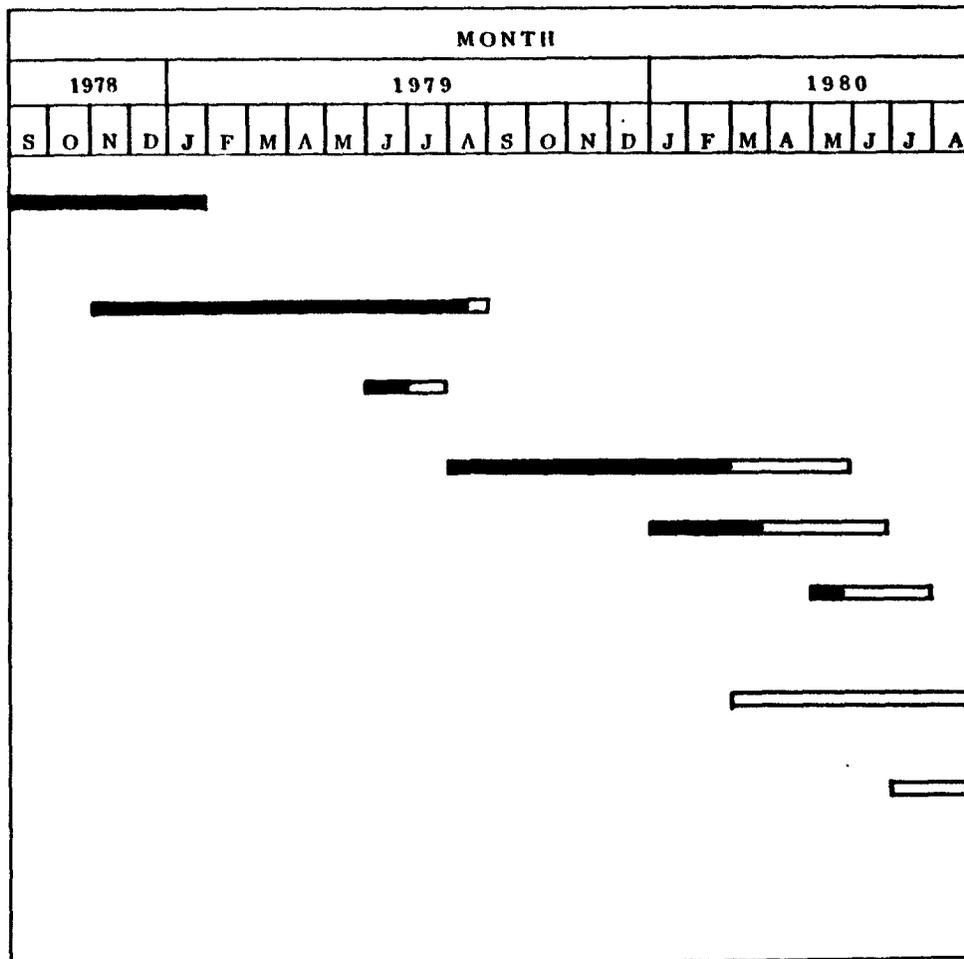
Preliminary rates for the reaction of  $\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$  have been measured over the temperature range of 294 - 1200 K. The values at lower temperatures are consistent with previous measurements and the temperature dependence appears to be Arrhenius-like.

### Task 3: Assessment of Rate Data To Determine Key NO Scavenger Species

We are continuing the assessment of the published experimental reaction rates and kinetic models relevant to the homogeneous chemistry of  $\text{NO}_x$  in combustor exhaust streams. The impact of our experimental results on proposed models is detailed in the technical discussion.

Subtasks

- 1.1 DEMONSTRATION OF APPARATUS CALIBRATION AND DETECTION EFFICIENCY
- 1.2 MEASUREMENT OF  $\text{NH}_x$  +  $\text{NO}$  RATES
- 3.1 ASSESSMENT OF RATE DATA TO DETERMINE KEY  $\text{NO}$  SCAVENGER SPECIES
- 2.1 RATE DATA FOR  $\text{NH}_x$  OXIDATION
- 4.1 CHEMICAL MODEL FOR  $\text{NO}$  CHEMISTRY
- 4.2 ASSESSMENT OF MEASURED RATE DATA FOR  $\text{NO}_x$  PRODUCTION AND SCAVENGING
- 3.2 TEST OF  $\text{NO}_x$  SCAVENGER CANDIDATES
- 5.1 CONCEPTUAL DESIGN FOR PILOT SCALE  $\text{NO}_x$  SCAVENGING TESTS



4

Figure 2.1 - Contract Subtask Schedule

Task 4: Chemical Model for NO Chemistry

A chemical reaction set containing approximately 50 reactions has been assembled. Initial computer modeling runs indicate that the key reaction is  $\text{NH}_2 + \text{NO} \rightarrow \text{products}$ , and that the identification of the products is critical in determining the chemistry of  $\text{NO}_x$ .

### 3. NH<sub>x</sub>/NO RATE MEASUREMENTS

#### 3.1 Task Goals and Milestones

The goals of this task are to: (1) demonstrate the efficient production of NH and NH<sub>2</sub> in the flow reactor using discharge flow techniques; (2) demonstrate the efficient detection of NH and NH<sub>2</sub> in the flow reactor using laser-induced resonance fluorescence; (3) equip the flow reactor with calibrated gas handling equipment to introduce NO, NH<sub>x</sub> and carrier gases; (4) demonstrate the use of the molecular beam mass spectrometer coupled to the flow reactor to detect NO, NH<sub>3</sub>, and other flow gases; and (5) utilize each of the subsystems to measure the rate of reaction of NO with NH, NH<sub>2</sub>, and NH<sub>3</sub> from room temperature to combustion temperatures.

The first three goals previously had been completed. In this last quarter, substantial progress has been made on the fifth and most important item, the rate measurements. The use of the mass spectrometer to identify reaction products will be attempted next month when the installation of an upgraded system will be completed.

#### 3.2 Technical Discussion

##### 3.2.1 Rate Measurements for the NH<sub>2</sub> + NO Reaction

In the previous quarterly<sup>(1)</sup> rate measurements for the reaction of NH<sub>2</sub> with NH<sub>3</sub> over the temperature range of 294-1200 K were discussed. Subsequently, measurements at additional temperatures were made, and the results for the complete set are illustrated in Fig. 3.1. The rate coefficient exhibits an increasing fall-off as the temperature is raised. Although not exhibiting Arrhenius-like behavior, the temperature dependence has been least-squares fit to the functional form

$$k(T) = A T^n e^{-b/T} .$$

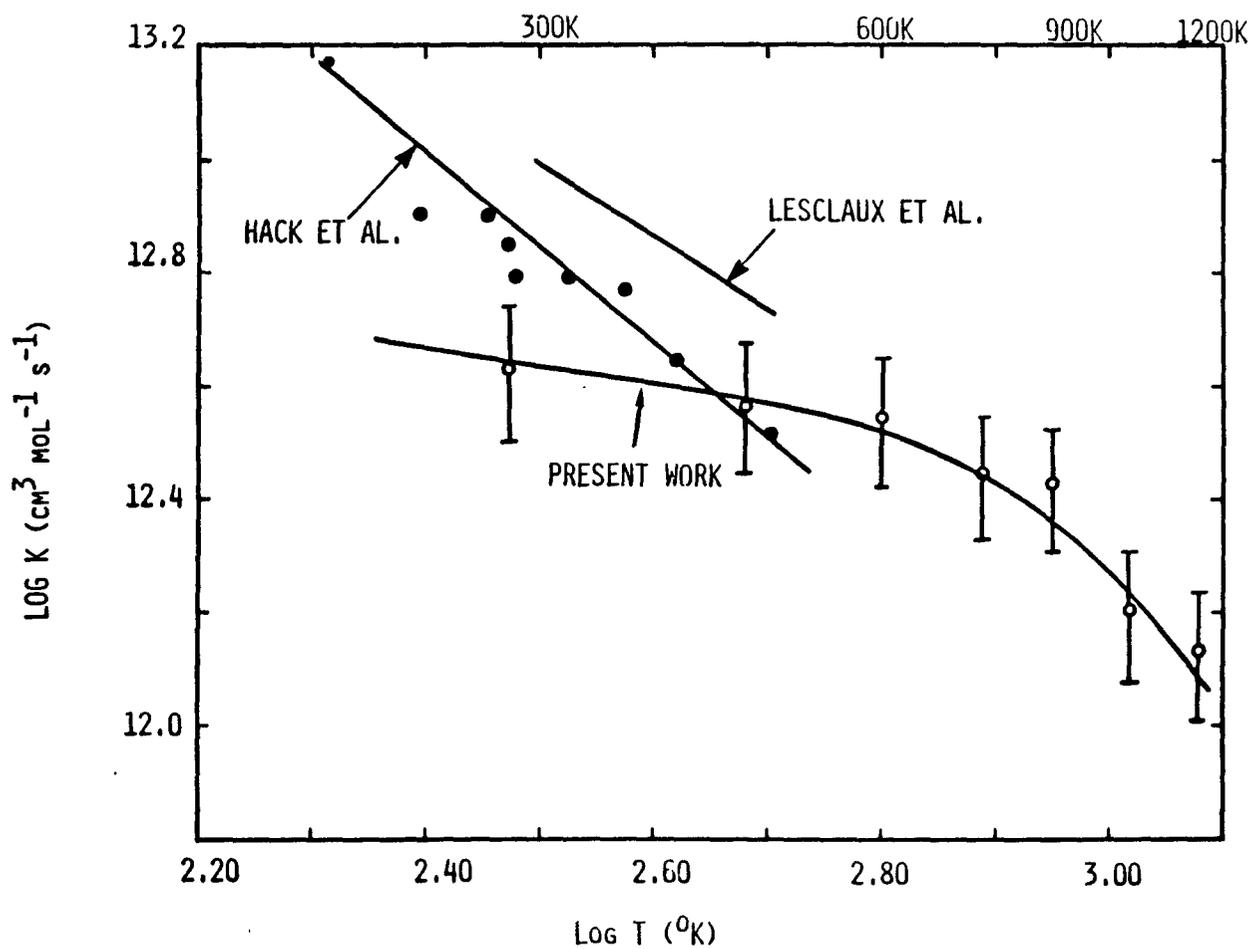


Figure 3.1. Temperature Dependence of Measured Rate Constants for  $\text{NH}_2 + \text{NO}$  Reaction

Although this form has no particular physical basis,<sup>(2)</sup> it is convenient to use and is the form used in most modeling codes, including the PACKAGE code. The best fit parameters are

$$A = 1.95 \times 10^{-4} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$b = 938 \text{ K}$$

$$n = -2.46 \quad .$$

### 3.2.2 Branching Ratio of $\text{NH}_2 + \text{NO}$ to OH Products

In the previous quarterly,<sup>(1)</sup> it was noted that a strong laser-induced fluorescence signal of OH was seen from the reaction of  $\text{NH}_2 + \text{NO}$ . An attempt to quantify the amount of OH produced leads to a lower limit of ~20%.

The calibration was performed in the following manner. Using the fast reaction of  $\text{H} + \text{NO}_2 \rightarrow \text{OH} + \text{NO}$ , a clean source of hydroxyl radicals is provided. Ammonia is introduced through the moveable injector, and quantitatively is converted to  $\text{NH}_2$  by the reaction  $\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$ . Using laser induced fluorescence to detect  $\text{NH}_2$ , and an OH resonance lamp to detect OH, we obtain the relative detection sensitivity of the apparatus to equal number densities of OH and  $\text{NH}_2$ . The only problem is that the laser beam has no clear exit path and scatters off the OH lamp, creating a large background which severely limits the S/N for the  $\text{NH}_2$  measurements.

The calibration procedure is:

1. Make OH from  $\text{H} + \text{NO}_2$ ,
2. Measure the signal of OH, defined as  $S_{\text{OH}}$ , for a set of known operating conditions,
3. Add excess  $\text{NH}_3$  to quantitatively convert all OH to  $\text{NH}_2$ ,
4. Measure the signal of  $\text{NH}_2$ , defined as  $S_{\text{NH}_2}$

$$S_{\text{OH}} = C_{\text{OH}} \times [\text{OH}]_{\text{calibration}} \quad (1a)$$

$$S_{\text{NH}_2} = C_{\text{NH}_2} \times [\text{NH}_2]_{\text{calibration}} \quad , \quad (1b)$$

where C is an apparatus constant which includes PMT response, transmission of filters, geometries, etc. for OH and NH<sub>2</sub>,

$$\frac{S_{OH}}{S_{NH_2}} = \frac{C_{OH} [OH]_{cal}}{C_{NH_2} [NH_2]_{cal}} \quad , \quad (2)$$

but

$$[OH]_{cal} = [NH_2]_{cal} \quad , \quad \text{and} \quad (3)$$

$$\frac{C_{OH}}{C_{NH_2}} = \frac{S_{OH}}{S_{NH_2}} \quad . \quad (4)$$

5. Now, the gases are changed and NH<sub>2</sub> is made from NH<sub>3</sub> + F.
6. Measure the signal of NH<sub>2</sub>, defined as I<sub>NH<sub>2</sub></sub> ,
7. Add excess NO through injector, quantitatively reacting all of the NH<sub>2</sub> → products, fraction (α) of which is OH,
8. Measure the signal of OH, defined as I<sub>OH</sub>.

therefore,

$$I_{NH_2} = C_{NH_2} \times [NH_2]_{rxn} \quad (5a)$$

$$I_{OH} = C_{OH} \times [OH]_{rxn} = C_{OH} \times \alpha [NH_2]_{rxn} \quad (5b)$$

$$\frac{I_{NH_2}}{I_{OH}} = \frac{C_{NH_2}}{\alpha C_{OH}} \quad (6)$$

but from Eq. (4) and rearranging Eq. (6),

$$\alpha = \frac{I_{OH}}{I_{NH_2}} \frac{S_{NH_2}}{S_{OH}} \quad (7)$$

A calibration step was performed before and after the reaction step to assure that the operating conditions remained steady. The value obtained for  $\alpha$  was  $0.2 \pm 0.1$ . There are a few assumptions that must be analyzed to validate this measurement.

1. Wall Removal: Since  $NH_2$  and OH have different rates of removal by the reactor walls, the assumption of quantitative conversion is violated. However, it can be shown that the difference actually cancels out in taking the ratios of S and I in expression Eq. (7).
2. Laser Frequency Drift: This cannot be measured except by noting that the calibration  $NH_2$  signal before and after remains approximately constant.
3. Quenching of Vibrationally Excited Products: Both the  $NH_2$  and OH detectors see molecules in the  $v = 0$  state only. If, during the calibration or reaction measurement, a species produced in  $v > 1$  is not quenched, the assumption of detecting quantitative conversion is violated. We have performed measurements showing the  $NH_2$  and OH produced in the source inlet are completely quenched. Since the distance of the injector from the detector region was only 10 cm, there might not have been time for sufficient quenching of the OH or  $NH_2$  produced by the addition of excess  $NH_3$  or NO, respectively. In other words, the values of  $S_{NH_2}$  and  $I_{ON}$  may have been too small, which leads to an underestimation in the value of  $\alpha$ . This could be corrected by adding the excess reagents at larger injector distances. However, wall removal of the products would be more severe, decreasing the already poor S/N for  $NH_2$ .

It is planned to repeat these measurements using laser induced fluorescence for both OH and NH<sub>2</sub>, which will lessen the S/N problem.

### 3.2.3 NH Radical Source

The development of a source for NH radicals has not been completely successful. The reaction of ammonia with excess fluorine atoms does produce NH, but in its first excited electronic state. The chemiluminescence overpowers the laser-induced fluorescence. Attempts to produce NH via direct dissociation of ammonia were unsuccessful. It may be possible to use the reaction of metastable argon, produced in the microwave discharge, with ammonia to form NH, as inferred by Stedman.<sup>(3)</sup>

### 3.3 Work Forecast

During the next quarter, we will attempt to narrow the limits on the fraction of OH produced from NH<sub>2</sub> + NO. A similar experiment will measure the fraction of H-atoms. The mass spectrometer will be used to look for other products, such as N<sub>2</sub>, N<sub>2</sub>O, as well as any complexes such as NH<sub>2</sub> NO. We will also proceed in the development of a usable source of NH radicals.

## 4. NH<sub>x</sub> OXIDATION MEASUREMENTS

### 4.1 Task Goal and Milestones

The goals of this task are to measure the rate constants for the reactions of NH, NH<sub>2</sub>, and NH<sub>3</sub> with oxidizing flame radicals from room temperatures to combustion temperatures. Using the mass spectrometer, the amount of branching to various product channels will also be measured.

The key oxidation reaction, NH<sub>3</sub> + OH → NH<sub>2</sub> + H<sub>2</sub>O, is presently being studied and is discussed below. When completed, the reactions of O and H with NH<sub>3</sub> and NH<sub>2</sub> will be investigated. We have chosen the reactions in order of probable importance to the overall NO<sub>x</sub> chemistry as determined from the modeling work of ourselves and others. (4)

### 4.2 Technical Discussion

#### Rate Measurements for the OH + NH<sub>3</sub> Reaction

The reaction of OH + NH<sub>3</sub> → NH<sub>2</sub> + N<sub>2</sub>O is proposed to be the key initiation step for the removal of NO by NH<sub>3</sub>. Previous rate measurements have been made in the temperature range 297 - 699 K. Perry, et al. (5) obtained a value for the rate coefficient of  $k = 2.93 \times 10^{-12} e^{-(1710 \pm 300)/RT} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  Hack, et al. (6) found values about 50% higher. The present work extends these measurements to 1200 K.

Hydroxyl radicals are generated by the fast reaction of H atoms (produced in a microwave discharge) and NO<sub>2</sub>. Anhydrous ammonia is admitted through the moveable injector and the rate of decay of OH is measured using an OH resonance lamp, made by flowing a stream of helium saturated in water vapor through a microwave discharge. Fluorescence is captured by a Hamamatsu R763 photomultiplier wired for photon counting. A 320 nm bandpass interference filter is used to reject unwanted light. The counts are amplified and shaped by a Pacific Precision Instruments Model 3262/AD4 Amplifier/Discriminator

and fed to a Monsanto Model 1505A Counter-Timer. Data are corrected for scattered light from the lamp and any other sources of background.

Initial experiments have been done at five temperatures between 294 and 1200 K. A sample of the data is shown in Figures 4.1 and 4.2. Although not yet corrected for diffusion and wall removal, the results indicate that the low temperature dependence can be extrapolated to higher temperatures.

Above 1000 K, background radiation increases dramatically and the wall removal of H atoms in the source also increases, resulting in a rapid deterioration of S/N. To overcome this, a tungsten hot-wire dissociator is being constructed which will produce H atoms at a position just upstream of the NO<sub>2</sub> mixing region. This should increase the number of OH radicals so that the signal will be enhanced. Presently, the rate measurements over the temperature range of 294 - 1200 K are being repeated and refined, and a final expression for the temperature dependent rate coefficient will be obtained shortly.

#### 4.3 Work Forecast

During the next quarter, we will measure the rates of reaction of H, O, and OH with NH<sub>3</sub> over the temperature range of 294 - 1200 K. We will use the mass spectrometer to identify reaction products when more than one product channel is open. The NH<sub>2</sub> oxidation measurements will also be started.

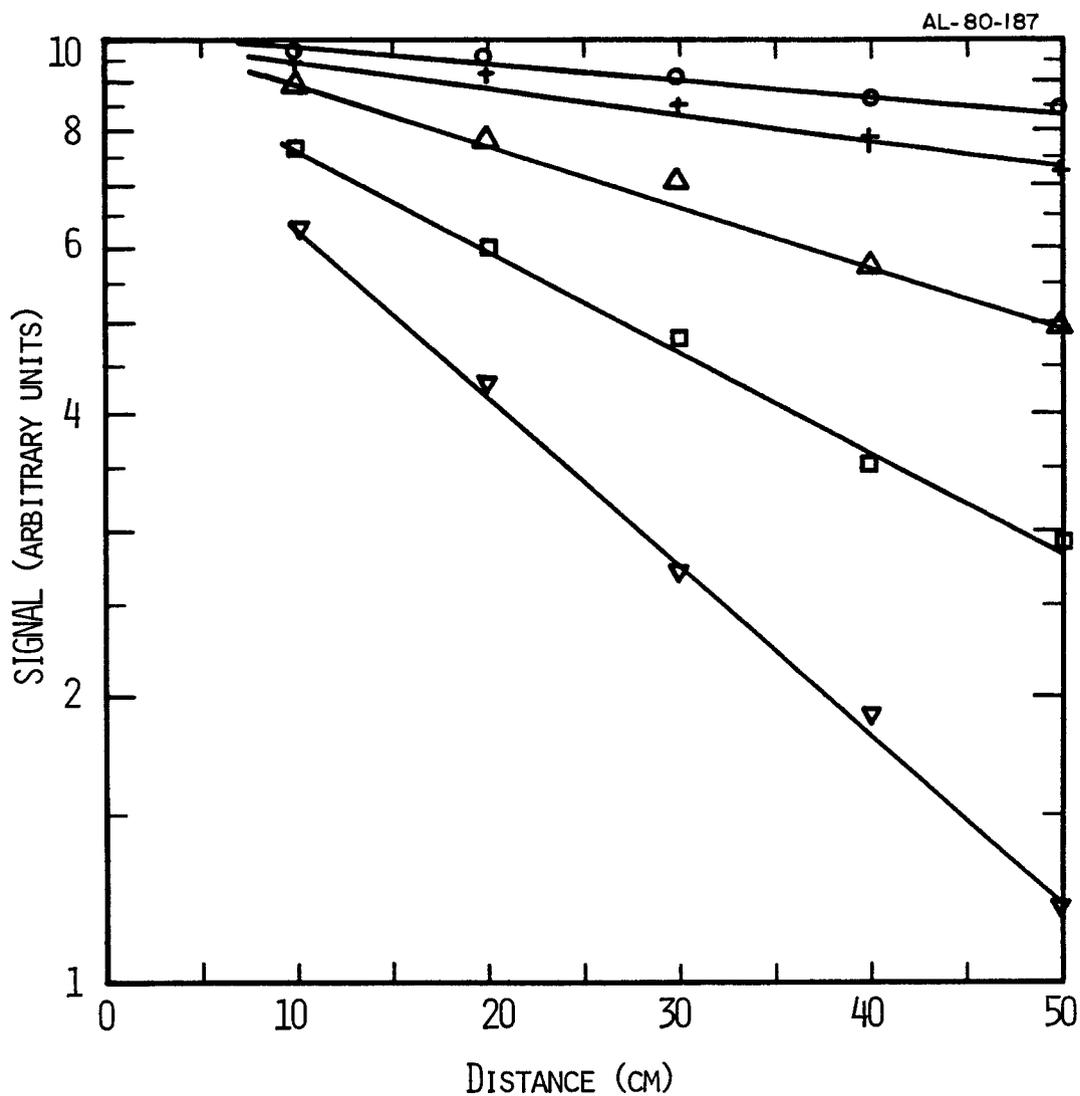


Figure 4.1 - Decay of  $[OH]$  versus Reaction Distance for Various Concentrations of  $NH_3$  at 850 K.  $[NH_3] = (\bullet) 1.48 \times 10^{13}$ ,  $(+)$   $3.25 \times 10^{13}$ ,  $(\Delta)$   $6.64 \times 10^{13}$ ,  $(\square)$   $1.06 \times 10^{14}$ ,  $(\nabla)$   $1.74 \times 10^{14}$  molecules  $cm^{-3}$ .

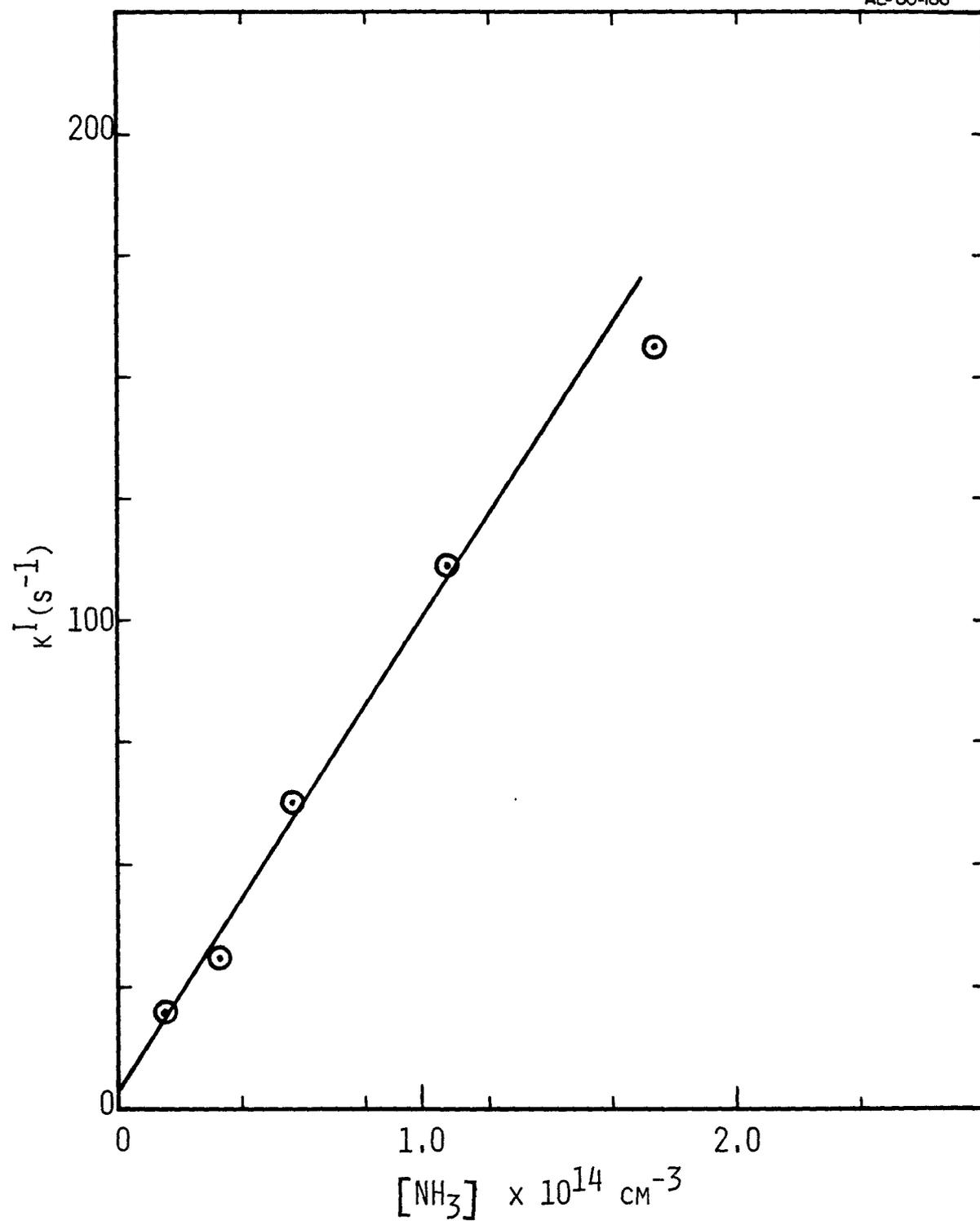


Figure 4.2 - First Order Removal of OH versus  $\text{NH}_3$  Concentration at 850 K

## 5. CHEMICAL MODEL FOR NO CHEMISTRY

### 5.1 Task Goals and Milestones

The goals of this task are to: (1) use the Aerodyne PACKAGE code to obtain a chemical model for the NO chemistry in coal combustor exhaust streams, and (2) to assess the impact of our measured kinetic data on models for NO production and scavenging.

During this quarter, a chemical reaction set containing the reactions which may have an influence on NO<sub>x</sub> chemistry at combustor exhaust temperatures has been assembled. Using a simplified set of initial conditions, it is demonstrated that the reaction of NH<sub>2</sub> + NO → products is crucial in determining the production and removal of NO.

### 5.2 Technical Discussion

#### Chemical Model for NO Chemistry

During this past quarter, modeling the chemistry of NO in combustion exhaust streams was initiated. The first goal is to devise a reasonable set of reaction steps which can reproduce the effects obtained experimentally. These are, in order of importance,

- 1) temperature dependence of NO removal upon addition of NH<sub>3</sub> ,
- 2) shift of this dependence toward lower temperatures upon addition of H<sub>2</sub> ,
- 3) initiation delay, and
- 4) self-inhibition effect.

We have chosen a set of initial conditions similar to those of Branch, et al.<sup>(4)</sup> which also are similar to a number of the experiments. The starting species are those produced by burning an O<sub>2</sub>/CH<sub>4</sub> mixture in excess argon at the desired temperature with an equivalence ratio of 0.93.

Once the model works for this simplified condition, the initial species will be those derived from the burning of coal under actual combustor conditions.

The initial reaction set assumes that certain species are not present at high temperatures. These include  $H_2O_2$ ,  $O_3$ ,  $NO_2$ , HCN, and  $N_2O$ , the last two having been observed at levels below 1 and 50 ppm, respectively.<sup>(7)</sup> Reactions of  $CO_2$  have also been ignored. The refinement of the model will probably include some reactions of  $CO_2$ ,  $NO_2$  and  $N_2O$ .

Presently, there are three groups of reactions in the model.

- 1)  $H_x - O_y$  Reactions: These include the interactions among H, OH,  $H_2O$ , and  $HO_2$ , including three body recombinations.
- 2)  $NH_x$  Oxidation Reactions: Included in this group are the reactions of N, NH,  $NH_2$ , and  $NH_3$  with H, OH, O, and  $O_2$ . As there are multiple product channels for some of these reactions, we have used all except those which are very endothermic, and thus, unlikely to contribute to the chemistry.
- 3) Reactions of NO and HNO: These reactions provide for the removal of NO and HNO. Included are the reactions of HNO and NO with  $NH_x$ , O, OH, and H where appropriate.

Rate values are obtained from a variety of sources, but generally come from critical reviews of rate data by Jensen and Jones,<sup>(8)</sup> Westley,<sup>(9)</sup> Levy<sup>(10)</sup> and NASA.<sup>(11)</sup> Experimental values are always preferred over theoretical estimates. Since the PACKAGE program incorporates the JANAF Thermochemical Tables, the reverse rates for all reactions are calculated from equilibrium constants and are also included in the modeling. As our experimental values for the key reactions become available, they are incorporated into the model.

From some very preliminary runs, it is apparent that the key reaction is  $NH_2 + NO$ , the products of which determine the gross features of the thermal de $NO_x$  process. If one naively assumes that  $H_2O$  and  $N_2$  are the principle

products, then no change in the NO concentration occurs. If  $\text{OH} + \text{H} + \text{N}_2$  are chosen as products, then the NO concentration is significantly decreased. This is the reason behind our attempts to experimentally measure all of the product channels of the reaction of  $\text{NH}_2 + \text{NO}$ .

### 5.3 Work Forecast

The modeling of the NO chemistry in combustor exhaust flows will continue as described in the previous section. During the next quarter, we expect to achieve significant progress towards completing a model for the NO chemistry. Once it can describe the observed behavior of the  $\text{NO}/\text{NH}_x$  system, we will modify it to predict the effect of other additives which may more efficiently remove NO.

## 6. REFERENCES

1. J.A. Silver, C.M. Gozewski, and C.E. Kolb, Fifth Quarterly Technical Summary Report, Rept. No. ARI-RP-49, Aerodyne Research, Inc., Bedford, MA 01730 (December 1979).
2. R.J. Cvetanović, D.L. Singleton, and G. Paraskevopoulos, *J. Phys. Chem.* 83, 50 (1979).
3. D.H. Stedman, *J. Chem. Phys.* 52, 3966 (1970).
4. M.C. Branch, James A. Miller, and Robert J. Kee, Western States Section Fall Combustion Meeting, Paper No. WSS 79-38 (1979).
5. R.A. Perry, R. Atkinson, and J.N. Pitts, Jr., *J. Chem. Phys.* 64, 3237 (1976).
6. W. Hack, K. Hoyerman and H. Gg. Wagner, *Ber. Bunsenges Phys. Chem.* 78, 380 (1974).
7. L.J. Muzio, J.K. Arand, EPRL Report No. FP-253, KVB, Inc., (1976).
8. D.E. Jensen and G.A. Jones, *Comb. and Flame* 32, 1 (1978).
9. F. Westley, NBSIR 79-1941 (1979).
10. J.M. Levy, J.P. Longwell, A.F. Sarofim, T.L. Corley, M. Heap, and T.J. Tyson, Proc. of the Third Stationary Source Combustion Symposium, Vol. IV, EPA-600/7-79-050d, p. 3 (1979).
11. NASA Panel for Data Evaluation, Chemical Kinetic and Photochemical Data for Use in Stratospheric Modelling, JPL Publication 79-27 (1979).