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September 27, 1974

Secretary, Technical Task Group on
Vinyl Chloride Research
Manufacturing Chemists Association
1825 Connecticut Avenue, N.W.
Washington, D.C. 20009

Attention: Dr. Kenneth D. Johnson

Subject: Proposal No. IITRI-75-68C
"The Role of Vinyl Chloride in
the Urban Industrial Environment"

Dear Dr. Johnson:

In response to your letter, dated August 6, 1974, IIT Research Institute is pleased to present a research program aimed toward the elucidation of possible health problems related to the presence of vinyl chloride in the atmosphere. The object of this proposed program is to find the answers as rapidly, facilely and thoroughly as possible, and each phase of the program will progress only if warranted from the results of the previous step.

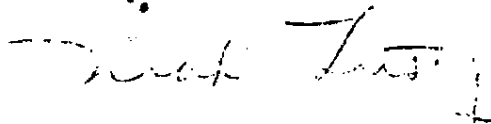
. A 6-man-month study is first presented with a cost estimate of \$35,000. This phase of the program is devoted to the gathering of information in the field regarding the concentration of vinyl chloride as well as species that may be formed from it in the ambient air surrounding several vinyl chloride plants. A careful search will be made for the presence of any harmful or even potentially harmful agents.

If the field testing shows the presence of undesirable intermediates and products and does not allow sufficient understanding of the processes leading to the formation of such substances, then a second phase of the program is suggested.

iii

This phase is designed to obtain an understanding of the photo- and thermochemical behavior of vinyl chloride in the urban-industrial atmosphere. Based on the results of the first phase work, carefully selected laboratory scale and smog chamber experiments will be devised to achieve this goal. Kinetic information will be obtained on the decomposition of vinyl chloride as well as on the formation of its reaction products. The smog chamber research may also include the examination of the behavior of vinyl chloride in a typical Chicago aerosol. An accurate understanding of the chemical properties of vinyl chloride in polluted air is vital in order to establish appropriate counter-measures against the accumulation of vinyl chloride or toxic matter formed from its presence. The duration of this part of the program is estimated to be one-man-year if carried out to its entirety. No cost estimate will be given at this time.

Respectfully submitted,
IIT RESEARCH INSTITUTE


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Approved by

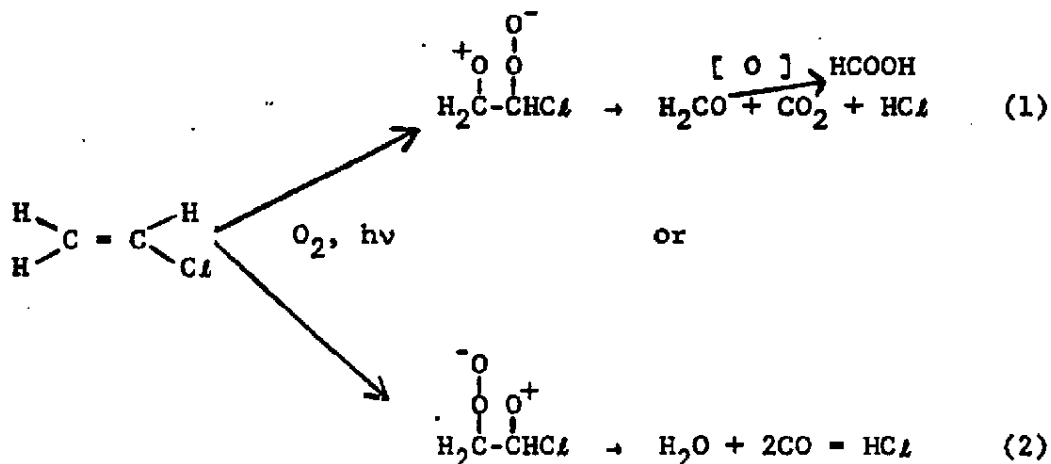
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THE ROLE OF VINYL CHLORIDE IN THE URBAN-INDUSTRIAL ENVIRONMENT

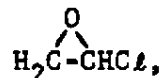
1. INTRODUCTION

The purpose of our proposed investigation is to ascertain the fate of vinyl chloride in urban-industrial air, particularly with respect to its toxic effect on human beings. The cause-effect relationship between vinyl chloride and cancer in workers, who are in daily contact with it, has recently become an important social issue. Possibly vinyl chloride may be a precursor to one or more carcinogens formed from it either in the atmosphere and/or in the human system. The important questions that must be answered are: (1) what happens to vinyl chloride once it enters the atmosphere, how long a time period does it remain intact, and (2) is it converted to potent carcinogens or otherwise hazardous substances or harmless agents.

Very little is known of its fate when it is present in the atmosphere other than its reported mild photoreactivity. However, Dr. P. Hanst¹ of the Environmental Protection Agency has performed smog chamber experiments and has found that vinyl chloride is photochemically converted to hydrogen chloride, water vapor, carbon monoxide, carbon dioxide, formaldehyde, and formic acid. The latter, formic acid, is a presumably an oxidation product of formaldehyde. These products can be explained, for the most part, as being derived via zwitter ion intermediates postulated by Criegee² from the ozonation of alkenes, i.e.,



According to Hanst¹, there is no evidence for the formation of an epoxide,



which has been postulated as a carcinogen. This epoxide may be formed by enzyme action on vinyl chloride when it is present in the human body, but confirmation of this point is not to be considered in the present work.

Because of Hanst's results, we propose proceeding directly to field tests as our first phase study and monitor for such constituents as vinyl chloride, hydrogen chloride, formaldehyde, formic acid etc. We will also perform a careful search for any air component that can be hazardous. If these results are not completely understood it may be necessary, with the agreement of IITRI and MCA, to conduct additional laboratory experiments.

2. WORK STATEMENT

2.1 Field Tests (Phase I)

- A large number of air samples will be collected and analyzed.
- Analytical techniques will be tested and developed to meet the program goals.

2.2 Laboratory and Smog Chamber Experiments (Phase II)

- If the objective of the program is not achieved by field testing, then, upon mutual agreement between MCA and IITRI, a variety of selected laboratory experiments will be conducted in order to determine the behavior of vinyl chloride towards known air pollutants.
- Analytical methods will be adapted to the continuous monitoring of the progress of the reactions.
- Reaction kinetics will be measured.
- These reactions will also be evaluated within a smog chamber.
- The smog chamber work will include the examination of the reactivity of vinyl chloride in a typical Chicago aerosol.

3. RATIONALE AND PROPOSED WORK

The results made available by Hanst¹ are very valuable because they provide us with the information needed to conduct field tests as our first stage of the program, since we know what substances for which to monitor. If, e.g., hydrogen chloride, formaldehyde etc. are present in greater than their normal atmospheric abundance and not produced from other sources than vinyl chloride plants, then these substances are the presumed products of this precursor, provided equations (1) and (2) are valid as being representative of the principal reaction paths. Conventional procedures for sampling and analysis should be adequate for this work, (see section 3.1.2). However, some effort would be required to determine the

stability and recovery of the vinyl chloride from the sampling collector. In addition, techniques already developed by IITRI for ambient air sampling and analysis will also be utilized in this program. We believe that the application of the gas chromatograph-mass spectrometer will be enormously beneficial to air constituent identification, for each of the numerous peaks expected on the gas chromatogram will be related to a mass spectral cracking pattern that can be used for identification purposes. Also available at IITRI is dual column chromatography which is one of the most refined techniques for resolving similar components in a mixture. If our analyses do not indicate the presence of known harmful agents or even potentially toxic substances, then the program can be re-evaluated at that time.

If, on the other hand, such substances are found, then it would be necessary to proceed to an in-depth examination to elucidate their nature and the processes leading to these materials with laboratory and smog chamber experimentation in order to conceive of procedures to retard their formation. Enough information needs to be accumulated in order to predict hazardous events in advance. To achieve this goal, information concerning the distribution of pollutants from a vinyl chloride facility, the chemical properties of these pollutants, plant production habit, and meteorological data must be correlated. Therefore, more samples need to be collected but under different weather or climate conditions and at various times relative to vinyl chloride production.

Consequently, the field testing will be conducted in the following manner. Initially, samples will be collected at three different plants, at the plant cite and at several instances from the plant simultaneously at various time intervals during the diurnal period. Approximately 30 samples will be collected at each plant vicinity. If unacceptable quantities of vinyl chloride or other hazardous substances

are identified, then the sampling will be performed once again toward the end of this phase of the program to check the initial results and also to take into consideration changes in weather or climatic conditions. Three plant sites will be selected to allow for the different nature of air pollutants in the environment of each plant. A portable weather station, developed by MRI, will be employed.

The laboratory and smog chamber experiments will be more time consuming and expensive and we will proceed to these studies only if it is felt (by agreement between IITRI and MCA) that the Field Monitoring Studies have not satisfactorily defined the problem and not answered the question as to the fate of vinyl chloride in the environment. Eventhough these studies may not be carried out, they will be discussed at the present time.

In the laboratory we plan to rapidly and as simply as possible demonstrate the gross chemical behavior of vinyl chloride individually or in combination with common air contaminants. For example, its thermo-(dark) and photochemical reactions with ozone, nitrogen oxides (NO_x) and various hydrocarbon derivatives including aldehydes etc. known to be present in the urban air will be studied on the laboratory scale using routine thermolysis and photolysis techniques. The information obtained from such experiments will permit kinetic and mechanistic interpretation of the reactions taking place. At the same time, techniques and methods for product identification and characterization will be developed. Particular scrutiny will be given to those agents which may be potential carcinogens or otherwise toxic. A number of analytical methods can be of general utility for detection and identification, such as gas chromatographic retention times gas chromatography-mass spectrometry combination, and several spectroscopic techniques (optical, nuclear magnetic resonance, electron paramagnetic resonance, mass spectroscopy), and wet

analytical procedures.

There can be differences between reactions taking place in the confines of a laboratory apparatus and those occurring in the open environment, i.e., in the former case surface contact can alter the course of reactions while in the latter the surface contact is minimized. Consequently, a simulation of the "open" environment can be obtained by use of a smog chamber. So the next step of Phase II will involve smog chamber studies of carefully selected reactions from the group considered above using vinyl chloride as the common substrate. Simulated sunlight will be applied. Analytical procedures will be adapted for the direct and continuous monitoring of products formed within the smog chamber, and comparisons will be made with the laboratory scale reactions.

Once the behavior of vinyl chloride is generally understood, more sophisticated experiments will be conducted involving vinyl chloride in a typical Chicago aerosol within the smog chamber; this aerosol will include not only molecular substances but also particulate and pollen matter. The same general analytical procedures will be applied to this phase of the research, except that the sensitivity of the techniques will be in the ppm and pphm range.

3.1 Field Monitoring Study

3.1.1 Field Sampling

Samples of air (between 90 and 180 samples) will be collected near three vinyl chloride facilities at various time intervals during the diurnal period and simultaneously at the plant cite and different distances from the plants. Samples will be analyzed at IITRI for vinyl chloride and other major components present. Those species which may be potentially harmful will be characterized by spectroscopic methods adapted to the determination of trace quantities. Sampling and

analytical techniques will be developed to satisfy the requirements of the program, although conventional procedures should generally apply. In addition several sampling methods developed at IITRI should be directly applicable to these studies, but, in this program as well as in others, preliminary sampling and recovery experiments will be required to determine the efficiency of the over-all method.

3.1.2 Analytical Methodology

Analytical procedures of high sensitivity for isolating and determining the organic and inorganic materials derived from vinyl chloride are well established. Some general methods also have been developed at IITRI for application to ventures similar to that proposed herein. All the procedures involve collection of gaseous substances by entrapment via absorption or adsorption in a matrix. The materials are then chemically or thermally desorbed and then measured by a technique using a two-column gas chromatograph coupled to a mass spectrometer or by chemical analysis. Furthermore, gaseous constituents in air can be identified in the ppm or even pphm range by a variety of spectroscopic techniques. Gas chromatograph-mass spectrometry is one very important tool that can be used for routine detection and identification at very low concentration levels. Optical spectra measurements (ultraviolet, visible, infrared) of ambient air can be obtained by placing gaseous samples either in cells containing mirrors to achieve long path lengths or by freezing the samples in a solid matrix at a low temperature. This analytical application has been used with success in other related studies. Some specific and relevant techniques already employed are described below.

3.1.2.1 Collection and Detection of Organic Vapors in Air

The organic components of air to be analyzed will be collected using method number P&CAM 127 developed by NIOHS. That is, organic vapors present in air are adsorbed on activated charcoal as a known column of air is drawn through the

pecially designed tube. The compounds adsorbed on the charcoal are desorbed by carbon disulfide. A aliquat of the desorbed sample is then analyzed by gas chromatography. Vinyl chloride present in the mixture can be detected in the ppm level using a 6' x 1/8" stainless steel column packed with 0.4% carbowax 1500 on Carbowax A.³ The analyses are performed at room temperature and a nitrogen flow rate of 20 cc/min and its retention time is 2 min. If increased resolution is required due to sample complexity an alternate two column gas chromatographic technique developed at this institute can be used. The procedure involves the transfer of the substances producing an individual peak to a secondary column where additional separation can take place. The two columns are of opposite polarity for maximum separation.

3.1.2.2 Collection and Detection of Gaseous Hydrogen Chloride in Air

Gaseous hydrogen chloride may be detected in the air in the ppm level using a technique developed by T. Okita⁴. A known volume of air is drawn through a combination millipore-sodium carbonate impregnated filter. The chloride collected on the filter was entrained in boiling water. The analyses of chloride was made colorimetrically using the Volhard method. It is important to note that organic chlorides such as vinyl chloride are not trapped on the filter.

3.2 Laboratory and Smog Chamber Experiments

3.2.1 Laboratory Experiments

The results of Phase I may necessitate an extended program if hazardous agents are found. To obtain more elaborate statistics, more air samples will be collected under varying weather conditions and plant production schedules and the data will be correlated according to these variables. Based on the findings from the Phase I work, several selected photo- and thermochemical reactions between vinyl chloride and the known air pollutants, individually, will be studied. These experi-

ments would be the fastest and easiest manner to obtain results. The progress of the reactions will be monitored continuously. The products will be identified and the reaction kinetics will be measured.

3.2.2 Smog Chamber Extension of Laboratory Scale Experiments

Because gas phase reactions on a laboratory scale may be inhomogeneous due to surface effects, it may prove advisable to examine some of the same reactions in a smog chamber where these surface catalyzed effects are minimized. These reactions would also be followed by monitoring devices and kinetic comparisons will be made.

3.2.3 Urban Aerosol Smog Chamber Experiments

Because aerosols contain particulates in addition to molecular species, there may be differences between the chemistry of a real air and that simulated in the discussion above (see 3.2.1 and 3.2.2). Consequently, it may be desirable to extend our study if there are still inconsistencies between the field observations and those from experiments described above. For the "real" air a typical Chicago aerosol will be employed.

4. TIME AND COST ESTIMATE

The cost for the first 6-man-month Phase I work (field monitoring) is estimated to be \$35,000. This figure includes staff, labor, material and travel costs and will not be exceeded without your approval. Phase II cannot be costed at this time.

5. BACKGROUND

Of particular importance to this study is the current program which we are conducting for the U.S. Environmental Protection Agency in which we are characterizing PAN-Type compounds as well as their modes of formation and decompo-

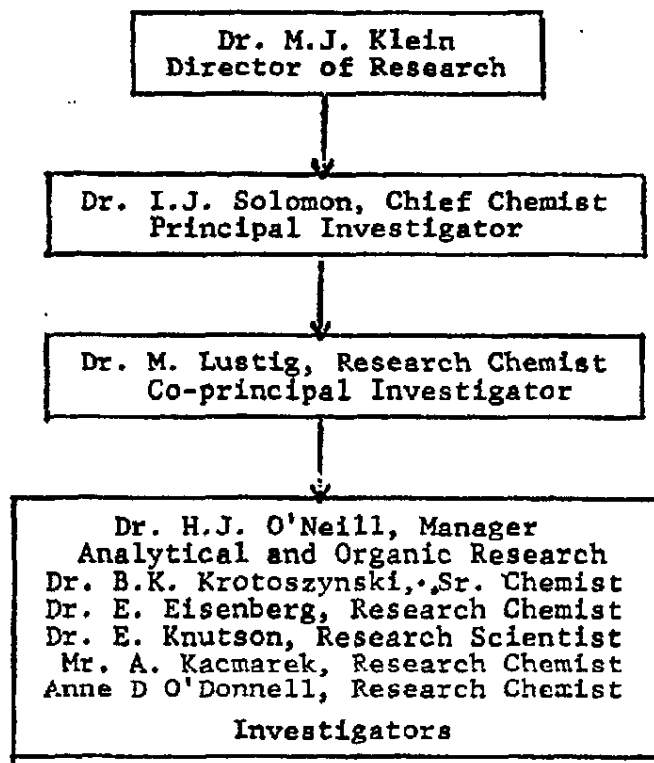
sition in photochemical smog. This particular research was initiated by in-house funding and later supported by the NSF and presently by the EPA. A new program under consideration by the NSF deals with the isolation and identification of the illusive NO_3 radical, a short-lived substance proposed to be present in any atmosphere containing NO_x . Additional pertinent information detailing our experience is enclosed.

6. PERSONNEL CAPABILITIES, FACILITIES, AND INSTRUMENTATION

6.1 Personnel

The research personnel that will be associated with this program are eminently qualified to perform the intended research. Refer to personnel chart below. Dr. I.J. Solomon, Principal Investigator, has been managing environmental oriented programs for several years. Dr. M. Lustig, Co-principal Investigator, has been performing research on a current EPA air pollution project involving the study of the formation, decomposition and characterization of PAN-Type compounds formed in a photochemical smog. Dr. H.J. O'Neill will direct the analysis studies for this program. He has directed projects involving collection and analysis of ambient air samples. Dr. B.K. Krotoszynski and Anne D. O'Donnell will be available for this project. These individuals are competent to perform the indicated analytical research. Mr. A. Kacmarek has conducted synthetic work on prior air pollution programs. Dr. W. Eisenberg is an organic photochemist whose background includes kinetic studies of primary photochemical processes, and Dr. E. Knutson is an Aerosol and Fine Particles Research Scientist and versed in smog chamber studies. More detailed information concerning these individuals may be found in the enclosures.

Personnel Chart



6.2 Facilities

Important to this study are two aerosol chambers at IITRI, one of which would be dedicated for use as a smog chamber in the proposed study at no cost to the Manufacturing Chemists Association. Since the study of vinyl chloride reactions may involve toxic reaction products, safety of laboratory personnel is a consideration. This aerosol chamber was specifically designed for the study of toxic aerosols. Both the chamber and the laboratory in which it is housed are operated under negative pressure. The chamber can be vented through a high efficiency

particulate filter, with provision for a charcoal bed gas absorber.

For the proposed application to the study of vinyl chloride reactions, the chamber will be equipped with a cylindrical gas reaction bag constructed of an appropriate polymer film. Ultraviolet (UV) irradiation will be accomplished by a battery of fluorescent "sun" lamps or "black" lamps mounted around the reaction bag. It is estimated that approximately 72 forty-watt lamps will provide the desired intensity.

The polymer film used to construct the gas reaction bag must be selected to have good UV transmission, good stability when exposed to UV and minimal surface chemical activity. Teflon is accepted as a lining material for smog chambers used in studies of photochemical smog reactions. Tests will be conducted to insure that Teflon does not emit halogenated hydrocarbon species which might interfere with the reactions of vinyl chloride.

Approximately 3 KW of electric power will be required for the UV lighting. It is anticipated that the massive steel construction and good thermal contact provided by the aerosol chamber in the photograph will prevent significant temperature rise in the volume of the chamber. The initial tests planned for the smog chamber will utilize air contaminated with high concentration of the common urban pollutants, as well as vinyl chloride.

Adequate laboratory space is available. Several photochemical apparatus for laboratory scale synthesis can be employed in this study. High vacuum facilities for the transfer and manipulation of gaseous substances are in routine service in the Chemistry Division of IITRI.

7. CONCLUSION

We have outlined a program intended to answer the pertinent questions regarding the behavior of vinyl chloride in polluted air. It is flexible and can be concluded at any stage depending on the results of the previous part and the requirements of the sponsor.

Bibliography

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2. R. Criegee, Record Chem. Progr., 18, 111 (1957).
3. Sepelco, Inc. Bellefonte, Pennsylvania, 16823, Bulletin 44, 1974.
4. T. Okita, K. Kaneker, T. Yanaka and R. Sugai, Atmospheric Environment, 8, 927 (1974).

SYNOPSIS OF PAST IITRI PROGRAMS RELATED TO THE PROPOSED
VINYL CHLORIDE STUDY

Development of Analytical Methods and Test Equipment for
Determination of Hydrocarbon Contaminants, Contract No.,
NAS8-2681

A monitor to continuously analyze the compressed gas supplies for non-condensable hydrocarbons, halocarbons and moisture at the 0.05 ppm level was developed and delivered.

Information Center for Organic Chemical Signatures, NSF,
Contract No. NSF-C514

The purpose of this program is to collect data to characterize the structure of organic compounds from which unknown compounds can be identified by matching signatures. Data from infrared, nuclear magnetic resonance, mass spectrometry and gas chromatography is being obtained and processed. The data is being indexed and prepared for computer (IBM 7094) input.

National Aeronautics and Space Administration (NASA) Technology
Utilization Survey on Air Pollution Monitoring Instrumentation,
NASA-Headquarters, Contract No. NASw-1716

Under this contract, Information Sciences Personnel conducted and published a technology survey on air pollution detection, monitoring, and control instrumentation, sensors, and techniques. Representatives of industry, academic and research institutions, as well as NASA were interviewed. The appropriate literature was searched to gather information on NASA-sponsored developments related to air pollution monitoring. Data was evaluated in terms of innovation to the state-of-the-art, and the dissemination of

Atmospheric Borane Monitor, Contract No. AF04(611)-7543

A small, portable instrument, sensitive to one part per hundred million, was developed. A small hydrogen-air flame was found to be a very efficient source for the excitation of the 2496 Å boron doublet.

Atmospheric Beryllium Monitor, Contract No. AF04(611)-7543

An instrument to monitor particulate beryllium oxide was designed and constructed. The sample is collected on continuous tape, such samples are irradiated with alpha particles, and the readout detected by a photomultiplier using scintillation counting techniques.

Continuous Analysis of Atmospheric Ozone, Contract No. AF19(604)-3834

A portable airborne analyzer was developed for detecting atmospheric ozone down to 0.1 ppm. The device uses the principle of catalytic decomposition of ozone which provides a thermal effect sensed by thermistors.

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Photochemical Reactivity of Vinyl Chloride

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AP00012014

The Photochemical Reactivity of Vinyl Chloride

	<u>Contents</u>	<u>Page</u>
1.	Introduction	1
2.	Photo-oxidation Experiments	2
3.	Hydroxyl Radical Attack on Vinyl Chloride	4
4.	Comparison of Reactivity Data with Other Investigators	7
5.	Products of Vinyl Chloride Photo-oxidation	7
6.	Eye Irritation	8
7.	Conclusions	9
8.	References	10
Table I	Rate parameters in photo-oxidation of vinyl chloride and some hydrocarbons	11
Table II	Relative photochemical reactivities	12
Fig. 1	Concentration time curves for the photo-oxidation of vinyl chloride in the presence of NO	13
Fig. 2	Plots showing the removal of olefin and NO during photo-oxidation	14
Fig. 3	Ozone formation during the photo-oxidation of hydrocarbons and vinyl chloride	15
Fig. 4	The effect of added vinyl chloride on the photo-dissociation of nitrous acid	16
Fig. 5	Plot of the rate data from the photolysis of HNO_2 -olefin mixtures according to equation (1)	17

1. Introduction

The formation of 'photochemical smog' in polluted atmospheres results from the oxidation of hydrocarbon substances in a photochemically initiated reaction involving oxides of nitrogen. The oxidation products characteristic of photochemical smog include oxidants (mainly ozone), aldehydes, CO, organic nitrogen compounds and nitric acid. The relative importance of the various hydrocarbons which are emitted into the atmosphere in producing photochemical smog in a given area depends on the rate at which they undergo photo-oxidation. Investigators have drawn up an empirical scale of reactivity which is based on the measurement of certain rate parameters for the oxidation of individual hydrocarbons in laboratory experiments, carried out under simulated atmospheric conditions. The parameters most widely used for comparison are

- (a) the rate of conversion of NO to NO₂
- (b) the rate of hydrocarbon consumption, and
- (c) the rate of ozone formation

The following general order of reactivity has been established^(1, 2)

Internal olefins	> polysubstituted benzenes	> terminal olefins	> mono alkyl benzenes	> paraffins
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The reactivity of a given hydrocarbon may be ascertained by comparing measured values of the above parameters with those for other hydrocarbons which have known reactivity.

Recent theories concerning the mechanism of the hydrocarbon-NO_x photo-oxidation have suggested that the major free radical species involved in the initial attack on the hydrocarbon is the hydroxyl radical, OH. There is accumulating experimental evidence which confirms this. In particular the rate of OH reaction with aliphatic hydrocarbons corresponds closely to the empirically determined photochemical reactivity for both unsaturated and saturated compounds. Although a similar correspondence is found for atomic oxygen and ozone reaction with olefins, the reactivity of O and O₃ with saturated hydrocarbons is too slow

to account for the observed photochemical reactivities of this class of hydrocarbons.

In order to determine the photochemical reactivity of vinyl chloride two series of experiments have been carried out. Firstly, the rates of photo-oxidation of ppm concentrations of vinyl chloride, ethylene, propylene and trans-2-butene in the presence of 1 ppm NO in air were measured and the rates compared. Secondly, the reactivity of these four olefins with hydroxyl radicals was measured by a technique recently developed in these laboratories⁽³⁾ which uses the photolysis of gaseous nitrous acid as a source of hydroxyl radicals.

2. Photo-oxidation Experiments

(a) Procedure

Mixtures containing part-per-million concentrations of olefins and nitric oxide in synthetic air were made up in a 200 l flexible bag constructed of Tedlar film. There was no detectable adsorption of olefins, NO or NO₂ on this material (loss rate $< 1\% \text{ hr}^{-1}$). Ozone loss rates were measurable ($\sim 10\% \text{ hr}^{-1}$) but not serious. The bag was irradiated by two banks of fluorescent lamps which had a broad spectral intensity in the blue-UV region (300 - 450 nm) with maximum intensity at 365 nm. The Tedlar film is transparent throughout this region. The light intensity was approximately 75% of that of natural sunlight (zenith $L = 40^\circ$) in this spectral range, as measured from the rate of photolysis of NO₂ in pure nitrogen ($k_d(\text{NO}_2) \simeq 0.27 \text{ min}^{-1}$).

Synthetic air was made up by introducing 50 l breathing grade oxygen to the bag and filling to 240 l with nitrogen (oxygen free grade). The trace gases, olefins and NO were added to the N₂ stream during filling. After allowing ten minutes for thorough mixing, the mixtures were irradiated and the concentrations of the olefin, the oxides of nitrogen NO and NO₂ and the ozone was determined as a function of time. The relative humidity of the air in the bag was approximately $20 \pm 3\%$ and the temperature $22 \pm 2^\circ\text{C}$.

Analysis of NO and NO₂ was carried out using a chemiluminescence NO_x analyser

(TECO Model 12A). Ozone was measured on a Nederbragt type ethylene chemiluminescence ozone detector, and the olefins were measured by gas chromatographic analysis using a flame ionisation detector. The minimum detectable concentrations using each of these techniques was of the order of 1 ppb and the precision at the 1 ppm level was better than $\pm 5\%$.

Materials: Nitric oxide was taken from a standard mixture containing 118 ppm NO in N_2 . Ethylene (99.8%), propylene (99%), trans-2-butene (99%) and vinyl chloride (99.9%) were taken from 'lecture bottle' cylinders (BDH Ltd). No impurity was detected either by gas chromatographic or infra-red spectroscopic analysis of the vinyl chloride.

(b) Results

A. Photo-oxidation of vinyl chloride in the presence of NO

Fig. 1 shows the concentration time curves for the reaction of 2.21 ppm C_2H_3Cl with 0.970 ppm NO under continuous irradiation. A typical, though rather slow, 'photochemical smog' type reaction is observed; after a short induction period, oxidation of NO to NO_2 commences with accompanying consumption of the vinyl chloride and as the NO is depleted, the concentration of ozone rises. Even after six hours irradiation, oxidation of NO was incomplete and only 26% of the vinyl chloride had been consumed. After prolonged irradiation (22 hours), 79% of the vinyl chloride had been consumed and the ozone concentration had increased to 0.60 ppm. Thus, significant ozone concentrations result from the photo-oxidation of vinyl chloride in air but only after a long period of irradiation.

B. Comparison of the rates of photo-oxidation of vinyl chloride with hydrocarbons

Similar experiments to those described above were carried out for ethylene, propylene and trans-2-butene with initial concentrations of 2.36, 1.67, 2.10 ppm respectively. Initial NO concentrations were 1.02,

0.91, 0.97 ppm respectively. Fig. 2 shows the concentration time curves for removal of NO and the olefins. Clearly the reactivities of trans-2-butene and propylene are much higher than that of vinyl chloride which is similar to ethylene. The absence of a noticeable induction period for NO oxidation with propylene arises from the presence of a higher initial concentration of NO₂ in this experiment ($(\text{NO}_2)_0 = 0.10$ ppm for C₃H₆ compared with < 0.03 for the other hydrocarbons). The same order of reactivity is also evident from the plots for ozone formation shown in Fig. 3.

A quantitative comparison of the photochemical reactivity can be made on the basis of a number of parameters. For the present discussion we will consider the following:-

- (A) The average rate of NO oxidation to 50% NO consumption
- (B) The amount of reactant consumed after a given time (4 hours)
- (C) The maximum rate of ozone formation
- (D) The final ozone concentration after essentially complete oxidation of NO.

The numerical values for these parameters, estimated from the concentration time curves are given in Table I.

On the basis of parameter A, the reactivity of vinyl chloride is rather close to that of ethylene but in terms of hydrocarbon reaction rate (B) vinyl chloride oxidation is significantly slower. Both compounds are considerably less reactive than propylene and trans-2-butene. For all four substances the final ozone concentration was approximately the same, showing that the chlorinated hydrocarbon, vinyl chloride, can potentially produce as much ozone as the 'reactive' olefins but only after a much longer reaction time.

3. Hydroxyl Radical Attack on Vinyl Chloride

(a) Procedure

Mixtures containing ~7 ppm gaseous nitrous acid together with approximately

0.3 ppm each of NO and NO₂, diluted in a N₂-O₂ mixture (2:1) were made up in the Tedlar bag. The mixture was drawn from this reservoir at a constant flow rate through a 27 cm³ cylindrical photolysis cell irradiated with 330 - 380 nm light from a mercury arc source. The concentrations of NO, NO₂ and HNO₂ at the inlet and outlet of the cell were measured and the rates of formation of NO and NO₂ (R_{NO} and R_{NO_2}) in the photolysis determined. Successive aliquots of vinyl chloride (or other olefins) were then added to the mixture and the effect of increasing olefin concentration on R_{NO} and R_{NO_2} determined. The maximum extent of photolysis of HNO₂ was approximately 4%.

(b) Results

Fig. 4 shows the effect of added vinyl chloride on the rates of NO, NO₂ and total NO + NO₂ formation in the photolysis of HNO₂. The rates are normalised to unit HNO₂ concentration. It will be seen that the addition of increasing amounts of vinyl chloride leads to a fall in the rate of NO formation, an increase in the rate of NO₂ formation and a less pronounced decrease in the total rate $R_{NO + NO_2}$. Similar effects were also obtained for the hydrocarbons ethylene, propylene and trans-2-butene.

The mechanistic interpretation of the results in Fig. 4 is complex and subject to considerable uncertainty. However, on the basis of the following simplified scheme, the data can give an estimate of the relative reactivity of the added hydrocarbons with OH.

In the absence of additive the photolysis of HNO₂ proceeds by



Thus equal rates of NO and NO₂ formation are expected in the photolysis. The slightly lower rate of NO₂ formation with zero C₂H₃Cl shown in Fig. 4 is due to the side reaction of NO₂ with OH to give HNO₃ which was not measured. When a compound, R, is present which reacts with OH radicals, reaction (3) then competes with reaction (2), *et*



The free radical product from (3) reacts with molecular oxygen which is present in great excess to yield a peroxy radical which can oxidise NO to NO₂



Some of the (P) $\dot{\text{O}}$ radicals may then be lost by recombination or undergo further reactions leading to the formation of NO₂. Some of the (P) $\dot{\text{O}}_2$ radicals may also be lost by recombination. The radical loss processes are reflected in the decline in the total rate $R_{\text{NO} + \text{NO}_2}$ with increasing additive (Fig. 4). In the simple case of R = CO, then (P) $\dot{\text{O}}_2$ and (P) $\dot{\text{O}}$ are HO₂ and OH respectively and it has been shown⁽³⁾ that the above mechanism fits the observations for the photolysis of HNO₂-CO mixtures. Furthermore, the relative rate constants for OH reaction can be obtained from a plot of the equation:

$$\frac{\Delta_{\text{NO}} + \Delta_{(\text{NO} + \text{NO}_2)}}{\beta_1 - \Delta_{(\text{NO} + \text{NO}_2)}} = \frac{k_3 [\text{R}]}{k_x [\text{NO}_x]} \approx \frac{k_3 [\text{R}]}{k_2 [\text{NO}_x]}$$

where Δ_{NO} and $\Delta_{(\text{NO} + \text{NO}_2)}$ represent the differences between the $R_{\text{NO}}/[\text{HNO}_2]$ and $R_{\text{NO} + \text{NO}_2}/[\text{HNO}_2]$ values respectively in the absence and presence of additive, β_1 is the dissociation rate of HNO₂, k_2 and k_3 are the rate constants for reactions (2) and (3) respectively* and $[\text{NO}_x] = [\text{NO} + \text{NO}_2 + \text{HNO}_2]$. Fig. 5 shows a plot of the data for vinyl chloride, C₂H₄, C₃H₆ and t-C₄H₈-2 according to equation (1). The slopes of the plots give a measure of the ratio k_3/k_2 , i.e. the relative reactivity of the hydrocarbons with OH. The order of reactivity is the same as that found in the photo-oxidation experiments.

By using the value of k_2 previously determined⁽³⁾, relative to the well known rate constant for the reaction of OH with CO, values of k_3 of 9.4×10^{-12} and 5.6×10^{-12} in cm³ molecule⁻¹ s⁻¹ units are derived for C₂H₄ and C₂H₃Cl respectively from the above slopes. Recent determinations of the absolute value of the rate constant for the reaction of OH with ethylene all lie in the region of 3×10^{-12} cm³ molecule⁻¹ s⁻¹⁽⁴⁾. The apparently higher value obtained in the present analysis almost certainly arises because more than one NO molecule is oxidised in the reactions following the attack of OH on C₂H₄. A comparison of

* k_x is a "human" rate constant - the rate constant for the reaction of (P) $\dot{\text{O}}$ with NO.

the k_3 values indicates a stoichiometry factor of about 3. The stoichiometry factor for vinyl chloride is unknown and therefore the rate constant value obtained can only be regarded as an upper limit. By analogy with ethylene the true value is probably a factor of 2 - 3 lower than the value given.

4. Comparison of Reactivity Data with Other Investigators

Table II shows a comparison of the relative reactivities of the substances under consideration with those obtained by other investigators which have been summarised by Altshuller and Bufalini⁽¹⁾. The OH reactivity data are compared with those of Morris and Niki⁽⁴⁾.

There is reasonably good agreement between the relative reactivities of the various substances based on A, the rate of NO oxidation and B, the consumption of reactant. The differences which are observed can probably be attributed to the different experimental conditions and measurement methods used in the various investigations. A close correspondence between relative reactivity toward OH and reactivity in the photochemical oxidation system is also evident. This correspondence has also been noted by Morris and Niki on the basis of their OH reaction measurements, with which the present estimates show good agreement considering the uncertainty in the stoichiometry mentioned above. It is also of interest to note that the reactivity of trichlorethylene is similar to that of vinyl chloride and ethylene.

5. Products of Vinyl Chloride Photo-oxidation

In the present study no investigation of the products of the photo-oxidation of vinyl chloride has been made. The nature of the expected major products may be deduced by analogy with ethylene for which the major products are formaldehyde, CO and CO₂. Thus fission of the C-C bond occurs in the oxidation reaction, and in addition to the other three products observed for C₂H₄, vinyl chloride would be expected to yield formyl chloride. Although formyl chloride has apparently never been isolated as a stable compound, it may be stable at very low concentrations

in air. Normally it decomposes to HCl and CO which will undergo further oxidation only slowly in the photochemical system.

6. Eye Irritation

While there is a strong correlation between the various chemical parameters used to characterise the reactivity of hydrocarbons in the photochemical system, no such correlation exists with the eye irritation index⁽²⁾. This is no doubt due to the widely differing lachrymatory effects of the products formed from quite similar starting materials. In the absence of experimental data, any attempt to assess the eye irritation index for vinyl chloride must therefore be largely speculative.

The only chlorinated compound for which the eye irritation index has been reported is trichloro-ethylene⁽¹⁾ and there is unfortunately some conflict between two separate investigations. Trichloro-ethylene lies between propylene and ethylene in photochemical reactivity and gives an eye-irritation index reported to be either somewhat greater than propylene⁽⁵⁾ or somewhat less than ethylene⁽⁶⁾. Taking the more pessimistic value, thought to be more realistic because of the possible formation of the strongly lachrymatory compounds phosgene and formyl chloride (the latter also being a potential product of vinyl chloride), and taking into account the somewhat lower photo-reactivity of vinyl chloride observed in the present investigation, then the data suggests that the eye-irritation index for vinyl chloride should be similar to that for propylene. Heuss and Glasson⁽²⁾ reported values of 0.3, 0.5, 1.2 and 3.0 for ethylene, trans-2-butene, propylene and 1,3-butadiene respectively, together with those for many other hydrocarbons. The eye-irritation was assessed by a panel after 4 mins. exposure as: none, light, moderate or severe and assigned numerical values of 0, 1, 2 and 3 respectively. It should be pointed out, however, that atmospheric measurements of eye irritants are almost an order of magnitude lower than laboratory concentrations resulting in equal eye-irritation, according to Schuck and Doyle⁽⁷⁾ and there is much uncertainty surrounding the subject.

7. Conclusions

The results discussed above show that

- (a) Vinyl chloride undergoes photo-oxidation in a similar manner to other hydrocarbon compounds when C_2H_2Cl-NO -air mixtures are exposed to UV radiation of wavelength and intensity similar to that of solar radiation near the earth's surface.
- (b) The photochemical reactivity of vinyl chloride, as measured from a number of rate parameters in the photo-oxidation reaction and also from its reactivity toward OH radicals, is similar to or slightly less than ethylene. Vinyl chloride is, therefore, only a moderately reactive precursor to photochemical smog, being less reactive than propylene and higher olefins, but more reactive than the normal paraffins.
- (c) The rate constant for the reaction of OH with vinyl chloride has an upper limit of $5.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300°K. The true value is probably a factor of 2 - 3 lower than this.

8. References

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2. J.M. Heuss and W.A. Glasson, 'Hydrocarbon Reactivity and Eye Irritation', Environ. Sci. and Tech. 2, 1109 - 1116 (1968).
3. R.A. Cox, to be published in J. Photochemistry.
4. E.D. Morris and H. Niki, 'Reactivity of Hydroxyl Radicals with Olefins', J. Phys. Chem. 75, 3640 - 3641 (1971).
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6. K.W. Wilson, G.J. Doyle, D.A. Hansen and R.D. Englert, Symposium of ACS Division of Organic Coating and Plastic Chemistry, New York, Sept. 1969. See also Environ. Sci. and Tech. 3, 896 (1969) and ibid p. 1224 together with Ref. 1 p. 48.
7. E.A. Schuck and G.J. Doyle, 'Photo-oxidation of Hydrocarbons in Mixtures Containing Oxides of Nitrogen and Sulphur Dioxide', Report No. 29, Air Pollution Foundation, San Marino, Calif. (1959) see also Ref. 1 p. 56.

TABLE I

Rate parameters in photo-oxidation of vinyl chloride and some hydrocarbons

Reactant	A $-d[NO]/dt$ (ppm/min $\times 10^2$)	B % reactant consumed after 4 hours	C $(d[O_3]/dt)_{max}$ (ppm/min $\times 10^2$)	D final $[O_3]$ (ppm)
Vinyl Chloride	0.31	13	$> 0.017^{\dagger}$	0.60 (1300 min)**
Ethylene	0.34	25	$> 0.17^{\dagger}$	0.47 (1300 min)
Propylene	1.40	88 (13)*	0.58	0.66 (240 min)
Trans-2-butene	3.0	> 100 (75)*	3.75	0.73 (80 min)

* hydrocarbon consumed after 30 minutes

 $\dagger$ maximum rate not achieved during reaction time used

** time at which final ozone concentration measured.

TABLE II

Relative photochemical reactivities*

Reactant	This work			Altshuller & Bufalini ⁽¹⁾		Morris & Niki ⁽⁴⁾
	A NO oxidation	B reactant consumption	C OH reactivity	A NO oxidation	B reactant consumption	C OH reactivity
C_2H_4	0.25	0.28	0.29	0.4	0.1	0.1
C_3H_6	1.0	1.0	1.0	1.0	1.0	1.0
$t-C_4H_8-2$	2.1	5.8	~ 3.0	2	~ 6	4.2
C_2H_3Cl	0.25	0.15	0.17	-	-	-
C_2HCl_3	-	-	-	0.5	0.45	-

*Reactivities are relative to propylene which is arbitrarily set at unity.

Fig. 1 Concentration time curves for the photo-oxidation of vinyl chloride in the presence of NO.

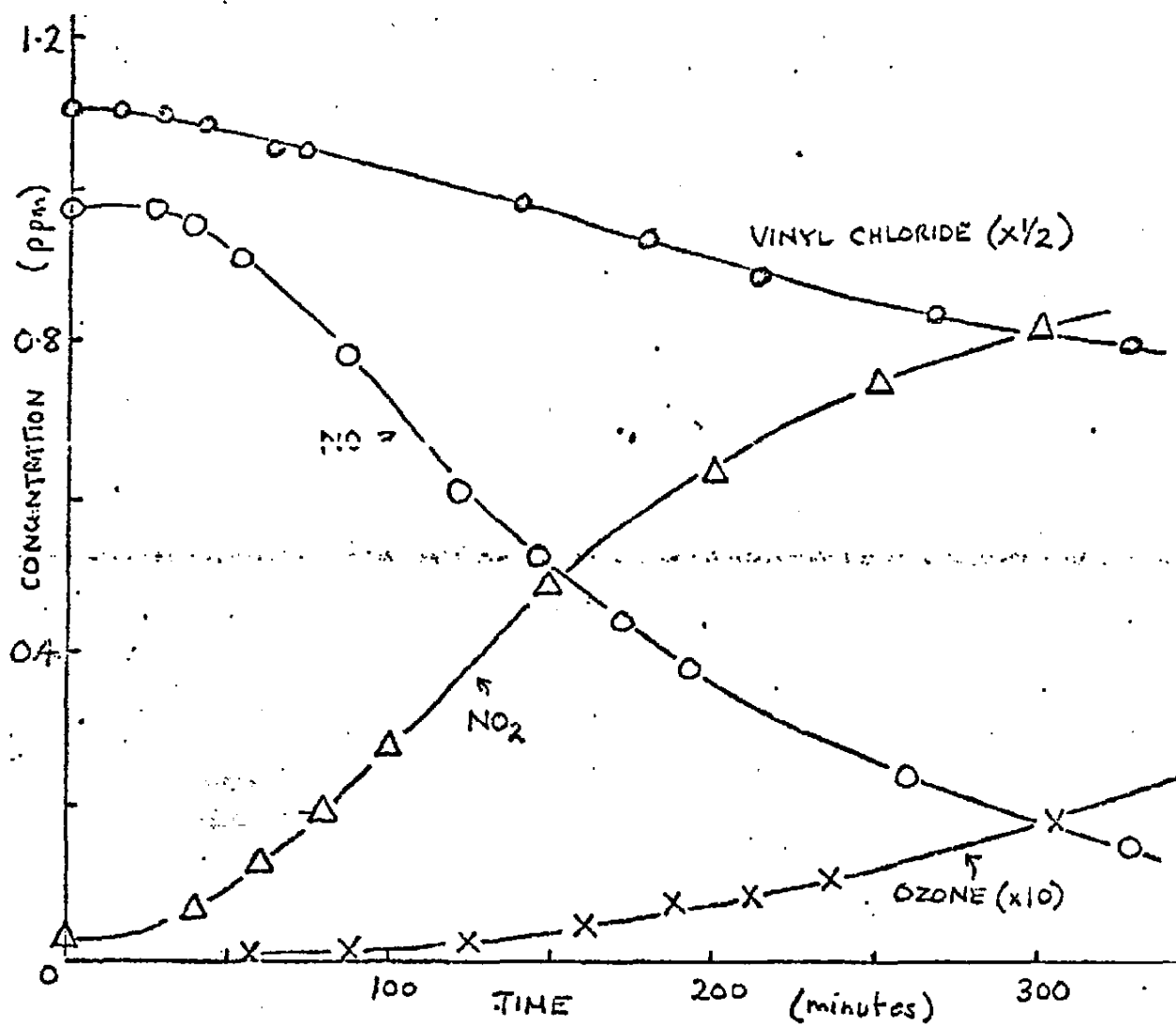


Fig. 2 Plots showing the removal of olefin (filled points) and NO (open points) during the photo-oxidation of vinyl chloride (O), ethylene (Δ), propylene ($\square$) and trans-2-butene ($\diamond$), in the presence of NO. The concentration axis for each hydrocarbon is shifted slightly so that the initial NO concentrations correspond to 0.97 ppm NO.

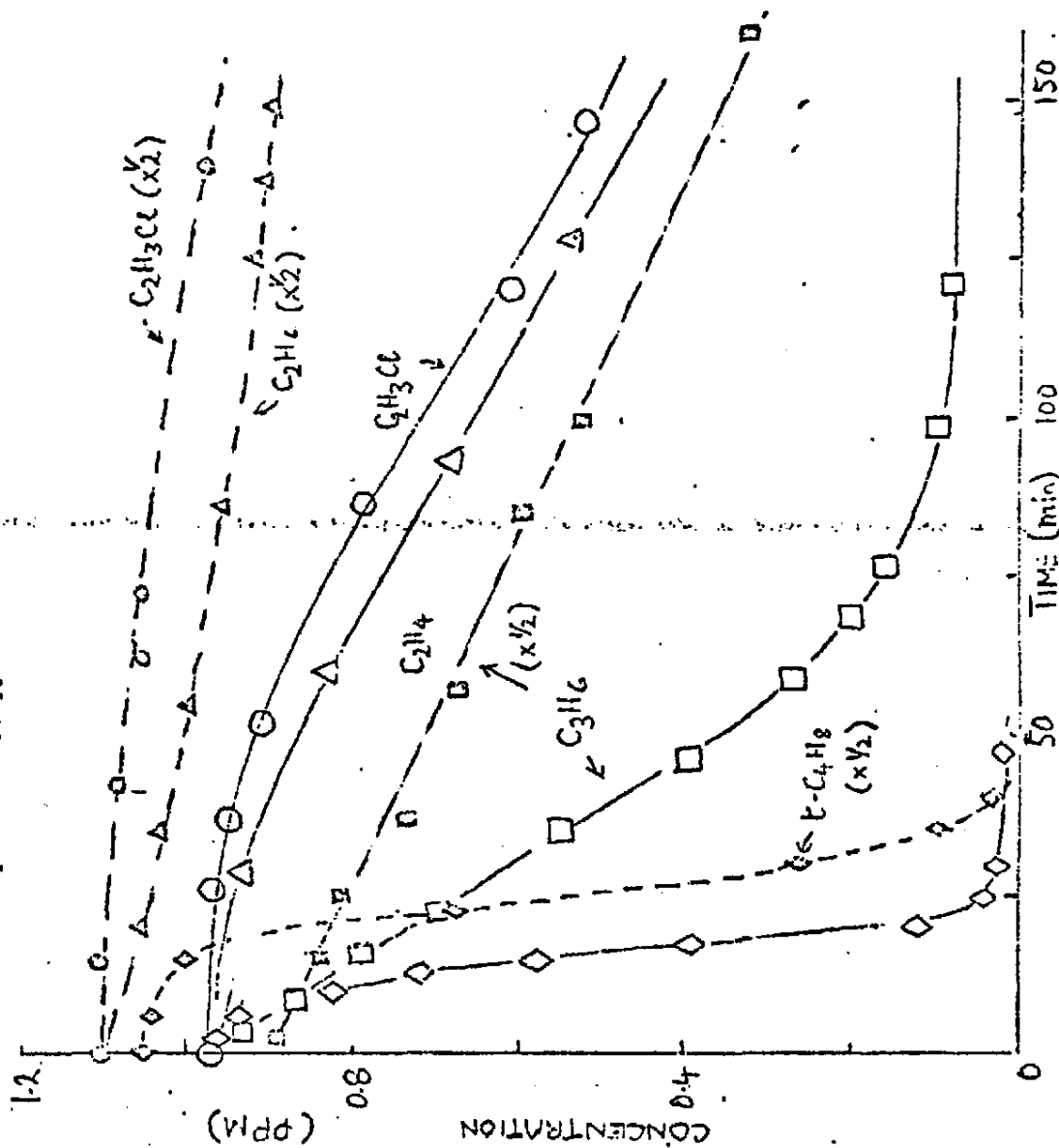


Fig. 3 Ozone formation during the photo-oxidation of hydrocarbons and vinyl chlorid (filled points).

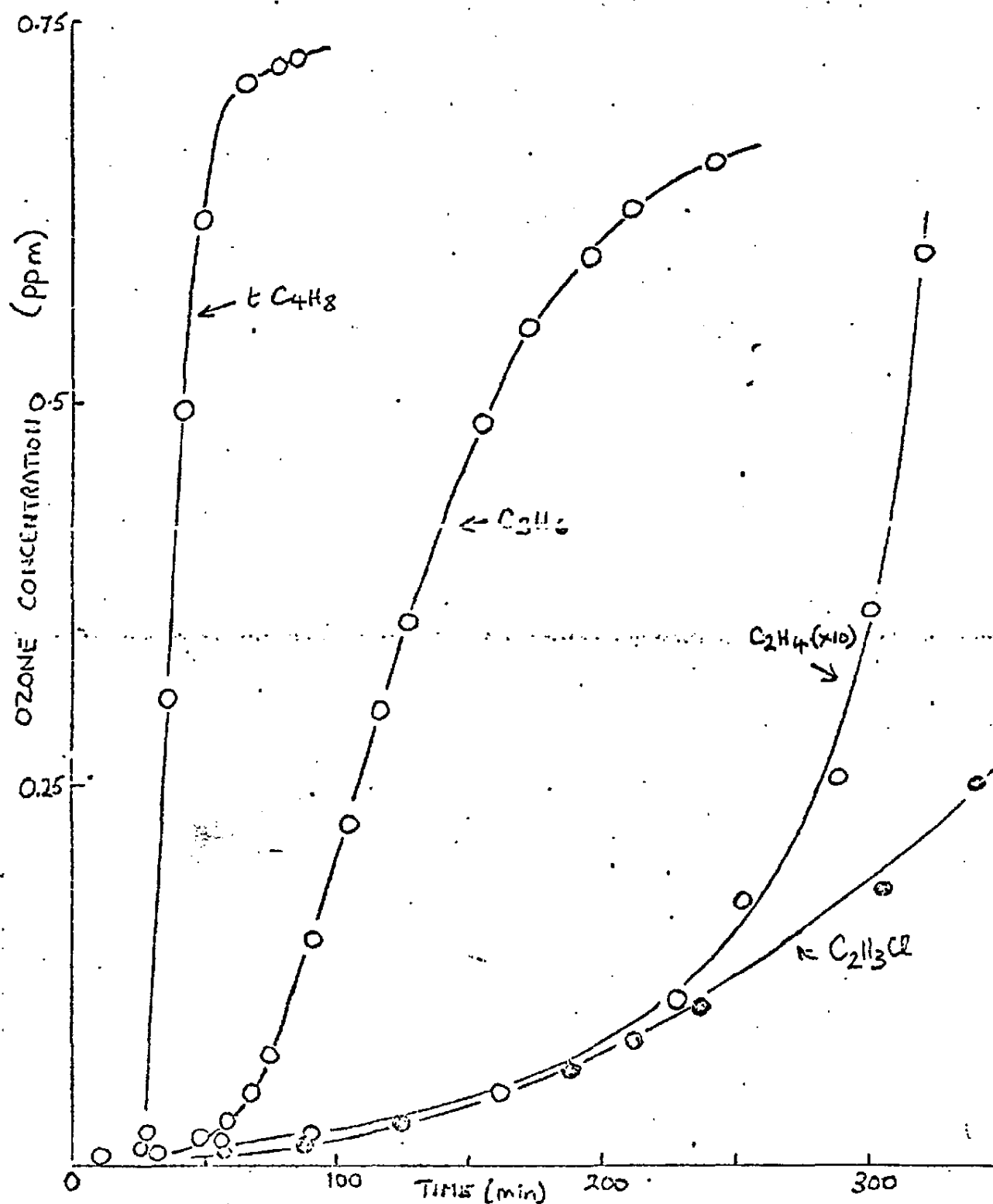


Fig. 4 The effect of added vinyl chloride on the photoassociation of nitrous acid. The plot shows the rates of formation of NO and NO₂ (R_{NO} and R_{NO_2}) and the total rate R_{NO+NO_2} , expressed per unit HNO₂ concentration as a function of the concentration ratio $[C_2H_3Cl]/[HNO_2]$.

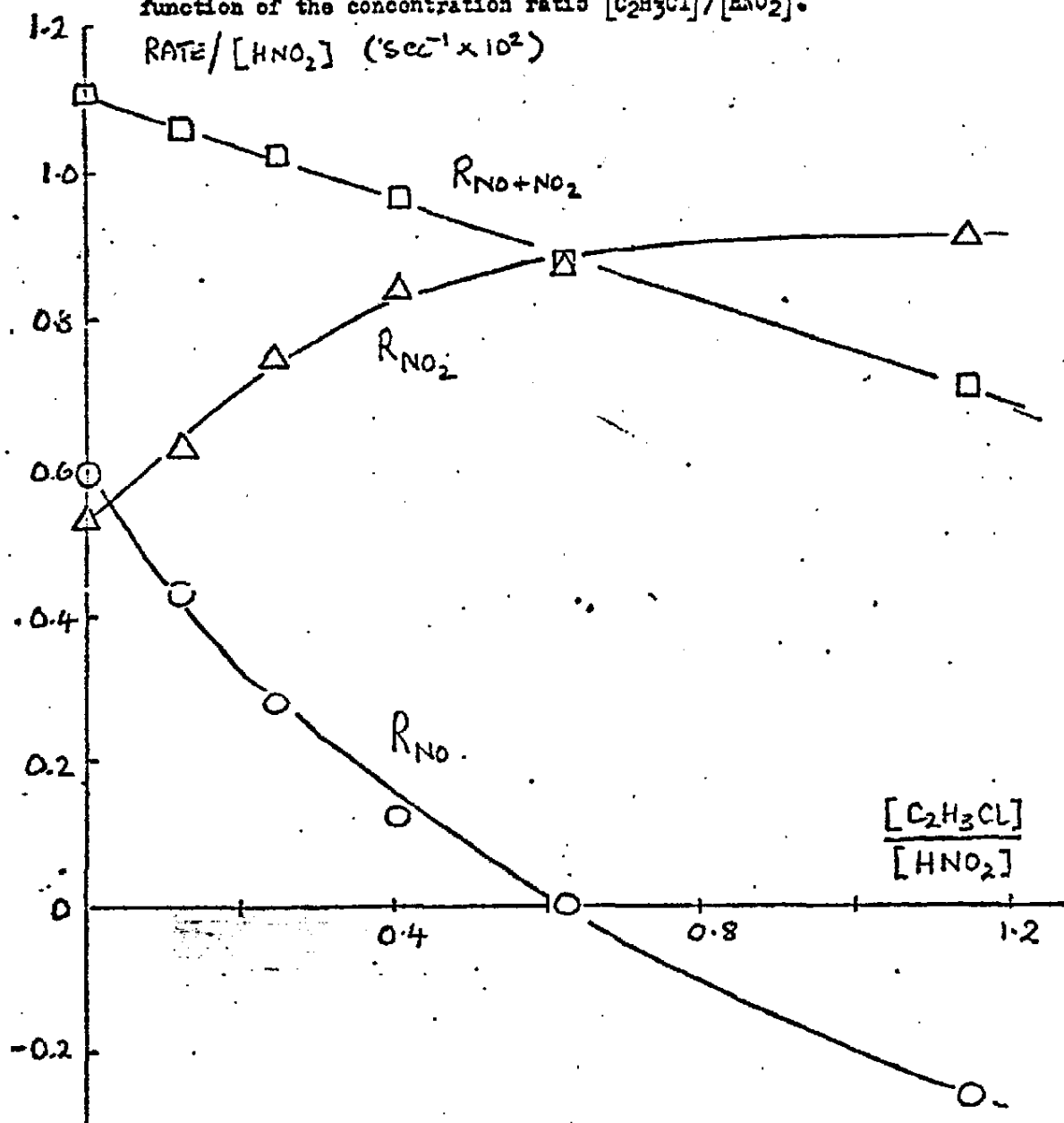
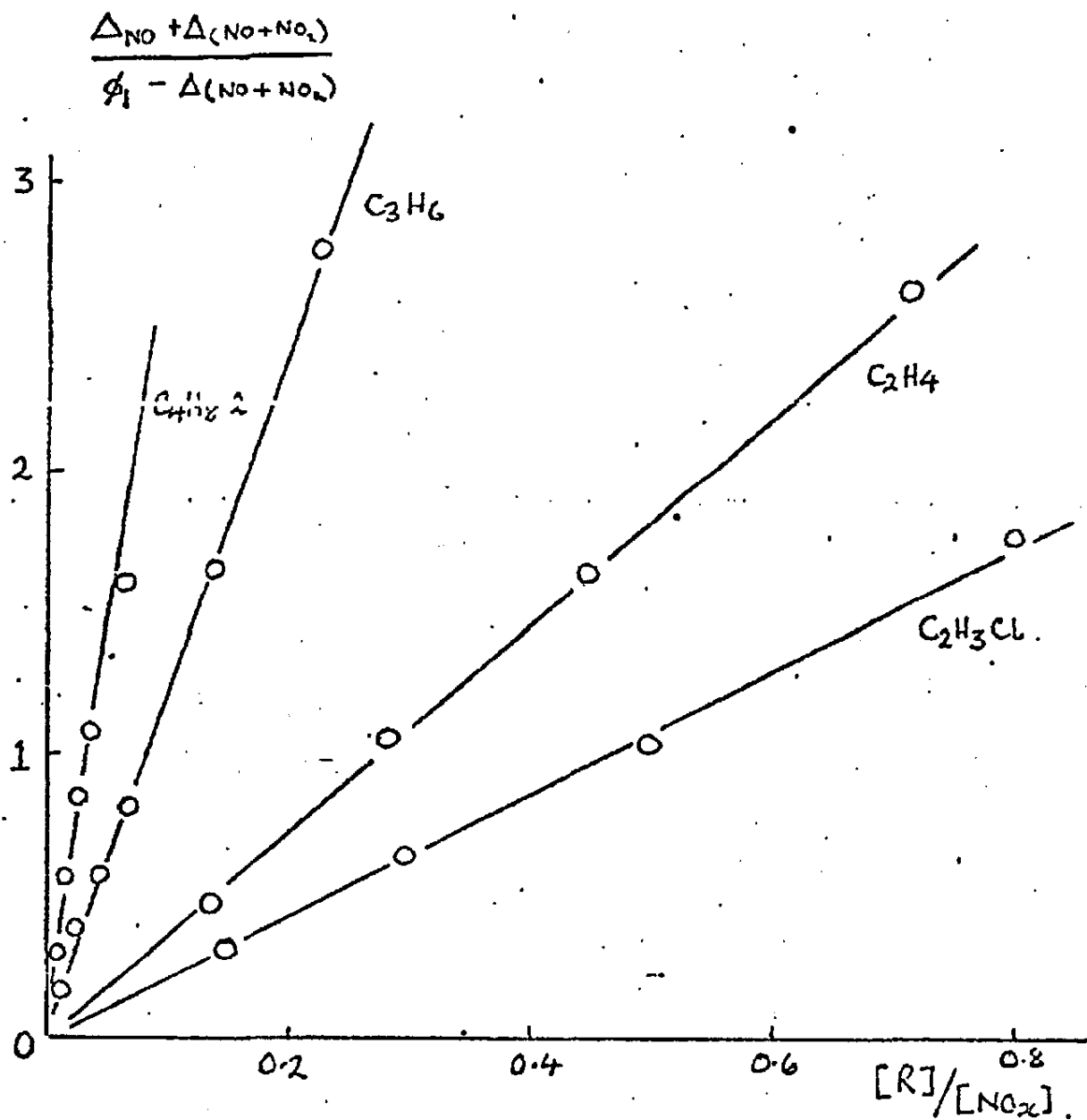


Fig. 5 Plot of the rate data from the photolysis of HNO_2 -olefin mixtures according to equation (1) (see text).



DRAFT

within a universe of different situations or within a range of situations established for local regulation purposes. Therefore, we have had to assume a general definition of incremental requirements.

A third major analytical issue is the extent to which NESHAP Regulations will apply to different steps in the production/consumption process and different size plants and operations. EPA has chosen, through economic impact analyses and other lines of reasoning, to exclude certain activities or groups from some regulations in the past. These exclusions have been made for reasons of emission rates, economic effects, or administrative costs. At the outset of our analysis, we reviewed the extent of potential emission sources associated with each chemical, ranging from the source of a raw material, to its refining or manufacture, to its fabrication or intermediate use, and finally to its end-use, consumption, or disposal. Again, without prescience of subsequent EPA regulation and EPA's economic impact analyses, we have had to make reasonable judgements of the extent to which NESHAP regulations will cover each production/consumption step.

2.4 Approach of This Study and Its Limitation

The proposed cost impact analysis methodology is one which builds upon previous work by both EPA and private industry relative to environmental regulation. It also reflects in some ways the specific issues involved in controlling hazardous air pollutants, the characteristics of the industries impacted, and the effects of having several regulations precede it.

The three chemicals selected for illustrating the methodology were chosen because they have been studied before in relation to other regulations. This enhanced our ability to focus on the analytical problems of anticipating the

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DRAFT

impact of NESHAP regulations in each of their relevant industries. It should be noted, however, that other pollutants which may be covered under Section 112 may require development of basic background information which was readily available for these three chemicals.

In preparing our analysis, we relied on these previous studies for an understanding of the impacted industries. To some degree, the studies were also sources of candidate control technologies. From other published materials, we developed generalized cost models for each of several leading control technologies. We then considered their cost and effectiveness in each major type of control situation. In order to enhance the experience of our staff in selecting a reasonable BACT assumption, we held discussions with knowledgeable representatives of AIHC member companies relative to these technologies, the chemicals in question, and their costs of application.

Once the appropriate control technologies and methodologies were identified for important control situations, we then calculated the capital, operating, and energy costs associated with anticipated NESHAP regulations. These calculations and a draft of this report were reviewed by AIHC for errors of logic, calculation, or omission.

2.5 Report Format

The first chapter or Executive Summary of this report is designed to serve the purposes of most readers, excepting those of AIHC and EPA. The remainder of the report is not intended to be encyclopedic. It reflects the work of less than two short months to analyze a reasonable estimate of cost impact for three chemicals using the proposed general methodology. Its purpose is to illustrate a methodological approach and a reasonable estimate of the level of impact which may result from regulations which are not yet in place. The information found

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3.0 COST IMPACT METHODOLOGY

There are several analytical methodologies which are usually associated with the economic assessments of developing environmental regulations. The one addressed in this report is development of a cost impact methodology within the limited time periods usually allowed for industry comments. Comparable cost impact methodologies will likely be used by EPA in their development of proposed regulations for specific chemicals. Finally, there are the more extensive methodologies of economic impact analyses. It is this, a full economic impact analysis, which should accompany EPA's proposed future NESHAP regulations.

The principal objective of this report is the development of a cost impact methodology for use by AIHC in responding to NESHAP regulations presently proposed and to those that will be proposed in the future. In developing the cost impact methodologies in this report, we have also outlined the components of an EPA economic impact analysis that should correspond to this kind of cost impact analysis.

3.1 Definition and Characterization of Impacted Industries

The definition of industries impacted by a NESHAP regulation must first begin with the identification of a specific air pollutant. Meaningful industry definition cannot be related to generic standards until those standards specify the control of a specific pollutant or the practices of a given industry. Hence, in this report, we have analyzed a selection of three chemicals by which we could identify illustrative costs of meeting either generic standards or pollutant-specific emission standards.

Given the identification of a specific chemical pollutant, the definition of impacted industries logically begins with those which produce those chemicals either as a primary product or as a byproduct. The extent to which impacted

DRAFT

here is taken largely from other reports, many of which far exceed this report in size and detail. More extended analyses, including those which address economic impact questions, will be appropriate as EPA performs its own regulatory analysis of each pollutant standard. More definitive cost impact analyses can be made by AIHC when specific regulations are proposed.

Chapter 3.0 describes the cost impact analysis methodology which has been recommended to AIHC in its response to future NESHAP proposed regulations.

Chapter 4.0 contains the generalized control costs models for available technologies which were used as alternatives in selecting BACT for each of the three chemicals.

Chapter 5.0 characterizes and categorizes each of the impacted industries associated with the three illustrative chemicals. Very little of this background information was developed specifically for this effort as most of the information was available from previous regulatory analyses.

Chapter 6.0 contains the results of illustrative cost impact analyses for the three chemicals.

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industries are further defined to include upstream or downstream industries depends to some degree on how the EPA regulation is written. If EPA proposals address a supplying industry, an intermediate using industry, or final use as part of a differentiated regulation, then those sectors become part of the impacted industries for the purpose of cost impact analysis. If the regulations are not industry-specific for each regulated chemical, then the cost impact analysis will require careful definition of the extent of expenditures needed by various industry sectors. Even where EPA regulations have specifically excluded control requirements for certain industry segments, it may be in the interest of industry (or in the public interest) to compare the quantities of pollutants being emitted from excluded sectors and the costs of their control to the quantities and costs associated with complying industries.

Industry definition is relatively straightforward in the cases of ambient air standards and New Source Performance Standards. In the former instance, it is necessary to identify the different types of industrial sources within an air quality control region. In the latter instance, the industry is self-defined by the category specified as the "source." In defining the industry under NESHAP regulation, the regulations may apply from the stage at which the chemical is extracted as a raw material or produced by chemical reactions, through all of the myriad handling and uses that it may encounter during the time it is to be considered a potentially hazardous air pollutant. In the analysis of NESHAP regulations, it will, consequently, be important to establish the cost impacts from the raw material sources through industrial production situations and as far forward to final occurrence or use as may be directly or indirectly governed by the regulation.

Industry characterization has become an established part of the analysis associated with EPA or other regulatory initiatives. Industry characterization must anticipate the important parameters along which control costs may vary within an industry and across which economic impacts may differ. As when analyzing the impact of other regulations, the industry characterization appropriate for a NESHAP cost impact analysis should address the following factors:

- description of extraction, production, and manufacturing processes;
- estimate of the industry's production and/or production capacity;
- description of user industries to which control will apply;
- inventory of the distribution of manufacturer's and user's facilities by size (or age) categories;
- estimates of sales volumes; and
- identification of major producers, users, and their locations.

In the illustrative analyses in this report, to demonstrate the methodology and the level of potential impact, it was not necessary to identify specific companies and locations. In subsequent analyses of actual NESHAP regulations, however, it will be necessary to identify the estimated production capacities and locations for specific companies. This kind of information will probably have been developed by EPA or their contractor as a part of the analysis supporting the proposed regulation, but it should also be a part of AIRC's analysis--if only to confirm the accuracy of EPA information.

The level of difficulty faced by AIHC in characterizing industries will vary with each chemical regulated under NESHAP. If a chemical has been studied for the purposes of previous regulations (e.g., OSHA), existing industry characterizations should be a good starting point for the analysis. This was one of the reasons why benzene, perchloroethylene, and vinyl chloride monomer were selected for analysis in this report. Industry characterization will be more difficult where the chemical emission has not been previously identified for control or regulatory examination. If EPA has not itself conducted a thorough survey of emission sources, for example, industry characterization by AIHC will not only involve substantial effort, but also require more time.

An important part of industry characterization is the categorization of impacted industries and users according to facility sizes, different processes, production mixes, etc. Often, the parameters of categorization will correspond to the industry categories along which regulations are themselves differentiated. Categories will also be suggested by the cost impact analysis and the variables which affect control costs. Finally, categorization should also reflect the industry subsectors which are likely to show differential economic impacts in the subsequent economic impact analyses, e.g., the small producer or user, the obsolescent process, the old facility, or the geographical location.

3.2 Description of Emission Control Situations

The emission control situations ultimately defined under NESHAP regulations will be principally responsible for establishing the control requirements and, obviously, the costs of compliance. If monitoring and maintenance-type regulations are established in lieu of emission control standards at specified points, the selection of the emission situations and the methods of estimating costs are drastically different. Furthermore, if emission rates from sources have already

DRAFT

been addressed by OSHA or other regulations (such as volatile organic chemicals), the costs for control under NESHAP will become incremental to those earlier incurred costs. Concomitantly, estimation of the magnitude of the emission reduction under NESHAP will require dealing with estimates of incremental reductions. Although EPA, in its proposed rulemaking of October 10, 1979 has proposed broad situations for control (e.g., fugitive emissions, chemical storage, chemical transfer and handling, waste, and process vents), it will often be difficult to define typical situations. This is especially true since there is likely to be a wide variance in the applicability of existing and future controls for site-specific reasons.

In addition to characterizing the control situations which must be addressed in the impacted industrial and user facilities, some relationship must be established which will characterize the magnitude of the control situations with typical production and consumption estimates. During the time periods typically allowed for industry comment on proposed regulations, it will be impractical to establish a complete and accurate survey of the number of control situations affected (e.g., the exact number of pumps, valves, process vents, storage tanks, etc.). It will, however, be important to develop reasonable estimates of the number of such control points in typical situations and to identify how the numbers may vary across types of situations. This judgment will not only be important for a realistic estimate of the costs of compliance, but also in differentiating the economic impacts of compliance between one situation and another. One such important distinction between control situations is between new and existing sources.

With the completion of the industry definition, industry characterization, and identification of control situations, the cost impact analysis has established

the basic population estimates in terms of the number of production and consumption sites, and the number of control points or situations for typical sites.

3.3. Generalized Control Cost Models

Chapter 4.0 describes the kinds of control technologies that are likely to be utilized in establishing the base for cost impact analyses of future NESHAP regulations. The major control technologies described therein are likely to be appropriate options for controlling the emissions of many chemicals. A principal portion of the work undertaken in this study was devoted to the use of control cost models as a means of judging best available technologies (BAT). As EPA identifies specific BAT technologies in future NESHAP regulations, that step will not be necessary in future analyses.

In addition to identifying the direct costs of control associated with compliance, control cost models should include cost credits or realistic benefits deriving from the recovery for reuse of byproducts, raw materials, reactants, or energy values. Obviously, the resulting control costs from compliance action are reduced by such benefits of control.

Generalized control cost models also provide the bases for considering alternative approaches to compliance. They serve as part of the basis on which the cost effectiveness of selecting different control options or control levels may be reviewed. Cost effectiveness can be judged according to the cost of control at different emission levels using a single technology or the cost of controls to achieve different emission levels using different technologies.

The control costs appropriate to NESHAP compliance fall into several groups. There are the traditional categories of capital and operating costs. These may vary according to whether they are in new source or existing source situations.

Operating cost categories include materials, supplies, energy, and labor. In addition to the capital and direct and indirect operating costs of control, NESHAP impacts encompass the costs of monitoring, and reporting. Finally, the costs of compliance with NESHAP regulations are a combination of the costs associated with the proposed generic standards, largely monitoring and maintenance costs, and those that may ultimately be related to process discharge standards of specific pollutants.

3.4 Cost Impact Calculation

The calculation of cost impact is straightforward. A generalized equation for this calculation is indicated in Figure 3-1. The number of production and consumption emission sources covered by a NESHAP regulation for a given chemical is the result of industry definition and characterization. These may be based on the actual number of facilities in each industry category or reflect the average size plant or facility corresponding to the number of plants and users in the industry. These numbers are then multiplied by appropriate factors that can be related to control costs. In Figure 3-1, it is assumed that the number and size of emission points in the chosen unit can be established. The cost of control associated with each type of emission point is then multiplied by the total number of like emission points. The overall costs of the NESHAP regulation for a given chemical is determined by summing these costs. Alternatively, a control cost function based on an average plant or user can be developed employing unit costs for control of the identified emission sources. That value, when multiplied by the total number of average size units, will give the total cost impact of the regulation.

The generic standards proposed on October 10, 1979 were presented on the basis that they "would rapidly effect reasonable control of emissions" and are,

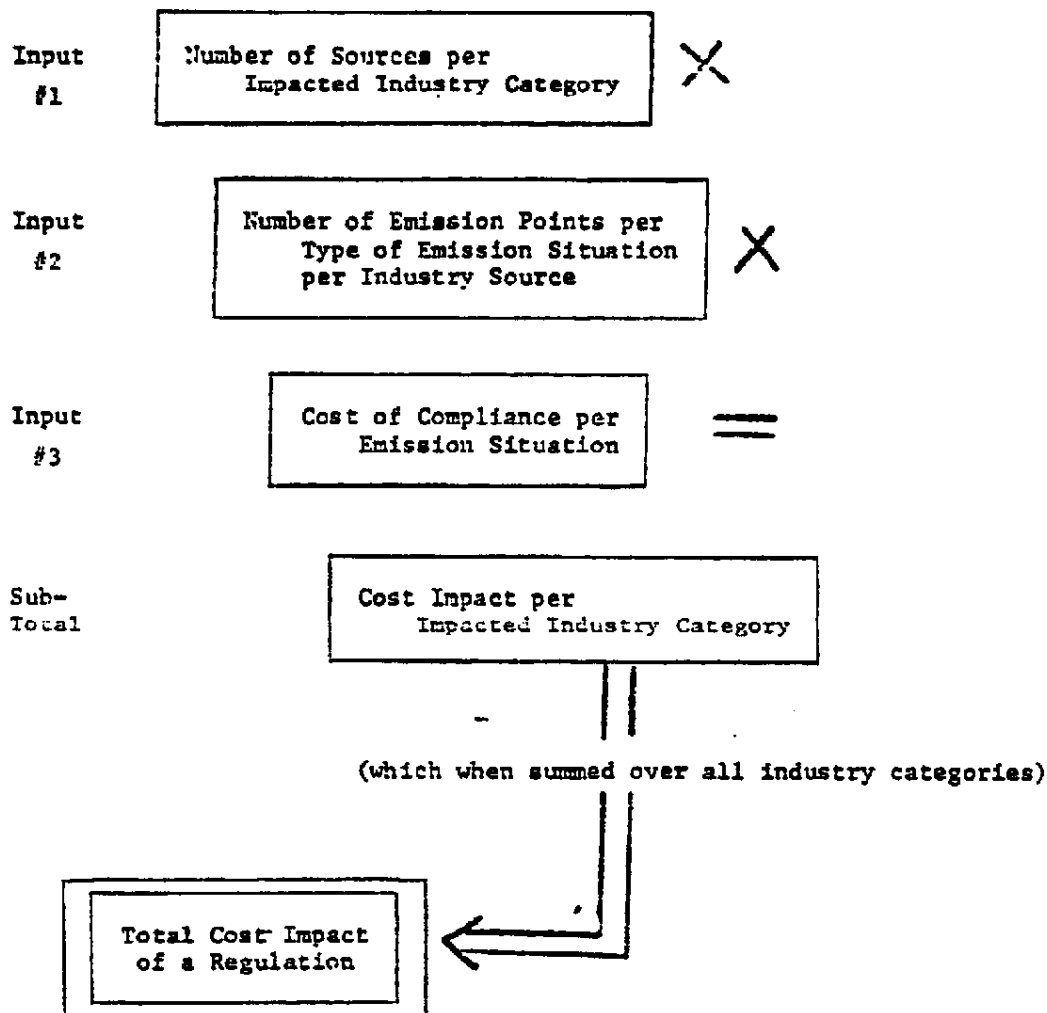


FIGURE 3-1 GENERALIZED CALCULATION OF COST IMPACT

DRAFT

consequently, related principally to monitoring and maintenance. It is not possible, however, to estimate at this time the costs of applying such generic standards in situations which are still to be associated with designated hazardous air pollutants. We have thus developed our analysis on the premises that final pollutant-specific standards will be developed on the basis of best available technology. It is recognized that the final standard may require control beyond best available technology. To obtain the best possible indication of potential future costs under NESHAP, we have provided the bases for assessing and anticipating BAT. To illustrate the cost impact methodologies, we have selected benzene, perchloroethylene, and vinyl chloride monomer as chemicals for application of cost estimating procedures.

Our approach to estimating the cost impact of a NESHAP regulation is presented in Figure 3-2. Figure 3-2 finds chemical pollutants listed down the vertical axis and the kinds of NESHAP regulations controlling their emissions across the horizontal axis. In the illustrative analyses in this report, we have addressed the cost impact for three chemicals according to a reasonable expectation of control requirements defined by the proposed generic standards and by future source-related categories requiring BAT for each pollutant. Cost impact is thus determined as the sum of impacts in a given row (associated with a given chemical) in the matrix. Cost impacts are not here related to the sum of impacts for vertical columns in the matrix (such as for the proposed generic standards). As control requirements can vary widely from one pollutant to another, it is not possible to extrapolate from the three chemicals analyzed here to a larger number of chemicals that may be eventually covered under NESHAP regulations. That reasoning argues that the economic impact of generic regulations cannot be evaluated in themselves until all pollutants to be covered by NESHAP are identified.

	Generic Standards			Process Standards			Control Cost
	#1	#2.....	"n"	#1	#2.....	"n"	
Pollutant "a"							Impact "a"
Pollutant "b"							Impact "b"
Pollutant "c"							Impact "c"
⋮							⋮
Pollutant "n"							Impact "n"

FIGURE 3-2 COST IMPACT DEFINITION MATRIX FOR NESHAP REGULATIONS

Thus, the most meaningful measure of generic standards will be found as they are part of the control regulations for a given set of chemical emissions.

In subsequent cost impact analyses, the costs of compliance can also be differentiated according to other financial parameters. Compliance costs can be discussed in terms of the cost of control per unit of production as it may vary by size of production or consumption facility. The cost of control can also be compared on a per-unit-of-production basis or per-installation basis according to the production process employed or the range of products produced. Implicit in the development of costs along impacted industry lines is the ability to distinguish the costs to be faced by manufacturers, formulators, users, consumers, or disposers.

Costs can also be compared in terms of different levels of emission volumes or emission rates. This cost-effectiveness comparison can provide the basis for suggesting alternative regulations or regulatory approaches. Finally, the costs of compliance may be compared to revenues, capital investment, or value added as a context for understanding the magnitude of cost impact. This is to be distinguished from analyses of price impact which result from the further step of economic impact analysis.

3.5 Relationship to Economic Impact Analysis

Estimates of the cost of compliance and cost impact are necessary foundations for the economic impact analyses which have traditionally accompanied environmental regulatory initiatives. They are also necessary for the determination of inflationary, energy, or economic analyses required by Executive Order 12044 and similar predecessors. Insofar as regulatory agencies have initiated economic impact analyses in the past, AIHC is not at this time contemplating independent development of analyses beyond the cost impact step. The thrust of the analysis