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HIGH ALTITUDE JET FUEL PHOTOCHEMISTRY

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In order to evaluate the potential for photochemical oxidant formation under simulated conditions of elevated altitudes a 2-year investigation has been carried out using a 5800- λ thermostatted, evacuable and Teflon-coated environmental chamber and solar simulator facility. This 2-year program consisted of the following studies:

- Irradiations of a series of JP-4/NO_x/air mixtures at simulated ground level, 10,000 ft and 20,000 ft altitude, together with the associated chamber characterization experiments.

- Irradiations of JP-4/NO_x/air mixtures, at atmospheric pressure over a range of temperatures and at room temperature over a range of pressures, to study separately the effects of temperature and pressure on the reactivity of this mixture.

- Irradiations of JP-8/NO_x/air mixtures at simulated ground level and 20,000 ft altitude.

- Determination of alkyl nitrate yields from irradiated n-pentane/NO_x/air and n-heptane/NO_x/air mixtures as a function of total pressure (60-740 torr) and temperature (~284°-~337°K). In addition, biacetyl yields from o-xylene and benzaldehyde and o-cresol yields from toluene were determined as a function of pressure (60-740 torr) at room temperature. These studies were carried out in order to obtain mechanistic data concerning the effects of temperature and pressure on the product distributions of the representative major constituents of JP-4 and JP-8 fuels.

The experimental data from the fuel/NO_x/air irradiations show that both JP-4 and JP-8 are photochemically unreactive when compared to commercial fuels such as unleaded gasoline. The data, when used in conjunction with data from the corresponding NO_x/air chamber characterization experiments, indicate that the reactivities of JP-4/NO_x/air mixtures measured in terms of their NO oxidation rates were essentially independent of temperature but increased with decreasing pressure. These data indicate that the reactivity of JP-4 and JP-8, with regard to NO oxidation rates, will increase with increasing altitude, although the maximum ozone yields may be only slightly affected.

These conclusions concerning the effects of temperature and pressure on the fuel reactivities are consistent with other data obtained in this investigation showing that the alkyl nitrate yields from n-pentane and n-heptane decreased with decreasing pressure and increasing temperature, while the yields of benzaldehyde and o-cresol from toluene, and of biacetyl from o-xylene, exhibited little or no pressure dependence.

PREFACE

This Report was prepared by the Statewide Air Pollution Research Center (SAPRC) of the University of California, Riverside, California 92521, under Contract Number F08635-80-C-0359, Program Element G2601F, with the Air Force Engineering and Services Center, Air Force Engineering and Services Laboratory, Tyndall Air Force Base, Florida 32403.

The work was performed between November 1980 and September 1982 under the direction of Dr. Authur M. Winer, Assistant Director of SAPRC and Principal Investigator, Dr. Roger Atkinson, co-investigator, and Dr. James N. Pitts, Jr., Director of SAPRC and co-investigator. Dr. William P. L. Carter, Ms. Sara M. Aschmann, Mr. William D. Long and Mr. Frank R. Burleson were members of the research staff of this program. Appreciation is expressed to Mr. Joseph P. Lick for assistance in processing the data and to Ms. Christy J. LaClaire, Ms. I. M. Minnich and Ms. Miriam Peterson for assistance in the preparation of this report.

Dr. Daniel A. Stone, AFESC/RDV, was Project Officer.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public, including foreign nationals.

This report has been reviewed and is approved for public release.

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TABLE OF CONTENTS

<u>Section</u>	<u>Title</u>	<u>Page</u>
I.	INTRODUCTION.....	1
II.	EFFECTS OF SIMULATED ALTITUDE ON THE PHOTOCHEMICAL REACTIVITY OF IRRADIATED JP-4/NO _x /AIR AND JP-8/NO _x /AIR MIXTURES.....	3
2.1	Introduction and Background.....	3
2.2	Experimental.....	8
2.2.1	Reaction Chamber.....	8
2.2.2	Analytical Techniques Employed.....	10
2.2.2.1	Total Pressure.....	10
2.2.2.2	Temperature.....	10
2.2.2.3	Ozone.....	10
2.2.2.4	Oxides of Nitrogen.....	13
2.2.2.5	Organic Reactants and Products.....	13
2.2.2.6	Formaldehyde.....	16
2.2.2.7	Light Intensity and Spectral Distribution.....	16
2.2.3	Operating Procedures.....	16
2.2.3.1	Procedures for Filling the Evacuable Chamber.....	16
2.2.3.2	Experimental Protocol.....	17
2.3	Results.....	19
2.3.1	Matrix of JP-4/NO _x /Air and JP-8/NO _x /Air Irradiations.....	19
2.3.2	Light Intensities and Spectral Distributions Used at the Three Simulated Altitudes (Ground Level, 10,000, and 20,000 Ft).....	20
2.3.3	Environmental Chamber Experiments.....	20
2.3.3.1	Chamber Characterization Runs.....	28

TABLE OF CONTENTS
(Concluded)

<u>Section</u>	<u>Title</u>	<u>Page</u>
	2.3.3.2 Results of Fuel/NO _x Runs.....	32
	2.4 Discussion.....	37
III.	TEMPERATURE AND PRESSURE EFFECTS ON ALKYL NITRATE FORMATION FROM THE NO _x PHOTOOXIDATIONS OF n-PENTANE AND n-HEPTANE.....	43
	3.1 Introduction.....	43
	3.2 Experimental.....	44
	3.3 Results.....	45
	3.4 Discussion.....	52
IV.	EFFECTS OF PRESSURE ON PRODUCT YIELDS IN THE NO _x PHOTO- OXIDATIONS OF SELECTED AROMATIC HYDROCARBONS.....	62
	4.1 Introduction.....	62
	4.2 Experimental.....	64
	4.3 Results.....	66
	4.4 Discussion.....	72
	4.4.1 Benzaldehyde and o-Cresol from Toluene.....	72
	4.4.2 Biacetyl from o-Xylene.....	76
	4.4.3 Conclusions.....	78
V.	RECOMMENDATIONS FOR FUTURE RESEARCH.....	79
	REFERENCES.....	80
	APPENDIX A.....	87

LIST OF FIGURES

<u>Figure</u>	<u>Title</u>	<u>Page</u>
1	Variation of the NO ₂ Photodissociation Rate Constant, k _{phot} , with Altitude for Selected Zenith Angles.....	4
2	SAPRC 5800- λ Evacuatable Chamber and Solar Simulator Facility.....	9
3	SAPRC 25-KW Solar Simulator.....	11
4	Technique for Injection of JP-4 into the 5800- λ Chamber.....	18
5	Transmission Spectra of 0.24-, 0.32-, and 0.64-cm Pyrex [®] Panes.....	22
6	Transmission Spectra of the Solar Simulator Output Through 0.64-cm, 0.64-cm + 0.32-cm, and 1.27-cm Thick Pyrex [®] Panes.....	23
7	Plots of the Combined 2- and 3-Pentyl Nitrate Yields Against the Amount of n-Pentane Consumed in CH ₃ ONO/NO/n-Pentane/air (or O ₂) Irradiations at 300 \pm 2 ^o K at 56, 154 \pm 1, 505, and 740 Torr Total Pressure.....	56
8	Plots of the n-Pentyl Nitrate Yields as a Function of Temperature and Pressure.....	59
9	Plots of the n-Heptyl Nitrate Yields as a Function of Temperature and Pressure.....	60
10	Plot of the Benzaldehyde and o-Cresol Yields from Irradiated Toluene/CH ₃ ONO/NO/Air (or O ₂) Mixtures as a Function of Total Pressure at \sim 303 ^o K. The Error Bars are the Two Least Squares Standard Deviations Given in Table 13.....	73
11	Plot of the Biacetyl Yields from Irradiated o-Xylene/CH ₃ ONO/NO/Air (or O ₂) Mixtures as a Function of Total Pressure at 301 \pm 2 ^o K. The Error Bars are the Two Least Squares Standard Deviations Given in Table 14.....	77

LIST OF TABLES

<u>Table</u>	<u>Title</u>	<u>Page</u>
1	Matrix of JP-4/NO _x /Air and JP-8/NO _x /Air Irradiations Carried Out.....	21
2	NO ₂ Photodissociation Rate Constants k _{phot} as a Function of Altitude and Zenith Angle.....	24
3	Chronological Order and Conditions of Experiments Carried Out for this Program.....	25
4	Conditions and Selected Results for NO _x /Air Irradiations Grouped by Temperature and Pressure Conditions.....	31
5	Photochemical Reactivity of JP-4/NO _x /Air Irradiations at Simulated Ground Level, 10,000 Ft, and 20,000 Ft Altitude, and of JP-8/NO _x /Air Irradiations at Simulated Ground Level and 20,000 Ft Altitude, and Selected Results of Associated NO _x /Air Irradiations.....	34
6	Photochemical Reactivity of JP-4 (100 ppmC)/NO _x (0.5 ppm)/Air (≤5% RH) Mixtures as a Function of Temperature and Pressure, and Selected Results of Associated NO _x /Air Irradiations.....	36
7	Experimental Data for the CH ₃ ONO/NO/n-Pentane/Air (or O ₂) Irradiations.....	46
8	Experimental Data for the CH ₃ ONO/NO/n-Heptane/Air (or O ₂) Irradiations.....	49
9	Pentyl Nitrate Yields from the Irradiation of CH ₃ ONO/n-Pentane/NO/Air (or O ₂) Mixtures.....	57
10	Heptyl Nitrate Yields from the Irradiation of CH ₃ ONO/n-Heptane/NO/Air (or O ₂) Mixtures.....	58
11	Experimental Data for the Toluene/CH ₃ ONO/NO/Air (or O ₂) Irradiations.....	67
12	Experimental Data for o-Xylene/CH ₃ ONO/NO/Air (or O ₂) Irradiations at 301±2°K.....	68
13	Benzaldehyde and o-Cresol Yields From the NO _x Photooxidation of Toluene.....	71
14	The Fraction of the OH Radical Reaction with o-Xylene Yielding Biacetyl as a Function of Pressure at 301±2°K.....	74
15	Comparison of the Present Benzaldehyde and o-Cresol Yields at ~303°K from the NO _x Photooxidation of Toluene with Previous Literature Values.....	74

SECTION I INTRODUCTION

Military jet aircraft flight procedures make it necessary to jettison excess fuel in certain in-flight operational situations. These fuel expulsions can be sizable (of the order of $5,000 \text{ lbs min}^{-1}$) (Reference 1), and in the presence of sunlight and NO_x emissions from engine exhaust can add to formation of ozone and other constituents of photochemical smog. Since these fuel dumping procedures are carried out at elevated altitudes, generally between 5,000 and 30,000 ft (Reference 1), the atmospheric properties involved are significantly different from those at ground level. For example, at 10,000 ft altitude the temperature and pressure are (References 2 and 3) $245\text{--}284^\circ\text{K}$ and 502-533 torr, respectively, while at 20,000 ft altitude the temperature and pressure are $228\text{--}266^\circ\text{K}$ and 330-365 torr, respectively. Furthermore, with increasing altitude the solar flux increases in intensity, with a corresponding shift towards a shorter wavelength cutoff (References 4 and 5), leading to enhanced photochemical activities (References 6 and 7).

To evaluate the combined effects of these atmospheric parameters on the potential for photochemical oxidant formation, the United States Air Force funded the Statewide Air Pollution Research Center (SAPRC) of the University of California at Riverside to carry out an environmental chamber study, using the SAPRC 5800-2 thermostatted, evacuable and Teflon[®]-coated chamber and solar simulator facility.

This 2-year program consisted of the following studies:

- Irradiations of a series of JP-4/ NO_x /air mixtures at simulated ground level, 10,000 ft and 20,000 ft altitude, together with the associated chamber characterization experiments.
- Irradiations of a JP-4/ NO_x /air mixture at atmospheric pressure at varying temperatures, and at room temperature at varying pressures, to study separately the effects of temperature and pressure on the reactivity of this mixture.
- Irradiations of JP-8/ NO_x /air mixtures at simulated ground level and 20,000 ft altitude.
- To obtain mechanistic data concerning the effects of temperature and pressure on the product distributions of the representative major

constituents of these fuels, alkyl nitrate yields from irradiated n-pentane/ NO_x /air and n-heptane/ NO_x /air mixtures were determined as a function of total pressure (60-740 torr) and temperature (~ 284 - $\sim 337^\circ\text{K}$). In addition, biacetyl yields from o-xylene and benzaldehyde and o-cresol yields from toluene were determined as a function of pressure (60-740 torr) at room temperature.

The data from these program elements provide empirical and mechanistic information concerning the chemistry occurring under the temperature and pressure conditions pertaining to the elevated altitudes encountered in jet fuel dumping. In the following sections the experimental procedures and the results obtained are described and discussed in detail.

SECTION II

EFFECTS OF SIMULATED ALTITUDE ON THE PHOTOCHEMICAL REACTIVITY OF IRRADIATED JP-4/NO_x/AIR AND JP-8/NO_x/AIR MIXTURES

2.1 INTRODUCTION AND BACKGROUND

As noted in Section I, the need to jettison excess fuel in the event of in-flight operational situations leads to the potential for photochemical air pollution formation. Since these fuel dumping procedures are carried out at elevated altitudes, the atmospheric properties involved are significantly different from those at ground level. The important physical atmospheric parameters are:

- Total pressure, which decreases with increasing altitude, and is in the range 502-533 torr at 10,000 ft and 330-365 torr at 20,000 ft altitude, depending on latitude and season (References 2 and 3).
- Temperature, which also decreases with increasing altitude in the troposphere (References 2 and 3) and is in the range 245-284°K at 10,000 ft and 228-266°K at 20,000 ft altitude, depending on latitude and season.
- Solar flux, which increases in intensity with increasing altitude with a corresponding shift towards a shorter wavelength cutoff (References 4 and 5), leading to enhanced photochemical activities (References 6 and 7).

Figure 1 shows, as an example, the variation of the calculated NO₂ photodissociation rate constant with altitude (0-14,000 ft) and zenith angle (Reference 5). This shows (a) the marked effect of altitude on the NO₂ photodissociation rate constant, and (b) that the major effect of zenith angle is for zenith angles >40°, with little effect for zenith angles between 0-40°.

To evaluate the combined effect of these atmospheric parameters on the potential for photochemical oxidant production, the chemical transformations of the jet fuels in question must be examined under conditions which closely approximate those at elevated altitudes. Although a considerable amount of experimental and computer modeling work has been carried out on the various aspects of air pollution at ground level, including studies of representatives of the various classes of compounds present in these jet fuels (References 8-15), and of the jet fuels themselves (Reference 16), no information is available as to the chemical transformations of these fuels under the atmospheric conditions at high altitudes.

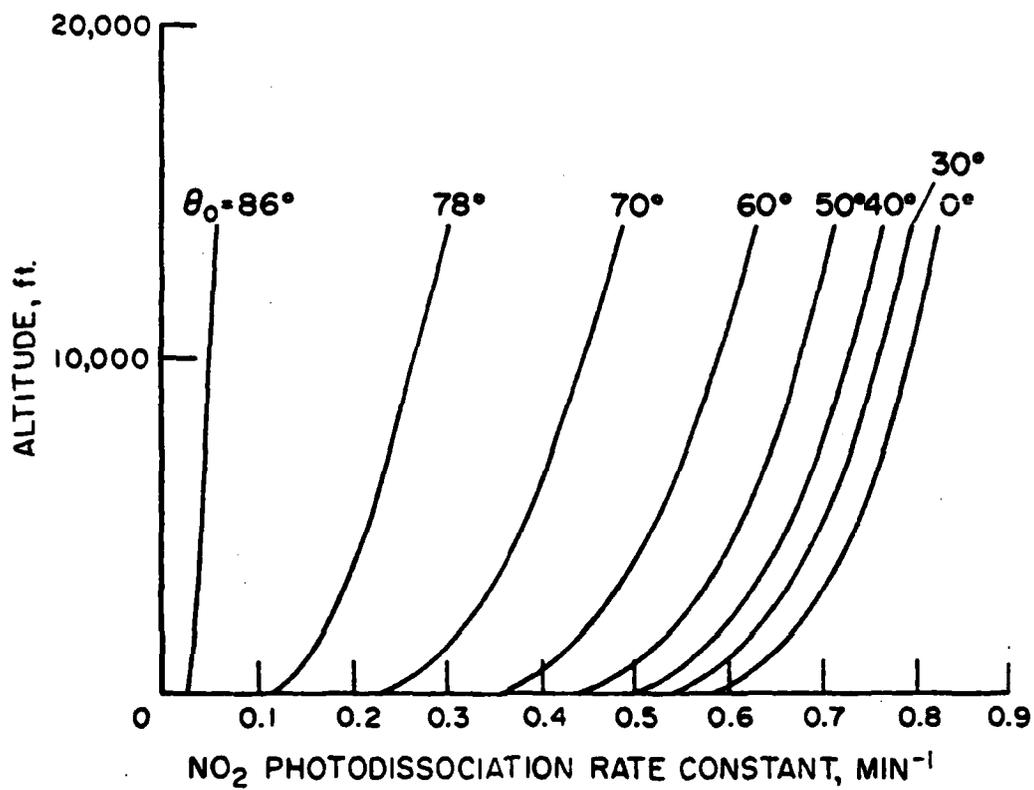


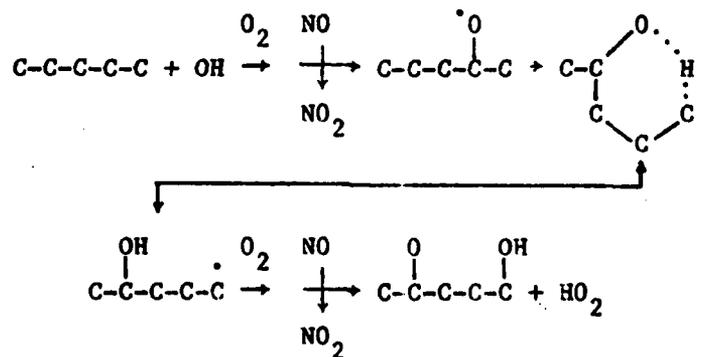
Figure 1. Variation of the NO₂ Photodissociation Rate Constant, k_{phot} , with Altitude for Selected Zenith Angles (from Reference 5).

The ambient troposphere is well mixed at elevated altitudes (e.g., 10,000-20,000 ft) and contains low levels of both hydrocarbons and NO_x . The hydrocarbon levels are ~1.6 ppm of methane (Reference 17), ~1 ppb of ethane, ~0.3 ppb of acetylene (Reference 18), with lower concentrations of higher hydrocarbons. Nitric oxide levels are <60 ppt (References 19-21) and while NO_2 levels are not accurately known they are certainly less than 1 ppb (Reference 22). Thus, the large quantities of hydrocarbons (HC) from dumping, in association with oxides of nitrogen ($\text{NO} + \text{NO}_2 \equiv \text{NO}_x$) from the exhaust, could represent a significant local perturbation on the atmospheric concentrations of HC and NO_x at high altitudes, relative to the background levels cited.

The primary distinction between the jet fuels and the hydrocarbons emitted into urban airsheds is that the latter include substantial quantities of alkenes and light alkanes, as well as aromatics. In contrast, the two jet fuels studied were complex mixtures comprised mainly of long chain alkanes and aromatics (Reference 16).

The aliphatic alkanes are known to react in atmospheric systems almost exclusively by hydroxyl (OH) radical attack. For the lower molecular weight alkanes this results in radical propagation reactions leading primarily to the formation of lower molecular weight aldehydes and ketones (References 11 and 23). However, from previous studies performed in our laboratories (References 11 and 24-26), for the $>\text{C}_4$ alkanes the following two additional reaction schemes have been shown to be important:

(1) In the case of alkanes with carbon chains longer than four, rapid isomerization of alkoxy radicals via intramolecular H-abstraction gives rise primarily to bifunctional products (References 11 and 24). For example;



In the case of higher molecular weight alkanes, these bifunctional products, having low vapor pressures, will probably end up in the aerosol phase. Thus, formation of organic aerosols, which are rich in hydroxyl and carbonyl groups but contain relatively few carboxylic acid groups, is predicted to be one important reaction channel for high molecular weight alkanes in the fuel mixtures.

(2) Studies in our laboratories (References 25 and 26) have shown that the higher molecular weight peroxy radicals formed following the reaction of OH radicals with alkanes in the presence of O_2 have a significant tendency to react with NO via a radical chain termination reaction forming organic nitrates



as opposed to the radical propagation reaction converting NO to NO_2



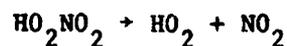
which is the dominant pathway for the lower molecular weight alkanes. Thus at 740 torr and $299 \pm 2^\circ K$ the rate constant ratios $k_1/(k_1 + k_2)$ increase monotonically from <0.01 for ethane to $\sim 0.30-0.35$ for n-heptane and n-octane (Reference 26). This process results not only in significant yields of alkyl nitrates, but also in a considerable amount of radical inhibition, tending to reduce rates of ozone formation and hydrocarbon consumption. In addition, the formation of alkyl nitrates removes active NO_x from the system, tending to reduce maximum ozone yields. The effects of temperature and pressure on these alkyl nitrate yields were also studied in this program for two n-alkanes and the data are described in detail in Section III.

The aromatic content of the fuel is expected to react differently than the aliphatics in atmospheric systems. Although formation of oxygenated aromatics and organic aerosols occurs to some extent (References 14 and 27-29), recent studies in our laboratories (References 14 and 30) and by others (References 31-33) have indicated that fragmentation is probably the major process. Among the products observed to be formed (References 30 and 31) are α -dicarbonyls, some of which are highly photoreactive. The photolysis of the α -dicarbonyls constitutes a significant radical source in

aromatic NO_x/air photooxidations. Again, the effects of pressure on certain product yields in the NO_x photooxidation of two representative aromatic hydrocarbons (toluene and o-xylene) were studied in this program and the data are described in detail in Section IV.

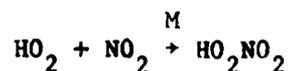
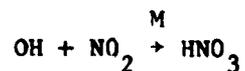
However, the available mechanistic information cited above was obtained at ground level atmospheric pressure and temperature (~740 torr, 300°K); the atmospheric conditions at elevated altitudes will have the following effects:

(1) A decrease in temperature will decrease many of the reaction rates involved in the atmospheric chemistry of these jet fuels. While for many reactions the changes will not be major (Reference 15), the formation of peroxy nitrates [pernitric acid (HO₂NO₂), alkylperoxy nitrates (RO₂NO₂), and acylperoxy nitrates (RCO₃NO₂)] will become much more important, since their thermal decomposition rate constants



are markedly temperature dependent (References 35-39). Such peroxy nitrates will act as sinks for NO_x and hence reduce O₃ formation rates (Reference 11).

(2) A decrease in total pressure will affect those reactions which are either third-order (e.g., O + O₂ + M → O₃ + M) or are in the fall-off region between second and third order kinetics, such as the NO_x removal and radical termination reactions (References 38, 40 and 41):



Hence, a reduction in total pressure may be expected to lead to a reduction in radical combination rate constants, and an enhanced photochemical activity.

(3) The increased solar light intensity and shift of the short wavelength cutoff to shorter wavelengths with increasing altitude (References 4 and 5) will increase the photodissociation rates of O_3 and of aldehydes and ketones leading to increased photochemical activity (References 6 and 7).

Some effects tend to enhance reactivities, while others reduce them, and it is not clear, a priori, which effects are more important. To assess these effects, sophisticated chamber experiments were carried out under temperature, pressure, light intensity and spectral distribution conditions closely simulating those characteristic of altitudes where the dumping of jet fuels takes place. To elucidate the influence of chamber wall effects, manifested by a variety of phenomena such as radical fluxes (References 11, 42 and 43), HNO_x wall adsorption and/or offgassing, etc. (Reference 44), it was also necessary to carry out detailed and carefully controlled characterization experiments under the same conditions of temperature and pressure.

The experimental techniques, the matrix of irradiations carried out, and the results obtained are described in detail in the following sections.

2.2 EXPERIMENTAL

2.2.1 Reaction Chamber

The reaction chamber used for this study was the 5800- λ SAPRC Teflon[®]-coated thermostatted evacuable environmental chamber equipped with a 25-KW solar simulator (Figure 2). The characteristics and operating procedures of this environmental chamber-solar simulator facility have been described in detail previously (Reference 45), and only the pertinent details will be discussed here.

The chamber is cylindrical, 3.96 m in length, 1.37 m in diameter, with an interior surface of FEP Teflon[®]-coated aluminum. The end-windows each consist of 16 quartz windows (30.5 cm x 30.5 cm x 2 cm) sealed to an aluminum grid structure by Viton O-rings (Reference 45). The exterior walls of the chamber are thermostatted via an external heating/cooling system to $\pm 1^\circ K$ over the temperature range 253-373^oK. In practice, with the solar simulator irradiating the chamber, the temperature variations are expected to be significantly higher and a useful lower temperature limit under such conditions is $\sim 260-265^\circ K$.

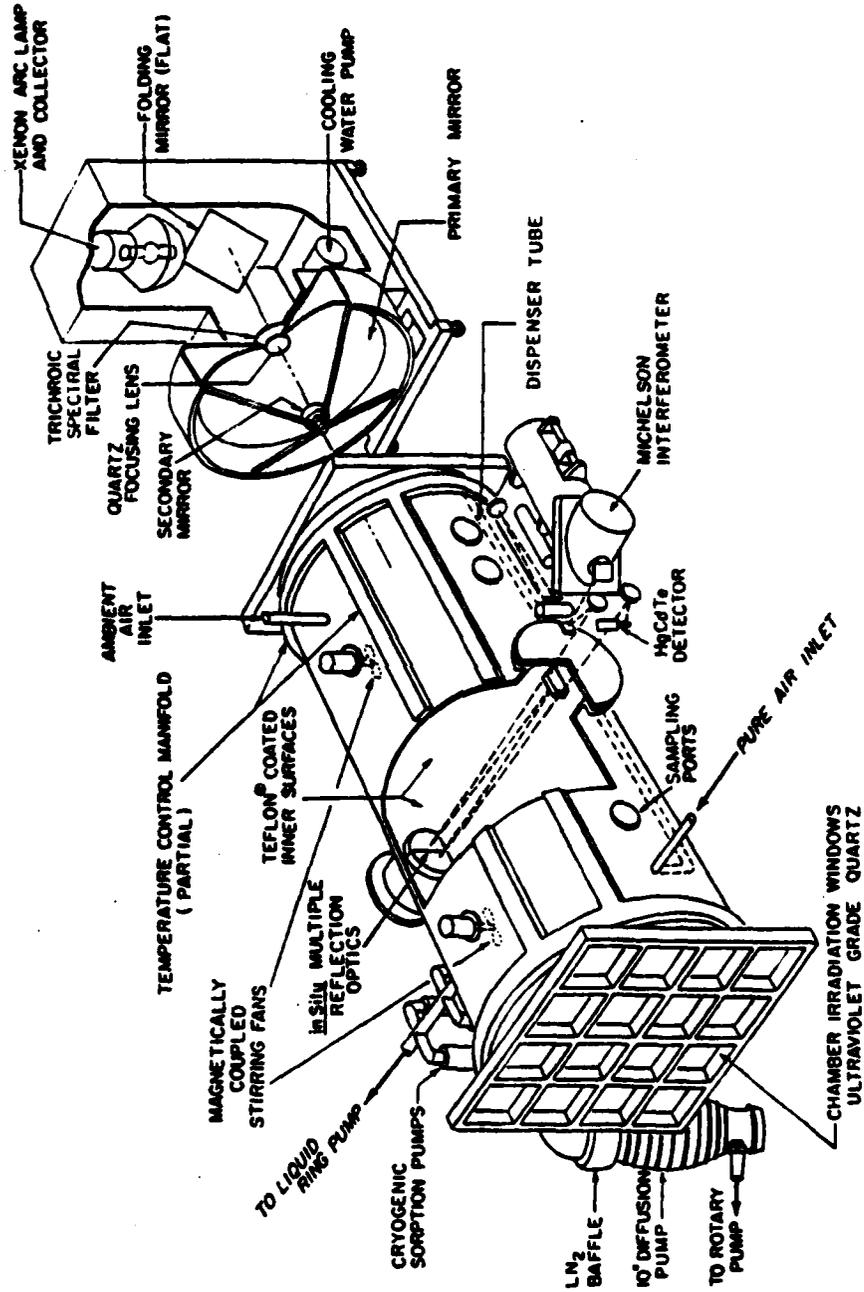


Figure 2. SAPRC 5800-2 Evacuatable Chamber and Solar Simulator Facility.

The solar simulator, employing a 25 KW point-source Xenon arc (Figure 3) provides a well-collimated light beam which, to a large extent, does not illuminate the chamber walls, thus minimizing surface photochemistry. In all experiments reported here, a Pyrex[®] pane (see Section 2.3) was placed in front of the quartz front window to obtain a spectral distribution applicable to that in the lower troposphere. The light intensity within the chamber was routinely monitored by measuring the rate of photolysis of NO₂ in N₂ (k_{phot}) by the method described by Holmes, et al. (Reference 46) with updated rate constants (Reference 47).

Between irradiations the chamber was evacuated overnight to $\sim 2 \times 10^{-5}$ torr (Reference 45).

2.2.2 Analytical Techniques Employed

Inorganic species, physical parameters, selected reactant hydrocarbons and selected organic products were monitored by the appropriate techniques, which are summarized below.

2.2.2.1 Total Pressure. The total pressure in the chamber was monitored by a Wallace and Tiernan Model 61A-1D-0800, two-turn, 0-800 torr absolute pressure gauge.

2.2.2.2 Temperature. The chamber gas temperature was monitored with a radiation-shielded iron-constant thermocouple. The leads from the thermocouple junction were sealed in a glass probe that projects into the dark space at the center of the chamber. A Doric Model DS-350 Thermocouple Indicator provided data in degrees Fahrenheit ([°]F) with an accuracy of $\pm 0.3^{\circ}$ F. Good gas-phase temperature control ($\pm 0.5^{\circ}$ K) was maintained during photolyses with a setting of the controller $2-3^{\circ}$ K below the desired temperature. Some radiation heating of the thermocouple probe occurred, although it was located in the dark space in the center of the chamber, and was further shielded with a foil cover. This heating has been estimated to be about 1° K by measuring the immediate temperature increase when the solar simulator is unshuttered.

2.2.2.3 Ozone. Ozone was monitored for the majority of experiments by two instruments: a Dasibi Model 1003AH ultraviolet absorption monitor at atmospheric pressure and a Monitor Labs Model 8410 chemiluminescence instrument at both atmospheric and reduced pressure. In addition, for a few irradiations a Meloy Labs chemiluminescence ozone analyzer was also used. The Dasibi ultraviolet absorption instrument cannot operate

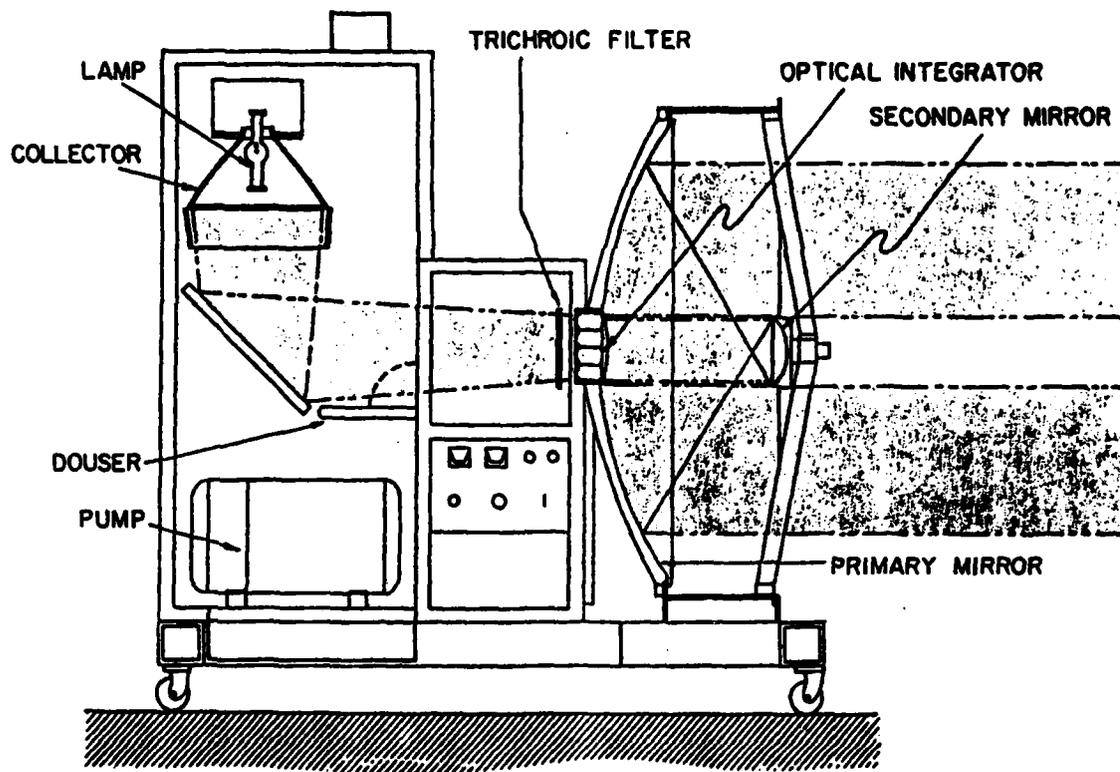


Figure 3. SAPRC 25-KW Solar Simulator.

with a negative pressure differential between the chamber and the ambient atmosphere, and thus could only be used at atmospheric pressure. This instrument, which was routinely calibrated by the California Air Resources Board against a longpath ultraviolet absorption primary standard apparatus, was used in turn to calibrate the Monitor Labs chemiluminescence analyzer and the Meloy Labs ozone analyzer at atmospheric pressure.

The Monitor Labs instrument was calibrated against the Dasibi Model 1003AH instrument at atmospheric pressure. For reduced pressures (i.e., 350 torr and 500 torr total pressures for simulated 10,000 ft and 20,000 ft altitudes) the Monitor Labs instrument, which operates by monitoring the chemiluminescence from the ozone-ethane reaction, was calibrated by (a) introducing and monitoring ≤ 1 ppm of O_3 into the reaction chamber at atmospheric pressure, (b) pumping the chamber to 500 torr total pressure and noting the Monitor Labs chemiluminescence reading, and (c) pumping to 350 torr total pressure and again noting the chemiluminescence response. Under these conditions, if the Monitor Labs instrument readings are R_{740} , R_{500} , and R_{350} at 740, 500, and 350 torr total pressure (and the instrument is calibrated correctly at 740 torr total pressure), then the (multiplicative) correction factors F_{500} and F_{350} are given by:

$$F_{500} = \frac{500}{740} \frac{R_{740}}{R_{500}}$$

and

$$F_{350} = \frac{350}{740} \frac{R_{740}}{R_{350}}$$

Values for F_{500} and F_{350} of 1.28 and 1.52 were obtained from such calibrations. A similar calibration was carried out for the Meloy Labs ozone analyzer.

The Dasibi Model 1003AH ultraviolet absorption analyzer yielded a small positive response to JP-4, and a larger response to JP-8, at the concentrations used in this study, in agreement with previous observations by Carter, et al. (Reference 16). No such interferences were observed by the Monitor Labs chemiluminescence instrument, which was used for the majority of the JP-4/ NO_x /air and JP-8/ NO_x /air irradiations carried out in this study.

2.2.2.4 Oxides of Nitrogen. Nitric oxide (NO) and total NO_x were monitored by a TECO Series 14 NO-NO_x chemiluminescence analyzer. With this instrument, NO is monitored directly, but total NO_x is measured by conversion to NO with a molybdenum catalyst. NO₂ is read as the difference between the two readings. This instrument was calibrated routinely, using an NBS calibration gas of known NO concentration. The gas was diluted to appropriate concentrations and the analyzer was then adjusted to give the correct reading. The instrument normally did not deviate more than 5% between calibration checks.

The analysis of NO₂ and NO_x is complicated by the fact that the converter has been shown (Reference 48) to convert PAN, organic nitrates, and HNO₃ to NO and, that such species give a positive interference in the NO₂ analysis (the NO data are unaffected). The conversion of PAN and organic nitrates has been shown to be essentially quantitative (Reference 48), and hence, in principle, NO₂ can be corrected by subtracting the measured PAN and organic nitrate concentrations. Although PAN was monitored in these experiments, organic nitrates could not be monitored with the techniques employed. Organic nitrates are known to be formed in significant yields in NO_x/air irradiations of the larger alkanes (Reference 26), which are present in JP-4 and JP-8 (Reference 16), and can be expected to cause significant interferences. For this reason, no attempt was made to correct the NO₂ data for these interferences. Thus, the NO₂ data obtained (NO₂-UNC) must be considered to be upper limits to the true NO₂ values.

As mentioned above, HNO₃, which is believed to be a major sink for NO_x in NO_x/air photooxidations, also interferes with NO₂ readings, although this interference is, in general, not quantitative (Reference 48). A nylon filter, which is known to efficiently remove gas phase HNO₃ (Reference 49), was thus placed in the sample line of the NO-NO_x monitor. This NO-NO_x analyzer was calibrated for operation at reduced pressures in a manner totally analogous to the ozone analyzer, as described in Section 2.2.2.3.

2.2.2.5 Organic Reactants and Products. Gas chromatography (GC) was used to monitor fuel components, background trace organics present in the pure matrix air, and a limited number of products. Except as noted below, flame ionization detection was used. For runs at atmospheric pressure, samples were taken (using 100 μl syringes) directly from the chamber. For runs at reduced pressure, samples were taken from a ~5 l

Pyrex[®] bulb which had been evacuated to $\leq 10^{-3}$ torr and which was then opened to the chamber and filled to atmospheric pressure by ultra-high purity N₂. In each case samples were injected manually into the various GC instruments. The syringes were flushed with the air being sampled at least two times prior to taking the analysis sample. Brief descriptions of each of the GC systems, the compounds monitored, and (where applicable) special procedures associated with them are given below.

The C₅+ hydrocarbon fuel components were monitored by capillary column gas chromatography employing a 30 m SE-52 coated fused silica capillary column. The procedure for injecting the gas sample onto the capillary column was very similar to that described by Carter, et al. (Reference 16). The 100 ml gas sample was flushed through an ~10 cm³ silylated Pyrex[®] loop, and the contents of this loop were then transferred over a 12 min time span to the head of column which was held at 183^oK. The GC oven temperature then rose to 223^oK over a 1.5 min time period, and was temperature programmed from 223-473^oK at 8^oK min⁻¹. This system was capable of monitoring most of the individual C₅-C₁₃ components of the two fuels studied in this program. However, because of the large number of individual components of the fuels, only concentrations of selected fuel components are reported.

Calibration factors for the various alkane and aromatic fuel components were obtained as follows. Stock calibration solutions were made by syringing the desired compounds into a weighed vial. Exact concentrations were obtained by weighing the vial on an Ainsworth Type 10 balance after the addition of each compound. In general, each stock solution was made up of six compounds. One microliter of each stock solution was added to a 46.75 l glass carboy. The carboy was cleaned before each calibration by heating it with a heat gun for 20 min on hot and 15 min on cool, then flushing the carboy with nitrogen for 1 hr. The compounds were added to the carboy the evening before a calibration so that the compounds would be completely mixed for the next morning. Calibration samples were then taken directly from the calibration carboy with a 100 ml all-glass gas-tight syringe.

Capillary column GC analyses of the fuel components were performed prior to the irradiation in each run and once an hour during the irradiation.

Aromatic hydrocarbons and C₂+ oxygenates were monitored using a 10 ft x 0.125 in stainless steel (SS) column packed with 10% Carbowax-600[®] on C-22 Firebrick[®] (100/120 mesh) operated at 343-348[°]K, with an N₂ flow rate of 50.5 ml min⁻¹. Samples were taken using cryogenic trapping techniques as described previously (Reference 9). Using this system, samples were taken prior to fuel injection only. Although this system was capable of monitoring the simpler C₂-C₅ aldehydes and ketones, in practice it could not be used for this purpose during fuel runs because of the interferences by larger hydrocarbon fuel components having similar retention times. For that reason, oxygenate data from this system are not reported for fuel runs. The primary use of this system was to assure that there was no significant oxygenate contamination in the pure air used in the runs in this study.

C₁ and C₂ hydrocarbons were monitored before fuel injection using a 5 ft x 0.125 in SS column packed with 100/120 mesh Porapak N,[®] held at 333[°]K and with an N₂ flow rate of 30 ml min⁻¹. This system was used primarily to determine that there were no significant contaminants in the matrix air, and, except for selected control and characterization runs, data are not reported. The sampling technique, calibration procedure, and discussions of the accuracy of this technique are given elsewhere (Reference 9).

C₃-C₆ hydrocarbons were monitored using a 34 ft x 0.125 in SS column packed with 10% 2,4-dimethylsulfolane (DMS) on C-22 Firebrick[®] held at 273[°]K, in series with 2 ft x 0.125 in stainless steel "soaker" columns containing 10% Carbowax-600[®] on C-22 Firebrick[®] (30/60 mesh). The N₂ flow rate was 26 ml min⁻¹. Again, because of problems with the long retention times of the fuel components, this GC system was only employed prior to fuel injection using the cryogenic trapping technique (Reference 9). However, this column was used to quantitatively analyze the propane and propene tracers introduced in the NO_x/air irradiations in order to monitor OH radical levels in the chamber, with samples being taken every 15 min (Reference 43).

Peroxyacetyl nitrate (PAN) was monitored using electron capture detection and an 18 in x 0.125 in Teflon[®] column of 5% Carbowax-400[®] on Chromasorb G[®] (80/100 mesh) operating at ambient temperature (Reference 9). Analyses were carried out by flushing a 1.95 ml loop with the sample

and then injecting the contents of the loop onto the column. The calibration of this system and factors affecting its accuracy are described elsewhere (Reference 9). For the majority of the runs, PAN data are reported on an hourly basis. In most fuel runs, other GC peaks were observed in the PAN chromatograms. These were probably alkyl nitrates, for which this system is also sensitive. However, because the exact identities of the compounds causing these peaks were not established, they are not reported on the data sheets.

2.2.2.6 Formaldehyde. Formaldehyde was monitored hourly during the irradiations using an improved chromatropic acid technique (References 9 and 45). Samples were taken at the rate of 1 l min^{-1} in a single bubbler containing 10 ml of distilled water. The developed solutions were read on a Beckman 35 spectrometer. A more detailed discussion of this technique, as it is employed in our laboratories, is given elsewhere (Reference 9).

2.2.2.7 Light Intensity and Spectral Distribution. The light intensity was monitored as the photolysis of NO_2 in N_2 (k_{phot}), as described by Holmes, et al. (Reference 46) and Winer, et al. (Reference 45). These NO_2 photolysis rate constants k_{phot} were determined periodically during this program. The light intensity was also monitored by an EG&G Model 550 radiometer fitted with an interference filter having a center wavelength of 350 nm, and between actinometry experiments the light intensity, as monitored by this radiometer, was held constant to $\pm 0.02 \text{ mW cm}^{-2}$. Spectral distributions were recorded, normally once each run, using a calibrated monochromator-photomultiplier tube system.

2.2.3 Operating Procedures

2.2.3.1 Procedures for Filling the Evacuatable Chamber. For the majority of the experiments the chamber was initially filled to ~ 10 torr total pressure with dry N_2 , and then NO and NO_2 in a $\sim 5 \text{ l}$ Pyrex[®] bulb attached to the vacuum line were flushed into the chamber by a stream of ultra-high purity nitrogen. The NO was purified by passage through a trap containing activated Linde Molecular Sieve 13X, while NO_2 was prepared by reaction of this purified NO with O_2 which had also been passed through activated Molecular Sieve 13X.

For the experiments where this injection procedure was not used, the NO and NO_2 were flushed into the chamber from the $\sim 5 \text{ l}$ Pyrex[®] bulb by a

stream of ultra-high purity N_2 either during the filling of the chamber with pure air, or after the chamber had been filled with pure air.

The jet fuels JP-4 and JP-8 (petroleum derived, supplied by the Fuels Branch, Fuels and Lubrication Division, Aero-Propulsion Laboratory, Wright-Patterson Air Force Base, Ohio) were injected using the procedures developed during a previous USAF-funded SAPRC program (Reference 16). For JP-4, the desired quantity of the liquid fuel (21 $\mu\ell$ for 5 ppmC to 430 $\mu\ell$ for 100 ppmC in the chamber) was placed in an ~ 1 ℓ bulb (Figure 4), fitted with high-vacuum greaseless stopcocks. The bulb was then flushed for ~ 15 min with N_2 at a flow rate of 5 $\ell \text{ min}^{-1}$, while being heated with a heat gun. After this time, all of the liquid fuel had disappeared, and tests (Reference 16) showed that reasonably complete and reproducible injections were obtained using this technique. Previous work in these laboratories (Reference 16) had shown that this technique was not satisfactory for less volatile fuels including JP-8, and that a different technique was necessary. A technique similar to that developed for this previous U.S. Air Force-funded program (Reference 16) was used. This consisted of heating a U-tube containing the required amount of the liquid JP-8 to $\sim 323^\circ\text{K}$ while passing a stream of N_2 through it at $\sim 5 \ell \text{ min}^{-1}$ for ~ 15 -30 min, while the chamber was under vacuum.

The chamber was filled with purified matrix air (Reference 50) to the desired pressure. For the two runs where the diluent gas was not air, but a synthetic N_2/O_2 mixture, the requisite pressures of ultra-high purity N_2 and O_2 were introduced into the chamber from cylinders.

For the NO_x /air irradiations involving the use of two organic tracers (propane and propene), the NO and NO_2 were injected as described above, while the desired amounts of the organic tracers propane and propene were introduced into the chamber from the vacuum gas handling system or via injection using all glass gas-tight syringes.

2.2.3.2 Experimental Protocol. After the chamber fill, samples were taken for background analyses of potential contaminants on the DMS, Porapak[®] columns, and on the PAN analyzer prior to irradiation. Providing that no anomalously high background levels of common contaminants in the pure air system (ethene and propene being the most reactive of these C_2 - C_4 alkanes and alkenes) were detected, then gas samples were taken just

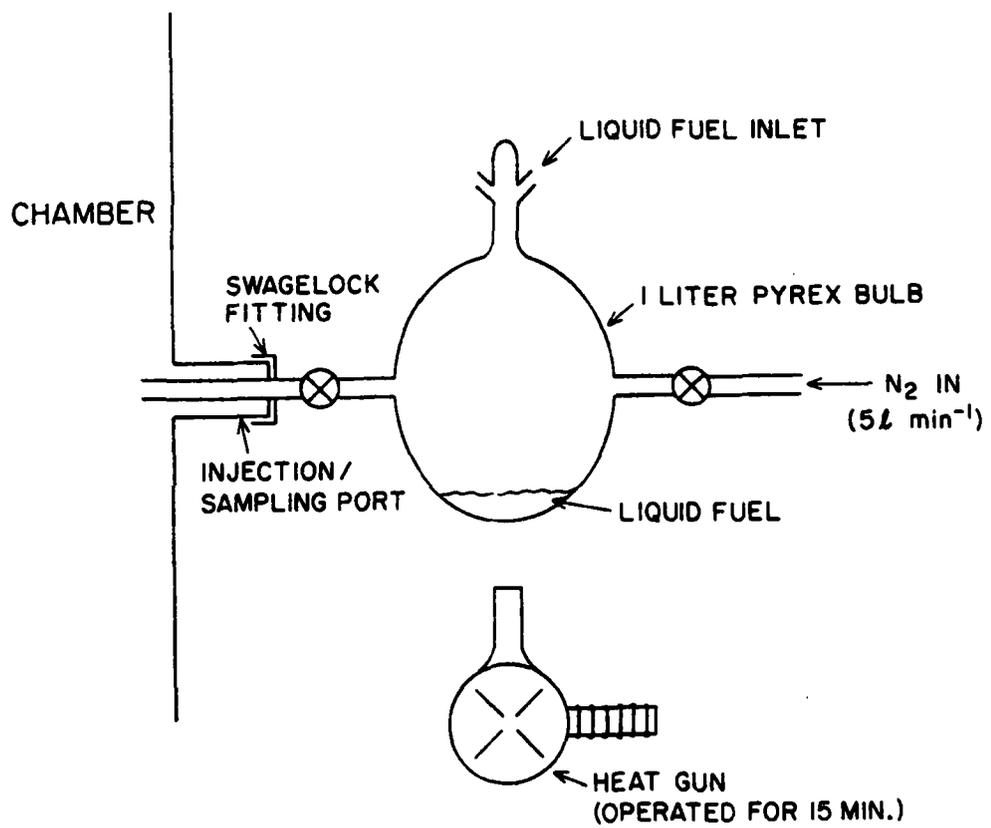


Figure 4. Technique for Injection of JP-4 into the 5800 l Chamber.

prior to the start of irradiation for analyses on all the gas chromatographic columns described above. A 20 μ gas sample for formaldehyde analysis was also taken prior to irradiation. Hourly samples were then taken during the irradiations.

For irradiations carried out at reduced pressure, samples were introduced from the chamber into an evacuated \sim 5 μ Pyrex[®] bulb, which was then pressurized to atmospheric pressure with ultra-high purity N₂. For the formaldehyde analyses, the gas from the chamber was pumped (at 1 μ min⁻¹ at atmospheric pressure) through the bubbler (Reference 9) and the bubbler was then pressurized to 1 atm.

The solar simulator was brought to the desired power at least 10 min prior to the start of irradiation.

2.3 RESULTS

2.3.1 Matrix of JP-4/NO_x/Air and JP-8/NO_x/Air Irradiations

In order to investigate the photochemical reactivity of JP-4 under conditions pertaining to elevated altitudes, the following sets of irradiations were carried out:

- Irradiations of JP-4/NO_x/air mixtures were conducted under temperature and pressure conditions designed to simulate ground level, 10,000 ft and 20,000 ft altitude. The relative light intensities and spectral distributions (see later) were adjusted to correspond to these altitudes at a zenith angle of 0°.

- An irradiation of a JP-4/NO_x/air mixture (100 ppmC JP-4, 0.5 ppm NO_x) was carried out at simulated 20,000 ft altitude, with the light intensity and spectral distribution adjusted to correspond, on a relative basis, to a zenith angle of 70°.

- A set of JP-4/NO_x/air irradiations was carried out at constant light intensity as a function of total pressure at 303°K, and as a function of temperature at 740 torr total pressure. The temperatures and pressures chosen were those used in the various simulated altitude experiments (i.e., 265, 284, and 303°K, and 350, 500, and 740 torr total pressure). These runs were designed to determine the effect of independently varying the total pressure and temperature on the photochemical reactivity.

- Three irradiations of JP-8/NO_x/air mixtures were carried out at simulated ground level and 20,000 ft altitude to ascertain that the effect

of simulated altitude on the photochemical reactivity of JP-8 paralleled that of JP-4.

The matrix of JP-4/NO_x/air and JP-8/NO_x/air irradiations carried out is given in Table 1.

2.3.2 Light Intensities and Spectral Distributions Used at the Three Simulated Altitudes (Ground Level, 10,000 and 20,000 Feet)

In order to study the effects of elevated altitudes, it is also necessary to simulate the changes in light intensity and spectral distribution between ground level, 10,000 ft and 20,000 ft altitudes. For photochemical purposes the most direct measure of light intensity is the NO₂ photodissociation rate constant k_{phot} , and Figure 1 shows the variation of k_{phot} with altitude for selected solar zenith angles, as taken from Peterson (Reference 5). The NO₂ photodissociation rates obtained at the various altitudes are given in Table 2. Since the evacuable chamber solar simulator cannot achieve NO₂ photodissociation rate constants in excess of 0.5-0.6 min⁻¹ for prolonged periods of time, these photodissociation rate constants were scaled by a factor of 0.6 to yield the values shown in Table 1.

The most important aspect of the spectral distribution of the photolyzing radiation is the short wavelength cutoff. From Peterson (Reference 4), the effect on the short wavelength cutoff of increasing altitude from ground level at 0° zenith angle is small, with, for instance, the ratio $I_{332.5 \text{ nm}}/I_{412.5 \text{ nm}}$ increasing by only 30%. In view of the relatively large effect on the short wavelength cutoff of using Pyrex® panes of differing thicknesses (Reference 6 and Figure 5) it was decided to use the 0.64 cm Pyrex® pane to simulate all runs carried out at 0° zenith angle, and to insert an additional 0.32 cm Pyrex® pane along with the 0.64 cm Pyrex® pane for the 70° zenith angle irradiation at simulated 20,000 ft. The spectral distribution of these two filters, uncorrected for monochromator-photomultiplier response, are shown in Figure 6, together with that for an unsolarized 1.27 cm Pyrex® pane.

2.3.3 Environmental Chamber Experiments

A chronological listing of the runs carried out, the initial concentrations, the relevant physical parameters and a description of the run type are given in Table 3. For the NO_x/air and jet fuel/NO_x/air irradiations simulating ground level, the pure matrix air was humidified

TABLE 1. MATRIX OF JP-4/NO_x/AIR AND JP-8/NO_x/AIR IRRADIATIONS CARRIED OUT.

EC Run No.	Initial Concentration JP-4 or JP-8 (ppmC)	NO _x (ppm)	Temperature (°K)	Total Pressure (torr)	k _{phot} (min ⁻¹)	Comments
JP-4						
489,492	50	0.5 ^a				
490	50	1.0	303	740	0.33	Simulated ground level 0° zenith angle
491	5	1.0				
515	100	0.5				
506	50	0.5				
508	50	1.0	284	500	0.44	Simulated 10,000 ft altitude, 0° zenith angle
509,510	100	0.5 ^a				
498,502	50	0.5 ^a				
497	50	1.0	265	350	0.47	Simulated 20,000 ft altitude, 0° zenith angle
500	100	0.5				
517	50	0.5	265	350	0.35 ^b	Simulated 20,000 ft altitude, 70° zenith angle
575	100	0.5	303	740		
578	100	0.5	303	500		
580,581	100	0.5	303	350	0.475	To investigate separately the effects of pressure and temperature on photochemical reactivity
588	100	0.5	284	740		
587	100	0.5	265	740		
JP-8						
592	50	0.5	303	740	0.34	Simulated ground level 0° zenith angle
591	100	0.5				
595	100	0.5	265	350	0.43	Simulated 20,000 ft altitude 0° zenith angle

^aDuplicated for test of reproducibility.

^bShort wavelength spectral distribution moved to the red to simulate 70° zenith angle.

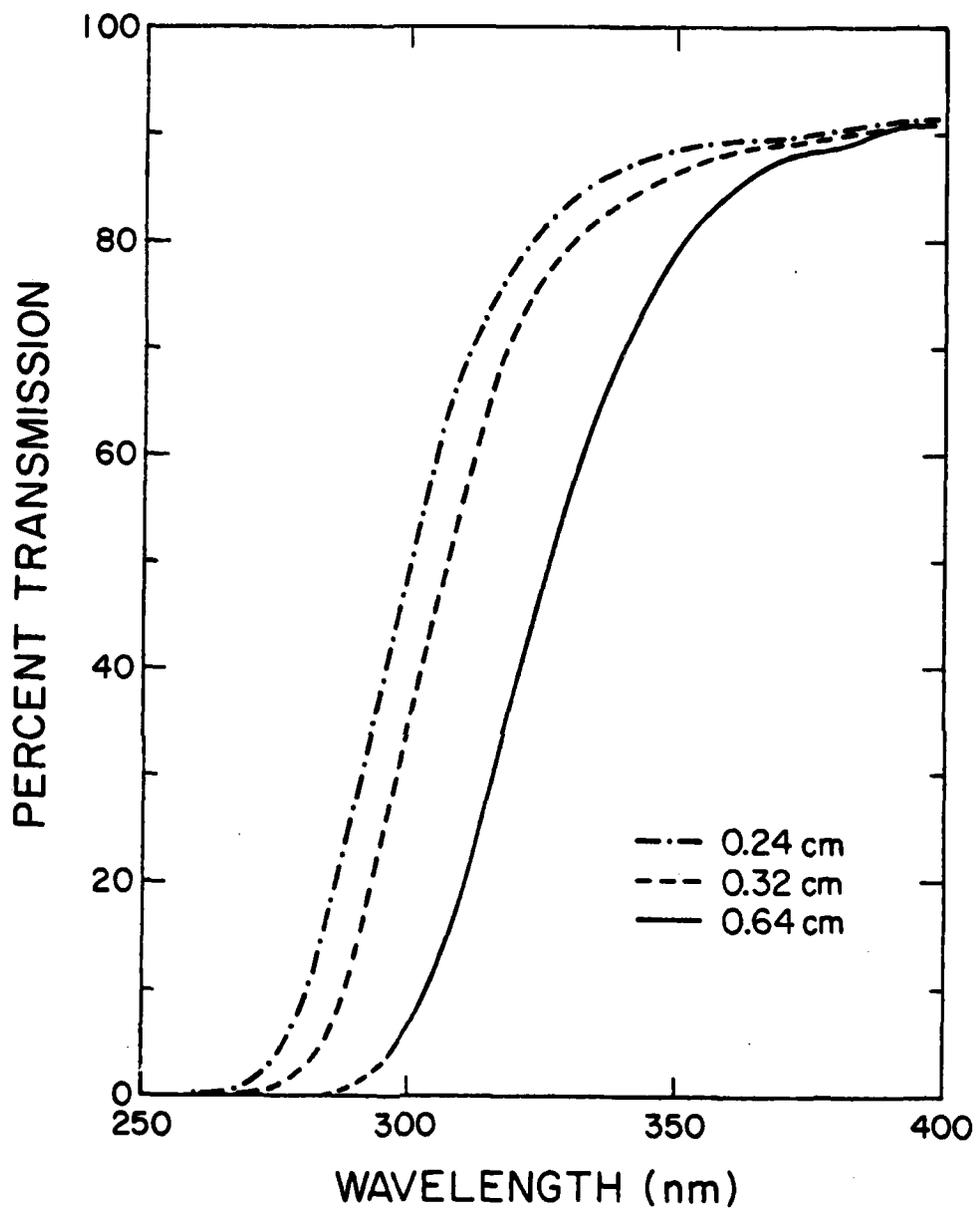


Figure 5. Transmission Spectra of 0.24, 0.32, and 0.64 cm Pyrex[®] Panes. (The 0.64 cm Pane had been Red-Shifted by ~10 nm Due to Prolonged Use Prior to the Spectrum Being Taken.) From Reference 6.

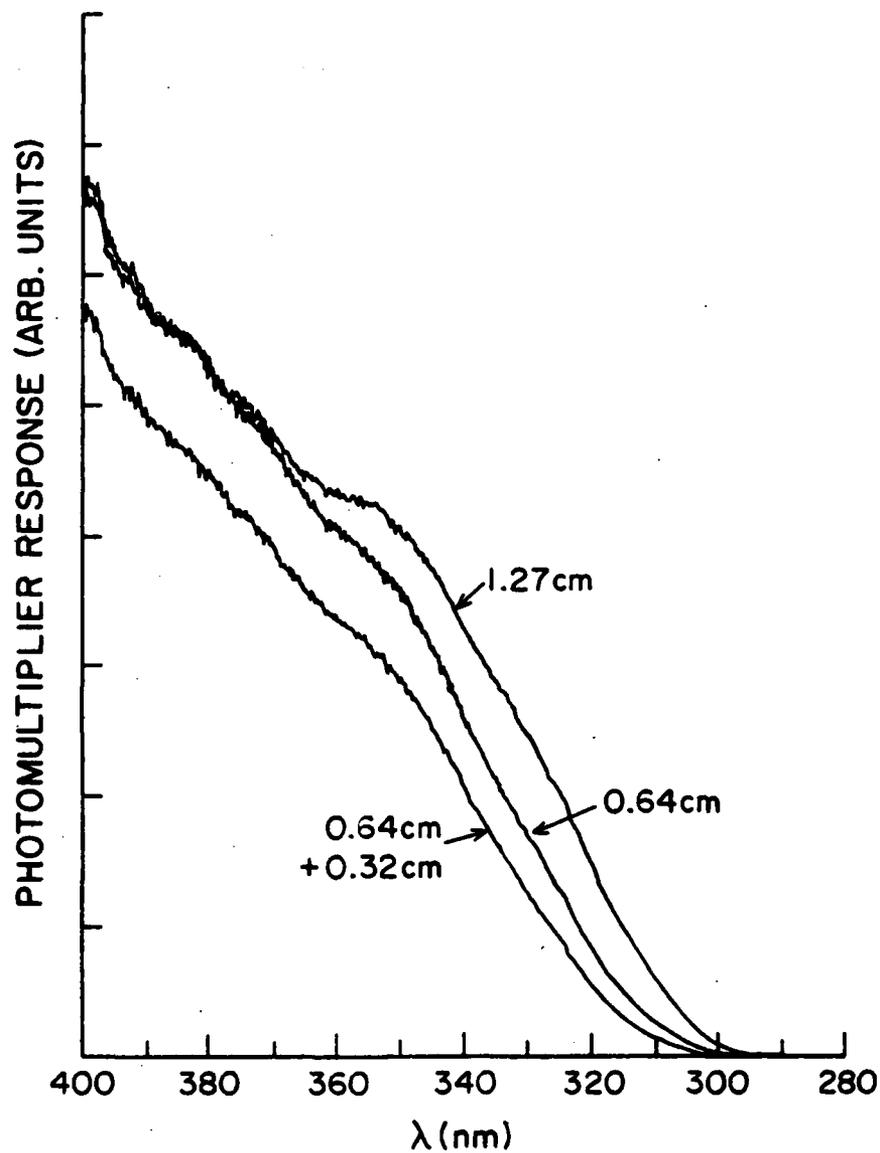


Figure 6. Transmission Spectra (Uncorrected for Detector Response) of the Solar Simulator Output through 0.64 cm, 0.64 cm + 0.32 cm, and 1.27 cm Thick Pyrex[®] Panes. (The 0.64 cm Pyrex[®] Pane has been Red-Shifted Substantially by Prolonged Irradiation.)

TABLE 2. NO₂ PHOTODISSOCIATION RATE CONSTANTS k_{phot} AS A FUNCTION OF ALTITUDE AND ZENITH ANGLE.

Altitude (ft)	NO ₂ Photodissociation Rate Constant k_{phot} (min ⁻¹)	
	Zenith Angle 0°	Zenith Angle 70°
0	0.57	0.23
10,000	0.79	0.44
20,000	0.84	0.52

(Reference 50) to ~50% RH since this approximates ambient atmospheric conditions. For the irradiations simulating 10,000 and 20,000 ft altitudes, dry ($\leq 5\%$ relative humidity based on 300°K) matrix air was used as the diluent gas.

Since chamber wall effects are known to be non-negligible in atmospheric simulation experiments, and since such effects may, in general, depend on temperature and pressure, a matrix of chamber characterization experiments was required to allow these effects to be taken into account. In general, chamber effects depend on the past history of the chamber as well as upon the conditions under which the experiments are carried out (Reference 43). However, our previous extensive experience with the SAPRC evacuable chamber has shown that reproducible results are obtained as long as the prior experiment in the chamber has been another hydrocarbon/NO_x/air photolysis. In this case no additional treatment of the chamber is required between experiments other than evacuation to $\leq 2 \times 10^{-5}$ torr. Therefore, following NO₂ actinometry runs, evacuated bakeouts, experiments in other SAPRC programs, exposure of the interior of the chamber to unusual contaminants, or other nonstandard chamber conditions, a "dummy" propene/NO_x/air conditioning run was performed to bring the chamber into a standard condition. These runs consisted of irradiating ~0.5 ppm propene and 0.5 ppm NO_x at 1 atm and 303°K for at least 4 hrs, followed by evacuation of the chamber to $\leq 2 \times 10^{-5}$ torr.

TABLE 3. CHRONOLOGICAL ORDER AND CONDITIONS OF EXPERIMENTS CARRIED OUT FOR THIS PROGRAM.

EC Run No.	Initial Concentration ^a			Average Temperature (°K)	Total Pressure (torr) ^b	k _{phot} (min ⁻¹) ^c	Radiometer (mW cm ⁻²)	Description
	JP-4 (ppmC)	NO (ppm)	NO ₂ (ppm)					
487		0.372	0.137	302.4	740 ^f	0.294	0.073	k _{phot} determination ^d
488		0.368	0.091	303.9	740 ^f	0.33	0.081	NO _x /air irradiation ^d
489	50	0.715	0.183	303.9	740 ^f	0.33	0.079	JP-4/NO _x /air irradiation, ground level
491	5	0.717	0.192	302.9	740 ^f	0.33	0.080	JP-4/NO _x /air irradiation, ground level
492	50	0.391	0.102	304.8	740 ^f	0.33	0.081	JP-4/NO _x /air irradiation, ground level
493		0.388	0.104	302.5	740 ^f	0.33	0.080	NO _x /air irradiation ^e
494						0.351	0.083	k _{phot} determination ^d
495						0.465	0.125	k _{phot} determination ^d
496		0.363	0.092	264.5	350	0.47	0.125	NO _x /air irradiation ^e
497	50	0.735	0.178	266.7	350	0.47	0.124	JP-4/NO _x /air irradiation, simulated 20,000 ft
498	50	0.361	0.086	265.9	350	0.47	0.125	JP-4/NO _x /air irradiation, simulated 20,000 ft
499		0.803	0.197	263.8	350	0.47	0.124	NO _x /air irradiation ^e
500	100	0.392	0.082	266.9	350	0.47	0.126	JP-4/NO _x /air irradiation, simulated 20,000 ft
501								Aborted after high ethene contamination observed, repeated as EC-502
502	50	0.354	0.069	268.0	350	0.47	0.125	JP-4/NO _x /air irradiation, simulated 20,000 ft
503		0.380	0.084	267.4	350	0.47	0.125	NO _x /air irradiation ^e
504						0.390	0.103	k _{phot} determination ^d
505		0.449	0.120	282.1	500	0.44	0.112	NO _x /air irradiation ^e
506	50	0.417	0.100	283.8	500	0.44	0.113	JP-4/NO _x /air irradiation, simulated 10,000 ft
507		0.814	0.191	283.3	500	0.44	0.112	NO _x /air irradiation ^e
508	50	0.786	0.210	283.3	500	0.44	0.113	JP-4/NO _x /air irradiation, simulated 10,000 ft
509	100	0.419	0.112	285.7	500	0.44	0.112	JP-4/NO _x /air irradiation, simulated 10,000 ft
510	100	0.419	0.112	283.4	500	0.44	0.112	JP-4/NO _x /air irradiation, simulated 10,000 ft
511		0.397	0.114	281.2	500	0.44	0.112	NO _x /air irradiation ^e
512						0.465	0.115	k _{phot} determination

TABLE 3. CHRONOLOGICAL ORDER AND CONDITIONS OF EXPERIMENTS CARRIED OUT FOR THIS PROGRAM (CONTINUED).

EC Run No.	Initial Concentration ^a		Average Temperature (°K)	Total Pressure (torr) ^b	k _{phot} ^c (min ⁻¹) ^c	Radiometer (mW cm ⁻²)	Description
	JP-4 (ppmC)	NO _x (ppm)					
513					0.310	0.080	k _{phot} determination ^d
514	0.410	0.090	302.5	740 ^f	0.31	0.081	NO _x /air irradiation ^e
515	100	0.104	303.1	740 ^f	0.31	0.081	JP-4/NO _x /air irradiation, ground level
516					0.354	0.076	k _{phot} determination ^d ; 0.64 cm + 0.32 cm Pyrex ^g filter panes in place
517	50	0.079	271.3	350	0.35	0.074	JP-4/NO _x /air irradiation, simulated 20,000 ft 70° zenith angle
518	0.365	0.090	268.8	350	0.35	0.073	NO _x /air irradiation ^e
519-571 A Series of NO _x -Air and NO _x -Isoprene, Methylvinylketone or Methacrolein-Air Irradiations Carried Out on Other Programs							
572					0.522	0.097	k _{phot} determination, followed by NO _x /propene/air conditioning run, followed by a dark O ₃ decay, with rate = 0.00048 min ⁻¹
573	0.402	0.085	304.4	740 ^f	0.475	0.082	NO _x /air irradiation ^e
574	0.441	0.126	305.3	740	0.475	0.082	NO _x /air irradiation ^e
575	100	0.079	306.4	740	0.475	0.082	JP-4/NO _x /air irradiation
576					0.475	0.082	k _{phot} determination ^d
577	0.480	0.079	305.1	500	0.475	0.082	NO _x /air irradiation ^e
578	0.470	0.084	304.4	500	0.475	0.082	JP-4/NO _x /air irradiation
579	0.464	0.094	303.8	350	0.475	0.082	NO _x /air irradiation
580	100	0.451	304.7	350	0.475	0.082	JP-4/NO _x /air irradiation
581	100	0.419	304.5	350	0.475	0.082	JP-4/NO _x /air irradiation
582	0.352	0.096	304.4	(200 N ₂ + 150 O ₂)	0.475	0.082	NO _x /air irradiation ^e
				(200 N ₂ + 150 O ₂)			

TABLE 3. CHRONOLOGICAL ORDER AND CONDITIONS OF EXPERIMENTS CARRIED OUT FOR THIS PROGRAM (CONCLUDED).

EC Run No.	Initial Concentration ^a		Average Temperature (°K)	Total Pressure (torr) ^b	k _{phot} (min ⁻¹) ^c	Radiometer (mW cm ⁻²)	Description
	JP-4 (ppmC)	NO (ppm)					
583					0.473	0.082	k _{phot} determination ^d
584		0.456	283.5	740	0.475	0.080	NO _x /air irradiation ^e
585	100	0.354	285.3	740	0.475	0.082	JP-4/NO _x /air irradiation - Malfunctioning NO analyzer meant this was really a 100 ppmC JP-4, ~1.0 ppm NO _x run
586		0.391	269.9	740	0.475	0.082	NO _x /air irradiation
587	100	0.402	271.7	740	~0.478	~0.088	JP-4/NO _x /air irradiation
588	100	0.362	285.0	740	0.475	0.082	JP-4/NO _x /air irradiation
589					0.346	0.060	k _{phot} determination ^d
590		0.427	302.5	740 ^f	0.34	0.059	NO _x /air irradiation
591	100	0.476	303.9	740 ^f	0.34	0.060	JP-8/NO _x /air irradiation, ground level
592	50	0.419	304.3	740 ^f	0.34	0.060	JP-8/NO _x /air irradiation, ground level
593					0.436	0.081	k _{phot} determination ^d
594	100	0.419	269.9	350	0.43	~0.080	NO _x /air irradiation
595	100	0.419	273.1	350	0.43	0.080	JP-8/NO _x /air irradiation, simulated 20,000 ft

^aReferenced to 303°K and 740 torr total pressure.

^bFor reduced pressure, nominal value; see data sheets for more detail.

^cBetween k_{phot} determinations, interpolated using radiometer readings.

^dFollowed by NO_x/propene/air conditioning irradiation.

^e~10 ppb levels of propene and propene tracers present to monitor OH radical concentrations.

^f~50% relative humidity. All other runs used dry air or dry O₂/N₂ mixtures.

Problems encountered with condensation on the chamber end-windows.

The detailed data sheets for the JP-4/NO_x/air and JP-8/NO_x/air irradiations are given in Appendix A. These data, and the results of the associated chamber characterization runs, are discussed in the following sections.

2.3.3.1 Chamber Characterization Runs. The most important chamber effects concern rates of ozone dark decay, chamber radical sources, and offgassing of reactive organics. The rate of ozone destruction on the chamber walls was measured following a propene/NO_x/air conditioning run (EC-572), and was found to be 0.00048 min⁻¹, in reasonable agreement with previous ozone decay rates measured in our chamber (Reference 11). The rates of offgassing of reactant organics and the chamber radical source were measured by conducting NO_x/air irradiations, which are described below.

In order to determine the extent of radical initiation from unknown sources, an effect which is known to be important in smog chamber systems (References 11, 42 and 43), and to obtain additional information about contaminant offgassing, at least one NO_x/air irradiation was carried out under the conditions employed for each of the altitudes and zenith angles to be simulated. These experiments consisted of adding ~0.4 ppm NO, ~0.1 ppm NO₂ and traces (~10 ppb) of propene and propane to pure air at the desired relative humidity and irradiating for 2 hrs. Since this system is almost completely unreactive in the absence of such effects (References 42 and 43), it is extremely sensitive to chamber effects related to radical initiation and to contamination effects related to reactive organics.

Radical initiation rates were obtained by equating the initiation rates to termination rates due to the OH + NO₂ reaction [the major termination mechanism in this system (Reference 43)], with the rate of the latter being estimated (Reference 43) from the known OH + NO₂ rate constant at the temperature and pressure of the experiment (References 15 and 47), and the measured NO₂ and OH radical levels. The OH radical levels were monitored by measuring the relative rates of decay of the two organic tracers (propene and propane), which were consumed essentially entirely by reaction with OH radicals except in certain experiments in which consumption of propene by reaction with O₃ and O(³P) had to be taken into account.



(3)



If propene and propane are the tracers, the relevant kinetic differential equations are:

$$d \ln[\text{propene}] / dt = -k_3 [OH] - k_4 [O_3] - k_5 [O(^3P)] \quad (I)$$

$$d \ln[\text{propane}] / dt = -k_6 [OH] \quad (II)$$

where k_3 and k_6 are the respective rate constants for the reaction of propene and propane with OH radicals, k_4 and k_5 are the rate constants for the reaction of propene with O_3 and $O(^3P)$ atoms, respectively, and the O_3 and $O(^3P)$ concentrations can be estimated based on the following assumptions. Since $O(^3P)$ is formed primarily from NO_2 photolysis and is consumed primarily by its rapid reaction with O_2 , it can, to a very good approximation, be considered to be in photostationary state governed by these two reactions, and thus:

$$[O(^3P)] \approx \frac{k_{\text{phot}} [NO_2]}{k_7 [O_2] [M]} \quad (III)$$

where k_{phot} and k_7 are the rate constants for the photolysis of NO_2 and for the third-order reaction of $O(^3P)$ atoms with O_2 respectively:



Similarly, O_3 is also formed by NO_2 photolysis and under the conditions of our experiments was consumed primarily by its rapid reaction with NO; thus it also can be assumed to be in photostationary state.

$$[O_3] \approx \frac{k_{\text{phot}} [NO_2]}{k_8 [NO]} \quad (IV)$$

where k_8 is the rate constant for the reaction of O_3 with NO.



Equations (I) through (IV) can be combined and rearranged to yield

$$[OH] = (k_3 - k_6)^{-1} \frac{d}{dt} \left(\ln \frac{[\text{propane}]}{[\text{propene}]} \right) - k_{\text{phot}} [NO_2] \left(A + \frac{B}{[NO]} \right) \quad (V)$$

where

$$A = \frac{k_5}{(k_3 - k_6) k_7 [O_2] [M]}$$

and

$$B = \frac{k_4}{(k_3 - k_6) k_8}$$

It can be seen from equation (V) that the correction for consumption of propene by reaction with O_3 and $O(^3P)$ atoms increases with $[NO_2]$ and $[NO_2]/[NO]$, respectively.

The radical flux, R_u , required to fit the data for a given run can be estimated from the fact that radical initiation and radical termination rates must balance. Since the only significant radical termination processes in this system are the reactions of OH radicals with NO and NO_2 , and since HONO is in photoequilibrium after ~60 min of irradiation (Reference 43), then

$$R_u = k_9 [OH]_{\text{avg}} [NO_2]_{\text{avg}}$$

where k_9 is the rate constant for the reaction of OH radicals with NO_2 ,



and $[OH]_{\text{avg}}$ and $[NO_2]_{\text{avg}}$ (the average OH radical and NO_2 concentrations for $t > 60$ min) are experimentally determined. It should be noted that, in general, the OH radical levels were approximately constant after the first hour.

The radical input rates estimated in this way for the second hour of the various runs are summarized in Table 4 along with the initial conditions and the observed OH radical concentrations. Since these rates are

TABLE 4. CONDITIONS AND SELECTED RESULTS FOR NO_x/AIR IRRADIATIONS GROUPED BY TEMPERATURE AND PRESSURE CONDITIONS.

EC Run No.	k _{phot} (min ⁻¹)	T (°K)	Pressure (torr)	Initial Concentration		10 ⁻⁶ x [OH] av (cm ⁻³) 0-60 min 60-120 min	Radical Flux (ppb min ⁻¹)	NO Oxidation Rate (ppb min ⁻¹)
				NO (ppm)	NO ₂ (ppm)			
488	0.33	302.4	740 ^b	0.372	0.137	2.3	0.23	0.3
493	0.33	302.5	740 ^b	0.388	0.104	1.6	0.17	0.4
514	0.31	302.5	740 ^b	0.410	0.090	2.5	0.24	0.7
590	0.34	302.5	740 ^b	0.427	0.114	3.7	0.40	0.9
573	0.475	304.4	740 ^b	0.402	0.085	3.4	0.38	0.5
574	0.475	305.0	740	0.441	0.126	1.8	0.16	0.2
577	0.475	305.1	500	0.480	0.079	1.5	0.10	0.5
579	0.475	303.8	350	0.404	0.094	1.4	0.11	0.4
582	0.475	304.4	350 ^c	0.352	0.096	1.8	0.07	0.3
584	0.475	283.5	740	0.456	0.119	0.6	0.08	0.1
505	0.44	282.1	500	0.449	0.120	1.4	0.09	0.2
507	0.44	283.3	500	0.814	0.191	0.3	0.10	0.4
511	0.44	281.2	500	0.397	0.114	1.0	0.07	0.2
586	0.475	269.9	740	0.391	0.139	0.5	0.03	0.2
496	0.47	264.5	350	0.363	0.092	1.0	0.05	0.2
499	0.47	263.8	350	0.803	0.197	0.5	0.05	0.1
503	0.47	267.4	350	0.380	0.084	1.3	0.05	0.2
518	0.35	268.8	350	0.365	0.090	0.6	0.03	0.1
594	0.43	269.9	350	0.419	0.086	0.3	0.09	0.1

^aCorrected for O(³P) atom and O₃ reactions (see text).

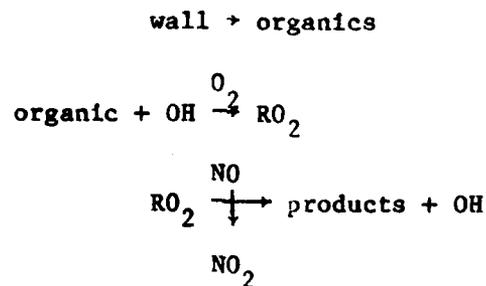
^b~50% relative humidity. All other irradiations were carried out with dry (~5% RH) matrix air.

^c200 torr N₂ + 150 torr O₂.

one to three orders-of-magnitude greater than the maximum rates of the known homogeneous radical initiation processes, such as O_3 or oxygenate photolysis or the reactions of propene with O_3 or $O(^3P)$ atoms (Reference 43), these values of R_u can be considered to measure the radical flux from unknown sources.

While some scatter exists in the data, the radical source normalized to the NO_2 photolysis rate constant k_{phot} (Reference 43) is reasonably consistent for irradiations carried out at similar initial NO_x concentrations, and under similar temperature and pressure conditions. Comparison of runs EC-574 through EC-582 ($\sim 303^\circ K$, dry air) and the irradiations at ~ 284 and $265^\circ K$ reveals no significant effect of total pressure on the radical source. Of most interest, however, is the observation that the radical source decreases with decreasing temperature, by approximately a factor of 2-3 from $303^\circ K$ to $265^\circ K$.

In addition to measuring the radical source, NO_x /air irradiations are also useful for determining whether there is any significant contamination by reactive organics. If such contamination existed, then NO oxidation would occur via the following reactions:



whereas if no such contamination existed, then the NO oxidation rate would be small, due primarily to reactions of the propene tracer and the CO present in the matrix air (Reference 43). The NO oxidation rates observed in these experiments are shown in Table 4. The rates observed are well within the range previously observed in the SAPRC evacuable chamber, and indicate that offgassing of reactive organics was not significant in these experiments (Reference 43).

2.3.3.2 Results of Fuel/ NO_x Runs. Detailed data tabulations for all of the fuel/ NO_x runs performed in this program are given in Appendix A. Selected relevant results of the simulated ground level, 10,000 ft

and 20,000 ft JP-4/NO_x/air and JP-8/NO_x/air runs are summarized in Table 5, and selected results of those experiments where the temperature and pressure were varied separately are given in Table 6. The specific results summarized include the maximum ozone concentration and the time at which the maximum occurred (for those runs where a maximum ozone level was reached), the NO oxidation rate ($-d[NO]/dt$) observed in the first hour of the irradiation, and the average OH radical concentration, estimated from the relative rates of decays of o-xylene and n-hexane observed in these runs. For comparison purposes, the OH radical levels and the radical input rates for the corresponding NO_x/air control irradiations are also given in these tables.

The experimental data shown in Table 5 indicate that the apparent reactivity of the fuel/NO_x mixtures, whether measured by the ultimate ozone yields or by the initial rate of oxidation of NO, decreases significantly with increasing simulated altitude, despite the fact that the overall light intensity increases. The results shown in Table 6 indicate that temperature is the dominant effect, since all aspects of reactivity decrease significantly when the temperature is decreased at constant pressure, while when the pressure is decreased at a constant temperature, the NO oxidation rate actually increases (although the maximum ozone yield decreased slightly).

The dominant effect of temperature observed in these experiments may be primarily due to the importance of temperature in determining the chamber-dependent radical input rate (Reference 43), since the decreased radical input rates caused by decreasing temperature would account for the reduced reactivity observed in these fuel/NO_x runs. Clearly, this must be considered when analyzing the results of these experiments in terms of their implications concerning the reactivity of these fuel/NO_x mixtures in the ambient atmosphere, where such chamber effects are presumably absent. On the other hand, the total pressure does not appear to be an important factor in determining radical input rates caused by chamber effects (Reference 43). Thus, our results may be of more direct applicability in assessing the effect of total pressure on fuel reactivity. Our data concerning the effects of temperature and pressure, and thus altitude, on the reactivity of fuel/NO_x mixtures are discussed in the following section.

TABLE 5. PHOTOCHEMICAL REACTIVITY OF JP-4/NO_x/AIR IRRADIATIONS AT SIMULATED GROUND LEVEL, 10,000 FEET, AND 20,000 FEET ALTITUDE, AND OF JP-8/NO_x/AIR IRRADIATIONS AT SIMULATED GROUND LEVEL AND 20,000 FEET ALTITUDE, AND SELECTED RESULTS OF ASSOCIATED NO_x/AIR IRRADIATIONS.

EC Run No.	Nominal Initial Fuel NO _x (ppmC)	Initial NO _x (ppm)	O ₂ maximum Conc. (ppm)	Time (hours)	Approx. Estimated [OH] (10 ⁶ cm ⁻³)	$\frac{-d[NO]}{dt}$ (0-60 min) (ppb min ⁻¹)	$\frac{-d[NO]}{dt}$ (0-60 min) (ppb min ⁻¹)	Associated NO _x /Air ^d		
							$\frac{-d[NO]}{dt}$ (0-60 min) (ppb min ⁻¹)	EC Run No.	[OH] (10 ⁶ cm ⁻³)	R _u (ppb min ⁻¹)
A. JP-4, Simulated ground level ^e										
489	50	0.5	0.47	5.25	0.4	4.7	21	488	2.5	0.23
492	50	0.5	0.52	5.0	-0.0	4.5	21	493	1.9	0.17
515	100	0.5	0.61	3.0	-0.0	6.4	28	514	2.7	0.24
491	5	1.0	-	>6.0	1.0	1.8	8			
490	50	1.0	-	>6.0	0.6	5.2	20			
B. JP-4, Simulated 10,000 feet ^f										
506	50	0.5	-	>6.0	0.3	3.4	43	505	1.4	0.09
509	100	0.5	0.42	6.0	0.1	4.2	54	511	1.1	0.07
510	100	0.5	0.45	>6.0	0.5	4.5	56			
508	50	1.0	-	>6.0	0.8	2.9	29	507	0.6	0.10
C. JP-4, Simulated 20,000 feet ^{g,h}										
498	50	0.5	-	>6.0	0.3	1.8	36	496	1.0	0.05
502	50	0.5	-	>6.0	0.1	1.8	36	503	1.2	0.05
500	100	0.5	-	>6.0	0.2	3.8	76			
517	50	1.0	-	>6.0	-0.0	2.6	52	499	0.5	0.05

TABLE 5. PHOTOCHEMICAL REACTIVITY OF JP-4/NO_x/AIR IRRADIATIONS AT SIMULATED GROUND LEVEL, 10,000 FEET, AND 20,000 FEET ALTITUDE, AND OF JP-8/NO_x/AIR IRRADIATIONS AT SIMULATED GROUND LEVEL AND 20,000 FEET ALTITUDE, AND SELECTED RESULTS OF ASSOCIATED NO_x/AIR IRRADIATIONS (CONCLUDED).

EC Run No.	Nominal Initial Concentration NO _x (ppmC)	O ₂ maximum ^a Conc. (ppm)	Time (hours)	Approx. Estimated ^b [OH] (10 ⁶ cm ⁻³)	-d[NO]/dt (0-60 min) (ppb min ⁻¹)	-d[NO]/R _u (0-60 min)	EC Run No.	Associated NO _x /Air ^d [OH] (10 ⁶ cm ⁻³)	R _u (ppb min ⁻¹)
D. JP-4, Simulated 20,000 feet, 70° zenith angle ^{g,1}									
517	50	-	>6.0	-0.0	1.3	43	518	0.6	0.03
E. JP-8, Simulated ground level ^e									
592	50	-	>6.0	-	2.1	5	590	3.7	0.40
591	100	0.49	5.0	-	3.2	8			
F. JP-8, Simulated 20,000 feet ^{g,j}									
595	100	-	>6.0	-	0.5	6	594	1.1	0.09

^aTime given is to nearest 0.25 hour. "u" indicates no maximum O₂ yield attained during the irradiation.
^bEstimated from slope of plot of $d(\ln[(o\text{-xylene})/(n\text{-hexane})])/dt$ using $k(\text{OH} + o\text{-xylene}) = 1.5 \times 10^{-11}$ cm³ molecule⁻¹ sec⁻¹ and $k(\text{OH} + n\text{-hexane}) = 1.7 \times 10^{-11}$ exp $(-650/RT)$ cm³ molecule⁻¹ sec⁻¹ (Reference 51). The uncertainty in absolute concentrations is approximately 0.5 x 10⁻⁶ cm⁻³.
^cR_u = radical input rate, taken from the results of the associated NO_x/air irradiations, except for the simulated ground level runs, where R_u was taken from regressions of plots of R_u vs [NO₂]_{avg} using a much larger set of NO_x/air irradiations (Reference 43).
^dFor a more complete summary of the results of these runs, see Table 4.
^eNominal 740 torr, 303°K, 50% relative humidity; NO₂ photolysis rate = 0.33 min⁻¹.
^fNominal 500 torr, 284°K, 5% relative humidity; NO₂ photolysis rate = 0.44 min⁻¹.
^gNominal 350 torr, 265°K, 5% relative humidity.
^hNO₂ photolysis rate = 0.47 min⁻¹.
ⁱNO₂ photolysis rate = 0.35 min⁻¹.
^jNO₂ photolysis rate = 0.43 min⁻¹.

TABLE 6. PHOTOCHEMICAL REACTIVITY OF JP-4(100 ppmC)/NO_x(0.5 ppm)/AIR (55% RH) MIXTURES AS A FUNCTION OF TEMPERATURE AND PRESSURE, AND SELECTED RESULTS OF ASSOCIATED NO_x/AIR IRRADIATIONS.

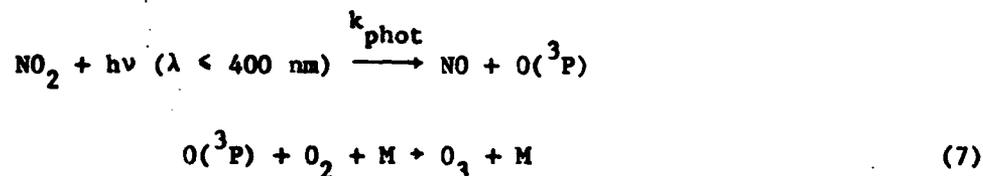
EC Run No.	Temperature (°K)	Pressure (torr)	O ₃ Conc. (ppm)	Maximum Time (hours)	Approx. Estimated [OH] (10 ⁶ cm ⁻³)	-d[NO]/dt (0-60 min) (ppb min ⁻¹)	-d[NO]/R _u ^c (0-60 min)	EC Run No.	Associated NO _x /Air ^d [OH] (10 ⁶ cm ⁻³)	R _u (ppb min ⁻¹)
587	272	740	-	>6.0	0.7	1.0	33	586	0.4	0.03
588	285	740	-	>6.0	0.7	4.7	59	584	0.8	0.08
575	303	740	0.72	2.75	<0.0	6.4	40	574	1.9	0.16
578	303	500	0.58	2.5	0.3	11 ^e	105	577	1.8	0.10
580	303	350	0.52	2.25	0.4	15 ^f	132	579	1.8	0.11
581	303	350 ^g	0.42	2.5	0.2	13 ^f	139	582 ^h	1.7	0.07

^aTime given is to nearest 0.25 hr. "u" indicates no maximum O₃ yield attained during the irradiation.
^bEstimated from slope of plot of $d(\ln[o\text{-xylenes}]/[n\text{-hexane}])/dt$ using $k(\text{OH} + o\text{-xylene}) = 1.5 \times 10^{-11}$ cm³ molecule⁻¹ sec⁻¹ and $k(\text{OH} + n\text{-hexane}) = 1.7 \times 10^{-11}$ exp (-650/RT) cm³ molecule⁻¹ sec⁻¹ (Reference 51). The uncertainty in absolute concentrations is approximately 0.5×10^{-6} cm⁻³.
^cR_u = radical input rate, taken from the results of the associated NO_x/air irradiations except for the simulated ground level runs, where R_u was taken from regressions of plots of R_u vs [NO₂]_{avg} using a much larger set of NO_x/air irradiations (Reference 43).
^dFor a more complete summary of the results of these runs, see Table 4.
^eFor t = 0-45 min only; significant O₃ formation occurred after 45 min.
^fFor t = 0-35 min only; significant O₃ formation occurred after 30 min.
^g200 torr N₂ + 150 torr O₂ used instead of air.

2.4 DISCUSSION

The release of aircraft fuels at high altitudes or near ground level may have a number of potentially significant atmospheric impacts in addition to ozone formation, such as the formation of toxic organic oxidation products and/or aerosol production (Reference 16). However, in this discussion we shall only consider reactivity relative to ozone formation, since this is the only aspect of reactivity which our present data address.

The direct cause of the formation of ozone in atmospheric systems is the photolysis of NO_2



and, according to our current understanding of atmospheric chemistry, there are no other significant primary sources of O_3 . If no other species are present, relatively little O_3 is formed, since O_3 reacts rapidly with NO



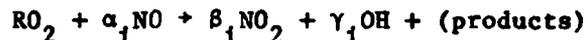
with the result that at the photostationary state O_3 is determined by the $[\text{NO}_2]/[\text{NO}]$ ratio.

$$[\text{O}_3] \approx \frac{k_{\text{phot}} [\text{NO}_2]}{k_8 [\text{NO}]} \quad (\text{IV})$$

In the presence of reactive organics, such as those in the aircraft fuels JP-4 and JP-8, intermediates are formed which convert NO to NO_2 and thus cause the $[\text{NO}_2]/[\text{NO}]$ ratio to increase, which in turn causes ozone formation to occur.

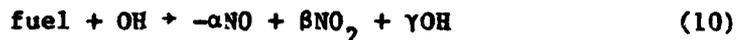
The major constituents of the two fuels studied here are the higher alkanes and aromatics, both of which are consumed in the atmosphere almost exclusively by reaction with hydroxyl radicals (Reference 51). The mechanisms for the atmospheric reactions of alkanes (References 11 and 15) and aromatics (References 14 and 15) are rather complex and, particularly for the aromatics, somewhat uncertain. However, the major overall processes in

both cases can be represented as indicated below:



where α_1 is the efficiency of the i th fuel component in oxidizing NO and thus causing O_3 formation, $(\alpha_1 - \beta_1)$ is its efficiency in removing active NO_x from the system, which has the effect of decreasing the maximum amount of O_3 which will be formed (since NO_x is required for O_3 formation), and $(1 - \gamma_1)$ is the efficiency of the fuel component in removing radicals from the system, which, if significant, will tend to decrease the overall rates of fuel consumption, NO oxidation and O_3 formation.

However, a large number of individual fuel components are present in JP-4 and JP-8, and their individual reactivity parameters are, in general, not known. Furthermore, because secondary reactions of some of the fuel oxidation products may also contribute to the observed reactivity, it is more useful to consider the overall process as indicated below.



The results of our experiments can then be examined in terms of the overall reactivity parameters α , $(\alpha - \beta)$, and $(1 - \gamma)$.

One important aspect of reactivity concerns the tendency of the reactions of the fuel to either inhibit or enhance radical levels. In particular, if the fuel components are oxidized to a significant extent to form species which undergo rapid photodecomposition to form radicals, or which react with ozone to form radicals, γ may be greater than 1. Thus, in principle, it is possible for a fuel to enhance radical levels. For example, toluene and other aromatics present in the fuels are known to form products which rapidly photolyze to produce radicals (References 14 and 15 and Section IV), and this obviously would tend to lead to higher radical levels. On the other hand, alkyl nitrate formation via the radical-terminating reaction,



is known to be important in the NO_x /air photooxidations of the heavier alkanes present in the fuels (References 25 and 26 and Section III), and this tends to lead to reduced radical levels. Since JP-4 and JP-8 contain both aromatics and heavier alkanes, it is difficult to predict, a priori, which of the above effects will be more important.

The estimated average OH radical levels observed in the JP-4/ NO_x /air smog chamber experiments (Tables 5 and 6) are highly scattered, but can be seen in most cases to be ~2-10 times lower than those observed in the corresponding NO_x /air irradiations performed with the same initial NO_x levels and reaction conditions (temperature, pressure, etc.). Thus it can be concluded that the presence of JP-4 in NO_x /air mixtures tends to reduce radical levels below what they would be if the fuel were absent, i.e., γ is significantly less than one. Because the major components of JP-8 have a carbon number too high for reliable monitoring with the GC techniques employed in this study (Reference 16), we could not obtain estimates of the OH radical levels in the runs containing JP-8. However, the fact that JP-8 is less reactive than JP-4 under all conditions studied, along with the fact that it contains similar types of constituents (although of higher molecular weight), strongly suggests that γ is also less than one for this fuel. The OH radical levels in the fuel runs are suppressed to such low values that their estimates are uncertain by at least a factor of two, and conclusions concerning the precise values of γ , or the effect of temperature and pressure on this parameter cannot be derived from the present data.

A better indication of the effect of temperature and pressure on the reactivity of the fuels can be obtained by examining their effects on the initial rates of NO oxidation, $-d[\text{NO}]/dt$, which are summarized in Tables 5 and 6. If, for the purposes of discussion, we (a) consider the fuel to consist of a single compound which reacts with OH radicals with a rate constant of k_f according to reaction (10), (b) assume reaction of the fuel is the major cause of NO oxidation, and (c) restrict our consideration to the initial period of the irradiation when $[\text{NO}] \gg [\text{O}_3]$ (and thus NO oxidation is manifested primarily by NO consumption rather than O_3 buildup), then we can write:

$$\frac{-d[\text{NO}]}{dt} \sim k_f [\text{fuel}] [\text{OH}]$$

If we further assume that the major radical source in these fuel/NO_x/air irradiations is the chamber radical source, represented by



(which occurs with a rate of R_u), and that the major radical sink, other than reactions of the fuel components [reaction (10)], is reaction of OH with NO₂,



then a steady state analysis for [OH] gives

$$[\text{OH}] \approx \frac{R_u}{k_9 [\text{NO}_2] + (1-\gamma)k_f [\text{fuel}]}$$

and, therefore, we can derive

$$\frac{-d[\text{NO}]}{dt} \frac{1}{R_u} = \frac{\alpha k_f [\text{fuel}]}{k_9 [\text{NO}_2] + (1-\gamma)k_f [\text{fuel}]} = \left\{ \frac{(1-\gamma)}{\alpha} + \frac{k_9}{\alpha k_f} \frac{[\text{NO}_2]}{[\text{fuel}]} \right\}^{-1} \quad (\text{VI})$$

Equation (VI) shows that the initial NO oxidation rate can be normalized by dividing by the chamber-dependent radical input rate (obtained from the corresponding NO_x/air irradiations) to obtain a quantity which does not depend on chamber effects, but rather depends only on the fuel reactivity parameters α, γ, and k_f, and the [NO₂]/[fuel] ratio. This then allows us to factor out, at least approximately, the effect of the chamber radical source.

The quantity $(\frac{-d[\text{NO}]}{dt}/R_u)$, which can be considered to be a measurement of the efficiency of the fuel in oxidizing NO and thus in forming ozone, is tabulated in Tables 5 and 6 for all the fuel/NO_x/air runs. Since the radical input rates generally show a ±50% scatter, these quantities must be considered to be uncertain by at least that amount. Despite these uncertainties, Table 5 indicates that the efficiency of both JP-4 and JP-8 in

oxidizing NO increases with the [fuel]/[NO_x] ratio, as predicted by equation (VI). Table 5 also indicates a progressive increase in the efficiency of JP-4 in oxidizing NO upon going from simulated ground level to simulated altitudes of 10,000 ft and 20,000 ft. It can also be seen from Table 5 that JP-8 is far less efficient in oxidizing NO than JP-4, and that there does not appear to be a significant change in efficiency of JP-8 in going from simulated ground level to simulated 20,000 ft altitude.

An indication of the effects of total pressure and of temperature, when varied independently of each other, can be obtained from the data in Table 6. The results of EC runs 575, 588, and 587 reveal that the NO oxidation efficiency does not depend strongly on temperature, and that the strong temperature dependence on overall reactivity observed in our chamber experiments can be attributed almost entirely to the temperature dependence of the chamber radical source. This suggests that in the atmosphere, in the absence of these chamber effects, the rate of ozone formation from fuel/NO_x mixtures may actually be relatively insensitive to temperature, contrary to what would be concluded from examining our data without due consideration of the role of chamber effects.

The data in Table 6 also indicate that the NO oxidation efficiency of JP-4 significantly increases when the pressure is decreased. This is because radical termination caused by formation of alkyl nitrates in the oxidation of the heavier alkane fuel constituents becomes less important as total pressure decreases. This is clearly shown by our direct measurements of the pressure effects on the alkyl nitrate yields discussed in Section III of this report. This suggests that in the troposphere, in the absence of the overwhelming effect of chamber radical sources, the rate of NO oxidation and ozone formation in fuel/NO_x mixtures will increase with altitude, primarily as a result of the pressure (as opposed to temperature) effects.

The above discussion has been concerned primarily with factors influencing the rate of ozone formation in fuel/NO_x irradiations, as opposed to the ultimate maximum O₃ yields which would be obtained if the irradiation were allowed to proceed for a sufficiently long time. Although the conditions in a majority of our experiments were such that the rate of NO oxidation and O₃ formation were too slow for the maximum ozone yield to be obtained in one day of simulated irradiation, several runs were sufficient-

ly reactive for ozone maximums to be observed. These runs reveal that despite significant differences in reactivity as defined by NO oxidation rates or NO oxidation efficiencies, the maximum O_3 yields from ground-level simulations in NO_x /air irradiation of JP-8 do not differ greatly from those obtained in corresponding runs employing JP-4. The maximum O_3 yield from JP-4/ NO_x /air irradiations seems to decrease slightly with increased simulated altitude (Table 5) and with decreasing pressure at constant temperature (Table 6), but the effect is relatively small, compared to the effects of varying these parameters on rates of NO oxidation and O_3 formation.

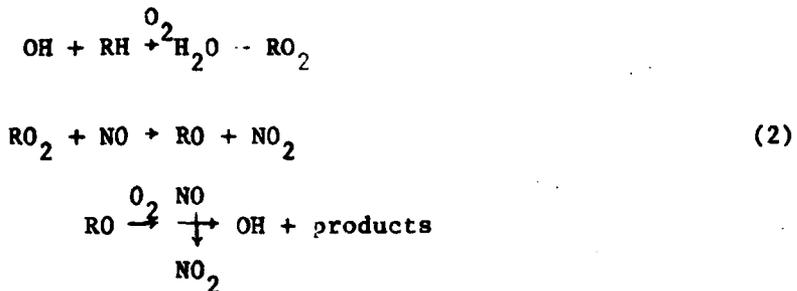
As indicated above, no ozone maximums were obtained in a majority of the experiments reported here; thus, the maximum O_3 yields obtained during those irradiations were determined primarily by how rapidly NO was oxidized. In the atmosphere, where there are (presumably) no unknown radical sources, radical levels may be lower than even the relatively low levels observed in our fuel/ NO_x runs, and O_3 yields are expected to be limited by its rate of formation under an even larger set of conditions than those observed in our environmental chamber. Therefore, unless the fuels are dumped under extremely NO_x -poor conditions, the ozone-forming potentials of these fuels in the open atmosphere are expected to be determined primarily by factors such as their NO oxidation efficiency, as opposed to their maximum O_3 yield potential. Finally, it should be stressed that both JP-4 and JP-8 are photochemically unreactive when compared to commercial fuels such as unleaded gasoline (Reference 16), or to other anthropogenic organics which are typically emitted to the atmosphere.

SECTION III

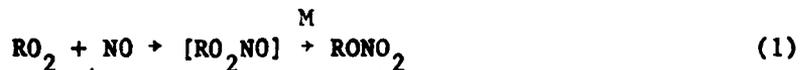
TEMPERATURE AND PRESSURE EFFECTS ON ALKYL NITRATE FORMATION
FROM THE NO_x PHOTOOXIDATIONS OF n-PENTANE AND n-HEPTANE

3.1 INTRODUCTION

The higher alkanes are important constituents of JP-4, JP-8 and other military and commercial fuels (Reference 16). Until recently, based on analogy with the reactions of the lower alkanes (Reference 15), the NO_x/air photooxidations of the higher alkanes have been thought to proceed primarily via the reaction sequence



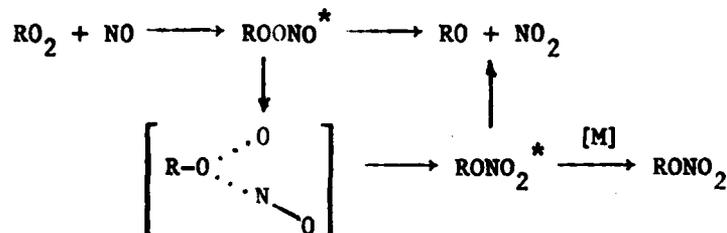
which exhibits essentially 100% radical propagation and involves no loss of NO_x from the system. However, Darnall, et al. (Reference 25) observed relatively high yields of alkyl nitrates in environmental chamber studies of the NO_x/air photooxidations of n-butane, n-pentane and n-hexane, which could only be attributed to their formation by the reaction pathway



This reaction represents both a radical and a NO_x sink, and could account for the relatively low radical levels observed in our chamber studies of JP-4 and JP-8 (Section II).

Recent investigations in our laboratories (Reference 26) have shown that the yields of alkyl nitrates formed in the NO_x/air photooxidations of the homologous series of n-alkanes ethane through n-octane at 299±2°K and 735 torr total pressure increase monotonically with the carbon number of the n-alkane from <1% for ethane to ~33% for n-octane, with the yields apparently approaching a limit of ~35% for the larger n-alkanes. The reaction pathway leading to alkyl nitrate formation is exothermic by ~57 kcal mole⁻¹ overall (Reference 52) and probably involves a three-member

transition state. The available data are consistent with the following mechanism (Reference 26)



where the asterisk denotes vibrational excitation. Hence, it may be expected that the alkyl nitrate yields from the NO_x photooxidation of the n-alkanes would exhibit pressure (and possibly temperature effects) with the yields decreasing with decreasing pressure.

Since the jet fuels JP-4 and JP-8 contain a large fraction of n-alkanes, a study of the temperature and pressure dependence of alkyl nitrate yields provides important information concerning the behavior of the fuels at elevated altitudes. Accordingly, the alkyl nitrate yields from the NO_x photooxidations of n-pentane and n-heptane have been determined as a function of both temperature (284-340°K) and total pressure (56-740 torr).

3.2 EXPERIMENTAL

As in the previous study from these laboratories (Reference 26), RO_2 radicals were formed in the presence of NO by the photolysis at >290 nm of methyl nitrite/NO/alkane/air (or O_2) mixtures with typical initial reactant concentrations being $\text{CH}_3\text{ONO} \sim (0.1-1.6) \times 10^{13}$ molecule cm^{-3} ; $\text{NO} \sim (2-3) \times 10^{13}$ molecule cm^{-3} ; and the alkane (n-pentane or n-heptane) $\sim (2-3) \times 10^{13}$ molecule cm^{-3} .

Irradiations were carried out in the SAPRC 5800-l Teflon[®]-coated evacuable, thermostatted, environmental chamber with irradiation being provided by the 25-KW solar simulator (Reference 45). Prior to each irradiation the chamber was evacuated to $\leq 2 \times 10^{-5}$ torr. Methyl nitrite, prepared as described previously (Reference 53), and NO were introduced into the chamber from a vacuum gas handling system. The chamber was then filled to the desired pressure with dry purified matrix air (References 45 and 50) or ultra-high purity O_2 . Known quantities of n-pentane or n-heptane were flushed into the chamber from a ~ 1 l Pyrex[®] bulb by a stream of ultra-high

purity N_2 . The chamber was maintained at the desired temperature by means of the chamber's heating/cooling system.

The n-alkanes were quantitatively analyzed by gas chromatography with flame ionization detection (GC-FID) using a 20 ft x 0.125 in stainless steel (SS) column of 5% DC703/G20M on 100/120 mesh AW, DMCS Chromosorb[®] G, operated at 333^oK without sample preconcentration. The pentyl nitrates were analyzed by GC-FID using a 10 ft x 0.125 in SS column of 10% Carbowax[®] 600 on C-22 Firebrick[®] (100/110 mesh), operated at 348^oK, while the heptyl nitrates were analyzed by GC-FID using a 5 ft x 0.125 in SS column of 5% Carbowax[®] 600 on C-22 Firebrick[®] (100/110 mesh), also operated at 348^oK. For these alkyl nitrate analyses 100 ml of gas sample was preconcentrated in a ~1 ml SS loop at liquid argon temperature prior to injection onto the column. Gas chromatographic retention times and calibration factors were determined as described previously (Reference 26).

Gas chromatographic analyses of the n-alkanes and of the alkyl nitrates were carried out prior to and during the irradiations. The irradiations were of ~60 min duration with gas chromatographic analyses being carried out every 15 min during this time period.

3.3 RESULTS

The temperature, pressure, initial reactant concentrations, and the observed amounts of n-alkane consumed and alkyl nitrate formed, as measured at various times during the irradiations, are given in Tables 7 and 8 for the $CH_3ONO/NO/n$ -pentane/air (or O_2) and the $CH_3ONO/NO/n$ -heptane/air (or O_2) irradiations, respectively.

These tables show that, within the experimental uncertainties, alkyl nitrate formation was observed without any apparent induction period, and that it increased linearly with the amount of n-alkane consumed. Furthermore, Tables 7 and 8 reveal that the alkyl nitrate yields are pressure and temperature dependent, decreasing with decreasing pressure and increasing temperature. These results are discussed in more detail in the following section.

TABLE 7. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-PENTANE/AIR (OR O₂) IRRADIATIONS.

EC Run No.	Temperature (°K)	Total Pressure (corr)	10 ⁻¹³ x Initial Conc. (molecule cm ⁻³)		10 ⁻¹² x -Δ(n-Pentane) (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)					
			CH ₃ ONO	NO		2-Pentyl	3-Pentyl	Total			
						Obs	Corr ^a	Obs	Corr ^a	Obs	Corr ^a
692	300±2	740	1.56	2.39	2.24	1.74	1.79	1.17	1.19	2.98	
						2.60	2.69	1.76	1.81	4.50	
						3.05	3.19	2.24	2.31	5.50	
693	300±2	352	1.42	2.42	2.13	3.31	3.50	2.33	2.41	5.91	
						0.88	0.90	0.67	0.68	.58	
						2.22	2.33	1.50	1.55	3.88	
694	300±2	155 ^b	1.36	2.36	2.30	2.26	2.41	1.67	1.74	4.15	
						2.55	2.74	1.83	1.91	4.65	
						4.57	4.48	0.86	0.88	2.36	
695	300±2	505	1.42	2.36	2.25	1.93	2.10	1.31	1.38	3.48	
						2.29	2.52	1.48	1.57	4.09	
						6.38	7.57				
696	300±2	153	0.61	2.36	2.28	2.86	1.41	1.00	1.02	2.43	
						4.07	2.29	1.64	1.69	4.07	
						5.19	2.57	2.74	1.93	2.00	4.74
697	300±2	56 ^b	0.36	2.36	2.27	2.95	3.17	2.05	2.14	5.31	
						0.64	0.65	0.40	0.40	1.05	
						1.12	1.16	0.83	0.86	2.02	
						1.10	1.14	0.86	0.88	2.02	
						1.52	1.62	1.02	1.07	2.69	
						0.64	0.67	0.50	0.52	1.19	
						1.02	1.10	0.69	0.72	1.82	
						1.00	1.10	0.71	0.76	1.86	
						1.26	1.41	0.91	0.98	2.39	

TABLE 7. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-PENTANE/AIR(OR O₂) IRRADIATIONS (CONTINUED).

EC Run No.	Temperature (°K)	Total Pressure (corr)	10 ⁻¹³ x Initial Conc. (molecule cm ⁻³)		10 ⁻¹² x -Δ(n-Pentane) (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)					
			CH ₃ ONO	NO		2-Pentyl Obs	2-Pentyl Corr ^a	3-Pentyl Obs	3-Pentyl Corr ^a	Total (Corr) ^a	
698	300±2	57 ^b	0.28	2.39	2.19	2.22	0.52	0.53	0.48	0.48	1.01
						3.62	0.81	0.84	0.52	0.53	1.37
						4.65	0.88	0.93	0.71	0.74	1.67
						5.50	0.98	1.05	0.69	0.72	1.77
699	328±2	740	1.30	2.15	2.38	3.62	1.45	1.50	1.02	1.05	2.55
						5.26	2.14	2.26	1.38	1.43	3.69
						6.17	2.55	2.74	1.74	1.81	4.55
						6.65	2.76	3.00	1.88	1.98	4.98
700	327±2	151	0.56	2.18	2.32	2.74	0.67	0.69	0.52	0.52	1.21
						5.07	1.10	1.17	0.81	0.83	2.00
						6.46	1.26	1.36	0.91	0.95	2.31
						7.91	1.60	1.76	1.19	1.26	3.02
701	326±2	400	1.26	2.19	2.31	3.36	1.17	1.21	0.74	0.76	1.97
						5.57	1.62	1.72	1.12	1.17	2.99
						6.36	2.05	2.22	1.38	1.45	3.67
						6.86	2.31	2.52	1.55	1.62	4.14
717	284±1	740	1.26	2.49	2.17	2.19	1.62	1.67	1.17	1.19	2.86
						3.26	2.52	2.62	1.86	1.91	4.53
						3.84	3.10	3.24	2.26	2.33	5.57
						4.12	3.50	3.69	2.57	2.64	6.33
718	284±1	356	0.72	2.52	2.12	1.45	0.86	0.88	0.60	0.61	1.49
						2.55	1.55	1.60	1.12	1.14	2.74
						3.31	2.02	2.10	1.52	1.57	3.67
						4.00	2.12	2.22	1.57	1.62	3.84

TABLE 7. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-PENTANE/AIR(OR O₂) IRRADIATIONS (CONCLUDED).

EC Run No.	Temperature (°K)	Total Pressure (torr)	10 ⁻¹³ x Initial Conc. (molecule cm ⁻³)		10 ⁻¹² x -δ(n-Pentane) (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)		Total (Corr) ^a			
			CH ₃ ONO	NO		2-Pentyl Obs	2-Pentyl Corr ^a		3-Pentyl Obs	3-Pentyl Corr ^a	
719	284±1	155	0.51	2.52	2.13	1.86	0.50	0.36	0.86		
						2.95	0.93	0.67	0.68	1.63	
						3.76	1.29	1.36	0.95	2.34	
720	337±3	740	0.74	2.12	2.52	4.10	1.45	1.52	1.07	1.10	2.62
						3.31	1.26	1.31	0.81	0.83	2.14
						4.95	1.91	2.00	1.29	1.33	3.33
						5.93	2.36	2.52	1.55	1.60	4.12
						6.41	2.60	2.79	1.74	1.81	4.60

^aCorrected for secondary re-irradiations with OH radicals (see text).

^bO₂ diluent gas.

TABLE 8. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-HEPTANE/ATR(O₂) IRRADIATIONS.

EC Run No.	Temperature (°K)	Total Pressure (corr)	10 ⁻¹³ x Initial Conc. (molecule cm ⁻³)		10 ⁻¹² x -Δ[n-Heptane] (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)		Total 4-Heptyl (Corr) ^a					
			CH ₃ ONO	NO		2-Heptyl Obs ^a	3-Heptyl Obs ^a		4-Heptyl Obs ^a				
702	300±2	740	1.36	2.38	2.28	3.29	2.60	2.74	4.10	4.26	1.79	1.86	8.86
						4.95	4.03	4.38	6.07	6.48	2.67	2.83	13.69
						6.00	5.05	5.62	7.57	8.22	3.36	3.62	17.46
703	300±2	353	1.00	2.36	2.17	2.86	1.83	1.93	2.72	2.81	1.21	1.26	6.00
						4.60	3.12	3.38	4.53	4.84	2.05	2.17	10.39
						5.96	3.74	4.19	5.48	5.98	2.55	2.76	12.93
704	300±2	160	0.58	2.36	2.22	2.57	1.00	1.05	1.48	1.52	0.67	0.69	3.26
						4.55	1.76	1.91	2.72	2.88	1.29	1.36	6.15
						5.26	2.36	2.60	3.60	3.86	1.57	1.67	8.13
705	300±2	56 ^b	0.28	2.36	2.19	6.26	2.57	2.88	4.19	4.60	1.81	1.95	9.43
						2.48	0.67	0.69	0.95	0.98	0.43	0.44	2.11
						4.26	1.26	1.36	1.86	1.98	0.83	0.88	4.22
706	323±2	740	1.32	2.21	2.46	5.84	1.69	1.88	2.50	2.72	1.10	1.19	5.79
						6.88	1.93	2.19	3.19	3.53	1.36	1.50	7.22
						4.84	2.57	2.76	3.81	4.05	1.72	1.81	8.62
707	324±2	356	0.67	2.21	2.31	7.05	3.81	4.29	5.48	6.00	2.43	2.64	12.93
						8.19	4.55	5.24	6.57	7.34	2.93	3.24	15.82
						8.84	5.12	6.00	7.46	8.43	3.36	3.76	18.19
						3.53	1.31	1.38	1.83	1.91	0.83	0.86	4.15
						5.26	2.57	2.81	3.45	3.69	1.52	1.62	8.12
						6.36	3.00	3.36	4.24	4.62	1.93	2.10	10.08
						7.38	3.26	3.74	4.74	5.26	2.12	2.33	11.33

TABLE 8. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-HEPTANE/AIR(OR O₂) IRRADIATIONS (CONTINUED).

EC Run No.	Temperature (°K)	Total Pressure (corr)	10 ⁻¹³ x Initial Conc. (molecule cm ⁻³)		10 ⁻¹² x -Δ[n-Heptane] (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)		Total (Corr) ^a					
			CH ₃ ONO	NO		2-Heptyl	3-Heptyl		4-Heptyl				
708	324±2	156	0.40	2.21	2.36	Obs	0.76	0.81	1.10	1.14	0.48	0.50	2.45
						Corr ^a	1.60	1.76	2.33	2.52	1.02	1.10	5.38
						Total	2.05	2.31	3.24	3.57	1.38	1.50	7.38
709	321±2	59 ^b	0.28	2.21	2.40	Obs	2.50	2.95	3.79	4.31	1.60	1.79	9.05
						Corr ^a	0.60	0.62	0.95	1.00	0.43	0.45	2.07
						Total	1.41	1.60	2.24	2.48	0.98	1.07	5.15
710	319±2	60 ^b	0.14	2.23	2.36	Obs	1.69	2.05	2.86	3.33	1.21	1.38	6.76
						Corr ^a	2.10	2.72	3.43	4.19	1.48	1.76	8.67
						Total	10.08	12.17					
711	284±1	740	1.41	2.49	2.30	Obs	0.31	0.31	0.55	0.57	0.24	0.24	1.12
						Corr ^a	0.95	1.02	1.55	1.64	0.64	0.67	3.33
						Total	1.29	1.45	2.26	2.48	0.93	1.00	4.93
712	285±1	349	1.08	2.49	2.14	Obs	1.72	2.00	3.00	3.38	1.26	1.41	6.79
						Corr ^a	2.02	2.12	3.48	3.60	1.60	1.64	7.36
						Total	3.62	3.91	5.86	6.22	2.69	2.83	12.96
713	283±1	159	0.75	2.52	2.18	Obs	4.50	4.93	7.15	7.67	3.19	3.41	16.01
						Corr ^a	5.12	5.67	8.08	8.74	3.64	3.91	18.32
						Total	1.52	1.60	2.50	2.60	1.12	1.17	5.37
						Obs	2.55	2.72	3.98	4.19	1.81	1.91	8.82
						Corr ^a	3.48	3.79	5.38	5.76	2.50	2.67	12.22
						Total	3.93	4.36	6.22	6.74	2.81	3.03	14.13
						Obs	0.98	1.02	1.69	1.74	0.76	0.79	3.55
						Corr ^a	1.91	2.05	3.12	3.31	1.41	1.48	6.84
						Total	5.41	5.81	4.12	4.45	1.88	2.02	9.28
						Obs	2.91	3.29	4.72	5.19	2.14	2.33	10.81
						Corr ^a							
						Total							

TABLE 8. EXPERIMENTAL DATA FOR THE CH₃ONO/NO/n-HEPTANE/AIR(OR O₂) IRRADIATIONS (CONCLUDED).

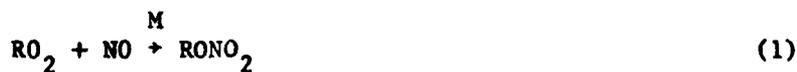
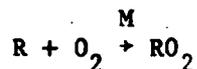
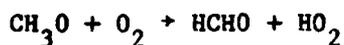
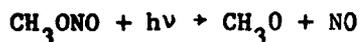
EC Run No.	Temperature (°K)	Total Pressure (torr)	10 ⁻¹³ x Initial Conc. CH ₃ ONO/NO n-Heptane (molecule cm ⁻³)		10 ⁻¹² x -Δ(n-Heptane) (molecule cm ⁻³)	10 ⁻¹¹ x Nitrate Yields (molecule cm ⁻³)							
			CH ₃ ONO	NO		2-Heptyl	3-Heptyl	4-Heptyl	Total				
			Obs	Corr ^a		Obs	Corr ^a	Obs	Corr ^a	Obs	Corr ^a	Obs	Corr ^a
714	284±1	58 ^b		0.35	2.48	2.11	0.64	0.67	1.02	1.05	0.45	0.48	2.20
						4.12	1.29	1.38	2.00	2.12	0.91	0.95	4.45
						5.19	1.60	1.76	2.62	2.83	1.14	1.21	5.80
						5.88	1.95	2.19	3.24	3.55	1.41	1.52	7.26
715	339±2	740		1.05	2.09	2.58	2.22	2.41	3.33	3.55	1.52	1.62	7.58
						7.77	3.26	3.69	4.98	5.48	2.26	2.41	11.58
						9.31	3.81	4.45	5.72	6.46	2.60	2.91	13.82
						10.41	4.67	5.60	6.24	7.19	2.81	3.19	15.98
716	342±2	160		0.64	2.07	4.55	1.36	1.50	2.00	2.14	0.91	0.98	4.62
						10.58	2.36	2.86	3.31	3.84	1.48	1.69	8.39
						13.27	2.81	3.67	4.00	4.93	1.81	2.19	10.79
						15.03	3.19	4.43	4.67	6.03	2.10	2.64	13.10

^aCorrected for secondary reactions with OH radicals (see text).

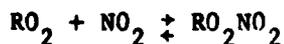
^bO₂ diluent gas.

3.4 DISCUSSION

As discussed previously (Reference 26), the major reactions occurring in the $\text{CH}_3\text{ONO}/\text{NO}/n\text{-alkane}/\text{air}$ photolysis system can be represented as follows:



In this system, the n -alkane and the alkyl nitrates are consumed essentially solely by reaction with OH radicals [Reactions (11) and (14)]. Reaction with NO, forming either the corresponding alkyl nitrate [Reaction (1)] or the alkoxy radical [Reaction (2)], is the only significant sink for the alkyl peroxy radicals formed from the reaction of OH radicals with the n -alkanes, since the reactions of alkyl peroxy radicals with NO_2 forming alkylperoxy nitrates



are insignificant due to the rapid back-decomposition of the alkylperoxy nitrates (References 11, 39 and 54).

In this system the formation of alkyl nitrates can occur either from the reaction of alkyl peroxy radicals with NO [Reaction (1)] or from the reaction of alkoxy radicals with NO₂ [Reaction (12)]. However, alkoxy radicals can also react with O₂ (References 15 and 55-62), decompose (References 15, 56-58 and 63), or isomerize (References 15, 24, 56 and 64-66) to ultimately give rise to products other than alkyl nitrates [shown overall as Reaction (13) above].

Upper limits for the contribution of Reaction (12) to the observed alkyl nitrate yields for these experiments can be estimated from the rate constants for the reactions of alkoxy radicals with NO₂ and O₂, and the NO₂ and O₂ concentrations. Alkoxy radicals react with NO₂ with a rate constant at atmospheric pressure of $k_{12} = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$, approximately independent of temperature (Reference 15). The rate constants for the reactions of alkoxy radicals with O₂ have received little direct attention, but Gutman, et al. (Reference 62) have recently determined absolute rate constants for the reaction of methoxy radicals with O₂ over the temperature range 413-608°K, and of ethoxy radicals with O₂ at 296 and 353°K. Furthermore, from thermochemical considerations, Gutman, et al. (Reference 62), estimated rate constants for other selected alkoxy radicals with O₂. For secondary alkoxy radicals the estimated rate constants are $\sim 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$, independent of temperature over the small range studied here. Assuming that all of the initially present NO and CH₃ONO form NO₂, the maximum yield of secondary alkyl nitrate formation from the reactions of RO radicals with NO₂ can be calculated to be 0.4% at 740 torr of air and 1.7% at 160 torr total pressure of air (the latter being the conditions most favoring nitrate formation from the reaction of RO radicals with NO₂). Since all of the initial nitrogenous species are not converted to NO₂ during NO_x/organic/air irradiations (Reference 11) and because the larger (>C₄) alkoxy radicals undergo significant decomposition and isomerization reactions (References 15, 24, 56-58 and 63-66), it may be concluded that less than 1% of the observed alkyl nitrate yields are due to the reaction of alkoxy radicals with NO₂ in the CH₃ONO/NO/n-alkane/air (or O₂) irradiations carried out in this study. This is negligible for these n-alkanes.

The conclusion that alkyl nitrate yields from the $RO + NO_2$ reactions are minor is supported by the excellent agreement in the pentyl nitrate yields observed from EC-696 (300 K, 153 torr total pressure of air) and EC-694 (300 K, 155 torr total pressure of O_2).

Clearly, the major source of alkyl nitrates observed in the present experiments is Reaction (1), and the observed alkyl nitrate yields should reflect the rate constant ratio $k_1/(k_1 + k_2) = \alpha$, since alkoxy radical formation [Reaction (2)] is the only significant process competing with Reaction (1) in the alkane photooxidation chain. However, to derive α from the observed alkyl nitrate product yields, a correction must be made for the secondary reactions of the alkyl nitrates. This was carried out as described below.

The sole loss process of the n-alkanes and the alkyl nitrates is via reaction with the OH radical, and hence

$$d[RH]/dt = -k_{11} [OH] [RH]$$

$$d[RONO_2]/dt = \alpha k_{11} [OH] [RH] - k_{14} [OH] [RONO_2]$$

where k_{11} and k_{14} are the rate constants for reactions (11) and (14), respectively, and α is the fraction of the reaction of $RO_2 + NO$ yielding alkyl nitrates. Under conditions where the OH radical concentration is constant, these equations can be integrated to yield

$$[RH]_t = [RH]_0 e^{-k_{11} [OH] t} \quad (VII)$$

and

$$[RONO_2]_t = [RH]_0 \frac{\alpha k_{11}}{(k_{11} - k_{14})} \left[e^{-k_{14} [OH] t} - e^{-k_{11} [OH] t} \right] \quad (VIII)$$

where $[RH]_0$ is the initial n-alkane concentration, $[OH]$ is the constant hydroxyl radical concentration, and $[RH]_t$ and $[RONO_2]_t$ are the alkane and alkyl nitrate concentrations, respectively, at time t . Equations (VII) and (VIII) may be combined to yield

$$\alpha = F \left\{ \frac{[\text{RONO}_2]_t}{\Delta [\text{RH}]_t} \right\} \quad (\text{IX})$$

where

$$F = \left(\frac{k_{11} - k_{14}}{k_{11}} \right) \left\{ \frac{1 - \left(\frac{[\text{RH}]_t}{[\text{RH}]_0} \right)}{\left(\frac{[\text{RH}]_t}{[\text{RH}]_0} \right)^{\frac{k_{14}}{k_{11}}} - \left(\frac{[\text{RH}]_t}{[\text{RH}]_0} \right)} \right\} \quad (\text{X})$$

and $\Delta [\text{RH}]_t = ([\text{RH}]_0 - [\text{RH}]_t)$.

Equations (IX) and (X) were used to correct each of the data points for each alkyl nitrate isomer given in Tables 7 and 8. F was calculated using the experimentally observed amounts of n -alkanes consumed and the values of k_{11} and k_{14} obtained from recent kinetic studies in these laboratories (References 67 and 68). The largest correction corresponded to a value of F of 1.39 for the 2-heptyl nitrate yield at 59% heptane reacted (Run EC-716, Table 8); in most cases these corrections were relatively minor.

Typical plots of the total corrected alkyl nitrate yields against the amount of n -alkane reacted are shown in Figure 7 for several n -pentane/ $\text{CH}_3\text{ONO}/\text{NO}/\text{air}$ (or O_2) irradiations at $300 \pm 2^\circ\text{K}$. It can be seen that, consistent with our assumption that the alkyl nitrates are a primary product in the n -alkane photooxidations, straight line plots with zero intercepts were obtained. Tables 9 and 10 list the least squares slopes obtained from such plots, which can be identified with the fraction, α , of the n -alkane reacted yielding the observed alkyl nitrates. In all cases the intercepts were within two least squares standard deviations of zero.

The yields of the 2- and 3-pentyl nitrates and of the 2-, 3-, and 4-heptyl nitrates determined here (0.125 ± 0.003 and 0.287 ± 0.016 , respectively) at $300 \pm 2^\circ\text{K}$ and 740 torr total pressure are in excellent agreement with the values 0.117 ± 0.013 and 0.293 ± 0.042 determined in our previous study (Reference 26) at $299 \pm 2^\circ\text{K}$ and 735 torr total pressure. Since these two studies were carried out in reaction chambers of greatly differing volume, 75 l (Reference 26) versus the present 5800 l, this excellent agreement indicates that the formation of the alkyl nitrates does not involve surface or heterogeneous effects. Furthermore, this agreement between the two sets of

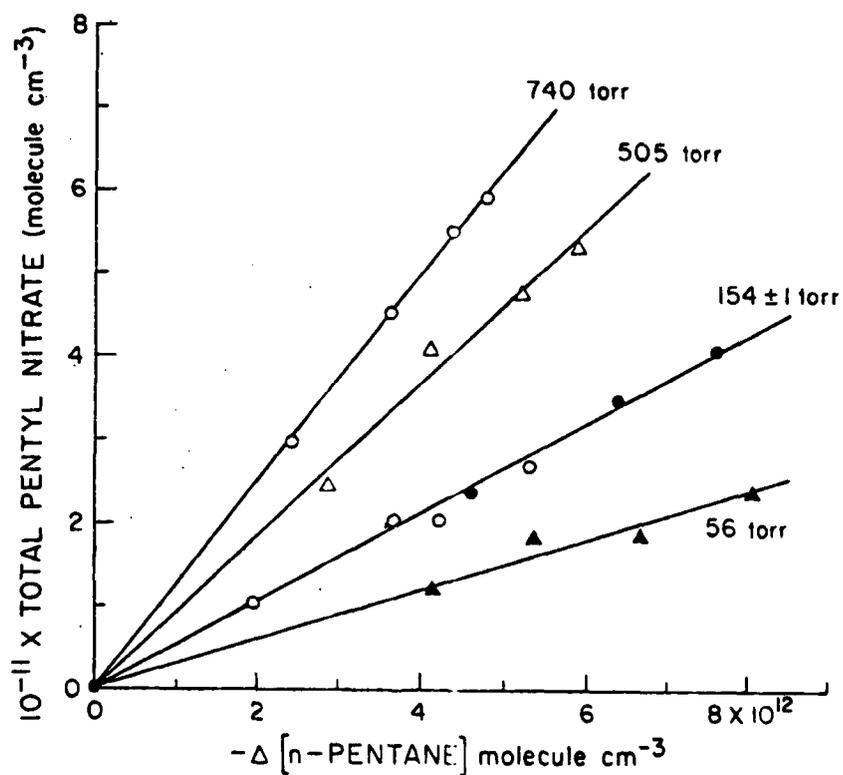


Figure 7. Plots of the Combined 2- and 3-Pentyl Nitrate Yields (Corrected for Secondary Reactions, See Text) Against the Amount of n-Pentane Consumed in $\text{CH}_3\text{ONO}/\text{NO}/\text{n-Pentane}/\text{Air}(\text{or } \text{O}_2)$ Irradiations at $300 \pm 2^\circ\text{K}$ at 56, 154 ± 1 , 505 and 740 Torr Total Pressure (○, △ - Air Diluent; ●, ▲ - O_2 Diluent).

TABLE 9. PENTYL NITRATE YIELDS FROM THE IRRADIATION OF
 $\text{CH}_3\text{ONO}/n\text{-PENTANE}/\text{NO}/\text{AIR}$ (OR O_2) MIXTURES.

Temperature (°K)	Total Pressure (torr)	Diluent Gas	Pentyl Nitrate Yield ^a
284±1	155	air	0.064±0.010
	356	air	0.101±0.014
	740	air	0.150±0.016
300±2	56	O_2	0.029±0.005
	57	O_2	0.032±0.008
	153	air	0.050±0.006
	155	O_2	0.054±0.003
	352	air	0.089±0.013
	505	air	0.092±0.010
	740	air	0.125±0.003
327±3	151	air	0.037±0.004
	400	air	0.058±0.008
	740	air	0.074±0.005
337±3	740	air	0.071±0.004

^a2- + 3-pentyl nitrates. Corrected for secondary reactions of the alkyl nitrates (see text). Error limits are two standard deviations of the least squares slopes of plots such as those shown in Figure 7.

data shows that systematic errors are likely to be small, since completely independent n-alkane and alkyl nitrate gas chromatographic calibrations were carried out for each study.

As shown in Tables 9 and 10 and Figures 8 and 9, the alkyl nitrate yields are both pressure and temperature dependent, with the yields increasing with increasing pressure and with decreasing temperature. While this is an expected result from the reaction pathways involved (see

TABLE 10. HEPTYL NITRATE YIELDS FROM THE IRRADIATION OF
 $\text{CH}_3\text{ONO}/n\text{-HEPTANE}/\text{NO}/\text{AIR}$ (OR O_2) MIXTURES.

Temperature ($^{\circ}\text{K}$)	Total Pressure (torr)	Diluent Gas	Heptyl Nitrate Yield ^a
284±2	58	O_2	0.121±0.018
	159	air	0.170±0.016
	349	air	0.257±0.038
	740	air	0.308±0.036
300±2	56	O_2	0.105±0.008
	160	air	0.152±0.018
	353	air	0.220±0.014
	740	air	0.287±0.016
322±4	59	O_2	0.071±0.006
	60	O_2	0.081±0.012
	156	air	0.105±0.014
	356	air	0.159±0.024
	740	air	0.199±0.024
341±4	160	air	0.085±0.008
	740	air	0.153±0.010

^a2- + 3- + 4-heptyl nitrates. Corrected for secondary reactions of the alkyl nitrates (see text). Error limits are two standard deviations of the least squares slopes of plots such as those shown in Figure 7.

introduction above), the temperature dependence of the alkyl nitrate yields are more extreme than may be expected, a priori, based on a simple chemical activation mechanism, and indicate that reactions of thermalized peroxy-nitrates (ROONO) may be significant.

The present data allow an assessment to be made of the effect of alkyl nitrate yields, and of the photochemical reactivities of the n-alkanes, as a function of altitude. Since the alkyl nitrate yields decrease with

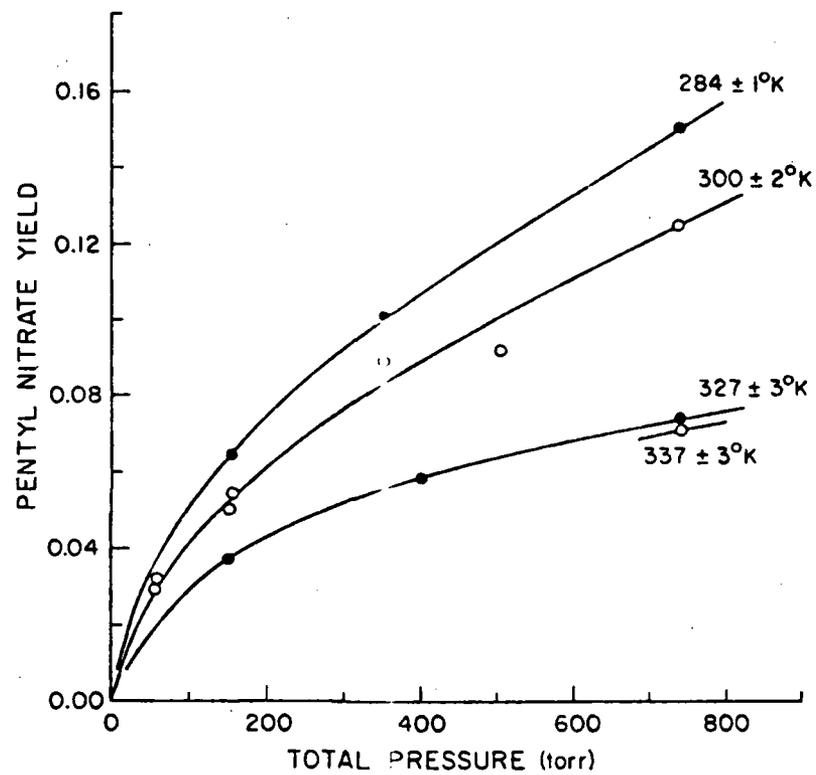


Figure 8. Plots of the n-Pentyl Nitrate Yields as a Function of Temperature and Pressure.

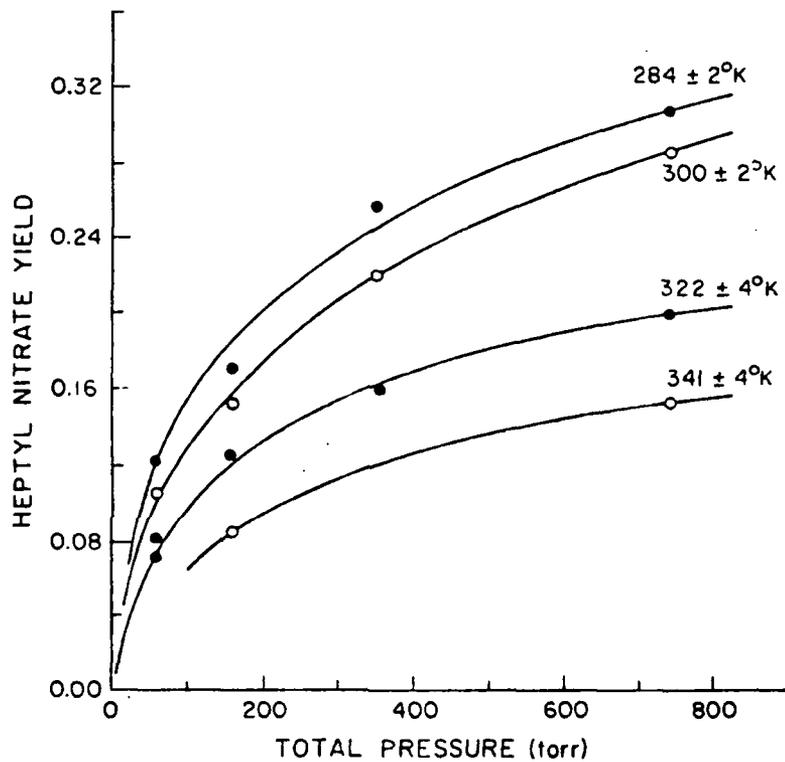


Figure 9. Plots of the n-Heptyl Nitrate Yields as a Function of Temperature and Pressure.

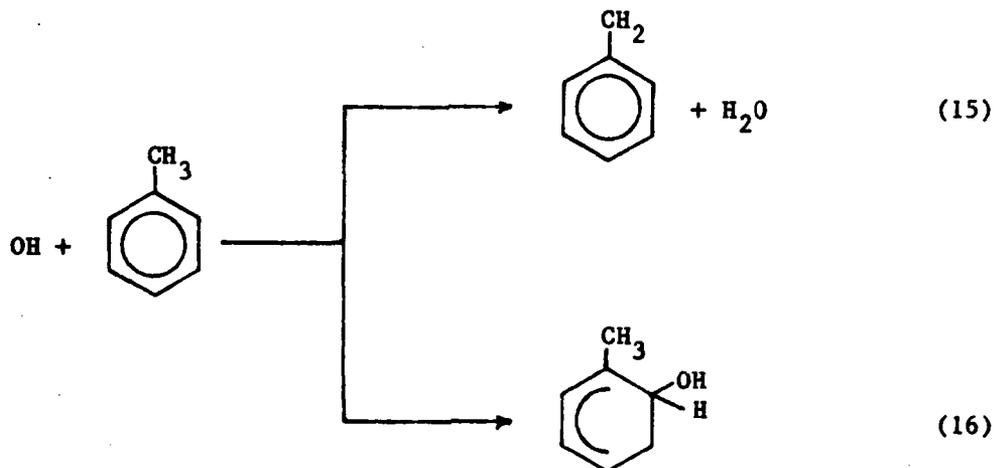
decreasing pressure, but increase with decreasing temperature, it is evident from Tables 7 and 8 that these yields will remain approximately constant with increasing altitude at least up to ~20,000 ft. Hence the influence of altitude on this reaction pathway will not have any significant effect on the photochemical reactivity of these n-alkane constituents of military jet fuels.

SECTION IV

EFFECTS OF PRESSURE ON PRODUCT YIELDS OF NO_x PHOTOOXIDATIONS OF SELECTED AROMATIC HYDROCARBONS

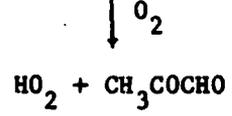
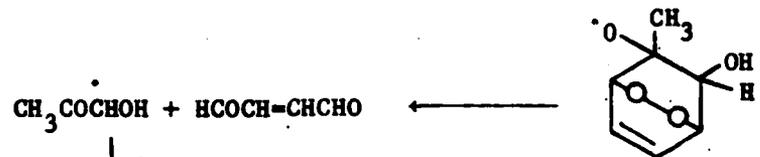
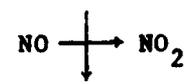
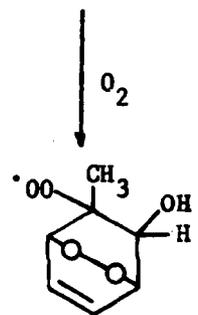
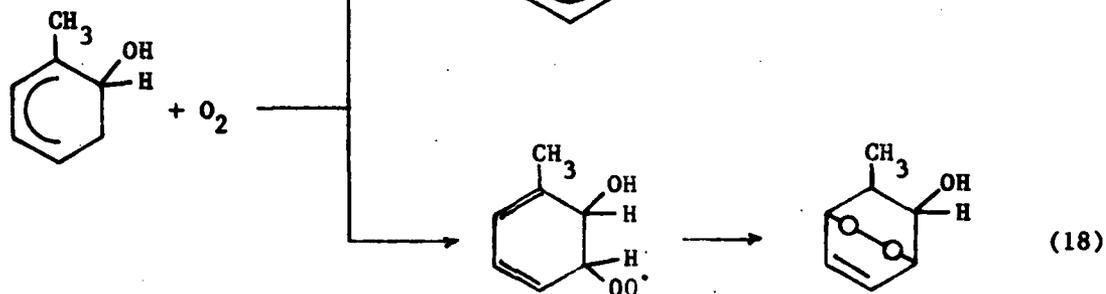
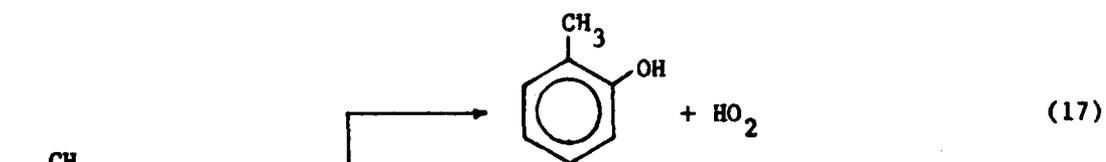
4.1 INTRODUCTION

Despite numerous studies of gas phase chemistry of the aromatic hydrocarbons (References 14, 27-34 and 69-74), the reaction pathways and product yields occurring after initial hydroxyl radical attack on aromatic hydrocarbons are still very poorly understood (References 14, 15, 34 and 51). The major atmospheric fate of aromatics, reaction with the OH radical, proceeds via two routes (References 15 and 51): H atom abstraction, mainly from the substituent methyl groups [Reaction (15)], and OH radical addition to the aromatic ring [Reaction (16)], which becomes reversible at elevated temperatures (References 51, 75 and 76). For example, for toluene the reactions are:



By analogy with the reactions of alkyl radicals (Reference 15), it is anticipated that under atmospheric conditions the benzyl-type radicals formed in reaction (15) will yield predominantly the aromatic aldehydes (References 14, 15, 27, 34, 51 and 74), while product and modeling studies (References 14, 15, 27, 30, 31, 34 and 74) have postulated that the hydroxycyclohexadienyl radicals formed in Reaction (16) will react with O₂ to yield phenolic compounds or add O₂ (Reference 14) to ultimately lead, at least in part, to ring cleavage. Again, taking the toluene system as an

example, the following reactions are expected:



Three temperature dependent kinetic studies (References 75-77) have derived rate constant ratios $k_{15}/(k_{15}+k_{16})$ at 298°K for a series of aromatic hydrocarbons, with values of $0.16^{+0.07}_{-0.05}$ (Reference 75) and $0.04^{+0.06}_{-0.02}$ (Reference 76) for toluene, while Kenley, et al. (Reference 74) have determined this rate constant ratio for several aromatic hydrocarbons from a

product analysis study carried out at low (6-12 torr) total pressure. From that (Reference 74) and other product studies (References 27, 28 and 71), reported benzaldehyde yields from toluene have ranged from 2.5% (Reference 28) to ~50% (Reference 71). Clearly, there are significant discrepancies in the previous data for toluene concerning the importance of the H-atom abstraction pathway [Reaction (15)], and also concerning the yield of benzaldehyde under atmospheric conditions.

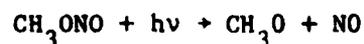
Furthermore, the relative importance of Reaction (18) has not been determined with certainty. Kenley, et al. (Reference 74) observed ~85% yields of the cresol isomers (mainly o-cresol) at 6-12 torr total pressure, and concluded that under their low pressure conditions the addition of O₂ to the OH-aromatic example results in the exclusive formation of phenolic products with Reaction (18) being negligible under these conditions. However, product studies at atmospheric pressure (References 14 and 28) have shown much lower yields of o-cresol [5% (Reference 28) to ~21% (Reference 14)] indicating alternate reaction pathways.

The observation of significant yields of α-dicarbonyls from o-xylene (References 30, 31 and 78) and other aromatic hydrocarbons (Reference 78), and of unsaturated 1,4-dicarbonyls from toluene (Reference 32) and 1,2,4-trimethylbenzene (Reference 33) also shows that ring cleavage, possibly via reaction (18) (References 14, 15 and 30) or its analogues, does indeed occur under atmospheric conditions. Thus, either there are discrepancies between the results of Kenley, et al. (Reference 74) and the other previous studies (References 27, 28 and 71), or there are significant pressure dependencies on the aromatic product yields.

In order to determine whether pressure effects could account for these divergent data, we have determined the yields of benzaldehyde and o-cresol from toluene, and of biacetyl from o-xylene, over the pressure range ~60-740 torr total pressure.

4.2 EXPERIMENTAL

Hydroxyl radicals were generated by the photolysis of methyl nitrite at $\lambda \geq 290$ nm in the presence of O₂:





In order to minimize O_3 and hence NO_3 formation, NO was also added to the reaction mixtures, which had initial concentrations of: toluene or o-xylene, $\sim(2-3) \times 10^{13}$ molecule cm^{-3} ; CH_3ONO , $\sim(2-5) \times 10^{12}$ molecule cm^{-3} ; and NO , $\sim(2-3) \times 10^{13}$ molecule cm^{-3} . Air or O_2 were used as diluent gases. Irradiations of mixtures of toluene (or o-xylene), CH_3ONO , and NO in air (or O_2) were carried out in the SAPRC 5800 l Teflon[®]-coated evacuable, thermostatted, environmental chamber with a 25 KW solar simulator (Reference 45). Prior to each irradiation the chamber was evacuated to $\leq 2 \times 10^{-5}$ torr. Methyl nitrite, prepared as described previously (Reference 53), and NO were introduced into the chamber from a vacuum gas handling system. The chamber was then filled to the desired pressure with dry purified matrix air (References 45 and 50) or ultra-high purity O_2 . The known quantities of toluene or o-xylene were flushed into the chamber from a ~ 1 l Pyrex[®] bulb by a stream of ultra-high purity N_2 . The chamber was maintained at the desired temperature by its heating/cooling system.

Toluene and o-xylene were quantitatively analyzed by gas chromatography with flame ionization detection (GC-FID) using a 10 ft x 0.125 in stainless steel (SS) column of 10% Carbowax[®] 600 on C-22 Firebrick[®] (100/120 mesh), operated at 348[°]K, with 100 μl of the sample being preconcentrated in a ~ 1 μl (SS) loop at liquid argon temperature prior to injection onto the column. Biscetyl was monitored by gas chromatography with electron capture detection using an 18 in x 0.125 in Teflon[®] column of 5% Carbowax[®] 400 on Chromasorb G[®] (80/110 mesh) operated at 300[°]K, without sample preconcentration. For these species, 100 μl gas samples were withdrawn into all-glass, gas-tight syringes from the chamber directly (for atmospheric pressure runs), or for runs at reduced pressure, from ~ 5 l Pyrex[®] bulbs which had been evacuated to $\leq 10^{-3}$ torr and which were then opened to the chamber and then filled to atmospheric pressure by ultra-high purity N_2 .

Benzaldehyde and o-cresol were monitored by GC-FID using a 6 ft x 0.25 in glass column packed with 80/100 Carbopack[®] C/0.1% SP-1000, temperature programmed from 423-523[°]K at 20[°]K min^{-1} . Gas samples from the

chamber of ~0.1 to 1 l volume were drawn through 0.25 in x 3.25 in glass traps packed with Tenax[®] GC 50/80 mesh. This sample was then transferred by the carrier gas at 523^oK from this trap to the column head which was at 423^oK, followed by the temperature programming of the column as noted above.

For the o-xylene/CH₃ONO/NO/air system, irradiations were of 80 min duration with analyses being carried out every 20 min. For the toluene-CH₃ONO/NO/air system however, because of the time involved in sampling via the Tenax[®] packed traps (~10-15 min), four 10 or 15 min irradiations of the same mixture were carried out during each experiment, with GC analyses being conducted at the end of each irradiation period.

4.3 RESULTS

Irradiations of toluene/CH₃ONO/NO/air (or O₂) and o-xylene/CH₃ONO/NO/air (or O₂) mixtures were carried out at ~303^oK over the pressure range ~60-740 torr total pressure, and a toluene/CH₃ONO/NO/air irradiation was also carried out at 323±2^oK and 740 torr total pressure. The initial reactant concentrations and the observed amounts of aromatic hydrocarbon consumed and product species formed, as measured at various times during the irradiations, are given in Tables 11 and 12 for the toluene and o-xylene systems, respectively.

In addition, irradiations of biacetyl/NO/air and biacetyl/CH₃ONO/NO/air mixtures were carried out at 303^oK and 740 torr total pressure to determine the photolytic lifetime of biacetyl under the experimental conditions employed in the aromatic hydrocarbon/CH₃ONO/NO/air irradiations. During these irradiations the biacetyl decays were strictly exponential, with first order decay rates of $(1.30 \pm 0.07) \times 10^{-4} \text{ sec}^{-1}$ for the biacetyl/CH₃ONO/NO/air experiment and $(1.26 \pm 0.04) \times 10^{-4} \text{ sec}^{-1}$ for the biacetyl/NO/air experiment (where the error limits are two least squares standard deviations of the slopes of the plots of ln[biacetyl] against irradiation time). Since the presence of CH₃ONO in one of the reactant mixtures is expected to significantly increase the OH radical concentrations, the excellent agreement of the biacetyl decays for these two irradiations shows that reaction with OH radicals is a minor loss process for biacetyl in the CH₃ONO/NO/air system. Thus the only significant loss process of biacetyl in these systems is via photolysis. This is consistent with the fact that

TABLE II. EXPERIMENTAL DATA FOR THE TOLUENE/CH₃ONO/NO/AIR(OR O₂) IRRADIATIONS.

EC Run No.	Temperature (°K)	Total Pressure (torr)	10 ⁻¹³ x Initial Conc (molecula cm ⁻³)		10 ⁻¹² x Δ(Toluene) (molecule cm ⁻³)	10 ⁻¹¹ x [Benzaldehyde] (molecule cm ⁻³)		10 ⁻¹¹ x [o-Cregol] (molecule cm ⁻³)	
			CH ₃ ONO	NO		Obs	Corr ^a	Obs	Corr ^a
728	306±2	740	0.49	2.40	2.39	2.29	2.62	2.38	3.74
						2.55	3.05	2.83	5.07
						2.91	3.62	3.29	6.65
729	302±2	360	0.49	2.37	2.26	1.33	1.62	1.73	2.16
						2.22	2.50	2.84	4.24
						2.70	3.16	3.56	5.99
						3.06	3.76	3.97	7.67
730	303±2	168	0.24	2.36	2.33	0.83	0.89	0.78	0.99
						1.19	1.34	0.81	1.20
						1.82	2.10	1.82	2.91
						2.03	2.36	1.82	2.98
731 ^b	302±1	62	0.24	2.35	2.42	1.08	1.18	1.12	1.52
						1.88	2.20	1.98	3.34
						2.34	2.83	2.57	4.76
						2.71	3.53	2.94	6.73
732	302±2	740	0.50	2.43	2.53	1.21	1.31	1.05	1.33
						1.88	2.12	1.76	2.64
						2.33	2.81	2.33	4.19
						2.64	3.24	2.48	4.76
733	302±1	161	0.24	2.37	2.41	0.98	1.01	0.79	0.89
						1.38	1.52	1.38	1.92
						2.17	2.46	2.33	3.54
						2.17	2.53	2.29	3.75
734	323±2	740	0.47	2.24	2.55	1.81	1.95	1.93	2.52
						2.83	3.26	3.12	4.98
						3.43	4.14	3.60	6.60
						3.95	4.95	4.14	8.53

^aCorrected for reaction with OH radicals (see text).

^bDiluent gas was O₂ in this irradiation.

TABLE 12. EXPERIMENTAL DATA FOR o-XYLENE/CH₃ONO/NO/AIR (OR O₂)
IRRADIATIONS AT 301±2°K.

EC Run No.	Total Pressure (torr)	10 ⁻¹³ x Initial Conc (molecule cm ⁻³)			10 ⁻¹² x -Δ[o-Xylene] (molecule cm ⁻³)	10 ⁻¹¹ x [Biacetyl] (molecule cm ⁻³)	
		CH ₃ ONO	NO	o-Xylene		Obs	Corr ^a
721	740	0.48	2.35	2.53	4.36	5.96	6.55
					7.17	7.41	9.05
					8.67	9.15	12.10
					9.79	9.36	13.77
722	347	0.24	2.37	2.34	2.95	4.29	4.62
					6.12	6.88	8.08
					7.69	7.96	10.29
					8.89	8.89	12.51
723	160	0.25	2.35	2.40	3.48	4.05	4.38
					6.29	6.19	7.31
					8.17	7.10	9.24
					10.41	7.88	11.17
724 ^b	67	0.25	2.34	2.43	5.55	5.53	6.03
					9.15	8.08	9.62
					12.03	9.36	12.24
					14.41	10.43	14.84

^aCorrected for photolysis (see text).

^bDiluent gas was O₂ for this irradiation.

the reaction of OH radicals with biacetyl is very slow [with a rate constant of $(2.4^{+0.8}_{-0.6}) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ at 298°K (References 30 and 51)], corresponding to a biacetyl lifetime due to reaction with OH radicals of ~100 hr at the OH radical concentrations ($\sim 1 \times 10^7 \text{ cm}^{-3}$) encountered in the o-xylene/CH₃ONO/NO/air irradiations.

Since biacetyl photolyzes rapidly (Reference 30) and benzaldehyde and o-cresol react with OH radicals more rapidly than toluene does (References 15 and 51), corrections must be made for these secondary reactions to derive the fraction of the OH radical reaction with the aromatics yielding biacetyl, benzaldehyde, and o-cresol. These corrections were made as described below.

Under the experimental conditions employed in the present study, the predominant loss process for benzaldehyde is via reaction with the OH radical, with photolysis (Reference 79) contributing $\leq 5\%$ of the OH radical reaction in consuming benzaldehyde. Similarly, the major loss process for o-cresol is also via reaction with the OH radical, reaction with O_3 (Reference 80) and the NO_3 radical (Reference 81) being of very minor importance under the experimental conditions employed. Since these two products from the NO_x photooxidation of toluene, benzaldehyde and o-cresol, are formed and lost via OH radical reactions, then

$$-d[\text{toluene}]/dt = (k_{15} + k_{16})[\text{OH}][\text{toluene}] \quad (\text{XI})$$

and

$$d[\text{product}]/dt = \alpha(k_{15} + k_{16})[\text{OH}][\text{toluene}] - k_{19}[\text{OH}][\text{product}] \quad (\text{XII})$$

where α is the fraction of the OH radical reaction with toluene yielding the product under consideration (either benzaldehyde or o-cresol), $(k_{15} + k_{16})$ is the overall rate constant for the reaction of OH radicals with toluene, and k_{19} is the rate constant for the reaction of OH radicals with benzaldehyde or o-cresol.



Under conditions where the OH radical concentration is constant, equations (XI) and (XII) can be integrated to obtain:

$$[\text{toluene}]_t = [\text{toluene}]_0 e^{-(k_{15} + k_{16})[\text{OH}]t} \quad (\text{XIII})$$

and

$$[\text{product}]_t = [\text{toluene}]_0 \left[\frac{\alpha(k_{15} + k_{16})}{[(k_{15} + k_{16}) - k_{19}]} \right] \left[e^{-k_{19}[\text{OH}]t} - e^{-(k_{15} + k_{16})[\text{OH}]t} \right] \quad (\text{XIV})$$

where $[\text{toluene}]_0$ is the initial toluene concentration, $[\text{OH}]$ is the constant hydroxyl radical concentration, and $[\text{toluene}]_t$ and $[\text{product}]_t$ are the toluene and product concentrations, respectively, at time t . Equations (XIII) and (XIV) can be combined to obtain

$$\alpha = F \left\{ \frac{[\text{product}]_t}{\Delta[\text{toluene}]_t} \right\} \quad (\text{XV})$$

where $[\text{product}]_t$ is the observed product yield at time t , $\Delta[\text{toluene}]_t$ is the amount of toluene consumed at time t , and F is the correction factor for reaction of the product with OH radicals:

$$F = \left(\frac{(k_{15} + k_{16}) - k_{19}}{(k_{15} + k_{16})} \right) \left\{ \frac{1 - \left(\frac{[\text{toluene}]_t}{[\text{toluene}]_{t_0}} \right)}{\left(\frac{[\text{toluene}]_t}{[\text{toluene}]_{t_0}} \right) \frac{k_{19}}{k_{15} + k_{16}} - \left(\frac{[\text{toluene}]_t}{[\text{toluene}]_{t_0}} \right)} \right\} \quad (\text{XVI})$$

Equation (XVI), which has been shown to be applicable even when the OH radical concentrations vary with time (Reference 26), was used to correct each of the data points for benzaldehyde and o-cresol in Table 11. F was calculated using the experimentally observed amounts of toluene consumed and the rate constant ratios $k_{19}/(k_{15} + k_{16}) = 7.0$ for o-cresol and 2.0 for benzaldehyde, both independent of temperature over the small temperature range employed in this study (302–323°K) (References 15 and 51). These correction factors were relatively minor for benzaldehyde ($F < 1.30$) but were much larger for o-cresol, with F being as high as 2.29 for the highest toluene conversion employed. For o-cresol, an uncertainty in the $k_{19}/(k_{15} + k_{16})$ ratio of ± 1 (i.e., 7 ± 1) led to a $\pm 10\%$ effect on the magnitude of F at the highest toluene conversions. Plots of the corrected benzaldehyde or o-cresol yield against the amount of toluene consumed yielded good straight lines, and Table 13 lists the least squares slopes obtained from these plots at the various temperatures and pressures employed. In all cases the

TABLE 13. BENZALDEHYDE AND o-CRESOL YIELDS FROM THE NO_x PHOTOOXIDATION OF TOLUENE.

Temperature (°K)	Total Pressure (torr)	Diluent Gas	Yield ^a	
			Benzaldehyde	o-Cresol
306±2	740	air	0.077±0.009	0.136±0.020
302±2	740	air	0.068±0.005	0.104±0.013
303±2	360	air	0.090±0.007	0.184±0.016
302±1	168	air	0.068±0.020	0.087±0.047
302±2	161	air	0.073±0.020	0.112±0.029
302±1	62	O ₂	0.065±0.007	0.121±0.027
323±2	740	air	0.095±0.003	0.162±0.018

^aCorrected for secondary reactions with OH radicals (see text). Indicated errors are two standard deviations of the slopes of plots of the corrected yields against the amount of toluene consumed.

least squares intercepts of such plots were within two standard deviations of zero.

For the case of biacetyl formation from o-xylene, equation (XVI) does not apply since, as noted above, the major biacetyl loss process is photolysis rather than reaction with the OH radical. In this case

$$\frac{d[\text{biacetyl}]}{dt} = \alpha(k_{15} + k_{16})[\text{OH}][\text{o-xylene}] - k_{20}[\text{biacetyl}] \quad (\text{XVII})$$

where α is the fraction of the OH radical reaction with o-xylene forming biacetyl, and k_{20} is the experimentally determined photolysis rate constant for biacetyl ($1.28 \times 10^{-4} \text{ sec}^{-1}$).



Integration of both sides of equation (XVII) leads to the expression

$$[\text{biacetyl}]_t + k_{20} \int_{t_0}^t [\text{biacetyl}] dt = \alpha \Delta[\text{o-xylene}]_t \quad (\text{XVIII})$$

where $[\text{biacetyl}]_t$ and $\Delta[\text{o-xylene}]_t$ are the observed biacetyl yields and the amount of o-xylene consumed, respectively, at time t. The quantity $\int_{t_0}^t [\text{biacetyl}] dt$ was obtained from the biacetyl-time concentration profiles. Each of the data points in Table 12 was corrected in this way for the biacetyl photolysis. Table 14 lists the fractions, α , of the reaction of OH radicals with o-xylene yielding biacetyl, these being the least squares analysis of plots of the corrected biacetyl yields against the amounts of o-xylene consumed. Again, in all cases the least squares intercepts of such plots were within two standard deviations of zero.

4.4 DISCUSSION

4.4.1 Benzaldehyde and o-Cresol from Toluene

The benzaldehyde and o-cresol yields determined in this work are plotted as a function of total pressure in Figure 10. Within the experimental uncertainties they are seen to be independent of pressure, with weighted least squares mean values of 0.073 ± 0.019 for benzaldehyde and 0.131 ± 0.066 for o-cresol (where the error limits are two weighted least squares standard deviations). Inclusion of the uncertainties in the gas chromatographic calibration factors leads to benzaldehyde and o-cresol yields of 0.073 ± 0.022 and 0.131 ± 0.072 , respectively, where the indicated errors are again two standard deviations.

Our results are compared with literature data in Table 15. For benzaldehyde the present datum is in between the reported values of O'Brien, et al. (Reference 28) and Kenley, et al. (Reference 74), with the benzaldehyde yield reported by Spicer and Jones (Reference 71) obviously being much too high. For o-cresol the present yield is in reasonable agreement with that derived from the environmental chamber-computer modeling study of Atkinson, et al. (Reference 14). However, the data of Kenley, et al. (Reference 74), which indicate that at low pressures and at high O_2/NO_x ratios the reaction of OH radicals with toluene yields ~15% benzaldehyde and ~68% o-cresol (together with ~17% of the other two cresol isomers), are in apparent conflict with our determination that the o-cresol yield is ~13%, independent of pressure over the range 62-740 torr. This discrepancy is possibly caused by the problems of sampling under the conditions employed by Kenley, et al. (Reference 74), since they report only a ~10%

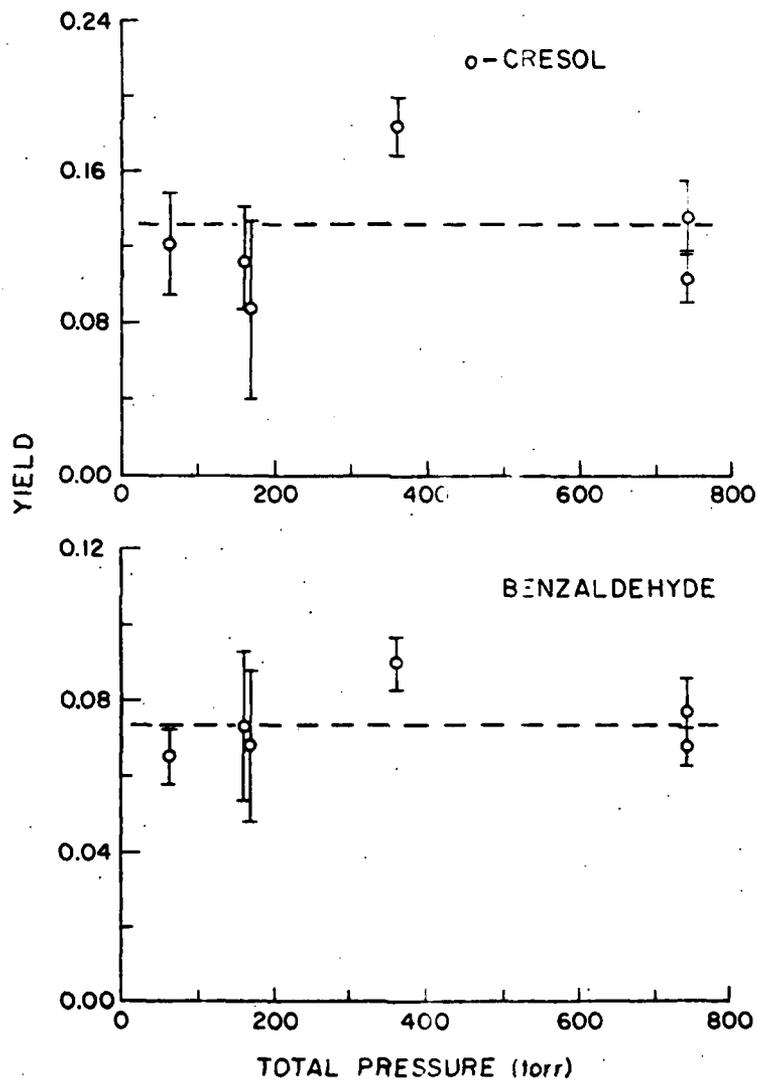


Figure 10. Plot of the Benzaldehyde and o-Cresol Yields from Irradiated Toluene/ $\text{CH}_3\text{ONO}/\text{NO}/\text{Air}$ (or O_2) Mixtures as a Function of Total Pressure at -303°K . The Error Bars are the Two Least Squares Standard Deviations Given in Table 13.

TABLE 14. THE FRACTION OF THE OH RADICAL REACTION WITH o-XYLENE YIELDING BIACETYL AS A FUNCTION OF PRESSURE AT 301±2°K.

Total Pressure (torr)	Diluent Gas	Biacetyl Yield ^a
740	a r	0.137±0.016
347	a r	0.135±0.012
160	a r	0.108±0.009
67	O ₂	0.102±0.004

^aCorrected for photolysis of biacetyl (see text). Error limits are two least squares standard deviations of the slopes of plots of the corrected biacetyl concentrations against the amount of o-xylene consumed.

TABLE 15. COMPARISON OF THE PRESENT BENZALDEHYDE AND o-CRESOL YIELDS AT ~303°K FROM THE NO_x PHOTOOXIDATION OF TOLUENE WITH PREVIOUS LITERATURE VALUES.

	Yield (%)		Reference
	Benzaldehyde	o-Cresol	
~25-35			27
15±2 ^a		68 ^{a,b}	74
~5			71
12 ^c		~21	14
2.5		5	28
7.3±2.2 ^d		13.1±7.2 ^d	This work

^aAt 6-12 torr total pressure.

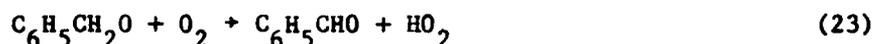
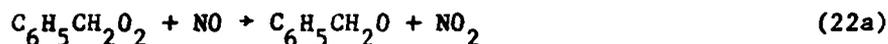
^bAt high O₂/NO₂ ratios (>2 x 10⁵).

^cValue obtained by using k₁₅/(k₁₅ + k₁₆) ratio of 0.156 from the literature (References 74 and 75) and assuming 25% benzyl nitrate formation from the C₆H₅CH₂O₂ + NO reaction.

^dIndependent of pressure over the range 62-740 torr.

sampling efficiency. However, further work at <50 torr total pressure is obviously necessary to definitely resolve this discrepancy.

While the reported benzaldehyde (and o-cresol) yields of Hoshino, et al. (Reference 27) and O'Brien, et al. (Reference 28) are in disagreement with the present data, the ratios of the o-cresol/benzaldehyde yields of 2.1 (Reference 27) and 2.0 (Reference 28) obtained in these studies are in good agreement with the ratio of 1.8 obtained in the present study. Under atmospheric conditions the benzyl radical is expected to react via the reaction sequence:



(reaction of benzoyl radicals with NO to form benzyl nitrite is of negligible importance due to the expected rapid photolysis of benzyl nitrite). At high O_2/NO_x ratios ($>2 \times 10^5$) benzyl nitrate formation via reaction (24) is negligible (Reference 74). Hence, under these conditions benzyl radicals will ultimately form benzaldehyde and benzyl nitrate via reaction (21), (22), and (23).

The fraction of reaction (22) forming benzyl nitrate is not known, but since the ratio $k_{22b}/(k_{22a} + k_{22b})$ is expected to decrease with decreasing pressure (Section III), the lack of a pressure dependence for the benzaldehyde yield indicates that benzyl nitrate formation is not a major process. This is in agreement with the data of Hoshino, et al. (Reference 27) which show that at atmospheric pressure the benzyl nitrate yields are ~12% of the benzaldehyde yields. Thus, the observed benzaldehyde yields should be close to, but somewhat lower (by ~10-15% due to benzyl nitrate formation) than the primary rate constant ratio $k_{15}/(k_{15} + k_{16})$ for the initial OH radical reaction with toluene (see Section 4.1). Indeed, the present benzaldehyde yield of 0.073 ± 0.022 is in between the $k_{15}/(k_{15} +$

k_{16}) ratios at 298°K of $0.16^{+0.07}_{-0.05}$ (Reference 75) and $0.04^{+0.06}_{-0.02}$ (Reference 76) reported from kinetic studies.

At 323±2°K, the benzaldehyde yield was observed to be somewhat higher than at ~303°K, although any increase is probably within the experimental errors. Such an increase in the benzaldehyde yield with increasing temperature is expected from the results of kinetic studies (References 51, 75 and 76), which indicate that the rate constant ratio $k_{15}/(k_{15} + k_{16})$ increases with temperature. The o-cresol yields do not, within the wide experimental uncertainties, appear to show any significant temperature dependence in the range 303-323°K.

4.4.2 Biacetyl from o-Xylene

The fraction of the OH radical reaction with o-xylene yielding biacetyl of 0.137 ± 0.016 determined in the present work is in good agreement with the value of 0.18 ± 0.04 obtained previously in these laboratories by Darnall, et al. (Reference 30), and is in agreement, within the large experimental error limits, with the value of 0.260 ± 0.102 reported by Takagi, et al. (Reference 31). Both of these previous studies employed the irradiation of o-xylene/NO/air mixtures. Thus, it is evident that at atmospheric pressure and ~300°K ~15% of the overall reaction of OH radicals with o-xylene yields biacetyl and previous work (Reference 30) has shown no effect of temperature on this biacetyl yield over the range 283-323°K.

However, the present data do suggest a small pressure effect, with the biacetyl yield decreasing by ~25% in going from 740 torr to 67 torr total pressure (Figure 11). If there is a pressure effect on the biacetyl yield, as these data suggest, then the specific reaction or reactions responsible for this pressure dependence are difficult to determine at this time, since several reactions in the sequence leading to ring cleavage could potentially be pressure dependent. For instance, the reaction of the OH-o-xylene adduct with O₂ to form the bicyclic intermediate (I) via Reaction (18) may be pressure dependent (but this is not the case for the formation of o-cresol from toluene), with Reaction (18) becoming more important at higher pressures. The possible formation of bicyclic nitrates via reaction path (a) is also likely to be pressure dependent, but would be contrary to the observed trend of increasing biacetyl yields with increasing pressure.

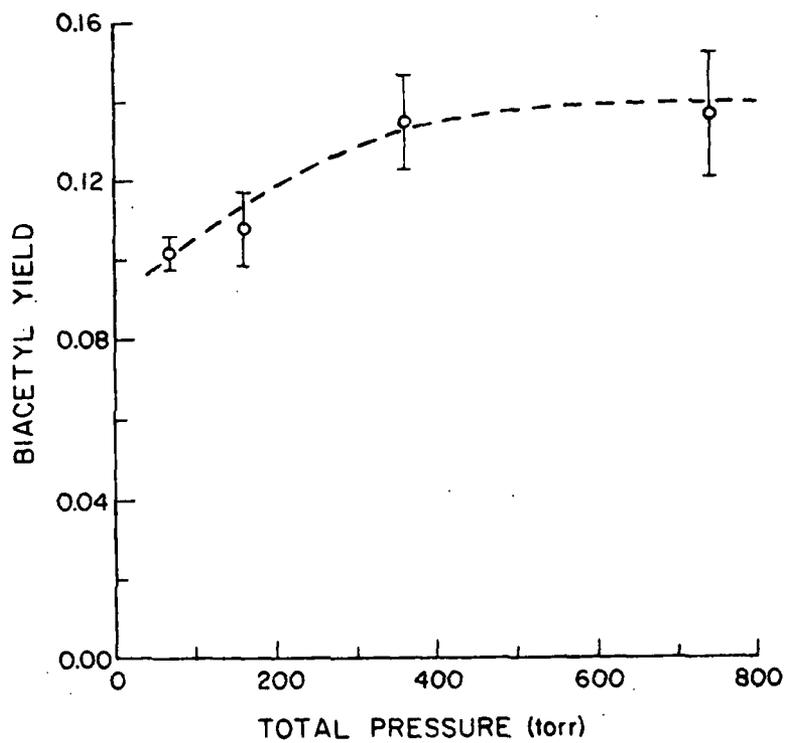
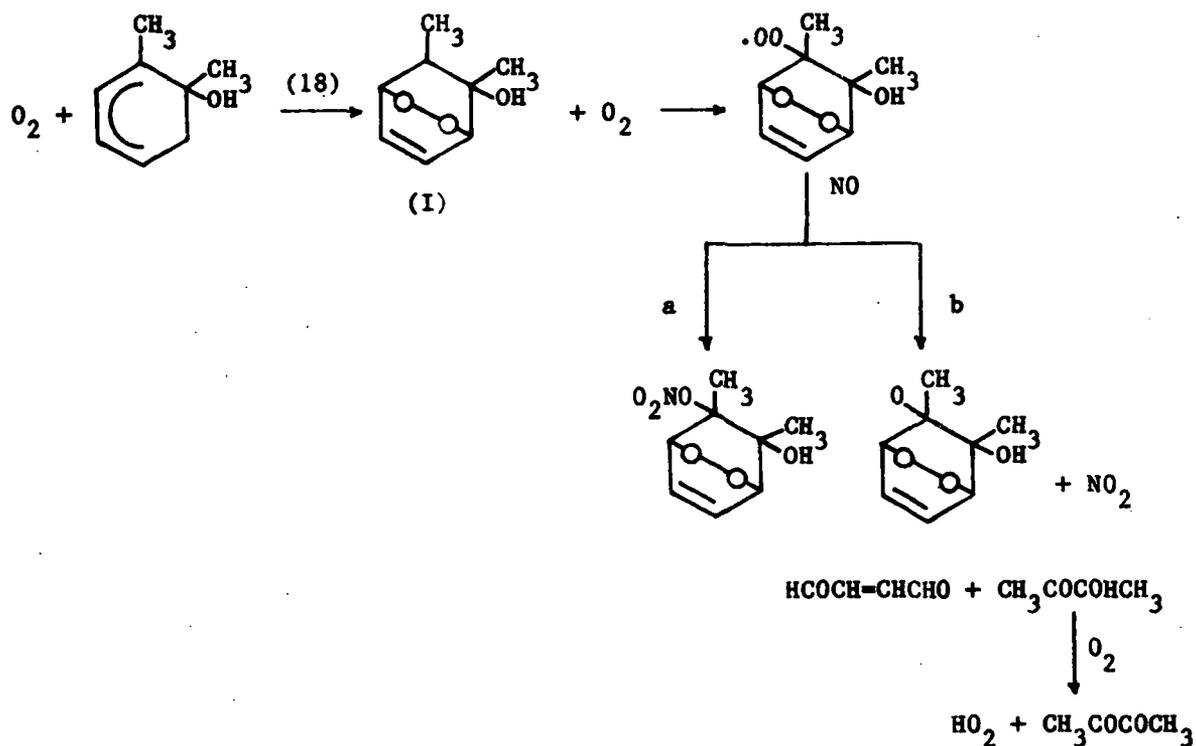


Figure 11. Plot of the Biacetyl Yields from Irradiated *o*-Xylene/ $\text{CH}_3\text{ONO}/\text{NO}/\text{Air}$ (or O_2) Mixtures as a Function of Total Pressure at $301 \pm 2^\circ\text{K}$. The Error Bars are the Two Least Squares Standard Deviations Given in Table 14.



Obviously much further work concerning the temperature and pressure dependencies of the individual elementary reactions is needed before any conclusions can be drawn as to the reactions responsible for any effects of pressure or temperature on observed final product yields.

4.4.3 Conclusions

The present data have determined the yields of benzaldehyde and o-cresol from toluene and of biacetyl from o-xylene as a function of pressure at $\sim 300^\circ K$. These data, which show no pressure dependence over the range 62-740 torr for benzaldehyde and o-cresol formation, and only a weak dependence for biacetyl formation over a similar pressure range, can now serve as much needed inputs to chemical kinetic computer modeling studies of the NO_x photooxidations of toluene and o-xylene.

SECTION V

RECOMMENDATIONS FOR FUTURE RESEARCH

From the data presented and discussed in Sections II, III, and IV above, it is evident that the most direct and time- and cost-effective approach to assessing the effects of altitude on the photochemical reactivity of military jet fuels is to investigate the atmospheric chemistry of individual fuel components, in a program analogous to the approach used in the investigations described in Sections III and IV above.

In particular, the following studies should be carried out:

- The yields of alkyl nitrates from the NO_x /air photooxidations of other n-alkanes as well as from representative branched and cyclic alkanes should be determined as functions of both temperature ($\sim 250\text{--}350^\circ\text{K}$) and pressure (≤ 50 torr to atmospheric pressure or greater).

- The products formed and reaction pathways occurring in the NO_x /air photooxidations of the important aromatic constituents of the military jet fuels should be studied again as a function of pressure and temperature.

From studies such as these, the detailed atmospheric chemistry of representative fuel components will be understood and can then be modeled using chemical kinetic computer models. Use of such models would provide cost- and time-effective predictive capabilities concerning the effect of altitude on the photochemical reactivity of present day or future fuels.

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APPENDIX A

AD-A125 035

HIGH ALTITUDE JET FUEL PHOTOCHEMISTRY(U) CALIFORNIA
UNIV RIVERSIDE STATEWIDE AIR POLLUTION RESEARCH CENTER
A M MINER ET AL. OCT 82 AFESC/ESL-TR-82-38

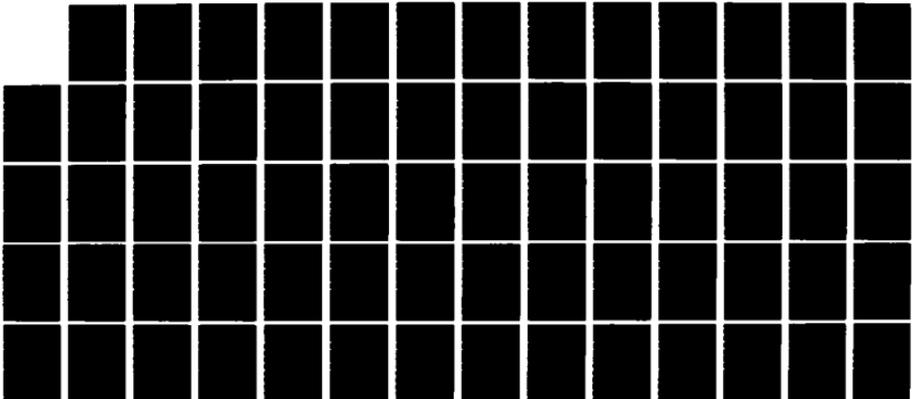
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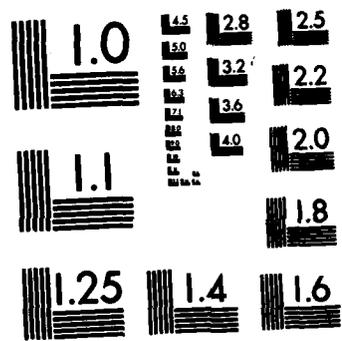


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DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

APPENDIX A

Detailed data sheets for the Fuel/NO_x/air irradiations carried out in this program.

The legend for the organics monitored is as follows:

PAN	Peroxyacetyl nitrate
HCHO	Formaldehyde
N-C5	n-Pentane
N-C6	n-Hexane
N-C7	n-Heptane
N-C8	n-Octane
N-C9	n-Nonane
BENZENE	Benzene
TOLUENE	Toluene
C2BENZ	Ethylbenzene
M-XYL	m-Xylene
I-C3-BZ	Isopropylbenzene
O-XYL	o-Xylene
N-C3-BZ	n-Propylbenzene
124TMEBZ	1,2,4-Trimethylbenzene
MECYC-C6	Methylcyclohexane
N-C10	n-Decane
N-C11	n-Undecane
C2-N	Ethyl nitrate
ME-N	Methyl nitrate
M+P-XYL	m- + p-Xylene
N-C12	n-Dodecane
N-C13	n-Tridecane
N-C14	n-Tetradecane

As discussed in the text, NO₂-UNC refers to the NO_x-NO data uncorrected for contributions due to PAN and other organic nitrates.

LC-489
JP-4 (PET); GROUND LEVEL
1981, FEB 9

0820: M02 INTO EC.
0831: M0 INTO EC.
0835: BEGIN 50Z R.M. PURE AIR FILL.
0943: START 315 MICROLITERS (50 PPMC) JP-4 FLUSH.

T=0 AT 1000 PSI

R1 = 0.330 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	DORIC-1	30.7	0.3	DEG C	MM, RELATIVE INTENSITY
					500 1.459
					430 1.143
					403 1.014
					380 0.825
					370 0.717
					360 0.588
					350 0.500
					340 0.368
					330 0.245
					320 0.109
					310 0.034
					300 0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
 1920 10'C-600 RM-1211 10' 10Z CARBOWAX-6001 FID
 2100 PN-1 RM 1211 POROPAK N 1 FID
 2200 DMS-1 RM-1211 DIMETHYLSULFOLANE1 FID
 2000 ECD-1 RM-1211 12' 5Z CARBOWAX-6001 ECD
 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY1 FID
 1530 T 14B-3 TECO 14B-3 NO-MOX NYLON FILTER ANALYZER
 1800 DORIC-1 DORIC TEMP INDICATOR, SN 41479
 1790 D-1790 BASIBI 1790 OZONE MONITOR
 8410 M03-8410 MONITOR LABS,CHEMLUM 03 ANALYZER MD 8410
 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS

EL-489
 JF-4 (PET) GROUND LEVEL
 1981, FEB 9

21-OCT-82
 PAGE 2

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	OZONE PPH M03-8410	NO PPH T 148-3	NO2-UNC PPH T 148-3	NOX-UNC PPH T 148-3	T DEG C DORTIC-1	PAN PPH ECD-1	MCHO PPH CA	M-C6 PPH SE-52C-2	M-C7 PPH SE-52C-2	M-C8 PPH SE-52C-2
1 850	-70								0.1917		0.0007
1 1000	0	A	0.368	0.091	0.461	30.7				0.2639	0.2518
1 1007	7							0.013			
1 1030	30		0.241	0.202	0.446	29.9	0.001				
1 1100	40		0.089	0.333	0.423	30.2	0.003	0.023	0.1681	0.2565	0.2469
1 1130	90		0.051	0.350	0.382	30.7	0.010				
1 1200	120		0.021	0.316	0.338	30.7	0.017	0.047	0.1237	0.2480	0.2353
1 1230	150		0.017	0.280	0.300	30.7	0.023				
1 1300	180		0.017	0.245	0.264	30.7	0.026	0.054		0.2422	0.2265
1 1330	210		0.017	0.211	0.230	30.9	0.033				
1 1400	240		0.020	0.190	0.209	30.9	0.037	0.070		0.2352	0.2201
1 1430	270		0.020	0.175	0.196	30.9	0.039				
1 1500	300		0.020	0.167	0.187	30.9	0.041				
1 1515	315		0.471								
1 1530	330		0.469	0.162	0.183	30.9	0.035				
1 1545	345		0.479								
1 1550	350		0.461								
1 1600	360		0.452	0.158	0.180	31.0	0.036	0.076		0.2072	0.1889

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	TOLUENE PPH SE-52C-2	C2BENZ PPH SE-52C-2	M-XYL PPH SE-52C-2	I-C3-BZ PPH SE-52C-2	O-XYL PPH SE-52C-2	M-C3-BZ PPH SE-52C-2	12ATMBZ PPH SE-52C-2	MECYC-C6 PPH SE-52C-2	M-C10 PPH SE-52C-2	M-C11 PPH SE-52C-2
1 850	-70										
1 1000	0		0.0009	0.0014	0.0012	0.0013	0.0011	0.0020		0.0013	0.0023
1 1100	40	0.3027	0.0263	0.0878	0.0179	0.0310	0.0318	0.0582	0.1861	0.0870	0.0652
1 1200	120	0.2964	0.0271	0.0858	0.0180	0.0309	0.0332	0.0612	0.1808	0.0934	0.0956
1 1300	180	0.2877	0.0250	0.0786	0.0161	0.0276	0.0303	0.0518	0.1753	0.0843	0.0745
1 1400	240	0.2745	0.0245	0.0750	0.0161	0.0272	0.0106	0.0500	0.1676	0.0835	0.0767
1 1500	300	0.2666	0.0245	0.0728	0.0167	0.0277	0.0300	0.0493	0.1630	0.0823	0.0798
1 1600	360	0.2021	0.0212	0.0632	0.0135	0.0245	0.0292	0.0428	0.1415	0.0718	0.0530

----- NO DATA TAKEN

EC-48Y
JP-4 (PET), GROUND LEVEL
1981, FEB Y

CLOCK TIME DAY NR.	ELAPSED TIME (MIN)	C2-N		ME-N	
		PPM	ECB-1	PPM	ECB-1
1 1030	30	0.0004	C	0.0000	
1 1100	60	0.0008		0.0000	
1 1130	90	0.0011		0.0000	
1 1200	120	0.0011		0.0001	
1 1230	150	0.0011		0.0001	
1 1300	180	0.0010		0.0001	
1 1330	210	0.0009		0.0001	
1 1400	240	0.0008		-----	
1 1430	270	0.0007		0.0001	
1 1500	300	0.0005		0.0001	
1 1530	330	0.0004		0.0001	
1 1600	360	0.0004		0.0001	

----- NO DATA TAKEN

NOTES

- A DASIBI DATA PRIOR TO 1-210 MIN. IS INCORRECT DUE TO MALFUNCTION.
- B TOLUENE DATA MAY BE HIGH ON SE-52C-2 BECAUSE OF INTERFERENCE.
- C EITHER C2-N OR C3-N-2

EC-490
JP-4 (PET), GROUND LEVEL
1981, FEB 10

0816: BEGIN PURE AIR FILL WITH "492 R.H.
0940: 215 MICROLITERS (50 PPMC) JP-4 FLUSHED INTO EC VIA SAMPLE PORT.
0952: STOP JP-4 BULB FLUSH.

T=0 AT 1000 PSI

K1 = 0.330 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	90RIC-1	30.7	0.6	BEG C	RELATIVE INTENSITY
ID	INST.	INITIAL CONC.		UNITS	500 1.474
MD	T 148-3	0.715	PPM		430 1.171
MD2-UNC	T 148-3	0.183	PPM		403 0.990
					380 0.824
					370 0.710
					360 0.592
					350 0.500
					340 0.374
					330 0.229
					320 0.116
					310 0.034
					300 0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2920 10'C-600 RM-1211 10' 10% CARBOMAX-600) FID
 2000 ECB-1 RM-1211 12' 5% CARBOMAX-400) ECD
 2200 BMS-1 RM-1211 DIMETHYLSULFOLANE) FID
 2100 PM-1 RM 1211 POROPAK M 1 FID
 2750 SE-52C-2 RM-1211 30H SE-52 QUARTZ CAPILLARY) FID
 1530 T 148-3 TECO 148-3 MO-NGX NYLON FILTER ANALYZER
 1800 DORIC-1 DORIC TEMP INDICATOR, SN 61479
 1790 D-1790 DASIBI 1790 OZONE MONITOR
 8410 M03-8410 MONITOR LABS,CHEMLUM O3 ANALYZER MD 8410
 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS

FI-454
H-4 (FEL), GROUND LEVEL
1981, FEB 10

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	MD	MD2-UNC	MDX-UNC	T	PAN	MCHO	I-C5	M-C4	M-C7
DAY HR.	(MIN)	MD3-8410	D-1790	T 148-3	T 148-3	T 148-3	DEG C	PPM	CA	DMS-1	SE-52C-2	SE-52C-2
							DORIC-1	ECD-1				
1 835	-85							0.000		0.0000		
1 905	-55							0.000				
1 1000	0	0.000	0.002	0.715	0.183	0.898	29.5	0.000	0.018		0.1981	0.2568
1 1006	6											
1 1030	30	0.002	0.000	0.571	0.285	0.856	29.6	0.001				
1 1100	60	0.010	0.000	0.405	0.429	0.834	30.0	0.002	0.026		0.1942	0.2468
1 1130	90	0.022	0.032	0.244	0.561	0.803	30.5	0.004				
1 1200	120	0.058	0.036	0.112	0.646	0.761	30.7	0.008	0.049		0.1830	0.2411
1 1230	150	0.142	0.124	0.058	0.454	0.712	30.9	0.014				
1 1300	180	0.232	0.215	0.034	0.457	0.641	31.0	0.021	0.070		0.1836	0.2303
1 1330	210	0.313	0.303	0.024	0.571	0.595	30.9	0.028				
1 1400	240	0.391	0.386	0.022	0.510	0.529	31.1	0.034	0.081		0.1855	0.2243
1 1430	270	0.469	0.474	0.020	0.441	0.461	31.2	0.041				
1 1455	295								0.089			
1 1500	300	0.537	0.542	0.015	0.378	0.395	31.1	0.048			0.1723	0.2169
1 1530	330	0.581	0.593	0.015	0.327	0.341	31.1	0.054				
1 1600	360	0.605	0.620	0.015	0.288	0.305	31.1	0.058	0.095		0.1601	0.1951
1 1630	390	0.615	0.630	0.015	0.266	0.275	31.2					

CLOCK TIME	ELAPSED TIME (MIN)	M-C8	M-C9	BENZENE	TOLUENE	C2BENZ	M-XYL	I-C3-B2	O-XYL	MECYC-C6	M-C10	M-C3-B2
DAY HR.	(MIN)	SE-52C-2										
1 905	-55											
1 1000	0	0.2417	0.1227	0.0879	0.2958	0.0249	0.0830	0.0160	0.0285	0.1855	0.0811	0.0292
1 1006	60	0.2322	0.1208	0.0861	0.2819	0.0250	0.0795	0.0159	0.0282	0.1771	0.0849	0.0321
1 1200	120	0.2225	0.1159	0.0823	0.2712	0.0243	0.0750	0.0157	0.0260	0.1694	0.0816	0.0310
1 1400	180	0.2115	0.1104	0.0791	0.2591	0.0231	0.0694	0.0154	0.0242	0.1615	0.0786	0.0284
1 1600	240	0.2040	0.1052	0.0743	0.2509	0.0224	0.0655	0.0145	0.0251	0.1554	0.0709	0.0289
1 1800	300	0.1943	0.1003	0.0735	0.2398	0.0214	0.0618	0.0137	0.0236	0.1478	0.0701	0.0272
1 1600	360	0.1753	0.0921	0.0669	0.2284	0.0190	0.0539	0.0112	0.0203	0.1322	0.0623	0.0248

NO DATA TAKEN

EC-490
JP-4 (PET), GROUND LEVEL
1981, FEB 10

CLOCK DAY HR.	ELAPSED TIME (MIN)	124TNEZ PPN SE-52C-2	M-C11 PPN SE-52C-2	ME-N PPN ECB-1	C2-N PPN ECB-1
1 835	-85	0.0010	0.0014	0.0000	0.0000
1 905	-55	0.0010	0.0014	0.0000	0.0000
1 1000	0	0.0536	0.0486	0.0000	0.0001 A
1 1030	30	0.0569	0.0666	0.0000	0.0004
1 1100	60	0.0569	0.0666	0.0000	0.0007
1 1130	90	0.0522	0.0670	0.0001	0.0010
1 1200	120	0.0522	0.0670	0.0001	0.0010
1 1230	150	0.0494	0.0715	0.0002	0.0010
1 1300	180	0.0494	0.0715	0.0003	0.0010
1 1330	210	0.0392	0.0649	0.0004	0.0010
1 1400	240	0.0392	0.0649	0.0004	0.0008
1 1430	270	0.0398	0.0597	0.0004	0.0007
1 1500	300	0.0398	0.0597	0.0004	0.0008
1 1530	330	0.0351	0.0466	0.0004	0.0008
1 1600	360	0.0351	0.0466	0.0004	0.0007

----- NO DATA TAKEN

NOTES

A TOLUENE DATA ON SE-52C-2 MAY BE HIGH BECAUSE OF INTERFERENCE.

EC-491
JP-4 (PET); GROUND LEVEL
1981 FEB. 11

0805: FILL TO -10 TORR WITH M2.
0815: M02 FLUSHED INTO EC WITH M2 TO -20 TORR.
0828: M0 FLUSHED INTO EC.
0832: PURE AIR FILL DEBUM. NET BULB: 72 FI DRY BULB: 96 FI 52X A.H.
0930: 21 MICROLITERS (5 PPHC) OF JP-4 INJECTED INTO EC.

T-0 AT 1015 PST

M1 = 0.330 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	DEB C	SPECTRAL DISTRIBUTION	
						MM.	RELATIVE INTENSITY
T	DORIC-1	57.5	29.5	DEB C		500	1.481
						430	1.165
						403	1.004
						380	0.852
						370	0.753
						360	0.612
						350	0.500
						340	0.371
						330	0.234
						320	0.120
						310	0.019
						300	0.000

INSTRUMENTS USED

- 3920 10°C-600 RH-1211 10' 10% CARBOWAX-600; FID
- 2750 SE-52C-2 RH-1211 30M SE-52 QUARTZ CAPILLARY; FID
- 2200 BMS-1 RH-1211 DIMETHYLBENZYLFLUORIDE; FID
- 2100 PM-1 RH 1211 POROPAK N 1 FID
- 1800 DORIC-1 DORIC TEMP INDICATOR, SN 61479
- 1530 T 148-3 TECO 148-3 NO-MOX NYLON FILTER ANALYZER
- 1790 B-1790 DASIBI 1790 OZONE MONITOR
- 8410 M03-8410 MONITOR LABS.CHEMLUM 03 ANALYZER MD 8410
- 2000 ECB-1 RH-1211 12' 5% CARBOWAX-600; ECD
- 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS

LC-491
JP-4 (PET), GROUND LEVEL
1981 FEB. 11

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	NO PPM	NO2-UNC PPM	NO2-UNC T 14B-3	NOX-UNC PPM	NOX-UNC T 14B-3	T DEG C	PAN PPM	HCHO PPM	N-C6 PPM	N-C7 PPM	N-C8 PPM
		B-1790	M03-8410	T 14B-3	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECB-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 850	-85	---	---	---	---	---	---	---	0.000	---	---	---	---	---
1 855	-80	---	---	---	---	---	---	---	---	0.014	---	---	---	---
1 935	-20	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1015	0	0.000	0.000	0.717	0.192	0.898	0.898	29.1	0.000	---	---	0.0201	0.0257	0.0240
1 1045	30	0.002	0.000	0.661	0.222	0.871	0.871	85.6	0.000	---	---	---	---	---
1 1115	60	0.002	0.002	0.607	0.258	0.861	0.861	30.9	0.000	0.016	---	0.0195	0.0245	0.0227
1 1145	90	0.000	0.002	0.554	0.292	0.832	0.832	87.8	0.000	---	---	---	---	---
1 1215	120	0.002	0.005	0.507	0.319	0.812	0.812	31.5	0.000	0.024	---	0.0186	0.0233	0.0215
1 1245	150	0.012	0.007	0.458	0.346	0.793	0.793	88.3	0.001	---	---	---	---	---
1 1315	180	0.007	0.005	0.412	0.373	0.771	0.771	31.4	0.001	0.033	---	0.0168	0.0200	0.0196
1 1345	210	0.012	0.007	0.373	0.385	0.747	0.747	88.6	0.001	---	---	---	---	---
1 1415	240	0.012	0.010	0.336	0.402	0.725	0.725	31.8	0.001	0.041	---	0.0170	0.0208	0.0183
1 1445	270	0.020	0.010	0.300	0.412	0.703	0.703	89.1	0.001	---	---	---	---	---
1 1515	300	0.017	0.010	0.266	0.427	0.678	0.678	32.0	0.002	0.044	---	0.0155	0.0176	0.0160
1 1545	330	0.024	0.022	0.236	0.432	0.656	0.656	89.3	0.002	---	---	---	---	---
1 1605	350	---	---	---	---	---	---	---	---	0.051	---	---	---	---
1 1615	360	0.022	0.020	0.212	0.432	0.632	0.632	32.1	0.002	---	---	0.0155	0.0182	0.0159

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	N-C9 PPM	BENZENE PPM	BENZENE PPM	TOLUENE PPM	C2BENZ PPM	N-XYL PPM	O-XYL PPM	MEDYC-C6 PPM	N-C10 PPM	I-C3-B2 PPM	N-C3-B2 PPM
		SE-52C-2	10'C-600	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 850	-85	---	0.000	---	---	---	---	---	---	---	---	---
1 855	-80	---	---	---	---	---	---	---	---	0.0011	---	---
1 1015	0	0.0121	---	0.0091	0.0259	0.0026	0.0091	0.0034	0.0182	0.0090	0.0012	0.0033
1 1115	60	0.0114	---	0.0081	0.0253	0.0025	0.0082	0.0030	0.0173	0.0081	0.0013	0.0033
1 1215	120	0.0191	---	0.0078	0.0230	0.0025	0.0074	0.0040	0.0140	0.0073	0.0014	0.0029
1 1315	180	0.0077	---	0.0075	0.0242	0.0020	0.0063	0.0021	0.0140	0.0069	0.0009	0.0027
1 1415	240	0.0092	---	0.0069	0.0208	0.0021	0.0059	0.0025	0.0140	0.0066	---	0.0025
1 1515	300	0.0083	---	0.0064	0.0180	0.0017	0.0049	0.0111	0.0120	0.0054	---	0.0022
1 1615	360	0.0079	---	0.0066	0.0166	0.0018	0.0048	0.0021	0.0121	0.0054	---	0.0022

NO DATA TAKEN

EL-491
JP-4 (PET), GROUND LEVEL
1981 FEB. 11

CLOCK TIME DAY HR. (MIN)	ELAPSED TIME (MIN)	124TMEZ SE-52C-2	N-C11 PPN SE-52C-2	ME-N PPN ECB-1
1 850	85	-----	-----	0.0000
1 855	80	0.0015	0.0024	-----
1 1015	0	0.0061	0.0088	0.0000
1 1045	30	-----	-----	0.0000
1 1115	60	0.0053	0.0073	0.0000
1 1145	90	-----	-----	0.0000
1 1215	120	0.0044	0.0040	0.0000
1 1245	150	-----	-----	0.0000
1 1315	180	0.0037	0.0040	0.0000
1 1345	210	-----	-----	0.0002
1 1415	240	0.0032	0.0059	0.0001
1 1445	270	-----	-----	0.0002
1 1515	300	0.0030	0.0041	0.0002
1 1545	330	-----	-----	0.0002
1 1615	360	0.0027	0.0044	0.0002

----- NO DATA TAKEN

NOTES

A TOLUENE DATA ON SE-52C-2 MAY BE HIGH BECAUSE OF INTERFERENCE.

EC-492
JP-4 (PET), GROUND LEVEL
1981 FEB. 12

0802: EC FILLED TO "10 TORR WITH N2.
0808: M02 FLUSHED INTO EC WITH N2.
0821: M0 FLUSHED INTO EC WITH N2.
0828: PURE AIR INTO EC. WET BULB TEMP: 70.5 F; DRY BULB TEMP: 85 F. 50% R.H.
0944: 215 MICROLITERS (50 PPMC) JP-4 INJECTED INTO EC.

T=0 AT 1015 PST

RI = 0.330 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	BORIC-1	31.7	1.4	DEG C	RELATIVE INTENSITY 500 1.468 430 1.135 403 0.977 360 0.799 370 0.723 360 0.590 350 0.500 340 0.344 330 0.237 320 0.113 310 0.017 300 0.000
ID	INST.	INITIAL CONC.	UNITS		
M0	T 14B-3	0.391	PPM		
M02-UNC	T 14B-3	0.102	PPM		

INSTRUMENTS USED

ID LABEL DESCRIPTION
1790 B-1790 DASIBI 1790 OZONE MONITOR
8410 M03-8410 MONITOR LABS 8410 O3 ANALYZER (CHEMIL.)
1530 T 14B-3 TECO 14B-3 NO-NOX ANALYZER
2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAP. GC; FID
2100 PM-1 RM-1211 POROPAK-M GC; FID
2200 DNS-1 CHAMPI DIMETHYLSULFOLANE GC; FID
2920 10'C-600 RM-1211 10' 10% CARBOWAX-600 GC; FID
2000 ECD-1 RM-1211 12' 5% CARBOWAX-400 GC; ECD
1800 BORIC-1 BORIC TEMPERATURE INDICATOR, SN 61479
3000 CA CHROMOTROPIC ACID MCHD ANALYSIS

EC-492
W-4 (PET), GROUND LEVEL
1981 FEB. 12

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	OZONE PPM	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	MCHO PPM	M-C6 PPM	M-C7 PPM	M-C8 PPM
DAY HR.		148-3	148-3	148-3	T 148-3	T 148-3	T 148-3	DORIC-1	EGD-1	CA	SE-52C-2	SE-52C-2	SE-52C-2
1 845	-90	---	---	---	---	---	---	---	0.000	0.014	---	---	---
1 1005	-10	---	---	---	---	---	---	---	---	---	---	---	---
1 1015	0	0.000	0.000	0.000	0.391	0.102	0.494	27.3	0.000	---	0.2073	0.2627	0.2440
1 1115	30	0.007	0.005	0.005	0.271	0.207	0.477	31.1	0.001	---	---	---	---
1 1115	60	0.024	0.014	0.014	0.118	0.338	0.454	31.0	0.003	0.025	0.2003	0.2550	0.2293
1 1145	90	0.110	0.092	0.092	0.034	0.388	0.423	31.4	0.005	---	---	---	---
1 1215	120	0.220	0.205	0.205	0.017	0.363	0.382	32.0	0.015	0.046	0.1961	0.2462	0.2191
1 1245	150	0.310	0.290	0.290	0.012	0.332	0.344	32.0	0.020	---	---	---	---
1 1315	180	0.391	0.374	0.374	0.010	0.295	0.305	32.3	0.027	---	0.1884	0.2324	0.2047
1 1325	190	---	---	---	---	---	---	---	---	0.060	---	---	---
1 1345	210	0.454	0.431	0.431	0.009	0.260	0.289	32.8	0.030	---	---	---	---
1 1415	240	0.505	0.495	0.495	0.001	0.229	0.238	32.5	0.037	0.068	0.1829	0.2251	0.2003
1 1445	270	0.522	0.515	0.515	0.007	0.207	0.216	32.1	0.041	---	---	---	---
1 1515	300	0.525	0.517	0.517	0.007	0.195	0.202	31.7	0.044	0.070	0.1809	0.2196	0.1973
1 1545	330	0.508	0.505	0.505	0.007	0.186	0.194	32.1	0.045	---	---	---	---
1 1605	350	---	---	---	---	---	---	---	---	0.077	---	---	---
1 1615	360	0.496	0.488	0.488	0.007	0.183	0.191	33.2	0.043	---	0.1634	0.2006	0.1770

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	BENZENE PPM	BENZENE PPM	BENZENE PPM	TOLUENE PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	124TMEBZ PPM	MECYC-C6 PPM
DAY HR.		SE-52C-2	10-C-600	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 845	-90	---	0.0002	---	---	---	---	---	---	---	---	---	---
1 905	-70	---	---	---	---	---	---	---	---	---	---	0.0013	---
1 1015	0	0.1254	---	0.0920	0.2977 A	0.0261	0.0843	0.0843	0.0153	0.0208	0.0284	0.0522	0.1857
1 1115	60	0.1170	---	0.0884	0.2458	0.0244	0.0784	0.0784	0.0138	0.0247	0.0270	0.0485	0.1776
1 1215	120	0.1148	---	0.0852	0.2717	0.0239	0.0747	0.0747	0.0131	0.0245	0.0277	0.0492	0.1715
1 1315	180	0.1058	---	0.0814	0.2315	0.0224	0.0685	0.0685	0.0139	0.0245	0.0259	0.0446	0.1615
1 1415	240	0.1019	---	0.0782	0.2200	0.0217	0.0648	0.0648	0.0139	0.0241	0.0247	0.0431	0.1553
1 1515	300	0.1020	---	0.0744	0.2448	0.0215	0.0639	0.0639	0.0133	0.0237	0.0250	0.0442	0.1523
1 1615	360	0.0847	---	0.0696	0.1949	0.0186	0.0557	0.0557	0.0106	0.0202	0.0127	0.0337	0.1388

----- NO DATA TAKEN

EC-492
JP-4 (PET), GROUND LEVEL
1981 FEB. 12

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	N-C10 PPM SE-52C-2	N-C11 PPM SE-52C-2	ME-N PPM ECD-1
1 845	-90	-----	-----	0.0000
1 905	-70	-----	0.0007	-----
1 1015	0	0.0815	0.0659	0.0000
1 1045	30	-----	-----	0.0000
1 1115	60	0.0767	0.0665	0.0000
1 1145	90	-----	-----	0.0000
1 1215	120	0.0788	0.0653	0.0000
1 1245	150	-----	-----	0.0000
1 1315	180	0.0711	0.0570	0.0000
1 1345	210	-----	-----	0.0000
1 1415	240	0.0680	0.0580	0.0001
1 1445	270	-----	-----	0.0001
1 1515	300	0.0711	0.0765	0.0001
1 1545	330	-----	-----	0.0001
1 1615	360	0.0569	0.0439	0.0001

----- NO DATA TAKEN

NOTES

A TOLUENE DATA MAY BE HIGH BECAUSE OF INTERFERENCE.

EC-497
JP-4 (PET), SIMULATED 20,000 FEET
1981, FEB 24

0738: ~0.2 PPM NO2 INTO EC.
0754: ~0.8 PPM MD INTO EC.
0758: BEGIN DRIEST PURE AIR FILL.
0829: 215 ML. (50 PPMC) OF JP-4 FLUSHED INTO EC.

EC DILUTION SCHEDULE

TIME	PR (TORR) BEFORE	PR (TORR) AFTER	TOUT	COOLANT
1006	341	352	22.4 F	2.9 F
1112	343	353	20.5 F	-5.9 F
1239	344	353	16.4 F	-12.0 F
1349	347	353	16.7 F	-10.8 F
1515	347	353	16.4 F	-11.7 F
1548	350	353	15.7 F	-12.0 F

T=0 AT 1000 PSI

N1 = 0.470 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	DEG C	SPECTRAL DISTRIBUTION
T	BORIC-1	-6.5	1.2	PPM		MM. RELATIVE INTENSITY
ID	INST.	INITIAL CONC.	UNITS			
NO	T 148-3	0.735	PPM			500 1.543
NO2-UNC	T 148-3	0.178	PPM			430 1.171
						403 0.995
						380 0.810
						370 0.711
						360 0.590
						350 0.500
						340 0.359
						330 0.232
						320 0.107
						310 0.023
						300 0.000

INSTRUMENTS USED

- 2920 10°C-600 RM-1211 10' 10X CARBOWAX-600; FID
- 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY; FID
- 2200 BMS-1 RM-1211 DIMETHYLSULFOLANE; FID
- 2100 PM-1 RM 1211 POROPAK N; FID
- 1530 T 148-3 TECO 148-3 NO-NOX NYLON FILTER ANALYZER
- 1800 BORIC-1 BORIC TEMP INDICATOR, SN 61479
- 8410 NO3-8410 MONITOR LABS-CHEMLUM O3 ANALYZER MD 8410
- 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS
- 2000 ECD-1 RM-1211 12' 5X CARBOWAX-600; ECD

EL-49/
JP-4 (NET). SIMULATED 20,000 FEET
1981, FEB 24

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO3-8410	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	HCHO PPM	N-C6 PPM	N-C6 PPM	N-C6 PPM	N-C7 PPM	N-C8 PPM
BAT NO.			T 14B-3	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECB-1	CA	SE-52C-2	DMS-1	SE-52C-2	SE-52C-2	SE-52C-2
1	901	-59	---	---	---	---	---	---	0.001	0.1793	0.1597	0.2333	0.2160	
1	930	-30	---	---	---	---	---	---	---	---	---	---	---	---
1	1000	0	-0.007	0.735	0.178	0.906	-7.8	---	---	0.1799	---	0.2341	0.2180	
1	1015	15	-0.004	0.698	0.202	0.898	-3.9	---	---	---	---	---	---	---
1	1030	30	0.000	0.647	0.223	0.869	-4.3	---	---	---	---	---	---	---
1	1045	45	0.000	0.610	0.236	0.848	-4.1	---	---	---	---	---	---	---
1	1100	60	0.000	0.578	0.253	0.833	-4.7	---	0.012	0.1730	---	0.2246	0.2087	---
1	1115	75	0.000	0.554	0.279	0.833	-5.0	---	---	---	---	---	---	---
1	1130	90	0.000	0.535	0.279	0.811	-5.7	---	---	---	---	---	---	---
1	1145	105	0.000	0.511	0.292	0.801	-6.2	---	---	---	---	---	---	---
1	1200	120	0.004	0.492	0.294	0.790	-6.4	---	0.026	0.1670	---	0.2161	0.2011	---
1	1215	135	0.004	0.479	0.301	0.780	-6.6	---	---	---	---	---	---	---
1	1230	150	0.004	0.466	0.305	0.769	-7.0	---	---	---	---	---	---	---
1	1245	165	0.004	0.453	0.312	0.762	-7.2	---	---	---	---	---	---	---
1	1300	180	0.004	0.440	0.312	0.752	-7.3	---	---	0.1619	---	0.2101	0.1945	---
1	1315	195	---	---	---	---	---	---	0.031	---	---	---	---	---
1	1330	210	0.004	0.428	0.314	0.741	-7.3	---	---	---	---	---	---	---
1	1345	225	0.007	0.415	0.318	0.732	-7.4	---	---	---	---	---	---	---
1	1400	240	0.007	0.402	0.320	0.723	-7.6	---	---	---	---	---	---	---
1	1415	255	0.000	0.393	0.318	0.711	-7.6	---	0.037	0.1568	---	0.2026	0.1870	---
1	1430	270	0.000	0.382	0.322	0.704	-7.0	---	---	---	---	---	---	---
1	1445	285	0.000	0.372	0.331	0.702	-6.0	---	---	---	---	---	---	---
1	1500	300	0.000	0.363	0.331	0.692	-6.4	---	---	---	---	---	---	---
1	1505	305	0.000	0.348	0.335	0.680	-6.9	---	0.039	0.1565	---	0.2023	0.1864	---
1	1515	315	---	---	---	---	---	0.003	---	---	---	---	---	---
1	1530	330	0.000	0.339	0.329	0.668	-7.4	---	---	---	---	---	---	---
1	1545	345	0.000	0.329	0.329	0.657	-7.4	---	---	---	---	---	---	---
1	1600	360	0.000	0.320	0.329	0.646	-7.7	---	0.041	---	---	---	---	---
1	1605	360	0.000	0.312	0.333	0.644	-6.4	0.007	---	0.1518	---	0.1955	0.1797	---

----- NO DATA TAKEN

EC-497
JP-4 (PET), SIMULATED 20,000 FEET
1981, FEB 24

CLOCK TIME	ELAPSED TIME (MIN)	N-C9 PPM	BENZENE PPM	SE-52C-2	TOLUENE PPM	10'C-600	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	0-XYL PPM	M-C3-BZ PPM	124THEBZ PPM	MECYC-C6 PPM
1 901	-59	0.1132	0.0298	SE-52C-2	0.2650 A	0.0482	0.0239	0.0774	0.0158	0.0279	0.0272	0.0517	0.1667
1 1000	0	0.1137	0.0304	0.2635	0.0517	0.0238	0.0764	0.0160	0.0277	0.0279	0.0279	0.0520	0.1672
1 1100	60	0.1094	0.0298	0.2542	0.0230	0.0728	0.0265	0.0152	0.0274	0.0274	0.0274	0.0494	0.1606
1 1200	120	0.1055	0.0285	0.2458	0.0218	0.0481	0.0255	0.0148	0.0262	0.0262	0.0262	0.0459	0.1550
1 1300	180	0.1017	0.0275	0.2378	0.0216	0.0452	0.0245	0.0142	0.0251	0.0251	0.0251	0.0437	0.1499
1 1400	240	0.0976	0.0270	0.2292	0.0208	0.0547	0.0233	0.0137	0.0237	0.0237	0.0237	0.0410	0.1443
1 1500	300	0.0945	0.0263	0.2291	0.0195	0.0600	0.0227	0.0130	0.0234	0.0234	0.0234	0.0381	0.1438
1 1600	360	0.0935	0.0260	0.2205	0.0200	0.0508	0.0219	0.0133	0.0233	0.0233	0.0233	0.0353	0.1381

CLOCK TIME	ELAPSED TIME (MIN)	N-C10 PPM	M-C11 PPM	ME-N PPM
1 901	-59	0.0770	0.0760	---
1 1000	0	0.0779	0.0793	---
1 1100	60	0.0752	0.0749	---
1 1200	120	0.0729	0.0698	---
1 1300	180	0.0693	0.0667	---
1 1400	240	0.0667	0.0646	---
1 1500	300	0.0650	0.0640	---
1 1505	305	---	0.0007	---
1 1600	360	0.0433	0.0620	0.0009

NO DATA TAKEN

NOTES

A TOLUENE DATA ON THE SE-52C-2 MAY BE HIGH BECAUSE OF INTERFERENCE.

EC-498
JP-4 (PET), SIMULATED 20,000 FEET
1981, FEB 25

0704: 0.1 PPM NO2 INTO EC.
0717: 0.4 PPM NO INTO EC.
0721: BEGIN BRIEST PURE AIR FILL TO 350 TORR. COOLANT: 12.5 TOUT: 32.0
0727: COOLANT: 10.4 F TOUT: 40.8 F
0800: 215 ML (50 PPMC) JP-4 FLUSHED INTO EC.

EC DILUTION SCHEDULE				
TIME	PR(TORR) BEFORE	PR(TORR) AFTER	TOUT	COOLANT
1035	345	353	18.0 F	-10.0 F
1139	346	353	16.9 F	-13.4 F
1254	349	353	15.5 F	-14.6 F
1354	349	353	15.3 F	-14.9 F
1448	349	353	15.0 F	-15.2 F

T=0 AT 930 PST

AJ = 0.470 MIM-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	DORIC-1	-7.3	1.2	DEG C	MM. RELATIVE INTENSITY
ID	INST.	INITIAL COMC.			
NO	T 14B-3	0.361	PPM		500 1.571
NO2-UNC	T 14B-3	0.086	PPM		430 1.215
					403 1.008
					380 0.833
					370 0.701
					360 0.596
					350 0.500
					340 0.368
					330 0.230
					320 0.117
					310 0.025
					300 0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2100 PM-1 RM 1211 POROPAK N / FID
 2200 DMS-1 RM-1211 DIMETHYLSULFOLANE / FID
 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY / FID
 1530 T 14B-3 TECO 14B-3 NO-MOX NYLON FILTER ANALYZER
 1800 DORIC-1 DORIC TEMP INDICATOR, 8M 61479
 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS
 8410 M03-8410 MONITOR LABS.CHEMLUM 03 ANALYZER MD 8410
 2000 ECD-1 RM-1211 12' 5X CARBOWAX-400 / ECD

EC-478
M-4 (FET), SIMULATED 20,000 FEET
1981, FEB 25

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	MCHO PPM	N-C6 PPM	N-C7 PPM	N-C8 PPM	N-C9 PPM
DAY NR.	(MIN)	M03-8410	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECD-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1	820	-70	-----	-----	-----	-----	-----	0.008	0.1709	0.2253	0.2108	0.1098
1	854	-34	-----	-----	-----	-----	-----	-----	0.1664	0.2217	0.2082	0.1088
1	930	0	0.000	0.086	0.446	-11.4	-----	-----	-----	-----	-----	-----
1	945	15	0.004	0.097	0.440	-5.1	-----	-----	-----	-----	-----	-----
1	1000	30	0.004	0.120	0.434	-5.7	-----	-----	-----	-----	-----	-----
1	1015	45	0.007	0.140	0.422	-6.0	-----	-----	-----	-----	-----	-----
1	1030	60	0.007	0.159	0.412	-6.3	-----	0.013	0.1634	0.2154	0.2034	0.1072
1	1045	75	0.011	0.176	0.403	-6.4	-----	-----	-----	-----	-----	-----
1	1100	90	0.019	0.185	0.392	-6.7	-----	-----	-----	-----	-----	-----
1	1115	105	0.022	0.195	0.382	-6.9	-----	-----	-----	-----	-----	-----
1	1130	120	0.026	0.202	0.376	-6.9	0.002	0.024	0.1610	0.2129	0.1998	0.1049
1	1145	135	0.030	0.206	0.365	-7.0	-----	-----	-----	-----	-----	-----
1	1200	150	0.033	0.208	0.356	-7.2	-----	-----	-----	-----	-----	-----
1	1215	165	0.033	0.215	0.349	-7.4	-----	-----	-----	-----	-----	-----
1	1230	180	0.037	0.215	0.343	-7.7	0.004	0.029	0.1573	0.2078	0.1942	0.1020
1	1245	195	0.037	0.215	0.334	-7.6	-----	-----	-----	-----	-----	-----
1	1300	210	0.044	0.215	0.328	-7.6	-----	-----	-----	-----	-----	-----
1	1315	225	0.044	0.215	0.322	-7.8	-----	-----	-----	-----	-----	-----
1	1330	240	0.048	0.215	0.315	-8.0	0.007	0.029	0.1545	0.2048	0.1905	0.1005
1	1345	255	0.048	0.215	0.309	-8.0	-----	-----	-----	-----	-----	-----
1	1400	270	0.052	0.215	0.304	-8.0	-----	-----	-----	-----	-----	-----
1	1415	285	0.059	0.213	0.298	-8.0	-----	-----	-----	-----	-----	-----
1	1430	300	0.059	0.213	0.292	-8.1	0.009	0.044	0.1504	0.2053	0.1837	0.0959
1	1445	315	0.063	0.211	0.285	-8.1	-----	-----	-----	-----	-----	-----
1	1500	330	0.063	0.208	0.281	-8.0	-----	-----	-----	-----	-----	-----
1	1515	345	0.067	0.208	0.276	-7.8	-----	0.031	-----	-----	-----	-----
1	1530	360	0.074	0.213	0.276	-5.8	0.010	-----	0.1481	0.1940	0.1796	0.0938

----- NO DATA TAKEN

EC-498
JP-4 (PET), SIMULATED 20,000 FEET
1981, FEB 25

CLOCK TIME	ELAPSED TIME (MIN)	BENZENE PPM	C2BENZ PPM	N-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	124TMBZ PPM	MECYC-C6 PPM	M-C10 PPM	N-C11 PPM	ME-N PPM
DAY HR.		SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	ECD-1
1 820	-70	0.0289	0.0230	0.0749	0.0156	0.0273	0.0270	0.0521	0.1618	0.0739	0.0750	-----
1 930	0	0.0276	0.0227	0.0741	0.0151	0.0269	0.0267	0.0519	0.1575	0.0752	0.0790	-----
1 1030	60	0.0268	0.0224	0.0716	0.0151	0.0260	0.0274	0.0496	0.1549	0.0747	0.0791	-----
1 1130	120	0.0267	0.0220	0.0689	0.0149	0.0253	0.0266	0.0473	0.1526	0.0727	0.0727	0.0000
1 1230	180	0.0262	0.0214	0.0664	0.0145	0.0246	0.0258	0.0450	0.1488	0.0707	0.0714	0.0001
1 1330	240	0.0260	0.0200	0.0560	0.0141	0.0236	0.0252	0.0438	0.1461	0.0703	0.0697	0.0002
1 1430	300	0.0251	0.0202	0.0614	0.0137	0.0230	0.0243	0.0398	0.1409	0.0657	0.0645	0.0003
1 1530	360	0.0251	0.0194	0.0520	0.0134	0.0223	0.0238	0.0398	0.1380	0.0648	0.0665	0.0003

----- NO DATA TAKEN

EC-500
JP-4 (PET), SIMULATED 20,000 FEET
1981, MAR 3

0800: MD2 INTO EC "0.1 PPM
0814: NO INTO EC
0825: 430 MICROLITERS (100 PPMC) JP-4 INJECTED
0830: FILLED WITH DRIEST PURE AIR TO 350 TURN

T=0 AT 1100 PSI

N1 = 0.470 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	-6.3	1.0	DEG C
HCHO	CA	0.034	0.013	PPM
ID	INST.	INITIAL CONC.	UNITS	
NO	T 14B-3	0.392	PPM	
MD2-UNC	T 14B-3	0.082	PPM	

SPECTRAL DISTRIBUTION

MN.	RELATIVE INTENSITY
500	1.610
430	1.221
403	1.038
380	0.845
370	0.718
340	0.593
350	0.500
340	0.374
330	0.220
320	0.112
310	0.024
300	0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2200 BMS-1 RM-1211 DIMETHYLSULFOLAME FID
- 2100 PM-1 RM 1211 POROPAK M F FID
- 2920 10'C-690 RM-1211 10' 102 CARBOMAX-600 FID
- 2750 SE-52C-2 GM-1211 30M SE-52 QUARTZ CAPILLARY FID
- 1530 T 14B-3 TECO 14B-3 NO-MOX NYLON FILTER ANALYZER
- 1800 DORIC-1 DORIC TEMP INDICATOR, SM 61479
- 8410 M03-B410 MONITOR LABS.CHEMLUM O3 ANALYZER MD B410
- 3000 CA CHRONOTROPIC ACID HCHO ANALYSIS

EC-500
JP-9 (PET), SIMULATED 20,000 FEET
1981, MAR 3

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	HCHO PPM	N-C4 PPM	N-C7 PPM	N-C8 PPM	N-C9 PPM	BENZENE PPM
DAY HR.		M03-8410	T 148-3	T 148-3	T 148-3	DORIC-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 850	-130	---	---	---	---	---	0.006	0.3677	0.4881	0.4577	0.2378	0.0616
1 1000	-60	---	---	---	---	---	---	0.3387	0.4492	0.4214	0.2194	---
1 1100	0	-0.004	0.392	0.082	0.480	-8.4	---	---	---	---	---	---
1 1115	15	0.000	0.334	0.124	0.466	-3.9	---	---	---	---	---	---
1 1130	30	0.004	0.257	0.180	0.444	-4.3	---	---	---	---	---	---
1 1145	45	0.015	0.206	0.212	0.425	-5.1	---	---	---	---	---	---
1 1200	60	0.024	0.165	0.234	0.404	-5.1	0.032	0.3302	0.4374	0.4088	0.2153	0.0532
1 1215	75	0.037	0.130	0.253	0.391	-5.4	---	---	---	---	---	---
1 1230	90	0.048	0.111	0.257	0.376	-5.8	---	---	---	---	---	---
1 1245	105	0.052	0.096	0.260	0.363	-6.2	---	---	---	---	---	---
1 1300	120	0.043	0.084	0.240	0.352	-6.2	0.042	0.3174	0.4184	0.3883	0.2030	0.0519
1 1315	135	0.070	0.075	0.257	0.337	-6.0	---	---	---	---	---	---
1 1330	150	0.078	0.064	0.257	0.326	-6.3	---	---	---	---	---	---
1 1345	165	0.085	0.058	0.253	0.318	-6.3	---	---	---	---	---	---
1 1400	180	0.093	0.051	0.251	0.309	-6.4	0.040	0.3061	0.4032	0.3740	0.1953	0.0521
1 1415	195	0.096	0.045	0.246	0.298	-6.7	---	---	---	---	---	---
1 1430	210	0.108	0.043	0.245	0.292	-6.7	---	---	---	---	---	---
1 1445	225	0.111	0.037	0.236	0.281	-6.7	---	---	---	---	---	---
1 1500	240	0.119	0.034	0.236	0.276	-6.9	0.040	0.3023	0.3970	0.3664	0.1888	0.0504
1 1515	255	0.130	0.030	0.231	0.266	-6.9	---	---	---	---	---	---
1 1530	270	0.133	0.028	0.225	0.260	-7.0	---	---	---	---	---	---
1 1545	285	0.137	0.026	0.223	0.253	-7.2	---	---	---	---	---	---
1 1600	300	0.148	0.021	0.216	0.245	-7.2	0.041	0.2999	0.3941	0.3647	0.1891	0.0510
1 1615	315	0.152	0.019	0.212	0.238	-7.0	---	---	---	---	---	---
1 1630	330	0.156	0.019	0.206	0.231	-7.2	---	---	---	---	---	---
1 1645	345	0.167	0.017	0.202	0.225	-7.0	---	---	---	---	---	---
1 1647	347	---	---	---	---	---	0.036	---	---	---	---	---
1 1700	360	0.174	0.015	0.200	0.219	-6.0	---	0.2959	0.3881	0.3602	0.1868	0.0493

----- NO DATA TAKEN

EC-500
JP-4 (PET), SIMULATED 20,000 FEET
1981, MAR 3

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	TOLUENE PPM SE-52C-2	TOLUENE PPM 10'C-600	C2BENZ PPM SE-52C-2	M-XYL PPM SE-52C-2	I-C3-BZ PPM SE-52C-2	O-XYL PPM SE-52C-2	M-C3-BZ PPM SE-52C-2	124TMBZ PPM SE-52C-2	MECYC-C6 PPM SE-52C-2	M-C10 PPM SE-52C-2	M-C11 PPM SE-52C-2
1 050	-130	0.5527 A	0.1068	0.0486	0.1622	0.0337	0.0575	0.0608	0.1151	0.3472	0.1659	0.1674
1 1100	0	0.5095	0.0998	0.0458	0.1315	0.0312	0.0536	0.0571	0.1071	0.3212	0.1540	0.1584
1 1200	40	0.4965	-----	0.0449	0.1427	0.0315	0.0515	0.0581	0.1035	0.3130	0.1531	0.1527
1 1300	120	0.4738	-----	0.0422	0.1319	0.0296	0.0487	0.0536	0.0949	0.2990	0.1428	0.1372
1 1400	180	0.4573	0.0858	0.0404	0.1251	0.0281	0.0467	0.0513	0.0889	0.2887	0.1357	0.1294
1 1500	240	0.4500	-----	0.0400	0.1236	0.0263	0.0453	0.0511	0.0820	0.2838	0.1292	0.1155
1 1600	300	0.4458	-----	0.0401	0.1223	0.0272	0.0451	0.0494	0.0835	0.2810	0.1296	0.1178
1 1700	360	0.4400	0.0876	0.0397	0.1200	0.0272	0.0445	0.0493	0.0822	0.2768	0.1287	0.1145

----- NO DATA TAKEN

NOTES

A TOLUENE DATA MAY BE HIGH DUE TO INTERFERENCE.

EC-502
JP-4 (PET), SIMULATED 20,000 FEET
1981, MAR 9

0714: 0.1 PPM NO2 INTO EC. 0.4 PPM NO INTO EC. DRY PURE AIR TO 350 TORR
0815: 215 MICROLITERS (50 PPMC) JPA INJECTED.
0945: T=0 PRESSURE: 351 TORR

EC DILUTION SCHEDULE

TIME	PR. BEFORE	PK. AFTER	COOLANT	TOUT
1238	344	353		
1338	349	353	-3.2	22.8
1512	349	353	-2	24.3

T=0 AT 945 PST

K1 = 0.470 MIN-1

SPECTRAL DISTRIBUTION

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	MM. INTENSITY
T	00RIC-1	-5.2	2.0	DEG C	500 1.610
					430 1.221
ID	INST.	INITIAL CONC.	UNITS		403 1.013
					380 0.845
MD	T 14B-3	0.354	PPM		370 0.742
MD2-UMC	T 14B-3	0.069	PPM		360 0.616
					350 0.500
					340 0.374
					330 0.242
					320 0.112
					310 0.024
					300 0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2200 DHS-1 RM-1211 DIMETHYLSULFOLANE I FID
- 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY I FID
- 4000 ECD-3 AF-LAB I 12' 5X CARBOMAX-600 I FID
- 2100 PM-3 RM 1211 PDROPAC M I FID
- 2720 10-C-600 RM-1211 10' 10X CARBOMAX-600 I FID
- 1530 T 14B-3 TECO 14B-3 NO-MOX NYLON FILTER ANALYZER
- 1800 00RIC-1 BORIC TEMP INDICATOR, SN 61479
- 8410 M03-8410 MONITOR LABS-CHEMLUM 03 ANALYZER MD 8410
- 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS

EC-302
JP-4 (PET), SIMULATED 20,000 FEET
1981, MAR 9

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO3-8410 PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEGC	MCHO CA	N-C6 PPM	N-C7 PPM	N-C8 PPM	N-C9 PPM	BENZENE PPM
DAY MR.	(MIN)		T 148-3	T 148-3	T 148-3	T 148-3	BORIC-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1	840	-65	---	---	---	---	---	0.005	0.1780	0.2284	0.2116	0.1086	0.0725
1	910	-35	---	---	---	---	---	---	0.1706	0.2201	0.2047	0.1066	0.0701
1	945	0	-0.007	0.354	0.049	0.425	-11.9	0.015	---	---	---	---	---
1	1000	15	0.000	0.333	0.082	0.416	-6.7	---	---	---	---	---	---
1	1015	30	0.000	0.309	0.100	0.412	-6.6	---	---	---	---	---	---
1	1030	45	0.000	0.275	0.127	0.403	-6.6	---	---	---	---	---	---
1	1045	60	0.007	0.245	0.150	0.397	-6.2	---	0.1695	0.2184	0.2020	0.1049	0.0693
1	1100	75	0.011	0.219	0.165	0.386	-6.0	---	---	---	---	---	---
1	1115	90	0.015	0.195	0.180	0.378	-5.8	---	---	---	---	---	---
1	1130	105	0.019	0.178	0.191	0.369	-6.2	---	---	---	---	---	---
1	1145	120	0.022	0.161	0.197	0.361	-6.4	---	0.1446	0.2122	0.1949	0.1015	0.0649
1	1150	125	---	---	---	---	---	0.020	---	---	---	---	---
1	1200	135	0.030	0.146	0.202	0.348	-6.6	---	---	---	---	---	---
1	1215	150	0.033	0.133	0.210	0.346	-6.4	---	---	---	---	---	---
1	1230	165	0.037	0.124	0.215	0.339	-5.9	---	---	---	---	---	---
1	1245	180	0.041	0.114	0.216	0.333	-5.4	0.033	0.1616	0.2080	0.1932	0.1024	0.0667
1	1300	195	0.044	0.103	0.223	0.328	-5.0	---	---	---	---	---	---
1	1315	210	0.044	0.094	0.225	0.322	-4.7	---	---	---	---	---	---
1	1330	225	0.054	0.088	0.227	0.318	-4.3	---	---	---	---	---	---
1	1345	240	0.059	0.079	0.227	0.309	-4.3	0.036	0.1401	0.2065	0.1887	0.0981	0.0656
1	1400	255	0.067	0.073	0.230	0.364	-3.8	---	---	---	---	---	---
1	1415	270	0.074	0.067	0.230	0.298	-3.6	---	---	---	---	---	---
1	1430	285	0.078	0.060	0.230	0.294	-3.3	---	---	---	---	---	---
1	1445	300	0.082	0.056	0.227	0.285	-3.2	0.041	0.1559	0.2008	0.1835	0.0955	0.0636
1	1500	315	0.089	0.049	0.225	0.276	-3.2	---	---	---	---	---	---
1	1515	330	0.093	0.045	0.225	0.275	-2.7	---	---	---	---	---	---
1	1530	345	0.104	0.041	0.223	0.266	-2.7	---	---	---	---	---	---
1	1535	350	---	---	---	---	---	0.038	---	---	---	---	---
1	1545	360	0.108	0.037	0.221	0.260	-2.7	---	0.1543	0.1983	0.1812	0.0944	0.0635

----- NO DATA TAKEN

EC-502
JP-4 (PET), SIMULATED 20,000 FEET
1981, MAR 9

CLOCK TIME	ELAPSED TIME (MIN)	TOLUENE PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	124TMEBZ PPM	MECYC-C6 PPM	N-C10 PPM	M-C11 PPM
1 840	-65	0.0527	0.0227	0.0735	0.0159	0.0276	0.0296	0.0499	0.1641	0.0707	0.0789
1 945	0	0.0517	0.0217	0.0715	0.0154	0.0262	0.0289	0.0493	0.1583	0.0707	0.0734
1 1045	60	-----	0.0213	0.0621	0.0147	0.0250	0.0251	0.0449	0.1365	0.0716	0.0770
1 1145	120	-----	0.0206	0.0659	0.0144	0.0243	0.0266	0.0472	0.1514	0.0700	0.0718
1 1245	180	0.0455	0.0214	0.0661	0.0149	0.0244	0.0274	0.0478	0.1492	0.0749	0.0780
1 1345	240	-----	0.0213	0.0642	0.0145	0.0241	0.0259	0.0446	0.1469	0.0702	0.0710
1 1445	300	-----	0.0195	0.0603	0.0138	0.0229	0.0252	0.0434	0.1429	0.0681	0.0721
1 1545	360	0.0464	0.0194	0.0592	0.0141	0.0225	0.0254	0.0432	0.1408	0.0677	0.0683

----- NO DATA TAKEN

EC-506
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 16

0730: -0.1 PPM NO2 FLUSHED INTO EC
0740: -0.4 PPM NO FLUSHED INTO EC
0743: DRY PURE AIR FILL TO 500 TORR
0757: 215 ML (50 PPMC) JP-4(PET) INJECTED.

EC DILUTION SCHEDULE

TIME	PR(TORR) BEFORE	PR(TORR) AFTER
1112	492	502
1152	495	502
1306	493	502
1356	495	502
1447	495	502

T=0 AT 945 PST

K1 = 0.440 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	BORIC-1	10.6	1.0	DEG C

ID	INST.	INITIAL CONC.	UNITS
NO	T 14B-3	0.417	PPM
NO2-UNC	T 14B-3	0.100	PPM

SPECTRAL DISTRIBUTION

MM.	RELATIVE INTENSITY
500	1.846
430	1.240
403	1.029
380	0.847
370	0.734
360	0.600
350	0.500
340	0.342
330	0.217
320	0.098
310	0.024
300	0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2920 10'C-400 RM-1211 10' 10% CARBONMAX-4001 FID
- 2200 BMS-1 RM-1211 DIMETHYLSULFOLANES FID
- 2100 PM-1 RM 1211 POROPAK N 1 FID
- 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY FID
- 2000 ECB-1 RM-1211 12' 5% CARBONMAX-4001 ECD
- 1800 BORIC-1 BORIC TEMP. INDICATOR, SN 61479
- 8410 MO3-9410 MONITOR LABS.CHEMLUM 03 ANALYZER MD 8410
- 1530 T 14B-3 TECO 14B-3 MO-NOX NYLON FILTER ANALYZER
- 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS

EC-506
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 16

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	MO2-UNC PPM	MOX-UNC PPM	T DEB C DORIC-1	PAN PPM ECD-1	MCHO PPM CA	M-C6 FPM SE-52C-2	M-C6 PPM BMS-1	M-C7 FPM SE-52C-2	M-C8 PPM SE-52C-2
1 815	-90	-----	-----	-----	-----	-----	-----	-----	0.1788	0.1679	0.2373	0.2215
1 945	0	-0.003	0.417	0.100	0.519	4.3	-----	-----	0.1736	-----	0.2293	0.2136
1 1000	15	0.000	0.378	0.135	0.513	9.7	-----	0.005	-----	-----	-----	-----
1 1015	30	0.003	0.324	0.180	0.504	10.1	-----	-----	-----	-----	-----	-----
1 1030	45	0.006	0.275	0.219	0.495	10.5	-----	-----	-----	-----	-----	-----
1 1045	60	0.015	0.216	0.265	0.482	10.5	-----	0.017	0.1694	-----	0.2327	0.2073
1 1100	75	0.024	0.165	0.303	0.469	10.6	-----	-----	-----	-----	-----	-----
1 1115	90	0.034	0.127	0.328	0.458	11.2	-----	-----	-----	-----	-----	-----
1 1130	105	0.051	0.095	0.341	0.438	10.5	-----	-----	-----	-----	-----	-----
1 1145	120	0.066	0.072	0.354	0.427	10.5	-----	0.059	0.1655	-----	0.2188	0.2036
1 1200	135	0.084	0.057	0.356	0.414	10.5	-----	-----	-----	-----	-----	-----
1 1215	150	0.105	0.044	0.358	0.405	10.4	-----	-----	-----	-----	-----	-----
1 1230	165	0.123	0.037	0.356	0.394	10.8	-----	-----	-----	-----	-----	-----
1 1245	180	0.141	0.031	0.353	0.385	10.6	-----	0.000	0.1611	-----	0.2122	0.1953
1 1300	195	0.159	0.025	0.348	0.373	10.9	-----	-----	-----	-----	-----	-----
1 1315	210	0.183	0.021	0.343	0.366	10.9	-----	-----	-----	-----	-----	-----
1 1330	225	0.207	0.017	0.336	0.354	11.0	-----	-----	-----	-----	-----	-----
1 1345	240	0.222	0.014	0.328	0.343	10.9	-----	-----	0.1549	-----	0.2037	0.1881
1 1400	255	0.243	0.011	0.320	0.334	10.9	-----	-----	-----	-----	-----	-----
1 1415	270	0.258	0.010	0.313	0.324	10.9	-----	-----	-----	-----	-----	-----
1 1430	285	0.276	0.010	0.307	0.318	11.0	-----	-----	-----	-----	-----	-----
1 1445	300	0.294	0.006	0.302	0.309	10.9	-----	0.033	0.1445	-----	0.1914	0.1771
1 1500	315	0.312	0.005	0.293	0.300	11.0	-----	-----	-----	-----	-----	-----
1 1515	330	0.327	0.005	0.284	0.292	11.0	-----	-----	-----	-----	-----	-----
1 1530	345	0.351	0.004	0.279	0.284	11.0	-----	-----	-----	-----	-----	-----
1 1535	350	-----	-----	-----	-----	-----	-----	0.023	-----	-----	-----	-----
1 1545	360	0.363	0.004	0.270	0.275	11.0	-----	-----	0.1498	-----	0.1942	0.1788

----- NO DATA TAKEN

EC-506
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 16

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	M-C9 PPM SE-52C-2	BENZENE PPM SE-52C-2	TOLUENE PPM SE-52C-2	TOLUENE PPM 10°C-600	C2BENZ PPM SE-52C-2	M-XYL PPM SE-52C-2	I-C3-B2 PPM SE-52C-2	O-XYL PPM SE-52C-2	M-C3-B2 PPM SE-52C-2	124TMEB2 PPM SE-52C-2	MIF-XYL PPM 10°C-600
1 815	-90	0.1145	0.0305	0.2700	A 0.0543	0.0241	0.0789	0.0134	0.0291	0.0307	0.0575	0.0579
1 945	0	0.1119	0.0282	0.2430	0.0444	0.0231	0.0743	0.0159	0.0275	0.0303	0.0540	0.0495
1 1045	60	0.1075	0.0286	0.2528	-----	0.0228	0.0632	0.0153	0.0262	0.0282	0.0519	-----
1 1145	120	0.1055	0.0274	0.2487	-----	0.0223	0.0693	0.0147	0.0252	0.0295	0.0472	-----
1 1245	180	0.1007	0.0245	0.2401	0.0514	0.0222	0.0581	0.0194	0.0230	0.0446	0.0522	0.0473
1 1345	240	0.9451	0.0258	0.2311	-----	0.0206	0.0424	0.0115	0.0235	0.0247	0.0416	-----
1 1445	300	0.0927	0.0249	0.2169	-----	0.0198	0.0513	0.0110	0.0219	0.0222	0.0413	-----
1 1545	360	0.0914	0.0247	0.2207	0.0429	0.0198	0.0503	0.0126	0.0221	0.0254	0.0394	0.0410

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	MECYC-C6 PPM SE-52C-2	M-C10 PPM SE-52C-2	M-C11 PPM SE-52C-2
1 815	-90	0.1705	0.0803	0.0794
1 945	0	0.1647	0.0798	0.0772
1 1045	60	0.1401	0.0774	0.0748
1 1145	120	0.1360	0.0744	0.0726
1 1245	180	0.1308	0.0753	0.0820
1 1345	240	0.1447	0.0682	0.0660
1 1445	300	0.1349	0.0644	0.0725
1 1545	360	0.1381	0.0647	0.0696

----- NO DATA TAKEN

NOTES

A TOLUENE DATA ON SE-52C-2 MAY BE HIGH BECAUSE OF INTERFERENCE.

LC-508
JP-4 (PFI), SIMULATED 10,000 FEEI
1981, MAR 18

0716: 0.2 PPM OF NO2 INTO EC
0729: 0.8 PPM OF NO INTO EC
0737: BEGIN PURE AIR FILL TO 500 TORR. AT 10% R.H.
0950: 215 MICROLITERS JP-4 INJECTED.
0950: FILLED TO 500 TORR.

EC MAKEUP AIR DILUTION SCHEDULE

TIME	PK(TORR) BEFORE	PR(TORR) AFTER
1026	493	503
1150	494	503
1311	493	503
1353	496	503
1507	496	503

I-O AT 930 PST

R1 = 0.440 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	10.1	1.3	DEG C

SPECTRAL DISTRIBUTION

WV	RELATIVE INTENSITY
430	1.587
435	1.207
463	1.001
380	0.820
370	0.708
340	0.600
350	0.500
340	0.362
330	0.217
320	0.098
310	0.026
300	0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
 1530 T 14B-3 TECO 14B-3 NO-NOX NYLON FILTER ANALYZER
 8410 M03-8410 MONITOR LABS-CHEMUM O3 ANALYZER MD 8410
 2200 DR8-1 RM-1211 DIMETHYLSULFOLANE) FID
 1800 DORIC-1 DORIC TEMP INDICATOR, SM 61479
 2000 ECD-1 RM-1211 12' 5% CARBOWAX-400) ECD
 2100 PN-1 RM 1211 POROPAK M 1 FID
 2920 10'C-600 RM-1211 10' 10% CARBOWAX-600) FID
 2750 SE-52C-2 RM-1211 30M SE-52 QUARTZ CAPILLARY) FID
 3000 CA CHROMOTROPIC ACID MCHD ANALYSIS

LC-508
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 18

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	FAN ECD-1	HCHO CA	N-C6 SE-52C-2	N-C6 DMS-1	N-C7 SE-52C-2	N-C8 SE-52C-2
1 805	-85	---	---	---	---	---	---	0.006	0.1781	0.1699	0.2414	0.2266
1 822	-68	---	---	---	---	---	---	---	---	---	---	---
1 930	0	0.000	0.780	0.210	0.984	5.0	0.000	---	0.1674	---	0.2265	0.2144
1 945	15	0.003	0.743	0.240	0.968	8.7	---	---	---	---	---	---
1 1000	30	0.003	0.702	0.275	0.959	8.7	---	---	---	---	---	---
1 1015	45	0.003	0.653	0.312	0.950	8.8	---	---	---	---	---	---
1 1030	40	0.009	0.610	0.352	0.942	9.4	0.000	0.017	0.1654	---	0.2233	0.2106
1 1045	75	0.009	0.567	0.373	0.924	9.7	---	---	---	---	---	---
1 1100	90	0.009	0.522	0.412	0.915	10.0	---	---	---	---	---	---
1 1115	105	0.012	0.483	0.438	0.904	10.2	---	---	---	---	---	---
1 1130	120	0.012	0.449	0.459	0.898	10.2	0.000	0.023	0.1595	---	0.2158	0.2013
1 1145	135	0.012	0.412	0.488	0.880	10.4	---	---	---	---	---	---
1 1200	150	0.021	0.382	0.502	0.874	10.5	---	---	---	---	---	---
1 1215	165	0.021	0.356	0.517	0.862	10.4	---	---	---	---	---	---
1 1230	180	0.021	0.328	0.534	0.853	10.5	0.006	---	0.1524	---	0.2057	0.1917
1 1245	195	0.021	0.303	0.550	0.842	10.5	---	---	---	---	---	---
1 1300	210	0.023	0.283	0.558	0.829	10.4	---	---	---	---	---	---
1 1315	225	0.029	0.260	0.571	0.818	10.8	---	---	---	---	---	---
1 1330	240	0.035	0.234	0.574	0.801	11.0	0.000	---	0.1513	---	0.2038	0.1905
1 1335	245	---	---	---	---	---	---	0.036	---	---	---	---
1 1345	255	0.038	0.219	0.574	0.781	11.2	---	---	---	---	---	---
1 1400	270	0.041	0.200	0.577	0.769	11.2	---	---	---	---	---	---
1 1415	285	0.044	0.180	0.582	0.752	10.9	---	---	---	---	---	---
1 1430	300	0.050	0.167	0.580	0.737	11.0	0.000	0.045	0.1483	---	0.2004	0.1862
1 1445	315	0.050	0.152	0.580	0.722	11.0	---	---	---	---	---	---
1 1500	330	0.059	0.137	0.580	0.708	11.2	---	---	---	---	---	---
1 1515	345	0.067	0.127	0.574	0.692	10.9	---	---	---	---	---	---
1 1520	350	---	---	---	---	---	---	0.042	---	---	---	---
1 1530	360	0.073	0.114	0.571	0.674	10.5	0.000	---	0.1404	---	0.1906	0.1782

----- NO DATA TAKEN

EC-508
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 18

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	BENZENE PPM	TOLUENE PPM	TOLUENE PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	1241MEZ PPM	M+P-XYL PPM
1 805	-85	0.1184	0.0309	0.2750 A	0.0569	0.0246	0.0809	0.0194	0.0297	0.0298	0.0586	0.0631
1 825	-85											
1 930	0	0.1162	0.0280	0.2401	0.0543	0.0233	0.0745	0.0187	0.0280	0.0284	0.0547	0.0552
1 1030	40	0.1116	0.0283	0.2555	0.0543	0.0230	0.0743	0.0203	0.0270	0.0332	0.1123	
1 1130	120	0.1051	0.0273	0.2445	0.0543	0.0225	0.0612	0.0180	0.0257	0.0283	0.0497	
1 1230	180	0.1013	0.0257	0.2356	0.0484	0.0220	0.0672	0.0189	0.0242	0.0278	0.0481	0.0463
1 1330	240	0.0995	0.0257	0.2330	0.0436	0.0213	0.0636	0.0165	0.0239	0.0271	0.0443	
1 1430	300	0.0979	0.0253	0.2284	0.0449	0.0220	0.0548	0.0167	0.0238	0.0250	0.0457	
1 1530	360	0.0933	0.0239	0.2179	0.0449	0.0203	0.0506	0.0199	0.0227	0.0260	0.0447	0.0384

CLOCK TIME	ELAPSED TIME (MIN)	M-C10 PPM	M-C11 PPM
1 805	-85	0.1738	0.0838
1 930	0	0.1634	0.0805
1 1030	40	0.1605	0.0894
1 1130	120	0.1541	0.0884
1 1230	180	0.1463	0.0819
1 1330	240	0.1448	0.0712
1 1430	300	0.1414	0.0711
1 1530	360	0.1349	0.0687

----- NO DATA TAKEN

NOTES

A TOLUENE DATA ON SE-52C-2 MAY BE HIGH DUE TO INTERFERENCE.

EC-509
JP-4 (PET), SIMULATED 10,000 FEET
1981 MARCH 19

0717: 0.1 PPM OF M02 INTO EC
0733: 0.4 PPM OF M0 INTO EC
0736: 430 ML (100 PPMC) OF JP-4 INJECTED
0746: FILLED TO 500 TORR

EC DILUTION SCHEDULE

TIME	PR(TORR) BEFORE	PR(TORR) AFTER
0950	498	503
1106	496	503
1158	496	503
1254	495	503
1349	496	503
1448	494	503

T=0 AT 915 PSI

K1 = 0.440 MIN-1

SPECTRAL DISTRIBUTION

MM.	RELATIVE INTENSITY
300	1.446
430	1.207
403	1.001
380	0.820
370	0.708
360	0.400
350	0.500
340	0.362
330	0.217
320	0.025
300	0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2750 SE-52C-2 RM-1219 30M SE-52 QUARTZ CAPILLARY FID
 2000 ECB-1 RM-1219 12' SE CARBOWAX-400/ ECD
 2720 10'-E-600 RM-1219 10' 10% CARBOWAX-600/ FID
 2200 BMS-1 RM-1219 DIMETHYLSULFOLANE/ FID
 2100 PM-1 RM 1219 POROPAK N / FID
 1800 BORGIC-1 BORGIC TEMP INDICATOR, SN 41479
 8410 M03-8410 MONITOR LABS.CHEMUM 03 ANALYZER MD 8410
 1530 T 14B-3 TECO 14B-3 MO-MOX NYLON FILTER ANALYZER
 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS

LC-509
JP-4 (PET), SIMULATED 10,000 FEET
1981 MARCH 19

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	MDX-UNC PPM	T 14B-3	MD2-UNC PPM	T 14B-3	MDX-UNC PPM	T 14B-3	DEG C	BORIC-1	PAN PPM	ECB-1	MCHO PPM	CA	M-C6 PPM	SE-52C-2	M-C7 PPM	SE-52C-2	M-C8 PPM	SE-52C-2	M-C9 PPM	SE-52C-2
1 805	-70															0.2214	0.4038	0.4038	0.424	0.424	0.2303		
1 842	-33													0.008									
1 915	0	0.000	0.419	0.112	0.519	0.112	0.519	0.519	3.9	3.9	0.000	0.000			0.2172	0.4013	0.4013	0.424	0.424	0.2413			
1 930	15	0.003	0.369	0.157	0.515	0.157	0.515	0.515	8.6	8.6													
1 945	30	0.009	0.307	0.208	0.502	0.208	0.502	0.502	9.4	9.4													
1 1000	45	0.015	0.227	0.273	0.489	0.273	0.489	0.489	9.5	9.5													
1 1015	60	0.033	0.165	0.319	0.476	0.319	0.476	0.476	10.1	10.1	0.004	0.004	0.027	0.027	0.2108	0.3903	0.3903	0.415	0.415	0.2332			
1 1030	75	0.051	0.091	0.352	0.459	0.352	0.459	0.459	10.6	10.6													
1 1045	90	0.075	0.082	0.373	0.444	0.373	0.444	0.444	11.0	11.0													
1 1100	105	0.099	0.060	0.378	0.431	0.378	0.431	0.431	11.3	11.3													
1 1115	120	0.129	0.049	0.371	0.414	0.371	0.414	0.414	11.4	11.4	0.011	0.011	0.036	0.036	0.2070	0.3809	0.3809	0.402	0.402	0.2362			
1 1130	135	0.153	0.041	0.367	0.400	0.367	0.400	0.400	11.0	11.0													
1 1145	150	0.180	0.032	0.358	0.382	0.358	0.382	0.382	11.4	11.4													
1 1200	165	0.204	0.032	0.343	0.365	0.343	0.365	0.365	11.4	11.4													
1 1215	180	0.228	0.026	0.334	0.349	0.334	0.349	0.349	11.2	11.2	0.019	0.019	0.033	0.033	0.2027	0.3694	0.3694	0.380	0.380	0.2064			
1 1230	195	0.246	0.024	0.319	0.334	0.319	0.334	0.334	11.3	11.3													
1 1245	210	0.267	0.019	0.309	0.319	0.309	0.319	0.319	11.4	11.4													
1 1300	225	0.288	0.019	0.298	0.307	0.298	0.307	0.307	11.6	11.6													
1 1315	240	0.303	0.017	0.285	0.294	0.285	0.294	0.294	11.4	11.4	0.022	0.022	0.040	0.040	0.1974	0.3617	0.3617	0.380	0.380	0.2136			
1 1330	255	0.327	0.017	0.273	0.281	0.273	0.281	0.281	11.6	11.6													
1 1345	270	0.345	0.015	0.268	0.268	0.268	0.268	0.268	11.6	11.6													
1 1400	285	0.340	0.015	0.249	0.255	0.249	0.255	0.255	11.6	11.6													
1 1415	300	0.375	0.015	0.240	0.245	0.240	0.245	0.245	11.6	11.6	0.028	0.028	0.042	0.042	0.1955	0.3571	0.3571	0.369	0.369	0.2127			
1 1430	315	0.393	0.013	0.231	0.236	0.231	0.236	0.236	11.7	11.7													
1 1445	330	0.402	0.013	0.225	0.230	0.225	0.230	0.230	11.9	11.9													
1 1500	345	0.414	0.013	0.216	0.221	0.216	0.221	0.221	12.0	12.0													
1 1505	350													0.044									
1 1515	360	0.417	0.013	0.212	0.215	0.212	0.215	0.215	12.0	12.0	0.023	0.023	0.044	0.044	0.1910	0.3494	0.3494	0.365	0.365	0.2003			
1 1530	375	0.414	0.009	0.206	0.208	0.206	0.208	0.208	53.9	53.9													

NO DATA TAKEN

LU-509
JP-4 (PET), SIMULATED 10,000 FEET
1981 MARCH 19

DAY HR.	TIME (MIN)	ELAPSED	BENZENE PPM	TOLUENE PPM	TOLUENE PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	12ATMBZ PPM	M+P-XYL PPM	MECYC-C6 PPM
1	805	-70	0.0831	0.4970	0.0880	0.0472	0.1525	0.0344	0.0371	0.0744	0.1245	0.1042	0.2926
1	915	0	0.0975	0.4919	0.0981	0.0486	0.1544	0.0373	0.0621	0.0887	0.1294	0.1115	0.2877
1	1015	60	0.0929	0.4814	0.0981	0.0496	0.1337	0.0396	0.0635	0.0939	0.1292	0.1115	0.2803
1	1115	120	0.0903	0.4690	0.0981	0.0492	0.1467	0.0431	0.0619	0.1009	0.1292	0.1115	0.2737
1	1215	180	0.0832	0.4486	0.0884	0.0425	0.1170	0.0310	0.0492	0.0589	0.1221	0.0957	0.2647
1	1315	240	0.0800	0.4445	0.0884	0.0456	0.1185	0.0370	0.0579	0.0860	0.1169	0.0957	0.2592
1	1415	300	0.0571	0.4342	0.0884	0.0494	0.1134	0.0379	0.0438	0.1005	0.1169	0.0957	0.2546
1	1515	360	0.0736	0.4288	0.0876	0.0428	0.1117	0.0380	0.0311	0.0637	0.0955	0.0894	0.2495

DAY HR.	TIME (MIN)	ELAPSED	M-C10 PPM	M-C11 PPM
1	805	-70	0.1679	0.1726
1	915	0	0.1742	0.1841
1	1015	60	0.1778	0.1939
1	1115	120	0.1777	0.1994
1	1215	180	0.1645	0.1808
1	1315	240	0.1640	0.0502
1	1415	300	0.1588	0.1790
1	1515	360	0.1458	0.1593

----- NO DATA TAKEN

NOTES

A TOLUENE DATA ON SE-52C-2 MAY BE HIGH BECAUSE OF INTERFERENCE.

EC-510
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 20

0724: 0.1 PPM M02 INJECTED INTO EC
0.4 PPM M0 INJECTED
430 MICROLITERS (100 PPMC) JP-4 INJECTED
FILL TO 500 TORR WITH 10% RM PURE AIR

EC DILUTION SCHEDULE

TIME	PR(TORR) BEFORE	PR(TORR) AFTER
1020	496	503
1156	493	503
1227	497	503
1326	495	503
1424	495	503

T=0 AT 915 PST

K1 = 0.440 MIN-1

SPECTRAL DISTRIBUTION

MN.	RELATIVE INTENSITY
500	1.667
430	1.233
463	1.052
380	0.833
370	0.743
340	0.603
350	0.500
340	0.380
330	0.228
320	0.103
310	0.028
300	0.000

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	10.2	1.9	DEG C

ID	INST.	INITIAL CONC.	UNITS
M0	T 14B-3	0.419	PPM
M02-UNC	T 14B-3	0.112	PPM

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2920 10'C-600 RM-1211 10' 10% CARBOWAX-600; FID
 2100 PM-1 RM 1211 POROPAK N 1 FID
 2200 DMS-1 RM-1211 DIMETHYLSULFOLANE; FID
 2750 SE-52C-2 RM-1211 30% SE-52 QUARTZ CAPILLARY; FID
 1800 DORIC-1 DORIC TEMP INDICATOR, SN 61479
 8410 M03-8410 MONITOR LABS.CHEMUM 03 ANALYZER MD 8410
 1530 T 14B-3 TECO 14B-3 MO-MOX NYLON FILTER ANALYZER
 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS

EC-510
JP-4 (PET), SIMULATED 10,000 FEET
1981, MAR 20

CLOCK TIME	ELAPSED TIME (MIN)	BENZENE PPM	TOLUENE PPM	TOLUENE PPM 10'C-600	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	12ATMEDZ RAW DATA SE-52C-2	M4F-XYL PPM 10'C-600	MECYC-C4 PPM SE-52C-2
1 915	-5	0.1108	0.5090	0.0985	0.0504	0.1383	0.0399	0.0657	0.0927	0.1331	0.0973	0.3130
1 915	0	0.0522	0.4847	0.1016	0.0439	0.1428	0.0313	0.0511	0.0583	0.1111	0.1073	0.3036
1 1015	60	0.0516	0.4743	-----	0.0430	0.1362	0.0311	0.0488	0.0555	0.1010	-----	0.2975
1 1115	120	0.0490	0.4638	-----	0.0417	0.1160	0.0324	0.0467	0.0590	0.0982	-----	0.2910
1 1215	180	0.0493	0.4647	0.0954	0.0421	0.1151	0.0282	0.0477	0.0610	0.0691	0.0947	0.2900
1 1315	240	0.0460	0.4402	-----	0.0400	0.1073	0.0317	0.0486	0.0551	0.0972	-----	0.2758
1 1415	300	0.0465	0.4391	-----	0.0409	0.1240	0.0293	0.0440	0.0546	0.0905	-----	0.2751
1 1515	360	0.0472	0.4302	0.0876	0.0387	0.1017	0.0272	0.0431	0.0506	0.0880	0.0847	0.2677

CLOCK TIME	ELAPSED TIME (MIN)	N-C10 PPM	M-C11 PPM
1 810	-5	0.1726	0.1802
1 915	0	0.1569	0.1729
1 1015	60	0.1472	0.1507
1 1115	120	0.1523	0.2354
1 1215	180	0.1298	0.1416
1 1315	240	0.1424	0.1519
1 1415	300	0.1362	0.1508
1 1515	360	0.1350	0.1478

----- NO DATA TAKEN

EC-515
JP-4 (PET), GROUND LEVEL
1981 APRIL 2

0811: 0.1 PPM NO2 INJECTED INTO EC
0822: 0.4 PPM NO INJECTED INTO EC
0825: 430 MICROLITERS (100 PPMC) INJECTED.
START PURE AIR FILL. DRY BULB TEMP: 85 F; WET BULB TEMP: 71 F
RH= 85X
1635: 500 MICROLITER BULB OZONE INJECTED

T=0 AT 1000 PST

K1 = 0.310 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	DORIC-1	29.9	0.8	DEG C	MM. RELATIVE INTENSITY
ID	INST.	INITIAL CONC.	UNITS		500 1.444
NO	T 14B-3	0.336	PPM		430 1.233
NO2-UNC	T 14B-3	0.084	PPM		403 1.023
					380 0.852
					370 0.734
					360 0.595
					350 0.500
					340 0.371
					330 0.234
					320 0.103
					310 0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2750 SE-52C-2 RM-121/ 30H SE-52 QUARTZ CAPILLARY FID
- 1530 T 14B-3 TECO 14B-3 NO-NOX NYLON FILTER ANALYZER
- 1800 DORIC-1 DORIC TEMP INDICATOR, SM 61479
- 2000 ECB-1 RM-121/ 12' 52 CARBONAX-400 ECD
- 2920 10'C-600 RM-121/ 10' 102 CARBONAX-600 FID
- 2200 DHS-1 RM-121/ DIMETHYLSULFOLANE FID
- 2100 PM-1 RM 121/ POROPAK M FID
- 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS
- 1790 D-1790 DASIBI 1790 OZONE MONITOR

EC-515
JP-4 (PET), GROUND LEVEL
1981 APRIL 2

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	HCHO PPM	N-C6 PPM	N-C6 PPM	N-C7 PPM	N-C8 PPM
DAY HR.	(MIN)	D-1790	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECD-1	CA	DMS-1	SE-52C-2	SE-52C-2	SE-52C-2
1	807	-113	---	---	---	---	---	0.002	0.3684	0.4087	0.5239	0.4891
1	1000	0	0.336	0.084	0.522	29.9	---	---	---	0.4020	0.5062	0.4770
1	1020	20	---	---	---	---	0.000	---	---	---	---	---
1	1030	30	0.002	0.225	0.500	28.8	---	---	---	---	---	---
1	1100	60	0.176	0.338	0.451	29.9	0.013	0.024	0.3887	0.4966	0.4632	---
1	1130	90	0.024	0.301	0.388	30.3	---	---	---	---	---	---
1	1200	120	0.010	0.301	0.388	30.3	---	---	---	---	---	---
1	1230	150	0.008	0.253	0.327	30.7	0.028	0.042	0.3895	0.4926	0.4480	---
1	1300	180	0.008	0.217	0.283	30.9	---	---	---	---	---	---
1	1330	210	0.008	0.194	0.253	30.9	0.034	0.069	0.3788	0.4763	0.4354	---
1	1400	240	0.008	0.181	0.239	30.9	---	---	---	---	---	---
1	1430	270	0.010	0.173	0.231	29.9	0.075 A	0.079	0.3652	0.4651	0.4236	---
1	1500	300	0.008	0.169	0.224	29.5	---	---	---	---	---	---
1	1530	330	0.008	0.162	0.217	29.1	0.069 A	0.056	0.3528	0.4480	0.4103	---
1	1550	350	0.008	0.158	0.209	29.0	---	---	---	---	---	---
1	1600	360	0.008	0.151	0.205	28.8	---	0.061	0.3538	0.4370	0.4035	---

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	M-C3-BZ PPM	124TMEBZ PPM	MECYC-C6 PPM	M-C10 PPM	M-C11 PPM
DAY HR.	(MIN)	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1	850	-70	0.2578	0.0517	0.1680	0.0364	0.0609	0.1266	0.3731	0.1860	0.1707
1	1000	0	0.2502	0.0514	0.1669	0.0371	0.0413	0.1267	0.3645	0.1824	0.1641
1	1100	60	0.2467	0.0513	0.1618	0.0394	0.0410	0.1270	0.3548	0.1875	0.1915
1	1200	120	0.2381	0.0497	0.1540	0.0365	0.0585	0.1248	0.3442	0.1833	0.1970
1	1300	180	0.2306	0.0483	0.1472	0.0358	0.0458	0.1147	0.3348	0.1742	0.1784
1	1400	240	0.2267	0.0465	0.1429	0.0363	0.0543	0.1225	0.3256	0.1743	0.1801
1	1500	300	0.2179	0.0459	0.1380	0.0342	0.0545	0.1088	0.3156	0.1675	0.1675
1	1600	360	0.2173	0.0449	0.1334	0.0356	0.0551	0.1103	0.3100	0.1655	0.1558

NO DATA TAKEN

NOTES

A PAN SAMPLE DILUTED 10:1. VALUES REPORTED HERE TAKE THIS INTO ACCOUNT.
B VALUE UNUSUALLY LARGE.

EC-517
JP-4 (PET), SIMULATED 20,000 FT., Z = 70
1981 APRIL 9

FILTER PANES - 1/4 INCH AND 1/8 INCH FUR 70 DEGREE ZENITH ANGLE SIMULATION.

0750: EC TO 400 MICRONS, MI-VAC OPENED
0759: MI-VAC CLOSED 500 MICRONS, M2 TO 10 TORR.
0802: 0.1 PPM M02 INTO EC
0814: 0.4 PPM M0 INTO EC
0818: 215 MICROLITERS (50 PPMC) JP-4 (PET) INJECTED.
0820: BEGIN DRY PURE AIR FILL TO 350 TORR.
0830: FILLED TO 350 TORR.
1250: PRESSURE ADJUST - 348 TO 352 TORR.
1500: PRESSURE ADJUST - 242 TO 352 TORR.

T=0 AT 1000 PSI

M1 = 0.350 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	DORIC-1	-1.9	2.6	DEG C	MM. RELATIVE INTENSITY
ID	INST.	INITIAL CONC.	UNITS		
M0	T 14B-3	0.352	PPM		500 1.788
M02-UNC	T 14B-3	0.079	PPM		430 1.299
					403 1.098
					380 0.881
					370 0.759
					340 0.615
					350 0.500
					340 0.349
					330 0.209
					320 0.071
					310 0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
2750 BE-52C-2 RM-1211 30M BE-52 QUARTZ CAPILLARY FID
1530 T 14B-3 TECO 14B-3 MO-MOX NYLON FILTER ANALYZER
1800 DORIC-1 DORIC TEMP INDICATOR, SN 61479
2920 10'C-000 RM-1211 10' 10% CARBOWAX-600 FID
2200 DHS-1 RM-1211 DIMETHYLSULFOLANES FID
2100 PH-1 RM 1211 POROPAK N 1 FID
3000 CA CHROMOTROPIC ACID MCHO ANALYSIS
8410 M03-8410 MONITOR LABS-CHEMLUN O3 ANALYZER MD 8410
2000 ECD-1 RM-1211 12' 5% CARBOWAX-400 ECD

EC-517
JP-4 (PET), SIMULATED 20,000 FT., Z = 70
1981 APRIL 9

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	HCHO PPM	N-C6 PPM	N-C6 FPM	N-C7 PPM	N-C8 PPM
DAY NR.		M03-0410	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECD-1	CA	DMS-1	SE-52C-2	SE-52C-2	SE-52C-2
1	845	-75	---	---	---	---	0.000	---	0.1613	0.1780	0.2274	0.2099
1	855	-65	---	---	---	---	---	0.004	---	---	---	---
1	906	-54	---	---	---	---	---	---	---	---	---	---
1	1000	0	0.000	0.079	0.436	-8.9	0.000	---	---	0.1725	0.2198	0.2024
1	1030	30	0.000	0.100	0.326	-2.6	---	---	---	---	---	---
1	1100	60	0.004	0.142	0.421	-0.8	0.001	0.013	0.1781	0.1727	0.2280	0.2109
1	1130	90	0.004	0.176	0.403	-2.1	---	---	---	---	---	---
1	1200	120	0.004	0.203	0.388	-1.8	0.002	0.017	0.1735	0.1727	0.2207	0.2036
1	1230	150	0.004	0.148	0.225	-1.3	---	---	0.1735	0.1735	0.2217	0.2019
1	1300	180	0.004	0.120	0.240	-1.0	0.009	0.031	0.1683	0.1683	0.2117	0.1943
1	1400	240	0.004	0.079	0.253	-0.8	0.013	0.042	0.1595	0.1595	0.2026	0.1861
1	1500	300	0.004	0.058	0.313	-0.7	0.018	0.048	---	---	---	---
1	1550	350	---	---	---	---	---	0.071	---	---	---	---
1	1600	360	0.007	0.037	0.294	0.9	0.022	---	0.1559	0.1559	0.1976	0.1812

CLOCK TIME	ELAPSED TIME (MIN)	BENZENE PPM	TOLUENE PPM	C2BENZ PPM	M-XYL PPM	I-C3-BZ PPM	O-XYL PPM	N-C3-BZ PPM	12ATMBZ PPM	M+P-XYL PPM	MECYC-C6 PPM
DAY NR.		SE-52C-2	10'C-600	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	10'C-600	SE-52C-2
1	845	-75	0.0298	---	0.0225	0.0741	0.0160	0.0285	0.0557	---	0.1627
1	1000	0	0.1032	0.0490	0.0211	0.0689	0.0140	0.0257	0.0493	---	0.1575
1	1100	60	0.1108	---	0.0224	0.0731	0.0163	0.0299	0.0561	---	0.1633
1	1200	120	0.1079	---	0.0232	0.0709	0.0171	0.0328	0.0558	---	0.1583
1	1300	180	0.1050	0.0501	0.0205	0.0675	0.0140	0.0279	0.0547	0.0500	0.1580
1	1400	240	0.1014	---	0.0215	0.0644	0.0151	0.0277	0.0502	---	0.1511
1	1500	300	0.0973	---	0.0206	0.0628	0.0147	0.0271	0.0471	---	0.1449
1	1600	360	0.0949	0.0438	0.0199	0.0528	0.0138	0.0244	0.0477	0.0426	0.1403

----- NO DATA TAKEN

EC-517
JP-4 (PET), SIMULATED 20,000 FT., 2 = 70
1981 APRIL 9

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	M-C10 PPH SE-52C-2	M-C11 PPH SE-52C-2
1 845	-75	0.0784	0.0806
1 1000	0	0.0724	0.0716
1 1100	40	0.0818	0.0844
1 1200	120	0.0933	0.0909
1 1300	180	0.0804	0.0887
1 1400	240	0.0759	0.0783
1 1500	300	0.0725	0.0741
1 1600	360	0.0714	0.0765

----- NO DATA TAKEN

EC-575
JP-4 (PET), GROUND LEVEL
1981 SEPTEMBER 3

0835: STOP PUMPING. 10 TORR. PURE AIR.
0847: 0.1 PPM NO2.
0849: 0.4 PPM NO.
0852: BEGIN ULTRA DRY PURE AIR FILL.
0918: BEGIN JP-4 N2 FLUSH (430 MICROLITERS).

I=0 AT 945 PST

N1 = 0.480 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	SPECTRAL DISTRIBUTION
T	DORIC-1	33.2	1.4	DEG C	RELATIVE INTENSITY
ID	INST.	INITIAL CONC.	UNITS		NM.
NO	T 14B-1	0.410	PPM		500 0.978
NO2-UNC	T 14B-1	0.088	PPM		430 0.957
					403 0.875
					380 0.755
					370 0.475
					340 0.584
					350 0.500
					340 0.382
					330 0.248
					320 0.124
					310 0.031
					300 0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
2750 SE-52C-2 RM-121 30M SE-52 QUARTZ CAP. GC FID
2100 PM-1 RM-121 POROPAK-N GC FID
2000 ECD-1 RM-121 12' 5% CARBOWAX-400 GC ECD
2200 BMS-1 RM-121 DIMETHYLSULFOLANE GC FID
2920 10'C-400 RM-121 10' 10% CARBOWAX-400 GC FID
1510 T 14B-1 TECO 14B-1 NO-NOX ANALYZER
3000 CA CHROMOTROPIC ACID HCHO ANALYSIS
1800 BORIC-1 BORIC TEMPERATURE INDICATOR, SN 61479
8410 MOJ-8410 MONITOR LABS 8410 O3 ANALYZER (CMENIL.)

LC-575
JP-4 (PET), GROUND LEVEL
1981 SEPTEMBER 3

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	MO2-UNC PPM	MOX-UNC PPM	T DORIC-1	PAN PPM	MCHO PPM	N-C6 PPM	N-C7 PPM	MECYC-C4 PPM	N-C8 PPM
1 945	0	0.020	0.410	0.088	0.998	31.6			0.4435	0.5213	0.3842	0.4811
1 952	7							0.008				
1 1000	15	0.015	0.341	0.146	0.491	31.8						
1 1015	30	0.022	0.173	0.299	0.477	29.8	0.003					
1 1030	45	0.112	0.027	0.415	0.445	29.8						
1 1045	60	0.303	0.004	0.400	0.407	30.8	0.040	0.015	0.4267	0.4926	0.3679	0.4537
1 1100	75	0.431	0.001	0.378	0.382	31.7						
1 1115	90	0.534	0.001	0.302	0.304	32.7	0.061					
1 1130	105	0.413	0.000	0.299	0.300	33.5						
1 1145	120	0.670	0.000	0.284	0.285	33.9	0.094	0.017	0.4174	0.4801	0.3586	0.4391
1 1200	135	0.705	0.000	0.271	0.272	34.2						
1 1215	150	0.723	0.000	0.261	0.262	34.3	0.096					
1 1230	165	0.725	0.000	0.252	0.255	34.0						
1 1245	180	0.721	0.000	0.246	0.249	34.0	0.113	0.069	0.4112	0.4713	0.3485	0.4315
1 1300	195	0.710	0.000	0.241	0.245	33.9						
1 1315	210	0.697	0.001	0.236	0.240	33.9	0.110					
1 1330	225	0.692	0.000	0.233	0.235	34.0						
1 1345	240	0.683	0.001	0.229	0.231	34.0	0.094	0.033	0.4005	0.4587	0.3385	0.4189
1 1400	255	0.677	0.000	0.224	0.227	33.9						
1 1415	270	0.668	0.000	0.222	0.224	33.9	0.094					
1 1430	285	0.657	0.000	0.217	0.219	34.0						
1 1445	300		0.000	0.213	0.214	34.0	0.092	0.029	0.3929	0.4493	0.3318	0.4113
1 1500	315		0.000	0.208	0.212	34.2						
1 1515	330		0.000	0.204	0.207	34.0	0.080					
1 1530	345	0.543	0.001	0.201	0.205	34.2						
1 1535	350							0.044				
1 1545	360	0.631	0.001	0.198	0.201	34.0	0.070		0.3848	0.4407	0.3250	0.4020

NO DATA TAKEN

EC-S75
JP-4 (PET), GROUND LEVEL
1981 SEPTEMBER 3

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	M-C10 PPM	M-C11 PPM	BENZENE PPM	O-XYL PPM	C2BENZ PPM	I-C3-BZ PPM	M-C3-BZ PPM	124TMBZ PPM
DAY HR.		SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 945	0	0.2392	0.1589	0.1756	0.0972	0.0452	0.1894	0.0458	0.0550	0.1143
1 1045	40	0.2351	0.1610	0.1815	0.0910	0.0454	0.1818	0.0483	0.0592	0.1119
1 1145	120	0.2252	0.1531	0.1687	0.0903	0.0423	0.1700	0.0460	0.0562	0.1086
1 1245	180	0.2225	0.1545	0.1779	0.0886	0.0419	0.1724	0.0457	0.0563	0.1066
1 1345	240	0.2151	0.1497	0.1730	0.0862	0.0397	0.1642	0.0484	0.0543	0.1080
1 1445	300	0.2112	0.1471	0.1730	0.0858	0.0384	0.1445	0.0453	0.0536	0.1078
1 1545	360	0.2041	0.1380	0.1571	0.0846	0.0370	0.1594	0.0457	0.0513	0.1026

----- NO DATA TAKEN

FC-576
JP-4 (PET), 500 TORR, 304 K
1981 SEPT. 10

0810: 10 TORR. PURE AIR INTO EC.
0.1 PPM NO2 INTO EC.
030 MICROLITERS JP-4 (PET) INTO EC.
0818: 0.4 PPM NO INTO EC.
0821: FILL TO 500 TORR WITH DRY PURE AIR.

CHAMBER MAKE UP AIR SCHEDULE

TIME	PH.	(TO)	PH.
0954	---	---	---
1120	490	---	503
1252	484	---	503
1345	483	---	503
1509	490	---	503
	485	---	503

1-0 AT 930 PDT

NI = 0.4/3 MIN-1

SPECTRAL DISTRIBUTION

WAVELENGTH (NM)	RELATIVE INTENSITY
500	1.235
430	1.073
403	0.942
380	0.796
370	0.677
360	0.595
350	0.500
340	0.371
330	0.253
320	0.120
310	0.019
300	0.000

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	31.2	0.4	DEG C

ID	INST.	INITIAL CONC.	UNITS
NO	T 14B-3	0.470	PPM
NO2-UNC	T 14B-3	0.084	PPM

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2750 SE-52C-2 RM-1211 JON SE-52 QUARTZ CAP. GC1 FID
 2000 ECB-1 RM-1211 12" SE CARBONAX-400 GC1 ECB
 1530 T 14B-3 TECO 14B-3 NO-MOX ANALYZER
 1000 DORIC-1 BORIC TEMPERATURE INDICATOR, SN 61479
 3000 CA CHERMOTROPIC ACID MCHG ANALYSIS
 0410 NO3-0410 MONITOR LABS 0410 O3 ANALYZER (CHERIL.)

80-576
JP-4 (PET), 500 TORR, 304 A
1981 SEPT. 10

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	I DEG C	PAN PPM	MCHO PPM	M-C6 PPM	M-C6 PPM	M-C6 PPM	M-C7 PPM	M-C8 PPM	M-C9 PPM
		M03-8410	T 148-3	T 148-3	D0KIC-1	ECD-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 911	-14		0.474	0.088	30.5		0.013						
1 915	-15												
1 930	0		0.470	0.084	29.7			0.4573	0.3969	0.4931	0.5363	0.2491	
1 945	15		0.361	0.182	29.8								
1 1000	30	0.000	0.130	0.392	30.8	0.003							
1 1015	45	0.181	0.021	0.453	31.0								
1 1030	60	0.333	0.017	0.425	31.4	0.045		0.4229	0.3629	0.4470	0.4878	0.2287	
1 1036	66						0.036						
1 1045	75	0.428	0.017	0.395	30.8								
1 1100	90	0.507	0.017	0.373	30.8								
1 1115	105	0.545	0.017	0.356	30.9								
1 1130	120	0.569	0.017	0.341	31.0	0.102	0.044	0.4155	0.3581	0.4352	0.4787	0.2215	
1 1145	135	0.585	0.017	0.330	31.2								
1 1200	150	0.585	0.017	0.322	31.3								
1 1215	165	0.585	0.015	0.315	31.4								
1 1230	180	0.580	0.017	0.312	31.3	0.112	0.050	0.4080	0.3459	0.4288	0.4683	0.2197	
1 1245	195	0.572	0.017	0.307	31.4								
1 1300	210	0.547	0.015	0.303	31.6								
1 1315	225	0.547	0.015	0.298	31.6								
1 1330	240	0.536	0.017	0.292	31.6	0.078	0.082	0.4004	0.3397	0.4180	0.4592	0.2078	
1 1345	255	0.539	0.017	0.288	32.0								
1 1400	270	0.515	0.017	0.285	31.4								
1 1415	285	0.507	0.017	0.281	31.4								
1 1430	300	0.507	0.017	0.274	31.7	0.078		0.3844	0.3246	0.4008	0.4403	0.2017	
1 1435	305						0.067						
1 1445	315	0.509	0.017	0.275	31.6								
1 1500	330	0.499	0.017	0.270	31.4								
1 1515	345	0.488	0.015	0.266	31.8								
1 1520	350						0.061						
1 1530	360	0.490	0.017	0.261	31.7	0.072		0.3721	0.3173	0.3906	0.4275	0.1981	

NO DATA TAKEN

CC-378
JP-4 (PET), 500 TORR, 304 K
1981 SEPT. 10

DAY HR.	(MIN)	CLOCK ELAPSED TIME	M-C10		M-C11		BENZENE		O-XYL		C2BENZ		I-C3-BZ		M-C3-BZ		124TMBZ		
			SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2	PPH	SE-52C-2
1	930	0	0.1457	0.1740	0.0999	0.0692	0.1911	0.0504	0.0613	0.1206									
1	1030	60	0.1560	0.1755	0.0911	0.0633	0.1772	0.0468	0.0574	0.1073									
1	1130	120	0.1508	0.1682	0.0902	0.0612	0.1738	0.0444	0.0548	0.1002									
1	1230	180	0.1508	0.1711	0.0894	0.0612	0.1688	0.0452	0.0588	0.1004									
1	1330	240	0.1407	0.1533	0.0928	0.0556	0.1613	0.0408	0.0503	0.0915									
1	1430	300	0.1379	0.1554	0.0840	0.0547	0.1589	0.0398	0.0492	0.0917									
1	1530	360	0.1348	0.1517	0.0838	0.0542	0.1559	0.0390	0.0484	0.0888									

----- NO DATA TAKEN

NOTES

THERE IS NO DMS, PH, OR C'400 DATA. THIS IS BECAUSE JP-4 WAS ALREADY IN THE CHAMBER AT THE PRE T=0 TIME, WHICH CAUSED THE PEAKS TO BE OBLITERATED.

EC-580
JP-4 (PET), 300 TORR.
1981 SEPT. 14

0826: BEGIN DRY PURE AIR FILL TO 350 TORR.
0847: 0.1 PPM M02 INJECTED.
0857: 0.4 PPM M0 INJECTED.
0901: 430 MICROLITERS JP-4 INJECTED.

MAKE UP AIR SCHEDULE

TIME	PR.	(TO)	PR.
1206	330		350
1232	342		352
1500	330		342

I=0 AT 9.30 PDI

A1 = 0.475 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	31.5	0.6	DEB C

ID	INST.	INITIAL CONC.	UNITS
M0	T 14B-3	0.451	PPM
M02-UNC	T 14B-3	0.071	PPM

SPECTRAL DISTRIBUTION

MM.	RELATIVE INTENSITY
500	1.235
430	1.048
403	0.915
380	0.784
370	0.680
360	0.586
350	0.500
340	0.372
330	0.238
320	0.121
310	0.033
300	0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2750 SE-52C-2 RH-1211 30M SE-52 QUARTZ CAP. GC) FID
- 2200 DHS-1 RH-1211 DIMETHYLSULFOLANE GC) FID
- 2190 PM-2 RH-1031 5' POROPAK-M GC) FID
- 2000 ECB-1 RH-1211 12' 5Z CARBOJAX-400 GC) ECD
- 2920 10°C-600 RH-1211 10' 10Z CARBOJAX-600 GC) FID
- 1212 D-1212 DASIBI 1212 OZONE MONITOR
- 1530 T 14B-3 TECO 14B-3 NO-MOX ANALYZER
- 1800 DORIC-1 DORIC TEMPERATURE INDICATOR, SN 41479
- 3000 CA CHROM OTROPIC ACID MCHO ANALYSIS

EC-580
JP-4 (PET), 300 TORR.
1981 SEPT. 14

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NO2-UNC T 14B-3	NOX-UNC PPM	NOX-UNC T 14B-3	PAN PPM	PAN ECD-1	HCHO PPM	HCHO CA CHROM	M-C6 PPM	M-C6 SE-52C-2	M-C7 PPM	M-C7 SE-52C-2	MECYC-C6 PPM	MECYC-C6 SE-52C-2	M-C8 PPM	M-C8 SE-52C-2	M-C9 PPM	M-C9 SE-52C-2	
1 930	0	0.027	0.451	0.071	0.531							0.4462	0.4462	0.5257	0.5257	0.3894	0.3894	0.4868	0.4868	0.2470	0.2470	
1 935	5									0.010												
1 945	15	0.027	0.279	0.225	0.511																	
1 1000	30	0.083	0.013	0.440	0.459																	
1 1015	45	0.198	0.000	0.397	0.406																	
1 1030	60	0.241	0.000	0.371	0.380			0.042		0.038		0.4466	0.4466	0.5374	0.5374	0.3989	0.3989	0.4932	0.4932	0.2539	0.2539	
1 1045	75	0.313	0.000	0.343	0.349																	
1 1100	90	0.337	0.000	0.324	0.330																	
1 1115	105	0.352	0.002	0.312	0.319																	
1 1130	120	0.349	0.002	0.303	0.309			0.100		0.056		0.4172	0.4172	0.4806	0.4806	0.3562	0.3562	0.4412	0.4412	0.2272	0.2272	
1 1145	135	0.359	0.004	0.296	0.303																	
1 1200	150	0.354	0.004	0.292	0.296																	
1 1215	165	0.327	0.002	0.288	0.294																	
1 1230	180									0.059												
1 1245	195	0.322	0.004	0.283	0.290			0.114				0.4053	0.4053	0.4667	0.4667	0.3447	0.3447	0.4266	0.4266	0.2176	0.2176	
1 1300	210	0.315	0.004	0.281	0.288																	
1 1315	225	0.320	0.004	0.276	0.283																	
1 1330	240	0.308	0.004	0.270	0.279																	
1 1345	255	0.310	0.004	0.275	0.275			0.110		0.054		0.3875	0.3875	0.4462	0.4462	0.3294	0.3294	0.4086	0.4086	0.2094	0.2094	
1 1400	270	0.305	0.004	0.266	0.266																	
1 1415	285	0.305	0.002	0.260	0.261																	
1 1430	300	0.305	0.002	0.249	0.255																	
1 1445	315	0.305	0.002	0.242	0.251			0.086				0.3721	0.3721	0.4276	0.4276	0.3147	0.3147	0.3896	0.3896	0.1953	0.1953	
1 1500	330	0.300	0.002	0.240	0.246																	
1 1515	345	0.293	0.002	0.236	0.242																	
1 1530	360	0.293	0.002	0.231	0.240																	
1 1530	360	0.290	0.006	0.234	0.240			0.057		0.077		0.3763	0.3763	0.4356	0.4356	0.3221	0.3221	0.3993	0.3993	0.2029	0.2029	

----- NO DATA TAKEN

LC-580
JP-4 (PET), 300 TORR.
1981 SEPT. 14

CLOCK TIME DAY HR. (MIN)	ELAPSED TIME (MIN)	N-C10 PPM SE-52C-2	N-C11 PPM SE-52C-2	BENZENE PPM SE-52C-2	O-XYL PPM SE-52C-2	C2BENZ PPM SE-52C-2	I-C3-BZ PPM SE-52C-2	M-C3-BZ PPM SE-52C-2	124TMBZ PPM SE-52C-2
1 930	0	0.1425	0.1478	0.0982	0.0497	0.1932	0.0513	0.0615	0.1182
1 1030	60	0.1698	0.1706	0.1015	0.0715	0.1989	0.0531	0.0651	0.1196
1 1130	120	0.1549	0.1712	0.0911	0.0631	0.1743	0.0471	0.0578	0.1055
1 1230	180	0.1482	0.1626	0.0894	0.0594	0.1697	0.0441	0.0546	0.1006
1 1330	240	0.1430	0.1610	0.0863	0.0498	0.1607	0.0424	0.0531	0.1079
1 1430	300	0.1297	0.1376	0.0832	0.0532	0.1546	0.0387	0.0480	0.0811
1 1530	360	0.1366	0.1451	0.0843	0.0558	0.1561	0.0407	0.0509	0.0860

----- NO DATA TAKEN

EC--SRI
JP-4 (PET), 350 TORR, 305 A
1981 SEPT. 15

0854: 200 TORR CYLINDER N2 INTO EC.
0853: 0.1 PPM M02 INTO EC.
0905: 0.4 PPM M0 INTO EC.
0908: 150 TORR, CYLINDER 02 INTO EC.
0923: BEGIN JP-4 FLUSH.
0927: 430 MICROLITERS JP-4 IN.
MAKE UP AIR SCHEDULE

TIME	PR	TO	PR
1111	347		352
1247	336		350
1324	344		350

T=0 AT 945 PDY
M1 = 0.475 MIM-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	REB C	MM. RELATIVE INTENSITY
T	BORIC-1	31.3	0.7			1.240
ID	INST.	INITIAL CONC.	UNITS			1.101
M0	T 14B-3	0.419	PPM			0.744
M02-UNC	T 14B-3	0.105	PPM			0.800
						0.700
						0.580
						0.500
						0.373
						0.237
						0.121
						0.019
						0.000

INSTRUMENTS USED

- ID LABEL DESCRIPTION
- 2750 SE-52C-2 RH-1211 20M SE-52 QUARTZ CAP. GC; FID
- 2200 BMS-1 RH-1211 DIMETHYLSULFOLANE GC; FID
- 2920 10'C-600 RH-1211 10' 10% CARBOWAX-600 GC; FID
- 2190 PM-2 RH-1033 S' POROPAK-N GC; FID
- 2000 ECB-1 RH-1211 12' 5% CARBOWAX-400 GC; ECD
- 1800 BORIC-1 DORIC TEMPERATURE INDICATOR, SN 61479
- 1530 T 14B-3 TECO 14B-3 MO-NIX ANALYZER
- 3000 CA CHROMOTROPIC ACID MCHO ANALYSIS
- 8410 M03-8410 MONITOR LABS 8410 03 ANALYZER (CHEMIL.)

EC-581
JP-4 (PET), 350 TORR, 305 A
1981 SEPT. 15

CLOCK TIME DAY HR. (MIN)	ELAPSED TIME (MIN)	OZONE PPM	NO PPM	NO2-UNC PPM	NOX-UNC PPM	T DEG C	PAN PPM	HCMD PPM	N-C6 PPM	N-C7 PPM	MECYC-C6 PPM	N-C8 PPM
		M03-8410	T 14B-3	T 14B-3	T 14B-3	DORIC-1	ECD-1	CA	SE-52C-2	SE-52C-2	SE-52C-2	SE-52C-2
1 942	-3							0.015				
1 945	0	0.031	0.419	0.105	0.519	30.1		0.059	0.4242	0.5219	0.3890	0.5028
1 1000	15	0.021	0.275	0.231	0.502	30.2						
1 1015	30	0.035	0.043	0.427	0.461	29.5						
1 1030	45	0.181	0.013	0.412	0.419	29.9						
1 1045	60	0.242	0.013	0.382	0.388	30.8	0.053	0.046	0.4087	0.4963	0.3684	0.4605
1 1100	75	0.314	0.013	0.358	0.363	31.6						
1 1115	90	0.356	0.013	0.339	0.346	32.3						
1 1130	105	0.398	0.013	0.322	0.328	31.7						
1 1145	120	0.412	0.013	0.309	0.313	31.3	0.104	0.094	0.3741	0.4531	0.3354	0.4226
1 1200	135	0.412	0.013	0.300	0.307	31.4						
1 1215	150	0.419	0.013	0.292	0.298	31.4						
1 1230	165	0.408	0.015	0.294	0.294	31.6						
1 1245	180	0.405	0.013	0.283	0.290	31.6	0.114		0.3817	0.4594	0.3413	0.4268
1 1300	195	0.391	0.015	0.281	0.288	31.6						
1 1315	210	0.391	0.015	0.275	0.283	31.4						
1 1330	225	0.377	0.017	0.275	0.281	31.4						
1 1345	240	0.377	0.017	0.266	0.275	31.4						
1 1400	255	0.381	0.017	0.261	0.270	31.6	0.102		0.3764	0.4547	0.3352	0.4216
1 1415	270	0.370	0.017	0.257	0.266	31.4						
1 1430	285	0.377	0.017	0.251	0.260	31.6						
1 1445	300	0.370	0.017	0.251	0.260	31.6	0.096	0.082	0.3626	0.4365	0.3225	0.4040
1 1500	315	0.349	0.017	0.249	0.255	31.7						
1 1515	330	0.356	0.017	0.245	0.253	31.6						
1 1530	345	0.349	0.017	0.245	0.253	31.8						
1 1538	353							0.096				
1 1545	360	0.345	0.017	0.238	0.246	31.6	0.080		0.3469	0.4184	0.3092	0.3877

----- NO DATA TAKEN

EC-581
JP-4 (PET), 350 TORR, 305 K
1981 SEPT. 15

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	M-C10 PPM	M-C11 PPM	BENZENE PPM	0-XYL PPM	C2BENZ PPM	I-C3-BZ PPM	M-C3-BZ PPM	124TNEBZ PPM
1 945	0	0.2459	0.1498	0.1768	0.0930	0.0825	0.2014	0.0593	0.0703	0.1386
1 1045	40	0.2388	0.1637	0.1815	0.0894	0.0657	0.1807	0.0484	0.0593	0.1277
1 1145	120	0.2208	0.1515	0.1699	0.0825	0.0622	0.1689	0.0457	0.0572	0.1209
1 1245	180	0.2227	0.1542	0.1744	0.0859	0.0620	0.1695	0.0459	0.0571	0.0998
1 1345	240	0.2183	0.1519	0.1733	0.0839	0.0602	0.1677	0.0445	0.0554	0.1004
1 1445	300	0.2095	0.1441	0.1620	0.0875	0.0584	0.1614	0.0432	0.0533	0.0913
1 1545	360	0.1980	0.1337	0.1464	0.0775	0.0549	0.1546	0.0402	0.0494	0.0861

----- M' DATA TAKEN

EC-587
JP-4 (PET), 740 TORR, 272 K
1981 SEPT. 23

0824: 10 TORR DRY PURE AIR, 0.1 PPM MD2.
0832: 0.4 PPM NO. BEGIN DRY PURE AIR FILL.
0900: FILLED.
0932: 430 MICROLITERS JP-4 (PET) INJECTED.

T=0 AT 1000 PSI

K1 = 0.475 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	-1.5	1.9	DEG C

ID	INST.	INITIAL	UNITS
MD	T 14B-3	0.432	PPM
MD2-UMC	T 14B-3	0.062	PPM

INSTRUMENTS USED

LV	LABEL	DESCRIPTION
2200	DMS-1	RM-1211 DIMETHYLSULFOLANE GC1 FID
2750	SE-52C-2	RM-1211 30M SE-52 QUARTZ CAP. GC1 FID
2100	PM-1	RM-121 POROPAK-N GC1 FID
2000	ECB-1	RM-1211 12" 5% CARBOMAX-400 GC1 ECD
2920	10'C-600	RM-1211 10' 10% CARBOMAX-600 GC1 FID
1800	DORIC-1	DORIC TEMPERATURE INDICATOR, SN 61479
1212	B-1212	DASIBI 1212 OZONE MONITOR
1530	T 14B-3	TECO 14B-3 NO-NOX ANALYZER
3000	CA	CHROMOTROPIC ACID HCHO ANALYSIS

LC-567
JP-4 (PET), 740 TORR, 272 K
1981 SEPT. 23

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPH	NO PPH	NO2-UNC PPH	NOX-UNC PPH	T DEG C	PAN PPH	MCMD PPH	M-C6 PPH	M-C7 PPH	MECYC-C6 PPH	M-C8 PPH
SAY NR.	(MIN)	D-1212	T 14B-3	T 14B-3	T 14B-3	BORIC-1	ECD-1	CA	8E-52C-2	8E-52C-2	8E-52C-2	8E-52C-2
1 945	-15	0.000	0.402	0.051	0.456	-6.8	---	---	---	---	---	---
1 1000	0	0.000	0.432	0.062	0.496	-7.3	---	0.000	0.3850	0.4657	0.3429	0.4312
1 1001	1	---	---	---	---	---	---	---	---	---	---	---
1 1015	15	0.000	0.426	0.076	0.504	0.9	---	---	---	---	---	---
1 1030	30	0.000	0.419	0.099	0.523	1.5	---	---	---	---	---	---
1 1045	45	0.000	0.394	0.104	0.501	1.9	---	---	---	---	---	---
1 1100	60	0.017	0.371	0.130	0.504	-1.7	---	---	0.3871	0.4676	0.3442	0.4322
1 1105	45	---	---	---	---	---	---	0.000	---	---	---	---
1 1115	75	0.022	0.340	0.159	0.501	-1.8	---	---	---	---	---	---
1 1130	90	0.022	0.305	0.194	0.500	-1.8	---	---	---	---	---	---
1 1145	105	0.024	0.264	0.217	0.483	-1.8	---	---	---	---	---	---
1 1200	120	0.037	0.238	0.266	0.504	-1.7	0.004	---	0.3763	0.4561	0.3364	0.4184
1 1215	135	0.037	0.200	0.292	0.494	-1.7	---	---	---	---	---	---
1 1230	150	0.039	0.168	0.312	0.482	-1.8	---	---	---	---	---	---
1 1245	165	0.049	0.139	0.330	0.471	-1.8	---	---	---	---	---	---
1 1300	180	0.054	0.122	0.343	0.465	-1.7	0.013	0.004	0.3684	0.4369	0.3262	0.4058
1 1315	195	0.043	0.099	0.354	0.454	-1.7	---	---	---	---	---	---
1 1330	210	0.048	0.085	0.362	0.448	-1.8	---	---	---	---	---	---
1 1345	225	0.073	0.074	0.361	0.435	-1.7	---	---	---	---	---	---
1 1400	240	0.083	0.062	0.362	0.426	-1.7	0.021	0.000	0.3657	0.4313	0.3208	0.3973
1 1415	255	0.090	0.056	0.358	0.417	-1.2	---	---	---	---	---	---
1 1430	270	0.100	0.050	0.341	0.412	-1.1	---	---	---	---	---	---
1 1445	285	0.105	0.041	0.357	0.402	-1.1	---	---	---	---	---	---
1 1500	300	0.120	0.039	0.355	0.396	-0.8	0.026	0.000	0.3588	0.4239	0.3183	0.3908
1 1515	315	0.122	0.033	0.354	0.390	-0.7	---	---	---	---	---	---
1 1530	330	0.134	0.029	0.351	0.383	-0.8	---	---	---	---	---	---
1 1545	345	0.139	0.028	0.343	0.374	-0.8	---	---	---	---	---	---
1 1550	350	---	---	---	---	---	---	0.000	---	---	---	---
1 1600	360	0.151	0.026	0.343	0.368	-1.2	0.034	---	0.3531	0.4175	0.3105	0.3838

----- NO DATA TAKEN

EC-587
JP-4 (PET), 740 TORR, 272 K
1981 SEPT. 23

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	M-C9 PPM SE-52C-2	M-C10 PPM SE-52C-2	M-C11 PPM SE-52C-2	BENZENE PPM SE-52C-2	O-XYL PPM SE-52C-2	C2BENZ PPM SE-52C-2	I-C3-BZ PPM SE-52C-2	M-C3-BZ PPM SE-52C-2	124THEBZ PPM SE-52C-2
1 1000	0	0.2222	0.1505	0.1598	0.0835	0.0430	0.1674	0.0460	0.0554	0.1104
1 1100	60	0.2249	0.1528	0.1672	0.0847	0.0648	0.1673	0.0476	0.0574	0.1111
1 1200	120	0.2148	0.1441	0.1584	0.0850	0.0594	0.1453	0.0442	0.0538	0.1043
1 1300	180	0.2079	0.1428	0.1559	0.0823	0.0564	0.1567	0.0424	0.0515	0.1001
1 1400	240	0.2023	0.1378	0.1494	0.0815	0.0543	0.1550	0.0410	0.0495	0.0955
1 1500	300	0.1980	0.1350	0.1455	0.0769	0.0528	0.1521	0.0397	0.0480	0.0931
1 1600	360	0.1944	0.1318	0.1409	0.0764	0.0516	0.1484	0.0391	0.0470	0.0911

----- NO DATA TAKEN

EC-588
JP-4 (PET), 740 TORR, 285 K
1981 SEPT. 24

0822: 0.1 PPM NO2.
0828: 0.4 PPM NO. FILL WITH DRY PURE AIR.
0853: 430 MICROLITERS JP-4 INJECTED.

T=0 AT 1000 PST

AI = 0.475 MIN-1

SPECTRAL DISTRIBUTION

MM.	RELATIVE INTENSITY
500	0.380
430	0.289
403	0.252
380	0.214
370	0.187
360	0.157
350	0.500
340	0.098
330	0.042
320	0.029
310	0.009
300	0.000

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	11.9	0.9	DEG C
ID	INST.	INITIAL CONC.	UNITS	
NO	T 14B-3	0.362		PPM
NO2-UMC	T 14B-3	0.094		PPM

INSTRUMENTS USED

ID LABEL DESCRIPTION
 2750 SE-52C-2 RH-1211 30M SE-52 QUARTZ CAP. GC1 FID
 2920 10°C-600 RH-1211 10' 10% CARBOMAX-600 GC1 FID
 2200 BMS-1 RH-1211 DIMETHYLSULFOLANE GC1 FID
 2100 PH-1 RH-121 FOROPAK-N GC1 FID
 2000 ECP-1 RH-1211 12" SE CARBOMAX-400 GC1 EGS
 1800 DORIC-1 DORIC TEMPERATURE INDICATOR, SN 61479
 1817 P-1070 BABI DI 1070 OZONE MONITOR
 1330 T 14B-3 TECO 14B-3 NO-NOX ANALYZER
 3000 CA CHROMOTROPIC ACID HCHO ANALYSIS

EL-588
JP-4 (PET), 740 TORR, 265 A
1981 SEPT. 24

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	D-1070	NO PPM	T 14B-3	MO2-UNC PPM	T 14B-3	MOX-UNC PPM	T 14B-3	DORIC-1	DEG C	FAN PPM	ECD-1	HCHO PPM	CA	0.017	N-C6 PPM	SE-52C-2	N-C7 PPM	SE-52C-2	MECYC-C6 PPM	SE-52C-2	N-C8 PPM	SE-52C-2	
1 952	0	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1000	8	---	---	0.362	---	0.094	---	0.458	---	13.7	---	---	---	---	---	---	0.4253	---	---	---	0.3816	---	---	0.4765	
1 1015	15	---	---	0.305	---	0.144	---	0.451	---	14.9	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1030	30	---	---	0.224	---	0.211	---	0.439	---	13.8	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1045	45	---	---	0.141	---	0.271	---	0.415	---	12.8	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1100	60	0.007	---	0.078	---	0.327	---	0.407	---	12.0	---	0.013	---	0.008	---	---	0.3984	---	---	---	0.3525	---	---	0.4375	
1 1115	75	0.044	---	0.042	---	0.344	---	0.389	---	11.9	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1130	90	0.088	---	0.051	---	0.351	---	0.378	---	11.8	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1145	105	0.124	---	0.032	---	0.339	---	0.358	---	11.6	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1200	120	0.163	---	0.013	---	0.338	---	0.354	---	11.6	---	0.037	---	0.013	---	---	0.3829	---	---	---	0.3373	---	---	0.4191	
1 1215	135	0.190	---	0.011	---	0.328	---	0.340	---	11.6	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1230	150	0.232	---	0.009	---	0.322	---	0.332	---	11.4	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1245	165	0.259	---	0.007	---	0.297	---	0.307	---	11.5	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1300	180	0.275	---	0.006	---	0.295	---	0.303	---	11.5	---	0.060	---	0.013	---	---	0.3877	---	---	---	0.3381	---	---	0.4158	
1 1315	195	0.284	---	0.004	---	0.294	---	0.301	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1330	210	0.315	---	0.005	---	0.289	---	0.294	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1345	225	0.334	---	0.005	---	0.284	---	0.294	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1400	240	0.364	---	0.005	---	0.273	---	0.280	---	11.5	---	0.074	---	0.017	---	---	0.3717	---	---	---	0.3250	---	---	0.4021	
1 1415	255	0.383	---	0.005	---	0.264	---	0.269	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1430	270	0.394	---	0.005	---	0.257	---	0.263	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1445	285	0.415	---	0.005	---	0.247	---	0.253	---	11.3	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1500	300	0.432	---	0.005	---	0.235	---	0.241	---	11.8	---	0.090	---	0.019	---	---	---	---	---	---	---	---	---	---	---
1 1515	315	0.447	---	0.005	---	0.229	---	0.235	---	11.5	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1530	330	0.454	---	0.004	---	0.222	---	0.228	---	11.5	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1545	345	0.466	---	0.005	---	0.214	---	0.222	---	11.8	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1550	350	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---
1 1600	360	0.483	---	0.005	---	0.211	---	0.217	---	11.6	---	0.092	---	0.017	---	---	0.3644	---	---	---	0.3166	---	---	0.3972	

NO DATA TAKEN

EC-588
JP-4 (PET), 740 TORR, 285 K
1981 SEPT. 24

CLOCK TIME	ELAPSED TIME (MIN)	M-C9 PPM	M-C10 PPM	M-C11 PPM	BENZENE PPM	O-XYL PPM	C2BENZ PPM	1-C3-B2 PPM	M-C3-B2 PPM	124THEDZ PPM
1 1000	0	0.2451	0.1690	0.1932	0.1009	0.0695	0.1940	0.0512	0.0422	0.1231
1 1100	40	0.2258	0.1543	0.1810	0.0873	0.0431	0.1740	0.0469	0.0575	0.1101
1 1200	120	0.2179	0.1510	0.1742	0.0815	0.0405	0.1464	0.0454	0.0557	0.1071
1 1300	180	0.2154	0.1486	0.1725	0.0872	0.0410	0.1414	0.0459	0.0559	0.1070
1 1400	240	0.2046	0.1422	0.1632	0.0803	0.0371	0.1552	0.0462	0.0512	0.0993
1 1400	340	0.2020	0.1372	0.1545	0.0787	0.0374	0.1558	0.0421	0.0516	0.0897

----- NO DATA TAKEN

EC-591
JP-8 (PET), GROUND LEVEL
1981 OCT. 7

0833: 0.1 PPM NO2 AND 0.4 PPM NO INTO EC.
306 MICROLITERS JP-8(PET) INTO EC.
0848: 502 R.H. PURE AIR FILL.
0900: FILLED.

T=0 AT 930 PST
A1 = 0.340 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS
T	DORIC-1	30.7	0.9	DEG C
ID	INST.	INITIAL CONC.	UNITS	
NO	T 14B-3	0.476	PPM	
NO2-UNC	T 14B-3	0.098	PPM	

SPECTRAL DISTRIBUTION

WV. INTENSITY	RELATIVE INTENSITY
500	1.705
430	1.240
403	1.023
380	0.873
370	0.734
360	0.600
350	0.500
340	0.342
330	0.217
320	0.098
310	0.026
300	0.000

INSTRUMENTS USED

ID	LABEL	DESCRIPTION
2650	VAR 3700	VARIAN GC1 30M SE-54 QUARTZ CAP. GC1 FID
1800	DORIC-1	DORIC TEMPERATURE INDICATOR, SN 61479
1212	B-1212	BASIBI 1212 OZONE MONITOR
1330	T 14B-3	TECO 14B-3 NO-NOX ANALYZER
3000	CA	CHROMOTROPIC ACID MCHO ANALYSIS

EC-591
JP-8 (PET), GROUND LEVEL
1981 OCT. 7

CLOCK TIME	ELAPSED TIME (MIN)	OZONE PPM	MO PPM	MO2-UNC PPM	MOX-UNC PPM	T DEG C	MCHO PPM	M-C9 PPM	M-C10 PPM	M-C11 PPM	M-C12 PPM	M-C13 PPM
DAY NR.		B-1212	T 14B-3	T 14B-3	T 14B-3	DORIC-1	CA	VAR 3700	VAR 3700	VAR 3700	VAR 3700	VAR 3700
1	928	-2					0.008					
1	930	0	0.041	0.098	0.571	28.3						
1	945	15	0.044	0.119	0.559	28.6						
1	1000	30	0.029	0.161	0.549	28.8						
1	1015	45	0.022	0.195	0.541	29.7						
1	1030	60	0.017	0.244	0.534	30.1	0.002	0.0257	0.0856	0.2829	0.3036	0.2264
1	1045	75	0.017	0.302	0.520	30.5						
1	1100	90	0.024	0.346	0.507	30.6						
1	1115	105	0.041	0.400	0.478	30.7						
1	1130	120	0.071	0.424	0.483	30.9	0.015	0.0257	0.0843	0.2947	0.3272	0.2469
1	1145	135	0.115	0.424	0.461	30.9						
1	1200	150	0.146	0.415	0.439	30.9						
1	1215	165	0.220	0.393	0.415	30.9						
1	1230	180	0.249	0.378	0.395	31.0	0.004	0.0243	0.0798	0.2745	0.3028	0.2344
1	1245	195	0.315	0.354	0.368	31.1						
1	1300	210	0.354	0.329	0.341	31.0						
1	1315	225	0.394	0.305	0.322	31.1						
1	1330	240	0.427	0.283	0.295	31.0	0.004	0.0241	0.0783	0.2708	0.2959	0.2327
1	1345	255	0.452	0.261	0.275	31.0						
1	1400	270	0.474	0.244	0.256	31.1						
1	1415	285	0.460	0.227	0.239	31.3						
1	1430	300	0.493	0.217	0.229	31.3	0.043	0.0235	0.0762	0.2673	0.2906	0.2297
1	1445	315	0.493	0.207	0.219	31.3						
1	1500	330	0.491	0.200	0.212	31.3						
1	1515	345	0.483	0.197	0.209	31.4						
1	1530	360	0.474	0.195	0.205	31.4	0.084	0.0224	0.0697	0.2172	0.1897	0.1077

MO DATA TAKEN

EC-591
JP-8 (PET), GROUND LEVEL
1981 OCT. 7

CLOCK TIME	ELAPSED TIME (MIN)	N-C14 PPH
BAY NR.	(MIN)	VAR 3700
1 930	0	----- A
1 1030	40	0.144
1 1130	120	0.121
1 1230	180	0.119
1 1330	240	0.124
1 1430	300	0.124
1 1530	360	0.044

----- NO DATA TAKEN

NOTES

A T-O ABORTED.

EC-592
JP-8 (PET), GROUND LEVEL
1981 OCT. 8

0847: 10 TORR. PURE AIR.
INJECTED 0.1 PPM NO2 AND 0.4 PPM NO.
INJECTED 193 MICROLITERS JP-8(PET).
50X R.N. PURE AIR FILL.

T=0 AT 930 P81

R1 = 0.140 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	MIN.	RELATIVE INTENSITY
T	DORIC-1	31.1	1.4	DEG C	500	1.744
ID	INST.	INITIAL CONC.		UNITS	430	1.272
NO	T 14D-3	0.419		PPM	403	1.077
NO2-UMC	T 14D-3	0.158		PPM	380	0.899
					376	0.740
					360	0.600
					350	0.500
					340	0.342
					330	0.217
					320	0.098
					310	0.024
					300	0.000

INSTRUMENTS USED

ID LABEL DESCRIPTION
2450 VAR 3700 VARIAN GC1 30H SE-54 QUARTZ CAP. GC1 FID
1000 DORIC-1 BORIC TEMPERATURE INDICATOR. SN 41479
1212 B-1212 BASIDI 1212 OZONE MONITOR
1530 T 14D-3 TECO 14D-3 NO-NOX ANALYZER
3000 CA CHROMOTROPIC ACID NCMD ANALYSIS

EC-592
JP-8 (PET), GROUND LEVEL
1981 OCT. 8

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	OZONE PPM B-1212	NO PPM T 14B-3	NO2-UNC PPM T 14B-3	NOX-UNC PPM T 14B-3	T DEG C DORIC-1	MCHO PPM CA	N-C9 PPM VAR 3700	N-C10 PPM VAR 3700	N-C11 PPM VAR 3700	N-C12 PPM VAR 3700	M-C13 PPM VAR 3700
1 930	0	0.088	0.419	0.158	0.578	28.6	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 935	5	0.024	0.402	0.166	0.566	28.7	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 945	15	0.022	0.373	0.180	0.556	28.7	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1000	30	0.017	0.339	0.209	0.549	29.2	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1015	45	0.012	0.295	0.249	0.541	29.8	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1030	60	0.010	0.253	0.280	0.534	30.1	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1045	75	0.010	0.205	0.322	0.524	30.4	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1100	90	0.017	0.151	0.361	0.512	30.9	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1115	105	0.029	0.109	0.373	0.505	31.0	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1130	120	0.051	0.073	0.419	0.493	31.0	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1145	135	0.078	0.051	0.427	0.478	30.9	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1200	150	0.110	0.034	0.427	0.461	31.0	0.006	0.0229	0.0602	0.1604	0.1762	0.1416
1 1215	165	0.149	0.024	0.422	0.444	31.3	0.008	0.0229	0.0602	0.1604	0.1762	0.1416
1 1230	180	0.185	0.020	0.410	0.424	31.3	0.008	0.0229	0.0602	0.1604	0.1762	0.1416
1 1245	195	0.225	0.017	0.393	0.410	31.3	0.008	0.0229	0.0602	0.1604	0.1762	0.1416
1 1300	210	0.266	0.015	0.375	0.390	31.3	0.013	0.0229	0.0602	0.1604	0.1762	0.1416
1 1315	225	0.295	0.012	0.358	0.371	31.4	0.013	0.0229	0.0602	0.1604	0.1762	0.1416
1 1330	240	0.327	0.012	0.341	0.351	31.4	0.013	0.0229	0.0602	0.1604	0.1762	0.1416
1 1345	255	0.361	0.012	0.322	0.332	31.6	0.013	0.0229	0.0602	0.1604	0.1762	0.1416
1 1400	270	0.393	0.010	0.302	0.312	32.0	0.013	0.0229	0.0602	0.1604	0.1762	0.1416
1 1415	285	0.422	0.012	0.285	0.292	32.6	0.010	0.0229	0.0602	0.1604	0.1762	0.1416
1 1430	300	0.454	0.010	0.268	0.275	33.3	0.010	0.0229	0.0602	0.1604	0.1762	0.1416
1 1445	315	0.481	0.010	0.251	0.258	34.2	0.010	0.0229	0.0602	0.1604	0.1762	0.1416
1 1500	330	0.500	0.010	0.239	0.246	33.1	0.015	0.0229	0.0602	0.1604	0.1762	0.1416
1 1515	345	0.508	0.010	0.224	0.231	31.9	0.015	0.0229	0.0602	0.1604	0.1762	0.1416
1 1520	350	0.508	0.010	0.224	0.231	31.9	0.015	0.0229	0.0602	0.1604	0.1762	0.1416
1 1530	360	0.508	0.010	0.224	0.231	31.9	0.015	0.0229	0.0602	0.1604	0.1762	0.1416

----- NO DATA TAKEN

EC-592
JP-8 (PET), GROUND LEVEL
1981 OCT. 8

CLOCK TIME DAY NR.	ELAPSED TIME (MIN)	N-C14 PPM VAR 3700
1 930	0	0.077
1 1030	40	0.055
1 1130	120	0.045
1 1230	180	0.045
1 1330	240	0.056
1 1430	300	0.039
1 1530	360	0.049

----- NO DATA TAKEN

EC-595
JP-8 (PET), SIMULATED 20,000 FEET
1981 OCT. 14

0820: FILL WITH DRY PURE AIR.
0832: INJECTED 386 MICROLITERS JP-8(PET).
0840: INJECTED 0.1 PPM NO2.
0855: INJECTED 0.4 PPM NO.
0915: T=0.

T=0 AT 915 PST

KJ = 0.430 MIN-1

ID	INST.	AVERAGE VALUE	S.DEV	UNITS	MM.	RELATIVE INTENSITY
T	DORIC-1	-0.1	1.4	DEG C	500	1.720
ID	INST.	INITIAL CONC.	UNITS		430	1.248
NO	T 14B-3	0.419	PPM		403	1.050
NO2-UNC	T 14B-3	0.077	PPM		380	0.972
					370	0.747
					360	0.618
					350	0.500
					340	0.362
					330	0.235
					320	0.110
					310	0.020
					300	0.000

SPECTRAL DISTRIBUTION

INSTRUMENTS USED

ID LABEL DESCRIPTION
2650 VAR 3700 VARIAN GCJ 30H SE-54 QUARTZ CAP. GCJ FID
1800 BORIC-1 DORIC TEMPERATURE INDICATOR, SM 61479
1017 B-1070 DASIBI 1070 OZONE MONITOR
1530 T 14B-3 TECO 14B-3 NO-NOX ANALYZER
1000 CA CHROMOTROPIC ACID MCHO ANALYSIS

EL-595
 JP-8 (PET), SIMULATED 20,000 FEET
 1981 OCT. 14

21-OCT-82
 PAGE 2

CLOCK TIME DAY HR.	ELAPSED TIME (MIN)	OZONE PPM D-1070	NO PPM T 14B-3	NO2-UNC		NOX-UNC		T DEG C DORIC-1	HCHO PPM CA	N-C9 PPM VAR 3700	N-C10 PPM VAR 3700	N-C11 PPM VAR 3700	N-C12 PPM VAR 3700	N-C13 PPM VAR 3700
				PPM T 14B-3	PPM T 14B-3	PPM T 14B-3	PPM T 14B-3							
1 915	0	0.000	0.419	0.077	0.498	-4.8								
1 930	15	0.000	0.414	0.084	0.498	-1.9								
1 945	30	0.000	0.408	0.088	0.498	-1.8								
1 1000	45	0.000	0.400	0.095	0.495	-1.6								
1 1015	60	0.000	0.389	0.097	0.488	-1.6								
1 1030	75	0.000	0.376	0.110	0.486	-1.4								
1 1045	90	0.000	0.367	0.118	0.484	-0.7								
1 1100	105	0.000	0.352	0.125	0.479	-0.7								
1 1115	120	0.000	0.337	0.133	0.473	-0.4								
1 1130	135	0.000	0.322	0.146	0.468	0.0								
1 1145	150	0.000	0.303	0.157	0.459	0.4								
1 1200	165	0.002	0.286	0.165	0.449	0.6								
1 1215	180	0.002	0.267	0.178	0.447	0.6								
1 1225	190	---	---	---	---	---								
1 1230	195	0.002	0.249	0.185	0.436	0.6								
1 1245	210	0.005	0.232	0.195	0.429	0.4								
1 1300	225	0.005	0.217	0.202	0.419	0.4								
1 1315	240	0.005	0.200	0.210	0.410	0.4								
1 1330	255	0.010	0.185	0.217	0.401	0.6								
1 1345	270	0.007	0.170	0.223	0.393	0.7								
1 1400	285	0.010	0.159	0.230	0.386	1.2								
1 1415	300	0.012	0.146	0.232	0.378	1.3								
1 1425	310	---	---	---	---	---								
1 1430	315	0.015	0.128	0.243	0.371	1.2								
1 1445	330	0.015	0.118	0.245	0.363	1.3								
1 1500	345	0.020	0.110	0.245	0.355	1.3								
1 1510	355	---	---	---	---	---								
1 1515	360	0.022	0.099	0.249	0.348	1.2								

NO DATA TAKEN

NOTES

- A ABORTED. RMT NOT ENGAGED.
- B ABORTED. RETENTION TIMES NOT IDENTIFIYABLE.
- C SAMPLE SKIPPED DUE TO SLOWNESS OF PROGRAM.

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END

FILMED

3-83

DTIC