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Project Summary

Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data

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A significant body of information is currently available to characterize the burden of possibly-hazardous organic chemicals (HOCs) in ambient environments. However, these data have not been accessible in an organized format, and no attempt had been made to study their significance or to integrate them into a useful and cohesive document. In this study, ambient data covering 151 chemicals were sought from 241 references primarily from the years 1970 through 1980. The data were collected and collated into a computer-accessible data base. The data were classified into four data-quality categories--excellent, good, acceptable, and questionable. The data were then analyzed to assess their reliability and usefulness in concentration trend analysis. Significant gaps were found in the available data. For any specific HOC, relatively little data are available with which health assessments or trend analysis can be made. Data acquisition has been limited primarily to a few geographical regions, and most sampling programs have been performed in the warmer months and during daylight hours.

Specific recommendations are made for future studies regarding data reporting. A strategy for an effective national monitoring program for HOCs in the atmosphere is presented.

A computer-compatible data tape listing all of the referenced atmospheric data has been prepared. The data tape contains information on each of the 132 chemicals for which data were actually obtained.

This Project Summary was developed by EPA's Environmental Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Significant quantities of organic chemicals are released into the ambient environment as a necessary outcome of day-to-day human activities. In recent years, it has become evident that many of these chemicals may be toxic at concentrations significantly higher than those found in the ambient atmosphere. The degree of risk associated with current exposures is a matter of active debate, and this effort focuses upon the gaseous organic chemicals in the ambient environment, especially those which may be hazardous. The term "hazardous organic chemicals" (HOCs) used here is not intended to imply that a proven human health hazard exists: in most cases toxicity studies are incomplete and entail extrapolation of animal data to humans.

This report attempts to integrate a diverse body of information on ambient concentrations of HOCs into a useful and cohesive document describing the species measured, the locations and times of the measurements, the concentrations which were observed, and the quality of the reported measurements. The objectives of the task were: (1) review, summarize and critically evaluate available (both published and unpublished) atmospheric data on HOCs in the air environ-

ment, (2) assess the extent, quality, reliability and representativeness of these data, (3) compile all "acceptable" data into a master data file and subject these data to comprehensive statistical analysis, and (4) identify major gaps in available data and recommend a research strategy for development of a measurement program to generate a national data base on HOCs in the air.

Procedure

A list of compounds to be included in the data base was developed, a literature search was conducted, and the gathered data were compiled into a computerized data base. Table 1 presents a listing of the 151 chemicals chosen as target compounds for this study. The chemicals were grouped into categories for organizational purposes in the study. The table also identifies certain chemicals as bacterial mutagens (BM) or suspected carcinogens (SC). This information was obtained from literature and studies which have evaluated large bodies of available data. Information about bacterial mutagenicity is based largely on the "Ames Salmonella Microsome Assay." Mutagenic tests are direct and simple, but the carcinogenicity information is based upon animal tests that include consideration of epidemiology and a critical and a comprehensive evaluation of carcinogen, mutagen, and other toxicological data. Evidence for the mutagenicity of toluene and the carcinogenicity of trichloroethylene is currently in some dispute for lack of sufficient data.

Compounds concentrated indoors (e.g., in industrial environments) as well as those concentrated in aquatic or soil environments (e.g., pesticides) or on aerosols were excluded from this study. In all, more than 17,000 data points from 241 references were incorporated into the data base.

All pertinent data were extracted from the literature reports and put into a com-

Table 1. *Target Hazardous Organic Chemicals in the Ambient Air*

Category A		Category B		Category C		Category D	
Name	Number	Name	Number	Name	Number	Name	Number
Benzene (SC)	001	Toluene	101	Dibromomethane	201	Methane	301
Methyl chloride (BM)	002	o-Xylene	102	Bromodichloromethane	202	Ethane	302
Methyl bromide (BM)	003	m/p-Xylene	103	Chlorodibromomethane	203	Ethylene	303
Methyl iodide (SC,BM)	004	Styrene (BM)	104	Dichlorodibromomethane	204	Acetylene	304
Methylene chloride (BM)	005	1,3 Butadiene (BM)	105	Bromoform	205	Propane	305
Chloroform (SC,BM)	006	n-Dodecane (SC)	106	1-Chloro-2-bromoethane	206	Propene	306
Carbon tetrachloride (SC)	007	n-Decane (SC)	107	Pentachloroethane	207	i-Butane	307
1,2 Dichloroethane (SC,BM)	008	n-Undecane (SC)	108	Bromopropane (isomers)	208	n-Butane	308
1,2 Dibromoethane (SC,BM)	009	n-Octadecane (SC)	109	Chlorobromopropane (isomers)	209	Butenes (isomers)	309
1,1,1 Trichloroethane (BM)	010	α-Pinene (BM)	110	1-Chloro-3-bromopropane	210	i-Pentane	310
1,1,2 Trichloroethane (SC)	011	Dodecylbenzene (BM)	111	Dibromochloropropane	211	n-Pentane	311
1,1,2,2 Tetrachloroethane (SC,BM)	012	Fluorcarbon-22 (BM)	112	1-Chloro-2,3-dibromopropane	212	i-Pentene	312
Hexachloroethane (SC)	013	Ethyl chloride	113	1,1 Dibromo-2-chloropropane	213	2-Methylpentane	313
1,2 Dichloropropane (BM)	014	1,1 Dichloroethane	114	Dichloropropene (isomers)	214	3-Methylpentane	314
Vinyl chloride (SC,BM)	015	1,1,1,2 Tetrachloroethane	115	1-Chloro-3 bromopropene	215	n-Hexane	315
Vinylidene chloride (SC,BM)	016	1,4 Dichlorobutane	116	Bromobenzene	216	2,4-Dimethyl pentane	316
(cis) 1,2 Dichloroethylene (BM)	017	1,2 Dibromopropane	117	Bromotoluene	217	Ethylbenzene	317
Trichloroethylene (SC,BM)	018	(trans) 1,2 dichloroethylene	118	Dichlorotoluene	218	1,3,5 Trimethylbenzene	318
Tetrachloroethylene (SC)	019	Benzaldehyde	119	Trichlorotoluene	219	1,2,4 Trimethylbenzene	319
Allyl chloride	020	Tolualdehyde (isomers)	120	Tetrachlorobenzene	220	1,2,3 Trimethylbenzene	320
Chloroprene (BM)	021	Phthalaldehyde (isomers)	121	Tetrachlorotoluene	221	Naphthalene	321
Hexachloro 1,3 butadiene (BM)	022	Phenol	122	Pentachlorobenzene	222	α-Methylnaphthalene	322
Monochlorobenzene (BM)	023	Peroxyacetyl nitrate	123	Chloronitrobenzene	223	Carbon tetrafluoride	323
o-Dichlorobenzene (BM)	024	Peroxypropionyl nitrate	124	Dichloronitrobenzene	224	Fluorocarbon-12	324
m-Dichlorobenzene (BM)	025	Peroxybenzoyl nitrate	125	Chloroaniline	225	Fluorocarbon-11	325
p-Dichlorobenzene (BM)	026	Diethyl sulphate (SC,BM)	126	Chlorobenzaldehyde	226	Fluorocarbon-113	326
Trichlorobenzene (BM)	027	Dimethyl sulphate (BM)	127	Epichlorohydrin	227	Fluorocarbon-114	327
Tetrachlorobenzene (BM)	028	Carbonyl sulfide	128	Maleic anhydride	228	Acetone	328
α-Chlorotoluene (SC,BM)	029	Carbon disulfide	129	1,4 Dioxane	229	Methylethyl ketone	329
Hexachlorocyclopentadiene (BM)	030	Tetramethyl lead	130	Aniline	230	Methyl isobutyl ketone	330
Ethylene oxide (BM)	031	Tetraethyl lead	131	Benzonitrile	231	Acetophenone	331
Propylene oxide (SC,BM)	032	Trimethyl ethyl lead	132	β-Chloro ethers	232	Propiophenone	332
Formaldehyde (SC,BM)	033	Dimethyl diethyl lead	133	Polychloronapthalenes	233	n-Heptane	333
Acetaldehyde	034	Methyl triethyl lead	134	Allyl bromide	234	n-Octane	334
Phosgene	035					n-Nonane	335
o-Cresol (SC)	036					4-Ethyl toluene	336
p-Cresol (SC)	037					Dimethyl sulfide	337
m-Cresol (SC)	038						
Acrolein (SC)	039						
bis-Chloromethyl ether (SC,BM)	040						
bis-(2-Chloroethyl) ether (SC)	041						
Acrylonitrile (SC,BM)	042						
Nitrobenzene	043						
Dimethyl nitrosamine (SC)	044						
Diethyl nitrosamine (SC)	045						
2-Nitropropane (SC)	046						

Key:

Category A: Ubiquitous toxic chemicals in urban ambient environment; Category B: Ubiquitous suspect toxic chemicals in urban ambient environment Category C: Toxic chemicals that are likely to be site specific and Category D: Chemicals considered to be nontoxic.

BM: Bacterial mutagens; SC: suspected carcinogens.

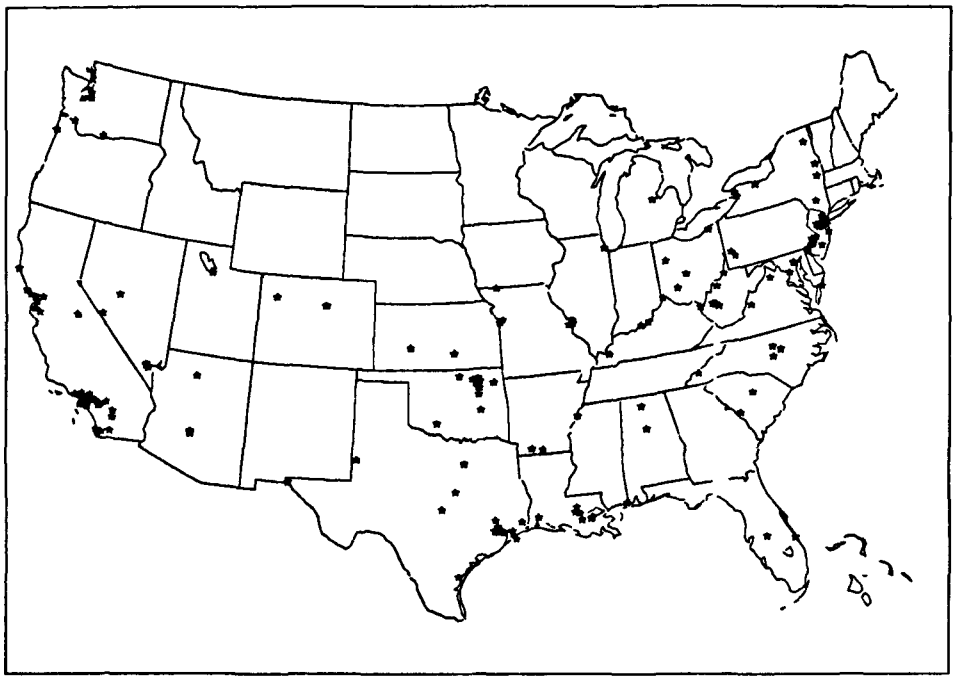

Figure 1. Sampling locations reporting data on any of the 151 target chemi-chemicals in this study. Sparse geographic coverage is obvious.

mon format for inclusion in the data base. Each entry in the data base includes: the bibliographic reference number; the latitude, longitude, street address, city and state of the sampling site; a site type code (remote, urban, etc.); the reported concentration (in parts per trillion and micrograms per cubic meter); a code for the units reported by the original investigator; the percent relative standard deviation of the reported values or of the measurement technique; a quality code describing the likely accuracy of the data; the number of samples averaged together to produce the data base line entry; codes for the sampling and analytical methods; the time average of the reported data; the maximum and minimum concentrations reported (in ppt); the date and time at which sampling began and ended, and the number of hours between sampling and analysis; the number of measurements below the detection limit; the reported detection limit; any comments necessary about the data.

The compiled data were analyzed for quality and quality codes were assigned based upon comments of the original researcher, the appropriateness of the analytic techniques, known limits of the techniques' accuracy and the magnitude of the reported concentrations. Although the assignment of quality codes was as objective as possible, a considerable amount of subjectivity was still needed in assigning many of the quality codes. The generalized characterization for the categories (excellent, good, acceptable, questionable) should not be construed as rigid, for while an error of a factor of two may be much too high for some compounds (e.g., benzene, methane), it may be acceptable for others (e.g., chlorobenzene). In short, the authors have integrated the available published and unpublished information, along with their own experiences, to arrive at a means of characterizing the quality of the available data.

Results

For each chemical the data are summarized and tabulated to show the number of data points, the average quality, the first quartile, the median, and the third quartile concentrations, for all of the data and the data grouped by sampling site classification (i.e., rural and remote, urban and suburban, source dominated). Appendices list minima, maxima, means and standard deviations for each location reported for each chemical. References are also listed so readers may access the original report for each location.

The full report also includes a brief analysis of the results for selected chemicals: benzene, methylene chloride, chloroform, carbon tetrachloride, 1,2-dichloroethane, 1,2-dibromoethane, 1,1,1-trichloroethane, trichloroethylene, tetrachloroethylene, hexachloro-1,3-butadiene, acetaldehyde, cresols, bis-chloroalkyl ethers, dimethyl nitrosamine, toluene, alpha-pinene, fluorocarbon-22, benzaldehyde, PAN, PBzN, and carbonyl sulfide. These chemicals are discussed for several reasons: the data show an interesting pattern, interest in the chemical is high, or some clarification or comment on the data was necessary.

Attempts to use the data for trend analysis showed that the data are too sparse within this data set to permit such a calculation. Even for one of the best data sets, benzene, trend analysis was impossible. No consistent sampling effort has been reported, and a much more complete, year-round data base must be assembled before trend analysis can be properly performed. The geographic sparsity of the data is illustrated in Figure 1, in which every location included in the data base has been marked with a star. Obviously, sampling for HOCs has been conducted in only a small portion of the geographic area.

Results and Recommendations

Although this data base contains a large quantity of data (more than 17,000 separate entries), it is only a beginning--a base to build upon. Even for the chemicals of greatest concern, relatively little data are available with which to assess potential risk or to develop control strategies.

Future studies should ensure the availability of "quality control" data, as well as the measurement data. The format used within the data base of this study could be used as a guide. During assembly of this data base, numerous omissions in data reporting were noted. Measurements are reported without any reference to error limits. Detection limits, where needed, are frequently not given, elapsed time between sample collection and analysis is rarely given, sampling and analytic procedures used are not always clearly defined. These data are essential to assessing the integrity of the measurements. Meteorological data should also be included.

To assure the usefulness of collected data, it should be available in a computer-compatible form, especially when a large volume of data is being reported. With the large number of studies being performed every day, this is the only way that the data can be quickly brought together, assessed, and analyzed.

The data collected for this study are primarily from the years 1970 through 1980. Every effort was made to compile all the available data; however, the size of

the task assures that data were missed. The missing data may add to the quantity of the data in the data base, but the general conclusions of this study will likely stand--more data are needed if valid human health-risk assessments, trend analysis, and models for control strategies are to be made.

The comprehensive analysis of the data base identified three specific shortcomings in the current HOC data base: (1) Much of the data available was collected to serve different objectives and is largely unsuited for the purposes of exposure characterization. Indeed, many of the reported studies are exploratory and qualitative in nature. (2) In some cases, inadequately field tested methods have been extensively applied, resulting in the collection of a body of data which is, at least in part, of poor or unknown quality. (3) The data coverage is extremely sparse and is often random in nature. To overcome the observed shortcomings, the authors recommend a three-step approach: (1) generate a data base mapping the spatial and temporal atmospheric distribution of HOCs for a preselected region, (2) characterize the primary and secondary emission patterns for the HOCs of interest within that region, and (3) compare the experimentally observed concentrations with predicted values based upon a modeling effort for the selected region which relates emissions to subsequent atmospheric concentrations. The authors also offer suggestions for carrying out the three-step strategy, specifically for selection of target areas and the siting strategy, the sampling strategy, selection of target chemicals and the analytical measurement strategy, and the quality assurance and quality control strategy.

In summary, a large number of potentially hazardous trace organic chemicals have been identified in the ambient environment. Available data are not sufficient to describe the atmospheric distributions of a majority of these chemicals. It is, therefore, impossible to assess exposures to these chemicals from past data. The data currently available on HOCs in ambient air have been compiled and summarized in a single document. A plan to overcome the gaps which now exists in the data has been described.

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The complete report consists of paper copy and magnetic tape, entitled "Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data," (Order No. PB 83-195 503; Cost: $19.00, subject to change) subject to change)
Data Tape Associated with the Report, (Order No. PB 83-195 511; Cost: $140.00, subject to change)
The above material is available only from:
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